



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 12:09 AM EDT

PDB ID : 8UGJ / pdb_00008ugj
EMDB ID : EMD-42227
Title : In-situ structure of typeB supercomplex in respiratory chain (composite)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-05
Resolution : 2.30 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:

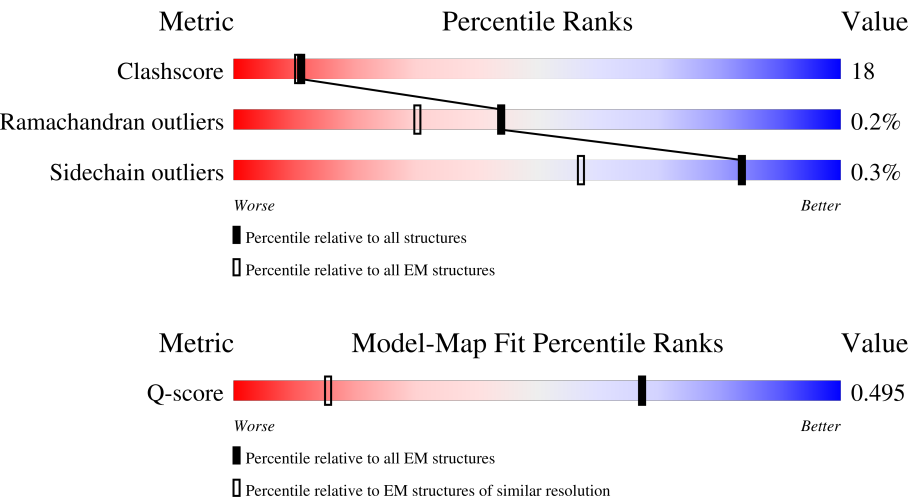
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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	12% 62% 37% .
2	1B	258	37% 23% 40%
3	1C	264	60% 19% 21%
4	1D	476	58% 32% 10%

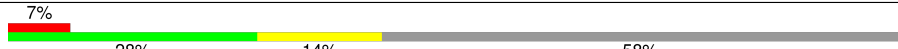
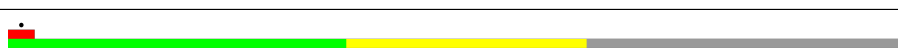
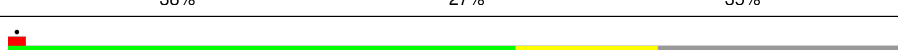
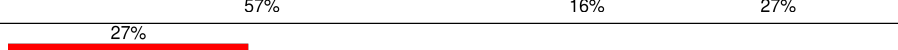
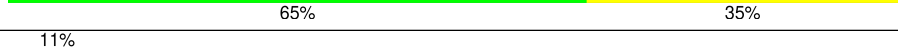
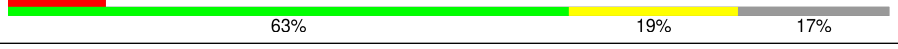
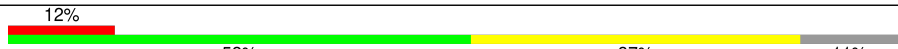
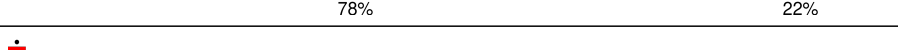
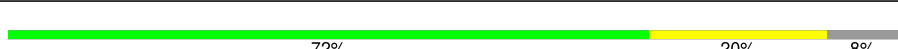
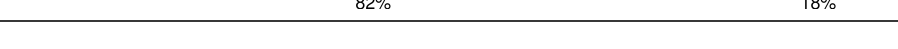
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Mol	Chain	Length	Quality of chain
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	

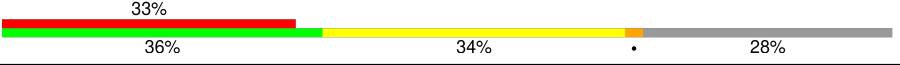
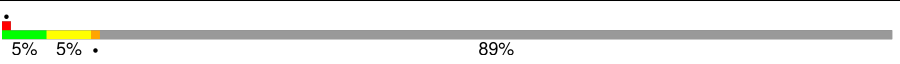
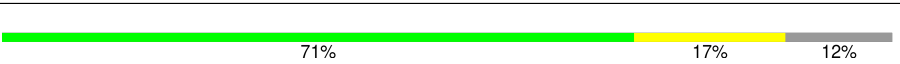
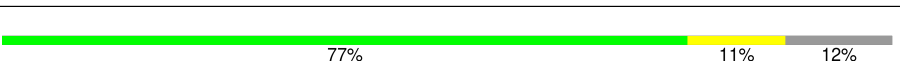
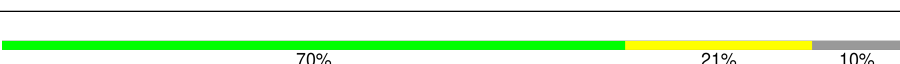
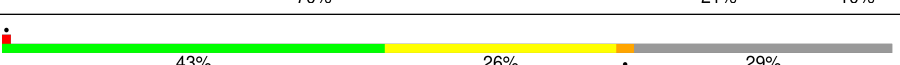
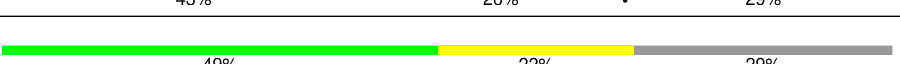
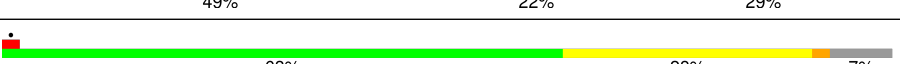
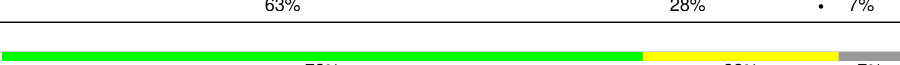
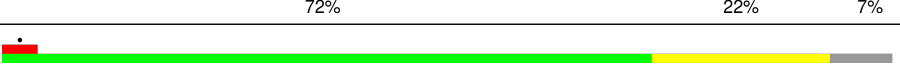
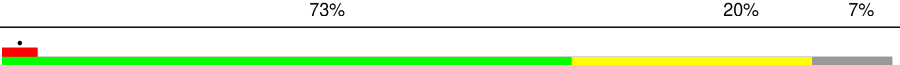
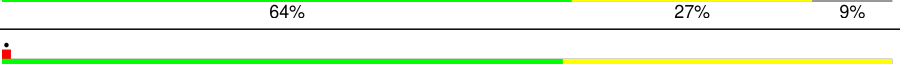
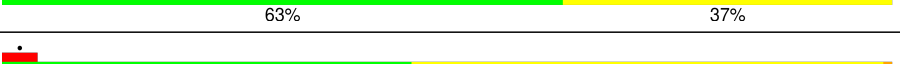
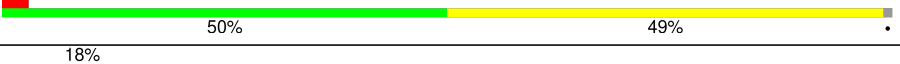
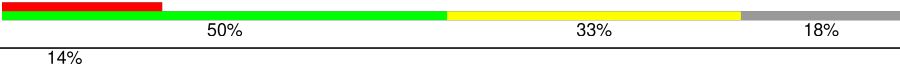
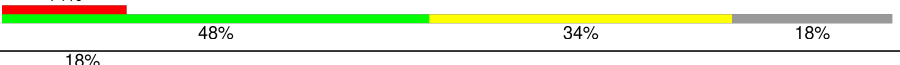
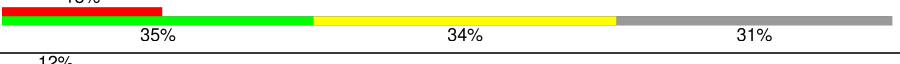
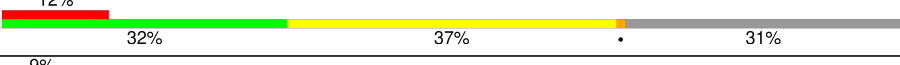
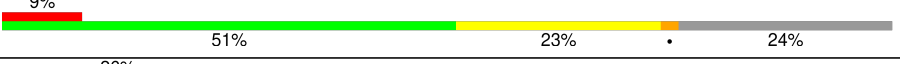
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Mol	Chain	Length	Quality of chain
29	1d	122	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	113	
44	1s	471	
45	3A	480	
45	3N	480	
46	3B	453	
46	3O	453	
47	3C	379	
47	3P	379	
48	3D	326	
48	3Q	326	
49	3E	274	

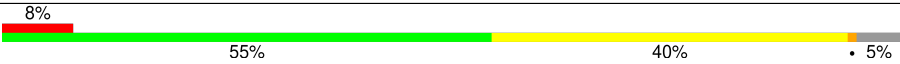
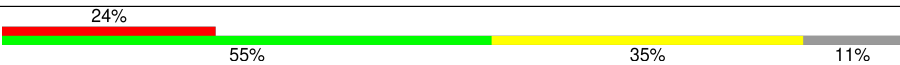
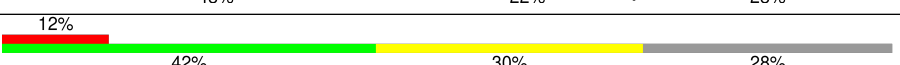
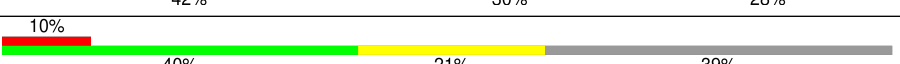
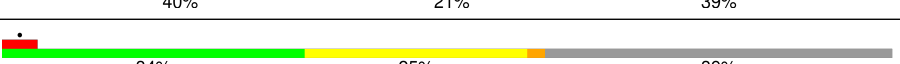
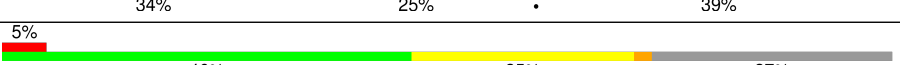
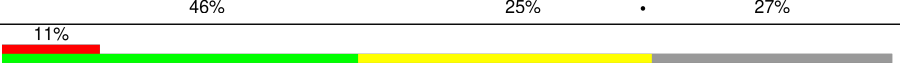
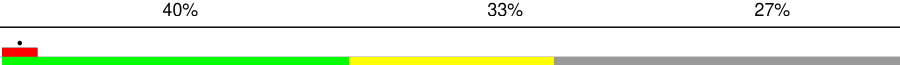
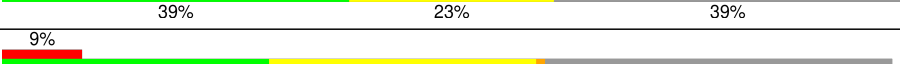
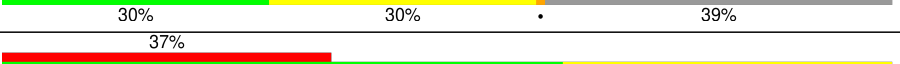
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Mol	Chain	Length	Quality of chain
49	3I	274	
49	3R	274	
49	3V	274	
50	3F	111	
50	3S	111	
51	3G	82	
51	3T	82	
52	3H	91	
52	3U	91	
53	3J	60	
53	3W	60	
54	3X	56	
54	3Y	56	
55	4A	514	
55	8A	514	
56	4B	229	
56	8B	229	
57	4C	261	
57	8C	261	
58	4D	169	
58	8D	169	
59	4E	152	
59	8E	152	
60	4F	128	
60	8F	128	

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Mol	Chain	Length	Quality of chain
61	4G	97	
61	8G	97	
62	4H	86	
62	8H	86	
63	4I	75	
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	SF4	1B	201	-	-	X	-
71	SF4	1F	502	-	-	X	-
71	SF4	1G	801	-	-	X	-
72	FES	1G	803	-	-	X	-
72	FES	3E	301	-	-	X	-
72	FES	3R	301	-	-	X	-
86	HEC	3D	501	X	-	-	-
86	HEC	3Q	501	X	-	-	-
91	CUA	8B	304	-	-	X	-

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 134346 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		

- 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		

- 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		

There are 2 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

- 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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1D	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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1c	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		

- 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		

- 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		

There are 29 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
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

- 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		

- 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		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	128	Total	C	N	O	S	0	0
			1100	723	194	181	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1i	0	ACE	-	acetylation	UNP A0A4X1UIV8

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	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		

- 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		

- 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		

- 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		

- 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 Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3J	56	Total	C	N	O		0	0
			464	305	82	77			
53	3W	56	Total	C	N	O		0	0
			464	305	82	77			

- 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		

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

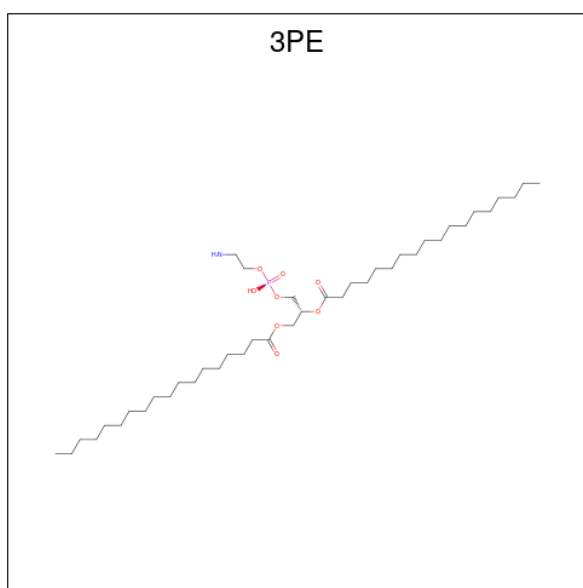
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

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 NDUF4.

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-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



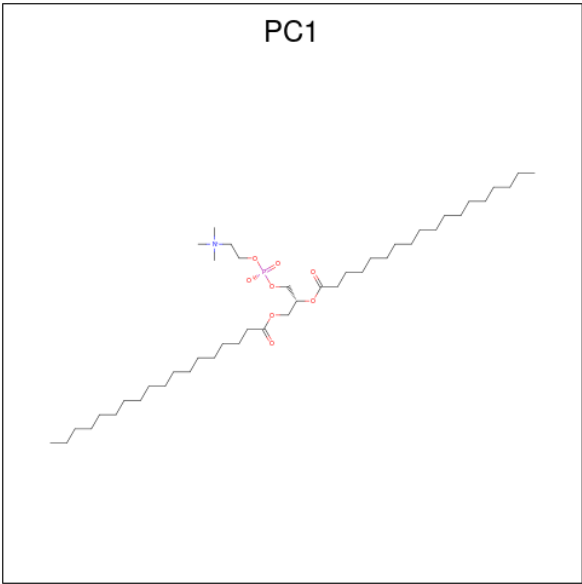
Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1K	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1M	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1M	1	Total	C	N	O	P	0
			50	40	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	1N	1	Total 49	C 39	N 1	O 8	P 1	0
69	1P	1	Total 35	C 25	N 1	O 8	P 1	0
69	1Y	1	Total 31	C 21	N 1	O 8	P 1	0
69	1Y	1	Total 40	C 30	N 1	O 8	P 1	0
69	1Y	1	Total 30	C 20	N 1	O 8	P 1	0
69	1Y	1	Total 33	C 23	N 1	O 8	P 1	0
69	1Y	1	Total 27	C 17	N 1	O 8	P 1	0
69	1d	1	Total 49	C 39	N 1	O 8	P 1	0
69	1j	1	Total 44	C 34	N 1	O 8	P 1	0
69	1m	1	Total 41	C 31	N 1	O 8	P 1	0
69	3A	1	Total 27	C 17	N 1	O 8	P 1	0
69	3A	1	Total 32	C 22	N 1	O 8	P 1	0
69	3C	1	Total 35	C 25	N 1	O 8	P 1	0
69	3C	1	Total 34	C 24	N 1	O 8	P 1	0
69	3D	1	Total 33	C 23	N 1	O 8	P 1	0
69	3G	1	Total 29	C 19	N 1	O 8	P 1	0
69	3N	1	Total 33	C 23	N 1	O 8	P 1	0
69	3N	1	Total 25	C 15	N 1	O 8	P 1	0
69	3P	1	Total 33	C 23	N 1	O 8	P 1	0
69	3R	1	Total 47	C 37	N 1	O 8	P 1	0
69	3Y	1	Total 30	C 20	N 1	O 8	P 1	0

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



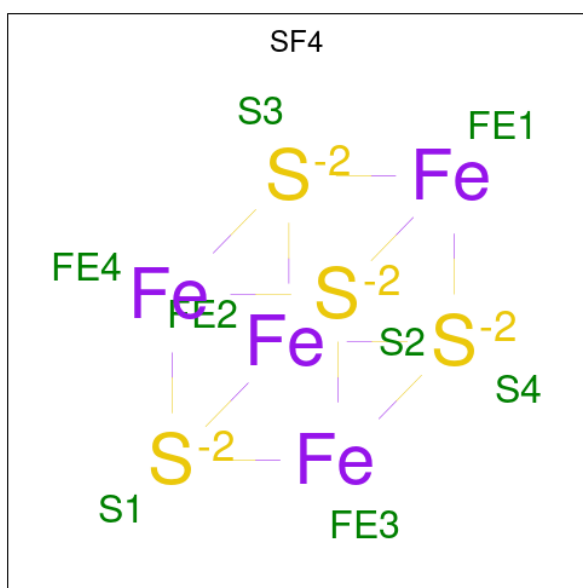
Mol	Chain	Residues	Atoms					AltConf
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1H	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	1M	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	1P	1	Total	C	N	O	P	0
			33	23	1	8	1	
70	1Y	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	

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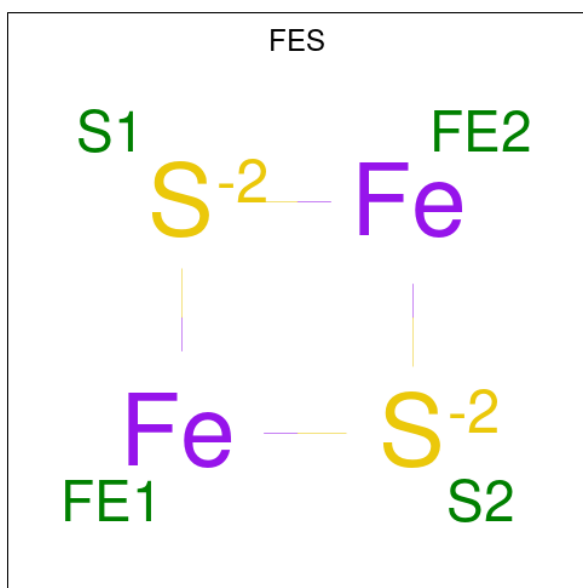
Mol	Chain	Residues	Atoms					AltConf
70	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	1q	1	Total	C	N	O	P	0
			49	39	1	8	1	
70	3J	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	3R	1	Total	C	N	O	P	0
			45	35	1	8	1	
70	3X	1	Total	C	N	O	P	0
			29	19	1	8	1	

- Molecule 71 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



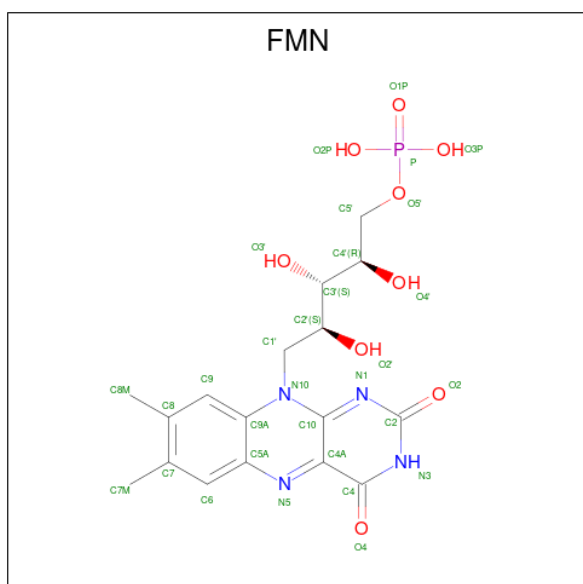
Mol	Chain	Residues	Atoms			AltConf
71	1B	1	Total	Fe	S	0
			8	4	4	
71	1F	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
72	1E	1	Total	Fe	S	0
			4	2	2	
72	1G	1	Total	Fe	S	0
			4	2	2	
72	3E	1	Total	Fe	S	0
			4	2	2	
72	3R	1	Total	Fe	S	0
			4	2	2	

- Molecule 73 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

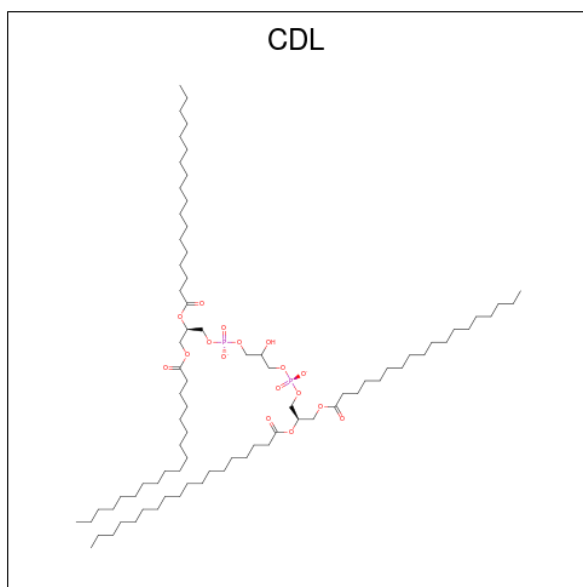


Mol	Chain	Residues	Atoms					AltConf
73	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
74	1G	1	Total	K	0
			1	1	

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



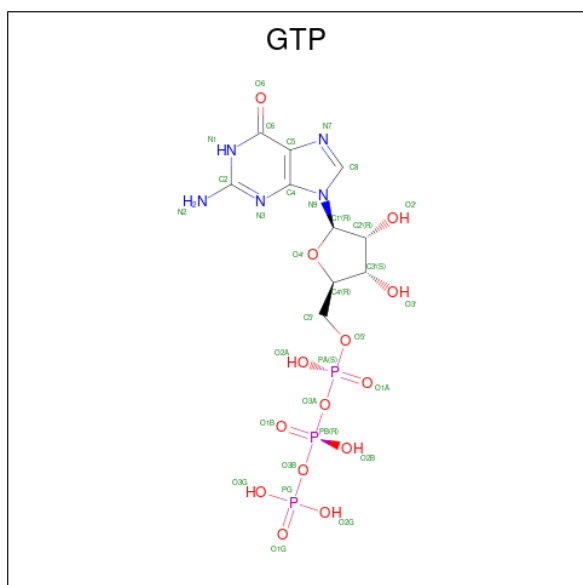
Mol	Chain	Residues	Atoms				AltConf
75	1H	1	Total	C	O	P	0
			51	32	17	2	
75	1L	1	Total	C	O	P	0
			76	57	17	2	
75	1N	1	Total	C	O	P	0
			62	43	17	2	
75	1X	1	Total	C	O	P	0
			86	67	17	2	
75	1d	1	Total	C	O	P	0
			65	46	17	2	
75	1h	1	Total	C	O	P	0
			80	61	17	2	
75	1q	1	Total	C	O	P	0
			61	42	17	2	
75	3A	1	Total	C	O	P	0
			58	39	17	2	

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Mol	Chain	Residues	Atoms				AltConf
75	3G	1	Total	C	O	P	0
			52	33	17	2	
75	3G	1	Total	C	O	P	0
			56	37	17	2	
75	3N	1	Total	C	O	P	0
			43	24	17	2	
75	3P	1	Total	C	O	P	0
			56	37	17	2	
75	3T	1	Total	C	O	P	0
			57	38	17	2	
75	4B	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	
75	4D	1	Total	C	O	P	0
			100	81	17	2	
75	8B	1	Total	C	O	P	0
			100	81	17	2	
75	8C	1	Total	C	O	P	0
			100	81	17	2	
75	8D	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 76 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

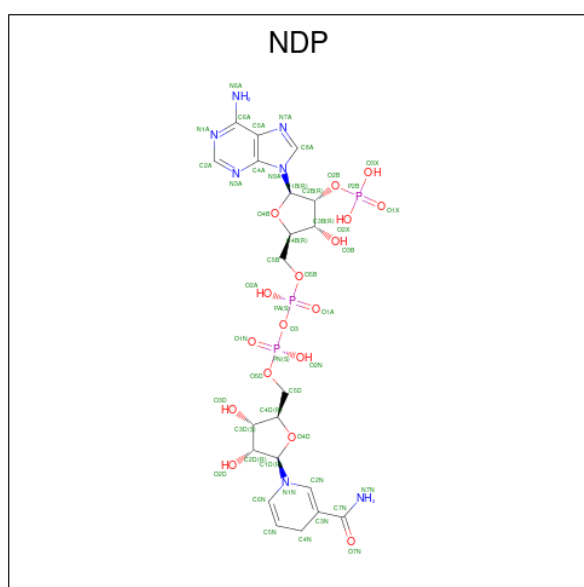


Mol	Chain	Residues	Atoms					AltConf
76	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 77 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
77	1O	1	Total	Mg	0
			1	1	
77	4A	1	Total	Mg	0
			1	1	
77	8A	1	Total	Mg	0
			1	1	

- Molecule 78 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
78	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 79 is ZINC ION (CCD ID: ZN) (formula: Zn).

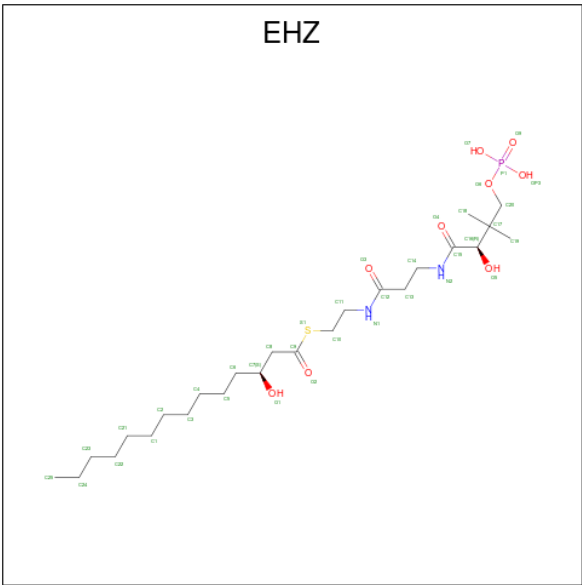
Mol	Chain	Residues	Atoms		AltConf
79	1R	1	Total	Zn	0
			1	1	
79	4F	1	Total	Zn	0
			1	1	

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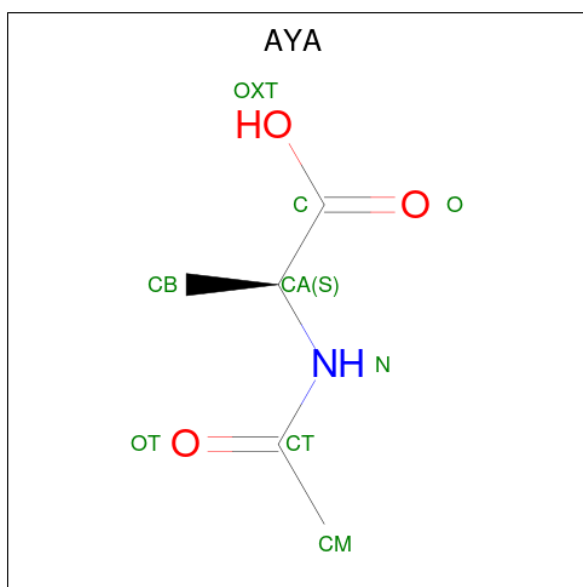
Mol	Chain	Residues	Atoms		AltConf
79	8F	1	Total	Zn	0
			1	1	

- Molecule 80 is {S}-[2-[3-[[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



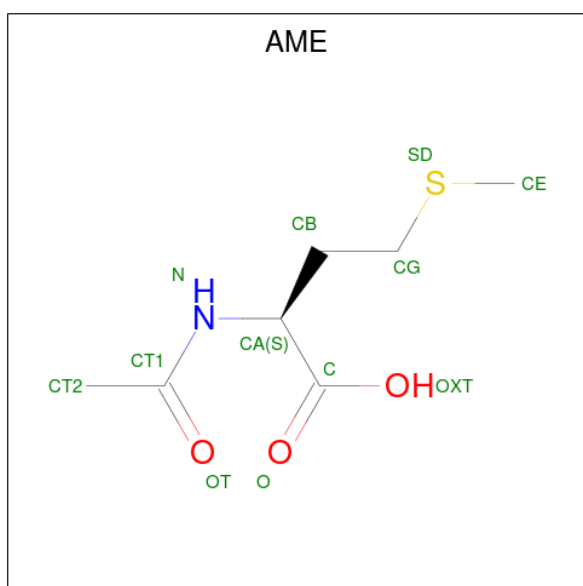
Mol	Chain	Residues	Atoms						AltConf
80	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 81 is N-ACETYLALANINE (CCD ID: AYA) (formula: C₅H₉NO₃).



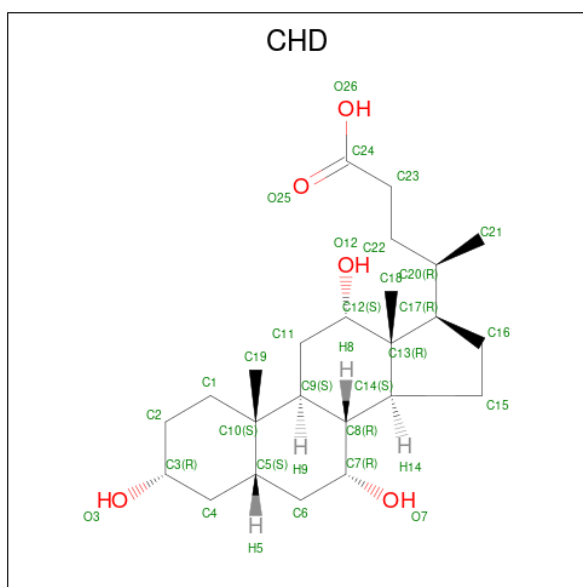
Mol	Chain	Residues	Atoms				AltConf
81	1Y	1	Total	C	N	O	0
			8	5	1	2	
81	1q	1	Total	C	N	O	0
			8	5	1	2	

- Molecule 82 is N-ACETYL METHIONINE (CCD ID: AME) (formula: $C_7H_{13}NO_3S$).



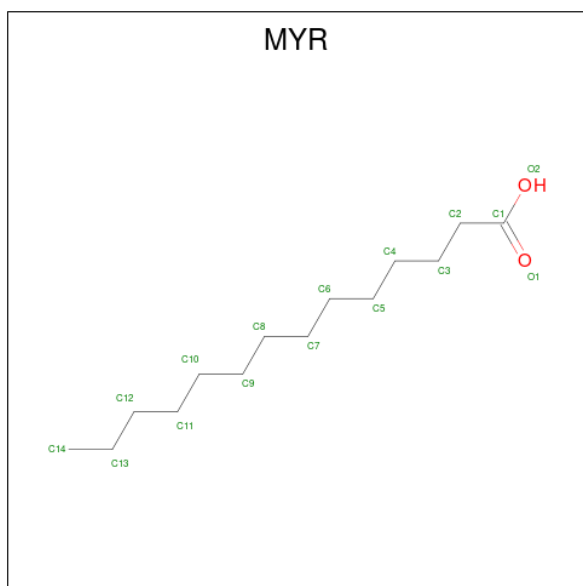
Mol	Chain	Residues	Atoms					AltConf
82	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 83 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



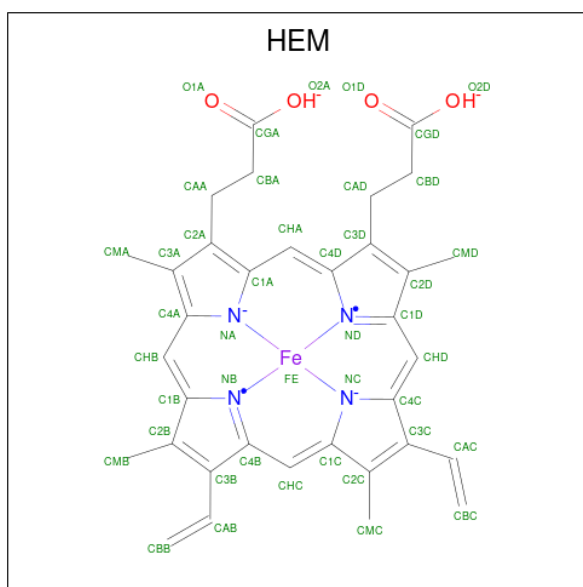
Mol	Chain	Residues	Atoms			AltConf
83	1i	1	Total	C	O	0
			29	24	5	

- Molecule 84 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



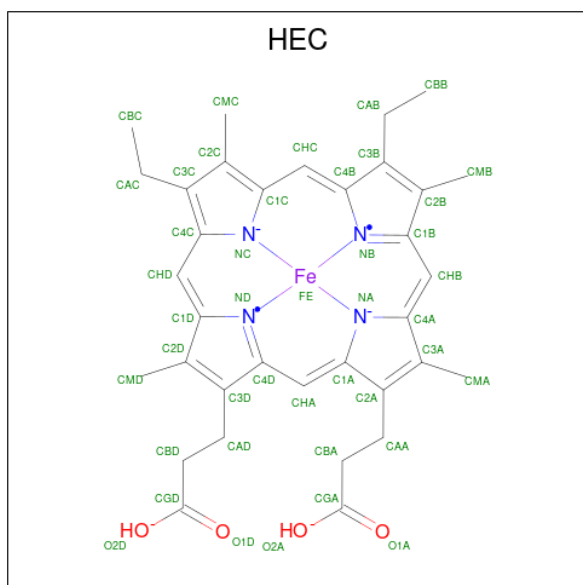
Mol	Chain	Residues	Atoms			AltConf
84	1l	1	Total	C	O	0
			15	14	1	

- Molecule 85 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



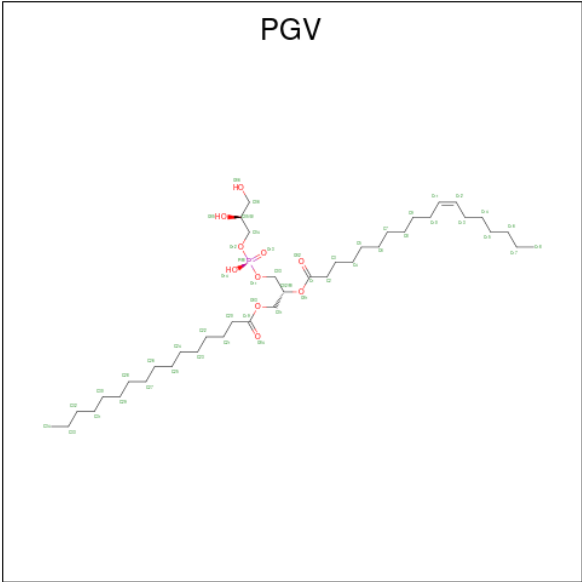
Mol	Chain	Residues	Atoms					AltConf
85	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
85	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
85	3P	1	Total 43	C 34	Fe 1	N 4	O 4	0
85	3P	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 86 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					AltConf
86	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
86	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 87 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



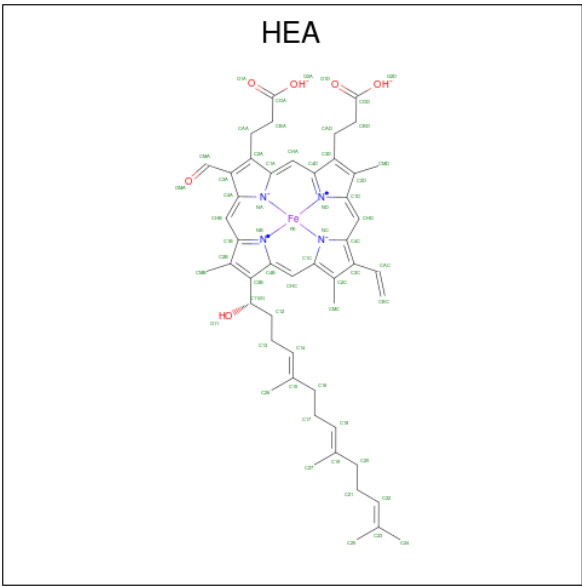
Mol	Chain	Residues	Atoms				AltConf
87	4A	1	Total	C	O	P	0
			51	40	10	1	
87	4A	1	Total	C	O	P	0
			51	40	10	1	
87	4A	1	Total	C	O	P	0
			51	40	10	1	
87	4B	1	Total	C	O	P	0
			51	40	10	1	
87	4B	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	

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Mol	Chain	Residues	Atoms				AltConf
87	4C	1	Total 51	C 40	O 10	P 1	0
87	4G	1	Total 51	C 40	O 10	P 1	0
87	4J	1	Total 51	C 40	O 10	P 1	0
87	4K	1	Total 51	C 40	O 10	P 1	0
87	4L	1	Total 51	C 40	O 10	P 1	0
87	4M	1	Total 51	C 40	O 10	P 1	0
87	8A	1	Total 51	C 40	O 10	P 1	0
87	8A	1	Total 51	C 40	O 10	P 1	0
87	8A	1	Total 51	C 40	O 10	P 1	0
87	8B	1	Total 51	C 40	O 10	P 1	0
87	8B	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8G	1	Total 51	C 40	O 10	P 1	0
87	8J	1	Total 51	C 40	O 10	P 1	0
87	8K	1	Total 51	C 40	O 10	P 1	0
87	8L	1	Total 51	C 40	O 10	P 1	0

- Molecule 88 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
88	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0
88	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0
88	8A	1	Total 60	C 49	Fe 1	N 4	O 6	0
88	8A	1	Total 60	C 49	Fe 1	N 4	O 6	0

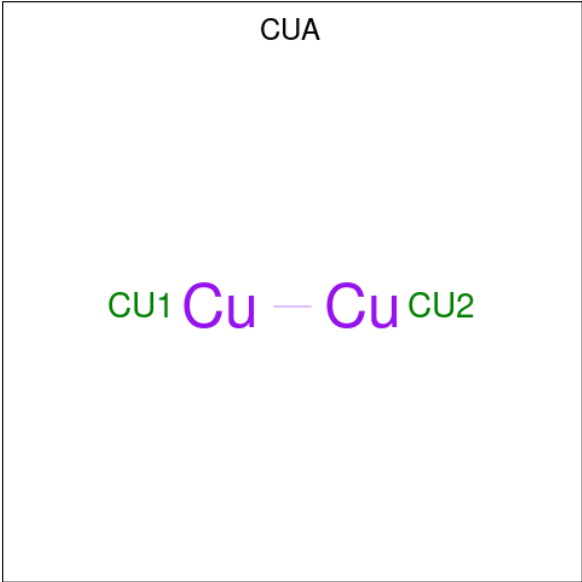
- Molecule 89 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 90 is SODIUM ION (CCD ID: NA) (formula: Na).

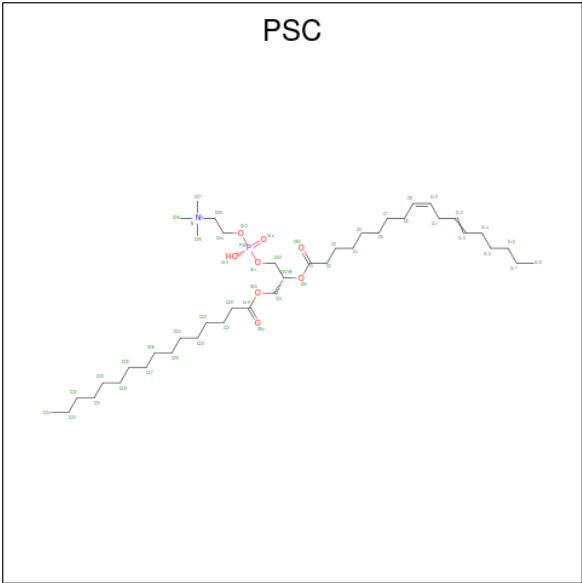
Mol	Chain	Residues	Atoms		AltConf
90	4A	1	Total	Na	0
			1	1	
90	8A	1	Total	Na	0
			1	1	

- Molecule 91 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



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

- Molecule 92 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).



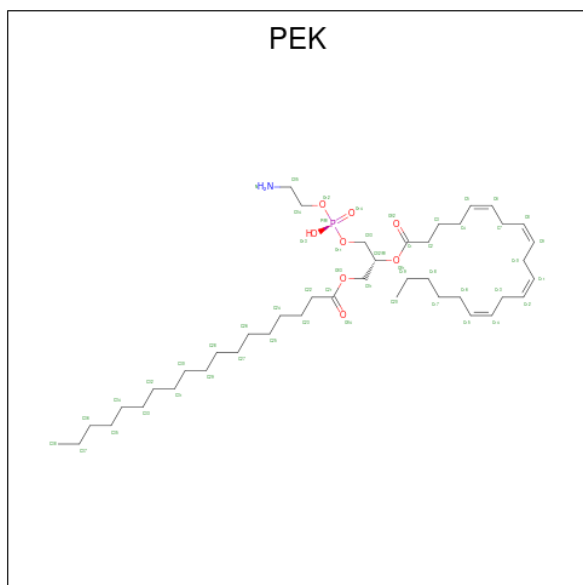
Mol	Chain	Residues	Atoms					AltConf
92	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	

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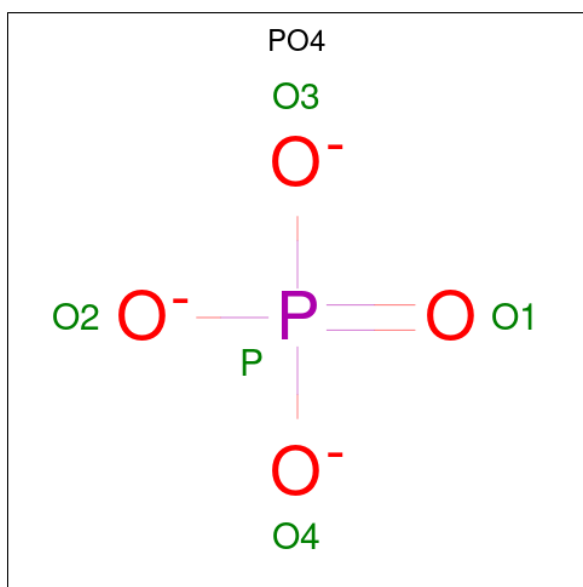
Mol	Chain	Residues	Atoms					AltConf
92	8B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 93 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
93	4C	1	Total	C	N	O	P	0
			52	42	1	8	1	
93	4G	1	Total	C	N	O	P	0
			53	43	1	8	1	
93	8C	1	Total	C	N	O	P	0
			52	42	1	8	1	
93	8G	1	Total	C	N	O	P	0
			53	43	1	8	1	

- Molecule 94 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

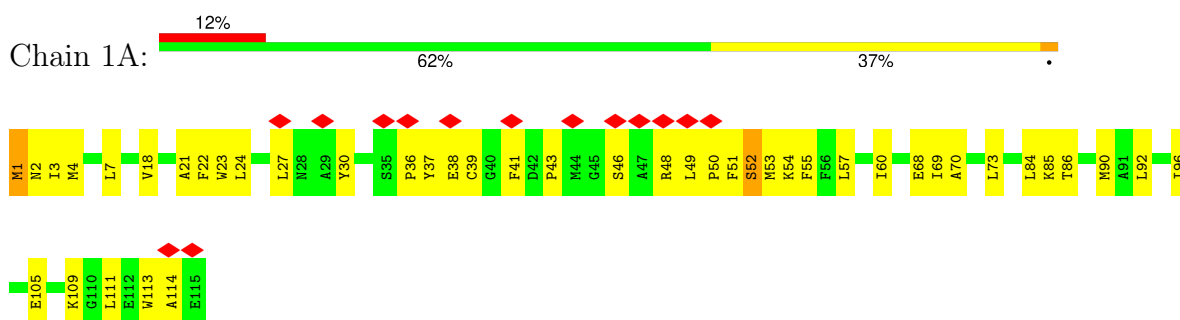


Mol	Chain	Residues	Atoms			AltConf
94	4H	1	Total	O	P	0
			5	4	1	
94	8H	1	Total	O	P	0
			5	4	1	

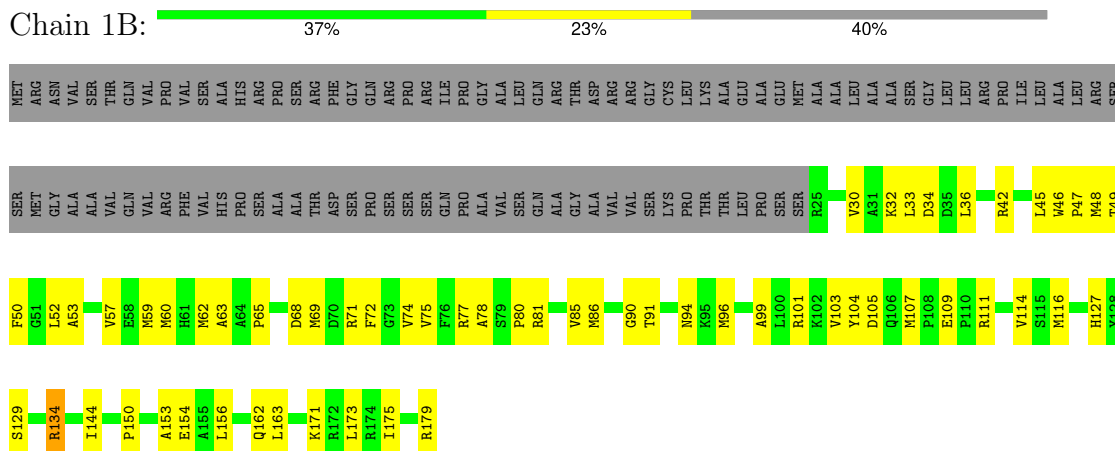
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

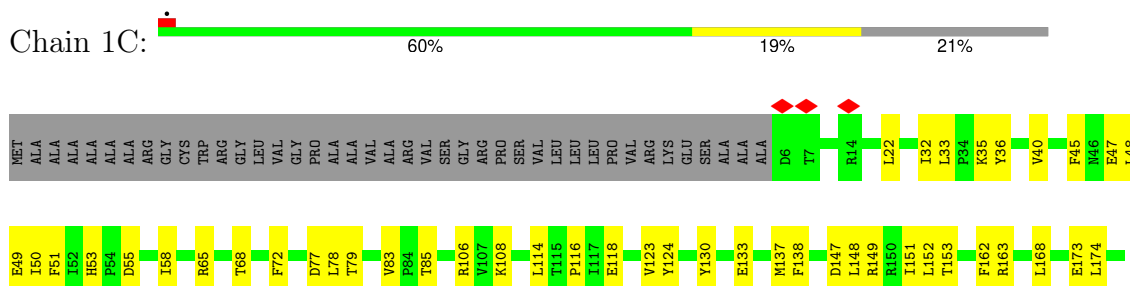
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

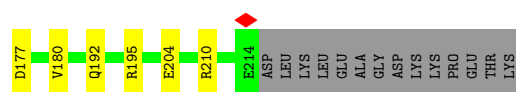


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

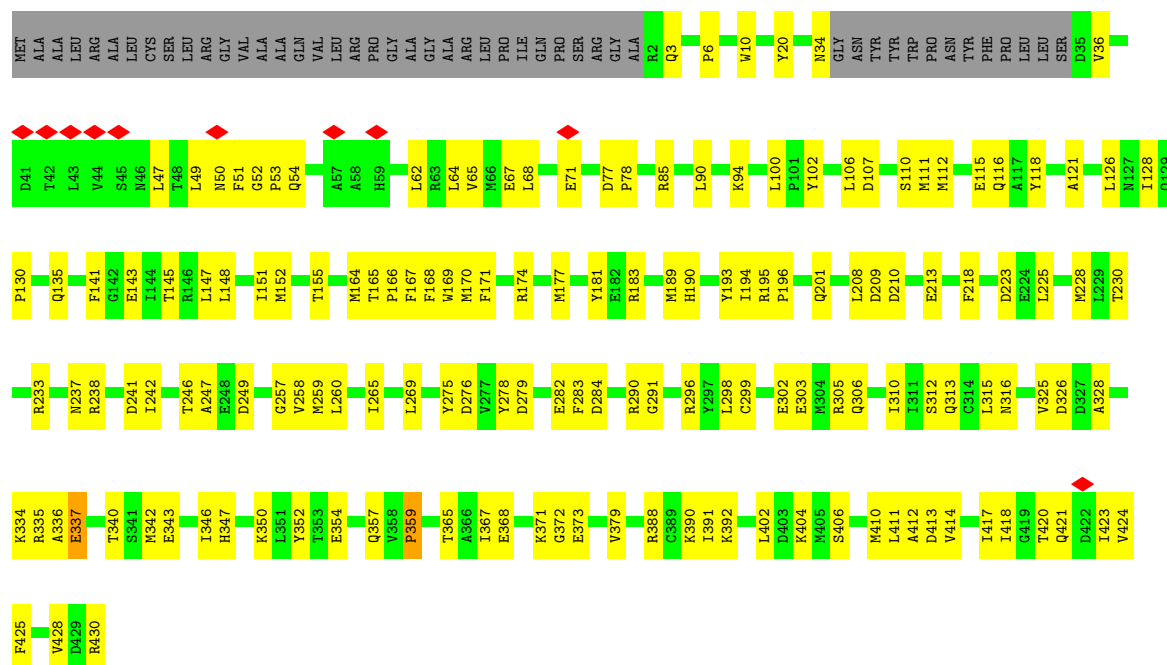


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

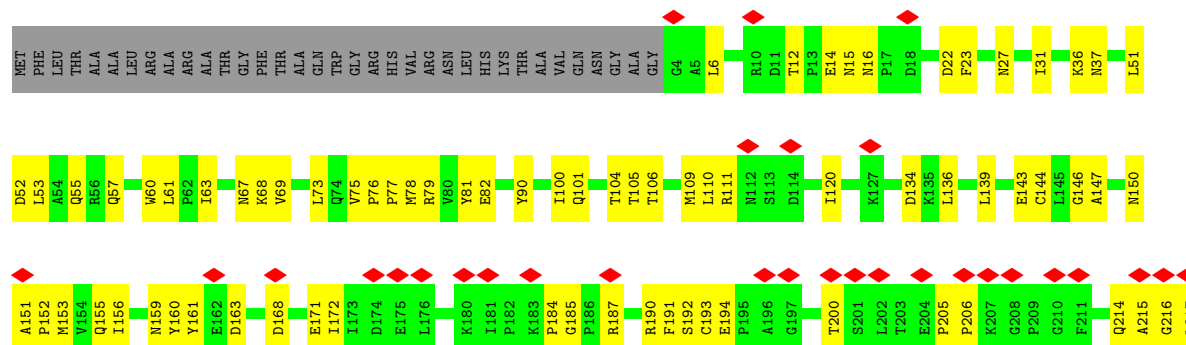




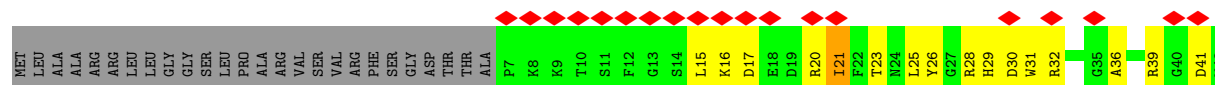
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

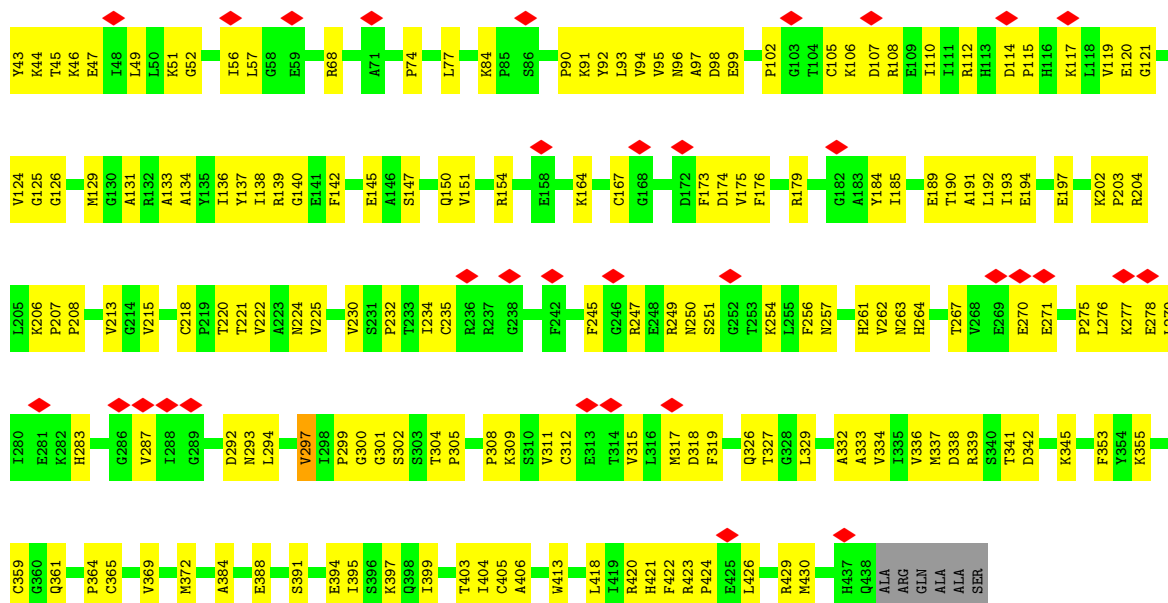


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



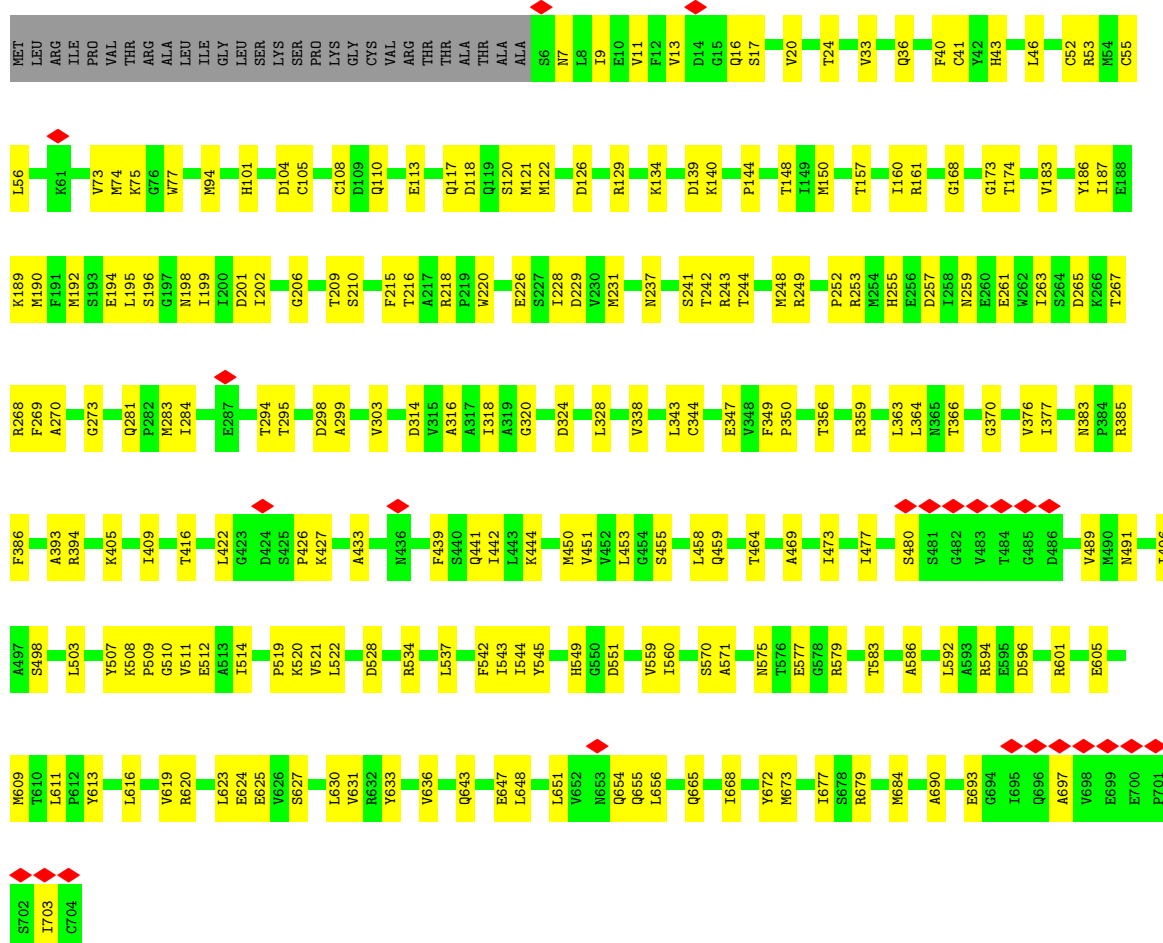
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



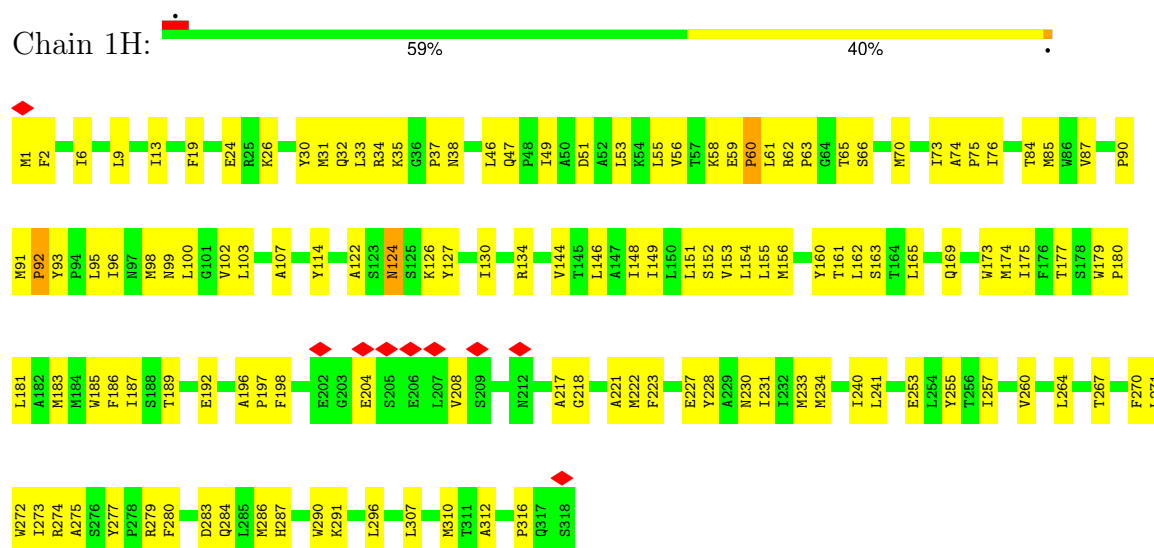


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

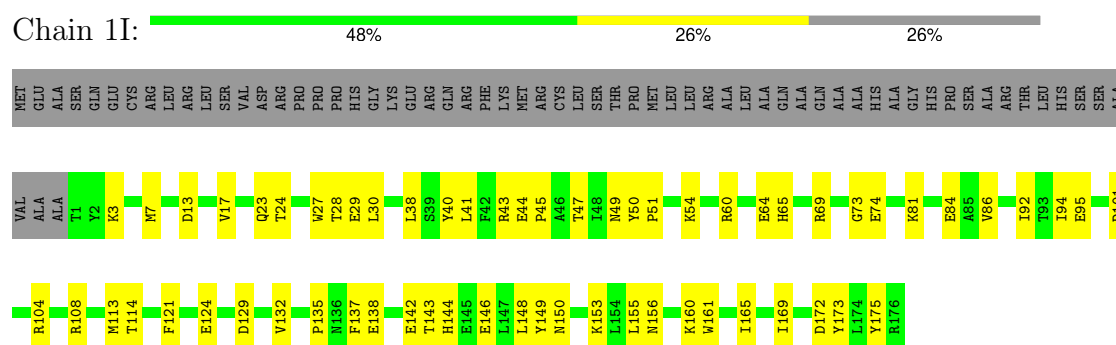
Chain 1G: 66% 30%



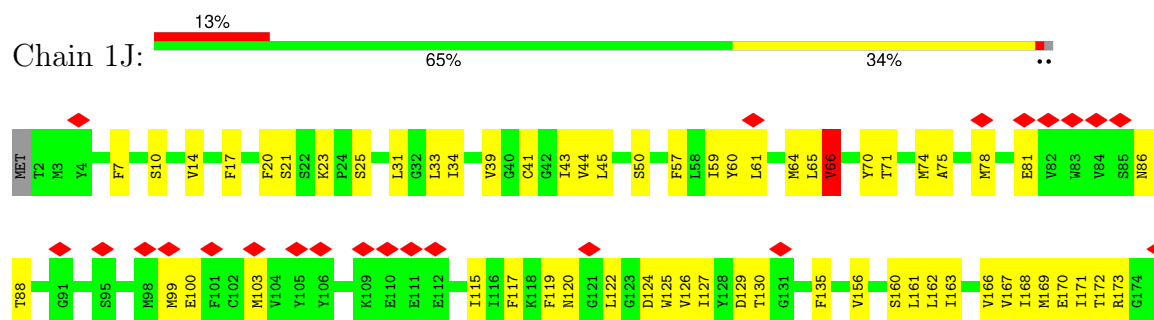
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



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



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

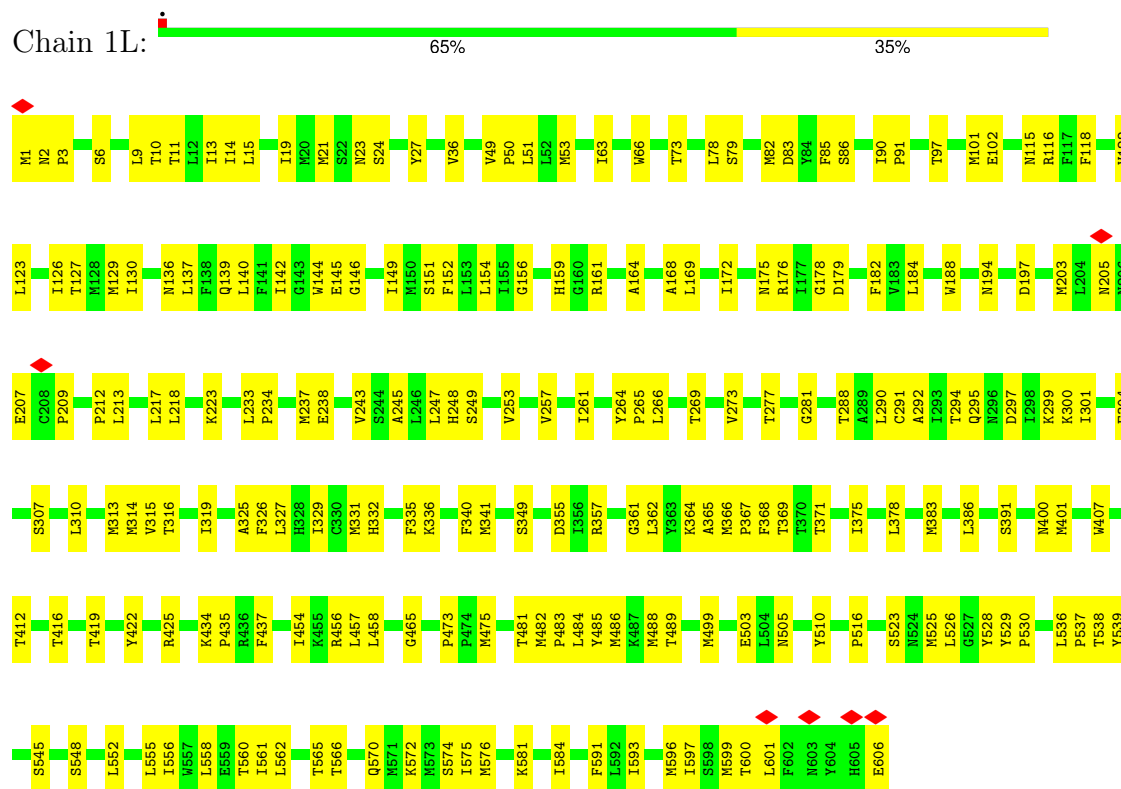


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

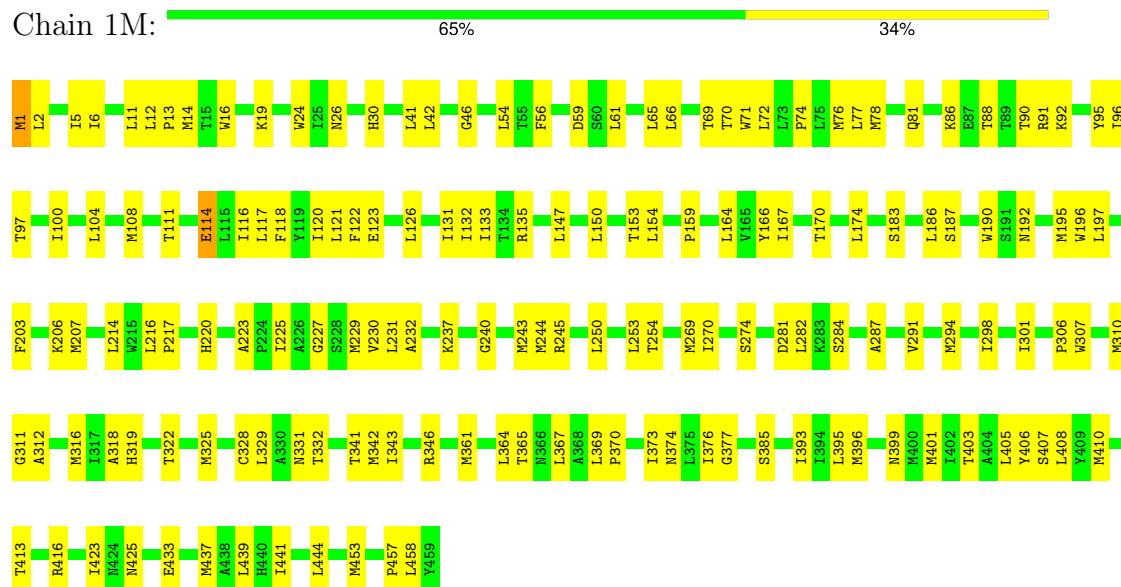




• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

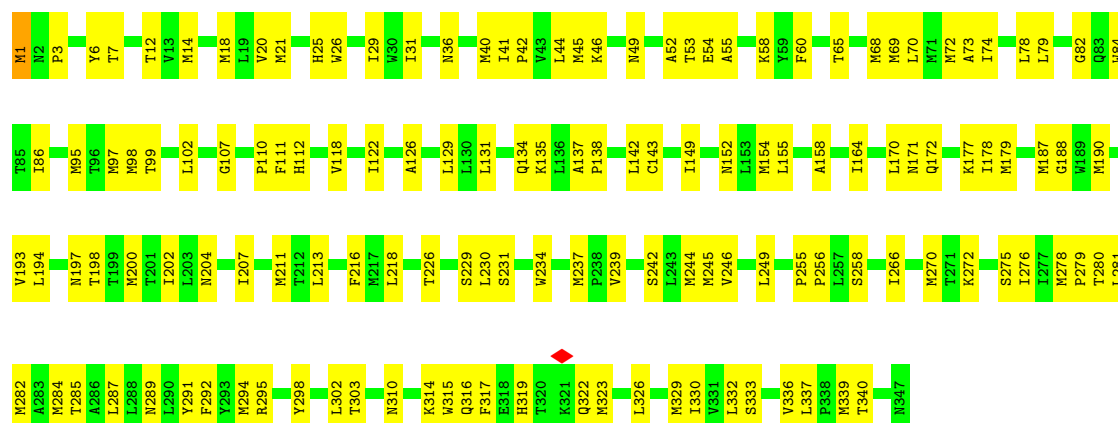


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



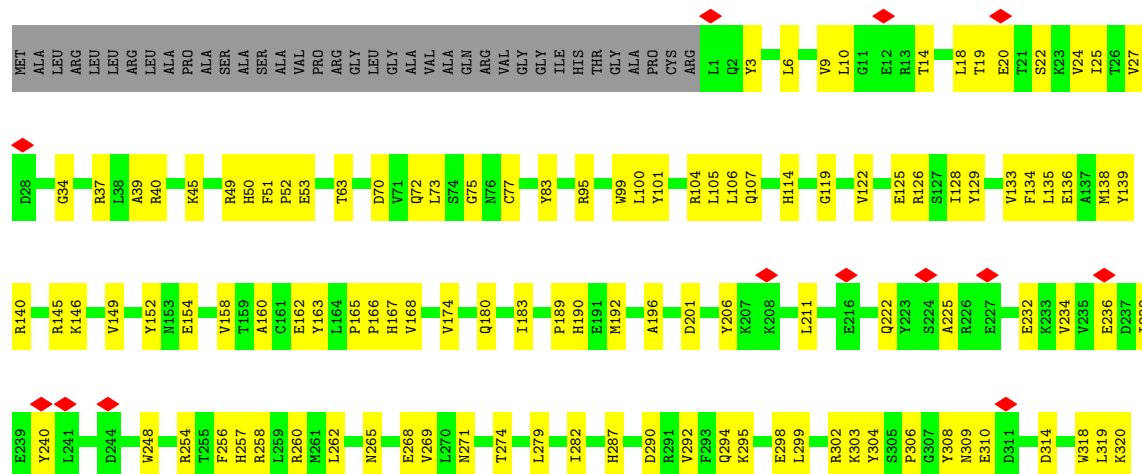
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N:  60% 40%



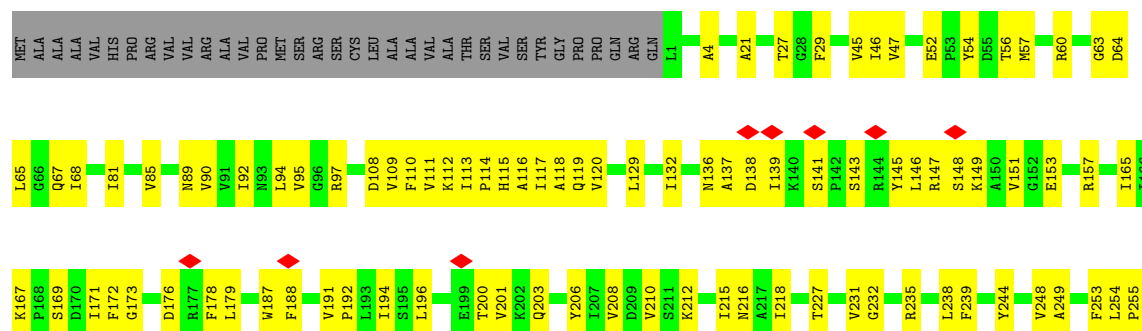
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 1O:  58% 32% 10%



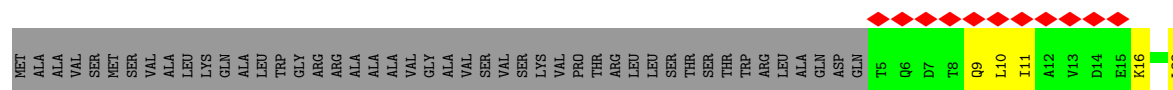
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:  60% 31% 9%

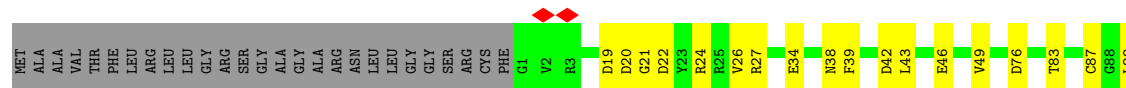




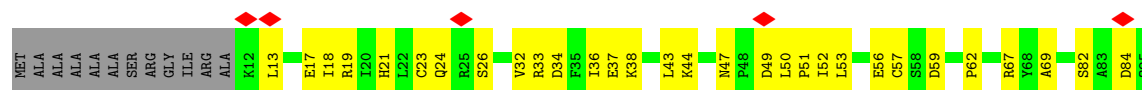
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



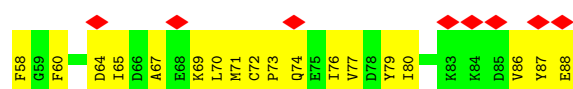
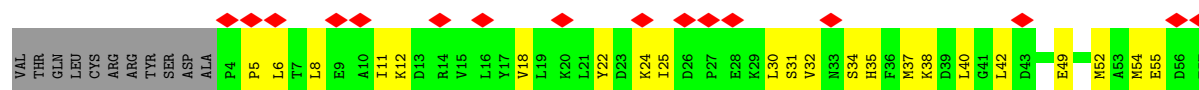
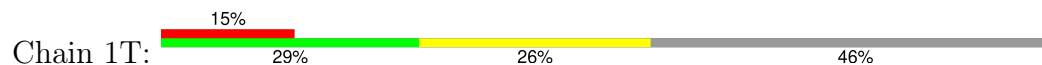
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



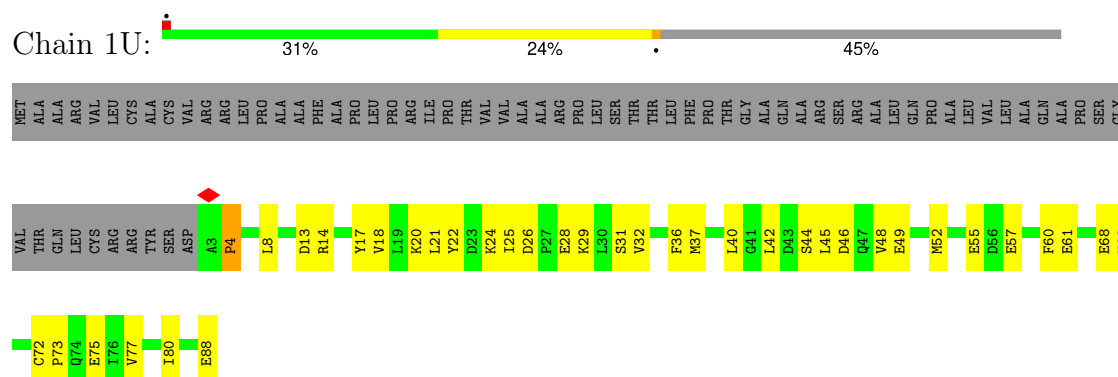
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



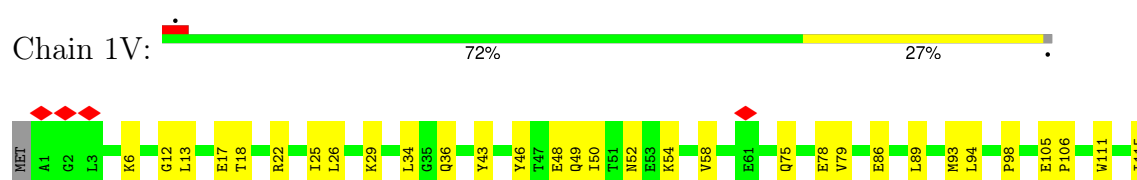
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



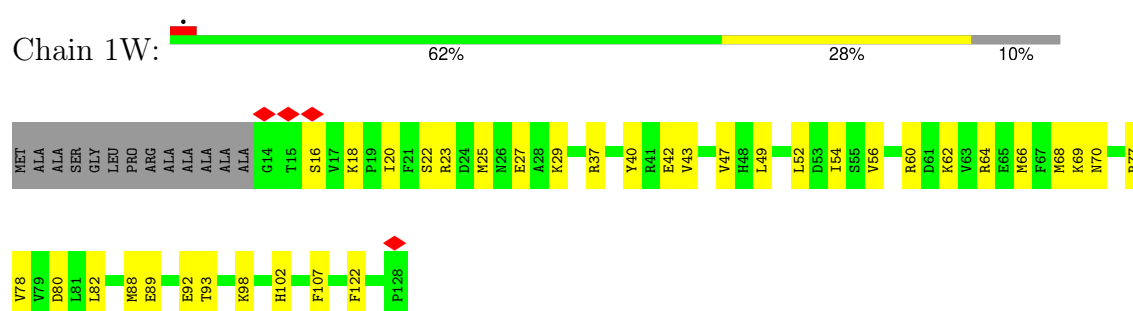
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



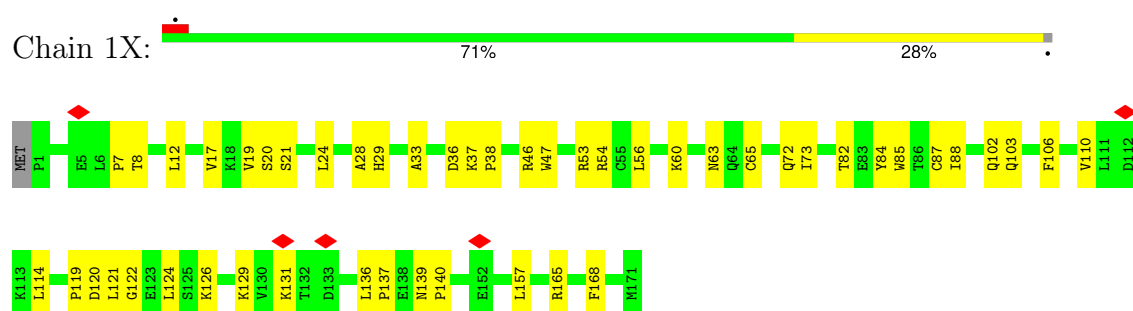
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



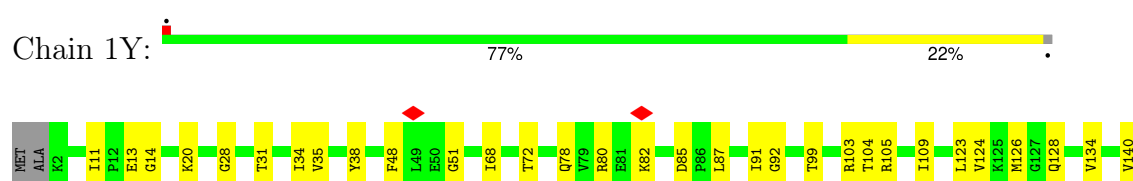
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



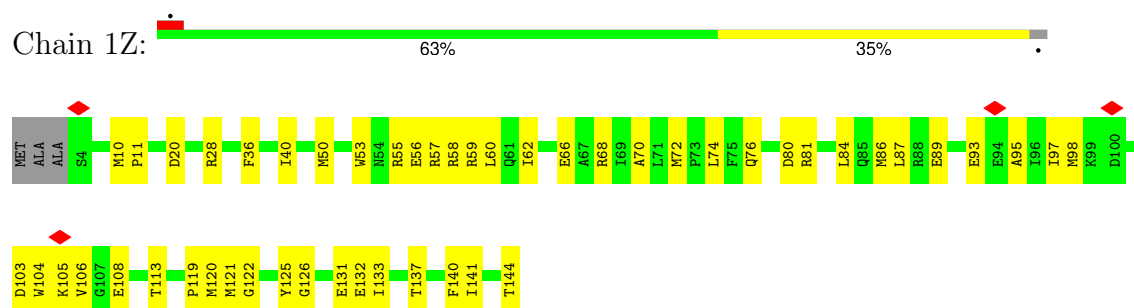
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



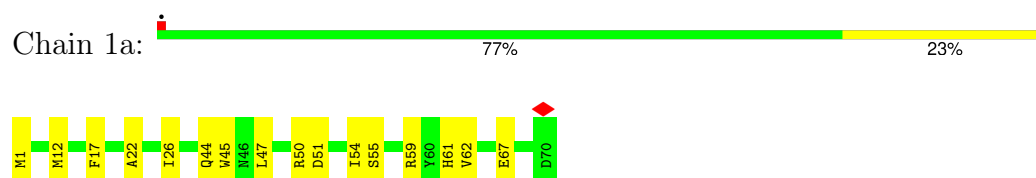
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



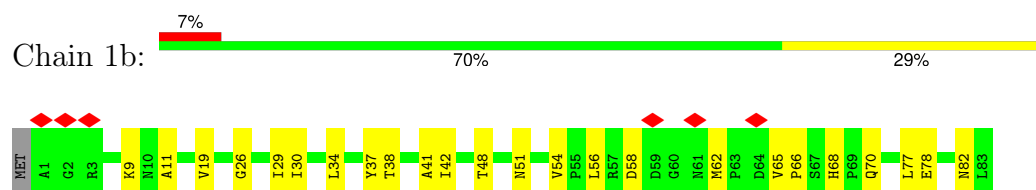
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



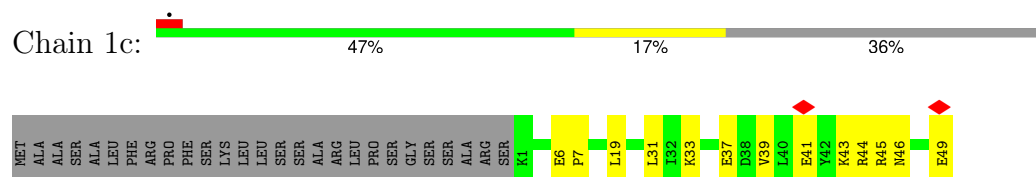
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



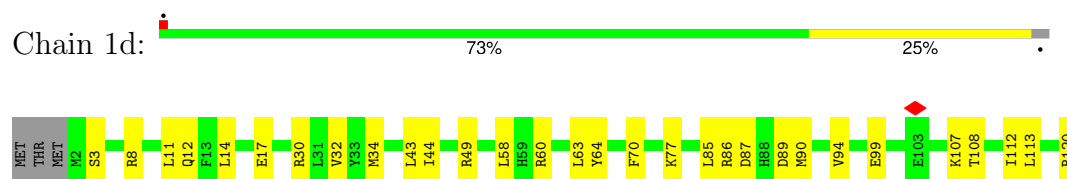
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



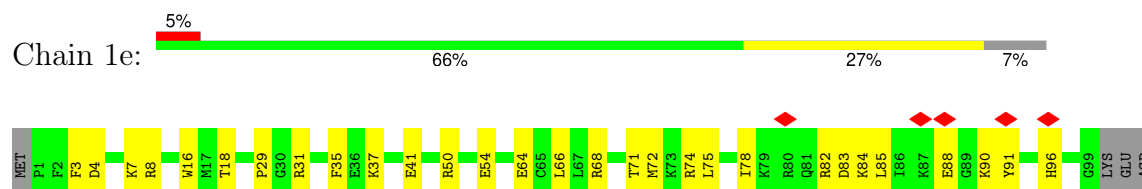
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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

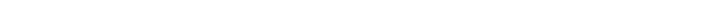


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



PRO
ARG
PRO

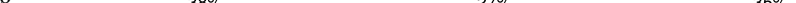
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 1f: 

MET	ALA	ALA	ALA	ALA	ILE	LEU	LYS	LEU	GLU	GLU	THR	ARG	GLY	GLY	GLY	GLU	LYS	CYS	ASP	LYS	ASN	GLN	GLY	VAL	LYS	GLY	ARG	ARG	PHE	MET	ILE	SER	ARG	SER	SER	PRO	HIS	LEU	ALA	ALA	PRO	ALA	ASN	GLY	ARG	ARG	SER	SER	PHE	ARG	ARG	ARG	TRP	TRP	LEU	LEU	GLY	SER
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[illegible]

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

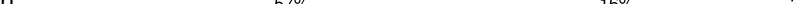
Chain 1g: 

MET	ALA	ALA	GLY	VAL	LEU	GLY	LEU	CYS	ALA	ARG	ARG	LEU	LEU	ALA	ALA	ALA	THR	ARG	GLY	LEU	PRO	ALA	ALA	ARG	VAL	ARG	TRP	TRP	GLU	SER	GLY	SER	SER	ARG	ALA	VAL	ILE	ALA	PRO	SER	SER	ALA	LEU	VAL	GLY	LYS	ARG	ARG	PRO	PRO	GLU	PRO	T23	T24	F25	L26	Q27	E28	F33
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N41	S44	D48	K49	D50	P51	I52	V53	D54	L55	M58	R59	F63	F66	S67	I68	V71	L72	G73	V77	L80	P81	D82	Y83	R84	E87	R90	A93	E94	R95	L96	V97	R100	L107	M108	N111	C112	F113	D114	K117	Q119	L120	P121
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ASP
GLU
ASP

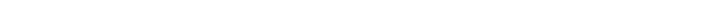
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h: 

MET	ALA	ALA	MET	MET	LEU	LEU	GLN	ARG	ALA	ALA	SER	VAL	THR	ALA	VAL	ALA	THR	LEU	SER	SER	ARG	ARG	ARG	LEU	GLY	THR	ARG	PHE	GLY	PHE	PHE	GLY	GLY	PHE	LEU	THR	HIS	GLY	PHE	PRO	LYS	THR	THR	GLY	ALA	PRO	VAL	ARG	HIS	SER	GLY	ASP	GLY	HIS	GLY	KE	111	K12	P13	639	140
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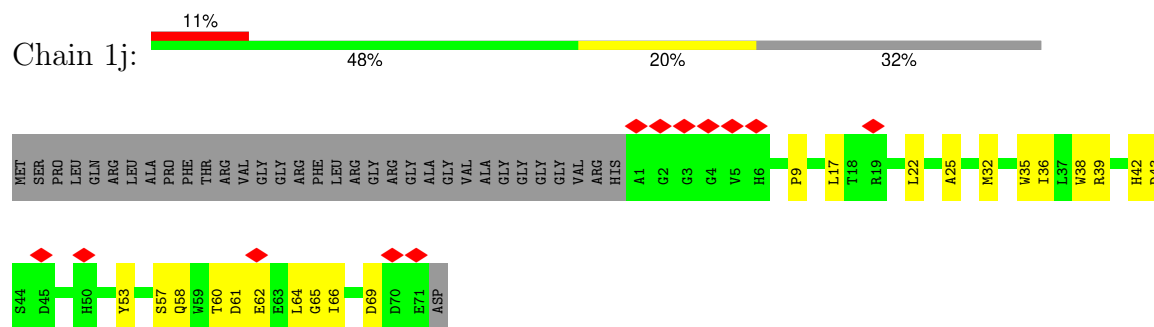
Category	Count
M44	100
V45	100
A50	100
D54	100
I55	100
P56	100
H63	100
H69	100
W74	100
A76	100
R77	100
F78	100
F79	100
Y80	100
D81	100
E84	100
E88	100
L94	100
Q95	100
I96	100
R104	100
L105	100
K106	100
E107	100
L108	100
E109	100
V110	100
R111	100
M114	100
R115	100
P121	100
D134	100
K138	100
T139	100
D142	100
M143	100

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

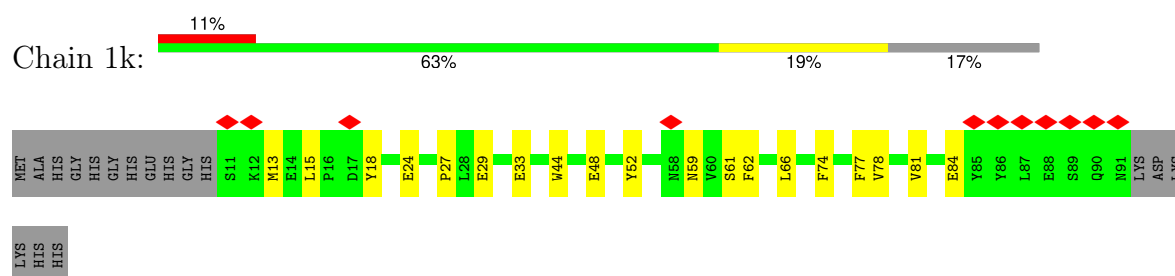
Chain 1i: 

H82	H83	H84	L85	K86	Y87	H88	V89	K92	P93	Y94	T95	V96	R99	K100	P105	T108	E111	V114	V115	M119	D124	Q125	H126	H127	ACE0	E7	K8	L9	Q13	L14	R15	E16	R19	E31	P36	R37	R38	V39	W40	P41	M42	E43	Q44	F45	W46	M47	F48	F49	L50	Q51	D52	G53	A54	P55	W56	K57	N58	V59	I60	Y61	K62	T63	Y64	R65	H66	S67	I68	F69	A70	T71	T72	H73	V74	P77	V78	W79	I80
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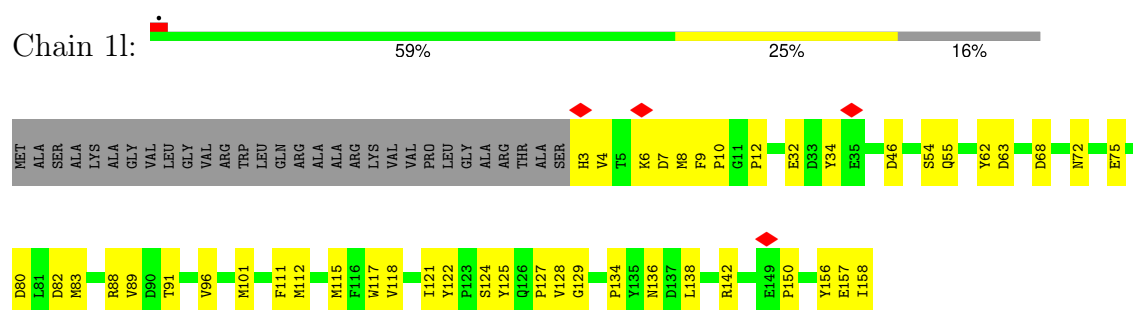
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



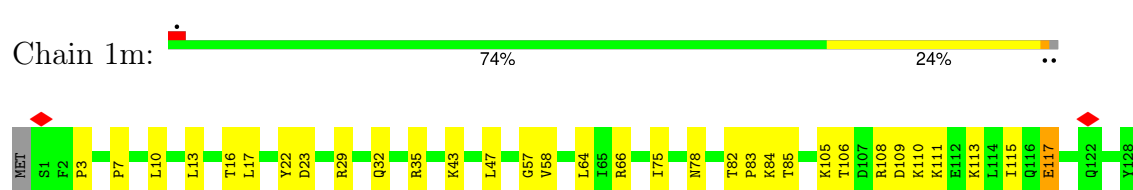
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



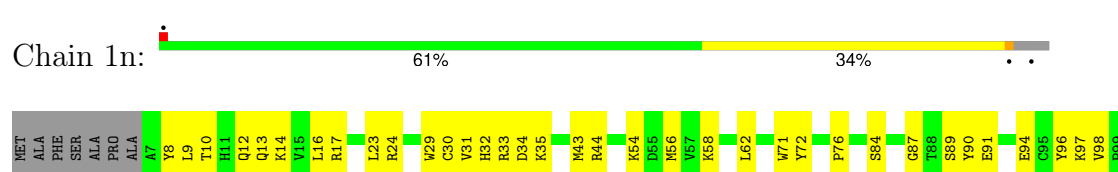
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

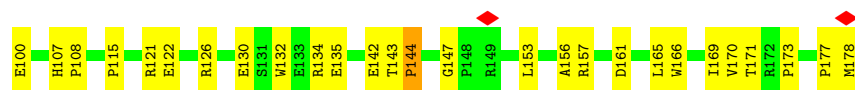


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

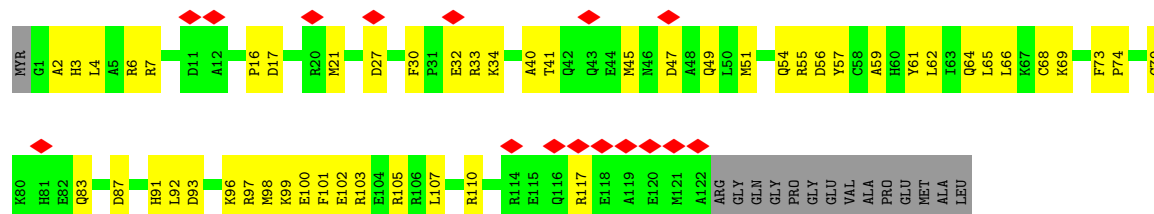


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

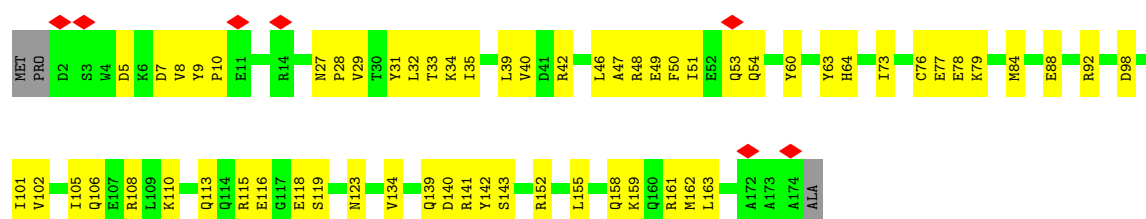




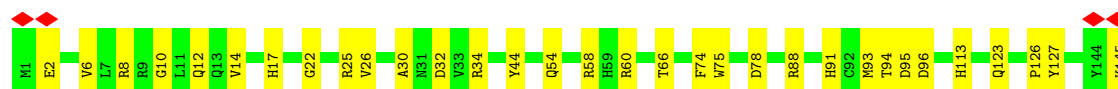
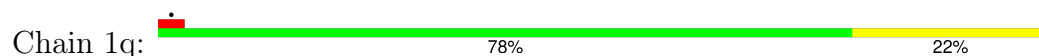
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



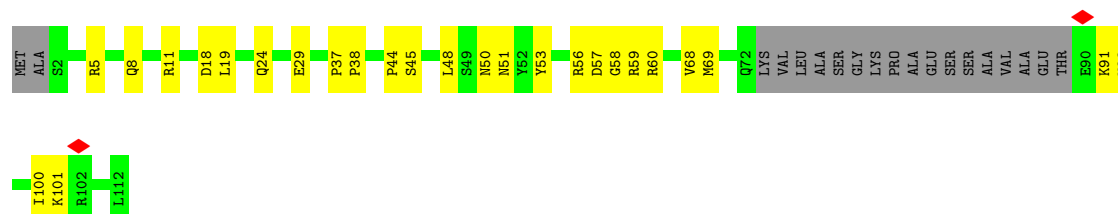
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

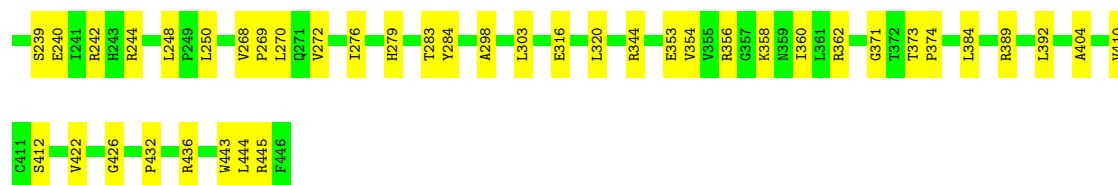


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



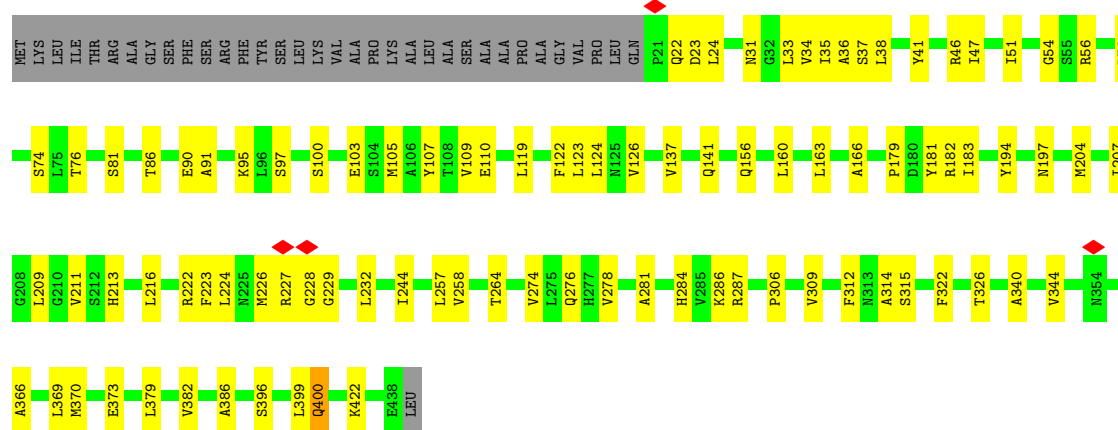
- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial





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

Chain 3B: 72% 21% 8%



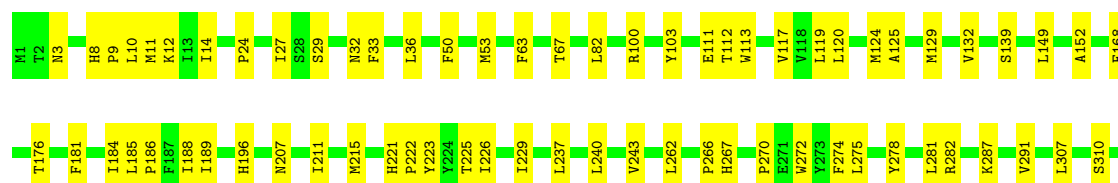
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3O: 72% 20% 8%



- Molecule 47: Cytochrome b

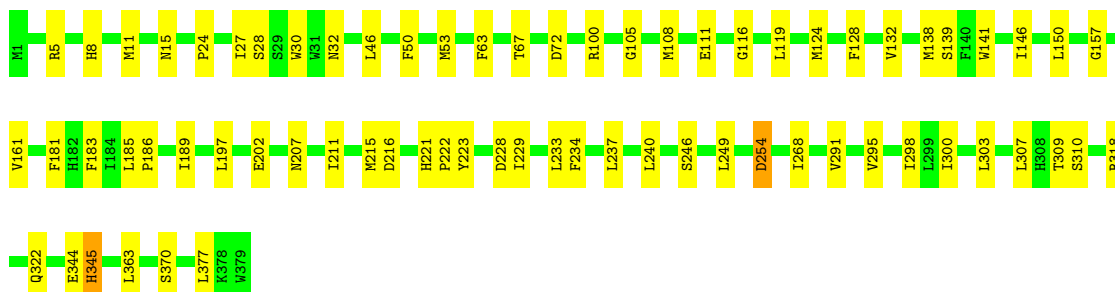
Chain 3C: 79% 21%





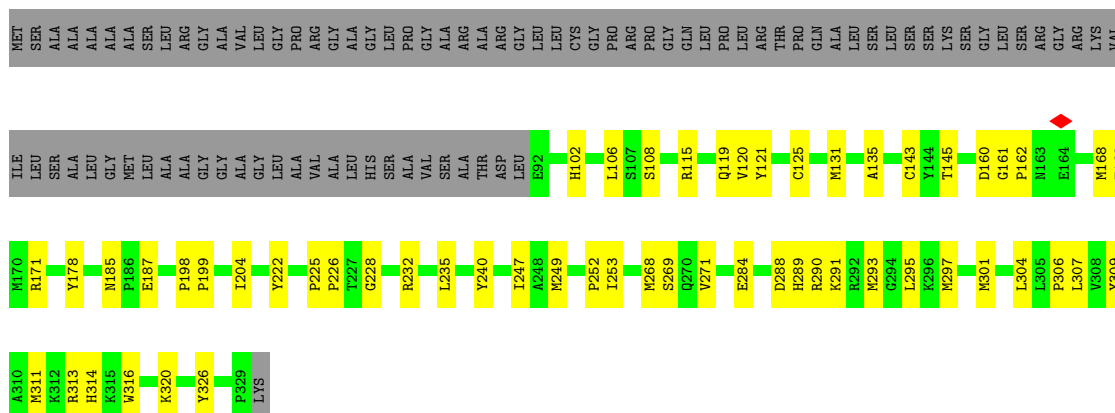
• Molecule 47: Cytochrome b

Chain 3P: 82% 18%



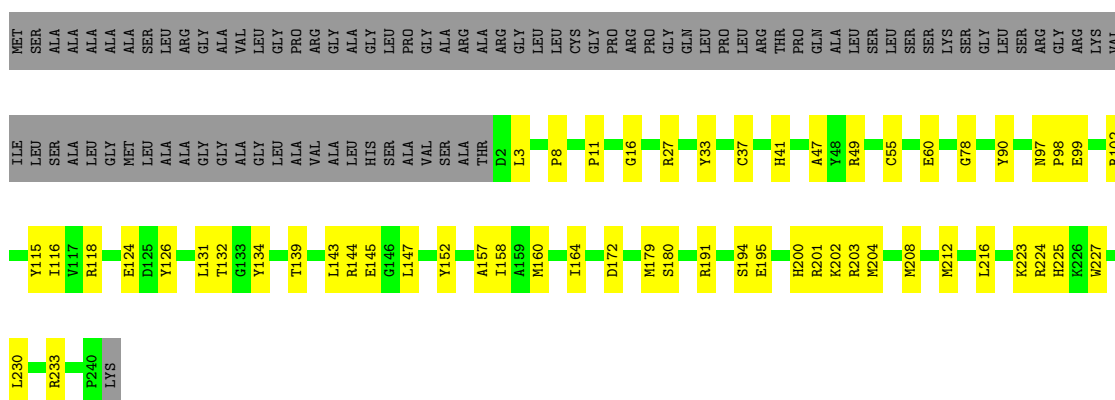
• Molecule 48: Cytochrome c1

Chain 3D: 55% 17% 27%

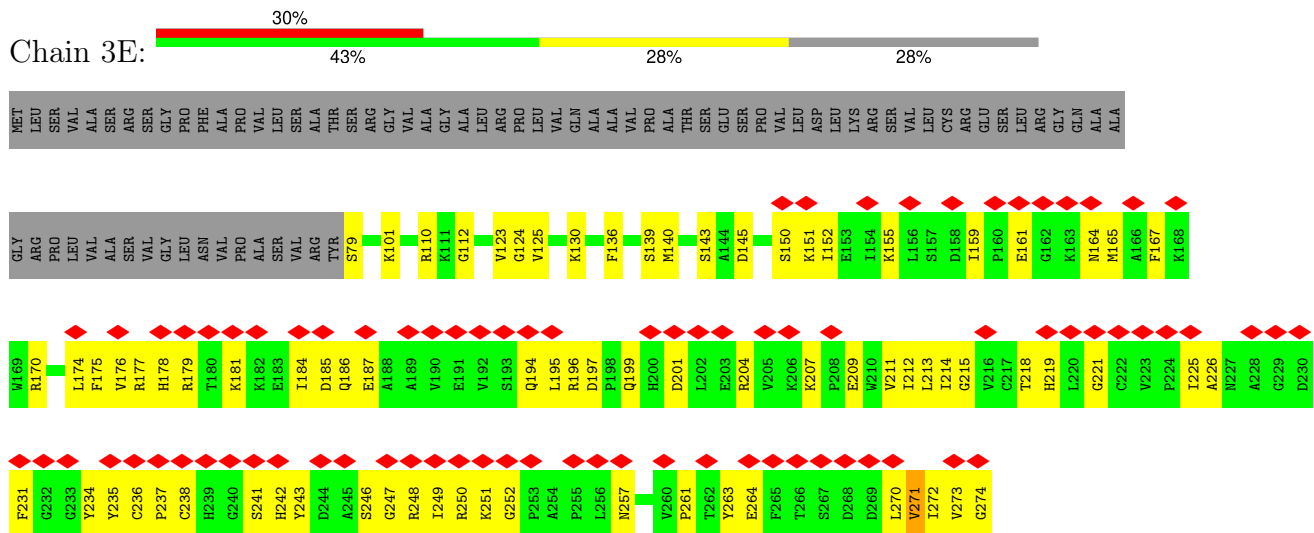


• Molecule 48: Cytochrome c1

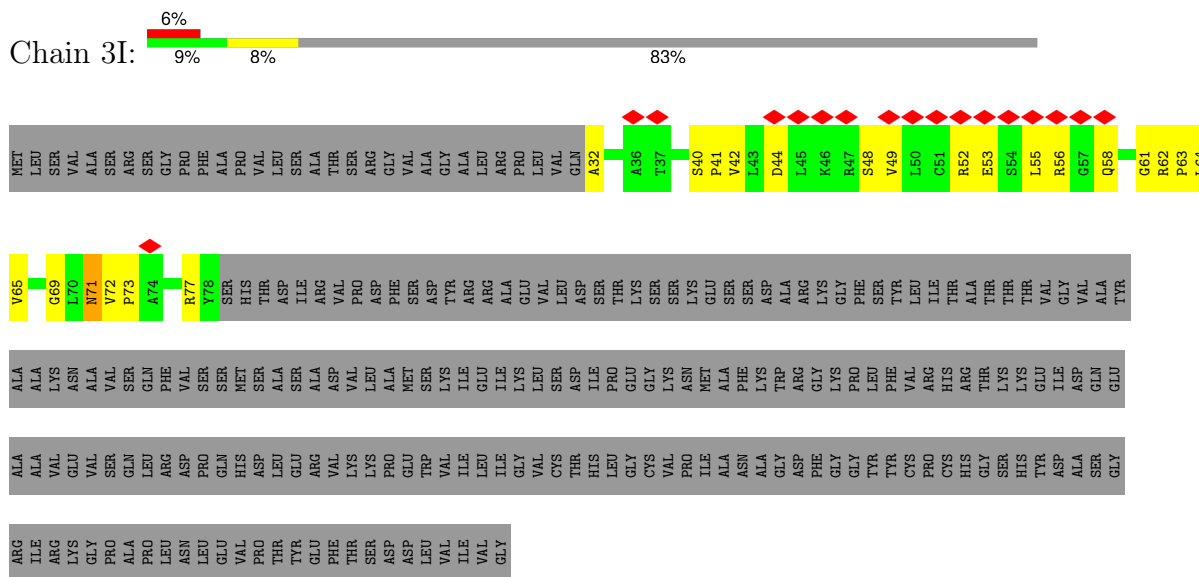
Chain 3Q: 56% 17% 27%



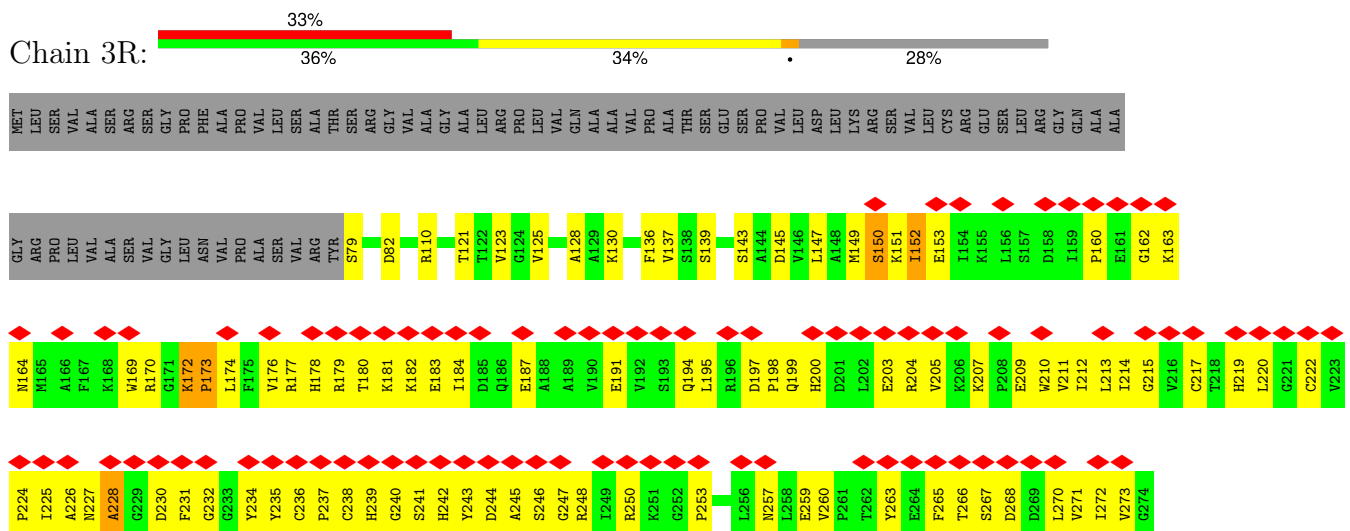
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

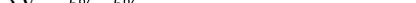


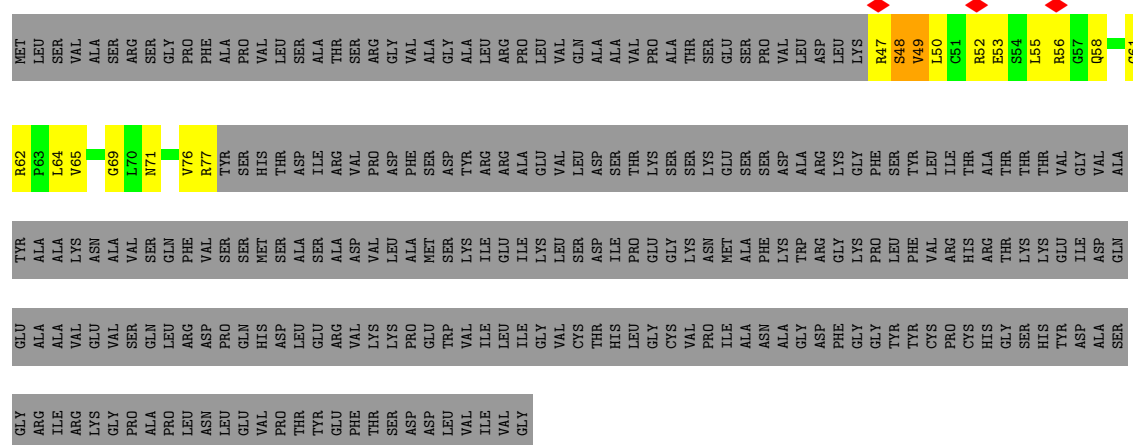
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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

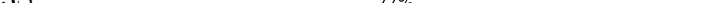


- Chain 3V:  5% 5% 89%

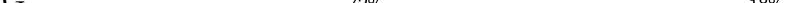


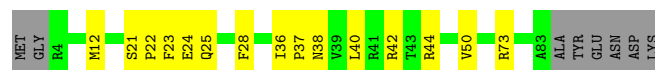
- Chain 3F:  71% 17% 12%

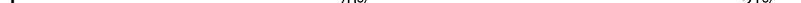


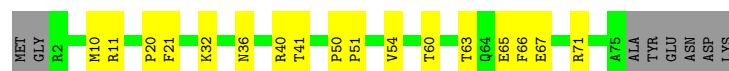
- Chain 3S:  77% 11% 12%

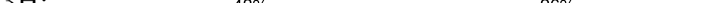


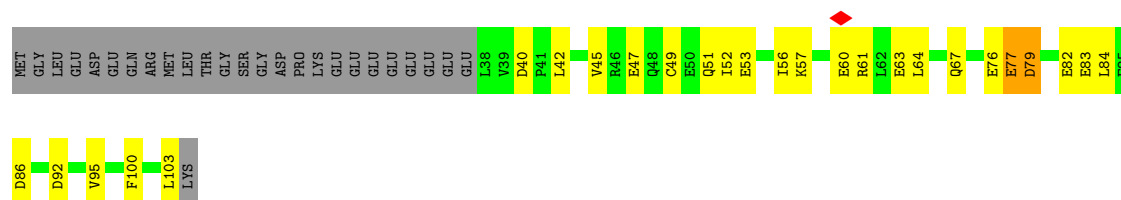
- Chain 3G: 



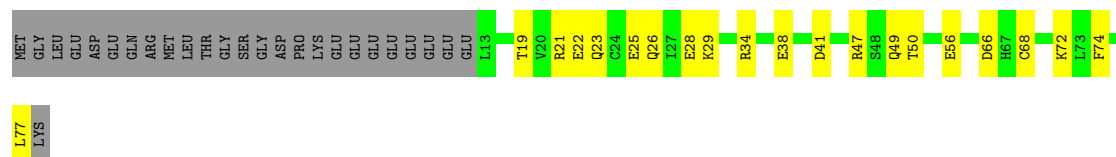
- Chain 3T: 



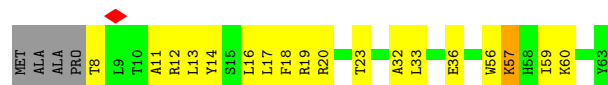
- Chain 3H: 



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



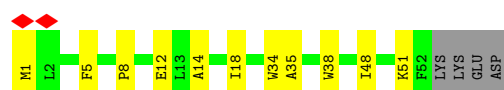
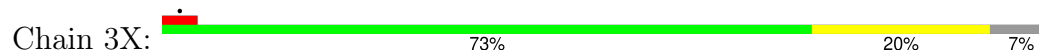
- Molecule 53: Complex III subunit 9



- Molecule 53: Complex III subunit 9



- Molecule 54: Cytochrome b-c1 complex subunit 10

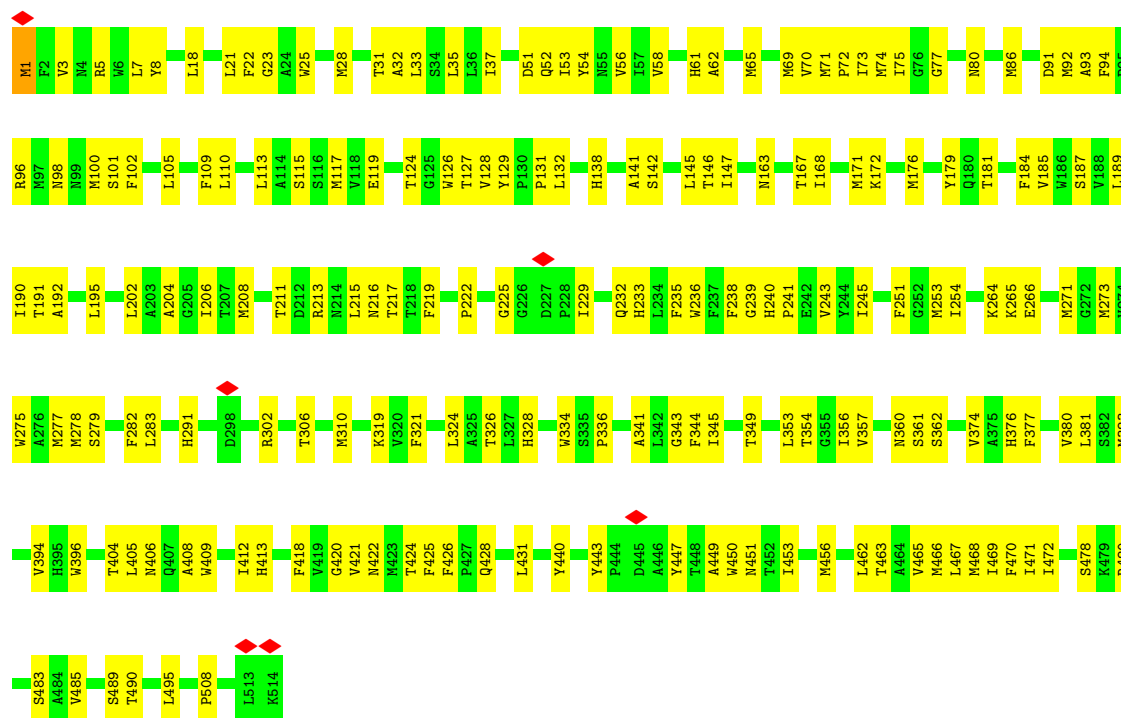


- Molecule 54: Cytochrome b-c1 complex subunit 10

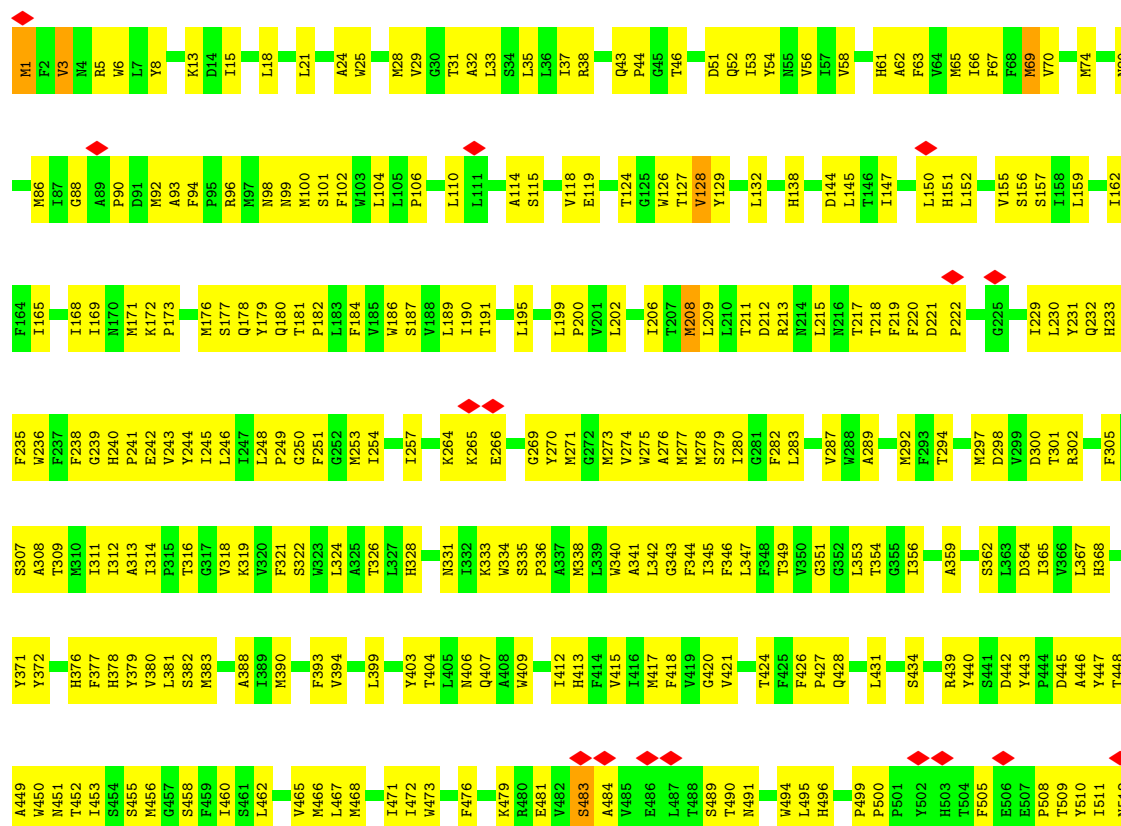


- Molecule 55: Cytochrome c oxidase subunit 1

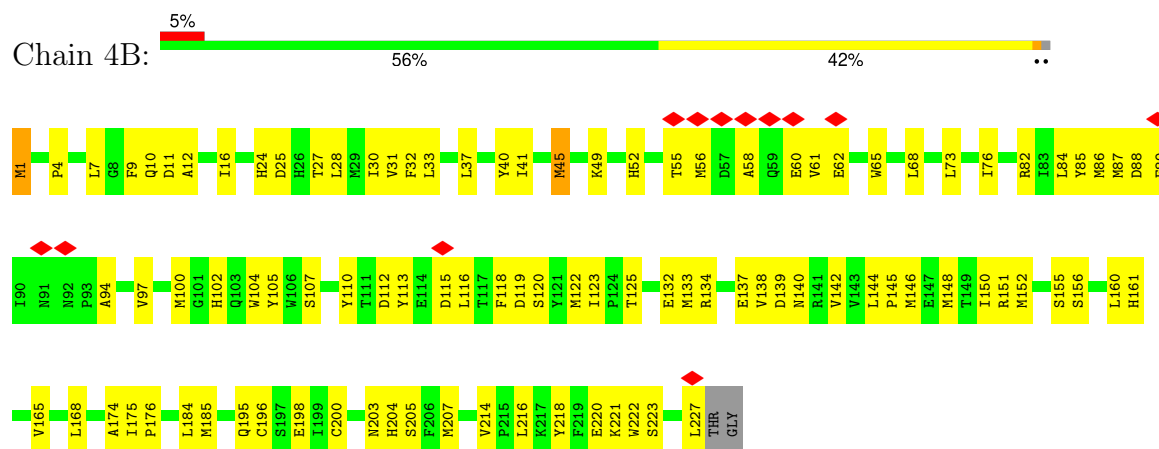




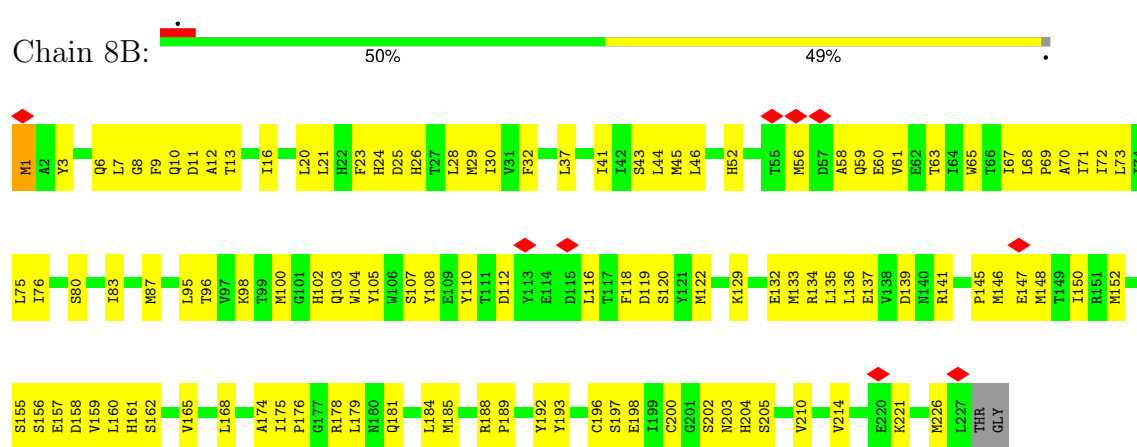
• Molecule 55: Cytochrome c oxidase subunit 1



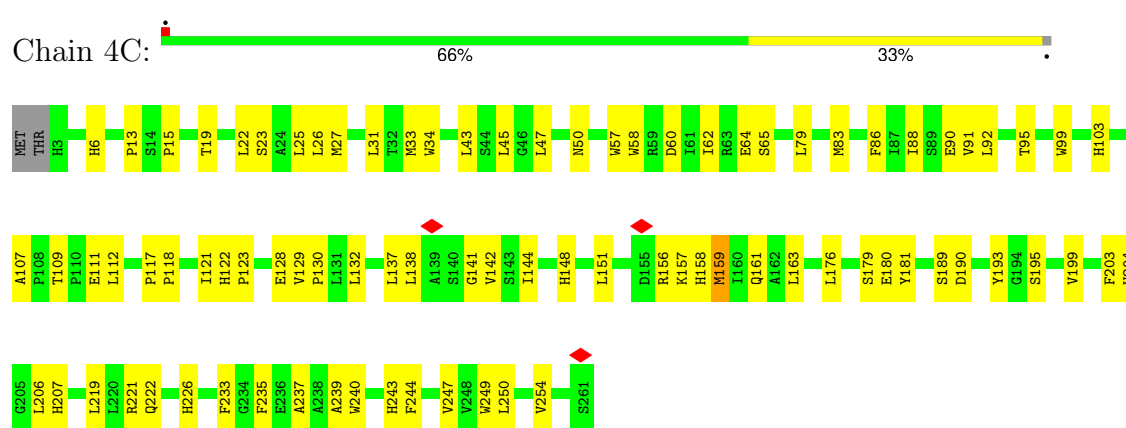
- Molecule 56: Cytochrome c oxidase subunit 2



- Molecule 56: Cytochrome c oxidase subunit 2

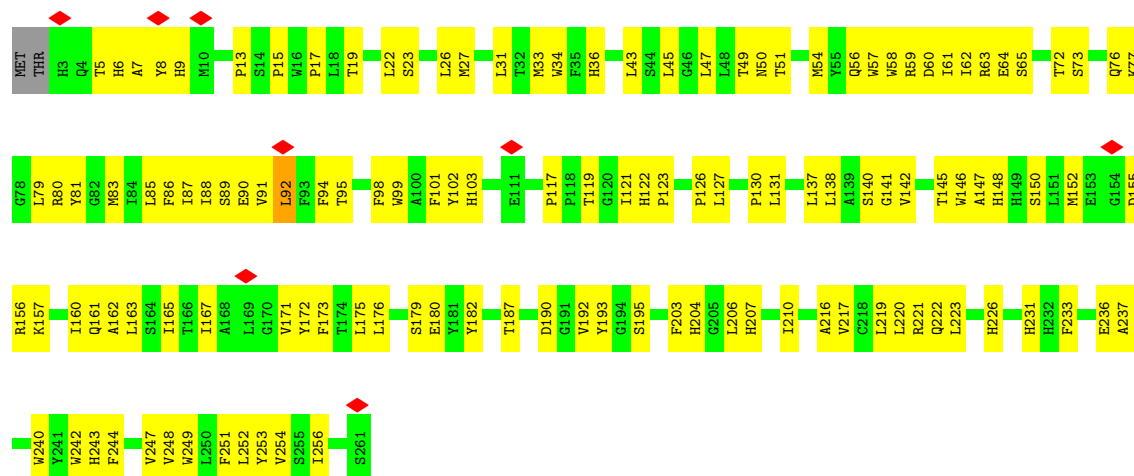


- Molecule 57: Cytochrome c oxidase subunit 3

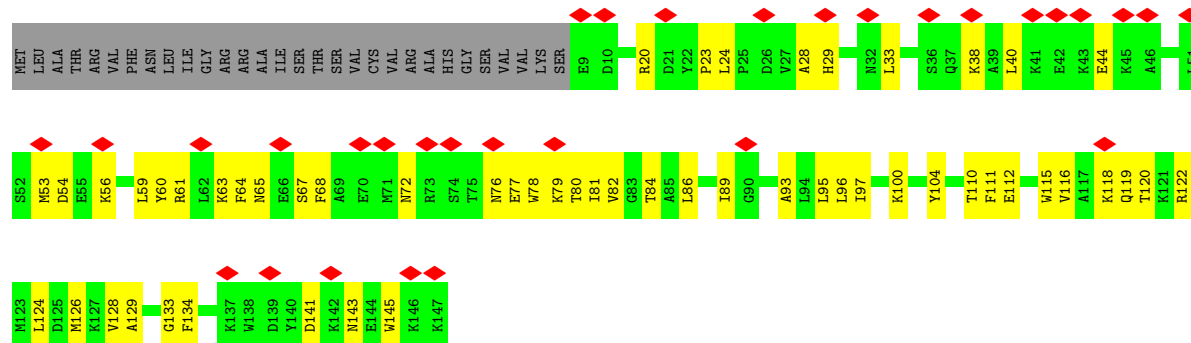


- Molecule 57: Cytochrome c oxidase subunit 3

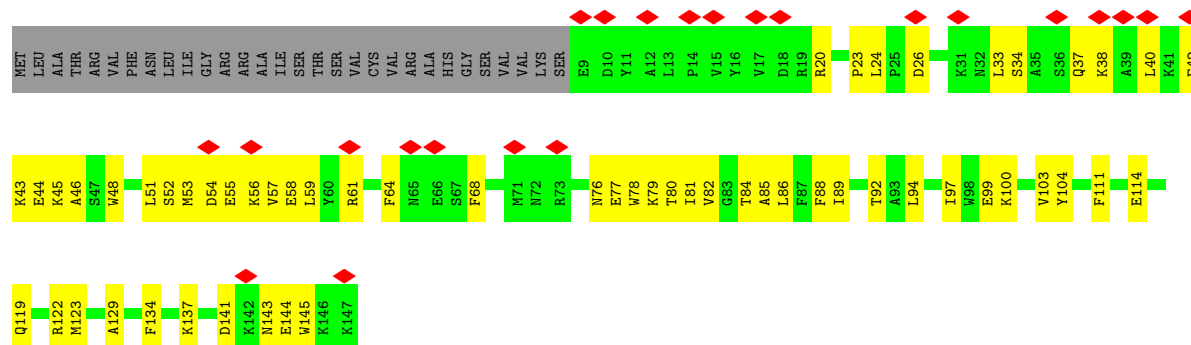




• Molecule 58: Cytochrome c oxidase subunit 4

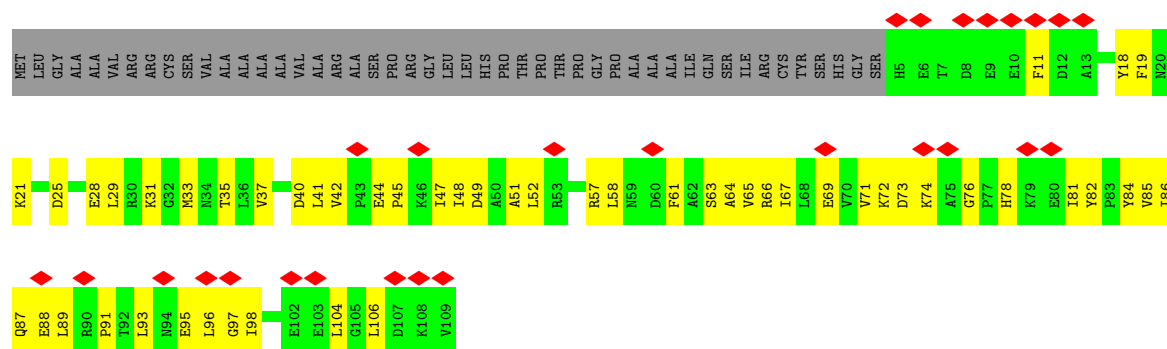


• Molecule 58: Cytochrome c oxidase subunit 4

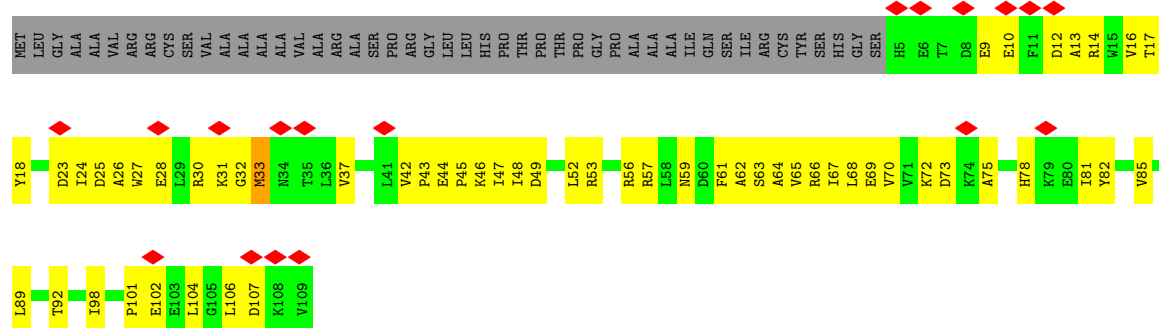


• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

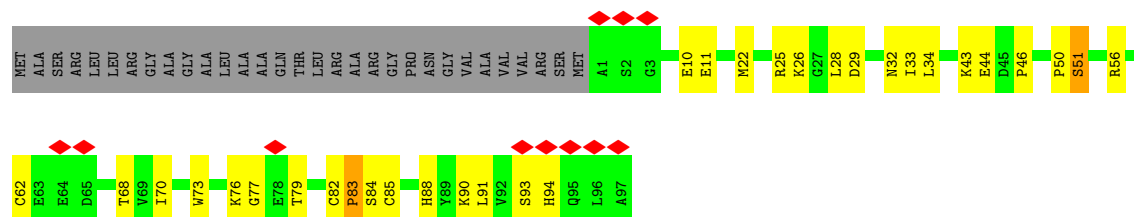




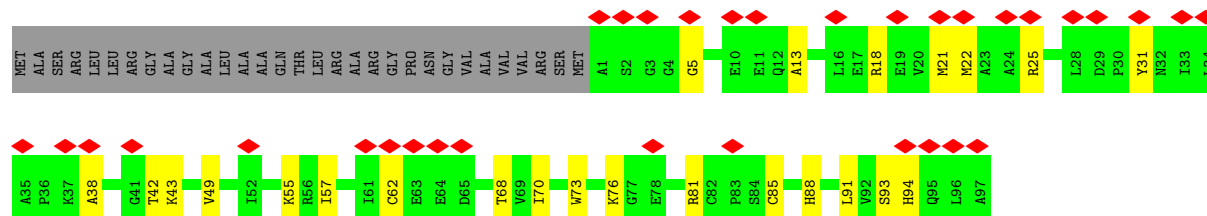
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial



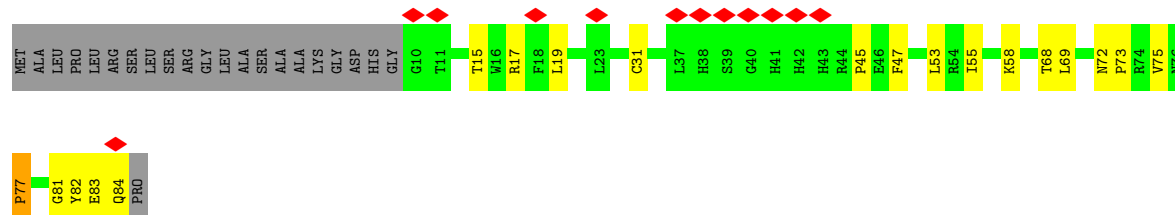
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



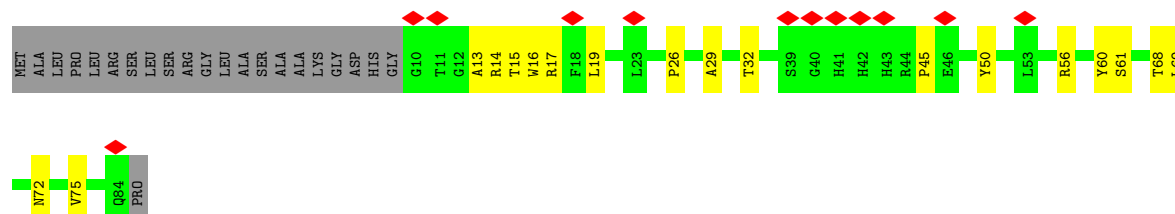
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



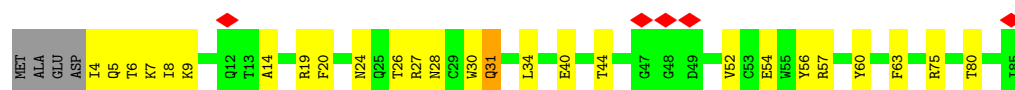
- Molecule 61: Cytochrome c oxidase subunit 6A2



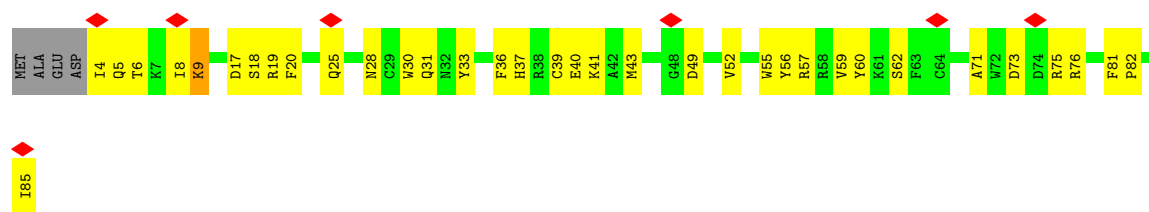
• Molecule 61: Cytochrome c oxidase subunit 6A2



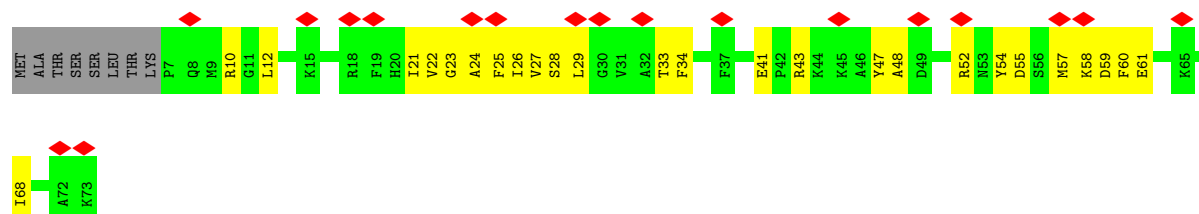
• Molecule 62: Cytochrome c oxidase subunit 6B1



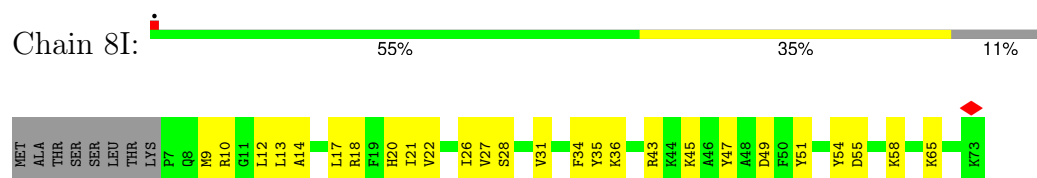
• Molecule 62: Cytochrome c oxidase subunit 6B1



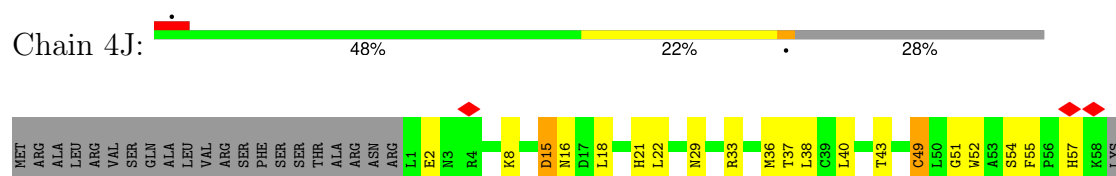
• Molecule 63: Cytochrome c oxidase subunit 6C



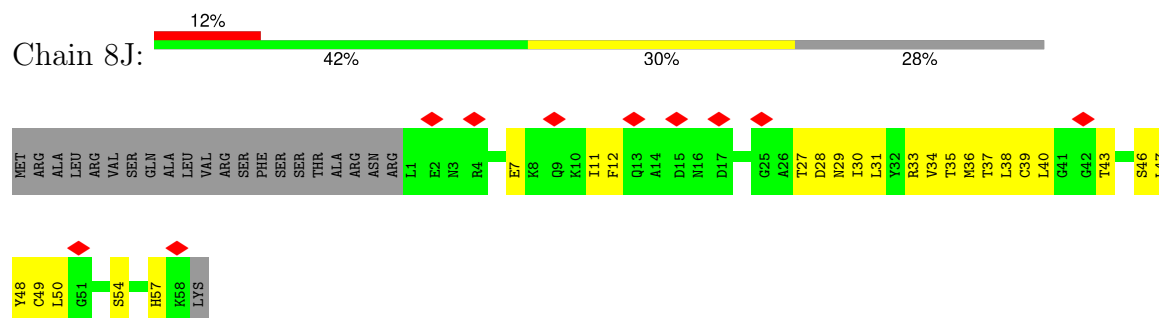
- Molecule 63: Cytochrome c oxidase subunit 6C



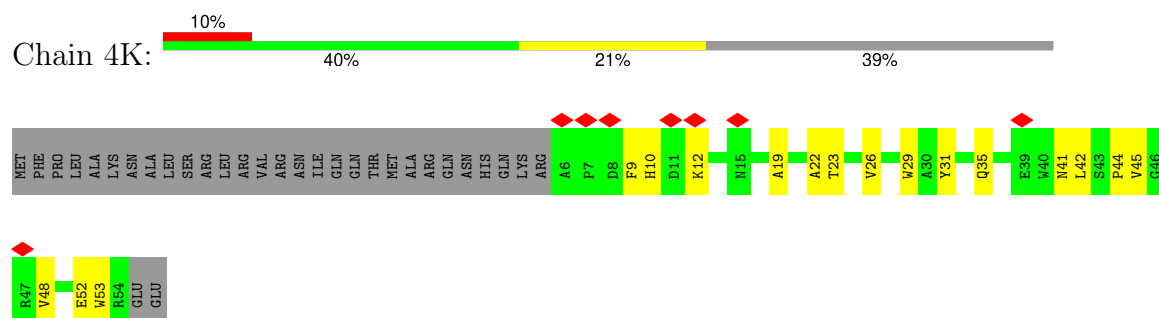
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



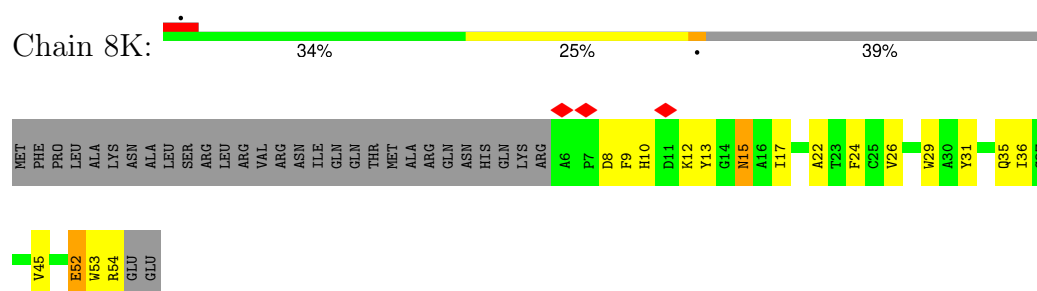
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 65: Cytochrome c oxidase subunit 7B



- Molecule 65: Cytochrome c oxidase subunit 7B



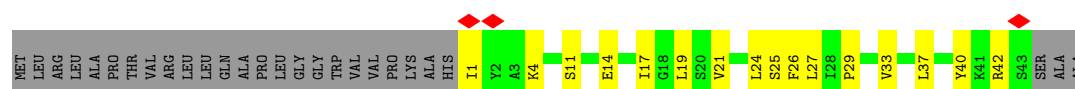
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



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



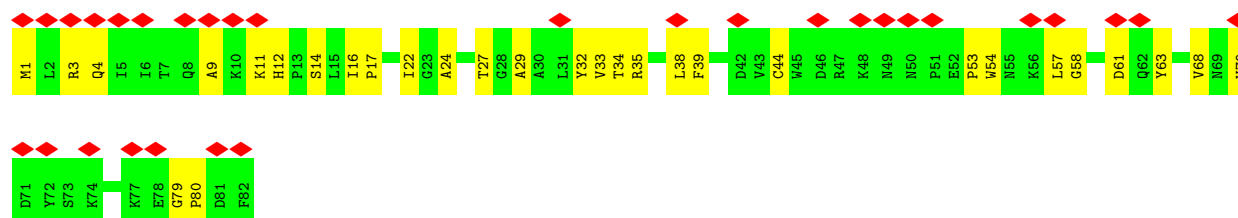
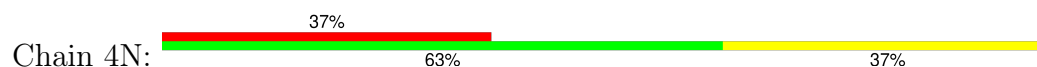
- Molecule 67: Cytochrome c oxidase subunit 8



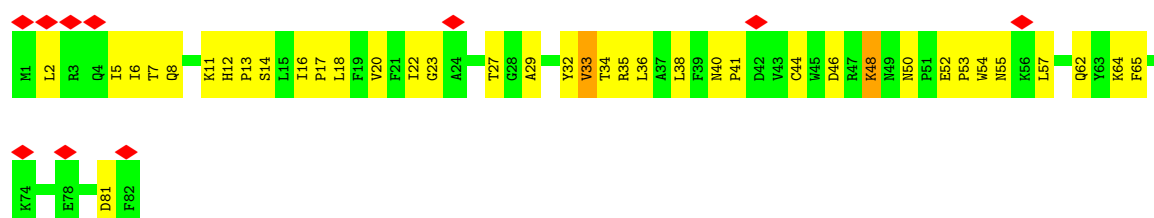
- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 68: Cytochrome c oxidase subunit NDUFA4



- Molecule 68: Cytochrome c oxidase subunit NDUFA4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	320000	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	1.149	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	572.0, 572.0, 572.0	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.21	0/930	0.43	0/1271
2	1B	0.18	0/1273	0.39	0/1722
3	1C	0.12	0/1791	0.31	0/2439
4	1D	0.18	1/3545 (0.0%)	0.33	0/4806
5	1E	0.16	0/1698	0.37	0/2311
6	1F	0.16	0/3401	0.36	0/4595
7	1G	0.14	0/5451	0.35	0/7387
8	1H	0.24	0/2566	0.42	2/3509 (0.1%)
9	1I	0.12	0/1443	0.31	0/1952
10	1J	0.17	0/1364	0.44	0/1850
11	1K	0.16	0/751	0.38	0/1018
12	1L	0.16	0/4939	0.36	0/6718
13	1M	0.15	0/3713	0.34	0/5063
14	1N	0.29	1/2765 (0.0%)	0.41	1/3758 (0.0%)
15	1O	0.14	0/2650	0.34	0/3588
16	1P	0.15	0/2828	0.34	0/3834
17	1Q	0.15	0/1070	0.36	0/1446
18	1R	0.14	0/755	0.32	0/1018
19	1S	0.17	0/711	0.44	0/956
20	1T	0.18	0/701	0.43	0/946
20	1U	0.29	0/706	0.47	1/954 (0.1%)
21	1V	0.17	0/946	0.33	0/1281
22	1W	0.17	0/995	0.36	0/1340
23	1X	0.14	0/1436	0.39	0/1938
24	1Y	0.11	0/1037	0.25	0/1404
25	1Z	0.16	0/1199	0.31	0/1617
26	1a	0.14	0/577	0.38	0/777
27	1b	0.16	0/664	0.36	0/912
28	1c	0.14	0/430	0.32	0/581
29	1d	0.11	0/1016	0.27	0/1374
30	1e	0.15	0/836	0.37	0/1118

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	1f	0.17	0/499	0.44	0/673
32	1g	0.16	0/858	0.39	0/1165
33	1h	0.16	0/1184	0.37	0/1603
34	1i	0.16	0/1138	0.38	0/1551
35	1j	0.17	0/627	0.36	0/858
36	1k	0.16	0/668	0.35	0/903
37	1l	0.15	0/1365	0.36	0/1867
38	1m	0.23	0/1092	0.35	0/1481
39	1n	0.39	2/1549 (0.1%)	0.62	2/2098 (0.1%)
40	1o	0.16	0/1069	0.41	0/1430
41	1p	0.13	0/1481	0.35	0/1997
42	1q	0.13	0/1253	0.31	0/1704
43	1r	0.29	1/777 (0.1%)	0.40	0/1051
44	1s	0.16	0/394	0.40	0/533
45	3A	0.13	0/3481	0.35	0/4722
45	3N	0.13	0/3496	0.32	0/4723
46	3B	0.13	0/3190	0.33	0/4317
46	3O	0.17	0/3175	0.35	0/4292
47	3C	0.16	0/3123	0.36	0/4269
47	3P	0.15	0/3122	0.33	0/4269
48	3D	0.14	0/1946	0.36	0/2641
48	3Q	0.13	0/1962	0.34	0/2663
49	3E	0.18	0/1551	0.46	0/2098
49	3I	1.51	4/344 (1.2%)	2.00	12/468 (2.6%)
49	3R	0.56	2/1551 (0.1%)	0.76	2/2098 (0.1%)
49	3V	1.68	2/225 (0.9%)	3.23	5/303 (1.7%)
50	3F	0.12	0/888	0.29	0/1193
50	3S	0.09	0/888	0.24	0/1193
51	3G	0.14	0/649	0.39	0/878
51	3T	0.15	0/649	0.35	0/878
52	3H	0.21	0/539	0.80	2/724 (0.3%)
52	3U	0.18	0/539	0.44	0/724
53	3J	0.40	0/476	0.57	0/641
53	3W	0.37	0/476	0.50	0/641
54	3X	0.12	0/445	0.32	0/608
54	3Y	0.14	0/437	0.38	0/598
55	4A	0.18	0/4156	0.34	0/5679
55	8A	0.29	1/4156 (0.0%)	0.46	2/5679 (0.0%)
56	4B	0.25	0/1865	0.43	0/2544
56	8B	0.23	0/1865	0.51	0/2544
57	4C	0.26	1/2179 (0.0%)	0.35	0/2981
57	8C	0.22	0/2179	0.40	0/2981
58	4D	0.16	0/1197	0.39	0/1617

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
58	8D	0.31	0/1197	0.51	0/1617
59	4E	0.23	0/871	0.51	0/1182
59	8E	0.29	0/871	0.52	0/1182
60	4F	0.27	0/749	0.61	1/1016 (0.1%)
60	8F	0.14	0/749	0.38	0/1016
61	4G	0.19	0/644	0.47	1/881 (0.1%)
61	8G	0.13	0/644	0.37	0/881
62	4H	0.15	0/708	0.36	0/956
62	8H	0.29	1/708 (0.1%)	0.45	0/956
63	4I	0.19	0/563	0.46	0/748
63	8I	0.25	0/563	0.46	0/748
64	4J	0.17	0/466	0.44	0/631
64	8J	0.18	0/466	0.47	0/631
65	4K	0.15	0/396	0.40	0/543
65	8K	0.27	0/396	0.56	0/543
66	4L	0.18	0/394	0.37	0/528
66	8L	0.27	0/394	0.51	1/528 (0.2%)
67	4M	0.23	0/349	0.49	0/477
67	8M	0.39	0/349	0.51	0/477
68	4N	0.17	0/680	0.39	0/921
68	8N	0.33	0/680	0.62	0/921
All	All	0.22	16/131727 (0.0%)	0.43	32/178746 (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
49	3V	0	1
68	8N	0	1
All	All	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	3V	49	VAL	C-N	22.83	1.70	1.33
49	3I	73	PRO	CG-CD	-19.98	0.82	1.50
49	3R	173	PRO	N-CD	16.16	1.70	1.47
49	3I	73	PRO	N-CD	13.25	1.66	1.47
14	1N	255	PRO	CA-C	-11.58	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1n	144	PRO	N-CD	10.97	1.63	1.47
49	3I	72	VAL	C-O	9.89	1.36	1.24
49	3R	173	PRO	CG-CD	-9.20	1.19	1.50
57	4C	159	MET	CG-SD	-8.28	1.60	1.80
49	3V	48	SER	C-N	-7.96	1.19	1.33
43	1r	37	PRO	CA-C	-6.68	1.48	1.51
55	8A	483	SER	CB-OG	-6.61	1.28	1.42
4	1D	359	PRO	CA-C	6.26	1.55	1.51
62	8H	9	LYS	CE-NZ	-5.53	1.32	1.49
39	1n	144	PRO	N-CA	-5.03	1.36	1.46
49	3I	73	PRO	CA-CB	-5.02	1.46	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	3V	49	VAL	O-C-N	-38.36	79.22	122.95
49	3R	173	PRO	CA-N-CD	-23.12	79.64	112.00
49	3I	73	PRO	CB-CG-CD	23.07	179.94	106.10
49	3V	49	VAL	CA-C-N	21.55	154.96	121.98
49	3V	49	VAL	C-N-CA	21.55	154.96	121.98
39	1n	144	PRO	CA-N-CD	-19.71	84.41	112.00
49	3I	73	PRO	N-CD-CG	-18.09	76.06	103.20
49	3V	48	SER	CA-C-N	-16.95	100.50	122.37
49	3V	48	SER	C-N-CA	-16.95	100.50	122.37
49	3I	41	PRO	CA-N-CD	-13.18	93.55	112.00
60	4F	83	PRO	CA-N-CD	-13.07	93.69	112.00
49	3I	73	PRO	CA-CB-CG	-13.03	79.75	104.50
49	3I	73	PRO	CA-N-CD	-11.93	95.30	112.00
52	3H	77	GLU	CA-C-N	11.12	141.71	121.70
52	3H	77	GLU	C-N-CA	11.12	141.71	121.70
14	1N	255	PRO	O-C-N	-9.00	116.92	121.15
8	1H	60	PRO	CA-N-CD	-7.86	101.00	112.00
49	3I	71	ASN	N-CA-C	-7.68	103.21	112.58
49	3I	41	PRO	N-CA-CB	-7.45	98.75	102.92
49	3I	41	PRO	N-CA-C	7.33	122.90	110.74
49	3R	172	LYS	C-N-CD	6.88	153.20	125.00
49	3I	40	SER	C-N-CD	-6.87	96.84	125.00
55	8A	208	MET	CB-CG-SD	6.42	131.97	112.70
20	1U	4	PRO	CA-N-CD	-6.38	103.06	112.00
61	4G	77	PRO	CA-N-CD	-6.15	103.39	112.00
55	8A	208	MET	CG-SD-CE	-5.91	87.90	100.90
49	3I	72	VAL	CA-C-O	-5.65	112.38	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	3I	72	VAL	C-N-CD	5.62	148.03	125.00
39	1n	143	THR	C-N-CD	5.44	147.32	125.00
66	8L	15	VAL	N-CA-C	-5.39	107.72	112.90
49	3I	41	PRO	N-CD-CG	-5.26	95.31	103.20
8	1H	124	ASN	CB-CA-C	-5.12	110.27	117.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
49	3V	48	SER	Mainchain
68	8N	48	LYS	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	79	0
2	1B	1242	0	1249	80	0
3	1C	1740	0	1691	40	0
4	1D	3452	0	3389	121	0
5	1E	1658	0	1662	67	0
6	1F	3325	0	3288	152	0
7	1G	5362	0	5388	173	0
8	1H	2504	0	2602	141	0
9	1I	1412	0	1366	62	0
10	1J	1329	0	1326	88	0
11	1K	750	0	798	57	0
12	1L	4818	0	4956	189	0
13	1M	3632	0	3836	146	0
14	1N	2712	0	2873	140	0
15	1O	2590	0	2556	92	0
16	1P	2751	0	2776	93	0
17	1Q	1047	0	1042	39	0
18	1R	741	0	704	16	0
19	1S	700	0	719	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	1T	689	0	687	42	0
20	1U	694	0	691	35	0
21	1V	927	0	972	25	0
22	1W	971	0	975	42	0
23	1X	1398	0	1378	45	0
24	1Y	1016	0	1020	31	0
25	1Z	1168	0	1161	58	0
26	1a	562	0	557	21	0
27	1b	643	0	645	23	0
28	1c	417	0	425	13	0
29	1d	985	0	978	29	0
30	1e	816	0	823	30	0
31	1f	487	0	498	20	0
32	1g	835	0	795	46	0
33	1h	1151	0	1164	32	0
34	1i	1100	0	1107	45	0
35	1j	601	0	546	36	0
36	1k	649	0	626	18	0
37	1l	1310	0	1204	43	0
38	1m	1062	0	1075	31	0
39	1n	1495	0	1434	53	0
40	1o	1045	0	1016	58	0
41	1p	1449	0	1416	62	0
42	1q	1212	0	1174	28	0
43	1r	759	0	783	29	0
44	1s	382	0	351	26	0
45	3A	3411	0	3308	72	0
45	3N	3424	0	3350	74	0
46	3B	3138	0	3116	68	0
46	3O	3124	0	3108	60	0
47	3C	3025	0	3090	73	0
47	3P	3024	0	3090	62	0
48	3D	1888	0	1834	49	0
48	3Q	1904	0	1849	50	0
49	3E	1518	0	1498	74	0
49	3I	340	0	359	18	0
49	3R	1518	0	1498	108	0
49	3V	224	0	241	19	0
50	3F	868	0	857	14	0
50	3S	868	0	857	9	0
51	3G	628	0	634	17	0
51	3T	628	0	634	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	3H	533	0	513	21	0
52	3U	533	0	513	18	0
53	3J	464	0	467	17	0
53	3W	464	0	467	15	0
54	3X	429	0	430	7	0
54	3Y	421	0	418	13	0
55	4A	4026	0	4005	196	0
55	8A	4026	0	4005	322	0
56	4B	1828	0	1836	122	0
56	8B	1828	0	1834	132	0
57	4C	2096	0	2027	100	0
57	8C	2096	0	2027	168	0
58	4D	1163	0	1143	79	0
58	8D	1163	0	1143	112	0
59	4E	852	0	845	73	0
59	8E	852	0	845	101	0
60	4F	734	0	718	34	0
60	8F	734	0	718	24	0
61	4G	617	0	585	17	0
61	8G	617	0	585	24	0
62	4H	687	0	645	23	0
62	8H	687	0	645	42	0
63	4I	550	0	560	32	0
63	8I	550	0	560	35	0
64	4J	456	0	459	35	0
64	8J	456	0	459	33	0
65	4K	383	0	366	22	0
65	8K	383	0	366	29	0
66	4L	381	0	380	27	0
66	8L	381	0	380	35	0
67	4M	338	0	345	30	0
67	8M	338	0	345	35	0
68	4N	660	0	664	29	0
68	8N	660	0	664	60	0
69	1A	47	0	71	3	0
69	1K	44	0	62	2	0
69	1L	91	0	136	8	0
69	1M	194	0	296	30	0
69	1N	49	0	75	5	0
69	1P	35	0	44	3	0
69	1Y	161	0	195	23	0
69	1d	49	0	75	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	1j	44	0	65	0	0
69	1m	41	0	59	0	0
69	3A	59	0	66	9	0
69	3C	69	0	86	9	0
69	3D	33	0	40	2	0
69	3G	29	0	32	1	0
69	3N	58	0	62	8	0
69	3P	33	0	40	0	0
69	3R	47	0	71	5	0
69	3Y	30	0	34	2	0
70	1A	70	0	88	7	0
70	1B	94	0	136	15	0
70	1H	102	0	161	12	0
70	1I	44	0	62	3	0
70	1M	79	0	109	10	0
70	1P	33	0	40	2	0
70	1Y	46	0	66	7	0
70	1d	39	0	52	8	0
70	1h	47	0	71	1	0
70	1q	49	0	75	4	0
70	3J	47	0	68	4	0
70	3R	45	0	64	4	0
70	3X	29	0	32	2	0
71	1B	8	0	0	2	0
71	1F	8	0	0	2	0
71	1G	16	0	0	3	0
71	1I	16	0	0	0	0
72	1E	4	0	0	0	0
72	1G	4	0	0	2	0
72	3E	4	0	0	2	0
72	3R	4	0	0	2	0
73	1F	31	0	19	4	0
74	1G	1	0	0	0	0
75	1H	51	0	46	1	0
75	1L	76	0	99	6	0
75	1N	62	0	68	3	0
75	1X	86	0	125	12	0
75	1d	65	0	77	6	0
75	1h	80	0	104	14	0
75	1q	61	0	66	2	0
75	3A	58	0	60	3	0
75	3G	108	0	104	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	3N	43	0	30	7	0
75	3P	56	0	56	9	0
75	3T	57	0	58	9	0
75	4B	100	0	156	14	0
75	4C	100	0	156	15	0
75	4D	100	0	156	17	0
75	8B	100	0	156	10	0
75	8C	100	0	156	16	0
75	8D	100	0	156	15	0
76	1O	32	0	12	3	0
77	1O	1	0	0	0	0
77	4A	1	0	0	0	0
77	8A	1	0	0	0	0
78	1P	48	0	26	2	0
79	1R	1	0	0	0	0
79	4F	1	0	0	0	0
79	8F	1	0	0	0	0
80	1T	37	0	0	0	0
80	1n	37	0	0	1	0
81	1Y	8	0	8	0	0
81	1q	8	0	8	2	0
82	1h	11	0	12	1	0
83	1i	29	0	39	0	0
84	1l	15	0	27	0	0
85	3C	86	0	60	2	0
85	3P	86	0	60	4	0
86	3D	42	0	32	2	0
86	3Q	43	0	32	3	0
87	4A	153	0	228	20	0
87	4B	102	0	151	8	0
87	4C	255	0	380	23	0
87	4G	51	0	76	5	0
87	4J	51	0	76	10	0
87	4K	51	0	76	2	0
87	4L	51	0	76	7	0
87	4M	51	0	76	3	0
87	8A	153	0	228	23	0
87	8B	102	0	151	11	0
87	8C	306	0	456	42	0
87	8G	51	0	76	8	0
87	8J	51	0	76	4	0
87	8K	51	0	76	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	8L	51	0	76	7	0
88	4A	120	0	108	10	0
88	8A	120	0	108	12	0
89	4A	1	0	0	0	0
89	8A	1	0	0	0	0
90	4A	1	0	0	0	0
90	8A	1	0	0	0	0
91	4B	2	0	0	1	0
91	8B	2	0	0	2	0
92	4B	52	0	80	8	0
92	8B	52	0	80	8	0
93	4C	52	0	72	5	0
93	4G	53	0	77	2	0
93	8C	52	0	72	5	0
93	8G	53	0	77	5	0
94	4H	5	0	0	0	0
94	8H	5	0	0	1	0
All	All	134346	0	135606	4915	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 18.

All (4915) 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)
56:8B:52:HIS:CD2	56:8B:56:MET:HE1	1.45	1.51
49:3V:49:VAL:C	49:3V:50:LEU:N	1.69	1.49
57:4C:151:LEU:HD13	57:4C:159:MET:SD	1.50	1.48
59:8E:72:LYS:HB2	59:8E:82:TYR:CE2	1.47	1.47
68:8N:7:THR:C	68:8N:11:LYS:HZ3	1.23	1.43
69:3A:503:3PE:H362	47:3C:11:MET:CE	1.58	1.33
56:4B:61:VAL:HG12	56:4B:65:TRP:CZ3	1.64	1.30
55:8A:483:SER:CA	67:8M:4:LYS:HZ1	1.44	1.30
55:8A:367:LEU:HD13	55:8A:372:TYR:CD2	1.68	1.28
56:8B:52:HIS:HD2	56:8B:56:MET:CE	1.45	1.28
69:3A:503:3PE:C36	47:3C:11:MET:HE2	1.63	1.28
5:1E:110:LEU:HB3	6:1F:261:HIS:NE2	1.49	1.27
66:4L:41:ARG:HG3	67:4M:40:TYR:CE2	1.71	1.25
56:8B:200:CYS:SG	91:8B:304:CUA:CU2	1.27	1.24
56:8B:196:CYS:SG	91:8B:304:CUA:CU1	1.26	1.23
15:1O:265:ASN:OD1	15:1O:268:GLU:HG2	1.36	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4B:86:MET:HA	56:4B:89:GLU:OE1	1.36	1.22
49:3R:173:PRO:CD	49:3R:173:PRO:N	1.70	1.22
56:8B:52:HIS:CD2	56:8B:56:MET:CE	2.19	1.22
55:4A:93:ALA:HA	55:4A:171:MET:CE	1.70	1.22
65:8K:38:ILE:HD11	65:8K:40:TRP:CZ2	1.76	1.21
49:3R:173:PRO:HD2	49:3R:173:PRO:O	1.39	1.19
2:1B:49:THR:HG23	2:1B:59:MET:HE1	1.23	1.19
62:8H:6:THR:HB	62:8H:9:LYS:NZ	1.58	1.17
8:1H:85:MET:HE3	8:1H:233:MET:CE	1.74	1.16
1:1A:18:VAL:HG23	8:1H:222:MET:HE2	1.21	1.16
1:1A:18:VAL:CG2	8:1H:222:MET:HE2	1.75	1.16
12:1L:140:LEU:HD22	12:1L:182:PHE:CZ	1.80	1.15
68:8N:7:THR:C	68:8N:11:LYS:NZ	2.04	1.15
57:8C:148:HIS:ND1	57:8C:152:MET:HE3	1.60	1.15
55:8A:483:SER:HB3	67:8M:4:LYS:NZ	1.60	1.14
55:8A:208:MET:HE1	55:8A:219:PHE:CG	1.81	1.14
58:8D:34:SER:N	58:8D:37:GLN:OE1	1.79	1.14
57:8C:148:HIS:HD1	57:8C:152:MET:HE3	1.10	1.14
58:4D:53:MET:HE1	59:4E:104:LEU:HD22	1.13	1.13
49:3R:152:ILE:HD11	49:3R:272:ILE:CG2	1.77	1.13
55:8A:483:SER:HA	67:8M:4:LYS:HZ1	1.08	1.12
20:1U:22:TYR:CE2	20:1U:24:LYS:NZ	2.17	1.12
59:4E:21:LYS:O	59:4E:57:ARG:NH1	1.83	1.11
65:8K:13:TYR:O	65:8K:17:ILE:HD12	1.49	1.11
55:8A:483:SER:CB	67:8M:4:LYS:NZ	2.14	1.09
45:3N:224:VAL:HG13	45:3N:225:GLU:H	0.97	1.09
55:8A:172:LYS:NZ	55:8A:178:GLN:OE1	1.86	1.09
55:8A:308:ALA:HA	55:8A:311:ILE:HD12	1.14	1.09
1:1A:105:GLU:HG3	10:1J:169:MET:HE1	1.25	1.07
57:4C:151:LEU:CD1	57:4C:159:MET:SD	2.43	1.07
55:8A:409:TRP:HB3	55:8A:471:ILE:HD13	1.30	1.07
55:4A:468:MET:HE2	55:4A:468:MET:HA	1.10	1.06
56:4B:62:GLU:HB3	56:4B:65:TRP:CZ2	1.90	1.06
58:8D:85:ALA:O	58:8D:89:ILE:HD12	1.56	1.05
55:4A:93:ALA:HA	55:4A:171:MET:HE1	1.07	1.05
12:1L:140:LEU:HD22	12:1L:182:PHE:HZ	0.98	1.05
49:3V:49:VAL:O	49:3V:50:LEU:N	1.90	1.05
8:1H:85:MET:HE3	8:1H:233:MET:HE2	1.05	1.04
57:4C:33:MET:HE3	64:4J:49:CYS:HB3	1.40	1.04
38:1m:113:LYS:O	38:1m:117:GLU:OE1	1.75	1.04
62:8H:6:THR:HB	62:8H:9:LYS:HZ3	1.08	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4B:61:VAL:CG1	56:4B:65:TRP:HZ3	1.71	1.03
6:1F:250:ASN:ND2	6:1F:318:ASP:HB2	1.73	1.03
19:1S:88:ARG:NH1	19:1S:88:ARG:O	1.91	1.03
55:8A:308:ALA:HA	55:8A:311:ILE:CD1	1.88	1.03
49:3R:152:ILE:HD11	49:3R:272:ILE:HG23	1.07	1.03
56:4B:61:VAL:HG12	56:4B:65:TRP:CE3	1.94	1.02
55:8A:483:SER:HB3	67:8M:4:LYS:HZ3	1.13	1.02
59:8E:72:LYS:CB	59:8E:82:TYR:HE2	1.71	1.02
55:8A:208:MET:CE	55:8A:219:PHE:CD2	2.43	1.01
11:1K:80:MET:HA	11:1K:80:MET:HE3	1.39	1.01
45:3A:118:GLN:HG2	45:3A:219:LEU:HD21	1.40	1.01
49:3R:173:PRO:HD2	49:3R:173:PRO:C	1.78	1.01
59:8E:72:LYS:CB	59:8E:82:TYR:CE2	2.43	1.00
59:8E:78:HIS:CE1	63:8I:12:LEU:CD1	2.44	1.00
68:8N:8:GLN:N	68:8N:11:LYS:HZ3	1.58	0.99
57:8C:60:ASP:HA	57:8C:63:ARG:HG3	1.44	0.99
66:4L:41:ARG:CG	67:4M:40:TYR:HE2	1.75	0.99
49:3V:64:LEU:HA	49:3V:77:ARG:O	1.62	0.99
55:4A:328:HIS:HB2	56:4B:45:MET:HE3	1.01	0.99
14:1N:149:ILE:HG21	14:1N:154:MET:CE	1.93	0.99
49:3R:173:PRO:CD	49:3R:173:PRO:O	2.10	0.99
60:4F:83:PRO:HD2	60:4F:84:SER:N	1.78	0.99
7:1G:439:PHE:CD1	7:1G:442:ILE:HD11	1.96	0.99
46:3B:396:SER:O	46:3B:400:GLN:HG3	1.62	0.99
6:1F:250:ASN:HD21	6:1F:318:ASP:CG	1.70	0.98
58:8D:77:GLU:O	58:8D:81:ILE:HD12	1.63	0.98
56:8B:52:HIS:CD2	56:8B:56:MET:SD	2.57	0.98
45:3N:224:VAL:CG1	45:3N:225:GLU:H	1.73	0.98
57:8C:59:ARG:NE	57:8C:63:ARG:HH21	1.60	0.98
37:1I:80:ASP:HB3	37:1I:83:MET:HE2	1.46	0.98
2:1B:86:MET:HE3	2:1B:107:MET:HE2	1.46	0.97
56:4B:62:GLU:HA	56:4B:65:TRP:CE2	1.99	0.97
55:8A:208:MET:HE1	55:8A:219:PHE:CB	1.94	0.97
13:1M:453:MET:HE2	32:1g:77:VAL:HG13	1.46	0.97
55:4A:328:HIS:CB	56:4B:45:MET:HE3	1.95	0.97
68:8N:7:THR:O	68:8N:11:LYS:NZ	1.94	0.96
1:1A:57:LEU:HD21	10:1J:172:THR:HG21	1.48	0.96
55:4A:28:MET:HA	55:4A:28:MET:HE3	1.47	0.96
55:8A:483:SER:CA	67:8M:4:LYS:NZ	2.28	0.95
58:8D:48:TRP:CZ3	59:8E:61:PHE:CD2	2.54	0.95
56:4B:62:GLU:HA	56:4B:65:TRP:CD2	2.02	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:144:PRO:HD2	39:1n:144:PRO:O	1.55	0.95
66:8L:18:LYS:NZ	66:8L:19:TRP:CZ2	2.34	0.95
55:8A:367:LEU:HD13	55:8A:372:TYR:CE2	2.00	0.95
55:4A:468:MET:HA	55:4A:468:MET:CE	1.97	0.94
59:4E:52:LEU:HD12	59:4E:98:ILE:HD12	1.48	0.94
65:8K:38:ILE:HD11	65:8K:40:TRP:CE2	2.02	0.94
45:3N:224:VAL:HG13	45:3N:225:GLU:N	1.75	0.94
66:8L:37:PHE:HB3	67:8M:33:VAL:HG11	1.49	0.94
2:1B:49:THR:CG2	2:1B:59:MET:HE1	1.98	0.94
66:4L:41:ARG:HG3	67:4M:40:TYR:HE2	1.04	0.94
55:8A:208:MET:HE1	55:8A:219:PHE:HB3	1.48	0.93
55:4A:468:MET:HE2	55:4A:468:MET:CA	1.98	0.93
55:4A:328:HIS:HB2	56:4B:45:MET:CE	1.95	0.93
62:8H:6:THR:CB	62:8H:9:LYS:NZ	2.32	0.93
57:8C:33:MET:HE2	64:8J:49:CYS:HB3	1.51	0.93
12:1L:73:THR:HG22	12:1L:194:ASN:HD21	1.29	0.93
16:1P:89:ASN:OD1	16:1P:90:VAL:HG12	1.69	0.93
20:1U:17:TYR:O	20:1U:21:LEU:HD23	1.69	0.93
55:8A:409:TRP:CB	55:8A:471:ILE:HD13	1.99	0.93
7:1G:101:HIS:CE1	71:1G:801:SF4:S3	2.61	0.92
56:4B:196:CYS:HG	91:4B:304:CUA:CU2	0.73	0.92
5:1E:216:GLY:C	5:1E:217:LEU:HD23	1.94	0.92
55:8A:308:ALA:CA	55:8A:311:ILE:HD12	2.00	0.92
55:8A:483:SER:CB	67:8M:4:LYS:HZ3	1.75	0.92
57:8C:122:HIS:CE1	61:8G:45:PRO:HB3	2.04	0.92
7:1G:570:SER:HA	7:1G:583:THR:O	1.69	0.92
55:8A:155:VAL:O	55:8A:159:LEU:HD12	1.69	0.92
14:1N:1:FME:O1	15:1O:258:ARG:NH1	2.01	0.92
17:1Q:39:VAL:HG21	17:1Q:108:ARG:HG3	1.50	0.92
55:4A:93:ALA:CA	55:4A:171:MET:HE1	1.98	0.92
14:1N:149:ILE:HG21	14:1N:154:MET:HE2	1.50	0.91
1:1A:1:FME:H	1:1A:4:MET:HE3	1.35	0.91
57:8C:148:HIS:CE1	57:8C:152:MET:HE3	2.04	0.91
1:1A:18:VAL:HG23	8:1H:222:MET:CE	1.99	0.91
8:1H:85:MET:CE	8:1H:233:MET:HE2	1.97	0.91
38:1m:117:GLU:OE1	38:1m:117:GLU:N	2.03	0.91
49:3R:173:PRO:CD	49:3R:173:PRO:C	2.33	0.91
61:8G:15:THR:O	61:8G:19:LEU:HD12	1.71	0.90
43:1r:57:ASP:OD2	43:1r:60:ARG:HB2	1.70	0.90
57:4C:129:VAL:CG1	57:4C:180:GLU:OE1	2.20	0.90
58:8D:99:GLU:OE2	58:8D:104:TYR:CE2	2.25	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:453:MET:HE1	32:1g:80:LEU:HD12	1.53	0.90
60:4F:83:PRO:HD2	60:4F:84:SER:H	1.34	0.90
62:8H:31:GLN:OE1	68:8N:54:TRP:NE1	2.05	0.89
58:8D:48:TRP:HZ3	59:8E:61:PHE:CD2	1.88	0.89
58:8D:68:PHE:CE1	59:8E:69:GLU:HB2	2.07	0.89
58:4D:96:LEU:HD23	58:4D:96:LEU:O	1.71	0.89
8:1H:156:MET:HE2	25:1Z:50:MET:HG2	1.53	0.88
40:1o:32:GLU:O	40:1o:34:LYS:NZ	2.05	0.88
12:1L:73:THR:CG2	12:1L:194:ASN:HD21	1.87	0.88
57:8C:182:TYR:HE2	87:8C:305:PGV:H042	1.38	0.88
46:3B:222:ARG:NE	46:3B:223:PHE:CE1	2.42	0.88
37:1l:12:PRO:HA	38:1m:78:ASN:OD1	1.73	0.88
61:4G:77:PRO:HD3	61:4G:82:TYR:CE1	2.08	0.88
39:1n:144:PRO:O	39:1n:144:PRO:CD	2.22	0.88
16:1P:108:ASP:HA	16:1P:112:LYS:HG2	1.56	0.87
55:8A:208:MET:CE	55:8A:219:PHE:CG	2.57	0.87
19:1S:43:LEU:CD1	19:1S:47:ASN:HD21	1.87	0.87
20:1U:22:TYR:CZ	20:1U:24:LYS:NZ	2.41	0.87
55:4A:91:ASP:OD1	55:4A:92:MET:N	2.06	0.87
58:4D:53:MET:CE	59:4E:104:LEU:HD22	2.04	0.87
57:8C:83:MET:HE2	57:8C:237:ALA:HB1	1.55	0.87
16:1P:115:HIS:NE2	16:1P:119:GLN:OE1	2.08	0.86
1:1A:27:LEU:HG	8:1H:59:GLU:HG3	1.55	0.86
10:1J:86:ASN:OD1	10:1J:88:THR:N	2.07	0.86
16:1P:147:ARG:HH12	59:8E:9:GLU:H	1.20	0.86
58:4D:77:GLU:HG3	65:4K:10:HIS:NE2	1.88	0.86
12:1L:161:ARG:HG2	12:1L:164:ALA:H	1.38	0.86
32:1g:120:LEU:HD22	41:1p:163:LEU:HD21	1.58	0.86
56:4B:61:VAL:CG1	56:4B:65:TRP:CZ3	2.49	0.86
49:3E:165:MET:HA	49:3E:165:MET:HE3	1.57	0.86
56:8B:58:ALA:HB2	92:8B:305:PSC:H031	1.56	0.86
3:1C:114:LEU:O	22:1W:20:ILE:HD11	1.76	0.86
8:1H:156:MET:SD	8:1H:174:MET:CE	2.64	0.86
12:1L:140:LEU:CD2	12:1L:182:PHE:CZ	2.58	0.86
55:4A:468:MET:HE1	55:4A:471:ILE:HD11	1.56	0.86
12:1L:140:LEU:CD2	12:1L:182:PHE:HZ	1.88	0.86
2:1B:49:THR:HG23	2:1B:59:MET:CE	2.06	0.86
34:1i:77:PRO:O	34:1i:81:ILE:HG12	1.76	0.86
59:4E:33:MET:HE3	59:4E:67:ILE:CG2	2.06	0.85
59:8E:78:HIS:CE1	63:8I:12:LEU:HD11	2.10	0.85
14:1N:149:ILE:HD13	14:1N:154:MET:HE1	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:88:ARG:NH2	19:1S:92:ASN:OD1	2.08	0.85
40:1o:41:THR:O	40:1o:45:MET:HB3	1.77	0.85
14:1N:270:MET:HE1	14:1N:282:MET:HE2	1.57	0.84
87:4M:101:PGV:H61	87:4M:101:PGV:H221	1.59	0.84
57:8C:50:ASN:OD1	57:8C:54:MET:HE2	1.77	0.84
58:8D:78:TRP:HA	58:8D:81:ILE:HD13	1.58	0.84
1:1A:68:GLU:HG2	10:1J:161:LEU:HD13	1.58	0.84
57:8C:148:HIS:CE1	57:8C:152:MET:CE	2.59	0.84
68:8N:8:GLN:HA	68:8N:11:LYS:NZ	1.92	0.84
68:8N:8:GLN:N	68:8N:11:LYS:NZ	2.22	0.84
34:1i:74:VAL:O	34:1i:78:VAL:HG12	1.77	0.84
37:1l:127:PRO:HG3	40:1o:3:HIS:HD2	1.42	0.84
6:1F:250:ASN:ND2	6:1F:318:ASP:CB	2.40	0.84
55:4A:412:ILE:HD13	58:4D:84:THR:OG1	1.76	0.84
55:8A:483:SER:CB	67:8M:4:LYS:HZ1	1.83	0.84
57:8C:122:HIS:HE1	61:8G:45:PRO:HB3	1.40	0.84
57:4C:45:LEU:HD11	64:4J:38:LEU:HD22	1.60	0.84
46:3B:222:ARG:HE	46:3B:223:PHE:HE1	1.26	0.84
56:8B:63:THR:HG22	56:8B:67:ILE:HD11	1.59	0.84
22:1W:23:ARG:O	22:1W:23:ARG:HD3	1.77	0.83
37:1l:127:PRO:HG3	40:1o:3:HIS:CD2	2.13	0.83
56:4B:61:VAL:HG12	56:4B:65:TRP:HZ3	1.09	0.83
55:8A:124:THR:CG2	55:8A:128:VAL:HA	2.08	0.83
7:1G:105:CYS:HA	7:1G:108:CYS:HB2	1.58	0.83
12:1L:584:ILE:HD11	14:1N:58:LYS:HG2	1.60	0.83
58:8D:97:ILE:HG22	65:8K:36:ILE:HD11	1.60	0.83
49:3R:239:HIS:CD2	49:3R:240:GLY:H	1.97	0.83
13:1M:19:LYS:HD2	31:1f:9:ASP:OD1	1.79	0.83
44:1s:42:GLN:N	44:1s:42:GLN:OE1	2.10	0.83
55:8A:69:MET:CE	88:8A:604:HEA:H272	2.08	0.83
49:3V:62:ARG:O	49:3V:77:ARG:NH2	2.11	0.83
22:1W:62:LYS:HD2	22:1W:66:MET:HE3	1.59	0.82
57:8C:27:MET:HE1	57:8C:50:ASN:HD22	1.43	0.82
55:8A:212:ASP:OD1	55:8A:219:PHE:HB2	1.79	0.82
57:4C:129:VAL:HG11	57:4C:180:GLU:OE1	1.77	0.82
59:4E:45:PRO:HB2	59:4E:88:GLU:HG3	1.61	0.82
59:8E:33:MET:CE	59:8E:67:ILE:HG22	2.09	0.82
58:4D:89:ILE:HG22	65:4K:29:TRP:HE1	1.44	0.82
59:8E:78:HIS:ND1	63:8I:12:LEU:HD11	1.95	0.82
9:1I:44:GLU:HG3	26:1a:1:MET:HE3	1.61	0.82
41:1p:158:GLN:HG2	41:1p:162:MET:CE	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8C:59:ARG:CD	57:8C:63:ARG:HH21	1.92	0.81
12:1L:525:MET:HE2	39:1n:76:PRO:HB3	1.60	0.81
27:1b:51:ASN:OD1	33:1h:139:THR:HG22	1.79	0.81
47:3C:9:PRO:HB3	47:3P:202:GLU:OE2	1.80	0.81
55:8A:250:GLY:O	55:8A:254:ILE:HG12	1.79	0.81
49:3R:232:GLY:HA3	49:3R:244:ASP:HA	1.61	0.81
56:8B:59:GLN:OE1	68:8N:14:SER:OG	1.97	0.81
1:1A:18:VAL:CG2	8:1H:222:MET:CE	2.57	0.81
55:4A:463:THR:HA	55:4A:466:MET:HE3	1.63	0.81
55:4A:462:LEU:HG	55:4A:466:MET:HE2	1.62	0.81
6:1F:17:ASP:HA	6:1F:20:ARG:HG2	1.61	0.80
49:3R:197:ASP:O	49:3R:248:ARG:NH2	2.14	0.80
55:4A:271:MET:HA	55:4A:271:MET:HE3	1.63	0.80
55:8A:208:MET:CE	55:8A:219:PHE:HB3	2.12	0.80
66:8L:18:LYS:NZ	67:8M:14:GLU:OE1	2.13	0.80
10:1J:99:MET:SD	10:1J:99:MET:C	2.64	0.80
55:8A:381:LEU:HD13	88:8A:604:HEA:HAC	1.61	0.80
59:8E:33:MET:HE1	59:8E:67:ILE:HG22	1.63	0.80
56:4B:133:MET:HE1	58:4D:119:GLN:HG3	1.64	0.80
61:4G:77:PRO:HD3	61:4G:82:TYR:CZ	2.16	0.80
35:1j:65:GLY:HA3	40:1o:30:PHE:CE1	2.16	0.80
55:8A:241:PRO:O	55:8A:245:ILE:HG13	1.82	0.80
62:8H:57:ARG:HA	62:8H:60:TYR:CE1	2.17	0.80
32:1g:112:CYS:HA	41:1p:141:ARG:HH21	1.46	0.80
57:8C:86:PHE:CZ	57:8C:90:GLU:OE2	2.35	0.80
56:8B:68:LEU:HA	56:8B:71:ILE:HD12	1.64	0.80
2:1B:81:ARG:HE	8:1H:61:LEU:CD2	1.95	0.80
55:8A:208:MET:SD	55:8A:219:PHE:CD2	2.75	0.80
2:1B:42:ARG:HH22	70:1B:203:PC1:H12	1.47	0.79
14:1N:270:MET:HE1	14:1N:282:MET:CE	2.12	0.79
12:1L:576:MET:HG2	69:1Y:202:3PE:H32	1.65	0.79
19:1S:18:ILE:HD11	19:1S:52:ILE:HG23	1.65	0.79
55:8A:124:THR:HG23	55:8A:128:VAL:HA	1.62	0.79
56:8B:59:GLN:NE2	68:8N:14:SER:H	1.81	0.79
16:1P:248:VAL:HG22	16:1P:334:VAL:HG21	1.65	0.79
39:1n:97:LYS:HG2	39:1n:177:PRO:HG3	1.65	0.79
48:3D:249:MET:HE3	48:3D:252:PRO:HG3	1.64	0.79
55:8A:483:SER:HA	67:8M:4:LYS:NZ	1.92	0.79
1:1A:105:GLU:CG	10:1J:169:MET:HE1	2.11	0.79
32:1g:55:LEU:O	32:1g:59:ARG:HG3	1.81	0.79
68:8N:18:LEU:O	68:8N:22:ILE:HD12	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:49:LEU:HD12	8:1H:126:LYS:HG3	1.65	0.79
59:4E:33:MET:HE3	59:4E:67:ILE:HG21	1.64	0.79
68:8N:8:GLN:CA	68:8N:11:LYS:NZ	2.46	0.79
66:4L:24:MET:HG3	87:4L:101:PGV:H201	1.65	0.78
15:1O:14:THR:O	15:1O:18:LEU:HD13	1.83	0.78
92:4B:305:PSC:H261	92:4B:305:PSC:H10	1.66	0.78
58:4D:53:MET:HE1	59:4E:104:LEU:CD2	2.05	0.78
56:8B:52:HIS:NE2	56:8B:56:MET:SD	2.56	0.78
4:1D:20:TYR:HB2	12:1L:575:ILE:HD11	1.65	0.78
87:4C:301:PGV:H162	93:4G:102:PEK:H162	1.65	0.78
57:8C:148:HIS:ND1	57:8C:152:MET:CE	2.45	0.78
4:1D:52:GLY:H	4:1D:53:PRO:HD3	1.49	0.78
7:1G:226:GLU:HG2	7:1G:253:ARG:HD3	1.64	0.78
52:3U:21:ARG:O	52:3U:25:GLU:HG3	1.84	0.78
55:4A:381:LEU:HD13	88:4A:604:HEA:HAC	1.66	0.78
52:3H:77:GLU:HA	52:3H:79:ASP:HB2	1.66	0.77
65:4K:52:GLU:N	65:4K:52:GLU:OE2	2.17	0.77
58:8D:34:SER:OG	58:8D:37:GLN:HG3	1.83	0.77
35:1j:38:TRP:CE3	35:1j:42:HIS:HE1	2.02	0.77
65:8K:52:GLU:OE1	65:8K:54:ARG:O	2.01	0.77
49:3R:199:GLN:HB2	49:3R:248:ARG:HH21	1.49	0.77
57:8C:119:THR:HG22	61:8G:50:TYR:CE2	2.19	0.77
58:8D:43:LYS:NZ	58:8D:46:ALA:HB3	1.99	0.77
58:8D:77:GLU:O	58:8D:81:ILE:CD1	2.32	0.77
26:1a:59:ARG:HE	26:1a:61:HIS:CE1	2.02	0.77
45:3A:172:GLU:OE1	45:3A:173:ASN:N	2.18	0.77
58:8D:78:TRP:HA	58:8D:81:ILE:CD1	2.13	0.77
59:8E:18:TYR:OH	59:8E:28:GLU:O	2.02	0.77
36:1k:29:GLU:OE1	36:1k:33:GLU:OE2	2.02	0.77
37:1l:80:ASP:HB3	37:1l:83:MET:CE	2.15	0.77
41:1p:88:GLU:O	41:1p:92:ARG:HG2	1.83	0.77
55:8A:69:MET:HE3	88:8A:604:HEA:H272	1.65	0.77
58:8D:68:PHE:CE1	59:8E:69:GLU:CB	2.67	0.77
23:1X:87:CYS:SG	23:1X:102:GLN:NE2	2.58	0.77
67:4M:29:PRO:O	67:4M:33:VAL:HG23	1.84	0.77
12:1L:176:ARG:HA	12:1L:179:ASP:OD2	1.85	0.77
55:8A:409:TRP:CB	55:8A:471:ILE:CD1	2.62	0.77
15:1O:189:PRO:HA	15:1O:192:MET:HG2	1.67	0.77
58:4D:64:PHE:CD2	59:4E:66:ARG:HD3	2.19	0.77
55:8A:208:MET:SD	55:8A:219:PHE:CE2	2.78	0.77
12:1L:23:ASN:HD22	75:1L:702:CDL:H321	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:86:ASN:OD1	10:1J:87:LYS:N	2.17	0.76
66:8L:26:THR:HG21	67:8M:21:VAL:HG22	1.65	0.76
17:1Q:9:GLN:HB3	22:1W:23:ARG:HH21	1.51	0.76
58:4D:82:VAL:O	58:4D:86:LEU:HD13	1.84	0.76
57:8C:6:HIS:CD2	57:8C:8:TYR:H	2.02	0.76
57:8C:47:LEU:CD2	87:8C:303:PGV:H12	2.15	0.76
25:1Z:59:ARG:O	25:1Z:62:ILE:HG22	1.86	0.76
30:1e:4:ASP:OD1	30:1e:7:LYS:HB3	1.86	0.76
87:8C:302:PGV:H162	93:8G:102:PEK:H162	1.66	0.76
55:8A:409:TRP:HB3	55:8A:471:ILE:CD1	2.15	0.76
4:1D:50:ASN:HA	4:1D:65:VAL:HA	1.66	0.76
8:1H:204:GLU:HG2	8:1H:279:ARG:HH22	1.49	0.76
58:4D:20:ARG:HD3	58:4D:72:ASN:HD21	1.50	0.76
6:1F:250:ASN:ND2	6:1F:318:ASP:CG	2.43	0.76
23:1X:122:GLY:HA3	27:1b:77:LEU:HD12	1.67	0.76
59:4E:85:VAL:O	59:4E:89:LEU:HD13	1.86	0.76
55:8A:362:SER:HA	56:8B:87:MET:HE1	1.67	0.76
6:1F:43:TYR:CE1	6:1F:44:LYS:HG3	2.21	0.76
1:1A:18:VAL:HG22	8:1H:222:MET:HE2	1.68	0.76
4:1D:328:ALA:HB3	7:1G:126:ASP:HB2	1.66	0.76
23:1X:36:ASP:OD2	27:1b:68:HIS:ND1	2.12	0.76
1:1A:90:MET:HA	1:1A:90:MET:HE3	1.67	0.75
12:1L:378:LEU:HD22	12:1L:383:MET:HE3	1.68	0.75
16:1P:249:ALA:HB2	16:1P:318:LEU:HD12	1.68	0.75
57:4C:151:LEU:HD22	57:4C:159:MET:HE1	1.68	0.75
56:8B:185:MET:HA	56:8B:185:MET:HE2	1.68	0.75
10:1J:17:PHE:HB3	11:1K:14:ILE:HD11	1.68	0.75
62:8H:6:THR:CA	62:8H:9:LYS:NZ	2.50	0.75
5:1E:144:CYS:O	6:1F:139:ARG:NH2	2.18	0.75
55:8A:393:PHE:HE2	55:8A:472:ILE:HD11	1.52	0.75
19:1S:43:LEU:HD11	19:1S:47:ASN:HD21	1.50	0.75
20:1T:49:GLU:OE2	22:1W:40:TYR:CZ	2.39	0.75
56:4B:94:ALA:HB3	56:4B:148:MET:SD	2.26	0.75
11:1K:36:MET:HE3	14:1N:68:MET:HG3	1.67	0.75
49:3R:200:HIS:HB3	49:3R:203:GLU:HG2	1.66	0.75
16:1P:4:ALA:HB2	18:1R:24:ARG:NH2	2.02	0.75
4:1D:269:LEU:HD11	4:1D:373:GLU:HG3	1.69	0.74
13:1M:46:GLY:HA2	32:1g:84:ARG:NH2	2.02	0.74
35:1j:69:ASP:HB3	40:1o:117:ARG:NH1	2.02	0.74
58:8D:34:SER:OG	58:8D:37:GLN:CD	2.30	0.74
55:4A:468:MET:HE1	55:4A:471:ILE:CD1	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:194:GLU:HG2	6:1F:28:ARG:HH21	1.50	0.74
66:4L:41:ARG:HG3	67:4M:40:TYR:CZ	2.19	0.74
57:8C:27:MET:HE1	57:8C:50:ASN:ND2	2.01	0.74
24:1Y:38:TYR:HB3	69:1Y:202:3PE:H232	1.67	0.74
26:1a:22:ALA:O	26:1a:26:ILE:HG12	1.88	0.74
75:4C:305:CDL:H822	75:4C:305:CDL:H612	1.69	0.74
14:1N:70:LEU:HG	14:1N:98:MET:HE2	1.69	0.74
19:1S:88:ARG:NH1	19:1S:92:ASN:OD1	2.19	0.74
40:1o:45:MET:HE1	40:1o:59:ALA:HB3	1.68	0.74
62:8H:73:ASP:OD1	62:8H:76:ARG:NH2	2.20	0.74
43:1r:11:ARG:HG3	43:1r:19:LEU:HD11	1.69	0.74
57:8C:33:MET:HE2	64:8J:49:CYS:CB	2.17	0.74
59:8E:69:GLU:HG2	59:8E:101:PRO:HG3	1.70	0.74
5:1E:76:PRO:HB2	5:1E:79:ARG:HG2	1.70	0.74
7:1G:648:LEU:HD21	19:1S:44:LYS:HG2	1.69	0.74
20:1T:18:VAL:HG21	20:1T:54:MET:HG3	1.69	0.74
14:1N:149:ILE:HG21	14:1N:154:MET:HE1	1.68	0.74
58:8D:77:GLU:HG2	58:8D:81:ILE:HD11	1.69	0.74
13:1M:307:TRP:HA	13:1M:310:MET:HE2	1.70	0.74
17:1Q:10:LEU:HD13	22:1W:16:SER:HB3	1.68	0.74
41:1p:158:GLN:HG2	41:1p:162:MET:HE2	1.68	0.74
61:4G:15:THR:O	61:4G:19:LEU:HD12	1.87	0.74
64:4J:21:HIS:CD2	64:4J:22:LEU:HD13	2.22	0.74
55:4A:222:PRO:HG2	56:4B:176:PRO:HB2	1.70	0.74
57:4C:151:LEU:CD2	57:4C:159:MET:HE1	2.17	0.74
48:3D:269:SER:OG	52:3H:42:LEU:HB2	1.88	0.73
51:3T:40:ARG:NH1	75:3T:101:CDL:OA3	2.20	0.73
55:4A:31:THR:HG21	55:4A:465:VAL:HG11	1.70	0.73
55:4A:306:THR:HG23	55:4A:310:MET:CE	2.18	0.73
12:1L:217:LEU:HD13	12:1L:277:THR:HG22	1.69	0.73
25:1Z:68:ARG:O	25:1Z:72:MET:HG3	1.87	0.73
59:8E:78:HIS:CE1	63:8I:12:LEU:HD12	2.23	0.73
2:1B:109:GLU:OE2	16:1P:54:TYR:OH	2.06	0.73
10:1J:34:ILE:HA	10:1J:61:LEU:HD11	1.70	0.73
13:1M:216:LEU:HD23	13:1M:291:VAL:HG22	1.69	0.73
48:3Q:139:THR:OG1	52:3U:41:ASP:OD1	2.07	0.73
55:4A:271:MET:HE3	55:4A:271:MET:CA	2.19	0.73
12:1L:297:ASP:HB3	12:1L:300:LYS:HB2	1.68	0.73
55:8A:333:LYS:HZ2	55:8A:335:SER:N	1.87	0.73
59:8E:85:VAL:O	59:8E:89:LEU:HG	1.88	0.73
2:1B:86:MET:HE3	2:1B:107:MET:CE	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:162:GLU:HG3	15:1O:262:LEU:HD22	1.70	0.73
35:1j:38:TRP:CD2	35:1j:42:HIS:CE1	2.77	0.73
56:4B:86:MET:CA	56:4B:89:GLU:OE1	2.27	0.73
57:4C:151:LEU:HD22	57:4C:159:MET:CE	2.19	0.73
59:4E:33:MET:HE3	59:4E:67:ILE:CB	2.18	0.73
68:8N:32:TYR:O	68:8N:34:THR:N	2.21	0.73
49:3R:172:LYS:HD2	49:3R:214:ILE:HG21	1.69	0.73
54:3Y:8:PRO:O	54:3Y:12:GLU:HG3	1.89	0.73
87:8A:601:PGV:H182	87:8A:601:PGV:H332	1.69	0.73
62:8H:6:THR:CB	62:8H:9:LYS:HZ1	2.02	0.73
66:8L:34:ALA:HA	66:8L:37:PHE:HD2	1.52	0.73
25:1Z:76:GLN:NE2	25:1Z:80:ASP:OD1	2.22	0.72
59:4E:48:ILE:CD1	59:4E:71:VAL:HG21	2.19	0.72
52:3H:61:ARG:NH2	52:3H:86:ASP:OD2	2.23	0.72
57:4C:33:MET:CE	64:4J:49:CYS:HB3	2.17	0.72
55:8A:74:MET:HE3	55:8A:249:PRO:HB2	1.69	0.72
6:1F:30:ASP:O	6:1F:39:ARG:NH2	2.23	0.72
8:1H:196:ALA:HB3	8:1H:197:PRO:HD3	1.71	0.72
13:1M:108:MET:HB3	13:1M:121:LEU:HD13	1.72	0.72
55:8A:110:LEU:HD11	87:8A:601:PGV:H181	1.71	0.72
69:1L:703:3PE:N	70:1M:505:PC1:O12	2.22	0.72
47:3C:229:ILE:HG23	70:3J:101:PC1:H3A1	1.71	0.72
46:3O:124:LEU:HD22	46:3O:224:LEU:HD21	1.71	0.72
62:4H:6:THR:HA	62:4H:9:LYS:HE2	1.71	0.72
55:8A:208:MET:HE3	55:8A:219:PHE:CD2	2.24	0.72
2:1B:81:ARG:HE	8:1H:61:LEU:HD23	1.54	0.72
7:1G:451:VAL:HG22	7:1G:489:VAL:HG12	1.72	0.72
49:3R:173:PRO:HG2	49:3R:215:GLY:O	1.89	0.72
49:3R:204:ARG:NH1	49:3R:246:SER:O	2.23	0.72
68:8N:8:GLN:HA	68:8N:11:LYS:CE	2.20	0.72
56:8B:59:GLN:CD	68:8N:14:SER:OG	2.33	0.72
2:1B:48:MET:HE2	2:1B:80:PRO:HG3	1.72	0.72
75:3P:504:CDL:HA61	75:3P:504:CDL:H532	1.71	0.72
10:1J:99:MET:HE3	10:1J:100:GLU:N	2.05	0.72
40:1o:45:MET:HE1	40:1o:59:ALA:CB	2.20	0.72
55:8A:483:SER:HB3	67:8M:4:LYS:CE	2.19	0.72
7:1G:477:ILE:HD11	7:1G:489:VAL:HG11	1.71	0.72
12:1L:528:TYR:CG	37:1l:101:MET:HG2	2.25	0.72
55:4A:353:LEU:HB3	56:4B:31:VAL:HG13	1.72	0.72
59:4E:33:MET:HE3	59:4E:67:ILE:HB	1.72	0.72
55:8A:222:PRO:HG2	56:8B:176:PRO:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8C:247:VAL:HG12	57:8C:251:PHE:HE1	1.54	0.72
64:8J:36:MET:HA	64:8J:39:CYS:SG	2.30	0.72
49:3R:150:SER:HB3	49:3R:170:ARG:H	1.53	0.71
55:4A:28:MET:HE2	67:4M:26:PHE:CE2	2.24	0.71
60:4F:83:PRO:CD	60:4F:84:SER:N	2.52	0.71
68:4N:32:TYR:O	68:4N:34:THR:N	2.23	0.71
20:1T:34:SER:HB3	20:1T:40:LEU:HD11	1.72	0.71
57:8C:127:LEU:HA	57:8C:131:LEU:HD11	1.71	0.71
20:1T:25:ILE:HD12	20:1T:40:LEU:HD22	1.71	0.71
69:1M:504:3PE:H3I1	14:1N:256:PRO:HD2	1.72	0.71
32:1g:120:LEU:HD23	32:1g:121:PRO:HD2	1.72	0.71
55:8A:367:LEU:CD1	55:8A:372:TYR:CE2	2.73	0.71
56:8B:45:MET:CE	92:8B:305:PSC:H81	2.20	0.71
56:8B:52:HIS:CG	56:8B:56:MET:HE1	2.19	0.71
56:8B:45:MET:HE1	92:8B:305:PSC:H81	1.73	0.71
66:8L:36:PRO:O	66:8L:40:VAL:HG23	1.91	0.71
55:8A:390:MET:HA	55:8A:390:MET:HE3	1.73	0.71
57:8C:27:MET:CE	57:8C:50:ASN:HD22	2.02	0.71
7:1G:110:GLN:HE21	17:1Q:45:MET:HB3	1.55	0.71
56:4B:58:ALA:HB2	92:4B:305:PSC:H031	1.71	0.71
6:1F:365:CYS:HB2	71:1F:502:SF4:S3	2.30	0.71
47:3P:111:GLU:OE1	47:3P:111:GLU:N	2.19	0.71
58:4D:63:LYS:HG2	58:4D:64:PHE:CE1	2.24	0.71
58:8D:44:GLU:OE2	59:8E:59:ASN:HB3	1.91	0.71
65:8K:13:TYR:O	65:8K:17:ILE:CD1	2.36	0.71
12:1L:503:GLU:HG3	64:4J:33:ARG:HE	1.55	0.71
14:1N:270:MET:HE3	14:1N:279:PRO:HG3	1.72	0.71
45:3A:269:PRO:HB2	45:3A:410:VAL:HG11	1.72	0.71
55:4A:28:MET:HE2	67:4M:26:PHE:HE2	1.56	0.71
59:4E:63:SER:O	59:4E:67:ILE:HG23	1.89	0.71
2:1B:86:MET:CE	2:1B:107:MET:HE2	2.20	0.71
10:1J:88:THR:HG23	69:1K:101:3PE:H232	1.72	0.71
15:1O:105:LEU:HA	15:1O:128:ILE:HD11	1.73	0.71
53:3W:10:TYR:HA	53:3W:14:PHE:HB2	1.73	0.71
55:4A:93:ALA:CA	55:4A:171:MET:CE	2.61	0.71
60:4F:76:LYS:HD3	60:4F:77:GLY:N	2.06	0.71
11:1K:80:MET:HA	11:1K:80:MET:CE	2.20	0.70
15:1O:24:VAL:HG23	15:1O:167:HIS:H	1.54	0.70
13:1M:423:ILE:HG12	38:1m:58:VAL:HG12	1.72	0.70
25:1Z:108:GLU:H	30:1e:74:ARG:NH2	1.89	0.70
68:8N:2:LEU:O	68:8N:6:ILE:HG12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:73:ALA:HB2	14:1N:97:MET:HB3	1.72	0.70
55:4A:176:MET:HE3	55:4A:181:THR:HG22	1.72	0.70
56:4B:30:ILE:HG21	56:4B:76:ILE:HD11	1.73	0.70
68:4N:11:LYS:O	68:4N:11:LYS:NZ	2.21	0.70
58:8D:68:PHE:CD1	59:8E:69:GLU:HB3	2.27	0.70
62:8H:6:THR:HA	62:8H:9:LYS:NZ	2.06	0.70
36:1k:24:GLU:OE1	36:1k:24:GLU:N	2.19	0.70
47:3C:103:TYR:HA	47:3C:315:MET:HE3	1.72	0.70
66:4L:41:ARG:O	66:4L:45:LEU:HD23	1.91	0.70
2:1B:104:TYR:O	2:1B:111:ARG:NH1	2.24	0.70
6:1F:164:LYS:N	44:1s:63:MET:HE1	2.05	0.70
14:1N:270:MET:HB3	14:1N:275:SER:HB3	1.72	0.70
8:1H:169:GLN:HG2	8:1H:174:MET:HG3	1.74	0.70
55:4A:383:MET:HE2	55:4A:421:VAL:HG13	1.74	0.70
55:8A:195:LEU:HG	55:8A:245:ILE:HG21	1.72	0.70
62:8H:36:PHE:O	62:8H:40:GLU:HG2	1.92	0.70
63:8I:65:LYS:HD2	63:8I:65:LYS:O	1.92	0.70
1:1A:36:PRO:HB2	1:1A:43:PRO:HG2	1.73	0.70
69:1M:502:3PE:H372	69:1M:502:3PE:H272	1.73	0.70
38:1m:111:LYS:O	38:1m:115:ILE:HG13	1.91	0.70
55:4A:96:ARG:NH2	57:4C:64:GLU:OE1	2.24	0.70
67:4M:17:ILE:O	67:4M:21:VAL:HG23	1.91	0.70
55:8A:333:LYS:NZ	55:8A:335:SER:CA	2.54	0.70
6:1F:276:LEU:HD13	6:1F:315:VAL:HG23	1.71	0.70
8:1H:32:GLN:OE1	8:1H:34:ARG:NH1	2.23	0.70
9:1I:150:ASN:HD21	42:1q:127:TYR:H	1.40	0.70
16:1P:89:ASN:OD1	16:1P:90:VAL:N	2.25	0.70
37:1I:158:ILE:HG12	40:1o:99:LYS:HB3	1.74	0.70
55:8A:367:LEU:CD1	55:8A:372:TYR:CD2	2.62	0.70
59:8E:63:SER:O	59:8E:67:ILE:HG23	1.92	0.70
6:1F:287:VAL:HG11	6:1F:294:LEU:HD12	1.73	0.70
23:1X:36:ASP:OD1	23:1X:37:LYS:N	2.25	0.70
87:4B:301:PGV:H22	75:4D:201:CDL:H312	1.74	0.70
63:4I:54:TYR:OH	63:4I:59:ASP:OD2	2.09	0.70
64:4J:2:GLU:N	64:4J:2:GLU:OE2	2.25	0.70
14:1N:6:TYR:CE2	14:1N:46:LYS:HD2	2.27	0.69
49:3E:159:ILE:HG12	49:3E:165:MET:HG2	1.73	0.69
49:3E:261:PRO:HB2	49:3E:273:VAL:HG11	1.73	0.69
87:4A:601:PGV:H332	87:4A:601:PGV:H162	1.72	0.69
13:1M:225:ILE:O	13:1M:229:MET:HG3	1.92	0.69
5:1E:55:GLN:HE22	5:1E:90:TYR:HA	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:28:GLU:OE1	17:1Q:28:GLU:N	2.25	0.69
53:3J:14:TYR:HA	53:3J:18:PHE:HB2	1.75	0.69
49:3R:239:HIS:HD2	49:3R:240:GLY:H	1.41	0.69
56:4B:62:GLU:CB	56:4B:65:TRP:CZ2	2.71	0.69
55:8A:333:LYS:HZ1	55:8A:335:SER:HA	1.58	0.69
68:8N:2:LEU:HA	68:8N:5:ILE:HG22	1.74	0.69
68:8N:50:ASN:HD21	68:8N:53:PRO:HB3	1.56	0.69
7:1G:101:HIS:HE1	71:1G:801:SF4:S3	1.94	0.69
10:1J:20:PHE:HE1	11:1K:32:CYS:HA	1.56	0.69
14:1N:332:LEU:HD21	75:1d:203:CDL:H431	1.74	0.69
6:1F:43:TYR:CD1	6:1F:44:LYS:HG3	2.28	0.69
6:1F:250:ASN:OD1	6:1F:250:ASN:O	2.11	0.69
7:1G:129:ARG:HB3	43:1r:48:LEU:HD22	1.74	0.69
34:1i:105:PRO:HG2	34:1i:119:MET:HE2	1.74	0.69
40:1o:74:PRO:HG3	41:1p:28:PRO:HD3	1.75	0.69
60:4F:83:PRO:CD	60:4F:84:SER:H	2.06	0.69
55:8A:176:MET:HE2	55:8A:181:THR:HG22	1.73	0.69
57:8C:23:SER:OG	57:8C:50:ASN:HB2	1.91	0.69
58:8D:48:TRP:NE1	59:8E:56:ARG:HD3	2.08	0.69
4:1D:249:ASP:OD2	4:1D:404:LYS:NZ	2.25	0.69
16:1P:138:ASP:HB3	16:1P:141:SER:HB2	1.74	0.69
20:1U:21:LEU:HD13	36:1k:18:TYR:OH	1.92	0.69
26:1a:1:MET:HE2	26:1a:1:MET:N	2.07	0.69
34:1i:100:LYS:O	40:1o:49:GLN:NE2	2.26	0.69
46:3B:166:ALA:HB2	46:3B:244:ILE:HG13	1.73	0.69
55:8A:242:GLU:HA	55:8A:245:ILE:HD12	1.75	0.69
87:8B:302:PGV:H91	87:8B:302:PGV:H251	1.74	0.69
68:8N:7:THR:O	68:8N:11:LYS:CE	2.40	0.69
15:1O:101:TYR:HE1	15:1O:128:ILE:HG23	1.58	0.69
29:1d:107:LYS:HB2	29:1d:112:ILE:HD11	1.73	0.69
64:4J:8:LYS:HA	64:4J:8:LYS:HE3	1.75	0.69
55:8A:393:PHE:CE2	55:8A:472:ILE:HD11	2.28	0.69
56:8B:16:ILE:O	56:8B:20:LEU:HD23	1.92	0.69
68:8N:8:GLN:CA	68:8N:11:LYS:HZ3	2.04	0.69
2:1B:62:MET:HE3	2:1B:69:MET:SD	2.33	0.69
12:1L:102:GLU:OE1	12:1L:456:ARG:NH2	2.25	0.69
12:1L:290:LEU:O	12:1L:523:SER:OG	2.10	0.69
22:1W:62:LYS:HD2	22:1W:66:MET:CE	2.22	0.69
23:1X:17:VAL:HG11	25:1Z:74:LEU:HD11	1.75	0.69
23:1X:29:HIS:HB3	23:1X:119:PRO:HD2	1.74	0.69
31:1f:47:GLU:OE1	31:1f:47:GLU:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:55:ARG:HH22	41:1p:119:SER:HB3	1.56	0.69
43:1r:29:GLU:OE2	43:1r:29:GLU:N	2.23	0.69
45:3A:118:GLN:CG	45:3A:219:LEU:HD21	2.20	0.69
47:3C:129:MET:HE1	47:3C:181:PHE:HB3	1.74	0.69
49:3R:162:GLY:H	49:3R:178:HIS:HB3	1.57	0.69
57:4C:90:GLU:OE2	57:4C:207:HIS:NE2	2.26	0.69
57:4C:176:LEU:HD12	57:4C:179:SER:OG	1.93	0.69
55:8A:495:LEU:HD11	60:8F:73:TRP:CD1	2.28	0.69
56:8B:25:ASP:O	56:8B:29:MET:HG3	1.92	0.69
20:1U:8:LEU:N	20:1U:88:GLU:OE2	2.26	0.69
29:1d:99:GLU:OE1	29:1d:99:GLU:N	2.26	0.69
52:3U:47:ARG:HG2	52:3U:50:THR:HB	1.75	0.69
59:4E:52:LEU:HD12	59:4E:98:ILE:CD1	2.22	0.69
59:4E:82:TYR:HA	59:4E:85:VAL:HG12	1.74	0.69
55:8A:379:TYR:CE1	55:8A:383:MET:HE1	2.27	0.69
59:8E:25:ASP:HB3	59:8E:28:GLU:OE2	1.93	0.69
1:1A:69:ILE:HD11	8:1H:144:VAL:HG13	1.75	0.69
7:1G:537:LEU:HD12	7:1G:543:ILE:HD11	1.74	0.69
56:8B:100:MET:SD	56:8B:155:SER:OG	2.50	0.69
87:8A:602:PGV:H221	87:8A:602:PGV:H61	1.74	0.68
58:8D:100:LYS:HA	58:8D:104:TYR:HD2	1.58	0.68
20:1T:12:LYS:HZ1	20:1T:32:VAL:HG13	1.58	0.68
25:1Z:59:ARG:O	25:1Z:62:ILE:CG2	2.42	0.68
55:4A:28:MET:HA	55:4A:28:MET:CE	2.22	0.68
55:8A:208:MET:CE	55:8A:219:PHE:CB	2.70	0.68
66:8L:20:ARG:NH1	66:8L:24:MET:HE2	2.08	0.68
13:1M:46:GLY:HA2	32:1g:84:ARG:CZ	2.24	0.68
16:1P:52:GLU:HG3	16:1P:54:TYR:H	1.58	0.68
57:4C:60:ASP:O	57:4C:64:GLU:HG3	1.94	0.68
59:4E:48:ILE:HD11	59:4E:71:VAL:CG2	2.24	0.68
55:8A:362:SER:HA	56:8B:87:MET:CE	2.23	0.68
62:8H:6:THR:HB	62:8H:9:LYS:HZ1	1.53	0.68
1:1A:27:LEU:HD22	70:1A:202:PC1:H122	1.76	0.68
1:1A:73:LEU:HD23	8:1H:151:LEU:HD12	1.74	0.68
12:1L:82:MET:HA	12:1L:82:MET:HE3	1.74	0.68
57:8C:77:LYS:HD2	57:8C:80:ARG:HD3	1.76	0.68
70:1H:403:PC1:H331	70:1H:403:PC1:H2A2	1.76	0.68
10:1J:74:MET:CE	10:1J:75:ALA:HB2	2.24	0.68
59:4E:48:ILE:HG21	59:4E:89:LEU:HD21	1.76	0.68
56:8B:141:ARG:HD3	56:8B:210:VAL:HG11	1.74	0.68
2:1B:101:ARG:NH1	2:1B:105:ASP:OD1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:190:MET:CG	7:1G:192:MET:HE3	2.24	0.68
13:1M:341:THR:HG21	38:1m:64:LEU:HD21	1.75	0.68
16:1P:264:ARG:HH12	16:1P:285:GLU:HB2	1.57	0.68
23:1X:46:ARG:NH2	33:1h:142:ASP:OD1	2.27	0.68
56:8B:133:MET:HE1	58:8D:123:MET:HG3	1.76	0.68
75:8C:306:CDL:H141	75:8C:306:CDL:H541	1.76	0.68
7:1G:672:TYR:HB3	7:1G:684:MET:HE3	1.74	0.68
12:1L:145:GLU:HA	12:1L:145:GLU:OE2	1.94	0.68
15:1O:45:LYS:HE3	15:1O:232:GLU:HG3	1.75	0.68
49:3I:32:ALA:N	49:3I:71:ASN:O	2.26	0.68
49:3V:65:VAL:H	49:3V:77:ARG:C	2.00	0.68
57:8C:65:SER:HB2	87:8C:307:PGV:H041	1.75	0.68
64:8J:39:CYS:O	64:8J:43:THR:HG23	1.94	0.68
15:1O:73:LEU:HD21	15:1O:295:LYS:HB3	1.76	0.68
59:8E:78:HIS:HE1	63:8I:12:LEU:CD1	2.03	0.68
12:1L:556:ILE:HD11	38:1m:75:ILE:HG22	1.76	0.68
25:1Z:108:GLU:H	30:1e:74:ARG:HH22	1.38	0.68
58:8D:48:TRP:HE1	59:8E:56:ARG:HH11	1.42	0.68
34:1i:68:ILE:O	34:1i:72:THR:HG22	1.95	0.67
13:1M:453:MET:HE2	32:1g:77:VAL:CG1	2.22	0.67
56:4B:132:GLU:HB3	56:4B:137:GLU:HG3	1.75	0.67
56:4B:161:HIS:CE1	56:4B:207:MET:HE1	2.30	0.67
57:8C:157:LYS:HA	57:8C:157:LYS:HE3	1.76	0.67
67:8M:18:GLY:O	67:8M:22:THR:HG23	1.93	0.67
39:1n:178:MET:HE2	39:1n:178:MET:HA	1.76	0.67
47:3C:125:ALA:O	47:3C:129:MET:HG3	1.94	0.67
23:1X:122:GLY:CA	27:1b:77:LEU:HD12	2.23	0.67
55:4A:22:PHE:CE2	55:4A:105:LEU:HB3	2.29	0.67
55:8A:15:ILE:HD11	55:8A:99:ASN:HA	1.76	0.67
56:8B:41:ILE:HG23	56:8B:45:MET:HE2	1.76	0.67
59:8E:75:ALA:HB1	59:8E:81:ILE:HD13	1.76	0.67
7:1G:324:ASP:HB3	7:1G:571:ALA:HB1	1.77	0.67
52:3U:49:GLN:OE1	52:3U:49:GLN:O	2.13	0.67
55:8A:124:THR:CG2	55:8A:128:VAL:HG22	2.25	0.67
55:8A:343:GLY:O	55:8A:347:LEU:HD22	1.94	0.67
55:8A:434:SER:O	56:8B:10:GLN:NE2	2.28	0.67
6:1F:364:PRO:HB2	6:1F:403:THR:HG22	1.75	0.67
7:1G:190:MET:SD	7:1G:192:MET:HE3	2.35	0.67
48:3D:284:GLU:OE2	48:3D:290:ARG:NH1	2.26	0.67
49:3R:176:VAL:HG22	49:3R:212:ILE:HG23	1.77	0.67
49:3V:53:GLU:HA	49:3V:56:ARG:HD2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:418:PHE:HE2	75:4D:201:CDL:HB21	1.58	0.67
57:4C:204:HIS:CE1	57:4C:249:TRP:HB2	2.30	0.67
87:8C:307:PGV:H152	87:8C:307:PGV:H291	1.77	0.67
66:8L:20:ARG:CZ	66:8L:24:MET:HE2	2.24	0.67
20:1U:28:GLU:OE2	20:1U:29:LYS:HG2	1.94	0.67
41:1p:5:ASP:HB3	41:1p:8:VAL:HG12	1.76	0.67
47:3C:8:HIS:HB3	47:3C:11:MET:HB2	1.77	0.67
49:3R:180:THR:O	49:3R:182:LYS:N	2.28	0.67
63:4I:55:ASP:OD1	63:4I:58:LYS:HB2	1.94	0.67
66:4L:41:ARG:CG	67:4M:40:TYR:CE2	2.57	0.67
58:8D:34:SER:OG	58:8D:37:GLN:CG	2.42	0.67
58:8D:81:ILE:HD12	58:8D:81:ILE:H	1.59	0.67
69:1M:502:3PE:H371	29:1d:43:LEU:HB3	1.77	0.67
36:1k:74:PHE:O	36:1k:78:VAL:HG22	1.95	0.67
56:8B:28:LEU:HG	63:8I:35:TYR:HE2	1.59	0.67
62:8H:57:ARG:HA	62:8H:60:TYR:HE1	1.58	0.67
66:8L:35:ALA:O	66:8L:39:ILE:HD12	1.95	0.67
12:1L:599:MET:HE1	14:1N:97:MET:SD	2.35	0.67
58:4D:20:ARG:CD	58:4D:72:ASN:HD21	2.08	0.67
55:8A:496:HIS:CE1	60:8F:57:ILE:HD11	2.30	0.67
49:3E:151:LYS:HG3	49:3E:152:ILE:HG23	1.75	0.67
55:8A:426:PHE:HZ	75:8B:303:CDL:H142	1.60	0.67
60:8F:18:ARG:HD3	60:8F:22:MET:HE3	1.77	0.67
22:1W:42:GLU:O	22:1W:42:GLU:OE2	2.14	0.66
55:8A:124:THR:HG21	55:8A:128:VAL:HG22	1.76	0.66
56:8B:13:THR:HA	56:8B:188:ARG:HH12	1.60	0.66
62:8H:71:ALA:O	62:8H:75:ARG:HG2	1.95	0.66
12:1L:499:MET:HE1	64:4J:37:THR:HG21	1.77	0.66
23:1X:121:LEU:HD11	25:1Z:62:ILE:HG23	1.76	0.66
33:1h:44:ASN:ND2	75:1h:202:CDL:OB9	2.28	0.66
55:8A:147:ILE:HG23	55:8A:206:ILE:HB	1.77	0.66
6:1F:224:ASN:ND2	73:1F:501:FMN:O2	2.29	0.66
12:1L:151:SER:HB2	12:1L:248:HIS:HE1	1.60	0.66
26:1a:44:GLN:HA	26:1a:47:LEU:HD12	1.76	0.66
45:3A:250:LEU:HD12	49:3I:44:ASP:HB2	1.76	0.66
45:3N:224:VAL:HG13	45:3N:225:GLU:OE1	1.94	0.66
3:1C:40:VAL:HG12	3:1C:50:ILE:HG23	1.78	0.66
41:1p:119:SER:O	41:1p:123:ASN:ND2	2.28	0.66
63:4I:23:GLY:O	63:4I:27:VAL:HG12	1.95	0.66
55:8A:407:GLN:OE1	55:8A:407:GLN:N	2.22	0.66
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:200:THR:HG21	6:1F:283:HIS:HA	1.77	0.66
8:1H:24:GLU:OE2	8:1H:274:ARG:NH1	2.29	0.66
45:3A:146:ARG:NH2	45:3A:308:GLN:OE1	2.29	0.66
48:3D:161:GLY:HA2	48:3D:168:MET:HE1	1.77	0.66
56:4B:216:LEU:HD22	56:4B:220:GLU:OE1	1.94	0.66
58:8D:40:LEU:CD2	58:8D:59:LEU:HD21	2.25	0.66
58:8D:43:LYS:HZ1	58:8D:46:ALA:HB3	1.61	0.66
2:1B:34:ASP:HB2	2:1B:173:LEU:HB2	1.76	0.66
9:1I:156:ASN:ND2	18:1R:34:GLU:OE1	2.27	0.66
20:1T:58:PHE:HD2	20:1T:80:ILE:HG21	1.58	0.66
26:1a:1:MET:HE2	26:1a:1:MET:H1	1.60	0.66
42:1q:60:ARG:HH22	42:1q:95:ASP:HA	1.60	0.66
48:3D:162:PRO:HB2	48:3Q:99:GLU:HG3	1.77	0.66
57:8C:86:PHE:CE1	57:8C:90:GLU:OE2	2.48	0.66
31:1f:5:GLN:O	31:1f:9:ASP:HB3	1.96	0.66
69:3A:503:3PE:H362	47:3C:11:MET:HE2	0.74	0.66
49:3R:209:GLU:HG2	49:3R:210:TRP:CD2	2.30	0.66
1:1A:60:ILE:HG21	10:1J:168:ILE:HG21	1.78	0.66
11:1K:55:LEU:HD13	30:1e:16:TRP:HE3	1.61	0.66
20:1T:70:LEU:HD23	20:1T:76:ILE:HG23	1.76	0.66
25:1Z:93:GLU:O	25:1Z:97:ILE:HG13	1.96	0.66
49:3R:266:THR:OG1	49:3R:270:LEU:O	2.14	0.66
55:8A:230:LEU:O	55:8A:234:LEU:HD22	1.95	0.66
58:8D:78:TRP:O	58:8D:82:VAL:HG23	1.95	0.66
6:1F:426:LEU:O	6:1F:430:MET:HG2	1.96	0.66
7:1G:226:GLU:OE1	17:1Q:36:ARG:NH2	2.28	0.66
11:1K:1:FME:O1	30:1e:72:MET:SD	2.54	0.66
13:1M:312:ALA:O	13:1M:316:MET:HG3	1.95	0.66
15:1O:63:THR:OG1	15:1O:302:ARG:NH2	2.29	0.66
55:4A:412:ILE:HG12	58:4D:81:ILE:HG23	1.76	0.66
87:8C:304:PGV:H221	87:8C:304:PGV:H31	1.78	0.66
62:8H:20:PHE:HB2	62:8H:28:ASN:HD21	1.61	0.66
4:1D:34:ASN:HB3	4:1D:36:VAL:HG22	1.77	0.66
6:1F:105:CYS:H	6:1F:257:ASN:ND2	1.93	0.66
13:1M:385:SER:CB	13:1M:396:MET:HE1	2.25	0.66
55:8A:93:ALA:HA	55:8A:171:MET:CE	2.26	0.66
7:1G:579:ARG:HG2	7:1G:636:VAL:HB	1.77	0.65
55:8A:232:GLN:HB3	55:8A:292:MET:HE2	1.78	0.65
3:1C:149:ARG:NH2	4:1D:77:ASP:OD2	2.29	0.65
62:4H:56:TYR:CZ	68:4N:80:PRO:HD2	2.31	0.65
57:8C:9:HIS:NE2	57:8C:64:GLU:OE2	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:127:HIS:O	2:1B:134:ARG:NH1	2.30	0.65
6:1F:25:LEU:HD11	6:1F:267:THR:HG22	1.78	0.65
11:1K:73:LEU:HD21	14:1N:41:ILE:HG13	1.78	0.65
45:3N:240:GLU:HG3	45:3N:422:VAL:HB	1.79	0.65
60:4F:70:ILE:HG21	60:4F:83:PRO:CD	2.26	0.65
3:1C:195:ARG:NH2	9:1I:92:ILE:O	2.29	0.65
55:8A:138:HIS:O	55:8A:213:ARG:NH2	2.29	0.65
70:1M:503:PC1:H272	70:1M:503:PC1:H371	1.78	0.65
55:8A:321:PHE:HA	55:8A:324:LEU:HD12	1.78	0.65
20:1T:35:HIS:CE1	20:1T:38:LYS:HE3	2.32	0.65
41:1p:158:GLN:O	41:1p:162:MET:HE3	1.97	0.65
70:1B:203:PC1:H341	70:1q:201:PC1:H352	1.77	0.65
7:1G:350:PRO:HB3	7:1G:464:THR:HG22	1.78	0.65
20:1T:12:LYS:NZ	20:1T:32:VAL:HG13	2.11	0.65
23:1X:72:GLN:HG2	23:1X:114:LEU:HD21	1.78	0.65
46:3O:28:ARG:HH22	46:3O:390:GLY:HA3	1.62	0.65
49:3V:77:ARG:O	49:3V:77:ARG:NE	2.30	0.65
54:3X:38:TRP:HA	70:3X:101:PC1:H32	1.78	0.65
87:4A:601:PGV:H62	64:4J:40:LEU:HD11	1.78	0.65
55:8A:33:LEU:HB3	55:8A:61:HIS:HB2	1.78	0.65
55:8A:232:GLN:HB3	55:8A:292:MET:CE	2.27	0.65
6:1F:185:ILE:HG12	6:1F:359:CYS:HB2	1.79	0.65
39:1n:12:GLN:HE22	39:1n:13:GLN:HG3	1.62	0.65
55:4A:406:ASN:HD22	55:4A:409:TRP:HD1	1.43	0.65
56:4B:89:GLU:HG2	68:4N:70:VAL:CG2	2.27	0.65
59:4E:48:ILE:HD13	59:4E:71:VAL:HG21	1.79	0.65
55:8A:151:HIS:NE2	55:8A:206:ILE:HG13	2.12	0.65
55:8A:333:LYS:HZ1	55:8A:335:SER:CA	2.10	0.65
57:8C:247:VAL:HG12	57:8C:251:PHE:CE1	2.32	0.65
59:8E:33:MET:HE1	59:8E:67:ILE:CG2	2.27	0.65
8:1H:31:MET:HE3	9:1I:41:LEU:HD22	1.79	0.65
26:1a:67:GLU:OE1	26:1a:67:GLU:N	2.25	0.65
75:1d:203:CDL:HA4	75:1d:203:CDL:H512	1.79	0.65
49:3R:209:GLU:OE2	49:3R:209:GLU:N	2.21	0.65
56:4B:61:VAL:O	56:4B:65:TRP:CE3	2.50	0.65
55:8A:298:ASP:OD2	55:8A:300:ASP:HB2	1.97	0.65
24:1Y:11:ILE:HG13	24:1Y:20:LYS:HE3	1.79	0.65
48:3D:160:ASP:HB2	48:3D:171:ARG:HG2	1.79	0.65
55:8A:190:ILE:HG23	87:8A:603:PGV:H252	1.79	0.65
55:8A:271:MET:HG3	68:8N:12:HIS:HE1	1.60	0.65
4:1D:34:ASN:HB2	15:1O:158:VAL:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:36:LYS:O	44:1s:65:GLN:NE2	2.30	0.64
12:1L:2:ASN:HB3	12:1L:3:PRO:HD2	1.79	0.64
12:1L:562:LEU:HD22	69:1N:901:3PE:H3B2	1.79	0.64
17:1Q:9:GLN:CB	22:1W:23:ARG:HH21	2.10	0.64
49:3E:231:PHE:HE1	49:3E:242:HIS:HB3	1.61	0.64
56:4B:28:LEU:HD21	75:4B:303:CDL:H561	1.77	0.64
55:8A:314:ILE:H	55:8A:314:ILE:HD12	1.62	0.64
75:8B:303:CDL:HB21	75:8B:303:CDL:HB61	1.78	0.64
66:8L:34:ALA:HA	66:8L:37:PHE:CD2	2.32	0.64
1:1A:27:LEU:HD13	70:1A:202:PC1:H132	1.78	0.64
14:1N:69:MET:HE3	14:1N:97:MET:CE	2.27	0.64
22:1W:25:MET:O	22:1W:29:LYS:HG3	1.97	0.64
52:3H:83:GLU:OE1	52:3H:83:GLU:N	2.26	0.64
49:3R:151:LYS:HD3	49:3R:152:ILE:HB	1.78	0.64
56:4B:89:GLU:OE2	68:4N:68:VAL:HB	1.97	0.64
59:4E:52:LEU:HD22	59:4E:67:ILE:HD11	1.79	0.64
65:4K:19:ALA:O	65:4K:23:THR:HG23	1.96	0.64
59:8E:81:ILE:H	59:8E:81:ILE:HD12	1.62	0.64
61:8G:29:ALA:O	61:8G:32:THR:HG22	1.98	0.64
1:1A:41:PHE:HB2	4:1D:51:PHE:CE2	2.31	0.64
5:1E:100:ILE:HD13	5:1E:156:ILE:HD12	1.78	0.64
13:1M:365:THR:HG21	13:1M:444:LEU:HD21	1.80	0.64
16:1P:92:ILE:HD11	16:1P:218:ILE:HD11	1.79	0.64
69:1d:201:3PE:H221	70:1d:202:PC1:H221	1.78	0.64
40:1o:56:ASP:OD1	40:1o:57:TYR:N	2.28	0.64
47:3P:32:ASN:ND2	47:3P:228:ASP:OD1	2.29	0.64
2:1B:33:LEU:HD13	70:1B:202:PC1:H381	1.80	0.64
20:1T:73:PRO:O	20:1T:77:VAL:HG23	1.97	0.64
47:3C:181:PHE:CE1	47:3P:53:MET:HE2	2.33	0.64
52:3H:45:VAL:HG12	52:3H:95:VAL:HG22	1.79	0.64
45:3N:141:ASN:HA	49:3V:47:ARG:HH21	1.61	0.64
59:4E:48:ILE:CG2	59:4E:89:LEU:HD21	2.27	0.64
59:8E:42:VAL:HG21	59:8E:81:ILE:HG21	1.78	0.64
12:1L:528:TYR:CD1	37:1l:101:MET:HG2	2.33	0.64
53:3J:36:GLU:OE1	54:3Y:34:TRP:NE1	2.30	0.64
75:4B:303:CDL:HB21	75:4B:303:CDL:HB61	1.79	0.64
7:1G:190:MET:HG2	7:1G:192:MET:HG2	1.80	0.64
12:1L:401:MET:SD	12:1L:482:MET:HG3	2.37	0.64
13:1M:54:LEU:HD21	33:1h:96:ILE:HD11	1.79	0.64
13:1M:118:PHE:O	13:1M:122:PHE:HB3	1.97	0.64
20:1U:25:ILE:HG12	20:1U:40:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3E:199:GLN:HB3	49:3E:204:ARG:HD3	1.78	0.64
46:3O:196:GLN:HA	46:3O:227:ARG:HD3	1.79	0.64
57:8C:59:ARG:CZ	57:8C:63:ARG:HH21	2.11	0.64
12:1L:194:ASN:ND2	41:1p:106:GLN:OE1	2.31	0.64
55:8A:409:TRP:HB2	55:8A:471:ILE:CD1	2.27	0.64
58:8D:77:GLU:HB2	65:8K:10:HIS:CD2	2.33	0.64
7:1G:620:ARG:NH1	7:1G:633:TYR:OH	2.31	0.64
43:1r:45:SER:O	43:1r:51:ASN:ND2	2.26	0.64
46:3O:28:ARG:NH2	46:3O:390:GLY:HA3	2.12	0.64
56:4B:115:ASP:OD1	56:4B:115:ASP:O	2.16	0.64
61:4G:83:GLU:OE1	61:4G:83:GLU:N	2.22	0.64
33:1h:63:HIS:NE2	33:1h:76:ALA:O	2.30	0.64
55:4A:35:LEU:HD21	55:4A:462:LEU:HB2	1.79	0.64
87:4B:302:PGV:H91	87:4B:302:PGV:H251	1.80	0.64
87:8A:601:PGV:H131	57:8C:22:LEU:HD21	1.80	0.64
87:8B:301:PGV:H22	75:8D:201:CDL:H312	1.80	0.64
34:1i:108:THR:HG22	34:1i:115:VAL:HB	1.79	0.64
57:4C:180:GLU:HA	57:4C:180:GLU:OE2	1.97	0.64
55:8A:407:GLN:NE2	87:8A:602:PGV:O05	2.31	0.64
68:8N:23:GLY:O	68:8N:27:THR:OG1	2.11	0.64
8:1H:156:MET:SD	8:1H:174:MET:HE3	2.36	0.63
46:3B:34:VAL:HG11	46:3B:386:ALA:HB1	1.81	0.63
51:3T:36:ASN:ND2	75:3T:101:CDL:OA4	2.31	0.63
58:4D:126:MET:HG2	63:4I:68:ILE:HG21	1.80	0.63
66:4L:28:TYR:CE2	87:4L:101:PGV:H302	2.33	0.63
15:1O:320:LYS:O	29:1d:60:ARG:NH2	2.30	0.63
46:3B:227:ARG:HG3	46:3B:229:GLY:H	1.64	0.63
45:3N:444:LEU:HB2	75:3N:502:CDL:HB31	1.80	0.63
68:8N:13:PRO:HA	68:8N:16:ILE:HG13	1.78	0.63
1:1A:37:TYR:CE2	2:1B:80:PRO:HD2	2.33	0.63
8:1H:223:PHE:O	8:1H:227:GLU:HG2	1.98	0.63
10:1J:130:THR:HG22	25:1Z:121:MET:HE2	1.79	0.63
14:1N:107:GLY:O	14:1N:187:MET:HE1	1.98	0.63
22:1W:29:LYS:HZ2	22:1W:29:LYS:HB3	1.63	0.63
24:1Y:35:VAL:HG23	69:1Y:202:3PE:H252	1.80	0.63
53:3J:20:ARG:HB2	53:3J:23:THR:HG22	1.81	0.63
55:8A:144:ASP:OD1	55:8A:213:ARG:NH1	2.30	0.63
15:1O:265:ASN:CG	15:1O:268:GLU:HG2	2.22	0.63
39:1n:13:GLN:O	39:1n:17:ARG:HG2	1.98	0.63
41:1p:29:VAL:O	41:1p:33:THR:HG23	1.97	0.63
65:4K:44:PRO:HB3	65:4K:48:VAL:HG21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:173:PRO:HB3	55:8A:511:ILE:HD13	1.81	0.63
59:8E:24:ILE:HD12	59:8E:25:ASP:H	1.63	0.63
60:8F:81:ARG:HG2	60:8F:88:HIS:CD2	2.34	0.63
7:1G:672:TYR:HD1	7:1G:684:MET:HE1	1.64	0.63
12:1L:6:SER:O	12:1L:10:THR:OG1	2.14	0.63
58:4D:77:GLU:HG2	58:4D:81:ILE:HD11	1.79	0.63
59:4E:41:LEU:O	59:4E:41:LEU:HD12	1.99	0.63
55:8A:271:MET:HG3	68:8N:12:HIS:CE1	2.32	0.63
55:8A:336:PRO:HB2	55:8A:394:VAL:HG11	1.80	0.63
66:8L:18:LYS:NZ	66:8L:19:TRP:CH2	2.66	0.63
8:1H:114:TYR:OH	10:1J:65:LEU:O	2.17	0.63
12:1L:159:HIS:HB2	13:1M:416:ARG:HB3	1.81	0.63
35:1j:65:GLY:CA	40:1o:30:PHE:CE1	2.82	0.63
52:3H:49:CYS:O	52:3H:52:ILE:HG12	1.99	0.63
75:3P:504:CDL:H151	75:3T:101:CDL:H521	1.80	0.63
57:4C:107:ALA:HB1	62:4H:27:ARG:HH21	1.64	0.63
58:4D:96:LEU:HD23	58:4D:96:LEU:C	2.22	0.63
59:4E:31:LYS:HE2	60:4F:83:PRO:O	1.99	0.63
55:8A:343:GLY:O	55:8A:347:LEU:CD2	2.46	0.63
70:1B:203:PC1:H3C1	8:1H:53:LEU:HD11	1.81	0.63
14:1N:280:THR:O	14:1N:284:MET:HG2	1.99	0.63
55:4A:273:MET:HE3	55:4A:319:LYS:HE3	1.80	0.63
59:4E:44:GLU:H	59:4E:47:ILE:HD11	1.64	0.63
56:8B:100:MET:HE2	56:8B:157:GLU:HG3	1.81	0.63
57:8C:87:ILE:O	57:8C:91:VAL:HG23	1.99	0.63
58:8D:48:TRP:NE1	59:8E:56:ARG:HH11	1.95	0.63
63:8I:22:VAL:O	63:8I:26:ILE:HG13	1.98	0.63
8:1H:156:MET:HE1	8:1H:177:THR:HG21	1.81	0.63
9:1I:146:GLU:OE2	42:1q:123:GLN:NE2	2.31	0.63
27:1b:56:LEU:O	27:1b:56:LEU:HD12	1.99	0.63
49:3I:71:ASN:O	49:3I:71:ASN:OD1	2.15	0.63
47:3P:8:HIS:HB3	47:3P:11:MET:HB2	1.80	0.63
53:3W:32:GLU:OE1	54:3X:34:TRP:NE1	2.32	0.63
58:4D:40:LEU:HD21	58:4D:59:LEU:HG	1.80	0.63
58:4D:56:LYS:NZ	59:4E:97:GLY:O	2.30	0.63
62:4H:6:THR:HA	62:4H:9:LYS:CE	2.29	0.63
75:8C:306:CDL:H212	75:8C:306:CDL:H311	1.80	0.63
68:8N:7:THR:O	68:8N:11:LYS:HD3	1.98	0.63
6:1F:250:ASN:ND2	6:1F:318:ASP:OD2	2.20	0.63
7:1G:36:GLN:NE2	17:1Q:47:SER:O	2.32	0.63
14:1N:207:ILE:HG22	14:1N:211:MET:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:23:GLY:O	31:1f:27:ASP:OD1	2.17	0.63
38:1m:105:LYS:O	38:1m:109:ASP:OD1	2.17	0.63
87:4A:603:PGV:H131	68:4N:22:ILE:HG21	1.79	0.63
56:8B:141:ARG:HD3	56:8B:210:VAL:CG1	2.28	0.63
12:1L:86:SER:O	12:1L:90:ILE:HG12	1.98	0.62
51:3T:63:THR:O	51:3T:67:GLU:OE2	2.17	0.62
59:4E:41:LEU:HD23	63:4I:10:ARG:HE	1.64	0.62
61:4G:68:THR:HG22	61:4G:69:LEU:H	1.63	0.62
87:4G:101:PGV:H261	87:4G:101:PGV:H92	1.81	0.62
69:1M:504:3PE:H281	14:1N:246:VAL:HG11	1.81	0.62
70:1M:505:PC1:H2D2	70:1M:505:PC1:H292	1.81	0.62
14:1N:6:TYR:HE2	14:1N:46:LYS:HD2	1.64	0.62
23:1X:19:VAL:O	26:1a:50:ARG:NH2	2.31	0.62
56:8B:52:HIS:HD2	56:8B:56:MET:HE1	0.88	0.62
57:8C:47:LEU:HD23	87:8C:303:PGV:H12	1.80	0.62
58:8D:24:LEU:HD11	59:8E:33:MET:HE2	1.80	0.62
1:1A:38:GLU:HB2	1:1A:43:PRO:HG3	1.79	0.62
13:1M:16:TRP:NE1	13:1M:97:THR:OG1	2.32	0.62
49:3E:123:VAL:HG13	53:3J:32:ALA:HA	1.81	0.62
75:8C:306:CDL:H822	75:8C:306:CDL:H612	1.81	0.62
4:1D:246:THR:HG23	21:1V:12:GLY:HA3	1.79	0.62
13:1M:325:MET:HE1	13:1M:441:ILE:HB	1.82	0.62
20:1T:54:MET:SD	20:1T:76:ILE:HG21	2.39	0.62
56:4B:41:ILE:O	56:4B:45:MET:HG2	2.00	0.62
55:8A:93:ALA:HA	55:8A:171:MET:HE1	1.80	0.62
57:8C:59:ARG:NE	57:8C:63:ARG:NH2	2.41	0.62
58:8D:53:MET:H	58:8D:53:MET:HE2	1.64	0.62
3:1C:116:PRO:HD2	22:1W:18:LYS:HE2	1.81	0.62
13:1M:147:LEU:HB3	69:1N:901:3PE:H332	1.81	0.62
29:1d:89:ASP:HB2	33:1h:121:PRO:HG2	1.82	0.62
65:8K:22:ALA:O	65:8K:26:VAL:HG12	2.00	0.62
19:1S:88:ARG:CZ	19:1S:92:ASN:OD1	2.48	0.62
38:1m:7:PRO:HB3	38:1m:13:LEU:HB2	1.82	0.62
57:4C:129:VAL:CB	57:4C:180:GLU:OE1	2.47	0.62
8:1H:156:MET:SD	8:1H:174:MET:HE1	2.40	0.62
31:1f:56:TRP:HE1	33:1h:88:GLU:HG3	1.64	0.62
63:4I:48:ALA:O	63:4I:52:ARG:HG3	1.99	0.62
57:8C:6:HIS:NE2	57:8C:8:TYR:HB2	2.14	0.62
57:8C:126:PRO:HA	57:8C:130:PRO:HG2	1.80	0.62
65:8K:38:ILE:O	65:8K:38:ILE:HG13	1.97	0.62
75:1N:902:CDL:H221	75:1N:902:CDL:H371	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:149:LEU:HG	47:3C:291:VAL:HG22	1.79	0.62
55:4A:241:PRO:O	55:4A:245:ILE:HG13	2.00	0.62
55:8A:254:ILE:HG13	55:8A:344:PHE:CD2	2.34	0.62
87:8A:603:PGV:H151	68:8N:22:ILE:HB	1.81	0.62
92:8B:305:PSC:H261	92:8B:305:PSC:H10	1.82	0.62
3:1C:22:LEU:HD12	3:1C:48:LEU:HB2	1.80	0.62
6:1F:197:GLU:OE1	6:1F:204:ARG:NH2	2.33	0.62
13:1M:108:MET:HE1	75:1X:201:CDL:H232	1.82	0.62
54:3X:14:ALA:O	54:3X:18:ILE:HG12	1.99	0.62
75:4C:305:CDL:H141	75:4C:305:CDL:H541	1.82	0.62
55:8A:510:TYR:CG	60:8F:49:VAL:HG23	2.34	0.62
57:8C:81:TYR:O	57:8C:85:LEU:HG	1.99	0.62
3:1C:40:VAL:HG23	43:1r:68:VAL:HG23	1.80	0.62
9:1I:7:MET:HG3	9:1I:7:MET:O	2.00	0.62
12:1L:316:THR:HA	12:1L:319:ILE:HG12	1.82	0.62
38:1m:105:LYS:O	38:1m:109:ASP:CG	2.43	0.62
55:4A:195:LEU:HG	55:4A:245:ILE:HD13	1.80	0.62
58:4D:54:ASP:C	58:4D:54:ASP:OD1	2.43	0.62
75:4D:201:CDL:H402	75:4D:201:CDL:H592	1.81	0.62
58:8D:84:THR:O	58:8D:88:PHE:HD1	1.82	0.62
7:1G:273:GLY:O	7:1G:549:HIS:NE2	2.29	0.61
16:1P:27:THR:HG21	16:1P:56:THR:HG22	1.82	0.61
47:3C:112:THR:O	47:3C:196:HIS:NE2	2.33	0.61
58:4D:120:THR:HG23	58:4D:134:PHE:HZ	1.65	0.61
55:8A:333:LYS:NZ	55:8A:335:SER:HA	2.14	0.61
55:8A:484:ALA:HB3	67:8M:2:TYR:HB2	1.81	0.61
35:1j:38:TRP:CE3	35:1j:42:HIS:CE1	2.85	0.61
49:3E:209:GLU:OE1	49:3E:209:GLU:N	2.24	0.61
45:3N:444:LEU:HD11	69:3N:503:3PE:H12	1.81	0.61
57:8C:22:LEU:O	57:8C:26:LEU:HG	2.00	0.61
7:1G:229:ASP:OD2	7:1G:231:MET:HG2	2.00	0.61
69:1Y:202:3PE:H341	69:1Y:203:3PE:H331	1.83	0.61
33:1h:41:THR:O	33:1h:45:VAL:HG23	2.00	0.61
57:8C:182:TYR:CE2	87:8C:305:PGV:H042	2.29	0.61
64:8J:27:THR:O	64:8J:31:LEU:HD12	1.99	0.61
1:1A:7:LEU:HD11	70:1H:403:PC1:H342	1.83	0.61
6:1F:21:ILE:HG23	6:1F:117:LYS:HZ1	1.66	0.61
75:1q:203:CDL:H181	75:1q:203:CDL:H331	1.82	0.61
53:3J:33:LEU:HD11	54:3Y:48:ILE:HG21	1.81	0.61
49:3R:214:ILE:N	49:3R:259:GLU:O	2.25	0.61
55:8A:333:LYS:NZ	55:8A:335:SER:HB3	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:8B:301:PGV:H05	75:8D:201:CDL:HA32	1.81	0.61
62:8H:25:GLN:NE2	62:8H:28:ASN:OD1	2.34	0.61
13:1M:6:ILE:HG12	75:1X:201:CDL:H652	1.82	0.61
19:1S:43:LEU:HD12	19:1S:47:ASN:HD21	1.66	0.61
20:1T:32:VAL:HG12	20:1T:74:GLN:HE21	1.65	0.61
46:3O:116:ILE:HG13	46:3O:120:MET:HE2	1.82	0.61
47:3P:377:LEU:HG	50:3S:20:TYR:HE2	1.66	0.61
64:4J:16:ASN:CG	64:4J:18:LEU:HD13	2.25	0.61
56:8B:133:MET:SD	58:8D:119:GLN:NE2	2.73	0.61
6:1F:21:ILE:HG21	6:1F:230:VAL:HG12	1.81	0.61
7:1G:11:VAL:HG11	7:1G:73:VAL:HB	1.82	0.61
19:1S:43:LEU:HD12	19:1S:43:LEU:O	2.00	0.61
49:3R:239:HIS:CE1	49:3R:253:PRO:HD2	2.36	0.61
55:4A:469:ILE:CD1	67:4M:26:PHE:CZ	2.83	0.61
55:8A:86:MET:HB3	55:8A:182:PRO:HG2	1.82	0.61
87:8A:601:PGV:H62	64:8J:40:LEU:HD11	1.82	0.61
57:8C:182:TYR:HE2	87:8C:305:PGV:C04	2.12	0.61
15:1O:294:GLN:O	15:1O:298:GLU:HG3	2.01	0.61
20:1T:5:PRO:HB2	20:1T:86:VAL:HG13	1.83	0.61
34:1i:86:LYS:HG2	34:1i:87:TYR:CE1	2.36	0.61
40:1o:21:MET:HE1	40:1o:101:PHE:HA	1.81	0.61
7:1G:347:GLU:HB2	7:1G:496:ILE:HD12	1.82	0.61
70:1I:203:PC1:H31	25:1Z:28:ARG:HG3	1.83	0.61
13:1M:71:TRP:CG	70:1M:505:PC1:H2C2	2.36	0.61
49:3E:261:PRO:HG2	49:3E:273:VAL:HG21	1.82	0.61
47:3P:216:ASP:OD1	47:3P:216:ASP:O	2.18	0.61
57:4C:86:PHE:HZ	87:4C:306:PGV:H301	1.65	0.61
3:1C:137:MET:HE1	3:1C:153:THR:HG23	1.82	0.61
7:1G:594:ARG:NH1	22:1W:122:PHE:O	2.34	0.61
75:3A:501:CDL:H151	75:3A:501:CDL:H321	1.82	0.61
52:3H:60:GLU:O	52:3H:64:LEU:HG	2.00	0.61
47:3P:132:VAL:HA	47:3P:139:SER:HB3	1.83	0.61
47:3P:215:MET:HB2	51:3T:10:MET:HE2	1.83	0.61
48:3Q:132:THR:HA	48:3Q:179:MET:HE3	1.83	0.61
57:8C:45:LEU:HD11	64:8J:38:LEU:HG	1.82	0.61
70:1A:202:PC1:H331	70:1A:202:PC1:H262	1.82	0.61
4:1D:52:GLY:N	4:1D:53:PRO:HD3	2.14	0.61
8:1H:253:GLU:O	8:1H:257:ILE:HD12	2.01	0.61
12:1L:90:ILE:HD12	12:1L:129:MET:SD	2.40	0.61
19:1S:24:GLN:HE22	19:1S:56:GLU:HG3	1.66	0.61
6:1F:91:LYS:HB2	6:1F:131:ALA:HA	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:104:ASP:O	7:1G:108:CYS:N	2.33	0.60
7:1G:284:ILE:HG23	7:1G:294:THR:HG21	1.83	0.60
15:1O:303:LYS:H	15:1O:309:ASN:HD21	1.47	0.60
35:1j:69:ASP:HB3	40:1o:117:ARG:HH12	1.67	0.60
36:1k:77:PHE:O	36:1k:81:VAL:HG13	2.01	0.60
37:1l:157:GLU:O	40:1o:33:ARG:NH2	2.32	0.60
58:8D:52:SER:OG	58:8D:54:ASP:OD1	2.19	0.60
62:8H:57:ARG:HA	62:8H:60:TYR:CD1	2.35	0.60
7:1G:46:LEU:O	17:1Q:116:LYS:NZ	2.34	0.60
13:1M:12:LEU:HD22	13:1M:97:THR:HG23	1.83	0.60
37:1l:138:LEU:O	37:1l:142:ARG:HB2	2.01	0.60
49:3E:161:GLU:HA	49:3E:178:HIS:HB3	1.82	0.60
64:4J:33:ARG:NH1	87:4J:101:PGV:H181	2.16	0.60
57:8C:233:PHE:HA	57:8C:236:GLU:OE1	2.01	0.60
58:8D:68:PHE:HE1	59:8E:69:GLU:HB2	1.61	0.60
4:1D:166:PRO:HG3	4:1D:228:MET:HG3	1.83	0.60
12:1L:596:MET:O	12:1L:600:THR:OG1	2.10	0.60
45:3A:354:VAL:HG21	45:3A:404:ALA:HA	1.83	0.60
55:4A:336:PRO:HB2	55:4A:394:VAL:HG11	1.83	0.60
55:8A:6:TRP:HE3	55:8A:18:LEU:HD21	1.66	0.60
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.84	0.60
13:1M:332:THR:HG22	13:1M:433:GLU:HG2	1.83	0.60
45:3N:173:ASN:HA	45:3N:176:LYS:HG2	1.84	0.60
46:3O:107:TYR:HB3	46:3O:123:LEU:HD11	1.84	0.60
58:4D:80:THR:HG21	65:4K:10:HIS:ND1	2.15	0.60
58:8D:48:TRP:HZ3	59:8E:61:PHE:CG	2.17	0.60
64:8J:30:ILE:O	64:8J:34:VAL:HG12	2.01	0.60
68:8N:5:ILE:HG23	68:8N:6:ILE:HD13	1.82	0.60
5:1E:52:ASP:OD2	6:1F:179:ARG:NH1	2.35	0.60
6:1F:105:CYS:H	6:1F:257:ASN:HD22	1.50	0.60
12:1L:288:THR:HG21	12:1L:307:SER:HB3	1.84	0.60
13:1M:243:MET:HE3	13:1M:301:ILE:HG21	1.82	0.60
16:1P:4:ALA:HB2	18:1R:24:ARG:HH21	1.65	0.60
25:1Z:86:MET:HE1	25:1Z:125:TYR:CE2	2.36	0.60
33:1h:74:TRP:O	33:1h:78:THR:HG22	2.02	0.60
49:3E:164:ASN:HB3	49:3E:177:ARG:HD3	1.84	0.60
49:3R:212:ILE:HD13	49:3R:271:VAL:HG21	1.83	0.60
55:4A:426:PHE:HZ	75:4B:303:CDL:H142	1.66	0.60
59:4E:33:MET:HE1	59:4E:67:ILE:HD12	1.83	0.60
68:8N:8:GLN:HA	68:8N:11:LYS:HE2	1.83	0.60
2:1B:150:PRO:HG3	4:1D:189:MET:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:165:THR:OG1	8:1H:275:ALA:O	2.19	0.60
7:1G:194:GLU:HG2	7:1G:195:LEU:HG	1.83	0.60
14:1N:95:MET:HE2	14:1N:149:ILE:HG23	1.84	0.60
48:3D:289:HIS:O	48:3D:293:MET:HG3	2.01	0.60
46:3O:212:SER:OG	46:3O:215:VAL:HG12	2.02	0.60
49:3R:239:HIS:CD2	49:3R:240:GLY:N	2.67	0.60
55:4A:33:LEU:HB3	55:4A:61:HIS:HB2	1.84	0.60
56:4B:112:ASP:OD1	56:4B:113:TYR:N	2.35	0.60
57:8C:59:ARG:CZ	57:8C:63:ARG:NH2	2.65	0.60
1:1A:92:LEU:O	1:1A:96:ILE:HG12	2.02	0.60
5:1E:37:ASN:ND2	44:1s:55:ASN:HD21	2.00	0.60
5:1E:110:LEU:HB3	6:1F:261:HIS:CD2	2.31	0.60
6:1F:31:TRP:HE1	44:1s:42:GLN:NE2	2.00	0.60
10:1J:7:PHE:CE1	11:1K:3:LEU:HD13	2.37	0.60
48:3D:228:GLY:HA3	52:3H:79:ASP:H	1.65	0.60
46:3O:49:LEU:HD21	46:3O:204:MET:HE3	1.83	0.60
58:4D:82:VAL:O	58:4D:86:LEU:CD1	2.50	0.60
55:8A:106:PRO:O	55:8A:110:LEU:HD13	2.01	0.60
57:8C:47:LEU:HD21	87:8C:303:PGV:H12	1.84	0.60
2:1B:81:ARG:NE	8:1H:61:LEU:HD21	2.17	0.60
4:1D:143:GLU:OE2	4:1D:278:TYR:OH	2.17	0.60
6:1F:125:GLY:O	6:1F:129:MET:HG3	2.01	0.60
7:1G:117:GLN:O	7:1G:121:MET:HG2	2.02	0.60
7:1G:316:ALA:HB3	7:1G:519:PRO:HG3	1.83	0.60
14:1N:339:MET:HE2	29:1d:34:MET:SD	2.41	0.60
37:1l:112:MET:HA	37:1l:112:MET:HE3	1.83	0.60
55:4A:80:ASN:OD1	55:4A:98:ASN:ND2	2.32	0.60
56:4B:102:HIS:NE2	56:4B:107:SER:OG	2.30	0.60
56:8B:95:LEU:HD12	56:8B:96:THR:N	2.16	0.60
57:8C:56:GLN:O	57:8C:60:ASP:OD1	2.19	0.60
57:8C:59:ARG:HD2	57:8C:63:ARG:HH21	1.66	0.60
61:8G:68:THR:HG22	61:8G:69:LEU:H	1.66	0.60
64:8J:48:TYR:CE1	87:8J:101:PGV:H032	2.36	0.60
1:1A:53:MET:CE	10:1J:172:THR:HG23	2.32	0.60
8:1H:156:MET:CG	8:1H:174:MET:HE1	2.32	0.60
10:1J:99:MET:CE	10:1J:100:GLU:N	2.65	0.60
69:1M:504:3PE:H2	14:1N:239:VAL:HG22	1.83	0.60
14:1N:142:LEU:HB3	14:1N:194:LEU:HD21	1.84	0.60
55:8A:124:THR:HG21	55:8A:128:VAL:HA	1.83	0.60
62:8H:17:ASP:OD1	62:8H:19:ARG:N	2.27	0.60
2:1B:91:THR:HG21	4:1D:85:ARG:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1K:101:3PE:H3C1	69:1K:101:3PE:H2C1	1.84	0.60
49:3E:219:HIS:HB3	72:3E:301:FES:S1	2.42	0.60
49:3R:123:VAL:HG13	53:3W:28:ALA:HA	1.84	0.60
55:4A:253:MET:HG2	55:4A:396:TRP:HZ3	1.65	0.60
57:4C:88:ILE:HG12	75:4C:305:CDL:H621	1.84	0.60
62:4H:19:ARG:C	62:4H:20:PHE:HD1	2.09	0.60
75:8C:306:CDL:H191	75:8C:306:CDL:H322	1.84	0.60
8:1H:175:ILE:O	8:1H:179:TRP:HB3	2.02	0.59
14:1N:266:ILE:HG22	14:1N:270:MET:HE2	1.83	0.59
15:1O:318:TRP:HB2	29:1d:58:LEU:HD12	1.82	0.59
51:3G:73:ARG:NH2	52:3H:82:GLU:HG2	2.16	0.59
49:3R:219:HIS:HB3	72:3R:301:FES:S1	2.42	0.59
55:4A:302:ARG:NH2	56:4B:88:ASP:OD1	2.35	0.59
64:8J:40:LEU:HD12	87:8J:101:PGV:H142	1.83	0.59
4:1D:130:PRO:HG2	4:1D:135:GLN:HE21	1.66	0.59
12:1L:378:LEU:HD12	35:1j:32:MET:HE1	1.85	0.59
20:1T:58:PHE:CD2	20:1T:80:ILE:HG21	2.36	0.59
32:1g:120:LEU:CD2	32:1g:121:PRO:HD2	2.32	0.59
55:4A:321:PHE:HA	55:4A:324:LEU:HD12	1.84	0.59
56:4B:33:LEU:HD12	63:4I:28:SER:HB2	1.84	0.59
68:4N:9:ALA:HB1	68:4N:16:ILE:CD1	2.32	0.59
55:8A:371:TYR:HD2	55:8A:428:GLN:HG2	1.65	0.59
55:8A:452:THR:HG22	55:8A:456:MET:HE2	1.84	0.59
56:8B:9:PHE:CE1	56:8B:24:HIS:CD2	2.90	0.59
65:8K:13:TYR:HB2	65:8K:17:ILE:HD11	1.83	0.59
1:1A:105:GLU:HG3	10:1J:169:MET:CE	2.17	0.59
6:1F:31:TRP:HE1	44:1s:42:GLN:HE22	1.50	0.59
6:1F:305:PRO:HD3	6:1F:413:TRP:HB3	1.84	0.59
12:1L:561:ILE:HG23	70:1Y:207:PC1:H2B2	1.84	0.59
13:1M:207:MET:HG3	13:1M:294:MET:HB3	1.82	0.59
14:1N:316:GLN:HA	15:1O:302:ARG:HH12	1.66	0.59
47:3C:149:LEU:HD11	47:3C:281:LEU:HD11	1.83	0.59
64:4J:36:MET:HB3	87:4J:101:PGV:H182	1.84	0.59
55:8A:100:MET:HE2	55:8A:104:LEU:HD21	1.84	0.59
55:8A:265:LYS:HB3	55:8A:490:THR:HG21	1.84	0.59
67:8M:24:LEU:HB3	67:8M:28:ILE:HD11	1.84	0.59
70:1B:202:PC1:H3G1	70:1B:203:PC1:H3E1	1.83	0.59
7:1G:383:ASN:ND2	7:1G:665:GLN:O	2.35	0.59
13:1M:453:MET:CE	32:1g:80:LEU:HD12	2.30	0.59
32:1g:118:ILE:HD11	41:1p:159:LYS:HG3	1.85	0.59
40:1o:27:ASP:N	40:1o:27:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:53:MET:HE2	47:3P:181:PHE:CZ	2.38	0.59
47:3C:270:PRO:HB2	47:3C:274:PHE:HB2	1.83	0.59
49:3R:235:TYR:HA	49:3R:242:HIS:HA	1.83	0.59
58:4D:95:LEU:HD21	67:4M:27:LEU:HD13	1.85	0.59
59:4E:45:PRO:HB2	59:4E:88:GLU:CG	2.31	0.59
57:8C:204:HIS:NE2	57:8C:249:TRP:HB2	2.16	0.59
58:8D:85:ALA:O	58:8D:89:ILE:CD1	2.41	0.59
2:1B:63:ALA:HB2	2:1B:69:MET:HE2	1.85	0.59
4:1D:259:MET:HE3	4:1D:421:GLN:HA	1.84	0.59
7:1G:243:ARG:HG2	7:1G:244:THR:HG23	1.84	0.59
10:1J:130:THR:HG22	25:1Z:121:MET:CE	2.33	0.59
12:1L:63:ILE:HD11	34:1i:85:LEU:HD22	1.84	0.59
12:1L:566:THR:O	12:1L:570:GLN:HG2	2.03	0.59
13:1M:116:ILE:O	13:1M:120:ILE:HG12	2.03	0.59
15:1O:3:TYR:HH	15:1O:257:HIS:HD1	1.49	0.59
47:3C:129:MET:HE1	47:3C:181:PHE:CB	2.32	0.59
5:1E:159:ASN:HB2	5:1E:184:PRO:HB3	1.82	0.59
7:1G:693:GLU:HB3	7:1G:697:ALA:HB2	1.84	0.59
12:1L:184:LEU:HD13	13:1M:393:ILE:HG21	1.83	0.59
35:1j:57:SER:OG	35:1j:58:GLN:OE1	2.19	0.59
40:1o:65:LEU:O	40:1o:69:LYS:HG3	2.02	0.59
45:3A:140:GLU:O	45:3A:143:SER:OG	2.20	0.59
46:3B:124:LEU:HD12	46:3B:223:PHE:HB2	1.85	0.59
55:4A:306:THR:HG23	55:4A:310:MET:HE1	1.83	0.59
56:4B:146:MET:HE2	56:4B:214:VAL:C	2.28	0.59
55:8A:5:ARG:HB2	66:8L:3:TYR:CE2	2.38	0.59
57:8C:206:LEU:O	57:8C:210:ILE:HG12	2.03	0.59
64:8J:33:ARG:O	64:8J:37:THR:HG22	2.03	0.59
68:8N:17:PRO:HD2	68:8N:18:LEU:H	1.66	0.59
20:1U:4:PRO:HD2	20:1U:4:PRO:O	2.02	0.59
56:4B:27:THR:O	56:4B:31:VAL:HG23	2.03	0.59
55:8A:51:ASP:OD2	56:8B:204:HIS:HB3	2.02	0.59
59:8E:44:GLU:HG2	59:8E:45:PRO:HD2	1.84	0.59
2:1B:86:MET:HE2	2:1B:103:VAL:HG23	1.84	0.59
14:1N:272:LYS:HD3	33:1h:108:LEU:HD21	1.84	0.59
24:1Y:85:ASP:OD2	24:1Y:87:LEU:HB3	2.03	0.59
40:1o:3:HIS:ND1	40:1o:4:LEU:HD23	2.16	0.59
42:1q:34:ARG:NH1	42:1q:54:GLN:OE1	2.35	0.59
46:3O:35:ILE:HD13	46:3O:206:LEU:HB3	1.85	0.59
87:8B:302:PGV:H62	68:8N:29:ALA:HB1	1.84	0.59
57:8C:7:ALA:HB2	60:8F:31:TYR:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:8N:16:ILE:O	68:8N:20:VAL:HG23	2.03	0.59
2:1B:144:ILE:HG13	2:1B:163:LEU:HB2	1.83	0.59
5:1E:151:ALA:HB1	5:1E:152:PRO:HD2	1.84	0.59
6:1F:129:MET:HE1	6:1F:221:THR:HB	1.83	0.59
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.38	0.59
16:1P:325:ARG:HG3	16:1P:326:TRP:CE2	2.38	0.59
53:3W:40:ASP:O	53:3W:44:GLU:HG3	2.02	0.59
56:4B:61:VAL:C	56:4B:65:TRP:CE3	2.81	0.59
87:4B:301:PGV:H312	75:4D:201:CDL:H462	1.85	0.59
59:4E:48:ILE:HD11	59:4E:71:VAL:HG21	1.84	0.59
61:4G:73:PRO:HA	61:4G:83:GLU:OE2	2.02	0.59
55:8A:157:SER:HB2	55:8A:199:LEU:HD11	1.85	0.59
75:8B:303:CDL:H811	75:8B:303:CDL:H262	1.84	0.59
87:8C:303:PGV:H332	93:8C:308:PEK:H322	1.85	0.59
2:1B:50:PHE:CE1	2:1B:103:VAL:HG21	2.38	0.59
14:1N:84:TRP:HB2	30:1e:18:THR:HA	1.83	0.59
34:1i:39:VAL:HG12	34:1i:44:GLN:HG3	1.85	0.59
45:3A:131:ARG:HD3	45:3A:175:ARG:HA	1.83	0.59
47:3P:237:LEU:HD13	48:3Q:212:MET:HG3	1.85	0.59
55:4A:343:GLY:HA2	87:4B:301:PGV:H062	1.84	0.59
59:4E:96:LEU:HD13	59:4E:98:ILE:HD11	1.84	0.59
56:8B:116:LEU:HD21	56:8B:226:MET:HE2	1.83	0.59
57:8C:6:HIS:HD2	57:8C:8:TYR:CD2	2.20	0.59
57:8C:60:ASP:O	57:8C:64:GLU:HG3	2.02	0.59
65:8K:38:ILE:HD11	65:8K:40:TRP:CH2	2.32	0.59
7:1G:157:THR:HB	7:1G:161:ARG:HE	1.67	0.58
11:1K:33:LEU:HA	11:1K:36:MET:HE2	1.84	0.58
24:1Y:104:THR:HG22	69:1Y:203:3PE:H11	1.85	0.58
34:1i:85:LEU:HD23	34:1i:89:VAL:HG21	1.85	0.58
46:3B:314:ALA:HA	49:3I:63:PRO:HD3	1.83	0.58
49:3E:125:VAL:HG21	70:3J:101:PC1:H362	1.85	0.58
49:3E:242:HIS:O	49:3E:250:ARG:N	2.35	0.58
55:4A:138:HIS:O	55:4A:213:ARG:NH2	2.36	0.58
57:8C:182:TYR:OH	87:8C:305:PGV:H05	2.03	0.58
58:8D:26:ASP:OD1	58:8D:26:ASP:N	2.36	0.58
58:8D:99:GLU:OE2	58:8D:104:TYR:CD2	2.55	0.58
61:8G:16:TRP:HA	61:8G:19:LEU:HD12	1.84	0.58
9:1I:43:ARG:HA	43:1r:11:ARG:HH21	1.68	0.58
13:1M:166:TYR:O	13:1M:170:THR:HG23	2.02	0.58
13:1M:329:LEU:O	13:1M:332:THR:OG1	2.21	0.58
14:1N:95:MET:HE2	14:1N:149:ILE:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:77:ASP:C	17:1Q:77:ASP:OD1	2.46	0.58
33:1h:50:ALA:HB2	41:1p:60:TYR:CE1	2.38	0.58
48:3Q:212:MET:HA	48:3Q:212:MET:HE3	1.86	0.58
55:4A:72:PRO:O	55:4A:77:GLY:N	2.33	0.58
56:4B:85:TYR:O	56:4B:89:GLU:OE1	2.21	0.58
60:4F:46:PRO:HG2	60:4F:90:LYS:HZ1	1.67	0.58
59:8E:64:ALA:O	59:8E:67:ILE:HG12	2.02	0.58
59:8E:66:ARG:O	59:8E:70:VAL:HG12	2.03	0.58
66:8L:19:TRP:CZ2	67:8M:14:GLU:OE1	2.55	0.58
10:1J:60:TYR:HE1	11:1K:37:MET:HE1	1.68	0.58
16:1P:143:SER:O	16:1P:147:ARG:HG3	2.02	0.58
47:3P:46:LEU:HD21	69:3R:302:3PE:H2C1	1.84	0.58
60:8F:22:MET:HE2	60:8F:22:MET:N	2.18	0.58
6:1F:326:GLN:O	6:1F:420:ARG:NH2	2.36	0.58
22:1W:49:LEU:O	22:1W:49:LEU:HD23	2.04	0.58
49:3I:62:ARG:HB2	49:3I:77:ARG:HH12	1.69	0.58
49:3V:77:ARG:C	49:3V:77:ARG:HE	2.11	0.58
58:4D:78:TRP:HA	58:4D:81:ILE:HD12	1.86	0.58
75:4D:201:CDL:H562	75:4D:201:CDL:H191	1.85	0.58
67:8M:32:TRP:O	67:8M:36:HIS:ND1	2.36	0.58
3:1C:83:VAL:HG12	3:1C:85:THR:HG22	1.84	0.58
9:1I:27:TRP:HB3	9:1I:30:LEU:HD12	1.86	0.58
23:1X:157:LEU:HD12	29:1d:17:GLU:HG2	1.84	0.58
38:1m:82:THR:HG22	38:1m:85:THR:HG23	1.85	0.58
46:3O:166:ALA:HB2	46:3O:244:ILE:HG13	1.85	0.58
47:3P:207:ASN:ND2	47:3P:211:ILE:O	2.36	0.58
54:3Y:38:TRP:HA	69:3Y:101:3PE:H11	1.84	0.58
55:4A:92:MET:HE2	55:4A:163:ASN:HD22	1.68	0.58
55:8A:420:GLY:O	55:8A:424:THR:OG1	2.19	0.58
58:8D:51:LEU:O	58:8D:56:LYS:NZ	2.33	0.58
8:1H:24:GLU:HA	8:1H:271:LEU:HD13	1.84	0.58
14:1N:242:SER:O	14:1N:246:VAL:HG23	2.03	0.58
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.38	0.58
17:1Q:22:LEU:HD23	22:1W:78:VAL:HG13	1.84	0.58
29:1d:8:ARG:NH2	70:1d:202:PC1:O14	2.36	0.58
35:1j:61:ASP:HA	35:1j:64:LEU:HB2	1.86	0.58
44:1s:43:HIS:CE1	44:1s:44:HIS:CE1	2.92	0.58
49:3E:187:GLU:OE1	49:3E:248:ARG:NH2	2.23	0.58
52:3H:47:GLU:O	52:3H:51:GLN:HG2	2.04	0.58
56:4B:97:VAL:HB	56:4B:152:MET:SD	2.43	0.58
57:4C:65:SER:HB2	87:4C:306:PGV:H041	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:4C:302:PGV:H332	93:4C:307:PEK:H322	1.86	0.58
58:4D:67:SER:HB3	59:4E:106:LEU:HB3	1.85	0.58
67:4M:42:ARG:O	67:4M:42:ARG:NE	2.27	0.58
68:8N:50:ASN:O	68:8N:50:ASN:OD1	2.21	0.58
19:1S:26:SER:O	19:1S:33:ARG:NH2	2.37	0.58
20:1U:14:ARG:HB3	20:1U:57:GLU:OE2	2.04	0.58
25:1Z:59:ARG:C	25:1Z:62:ILE:HG22	2.28	0.58
87:4A:601:PGV:H341	87:4L:101:PGV:H152	1.85	0.58
60:8F:43:LYS:HA	60:8F:88:HIS:HD1	1.68	0.58
2:1B:69:MET:HB2	2:1B:74:VAL:HB	1.85	0.58
10:1J:74:MET:C	10:1J:74:MET:SD	2.87	0.58
10:1J:74:MET:HE3	10:1J:75:ALA:HB2	1.86	0.58
12:1L:3:PRO:HG2	12:1L:53:MET:HE1	1.84	0.58
19:1S:23:CYS:SG	19:1S:59:ASP:N	2.77	0.58
48:3Q:147:LEU:HD12	48:3Q:157:ALA:HB1	1.85	0.58
48:3Q:203:ARG:NH2	53:3W:53:LYS:NZ	2.51	0.58
55:4A:28:MET:HE3	55:4A:28:MET:CA	2.23	0.58
55:4A:310:MET:HG2	56:4B:73:LEU:HD12	1.84	0.58
55:4A:443:TYR:O	56:4B:134:ARG:NH2	2.37	0.58
64:4J:15:ASP:OD1	64:4J:15:ASP:N	2.37	0.58
55:8A:6:TRP:CE3	55:8A:18:LEU:HD21	2.38	0.58
56:8B:25:ASP:OD2	63:8I:43:ARG:NE	2.35	0.58
58:8D:48:TRP:HE1	59:8E:56:ARG:CD	2.17	0.58
60:8F:21:MET:O	60:8F:25:ARG:HG2	2.04	0.58
87:8L:101:PGV:H131	87:8L:101:PGV:H311	1.85	0.58
6:1F:46:LYS:NZ	6:1F:167:CYS:O	2.32	0.58
7:1G:118:ASP:OD2	17:1Q:46:GLN:NE2	2.37	0.58
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.39	0.58
34:1i:99:ARG:NH1	40:1o:49:GLN:OE1	2.37	0.58
48:3D:307:LEU:O	48:3D:311:MET:HG3	2.03	0.58
55:4A:113:LEU:O	55:4A:117:MET:HG2	2.04	0.58
55:4A:215:LEU:HD11	93:4C:307:PEK:H271	1.85	0.58
7:1G:198:ASN:OD1	7:1G:268:ARG:NH2	2.36	0.58
14:1N:20:VAL:HG13	14:1N:29:ILE:HG23	1.86	0.58
14:1N:149:ILE:CG2	14:1N:154:MET:HE2	2.32	0.58
18:1R:38:ASN:HB3	18:1R:43:LEU:HD11	1.86	0.58
75:1X:201:CDL:H452	75:1X:201:CDL:H251	1.85	0.58
50:3F:82:MET:HE3	50:3F:83:ARG:HG3	1.86	0.58
46:3O:46:ARG:HG2	46:3O:379:LEU:HD22	1.85	0.58
51:3T:65:GLU:C	51:3T:65:GLU:OE1	2.47	0.58
68:4N:9:ALA:HB1	68:4N:16:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:8C:306:CDL:HB61	75:8C:306:CDL:H542	1.86	0.58
59:8E:28:GLU:CD	59:8E:28:GLU:H	2.12	0.58
59:8E:107:ASP:N	59:8E:107:ASP:OD1	2.37	0.58
87:8G:101:PGV:H282	87:8G:101:PGV:H102	1.86	0.58
67:8M:17:ILE:O	67:8M:21:VAL:HG12	2.03	0.58
5:1E:101:GLN:OE1	5:1E:155:GLN:NE2	2.37	0.57
7:1G:126:ASP:OD1	43:1r:56:ARG:NH1	2.36	0.57
14:1N:95:MET:HE2	14:1N:149:ILE:HG12	1.85	0.57
35:1j:17:LEU:HD23	35:1j:22:LEU:HD21	1.85	0.57
45:3N:42:ASP:HB2	45:3N:194:ARG:HB3	1.86	0.57
47:3P:233:LEU:HG	48:3Q:212:MET:HE1	1.86	0.57
49:3R:199:GLN:HB2	49:3R:248:ARG:NH2	2.17	0.57
55:4A:456:MET:HG2	58:4D:96:LEU:CD1	2.34	0.57
66:4L:18:LYS:NZ	67:4M:14:GLU:OE1	2.34	0.57
55:8A:491:ASN:HB3	55:8A:494:TRP:HD1	1.68	0.57
57:8C:117:PRO:HG2	57:8C:123:PRO:HG3	1.87	0.57
1:1A:37:TYR:OH	4:1D:54:GLN:OE1	2.21	0.57
8:1H:273:ILE:HG23	8:1H:277:TYR:CD2	2.40	0.57
12:1L:481:THR:OG1	40:1o:91:HIS:ND1	2.29	0.57
20:1U:36:PHE:HA	20:1U:40:LEU:HB2	1.86	0.57
32:1g:118:ILE:HD12	41:1p:155:LEU:HD11	1.86	0.57
44:1s:63:MET:HG3	44:1s:64:PRO:HD2	1.85	0.57
2:1B:81:ARG:HE	8:1H:61:LEU:HD21	1.69	0.57
14:1N:207:ILE:O	14:1N:211:MET:HG3	2.04	0.57
19:1S:52:ILE:H	19:1S:52:ILE:HD12	1.69	0.57
35:1j:38:TRP:CE2	35:1j:42:HIS:CE1	2.91	0.57
57:4C:92:LEU:O	57:4C:95:THR:OG1	2.23	0.57
58:4D:78:TRP:CD1	75:4D:201:CDL:H202	2.39	0.57
56:8B:59:GLN:HE21	68:8N:13:PRO:HD2	1.67	0.57
57:8C:43:LEU:HD21	87:8C:303:PGV:H262	1.85	0.57
12:1L:142:ILE:HG21	75:1L:702:CDL:H641	1.85	0.57
13:1M:453:MET:CE	32:1g:77:VAL:HG13	2.28	0.57
39:1n:170:VAL:HG13	39:1n:171:THR:HG23	1.86	0.57
45:3A:142:ASP:OD1	49:3E:79:SER:N	2.38	0.57
55:4A:190:ILE:HG23	87:4A:603:PGV:H252	1.85	0.57
55:8A:37:ILE:HD11	55:8A:58:VAL:HA	1.87	0.57
58:8D:40:LEU:HD21	58:8D:59:LEU:HD21	1.84	0.57
62:8H:81:PHE:HD1	62:8H:82:PRO:HD2	1.69	0.57
11:1K:1:FME:SD	14:1N:79:LEU:HD21	2.45	0.57
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.33	0.57
14:1N:258:SER:HB2	14:1N:336:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3B:22:GLN:OE1	46:3B:41:TYR:HE2	1.86	0.57
75:3G:103:CDL:H121	75:3G:103:CDL:H512	1.86	0.57
46:3O:97:SER:HA	49:3V:69:GLY:HA2	1.85	0.57
56:4B:151:ARG:NH2	62:4H:14:ALA:O	2.37	0.57
55:8A:5:ARG:HB2	66:8L:3:TYR:HE2	1.70	0.57
55:8A:101:SER:OG	55:8A:156:SER:O	2.20	0.57
55:8A:510:TYR:CD1	60:8F:49:VAL:HG23	2.38	0.57
87:8C:301:PGV:H281	87:8C:307:PGV:H312	1.86	0.57
5:1E:37:ASN:C	44:1s:65:GLN:HE22	2.12	0.57
8:1H:91:MET:O	8:1H:93:TYR:N	2.37	0.57
16:1P:200:THR:HB	16:1P:238:LEU:HB2	1.87	0.57
16:1P:216:ASN:ND2	16:1P:303:LEU:O	2.37	0.57
45:3A:305:GLN:OE1	49:3I:42:VAL:HG12	2.04	0.57
46:3B:365:LYS:HG2	46:3B:399:LEU:HD22	1.87	0.57
75:3G:102:CDL:OA7	75:3G:102:CDL:O1	2.23	0.57
55:4A:51:ASP:OD2	56:4B:205:SER:OG	2.21	0.57
59:4E:41:LEU:HD12	59:4E:41:LEU:C	2.29	0.57
60:4F:51:SER:HB3	60:4F:91:LEU:CD2	2.34	0.57
57:8C:157:LYS:HZ1	87:8C:302:PGV:H02	1.69	0.57
12:1L:142:ILE:HG12	13:1M:370:PRO:HB2	1.87	0.57
35:1j:69:ASP:HB3	40:1o:117:ARG:CZ	2.34	0.57
40:1o:69:LYS:HG2	40:1o:79:CYS:SG	2.44	0.57
70:1q:201:PC1:H2G2	70:1q:201:PC1:H3B2	1.87	0.57
55:4A:456:MET:HE2	58:4D:96:LEU:HD13	1.86	0.57
55:8A:127:THR:HA	55:8A:235:PHE:HE2	1.69	0.57
55:8A:343:GLY:HA2	87:8B:301:PGV:H062	1.86	0.57
1:1A:27:LEU:HD11	8:1H:60:PRO:HD3	1.86	0.57
4:1D:151:ILE:HD12	4:1D:177:MET:HE1	1.87	0.57
7:1G:215:PHE:HB3	9:1I:104:ARG:HG3	1.86	0.57
43:1r:57:ASP:OD1	43:1r:58:GLY:N	2.38	0.57
45:3N:269:PRO:HB2	45:3N:410:VAL:HG11	1.87	0.57
56:4B:62:GLU:CA	56:4B:65:TRP:CE2	2.81	0.57
59:4E:82:TYR:CE1	59:4E:86:ILE:HG13	2.40	0.57
55:8A:13:LYS:HE2	55:8A:500:PRO:HB2	1.86	0.57
55:8A:179:TYR:OH	87:8A:603:PGV:O02	2.21	0.57
57:8C:156:ARG:HH22	57:8C:223:LEU:HA	1.70	0.57
4:1D:299:CYS:O	4:1D:303:GLU:HG2	2.04	0.57
5:1E:159:ASN:ND2	5:1E:161:TYR:OH	2.37	0.57
6:1F:28:ARG:NH1	44:1s:35:ASN:O	2.38	0.57
6:1F:262:VAL:HA	6:1F:287:VAL:HA	1.85	0.57
7:1G:55:CYS:HB3	72:1G:803:FES:S2	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:439:PHE:CE1	7:1G:442:ILE:HD11	2.38	0.57
12:1L:539:TYR:HB2	37:1L:89:VAL:HG21	1.87	0.57
13:1M:319:HIS:HA	13:1M:322:THR:HG22	1.86	0.57
46:3B:47:ILE:HD11	46:3B:211:VAL:HG11	1.86	0.57
55:4A:124:THR:HG22	55:4A:132:LEU:HG	1.87	0.57
57:8C:161:GLN:O	57:8C:165:ILE:HG12	2.05	0.57
6:1F:106:LYS:O	6:1F:110:ILE:HG22	2.04	0.57
13:1M:153:THR:HG22	13:1M:206:LYS:HG2	1.87	0.57
14:1N:314:LYS:NZ	15:1O:274:THR:OG1	2.28	0.57
19:1S:82:SER:OG	19:1S:84:ASP:OD1	2.23	0.57
33:1h:69:HIS:NE2	75:1h:202:CDL:OA4	2.33	0.57
35:1j:9:PRO:HB2	36:1k:13:MET:HE1	1.85	0.57
46:3B:23:ASP:OD1	46:3B:24:LEU:N	2.37	0.57
53:3J:13:LEU:HD23	53:3J:17:LEU:HD12	1.87	0.57
55:4A:179:TYR:OH	87:4A:603:PGV:O02	2.20	0.57
55:4A:377:PHE:HA	55:4A:380:VAL:HG22	1.87	0.57
57:4C:23:SER:HB3	57:4C:50:ASN:HB2	1.87	0.57
57:4C:121:ILE:HG21	57:4C:193:TYR:HD2	1.69	0.57
75:4C:305:CDL:H542	75:4C:305:CDL:HB61	1.87	0.57
55:8A:460:ILE:CG1	58:8D:92:THR:HG21	2.35	0.57
55:8A:481:GLU:OE1	66:8L:7:PRO:HG2	2.05	0.57
57:8C:85:LEU:HA	57:8C:88:ILE:HD12	1.86	0.57
62:8H:6:THR:HA	62:8H:9:LYS:HZ1	1.69	0.57
68:8N:34:THR:O	68:8N:38:LEU:HG	2.05	0.57
8:1H:90:PRO:HD2	8:1H:240:ILE:HD13	1.86	0.56
24:1Y:123:LEU:HB3	69:1Y:204:3PE:H261	1.85	0.56
34:1i:41:PRO:HA	34:1i:44:GLN:HB2	1.86	0.56
39:1n:100:GLU:OE1	39:1n:121:ARG:NH1	2.38	0.56
43:1r:51:ASN:O	43:1r:56:ARG:NH2	2.37	0.56
47:3P:309:THR:OG1	47:3P:370:SER:OG	2.21	0.56
56:4B:9:PHE:HE1	56:4B:24:HIS:CD2	2.23	0.56
55:8A:495:LEU:O	55:8A:495:LEU:HD12	2.05	0.56
57:8C:90:GLU:HB2	57:8C:244:PHE:CE2	2.40	0.56
64:8J:7:GLU:OE1	64:8J:7:GLU:N	2.27	0.56
5:1E:168:ASP:O	5:1E:171:GLU:HG3	2.05	0.56
9:1I:101:ASP:OD1	9:1I:101:ASP:N	2.35	0.56
12:1L:9:LEU:O	12:1L:13:ILE:HG12	2.03	0.56
47:3C:176:THR:OG1	47:3P:53:MET:O	2.21	0.56
55:4A:374:VAL:HA	55:4A:377:PHE:CE2	2.40	0.56
56:4B:110:TYR:HB2	56:4B:116:LEU:HB3	1.86	0.56
57:4C:129:VAL:HB	57:4C:180:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:208:MET:O	55:8A:211:THR:OG1	2.23	0.56
57:8C:58:TRP:CZ3	87:8C:307:PGV:H71	2.39	0.56
3:1C:40:VAL:HG22	43:1r:69:MET:HB3	1.86	0.56
4:1D:237:ASN:HB3	8:1H:284:GLN:CD	2.30	0.56
6:1F:297:VAL:HG22	6:1F:336:VAL:HG12	1.86	0.56
10:1J:130:THR:HA	25:1Z:121:MET:HE2	1.87	0.56
10:1J:167:VAL:HG22	14:1N:42:PRO:HG2	1.85	0.56
13:1M:207:MET:HG2	13:1M:298:ILE:HG13	1.87	0.56
16:1P:171:ILE:HG12	16:1P:210:VAL:HG21	1.86	0.56
16:1P:335:LYS:H	16:1P:335:LYS:HD3	1.70	0.56
30:1e:88:GLU:HB2	30:1e:90:LYS:HZ2	1.70	0.56
32:1g:100:ARG:HD2	32:1g:107:LEU:HA	1.86	0.56
45:3N:354:VAL:HG21	45:3N:404:ALA:HA	1.87	0.56
46:3O:34:VAL:HG11	46:3O:386:ALA:HB1	1.87	0.56
49:3R:236:CYS:HB2	49:3R:241:SER:O	2.05	0.56
55:4A:362:SER:HA	56:4B:87:MET:CE	2.35	0.56
59:4E:31:LYS:HD2	59:4E:35:THR:HG23	1.85	0.56
61:4G:84:GLN:OE1	61:4G:84:GLN:N	2.38	0.56
55:8A:162:ILE:HG23	57:8C:85:LEU:HD12	1.87	0.56
56:8B:69:PRO:O	56:8B:73:LEU:HD22	2.05	0.56
59:8E:12:ASP:O	59:8E:16:VAL:HG23	2.04	0.56
59:8E:81:ILE:O	59:8E:85:VAL:HG12	2.06	0.56
68:8N:33:VAL:HA	68:8N:36:LEU:HD12	1.86	0.56
1:1A:113:TRP:HZ2	8:1H:286:MET:HG3	1.68	0.56
6:1F:245:PHE:O	6:1F:251:SER:OG	2.22	0.56
10:1J:86:ASN:HD22	11:1K:23:ARG:HH22	1.52	0.56
11:1K:47:ILE:CD1	14:1N:79:LEU:HB2	2.36	0.56
13:1M:190:TRP:CE3	24:1Y:126:MET:HE2	2.41	0.56
23:1X:106:PHE:O	23:1X:110:VAL:HG22	2.04	0.56
48:3Q:116:ILE:HG12	86:3Q:501:HEC:HMA3	1.87	0.56
55:4A:271:MET:HA	55:4A:271:MET:CE	2.30	0.56
56:8B:133:MET:HE1	58:8D:123:MET:CG	2.35	0.56
2:1B:81:ARG:NE	8:1H:61:LEU:CD2	2.67	0.56
12:1L:136:ASN:HA	12:1L:197:ASP:HA	1.86	0.56
13:1M:167:ILE:HG12	13:1M:195:MET:CE	2.35	0.56
15:1O:168:VAL:HG11	15:1O:238:ILE:HD12	1.87	0.56
55:4A:225:GLY:HA3	57:4C:112:LEU:HD13	1.88	0.56
57:4C:190:ASP:HB3	61:4G:53:LEU:HD22	1.88	0.56
58:4D:29:HIS:CE1	58:4D:65:ASN:CG	2.84	0.56
68:8N:7:THR:O	68:8N:11:LYS:CD	2.53	0.56
1:1A:37:TYR:HE2	2:1B:80:PRO:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:1:FME:HE3	13:1M:111:THR:HG21	1.87	0.56
15:1O:279:LEU:HD13	15:1O:282:ILE:HD11	1.87	0.56
39:1n:134:ARG:HD2	39:1n:161:ASP:HB3	1.88	0.56
41:1p:116:GLU:HG3	41:1p:123:ASN:HB2	1.87	0.56
43:1r:8:GLN:HA	43:1r:11:ARG:HD2	1.88	0.56
47:3C:132:VAL:HA	47:3C:139:SER:HB3	1.87	0.56
46:3O:157:ALA:O	46:3O:161:GLU:HG2	2.05	0.56
49:3R:210:TRP:CZ3	49:3R:267:SER:HA	2.41	0.56
57:8C:216:ALA:O	57:8C:220:LEU:HD13	2.06	0.56
57:8C:221:ARG:NH1	87:8C:307:PGV:O13	2.38	0.56
75:8C:306:CDL:H342	75:8C:306:CDL:H401	1.88	0.56
63:8I:10:ARG:NH1	63:8I:10:ARG:HB2	2.20	0.56
3:1C:151:ILE:HG23	3:1C:152:LEU:HG	1.86	0.56
7:1G:318:ILE:HD11	7:1G:522:LEU:HD21	1.87	0.56
69:1M:501:3PE:H281	14:1N:280:THR:HG21	1.87	0.56
14:1N:218:LEU:HB3	14:1N:244:MET:HE2	1.88	0.56
17:1Q:27:GLU:OE2	17:1Q:27:GLU:N	2.26	0.56
23:1X:7:PRO:HG2	25:1Z:84:LEU:HD13	1.86	0.56
24:1Y:128:GLN:HE21	69:1Y:204:3PE:P	2.28	0.56
47:3C:207:ASN:ND2	47:3C:211:ILE:O	2.28	0.56
48:3Q:158:ILE:HG12	48:3Q:160:MET:H	1.71	0.56
55:4A:450:TRP:HH2	75:4B:303:CDL:H771	1.71	0.56
57:4C:34:TRP:HZ3	93:4C:307:PEK:H272	1.70	0.56
55:8A:297:MET:O	55:8A:302:ARG:NH1	2.39	0.56
7:1G:364:LEU:HD12	7:1G:491:ASN:HB3	1.86	0.56
10:1J:31:LEU:O	10:1J:34:ILE:HG13	2.05	0.56
13:1M:26:ASN:OD1	31:1f:13:HIS:NE2	2.38	0.56
13:1M:78:MET:HE1	13:1M:439:LEU:HD12	1.88	0.56
19:1S:88:ARG:HH22	19:1S:92:ASN:CG	2.12	0.56
48:3Q:172:ASP:OD1	48:3Q:172:ASP:N	2.36	0.56
49:3R:152:ILE:CD1	49:3R:272:ILE:CG2	2.69	0.56
55:4A:70:VAL:O	55:4A:74:MET:HB2	2.06	0.56
55:4A:306:THR:HG23	55:4A:310:MET:HE3	1.88	0.56
87:4C:306:PGV:H291	87:4C:306:PGV:H152	1.86	0.56
55:8A:104:LEU:HD12	55:8A:152:LEU:CD1	2.35	0.56
55:8A:476:PHE:HB3	66:8L:21:LEU:HD21	1.87	0.56
56:8B:95:LEU:HD12	56:8B:96:THR:H	1.69	0.56
87:8B:301:PGV:H312	75:8D:201:CDL:H462	1.88	0.56
75:8C:306:CDL:H581	75:8C:306:CDL:H761	1.87	0.56
58:8D:76:ASN:HB3	58:8D:79:LYS:HE2	1.88	0.56
59:8E:33:MET:HE2	59:8E:67:ILE:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:8J:28:ASP:OD1	64:8J:29:ASN:N	2.39	0.56
67:8M:20:SER:O	67:8M:24:LEU:HD23	2.06	0.56
7:1G:105:CYS:HA	7:1G:108:CYS:CB	2.33	0.56
12:1L:606:GLU:OE1	12:1L:606:GLU:N	2.39	0.56
16:1P:179:LEU:H	16:1P:179:LEU:HD23	1.71	0.56
58:4D:118:LYS:HE3	65:4K:53:TRP:HA	1.88	0.56
55:8A:428:GLN:HA	55:8A:431:LEU:HD12	1.88	0.56
55:8A:460:ILE:HG12	58:8D:92:THR:HG21	1.86	0.56
57:8C:247:VAL:O	57:8C:251:PHE:HD1	1.88	0.56
63:8I:43:ARG:O	63:8I:47:TYR:HD1	1.89	0.56
68:8N:8:GLN:HA	68:8N:11:LYS:HZ1	1.69	0.56
4:1D:237:ASN:HB3	8:1H:284:GLN:NE2	2.21	0.56
6:1F:384:ALA:HB1	6:1F:388:GLU:HG3	1.88	0.56
8:1H:189:THR:HG22	8:1H:270:PHE:HZ	1.69	0.56
12:1L:341:MET:HE1	12:1L:457:LEU:HD12	1.86	0.56
14:1N:237:MET:HE1	14:1N:319:HIS:CD2	2.41	0.56
15:1O:232:GLU:O	15:1O:236:GLU:HG2	2.05	0.56
38:1m:117:GLU:N	38:1m:117:GLU:CD	2.63	0.56
46:3B:46:ARG:NH2	46:3B:110:GLU:OE1	2.39	0.56
56:4B:37:LEU:O	56:4B:41:ILE:HD12	2.06	0.56
56:4B:62:GLU:HB3	56:4B:65:TRP:CH2	2.40	0.56
55:8A:333:LYS:CE	55:8A:335:SER:HB3	2.36	0.56
57:8C:179:SER:OG	57:8C:180:GLU:OE1	2.24	0.56
61:8G:15:THR:C	61:8G:19:LEU:HD12	2.30	0.56
65:8K:42:LEU:HD11	87:8K:101:PGV:H202	1.88	0.56
66:8L:28:TYR:CE2	87:8L:101:PGV:H302	2.41	0.56
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.87	0.55
12:1L:209:PRO:HB2	12:1L:213:LEU:HG	1.88	0.55
13:1M:90:THR:HG21	69:1M:504:3PE:H12	1.87	0.55
48:3D:204:ILE:HG12	86:3D:501:HEC:HMA3	1.87	0.55
48:3D:247:ILE:HG12	48:3D:249:MET:H	1.71	0.55
59:4E:37:VAL:HG13	59:4E:74:LYS:HD3	1.89	0.55
55:8A:232:GLN:C	55:8A:292:MET:HE1	2.31	0.55
56:8B:3:TYR:CZ	56:8B:6:GLN:HG3	2.41	0.55
62:8H:30:TRP:NE1	94:8H:101:PO4:O2	2.37	0.55
66:8L:33:PHE:O	66:8L:37:PHE:CE2	2.60	0.55
7:1G:228:ILE:H	7:1G:583:THR:HG22	1.70	0.55
7:1G:359:ARG:O	7:1G:363:LEU:HG	2.06	0.55
10:1J:74:MET:HE1	10:1J:75:ALA:HB2	1.86	0.55
12:1L:327:LEU:O	12:1L:331:MET:HG2	2.06	0.55
12:1L:366:MET:HB3	12:1L:369:THR:HB	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1M:502:3PE:H391	69:1M:502:3PE:H291	1.89	0.55
14:1N:95:MET:CE	14:1N:149:ILE:HG12	2.36	0.55
18:1R:42:ASP:O	18:1R:46:GLU:HG3	2.05	0.55
24:1Y:78:GLN:HE22	51:3T:60:THR:HG21	1.70	0.55
24:1Y:128:GLN:HG2	69:1Y:204:3PE:N	2.21	0.55
24:1Y:140:VAL:O	33:1h:115:ARG:NH1	2.38	0.55
32:1g:28:GLU:HA	32:1g:28:GLU:OE2	2.06	0.55
45:3A:91:THR:HG23	45:3A:93:GLU:H	1.72	0.55
47:3C:196:HIS:HE1	85:3C:502:HEM:ND	2.03	0.55
46:3O:365:LYS:HG2	46:3O:399:LEU:HD22	1.88	0.55
52:3U:34:ARG:O	52:3U:38:GLU:HG3	2.06	0.55
55:4A:52:GLN:O	55:4A:56:VAL:HG13	2.07	0.55
55:4A:117:MET:SD	66:4L:39:ILE:HG12	2.47	0.55
75:4C:305:CDL:H581	75:4C:305:CDL:H761	1.88	0.55
59:4E:64:ALA:O	59:4E:67:ILE:HG12	2.07	0.55
60:4F:22:MET:O	60:4F:26:LYS:HG2	2.05	0.55
55:8A:80:ASN:OD1	55:8A:98:ASN:ND2	2.36	0.55
55:8A:377:PHE:O	55:8A:381:LEU:HB2	2.06	0.55
57:8C:182:TYR:O	61:8G:72:ASN:ND2	2.39	0.55
6:1F:261:HIS:CE1	6:1F:341:THR:OG1	2.59	0.55
7:1G:216:THR:CG2	7:1G:248:MET:HE3	2.36	0.55
7:1G:283:MET:HB2	7:1G:560:ILE:HB	1.88	0.55
47:3P:215:MET:HB2	51:3T:10:MET:CE	2.37	0.55
49:3R:209:GLU:HG2	49:3R:210:TRP:CE3	2.41	0.55
58:4D:63:LYS:HB3	58:4D:64:PHE:CD1	2.41	0.55
63:8I:17:LEU:O	63:8I:21:ILE:HG12	2.06	0.55
10:1J:23:LYS:HE3	11:1K:21:MET:O	2.07	0.55
13:1M:66:LEU:O	13:1M:70:THR:HG23	2.06	0.55
28:1c:33:LYS:O	28:1c:37:GLU:HG2	2.07	0.55
33:1h:13:PRO:HD3	39:1n:98:VAL:HG21	1.87	0.55
35:1j:32:MET:O	35:1j:36:ILE:HG12	2.06	0.55
55:4A:508:PRO:HG2	60:4F:32:ASN:HD22	1.71	0.55
56:4B:134:ARG:HB2	58:4D:110:THR:HG21	1.88	0.55
6:1F:250:ASN:HD21	6:1F:318:ASP:CB	2.11	0.55
7:1G:366:THR:HG21	7:1G:450:MET:CE	2.35	0.55
23:1X:33:ALA:HB2	23:1X:119:PRO:HG3	1.88	0.55
23:1X:63:ASN:OD1	25:1Z:81:ARG:NH2	2.40	0.55
49:3E:136:PHE:O	49:3E:139:SER:OG	2.21	0.55
1:1A:3:ILE:HG21	70:1H:403:PC1:H221	1.89	0.55
4:1D:209:ASP:O	4:1D:213:GLU:HG2	2.07	0.55
4:1D:282:GLU:O	4:1D:313:GLN:NE2	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:111:ARG:HB2	5:1E:152:PRO:HD3	1.89	0.55
5:1E:146:GLY:HA3	6:1F:142:PHE:HZ	1.71	0.55
7:1G:160:ILE:HD11	7:1G:183:VAL:HG13	1.89	0.55
7:1G:216:THR:HG22	7:1G:248:MET:HE3	1.89	0.55
11:1K:47:ILE:HD11	14:1N:79:LEU:HB2	1.87	0.55
12:1L:49:VAL:HG13	41:1p:32:LEU:HD13	1.87	0.55
27:1b:26:GLY:O	27:1b:30:ILE:HG23	2.06	0.55
34:1i:85:LEU:HA	34:1i:89:VAL:HB	1.88	0.55
46:3B:109:VAL:HB	46:3B:119:LEU:HD12	1.89	0.55
47:3C:266:PRO:HG3	49:3R:220:LEU:HD21	1.89	0.55
45:3N:86:LEU:HD13	45:3N:99:ILE:HG12	1.87	0.55
57:4C:121:ILE:HG21	57:4C:193:TYR:CD2	2.41	0.55
56:8B:9:PHE:HE1	56:8B:24:HIS:CD2	2.23	0.55
56:8B:118:PHE:HD2	56:8B:226:MET:HE1	1.72	0.55
62:8H:6:THR:CA	62:8H:9:LYS:HZ1	2.18	0.55
13:1M:65:LEU:O	13:1M:69:THR:HG23	2.06	0.55
36:1k:48:GLU:HG2	39:1n:33:ARG:HB3	1.88	0.55
43:1r:101:LYS:N	43:1r:101:LYS:HD2	2.22	0.55
75:3A:501:CDL:H132	69:3A:503:3PE:H372	1.89	0.55
45:3N:412:SER:HB3	53:3W:15:ARG:HH22	1.71	0.55
57:4C:157:LYS:O	57:4C:161:GLN:HG3	2.07	0.55
58:4D:64:PHE:CE2	59:4E:66:ARG:HD3	2.41	0.55
55:8A:264:LYS:NZ	55:8A:326:THR:O	2.33	0.55
87:8A:602:PGV:H71	58:8D:84:THR:HG21	1.89	0.55
59:8E:72:LYS:HB2	59:8E:82:TYR:CD2	2.28	0.55
61:8G:61:SER:O	61:8G:61:SER:OG	2.24	0.55
68:8N:36:LEU:HA	68:8N:40:ASN:OD1	2.07	0.55
70:1M:503:PC1:H282	69:1M:506:3PE:H262	1.88	0.55
33:1h:84:GLU:O	33:1h:88:GLU:HG2	2.07	0.55
48:3Q:118:ARG:HG3	48:3Q:194:SER:HB3	1.87	0.55
55:4A:383:MET:HE3	55:4A:421:VAL:HG22	1.87	0.55
8:1H:146:LEU:HD11	8:1H:192:GLU:HG3	1.89	0.55
20:1T:12:LYS:HZ1	20:1T:32:VAL:HA	1.72	0.55
25:1Z:103:ASP:OD1	25:1Z:103:ASP:N	2.40	0.55
55:4A:37:ILE:HD11	55:4A:58:VAL:HA	1.89	0.55
55:8A:144:ASP:OD2	57:8C:36:HIS:NE2	2.40	0.55
12:1L:213:LEU:HB3	12:1L:273:VAL:HG11	1.87	0.55
13:1M:195:MET:HB2	69:1M:501:3PE:H221	1.88	0.55
69:1M:502:3PE:H2E2	69:1M:504:3PE:H2C2	1.89	0.55
70:1M:505:PC1:H322	75:1h:202:CDL:H111	1.88	0.55
14:1N:14:MET:O	14:1N:18:MET:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:37:ARG:NH2	15:1O:40:ARG:HD2	2.22	0.55
20:1U:22:TYR:HB3	20:1U:25:ILE:HD12	1.89	0.55
29:1d:3:SER:HB2	70:1d:202:PC1:H131	1.89	0.55
35:1j:69:ASP:OD1	40:1o:110:ARG:HG3	2.07	0.55
41:1p:105:ILE:HG13	41:1p:134:VAL:HG21	1.87	0.55
46:3B:107:TYR:HB3	46:3B:123:LEU:HD11	1.88	0.55
49:3I:49:VAL:HG11	49:3I:55:LEU:HD13	1.88	0.55
49:3R:239:HIS:HD2	49:3R:240:GLY:N	2.04	0.55
50:3S:52:GLU:OE2	51:3T:11:ARG:NH1	2.40	0.55
56:4B:49:LYS:HZ1	59:4E:76:GLY:C	2.15	0.55
55:8A:44:PRO:HD3	55:8A:448:THR:HG23	1.88	0.55
56:8B:59:GLN:HE21	68:8N:13:PRO:CD	2.20	0.55
58:8D:144:GLU:N	58:8D:144:GLU:OE1	2.40	0.55
4:1D:257:GLY:HA3	4:1D:372:GLY:HA2	1.90	0.54
54:3X:1:MET:HA	54:3X:5:PHE:CE2	2.42	0.54
59:4E:25:ASP:OD1	59:4E:28:GLU:CD	2.50	0.54
70:1A:202:PC1:H11	8:1H:62:ARG:HH22	1.72	0.54
4:1D:279:ASP:OD1	4:1D:279:ASP:N	2.40	0.54
4:1D:336:ALA:O	4:1D:340:THR:HG23	2.06	0.54
13:1M:2:LEU:HD21	75:1X:201:CDL:H552	1.88	0.54
13:1M:16:TRP:CE2	69:1M:502:3PE:H281	2.42	0.54
20:1U:46:ASP:OD1	39:1n:44:ARG:NH1	2.40	0.54
34:1i:86:LYS:HG2	34:1i:87:TYR:CD1	2.42	0.54
49:3E:179:ARG:HE	49:3E:211:VAL:HB	1.71	0.54
56:4B:52:HIS:CD2	59:4E:40:ASP:HB2	2.42	0.54
57:4C:250:LEU:O	57:4C:254:VAL:HG23	2.07	0.54
55:8A:90:PRO:HG3	57:8C:6:HIS:CD2	2.41	0.54
55:8A:417:MET:O	55:8A:421:VAL:HG22	2.07	0.54
55:8A:447:TYR:O	55:8A:451:ASN:ND2	2.41	0.54
92:8B:305:PSC:H251	63:8I:21:ILE:HG13	1.89	0.54
67:8M:38:ASP:C	67:8M:38:ASP:OD1	2.50	0.54
6:1F:99:GLU:O	6:1F:139:ARG:NH1	2.39	0.54
7:1G:601:ARG:NH1	7:1G:605:GLU:OE1	2.39	0.54
16:1P:147:ARG:NH1	59:8E:9:GLU:H	1.99	0.54
29:1d:86:ARG:O	29:1d:90:MET:HB2	2.06	0.54
49:3E:176:VAL:HG22	49:3E:212:ILE:HD12	1.89	0.54
48:3Q:223:LYS:NZ	75:3T:101:CDL:OB4	2.37	0.54
55:4A:275:TRP:CE3	87:4A:603:PGV:H12	2.42	0.54
59:4E:82:TYR:O	59:4E:86:ILE:HG12	2.07	0.54
55:8A:52:GLN:O	55:8A:56:VAL:HG13	2.07	0.54
58:8D:48:TRP:HH2	59:8E:61:PHE:HA	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:354:GLU:OE2	4:1D:357:GLN:NE2	2.40	0.54
6:1F:107:ASP:OD1	6:1F:108:ARG:N	2.40	0.54
7:1G:110:GLN:HG3	7:1G:113:GLU:HG3	1.90	0.54
10:1J:86:ASN:OD1	10:1J:86:ASN:C	2.49	0.54
13:1M:126:LEU:HD23	13:1M:150:LEU:HD12	1.87	0.54
33:1h:110:VAL:HG12	33:1h:114:MET:CE	2.37	0.54
55:4A:468:MET:CE	55:4A:468:MET:CA	2.73	0.54
1:1A:55:PHE:CD1	10:1J:70:TYR:OH	2.61	0.54
4:1D:3:GLN:NE2	13:1M:135:ARG:O	2.33	0.54
4:1D:100:LEU:HD22	4:1D:195:ARG:HD3	1.89	0.54
4:1D:151:ILE:HD11	4:1D:218:PHE:CZ	2.43	0.54
7:1G:189:LYS:HD3	7:1G:190:MET:O	2.08	0.54
13:1M:5:ILE:HG23	13:1M:104:LEU:HD11	1.88	0.54
13:1M:306:PRO:O	13:1M:310:MET:HG3	2.07	0.54
34:1i:52:ASP:HB3	34:1i:57:LYS:HE3	1.88	0.54
37:1l:68:ASP:OD1	37:1l:68:ASP:N	2.39	0.54
92:8B:305:PSC:H011	63:8I:17:LEU:HD21	1.90	0.54
1:1A:21:ALA:HB1	8:1H:218:GLY:HA3	1.88	0.54
15:1O:22:SER:OG	15:1O:119:GLY:O	2.25	0.54
75:1X:201:CDL:H531	75:1X:201:CDL:H352	1.88	0.54
46:3B:197:ASN:HB3	46:3B:232:LEU:HB2	1.89	0.54
47:3C:149:LEU:HD21	47:3C:281:LEU:HD13	1.90	0.54
49:3E:165:MET:HA	49:3E:165:MET:CE	2.30	0.54
55:4A:1:FME:SD	87:4A:601:PGV:H211	2.47	0.54
55:4A:483:SER:HB3	67:4M:4:LYS:HG3	1.89	0.54
58:4D:77:GLU:HG3	65:4K:10:HIS:CE1	2.40	0.54
68:4N:24:ALA:HA	68:4N:27:THR:HG22	1.89	0.54
55:8A:298:ASP:OD2	55:8A:301:THR:N	2.38	0.54
57:8C:63:ARG:HD3	64:8J:12:PHE:CE2	2.43	0.54
58:8D:114:GLU:OE2	58:8D:114:GLU:N	2.26	0.54
7:1G:551:ASP:OD2	7:1G:679:ARG:NE	2.41	0.54
46:3B:286:LYS:HG2	46:3B:287:ARG:HG3	1.90	0.54
46:3B:312:PHE:HA	49:3I:61:GLY:HA2	1.89	0.54
48:3Q:216:LEU:HB3	75:3T:101:CDL:H562	1.90	0.54
55:8A:406:ASN:HD22	55:8A:409:TRP:HD1	1.56	0.54
62:8H:20:PHE:CB	62:8H:28:ASN:HD21	2.21	0.54
2:1B:173:LEU:HD11	70:1B:202:PC1:H252	1.90	0.54
12:1L:13:ILE:HD11	75:1h:202:CDL:H401	1.89	0.54
13:1M:364:LEU:HD13	13:1M:369:LEU:HD22	1.89	0.54
14:1N:213:LEU:HD13	14:1N:329:MET:HE3	1.90	0.54
21:1V:36:GLN:OE1	21:1V:94:LEU:HD21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:47:VAL:HA	22:1W:52:LEU:HD12	1.89	0.54
69:1d:201:3PE:O13	69:1d:201:3PE:H31	2.08	0.54
42:1q:25:ARG:HD2	42:1q:74:PHE:HZ	1.71	0.54
53:3J:12:ARG:O	53:3J:16:LEU:HG	2.08	0.54
55:4A:191:THR:HG23	55:4A:245:ILE:HG23	1.88	0.54
75:4C:305:CDL:H191	75:4C:305:CDL:H322	1.90	0.54
62:4H:31:GLN:HA	62:4H:31:GLN:HE21	1.72	0.54
55:8A:242:GLU:O	55:8A:246:LEU:HG	2.07	0.54
56:8B:104:TRP:CG	56:8B:203:ASN:HB2	2.43	0.54
10:1J:14:VAL:HA	10:1J:17:PHE:HB2	1.90	0.54
12:1L:407:TRP:HE1	37:1l:112:MET:HE3	1.73	0.54
75:1L:702:CDL:H142	13:1M:361:MET:HE1	1.89	0.54
25:1Z:105:LYS:HB2	25:1Z:108:GLU:HB2	1.89	0.54
34:1i:83:TYR:HE1	41:1p:48:ARG:HD3	1.73	0.54
42:1q:8:ARG:O	42:1q:12:GLN:HG3	2.08	0.54
47:3C:237:LEU:HD13	48:3D:301:MET:HG3	1.90	0.54
51:3G:21:SER:HB2	51:3G:24:GLU:HG2	1.90	0.54
46:3O:29:LEU:HD12	46:3O:33:LEU:HB3	1.89	0.54
57:4C:27:MET:HE1	57:4C:50:ASN:ND2	2.23	0.54
57:4C:138:LEU:O	57:4C:142:VAL:HG23	2.08	0.54
60:4F:51:SER:HB3	60:4F:91:LEU:HD21	1.88	0.54
62:4H:27:ARG:HG2	62:4H:27:ARG:HH11	1.73	0.54
55:8A:28:MET:HG3	66:8L:29:PHE:HD1	1.73	0.54
58:8D:99:GLU:OE1	58:8D:103:VAL:HG21	2.07	0.54
59:8E:52:LEU:HD22	59:8E:98:ILE:HD13	1.89	0.54
59:8E:52:LEU:HD23	59:8E:67:ILE:HD11	1.89	0.54
62:8H:5:GLN:HG2	62:8H:6:THR:HG23	1.89	0.54
6:1F:134:ALA:HB3	6:1F:175:VAL:HG12	1.90	0.54
7:1G:356:THR:HG22	7:1G:503:LEU:HG	1.89	0.54
21:1V:34:LEU:HD13	21:1V:48:GLU:HG2	1.90	0.54
30:1e:37:LYS:O	30:1e:41:GLU:HG3	2.07	0.54
47:3C:229:ILE:HG21	70:3J:101:PC1:H351	1.89	0.54
48:3D:235:LEU:HD11	49:3R:238:CYS:HA	1.89	0.54
55:4A:8:TYR:OH	64:4J:36:MET:HE3	2.08	0.54
66:4L:17:ASN:HB3	66:4L:20:ARG:HB3	1.90	0.54
55:8A:86:MET:HE1	55:8A:184:PHE:HB3	1.89	0.54
55:8A:333:LYS:HZ1	55:8A:335:SER:CB	2.21	0.54
57:8C:54:MET:HE1	87:8C:303:PGV:H181	1.89	0.54
3:1C:53:HIS:ND1	3:1C:55:ASP:OD1	2.41	0.53
4:1D:165:THR:HG23	8:1H:32:GLN:HG2	1.90	0.53
7:1G:324:ASP:OD1	7:1G:324:ASP:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:140:LEU:CD2	12:1L:182:PHE:CE2	2.91	0.53
12:1L:175:ASN:O	12:1L:179:ASP:OD2	2.25	0.53
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.42	0.53
14:1N:20:VAL:HG11	14:1N:137:ALA:HB1	1.91	0.53
16:1P:46:ILE:O	16:1P:46:ILE:HG22	2.07	0.53
45:3A:412:SER:HB3	53:3J:19:ARG:NH2	2.23	0.53
45:3N:412:SER:O	53:3W:15:ARG:NH2	2.41	0.53
49:3R:173:PRO:CD	49:3R:215:GLY:O	2.57	0.53
55:4A:273:MET:CE	55:4A:319:LYS:HE3	2.37	0.53
55:8A:307:SER:O	55:8A:311:ILE:CD1	2.56	0.53
55:8A:499:PRO:HG3	66:8L:10:ASN:HD21	1.73	0.53
2:1B:48:MET:HE2	2:1B:80:PRO:CG	2.37	0.53
13:1M:220:HIS:CE1	13:1M:231:LEU:HB3	2.44	0.53
15:1O:303:LYS:H	15:1O:309:ASN:ND2	2.06	0.53
21:1V:49:GLN:HE22	43:1r:92:LYS:HB3	1.72	0.53
22:1W:56:VAL:HG12	22:1W:60:ARG:HD2	1.88	0.53
30:1e:64:GLU:O	30:1e:68:ARG:HD2	2.08	0.53
32:1g:41:ASN:HB3	32:1g:44:SER:HB2	1.89	0.53
75:1h:202:CDL:H562	34:1i:79:TRP:HB3	1.91	0.53
47:3P:108:MET:HA	47:3P:108:MET:HE3	1.90	0.53
48:3Q:203:ARG:HH22	53:3W:53:LYS:NZ	2.06	0.53
3:1C:33:LEU:HD13	21:1V:98:PRO:HB3	1.91	0.53
8:1H:307:LEU:HD12	8:1H:310:MET:HE2	1.89	0.53
9:1I:84:GLU:HB2	9:1I:94:ILE:HD12	1.89	0.53
37:1l:124:SER:O	37:1l:124:SER:OG	2.22	0.53
47:3P:345:HIS:CE1	51:3T:65:GLU:OE2	2.61	0.53
54:3X:8:PRO:O	54:3X:12:GLU:HG3	2.07	0.53
57:4C:129:VAL:HG11	57:4C:180:GLU:CD	2.34	0.53
56:8B:188:ARG:HG2	63:8I:54:TYR:CE2	2.43	0.53
57:8C:203:PHE:O	57:8C:207:HIS:ND1	2.28	0.53
64:8J:11:ILE:HG22	64:8J:12:PHE:CD1	2.44	0.53
14:1N:95:MET:HE3	14:1N:99:THR:OG1	2.08	0.53
16:1P:203:GLN:OE1	16:1P:235:ARG:NH1	2.42	0.53
19:1S:50:LEU:O	19:1S:52:ILE:HD12	2.08	0.53
41:1p:31:TYR:O	41:1p:35:ILE:HG12	2.08	0.53
46:3B:56:ARG:HD2	46:3B:103:GLU:HG2	1.89	0.53
46:3B:76:THR:HG23	46:3B:81:SER:HA	1.91	0.53
48:3Q:16:GLY:O	48:3Q:202:LYS:NZ	2.33	0.53
48:3Q:195:GLU:OE2	48:3Q:201:ARG:NE	2.41	0.53
49:3R:195:LEU:HD22	49:3R:250:ARG:HA	1.90	0.53
66:4L:15:VAL:HG12	66:4L:21:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:8B:152:MET:HE2	56:8B:152:MET:HA	1.89	0.53
59:8E:52:LEU:HD21	59:8E:68:LEU:HD11	1.91	0.53
63:8I:55:ASP:HB3	63:8I:58:LYS:HB3	1.90	0.53
5:1E:147:ALA:HB3	5:1E:153:MET:HE3	1.90	0.53
13:1M:61:LEU:HD22	13:1M:244:MET:HE2	1.89	0.53
14:1N:40:MET:HE1	14:1N:129:LEU:HB3	1.91	0.53
32:1g:108:MET:HE1	41:1p:98:ASP:HB3	1.90	0.53
46:3B:222:ARG:CD	46:3B:223:PHE:CE1	2.92	0.53
87:4G:101:PGV:H102	87:4G:101:PGV:H282	1.91	0.53
55:8A:5:ARG:HD2	66:8L:3:TYR:CD2	2.43	0.53
55:8A:328:HIS:CE1	63:8I:13:LEU:HD21	2.43	0.53
12:1L:483:PRO:HG3	35:1j:53:TYR:CZ	2.44	0.53
14:1N:149:ILE:CD1	14:1N:154:MET:HE1	2.34	0.53
19:1S:82:SER:O	19:1S:86:VAL:HG23	2.08	0.53
69:1Y:202:3PE:H342	69:1Y:203:3PE:H231	1.91	0.53
45:3A:304:CYS:HB3	45:3A:334:MET:HE2	1.89	0.53
45:3N:171:SER:OG	49:3R:82:ASP:OD2	2.25	0.53
55:4A:100:MET:HE2	57:4C:57:TRP:CH2	2.44	0.53
58:4D:100:LYS:HA	58:4D:104:TYR:HD2	1.72	0.53
55:8A:307:SER:O	55:8A:311:ILE:HD11	2.08	0.53
56:8B:70:ALA:HA	56:8B:73:LEU:HD23	1.90	0.53
70:1A:202:PC1:O22	16:1P:187:TRP:CH2	2.62	0.53
6:1F:102:PRO:HD2	6:1F:302:SER:HB3	1.91	0.53
6:1F:292:ASP:O	6:1F:339:ARG:NH1	2.41	0.53
7:1G:672:TYR:HD1	7:1G:684:MET:CE	2.20	0.53
8:1H:46:LEU:HD23	8:1H:49:ILE:HD12	1.90	0.53
12:1L:526:LEU:HD12	12:1L:530:PRO:HG2	1.90	0.53
69:1M:506:3PE:H332	69:1M:506:3PE:H241	1.90	0.53
15:1O:25:ILE:HG23	15:1O:168:VAL:HB	1.90	0.53
23:1X:136:LEU:HD23	23:1X:137:PRO:HD2	1.91	0.53
25:1Z:10:MET:HE3	25:1Z:11:PRO:HD2	1.91	0.53
39:1n:94:GLU:HA	39:1n:97:LYS:HG3	1.91	0.53
41:1p:47:ALA:O	41:1p:51:ILE:HG13	2.09	0.53
41:1p:50:PHE:O	41:1p:54:GLN:HG2	2.08	0.53
43:1r:91:LYS:HD3	43:1r:92:LYS:N	2.23	0.53
47:3C:221:HIS:O	47:3C:225:THR:OG1	2.24	0.53
47:3P:128:PHE:CD1	47:3P:146:ILE:HD11	2.43	0.53
55:4A:447:TYR:O	55:4A:451:ASN:ND2	2.42	0.53
56:4B:160:LEU:HB3	56:4B:198:GLU:HG2	1.91	0.53
57:4C:88:ILE:O	57:4C:92:LEU:HD23	2.08	0.53
57:4C:221:ARG:HB3	57:4C:226:HIS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:4C:303:PGV:H221	87:4C:303:PGV:H31	1.91	0.53
57:8C:172:TYR:HE2	93:8G:102:PEK:H181	1.74	0.53
58:8D:53:MET:H	58:8D:53:MET:CE	2.22	0.53
62:8H:39:CYS:O	62:8H:43:MET:HG2	2.08	0.53
64:8J:35:THR:O	64:8J:39:CYS:SG	2.67	0.53
7:1G:295:THR:HG23	7:1G:298:ASP:H	1.74	0.53
9:1I:60:ARG:HG2	9:1I:172:ASP:OD2	2.09	0.53
16:1P:201:VAL:HG12	16:1P:290:SER:HB3	1.90	0.53
41:1p:98:ASP:OD2	41:1p:142:TYR:OH	2.24	0.53
45:3A:304:CYS:CB	45:3A:334:MET:HE2	2.39	0.53
48:3D:185:ASN:OD1	48:3D:187:GLU:N	2.42	0.53
51:3G:42:ARG:HD2	75:3G:102:CDL:OB3	2.09	0.53
45:3N:140:GLU:O	45:3N:143:SER:OG	2.25	0.53
58:4D:145:TRP:CD1	58:4D:145:TRP:H	2.24	0.53
55:8A:65:MET:SD	55:8A:69:MET:SD	3.07	0.53
56:8B:60:GLU:CD	56:8B:60:GLU:H	2.17	0.53
57:8C:138:LEU:O	57:8C:142:VAL:HG23	2.08	0.53
58:8D:48:TRP:CD1	59:8E:56:ARG:HD3	2.44	0.53
75:8D:201:CDL:H371	75:8D:201:CDL:H561	1.90	0.53
6:1F:96:ASN:OD1	6:1F:192:LEU:HD13	2.09	0.53
6:1F:164:LYS:HB2	44:1s:63:MET:HE1	1.89	0.53
13:1M:123:GLU:OE1	13:1M:123:GLU:HA	2.09	0.53
21:1V:46:TYR:O	21:1V:50:ILE:HG13	2.09	0.53
22:1W:23:ARG:O	22:1W:23:ARG:CD	2.53	0.53
48:3D:106:LEU:HD22	48:3D:295:LEU:HB2	1.90	0.53
46:3O:240:ARG:O	46:3O:421:ARG:NH1	2.42	0.53
48:3Q:152:TYR:OH	52:3U:66:ASP:OD2	2.20	0.53
49:3V:49:VAL:O	49:3V:49:VAL:HG23	2.09	0.53
55:4A:100:MET:HE2	57:4C:57:TRP:CZ3	2.43	0.53
57:4C:117:PRO:HG2	57:4C:123:PRO:HG3	1.89	0.53
75:4C:305:CDL:H401	75:4C:305:CDL:H342	1.91	0.53
63:4I:22:VAL:O	63:4I:26:ILE:HG12	2.09	0.53
56:8B:59:GLN:CD	68:8N:14:SER:HG	2.04	0.53
56:8B:150:ILE:HB	56:8B:184:LEU:HB3	1.90	0.53
58:8D:48:TRP:CE3	59:8E:61:PHE:CD2	2.96	0.53
1:1A:53:MET:O	1:1A:57:LEU:HD23	2.09	0.53
2:1B:86:MET:CE	2:1B:103:VAL:HG23	2.39	0.53
7:1G:544:ILE:HG23	7:1G:559:VAL:HG23	1.91	0.53
8:1H:2:PHE:O	8:1H:6:ILE:HG13	2.09	0.53
8:1H:70:MET:HA	8:1H:73:ILE:HG22	1.90	0.53
12:1L:213:LEU:HB2	12:1L:273:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:282:LEU:HG	13:1M:342:MET:HG3	1.91	0.53
42:1q:6:VAL:HG12	75:1q:203:CDL:HA61	1.90	0.53
48:3Q:134:TYR:OH	48:3Q:160:MET:HB3	2.09	0.53
49:3R:173:PRO:CG	49:3R:215:GLY:O	2.56	0.53
55:8A:186:TRP:O	55:8A:190:ILE:HG12	2.09	0.53
55:8A:187:SER:O	55:8A:191:THR:OG1	2.17	0.53
58:8D:48:TRP:CH2	59:8E:61:PHE:HA	2.44	0.53
65:8K:31:TYR:HA	65:8K:35:GLN:HG3	1.91	0.53
4:1D:258:VAL:HG12	4:1D:296:ARG:HG2	1.91	0.52
6:1F:312:CYS:HA	6:1F:315:VAL:HG22	1.90	0.52
7:1G:122:MET:HA	43:1r:60:ARG:HH22	1.74	0.52
7:1G:237:ASN:H	7:1G:259:ASN:ND2	2.07	0.52
37:1l:96:VAL:HB	37:1l:101:MET:HE3	1.91	0.52
47:3C:11:MET:HA	47:3C:11:MET:HE3	1.91	0.52
75:4B:303:CDL:H321	63:4l:34:PHE:CE1	2.43	0.52
55:8A:165:ILE:O	55:8A:169:ILE:HG13	2.09	0.52
55:8A:333:LYS:NZ	55:8A:335:SER:CB	2.72	0.52
9:1I:28:THR:HG22	70:1I:203:PC1:H221	1.91	0.52
9:1I:148:LEU:HD23	17:1Q:70:MET:HG3	1.91	0.52
10:1J:86:ASN:ND2	11:1K:23:ARG:HH12	2.07	0.52
14:1N:298:TYR:O	14:1N:303:THR:OG1	2.19	0.52
16:1P:260:HIS:O	16:1P:264:ARG:HG2	2.08	0.52
25:1Z:59:ARG:HA	25:1Z:62:ILE:HG22	1.92	0.52
39:1n:91:GLU:HB2	39:1n:94:GLU:HG3	1.91	0.52
50:3F:108:GLU:OE2	50:3F:111:ARG:NH1	2.42	0.52
55:4A:264:LYS:NZ	55:4A:326:THR:O	2.37	0.52
64:4J:21:HIS:CD2	64:4J:22:LEU:CD1	2.90	0.52
55:8A:69:MET:HE1	88:8A:604:HEA:H18	1.91	0.52
67:8M:31:GLY:O	67:8M:35:SER:OG	2.19	0.52
5:1E:194:GLU:HG3	6:1F:26:TYR:CD2	2.44	0.52
12:1L:188:TRP:CE3	12:1L:212:PRO:HG3	2.44	0.52
12:1L:375:ILE:HD12	12:1L:458:LEU:HD11	1.90	0.52
13:1M:11:LEU:HB3	13:1M:100:ILE:HD13	1.90	0.52
16:1P:173:GLY:H	16:1P:176:ASP:HB3	1.73	0.52
16:1P:268:ARG:HH12	16:1P:272:VAL:HG22	1.74	0.52
25:1Z:62:ILE:O	25:1Z:66:GLU:HG3	2.09	0.52
33:1h:39:GLY:HA3	70:1h:203:PC1:H2E1	1.91	0.52
49:3E:249:ILE:HG23	49:3E:249:ILE:O	2.09	0.52
45:3N:279:HIS:ND1	45:3N:284:TYR:OH	2.24	0.52
58:4D:95:LEU:HD21	67:4M:27:LEU:CD1	2.39	0.52
62:4H:8:ILE:HG13	62:4H:9:LYS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:338:MET:HE3	55:8A:341:ALA:HB3	1.90	0.52
58:8D:24:LEU:CD1	59:8E:33:MET:HE2	2.39	0.52
58:8D:48:TRP:HE1	59:8E:56:ARG:HD3	1.74	0.52
58:8D:78:TRP:CD1	75:8D:201:CDL:H202	2.45	0.52
61:8G:56:ARG:HH21	61:8G:60:TYR:HE2	1.56	0.52
4:1D:155:THR:HB	4:1D:167:PHE:HA	1.91	0.52
4:1D:183:ARG:NH1	4:1D:210:ASP:OD2	2.29	0.52
6:1F:406:ALA:HB3	73:1F:501:FMN:HM82	1.90	0.52
8:1H:197:PRO:HD2	8:1H:198:PHE:CD2	2.44	0.52
14:1N:143:CYS:SG	14:1N:198:THR:HG23	2.49	0.52
14:1N:190:MET:HG3	14:1N:204:ASN:HD22	1.75	0.52
15:1O:268:GLU:HA	15:1O:271:ASN:HB2	1.91	0.52
16:1P:97:ARG:NH2	78:1P:402:NDP:O1A	2.40	0.52
25:1Z:108:GLU:N	30:1e:74:ARG:HH22	2.07	0.52
45:3N:36:THR:HG21	45:3N:373:THR:HA	1.92	0.52
45:3N:276:ILE:HD11	45:3N:354:VAL:HA	1.91	0.52
45:3N:298:ALA:HA	45:3N:303:LEU:HB2	1.90	0.52
75:3P:504:CDL:HB22	51:3T:40:ARG:HH21	1.75	0.52
87:4G:101:PGV:H011	87:4G:101:PGV:H51	1.92	0.52
62:4H:57:ARG:HA	62:4H:60:TYR:CD1	2.44	0.52
87:8C:304:PGV:H231	87:8C:304:PGV:H271	1.92	0.52
1:1A:55:PHE:HZ	8:1H:134:ARG:HE	1.58	0.52
7:1G:320:GLY:O	7:1G:498:SER:OG	2.26	0.52
9:1I:69:ARG:NH1	9:1I:73:GLY:O	2.42	0.52
38:1m:16:THR:O	38:1m:22:TYR:HE2	1.93	0.52
46:3B:207:ILE:HG12	46:3B:382:VAL:HG12	1.92	0.52
50:3F:47:ASP:OD1	50:3F:101:TYR:OH	2.27	0.52
48:3Q:145:GLU:HA	48:3Q:145:GLU:OE2	2.09	0.52
49:3R:205:VAL:HB	49:3R:211:VAL:HG23	1.90	0.52
49:3R:225:ILE:HG12	49:3R:237:PRO:HG3	1.92	0.52
50:3S:108:ALA:O	54:3Y:9:ARG:NE	2.37	0.52
55:4A:126:TRP:HZ3	88:4A:605:HEA:HBD2	1.74	0.52
55:4A:408:ALA:O	55:4A:412:ILE:HG13	2.09	0.52
87:4A:602:PGV:H281	87:4C:306:PGV:H312	1.90	0.52
58:4D:78:TRP:O	58:4D:82:VAL:HG23	2.10	0.52
56:8B:160:LEU:HD11	56:8B:175:ILE:HG23	1.92	0.52
57:8C:243:HIS:O	57:8C:247:VAL:HG23	2.08	0.52
64:8J:43:THR:O	64:8J:47:LEU:HG	2.09	0.52
2:1B:62:MET:HB2	2:1B:153:ALA:HB1	1.92	0.52
4:1D:50:ASN:HB3	4:1D:65:VAL:HG13	1.92	0.52
4:1D:68:LEU:HD21	4:1D:411:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:43:HIS:HB3	7:1G:46:LEU:HB2	1.90	0.52
8:1H:187:ILE:HD11	70:1H:402:PC1:H271	1.91	0.52
9:1I:49:ASN:ND2	42:1q:30:ALA:O	2.40	0.52
12:1L:407:TRP:HE1	37:1l:112:MET:CE	2.22	0.52
69:1M:501:3PE:H31	14:1N:276:ILE:HG21	1.92	0.52
17:1Q:27:GLU:HA	17:1Q:30:ILE:HG22	1.91	0.52
49:3E:263:TYR:HB3	49:3E:273:VAL:HG13	1.92	0.52
45:3N:14:THR:HG21	45:3N:389:ARG:HB3	1.90	0.52
46:3O:76:THR:HG23	46:3O:81:SER:HA	1.90	0.52
49:3R:125:VAL:HG21	70:3R:303:PC1:H361	1.91	0.52
49:3R:209:GLU:OE1	49:3R:210:TRP:CZ3	2.63	0.52
59:4E:25:ASP:C	59:4E:58:LEU:HD11	2.34	0.52
65:8K:15:ASN:N	65:8K:15:ASN:OD1	2.42	0.52
7:1G:252:PRO:HG3	7:1G:263:ILE:HG12	1.92	0.52
12:1L:484:LEU:HD21	12:1L:488:MET:HE2	1.91	0.52
15:1O:240:TYR:OH	21:1V:22:ARG:NH2	2.39	0.52
16:1P:208:VAL:O	16:1P:212:LYS:HG3	2.09	0.52
23:1X:82:THR:HA	23:1X:85:TRP:CD1	2.44	0.52
23:1X:120:ASP:OD1	23:1X:121:LEU:N	2.41	0.52
39:1n:9:LEU:HD23	39:1n:14:LYS:HG2	1.92	0.52
45:3A:412:SER:HB3	53:3J:19:ARG:HH21	1.74	0.52
47:3C:82:LEU:HD12	47:3C:243:VAL:HG21	1.92	0.52
69:3C:504:3PE:H2A1	49:3R:130:LYS:HA	1.92	0.52
46:3O:169:ARG:HG3	46:3O:240:ARG:HB3	1.91	0.52
56:4B:89:GLU:HG2	68:4N:70:VAL:HG22	1.90	0.52
59:4E:21:LYS:C	59:4E:57:ARG:HH12	2.03	0.52
62:4H:40:GLU:O	62:4H:44:THR:HG23	2.10	0.52
55:8A:94:PHE:HE1	57:8C:79:LEU:HD22	1.74	0.52
57:8C:92:LEU:O	57:8C:95:THR:OG1	2.26	0.52
4:1D:238:ARG:NH2	4:1D:412:ALA:HB1	2.25	0.52
9:1I:150:ASN:ND2	42:1q:127:TYR:O	2.42	0.52
10:1J:156:VAL:O	10:1J:160:SER:OG	2.20	0.52
14:1N:25:HIS:O	14:1N:29:ILE:HG12	2.10	0.52
15:1O:53:GLU:OE2	15:1O:126:ARG:NH1	2.43	0.52
19:1S:94:LEU:HD12	19:1S:94:LEU:O	2.09	0.52
23:1X:82:THR:HA	23:1X:85:TRP:NE1	2.25	0.52
45:3A:324:PHE:HB2	45:3A:334:MET:CE	2.39	0.52
49:3E:185:ASP:OD1	49:3E:186:GLN:N	2.43	0.52
46:3O:35:ILE:HG23	46:3O:216:LEU:HD23	1.90	0.52
49:3R:248:ARG:CZ	49:3R:257:ASN:HD22	2.23	0.52
55:4A:86:MET:HE1	55:4A:184:PHE:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:287:VAL:HG21	55:8A:312:ILE:HD11	1.91	0.52
55:8A:456:MET:HE1	65:8K:40:TRP:CH2	2.45	0.52
87:8A:602:PGV:H261	87:8A:602:PGV:H102	1.90	0.52
57:8C:119:THR:HG21	62:8H:82:PRO:HA	1.92	0.52
63:8I:45:LYS:HE2	63:8I:49:ASP:OD2	2.10	0.52
68:8N:62:GLN:NE2	68:8N:64:LYS:O	2.34	0.52
2:1B:47:PRO:HB3	2:1B:85:VAL:HG13	1.92	0.52
12:1L:249:SER:OG	12:1L:336:LYS:HG3	2.10	0.52
12:1L:357:ARG:HG2	39:1n:31:VAL:HG22	1.91	0.52
69:1Y:202:3PE:H391	69:1Y:203:3PE:H261	1.91	0.52
80:1n:201:EHZ:O1	80:1n:201:EHZ:S1	2.68	0.52
40:1o:17:ASP:O	40:1o:21:MET:HG2	2.10	0.52
49:3E:219:HIS:C	49:3E:221:GLY:H	2.16	0.52
45:3N:57:TYR:OH	45:3N:137:GLU:OE1	2.20	0.52
45:3N:195:MET:SD	45:3N:219:LEU:HD21	2.50	0.52
55:4A:115:SER:HB2	55:4A:145:LEU:HB2	1.92	0.52
55:4A:278:MET:HG2	87:4A:603:PGV:H241	1.92	0.52
55:4A:413:HIS:CD2	55:4A:468:MET:HE3	2.44	0.52
92:4B:305:PSC:H251	63:4I:21:ILE:HG13	1.92	0.52
55:8A:127:THR:HA	55:8A:235:PHE:CE2	2.45	0.52
55:8A:169:ILE:HG21	75:8C:306:CDL:HA62	1.92	0.52
57:8C:23:SER:HB2	57:8C:49:THR:HG23	1.91	0.52
57:8C:59:ARG:HD2	57:8C:63:ARG:NH2	2.24	0.52
59:8E:53:ARG:NH1	59:8E:92:THR:HG23	2.25	0.52
62:8H:75:ARG:HH11	62:8H:75:ARG:HG3	1.75	0.52
1:1A:68:GLU:CG	10:1J:161:LEU:HD13	2.35	0.52
5:1E:14:GLU:N	5:1E:14:GLU:OE2	2.42	0.52
6:1F:299:PRO:O	6:1F:334:VAL:HG12	2.10	0.52
12:1L:561:ILE:HD12	70:1Y:207:PC1:H291	1.91	0.52
16:1P:137:ALA:HA	16:1P:146:LEU:HB3	1.92	0.52
37:1l:115:MET:HA	37:1l:118:VAL:HG12	1.91	0.52
41:1p:141:ARG:HG3	41:1p:142:TYR:CE1	2.45	0.52
48:3D:222:TYR:OH	48:3D:249:MET:HB3	2.09	0.52
45:3N:224:VAL:CG1	45:3N:225:GLU:N	2.43	0.52
50:3S:35:ASP:OD1	50:3S:89:TYR:OH	2.22	0.52
59:4E:33:MET:CE	59:4E:67:ILE:HG21	2.38	0.52
56:8B:44:LEU:HD11	63:8I:20:HIS:CD2	2.45	0.52
56:8B:72:ILE:O	56:8B:76:ILE:HG13	2.09	0.52
87:8C:301:PGV:H242	87:8C:301:PGV:H22	1.92	0.52
4:1D:260:LEU:HD22	4:1D:265:ILE:HD13	1.92	0.51
4:1D:410:MET:HE2	8:1H:283:ASP:OD1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:120:GLU:HG3	6:1F:232:PRO:HG2	1.92	0.51
6:1F:309:LYS:HA	6:1F:312:CYS:SG	2.50	0.51
11:1K:26:LEU:O	11:1K:30:LEU:HG	2.10	0.51
12:1L:10:THR:O	12:1L:14:ILE:HG23	2.10	0.51
16:1P:203:GLN:NE2	16:1P:232:GLY:O	2.43	0.51
38:1m:23:ASP:HB2	45:3N:230:ALA:HB3	1.91	0.51
38:1m:82:THR:OG1	38:1m:83:PRO:HD2	2.10	0.51
40:1o:51:MET:HA	41:1p:118:GLU:HG2	1.91	0.51
40:1o:54:GLN:HB3	40:1o:62:LEU:HD13	1.92	0.51
58:4D:44:GLU:HG3	58:4D:59:LEU:HD11	1.92	0.51
55:8A:294:THR:HG22	55:8A:365:ILE:HD13	1.92	0.51
55:8A:418:PHE:CE2	87:8B:301:PGV:H061	2.45	0.51
56:8B:3:TYR:CE1	56:8B:6:GLN:HG3	2.44	0.51
56:8B:41:ILE:O	56:8B:45:MET:HG2	2.08	0.51
56:8B:116:LEU:HD21	56:8B:226:MET:CE	2.40	0.51
57:8C:83:MET:O	57:8C:87:ILE:HG13	2.10	0.51
1:1A:55:PHE:HD1	10:1J:70:TYR:OH	1.93	0.51
3:1C:68:THR:N	21:1V:86:GLU:OE1	2.41	0.51
4:1D:106:LEU:HD13	4:1D:391:ILE:HG21	1.93	0.51
6:1F:140:GLY:O	6:1F:179:ARG:NH2	2.43	0.51
8:1H:99:ASN:N	70:1H:403:PC1:O12	2.30	0.51
70:1M:505:PC1:H341	75:1h:202:CDL:H311	1.91	0.51
14:1N:291:TYR:CE2	69:1N:901:3PE:H322	2.45	0.51
39:1n:96:TYR:HB2	39:1n:177:PRO:HG2	1.92	0.51
43:1r:18:ASP:C	43:1r:18:ASP:OD1	2.54	0.51
47:3C:262:LEU:HD11	49:3R:172:LYS:HA	1.93	0.51
45:3N:204:GLU:HB2	45:3N:207[B]:GLN:HG2	1.93	0.51
57:4C:47:LEU:HD22	87:4C:302:PGV:H12	1.91	0.51
58:4D:72:ASN:HB3	75:4D:201:CDL:H832	1.91	0.51
55:8A:211:THR:HA	55:8A:215:LEU:HD13	1.91	0.51
56:8B:44:LEU:HD11	63:8I:20:HIS:CG	2.45	0.51
56:8B:118:PHE:HB3	56:8B:226:MET:HE1	1.91	0.51
1:1A:55:PHE:CE1	8:1H:134:ARG:HD3	2.46	0.51
8:1H:156:MET:CE	25:1Z:50:MET:HG2	2.35	0.51
12:1L:368:PHE:HE2	12:1L:454:ILE:HB	1.75	0.51
15:1O:50:HIS:HE2	15:1O:125:GLU:CD	2.18	0.51
24:1Y:13:GLU:N	24:1Y:13:GLU:OE1	2.43	0.51
35:1j:65:GLY:N	40:1o:30:PHE:HE1	2.09	0.51
46:3B:38:LEU:HB3	46:3B:209:LEU:HD12	1.91	0.51
48:3D:309:TYR:OH	75:3G:103:CDL:OB3	2.25	0.51
55:4A:71:MET:HA	55:4A:75:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:167:THR:HA	55:4A:171:MET:HG3	1.92	0.51
55:4A:216:ASN:ND2	61:4G:58:LYS:O	2.32	0.51
57:4C:158:HIS:HE1	61:4G:17:ARG:NH2	2.08	0.51
75:4C:305:CDL:H251	75:4C:305:CDL:H371	1.93	0.51
64:4J:36:MET:CG	87:4J:101:PGV:H182	2.40	0.51
68:4N:38:LEU:C	68:4N:39:PHE:HD1	2.18	0.51
55:8A:218:THR:HG23	57:8C:192:VAL:HG22	1.92	0.51
56:8B:156:SER:OG	56:8B:159:VAL:O	2.26	0.51
57:8C:163:LEU:O	57:8C:167:ILE:HG13	2.10	0.51
5:1E:78:MET:HE3	7:1G:173:GLY:HA3	1.92	0.51
5:1E:106:THR:O	5:1E:110:LEU:HG	2.10	0.51
24:1Y:128:GLN:NE2	69:1Y:204:3PE:O14	2.43	0.51
46:3B:24:LEU:HD23	46:3B:38:LEU:HB2	1.91	0.51
49:3E:235:TYR:OH	48:3Q:144:ARG:NE	2.37	0.51
55:4A:204:ALA:O	55:4A:208:MET:HG3	2.10	0.51
55:4A:357:VAL:O	55:4A:360:ASN:ND2	2.44	0.51
56:4B:133:MET:HA	56:4B:133:MET:HE2	1.93	0.51
55:8A:96:ARG:HH21	57:8C:61:ILE:HG13	1.76	0.51
55:8A:240:HIS:O	55:8A:243:VAL:HB	2.10	0.51
56:8B:75:LEU:O	56:8B:75:LEU:HD23	2.10	0.51
56:8B:102:HIS:NE2	56:8B:107:SER:OG	2.37	0.51
58:8D:64:PHE:CE2	59:8E:62:ALA:HB1	2.45	0.51
1:1A:48:ARG:H	8:1H:126:LYS:HZ1	1.57	0.51
1:1A:50:PRO:HA	8:1H:130:ILE:HD11	1.92	0.51
6:1F:151:VAL:HG23	6:1F:154:ARG:HH21	1.76	0.51
8:1H:65:THR:O	8:1H:124:ASN:ND2	2.36	0.51
10:1J:17:PHE:HA	10:1J:20:PHE:CD2	2.46	0.51
10:1J:65:LEU:O	10:1J:66:VAL:HG23	2.10	0.51
11:1K:96:LEU:HD12	14:1N:54:GLU:HG2	1.93	0.51
13:1M:72:LEU:O	13:1M:76:MET:HG3	2.10	0.51
13:1M:306:PRO:HA	13:1M:458:LEU:HD22	1.91	0.51
14:1N:211:MET:HG2	14:1N:333:SER:HB2	1.93	0.51
44:1s:43:HIS:HA	44:1s:46:TYR:CE1	2.45	0.51
55:4A:18:LEU:HB3	55:4A:102:PHE:CZ	2.45	0.51
59:4E:84:TYR:HA	59:4E:87:GLN:HG2	1.92	0.51
60:4F:25:ARG:HG2	60:4F:25:ARG:HH11	1.76	0.51
57:8C:72:THR:HG22	57:8C:73:SER:H	1.76	0.51
57:8C:137:LEU:HG	57:8C:173:PHE:CD2	2.45	0.51
58:8D:85:ALA:C	58:8D:89:ILE:HD12	2.34	0.51
87:8G:101:PGV:H51	87:8G:101:PGV:H011	1.91	0.51
3:1C:65:ARG:NH1	3:1C:123:VAL:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:156:MET:CG	8:1H:174:MET:CE	2.89	0.51
37:1l:80:ASP:CB	37:1l:83:MET:CE	2.88	0.51
49:3R:199:GLN:CB	49:3R:248:ARG:HH21	2.20	0.51
55:4A:428:GLN:HA	55:4A:431:LEU:HD12	1.92	0.51
57:4C:163:LEU:HB3	57:4C:219:LEU:HD13	1.93	0.51
57:4C:243:HIS:O	57:4C:247:VAL:HG23	2.11	0.51
58:4D:129:ALA:HB3	58:4D:134:PHE:H	1.76	0.51
63:4I:34:PHE:C	63:4I:34:PHE:CD1	2.89	0.51
55:8A:18:LEU:HB3	55:8A:102:PHE:CZ	2.45	0.51
55:8A:338:MET:HE3	55:8A:338:MET:O	2.11	0.51
87:8A:602:PGV:H342	67:8M:23:PHE:HD2	1.75	0.51
56:8B:162:SER:HB3	56:8B:197:SER:H	1.76	0.51
58:8D:55:GLU:HA	58:8D:58:GLU:HG3	1.93	0.51
2:1B:52:LEU:HB2	2:1B:90:GLY:HA3	1.91	0.51
4:1D:246:THR:HB	4:1D:249:ASP:HB2	1.92	0.51
8:1H:85:MET:HE2	8:1H:233:MET:HG3	1.92	0.51
12:1L:9:LEU:HD12	34:1i:85:LEU:HD11	1.92	0.51
13:1M:12:LEU:HB2	13:1M:13:PRO:HD3	1.91	0.51
15:1O:234:VAL:O	15:1O:238:ILE:HG12	2.09	0.51
37:1l:121:ILE:HG13	37:1l:122:TYR:CD1	2.46	0.51
40:1o:103:ARG:HD3	40:1o:107:LEU:HD12	1.91	0.51
49:3E:238:CYS:HB3	72:3E:301:FES:S2	2.50	0.51
46:3O:319:SER:OG	46:3O:320:GLY:N	2.43	0.51
48:3Q:131:LEU:HB3	48:3Q:164:ILE:HD11	1.93	0.51
55:4A:404:THR:O	55:4A:480:ARG:NH1	2.44	0.51
55:8A:202:LEU:HD22	55:8A:238:PHE:CE2	2.45	0.51
56:8B:41:ILE:CG2	56:8B:45:MET:HE2	2.39	0.51
11:1K:55:LEU:HD13	30:1e:16:TRP:CE3	2.45	0.51
12:1L:78:LEU:HD11	75:1L:702:CDL:H662	1.93	0.51
12:1L:261:ILE:HD12	12:1L:326:PHE:HB2	1.93	0.51
15:1O:73:LEU:HD13	15:1O:299:LEU:HD11	1.92	0.51
32:1g:90:ARG:O	32:1g:94:GLU:HG3	2.11	0.51
59:4E:19:PHE:HD2	59:4E:51:ALA:HA	1.75	0.51
55:8A:38:ARG:HD3	55:8A:455:SER:HA	1.92	0.51
55:8A:150:LEU:HD12	55:8A:202:LEU:HD21	1.91	0.51
55:8A:442:ASP:OD2	56:8B:134:ARG:NH1	2.40	0.51
56:8B:52:HIS:HD2	56:8B:56:MET:SD	2.12	0.51
57:8C:77:LYS:O	57:8C:80:ARG:HG2	2.10	0.51
3:1C:77:ASP:OD1	3:1C:78:LEU:N	2.44	0.51
4:1D:233:ARG:NH2	9:1I:23:GLN:O	2.44	0.51
6:1F:337:MET:HB3	6:1F:341:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:167:VAL:HG13	14:1N:42:PRO:HG3	1.92	0.51
12:1L:253:VAL:HB	12:1L:310:LEU:HD11	1.92	0.51
16:1P:95:VAL:HG11	16:1P:113:ILE:HG21	1.92	0.51
45:3A:172:GLU:OE1	45:3A:172:GLU:C	2.54	0.51
49:3V:77:ARG:C	49:3V:77:ARG:NE	2.69	0.51
55:4A:254:ILE:HD12	55:4A:341:ALA:HA	1.93	0.51
60:4F:26:LYS:HB2	60:4F:28:LEU:HD12	1.93	0.51
65:4K:31:TYR:O	65:4K:35:GLN:HB2	2.11	0.51
55:8A:349:THR:O	55:8A:353:LEU:HG	2.10	0.51
57:8C:34:TRP:HZ3	93:8C:308:PEK:H272	1.74	0.51
57:8C:231:HIS:CD2	87:8C:307:PGV:H042	2.46	0.51
59:8E:16:VAL:HG23	59:8E:47:ILE:HG22	1.92	0.51
7:1G:140:LYS:O	7:1G:148:THR:OG1	2.29	0.51
8:1H:33:LEU:HD22	9:1I:40:TYR:HE2	1.76	0.51
24:1Y:134:VAL:HG11	69:1Y:205:3PE:H222	1.92	0.51
32:1g:24:ILE:HG12	32:1g:26:LEU:O	2.11	0.51
44:1s:43:HIS:HA	44:1s:46:TYR:CD1	2.45	0.51
45:3A:97:TYR:HH	45:3A:190:TYR:HH	1.59	0.51
69:3C:504:3PE:H11	49:3R:137:VAL:HG12	1.93	0.51
48:3Q:180:SER:HB2	52:3U:77:LEU:HD11	1.92	0.51
49:3R:243:TYR:HA	49:3R:248:ARG:O	2.11	0.51
49:3R:260:VAL:HG13	49:3R:263:TYR:HE1	1.76	0.51
87:4B:302:PGV:H62	68:4N:29:ALA:HB1	1.92	0.51
75:4C:305:CDL:H311	75:4C:305:CDL:H212	1.91	0.51
60:4F:70:ILE:HG21	60:4F:83:PRO:HD3	1.92	0.51
55:8A:240:HIS:HA	55:8A:243:VAL:HB	1.92	0.51
65:8K:38:ILE:CD1	65:8K:40:TRP:CE2	2.86	0.51
4:1D:64:LEU:HD11	4:1D:418:ILE:HD11	1.93	0.50
5:1E:100:ILE:HB	5:1E:139:LEU:HA	1.93	0.50
6:1F:300:GLY:O	6:1F:304:THR:OG1	2.18	0.50
7:1G:673:MET:SD	7:1G:679:ARG:HA	2.51	0.50
15:1O:165:PRO:O	15:1O:248:TRP:NE1	2.38	0.50
16:1P:45:VAL:HB	16:1P:68:ILE:HG13	1.94	0.50
16:1P:176:ASP:OD1	16:1P:178:PHE:N	2.37	0.50
21:1V:89:LEU:O	21:1V:93:MET:HG2	2.10	0.50
22:1W:88:MET:O	22:1W:92:GLU:HG3	2.11	0.50
32:1g:68:ILE:HG23	32:1g:72:LEU:HD12	1.93	0.50
34:1i:15:ARG:HD2	34:1i:19:ARG:HH22	1.76	0.50
37:1l:80:ASP:CB	37:1l:83:MET:HE2	2.30	0.50
44:1s:46:TYR:HD2	44:1s:50:THR:HG21	1.76	0.50
46:3B:109:VAL:HG13	46:3B:123:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:443:TRP:HB3	45:3N:445:ARG:HG2	1.92	0.50
47:3P:186:PRO:HA	47:3P:189:ILE:HD12	1.93	0.50
55:8A:473:TRP:CD1	66:8L:22:LEU:HD13	2.46	0.50
56:8B:118:PHE:CD2	56:8B:226:MET:HE1	2.46	0.50
57:8C:119:THR:HG22	61:8G:50:TYR:HE2	1.72	0.50
57:8C:182:TYR:CE2	87:8C:305:PGV:C04	2.92	0.50
5:1E:105:THR:O	5:1E:109:MET:N	2.36	0.50
10:1J:45:LEU:HD23	10:1J:50:SER:HA	1.93	0.50
12:1L:73:THR:HG22	12:1L:73:THR:O	2.10	0.50
17:1Q:77:ASP:OD1	17:1Q:77:ASP:O	2.29	0.50
19:1S:88:ARG:NH1	19:1S:88:ARG:C	2.67	0.50
20:1T:22:TYR:HE2	20:1T:24:LYS:HB2	1.76	0.50
24:1Y:68:ILE:HG13	24:1Y:99:THR:HG21	1.93	0.50
34:1i:67:SER:O	34:1i:71:VAL:HG22	2.11	0.50
39:1n:56:MET:HE2	45:3N:228:VAL:HG11	1.93	0.50
42:1q:88:ARG:HG2	42:1q:93:MET:HB2	1.94	0.50
46:3B:264:THR:HB	46:3B:315:SER:HB3	1.92	0.50
56:4B:104:TRP:NE1	56:4B:200:CYS:O	2.42	0.50
58:4D:54:ASP:OD1	58:4D:54:ASP:O	2.29	0.50
59:4E:78:HIS:CE1	63:4I:12:LEU:HD23	2.46	0.50
57:8C:244:PHE:CD1	57:8C:244:PHE:C	2.90	0.50
58:8D:68:PHE:HZ	59:8E:66:ARG:HG3	1.76	0.50
13:1M:114:GLU:OE1	23:1X:168:PHE:HB3	2.12	0.50
13:1M:373:ILE:HA	13:1M:376:ILE:HD12	1.92	0.50
15:1O:34:GLY:N	76:1O:401:GTP:O3G	2.32	0.50
43:1r:57:ASP:OD1	43:1r:57:ASP:C	2.54	0.50
45:3A:276:ILE:HD11	45:3A:354:VAL:HA	1.93	0.50
46:3B:276:GLN:HG2	46:3B:281:ALA:HB2	1.93	0.50
75:3N:502:CDL:HB32	75:3N:502:CDL:H112	1.93	0.50
49:3R:222:CYS:HB2	72:3R:301:FES:S2	2.51	0.50
55:8A:165:ILE:CG2	55:8A:169:ILE:HD11	2.41	0.50
56:8B:155:SER:HB3	56:8B:179:LEU:HD12	1.94	0.50
75:8C:306:CDL:H631	75:8C:306:CDL:H821	1.93	0.50
8:1H:272:TRP:CZ2	9:1I:38:LEU:HB2	2.47	0.50
14:1N:190:MET:HG3	14:1N:204:ASN:ND2	2.26	0.50
69:1Y:203:3PE:H262	70:1Y:207:PC1:H3E2	1.93	0.50
25:1Z:58:ARG:NH2	27:1b:48:THR:OG1	2.39	0.50
47:3P:240:LEU:HB3	48:3Q:208:MET:HE2	1.93	0.50
56:4B:223:SER:O	56:4B:227:LEU:HG	2.12	0.50
65:4K:22:ALA:O	65:4K:26:VAL:HG23	2.11	0.50
55:8A:24:ALA:O	55:8A:28:MET:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:269:GLY:O	55:8A:273:MET:HG3	2.11	0.50
57:8C:87:ILE:HG23	57:8C:244:PHE:CD2	2.46	0.50
5:1E:51:LEU:HD23	5:1E:69:VAL:HG21	1.92	0.50
6:1F:31:TRP:HH2	6:1F:151:VAL:HG13	1.77	0.50
6:1F:191:ALA:HB2	6:1F:203:PRO:HG3	1.94	0.50
7:1G:623:LEU:HD22	7:1G:630:LEU:HD22	1.93	0.50
8:1H:267:THR:O	8:1H:271:LEU:HG	2.12	0.50
10:1J:71:THR:HG21	11:1K:75:LEU:HD22	1.94	0.50
12:1L:529:TYR:HB3	12:1L:530:PRO:HD3	1.93	0.50
15:1O:128:ILE:HG21	15:1O:160:ALA:HB2	1.94	0.50
23:1X:19:VAL:HG23	23:1X:24:LEU:HG	1.93	0.50
23:1X:46:ARG:NH1	25:1Z:80:ASP:OD2	2.45	0.50
23:1X:139:ASN:OD1	23:1X:139:ASN:O	2.30	0.50
32:1g:52:ILE:HG23	32:1g:53:VAL:HG13	1.94	0.50
40:1o:45:MET:SD	40:1o:55:ARG:HG2	2.52	0.50
43:1r:92:LYS:N	43:1r:92:LYS:HD2	2.26	0.50
47:3C:24:PRO:HB2	47:3C:27:ILE:HG23	1.93	0.50
53:3J:12:ARG:HH22	61:8G:14:ARG:HE	1.59	0.50
46:3O:197:ASN:HB3	46:3O:232:LEU:HB2	1.91	0.50
55:8A:43:GLN:HG3	55:8A:44:PRO:HD2	1.93	0.50
55:8A:362:SER:CA	56:8B:87:MET:HE1	2.40	0.50
58:8D:89:ILE:HG22	65:8K:29:TRP:HE1	1.77	0.50
58:8D:145:TRP:H	58:8D:145:TRP:CD1	2.28	0.50
59:8E:43:PRO:HB2	59:8E:48:ILE:HD11	1.94	0.50
59:8E:78:HIS:ND1	63:8I:12:LEU:CD1	2.65	0.50
67:8M:24:LEU:O	67:8M:28:ILE:HG13	2.11	0.50
1:1A:113:TRP:CZ2	8:1H:286:MET:HG3	2.47	0.50
2:1B:69:MET:HA	2:1B:72:PHE:HD2	1.77	0.50
2:1B:154:GLU:HG2	9:1I:50:TYR:CE1	2.45	0.50
5:1E:146:GLY:HA3	6:1F:142:PHE:CZ	2.45	0.50
6:1F:342:ASP:HB3	6:1F:345:LYS:HB3	1.94	0.50
12:1L:21:MET:HE3	12:1L:24:SER:OG	2.12	0.50
12:1L:149:ILE:HG13	13:1M:369:LEU:HD13	1.94	0.50
16:1P:192:PRO:HB2	16:1P:263:TYR:OH	2.12	0.50
20:1U:26:ASP:OD1	20:1U:28:GLU:HG3	2.11	0.50
24:1Y:48:PHE:HA	69:1Y:206:3PE:H222	1.93	0.50
25:1Z:95:ALA:HB2	25:1Z:106:VAL:HG21	1.94	0.50
25:1Z:98:MET:HE2	30:1e:78:ILE:HA	1.93	0.50
69:1d:201:3PE:H252	69:1d:201:3PE:H362	1.93	0.50
34:1i:44:GLN:HA	34:1i:47:ASN:HD21	1.77	0.50
46:3B:95:LYS:HG3	49:3I:32:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:3H:100:PHE:HA	52:3H:103:LEU:HB2	1.93	0.50
49:3R:179:ARG:HH21	49:3R:184:ILE:HG23	1.76	0.50
58:4D:89:ILE:HG22	65:4K:29:TRP:NE1	2.20	0.50
56:8B:6:GLN:NE2	56:8B:8:GLY:O	2.44	0.50
56:8B:59:GLN:OE1	56:8B:59:GLN:HA	2.11	0.50
57:8C:187:THR:N	57:8C:190:ASP:OD2	2.30	0.50
58:8D:123:MET:HE2	58:8D:134:PHE:CE2	2.46	0.50
58:8D:137:LYS:HD2	65:8K:45:VAL:HG21	1.94	0.50
58:8D:141:ASP:O	58:8D:143:ASN:N	2.44	0.50
1:1A:54:LYS:HG2	1:1A:114:ALA:H	1.77	0.50
6:1F:110:ILE:HD12	6:1F:114:ASP:HB2	1.94	0.50
7:1G:231:MET:HE3	7:1G:270:ALA:HB3	1.94	0.50
7:1G:409:ILE:HD11	7:1G:422:LEU:HD12	1.93	0.50
10:1J:119:PHE:CE1	11:1K:1:FME:HE2	2.46	0.50
12:1L:118:PHE:O	12:1L:122:VAL:HG23	2.11	0.50
69:1L:701:3PE:H242	69:1L:701:3PE:H322	1.93	0.50
15:1O:24:VAL:HG23	15:1O:166:PRO:HA	1.94	0.50
20:1T:8:LEU:HD23	20:1T:88:GLU:HB3	1.93	0.50
24:1Y:28:GLY:HA2	69:1Y:203:3PE:H2B2	1.93	0.50
25:1Z:125:TYR:HB3	25:1Z:133:ILE:HG22	1.93	0.50
37:1L:125:TYR:OH	40:1O:7:ARG:HD3	2.12	0.50
46:3O:52:LYS:O	46:3O:203:ARG:NH2	2.36	0.50
49:3R:204:ARG:HH22	49:3R:213:LEU:HD23	1.77	0.50
55:8A:110:LEU:CD1	87:8A:601:PGV:H181	2.41	0.50
1:1A:53:MET:HE2	10:1J:172:THR:HG23	1.93	0.50
6:1F:254:LYS:HD3	6:1F:332:ALA:HB2	1.93	0.50
10:1J:167:VAL:O	10:1J:171:ILE:HG13	2.11	0.50
12:1L:473:PRO:HG2	12:1L:475:MET:HE3	1.94	0.50
69:1Y:202:3PE:H31	69:1Y:202:3PE:H242	1.93	0.50
25:1Z:121:MET:HG3	25:1Z:137:THR:HG22	1.94	0.50
32:1g:95:ARG:HH11	32:1g:95:ARG:HG3	1.77	0.50
46:3B:369:LEU:HD11	46:3B:399:LEU:HD11	1.94	0.50
45:3N:34:THR:HG22	45:3N:102:LEU:HD23	1.94	0.50
47:3P:234:PHE:HD2	75:3T:101:CDL:H762	1.75	0.50
55:4A:265:LYS:HB3	55:4A:490:THR:HG21	1.94	0.50
87:4C:303:PGV:H231	87:4C:303:PGV:H271	1.94	0.50
63:4I:29:LEU:O	63:4I:33:THR:OG1	2.22	0.50
56:8B:12:ALA:HB2	56:8B:21:LEU:HD12	1.93	0.50
57:8C:147:ALA:HB2	57:8C:162:ALA:HB3	1.94	0.50
62:8H:55:TRP:O	62:8H:59:VAL:HG12	2.11	0.50
5:1E:134:ASP:OD1	5:1E:136:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:194:GLU:HG2	6:1F:28:ARG:NH2	2.23	0.50
7:1G:229:ASP:OD2	7:1G:267:THR:HG23	2.12	0.50
15:1O:104:ARG:NH2	76:1O:401:GTP:N7	2.59	0.50
16:1P:139:ILE:HD12	59:8E:9:GLU:OE1	2.11	0.50
34:1i:14:LEU:HD22	39:1n:169:ILE:HD11	1.93	0.50
50:3S:14:GLU:OE1	50:3S:14:GLU:N	2.38	0.50
56:4B:110:TYR:HE2	56:4B:118:PHE:HE2	1.59	0.50
55:8A:69:MET:HE3	88:8A:604:HEA:C27	2.40	0.50
55:8A:155:VAL:C	55:8A:159:LEU:HD12	2.35	0.50
55:8A:483:SER:N	67:8M:4:LYS:HZ1	2.05	0.50
55:8A:496:HIS:CE1	60:8F:57:ILE:CD1	2.95	0.50
69:1A:201:3PE:H3A2	27:1b:19:VAL:HG23	1.94	0.49
7:1G:385:ARG:HE	7:1G:416:THR:HG23	1.77	0.49
7:1G:624:GLU:HB2	7:1G:631:VAL:HG21	1.94	0.49
10:1J:129:ASP:OD2	11:1K:52:HIS:NE2	2.45	0.49
11:1K:27:MET:HE1	11:1K:78:LEU:HD22	1.94	0.49
69:1L:701:3PE:H221	37:1l:88:ARG:HA	1.92	0.49
13:1M:92:LYS:O	13:1M:96:ILE:HG12	2.12	0.49
13:1M:131:ILE:HD12	14:1N:302:LEU:HD21	1.94	0.49
16:1P:113:ILE:O	16:1P:117:ILE:HG12	2.12	0.49
20:1T:11:ILE:HG23	20:1T:58:PHE:HE2	1.77	0.49
27:1b:34:LEU:O	27:1b:34:LEU:HD12	2.11	0.49
30:1e:83:ASP:OD1	30:1e:84:LYS:N	2.45	0.49
35:1j:42:HIS:NE2	36:1k:84:GLU:OE1	2.45	0.49
48:3D:240:TYR:OH	52:3H:92:ASP:OD2	2.26	0.49
46:3O:51:ILE:HG12	46:3O:204:MET:HG2	1.94	0.49
46:3O:109:VAL:HG13	46:3O:123:LEU:HD13	1.93	0.49
48:3Q:200:HIS:O	48:3Q:204:MET:HG3	2.12	0.49
75:4B:303:CDL:H321	63:4I:34:PHE:HE1	1.76	0.49
59:4E:93:LEU:HB3	59:4E:98:ILE:O	2.11	0.49
55:8A:35:LEU:HG	55:8A:462:LEU:HD22	1.94	0.49
56:8B:105:TYR:HE2	56:8B:119:ASP:OD2	1.95	0.49
56:8B:139:ASP:N	56:8B:139:ASP:OD1	2.43	0.49
56:8B:161:HIS:HB2	56:8B:174:ALA:HB3	1.94	0.49
57:8C:59:ARG:HG2	57:8C:63:ARG:HE	1.77	0.49
57:8C:210:ILE:HG21	87:8C:307:PGV:H281	1.93	0.49
64:8J:28:ASP:HA	64:8J:31:LEU:CD1	2.42	0.49
1:1A:111:LEU:HD13	8:1H:290:TRP:HB3	1.94	0.49
7:1G:350:PRO:HD3	7:1G:458:LEU:HD13	1.94	0.49
7:1G:366:THR:HG22	7:1G:370:GLY:HA3	1.94	0.49
9:1I:44:GLU:OE1	81:1q:202:AYA:HM3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:99:MET:SD	10:1J:99:MET:O	2.70	0.49
11:1K:48:ILE:HG23	11:1K:53:PHE:HB3	1.94	0.49
13:1M:14:MET:HE1	13:1M:30:HIS:CG	2.47	0.49
20:1T:72:CYS:O	20:1T:76:ILE:HG13	2.12	0.49
34:1i:114:GLU:OE1	34:1i:114:GLU:N	2.41	0.49
35:1j:65:GLY:N	40:1o:30:PHE:CE1	2.80	0.49
47:3C:29:SER:HB2	75:3G:103:CDL:H731	1.94	0.49
49:3E:164:ASN:HA	49:3E:177:ARG:HB2	1.94	0.49
47:3P:67:THR:HG22	48:3Q:115:TYR:HE2	1.77	0.49
49:3R:179:ARG:HG3	49:3R:184:ILE:HG12	1.93	0.49
87:4A:602:PGV:H242	87:4A:602:PGV:H22	1.94	0.49
57:4C:118:PRO:HB2	57:4C:121:ILE:HD12	1.94	0.49
58:4D:111:PHE:HE2	65:4K:41:ASN:HB2	1.77	0.49
55:8A:338:MET:HE2	55:8A:342:LEU:HG	1.93	0.49
55:8A:449:ALA:O	55:8A:453:ILE:HG12	2.12	0.49
56:8B:188:ARG:NH1	63:8I:51:TYR:OH	2.45	0.49
68:8N:18:LEU:CD1	68:8N:22:ILE:HD11	2.42	0.49
5:1E:150:ASN:HA	5:1E:190:ARG:HH12	1.77	0.49
14:1N:152:ASN:ND2	69:1Y:205:3PE:O12	2.45	0.49
40:1o:102:GLU:OE2	40:1o:105:ARG:NH1	2.45	0.49
45:3A:273:ALA:HB1	45:3A:345:LEU:HD13	1.94	0.49
46:3B:366:ALA:O	46:3B:370:MET:HG3	2.11	0.49
47:3C:267:HIS:ND1	47:3C:267:HIS:O	2.45	0.49
47:3C:310:SER:HB2	47:3C:370:SER:HB3	1.94	0.49
55:4A:23:GLY:HA3	55:4A:73:ILE:HG13	1.94	0.49
55:4A:240:HIS:O	55:4A:243:VAL:HB	2.12	0.49
57:4C:244:PHE:HA	75:4C:305:CDL:H832	1.93	0.49
55:8A:242:GLU:HA	55:8A:245:ILE:CD1	2.40	0.49
57:8C:244:PHE:HA	75:8C:306:CDL:H832	1.94	0.49
68:8N:22:ILE:HD12	68:8N:22:ILE:H	1.78	0.49
1:1A:85:LYS:HG3	1:1A:86:THR:H	1.78	0.49
7:1G:444:LYS:NZ	7:1G:480:SER:HB2	2.27	0.49
9:1I:132:VAL:HG21	9:1I:165:ILE:HD12	1.94	0.49
10:1J:135:PHE:CD2	25:1Z:68:ARG:HD3	2.47	0.49
23:1X:124:LEU:HD21	25:1Z:70:ALA:HB2	1.94	0.49
34:1i:92:LYS:HD3	34:1i:95:THR:CG2	2.43	0.49
38:1m:47:LEU:HB3	39:1n:165:LEU:HD13	1.94	0.49
40:1o:68:CYS:SG	40:1o:79:CYS:HB2	2.51	0.49
46:3B:137:VAL:O	46:3B:141:GLN:HG2	2.12	0.49
48:3D:185:ASN:OD1	48:3D:185:ASN:C	2.56	0.49
45:3N:8:LEU:HD22	45:3N:392:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:358:LYS:O	45:3N:362:ARG:HG3	2.13	0.49
55:4A:362:SER:HA	56:4B:87:MET:HE3	1.94	0.49
57:4C:15:PRO:HB2	64:4J:36:MET:HE1	1.94	0.49
75:4D:201:CDL:H371	75:4D:201:CDL:H561	1.94	0.49
59:4E:52:LEU:CD2	59:4E:67:ILE:HD11	2.42	0.49
55:8A:274:VAL:O	55:8A:278:MET:HG3	2.12	0.49
55:8A:445:ASP:OD1	55:8A:446:ALA:N	2.45	0.49
57:8C:79:LEU:HB3	57:8C:233:PHE:CE2	2.46	0.49
57:8C:121:ILE:HG21	57:8C:193:TYR:HD2	1.77	0.49
58:8D:34:SER:OG	58:8D:37:GLN:OE1	2.30	0.49
3:1C:49:GLU:HG2	3:1C:106:ARG:HE	1.78	0.49
5:1E:216:GLY:O	5:1E:217:LEU:HD23	2.13	0.49
6:1F:261:HIS:HE1	6:1F:341:THR:OG1	1.93	0.49
10:1J:120:ASN:OD1	10:1J:122:LEU:N	2.45	0.49
13:1M:216:LEU:HB3	13:1M:217:PRO:HD3	1.94	0.49
15:1O:49:ARG:HH21	15:1O:51:PHE:HE1	1.60	0.49
15:1O:139:TYR:CZ	15:1O:146:LYS:HD3	2.47	0.49
39:1n:161:ASP:OD1	39:1n:161:ASP:C	2.55	0.49
45:3A:8:LEU:HD22	45:3A:392:LEU:HB3	1.94	0.49
46:3B:156:GLN:NE2	49:3I:58:GLN:O	2.46	0.49
48:3D:121:TYR:CZ	48:3D:131:MET:HG3	2.47	0.49
48:3D:316:TRP:O	48:3D:320:LYS:HG2	2.13	0.49
49:3E:194:GLN:NE2	49:3E:194:GLN:O	2.45	0.49
46:3O:137:VAL:O	46:3O:141:GLN:HG2	2.13	0.49
55:4A:468:MET:CE	55:4A:471:ILE:HD11	2.36	0.49
87:4A:602:PGV:O14	57:4C:57:TRP:NE1	2.39	0.49
56:4B:148:MET:HE1	56:4B:216:LEU:HD21	1.94	0.49
55:8A:445:ASP:O	55:8A:448:THR:OG1	2.24	0.49
62:8H:8:ILE:HD11	62:8H:55:TRP:HB2	1.94	0.49
4:1D:357:GLN:O	43:1r:59:ARG:NH1	2.45	0.49
8:1H:100:LEU:HD13	8:1H:103:LEU:HD12	1.93	0.49
11:1K:27:MET:HE2	11:1K:78:LEU:HD13	1.94	0.49
13:1M:385:SER:OG	13:1M:396:MET:HE1	2.13	0.49
16:1P:21:ALA:HA	16:1P:90:VAL:O	2.11	0.49
20:1T:11:ILE:HG23	20:1T:58:PHE:CE2	2.47	0.49
21:1V:75:GLN:O	21:1V:78:GLU:HG2	2.13	0.49
28:1c:19:LEU:HB3	75:1d:203:CDL:H122	1.95	0.49
35:1j:53:TYR:CE1	40:1o:98:MET:HE1	2.47	0.49
46:3O:312:PHE:HA	49:3V:61:GLY:HA2	1.93	0.49
56:4B:160:LEU:HD11	56:4B:175:ILE:HG23	1.93	0.49
57:4C:58:TRP:CZ3	87:4C:306:PGV:H71	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:4I:57:MET:O	63:4I:57:MET:HE3	2.11	0.49
55:8A:29:VAL:HG13	66:8L:36:PRO:HG3	1.94	0.49
1:1A:48:ARG:HE	10:1J:78:MET:HA	1.78	0.49
6:1F:202:LYS:HE2	6:1F:361:GLN:HB2	1.94	0.49
13:1M:122:PHE:CE1	13:1M:206:LYS:HD3	2.46	0.49
16:1P:165:ILE:HB	16:1P:227:THR:HG23	1.95	0.49
16:1P:172:PHE:HB2	16:1P:179:LEU:CD2	2.43	0.49
19:1S:49:ASP:N	19:1S:49:ASP:OD1	2.45	0.49
20:1U:13:ASP:O	20:1U:17:TYR:HB2	2.13	0.49
23:1X:38:PRO:HG3	23:1X:65:CYS:SG	2.53	0.49
28:1c:44:ARG:C	28:1c:44:ARG:HD3	2.38	0.49
47:3P:157:GLY:O	47:3P:161:VAL:HG23	2.13	0.49
56:4B:25:ASP:OD2	63:4I:43:ARG:NE	2.42	0.49
59:4E:11:PHE:CE2	59:4E:41:LEU:HD21	2.47	0.49
60:4F:93:SER:O	60:4F:94:HIS:HB3	2.11	0.49
56:8B:59:GLN:HE21	68:8N:13:PRO:N	2.10	0.49
59:8E:9:GLU:HA	59:8E:12:ASP:HB2	1.94	0.49
2:1B:71:ARG:HH21	8:1H:38:ASN:HD21	1.60	0.49
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.94	0.49
6:1F:98:ASP:OD1	6:1F:139:ARG:HD2	2.13	0.49
7:1G:194:GLU:OE1	7:1G:194:GLU:N	2.29	0.49
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.47	0.49
70:1M:503:PC1:H2	70:1M:503:PC1:H221	1.53	0.49
20:1U:48:VAL:HG12	20:1U:52:MET:SD	2.53	0.49
22:1W:69:LYS:NZ	22:1W:69:LYS:HB3	2.28	0.49
22:1W:98:LYS:HB3	22:1W:102:HIS:HB2	1.93	0.49
75:3A:501:CDL:H152	69:3A:503:3PE:H381	1.95	0.49
49:3E:197:ASP:N	49:3E:197:ASP:OD1	2.44	0.49
75:3G:103:CDL:H522	75:3G:103:CDL:H562	1.93	0.49
45:3N:80:GLU:OE2	46:3O:292:THR:OG1	2.21	0.49
49:3R:121:THR:O	49:3R:125:VAL:HG23	2.12	0.49
87:4C:304:PGV:H222	87:4C:304:PGV:H21	1.94	0.49
55:8A:54:TYR:O	55:8A:58:VAL:HG23	2.13	0.49
59:8E:18:TYR:HE2	59:8E:32:GLY:HA3	1.77	0.49
61:8G:14:ARG:HD2	61:8G:17:ARG:HD3	1.95	0.49
63:8I:27:VAL:O	63:8I:31:VAL:HG13	2.13	0.49
66:8L:21:LEU:O	66:8L:25:MET:HG3	2.12	0.49
5:1E:217:LEU:HD23	5:1E:217:LEU:N	2.28	0.49
10:1J:120:ASN:OD1	10:1J:120:ASN:C	2.56	0.49
75:1N:902:CDL:OA4	75:1N:902:CDL:O1	2.27	0.49
18:1R:49:VAL:HG22	18:1R:90:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:84:TYR:CZ	23:1X:88:ILE:HD11	2.48	0.49
33:1h:110:VAL:CG1	33:1h:114:MET:HE2	2.42	0.49
37:1l:91:THR:HG22	38:1m:10:LEU:HA	1.95	0.49
49:3E:241:SER:HA	49:3E:252:GLY:HA3	1.94	0.49
46:3O:258:VAL:HA	46:3O:323:GLY:HA3	1.94	0.49
46:3O:299:VAL:HG11	46:3O:336:VAL:HG13	1.95	0.49
56:4B:150:ILE:HB	56:4B:184:LEU:HB3	1.95	0.49
63:4I:41:GLU:OE1	63:4I:41:GLU:CA	2.60	0.49
63:4I:41:GLU:OE1	63:4I:41:GLU:HA	2.11	0.49
55:8A:63:PHE:CE1	55:8A:150:LEU:HD21	2.48	0.49
4:1D:223:ASP:HB3	4:1D:305:ARG:HH22	1.78	0.49
6:1F:74:PRO:HB2	6:1F:77:LEU:HB2	1.94	0.49
7:1G:20:VAL:HG21	7:1G:73:VAL:HG21	1.95	0.49
8:1H:92:PRO:HD3	8:1H:255:TYR:CD1	2.48	0.49
10:1J:120:ASN:OD1	10:1J:122:LEU:HB2	2.12	0.49
13:1M:2:LEU:HD13	31:1f:26:LEU:HD23	1.93	0.49
14:1N:44:LEU:HD22	14:1N:122:ILE:HD13	1.94	0.49
14:1N:172:GLN:NE2	14:1N:177:LYS:HD3	2.28	0.49
15:1O:77:CYS:HB3	15:1O:95:ARG:HG2	1.95	0.49
19:1S:17:GLU:OE1	19:1S:19:ARG:HD3	2.12	0.49
23:1X:126:LYS:HE3	27:1b:66:PRO:HG3	1.95	0.49
27:1b:56:LEU:HD11	27:1b:65:VAL:HG21	1.95	0.49
46:3B:204:MET:HE1	46:3B:224:LEU:HD22	1.95	0.49
46:3O:203:ARG:NH1	46:3O:232:LEU:O	2.46	0.49
56:4B:61:VAL:C	56:4B:65:TRP:CZ3	2.91	0.49
57:4C:90:GLU:OE1	87:4C:306:PGV:H321	2.12	0.49
59:4E:96:LEU:CD1	59:4E:98:ILE:HD11	2.43	0.49
55:8A:275:TRP:CE3	87:8A:603:PGV:H12	2.48	0.49
55:8A:443:TYR:O	56:8B:134:ARG:NH2	2.46	0.49
57:8C:95:THR:HA	57:8C:98:PHE:HD2	1.78	0.49
57:8C:102:TYR:HE2	87:8C:304:PGV:H12	1.76	0.49
69:1A:201:3PE:H2A2	69:1A:201:3PE:H2E1	1.94	0.48
10:1J:163:ILE:HG21	14:1N:12:THR:HG21	1.95	0.48
12:1L:332:HIS:HA	12:1L:335:PHE:CE2	2.48	0.48
26:1a:50:ARG:O	26:1a:54:ILE:HG23	2.12	0.48
36:1k:48:GLU:N	36:1k:48:GLU:OE2	2.46	0.48
47:3P:246:SER:HB2	47:3P:249:LEU:HB2	1.95	0.48
48:3Q:203:ARG:NH2	53:3W:53:LYS:HZ1	2.11	0.48
49:3R:172:LYS:CB	49:3R:214:ILE:HD12	2.43	0.48
55:4A:92:MET:HE2	55:4A:163:ASN:ND2	2.27	0.48
75:4B:303:CDL:H631	75:4B:303:CDL:H141	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:333:LYS:HZ2	55:8A:335:SER:CA	2.22	0.48
56:8B:29:MET:CE	63:8I:36:LYS:HG3	2.43	0.48
59:8E:13:ALA:O	59:8E:17:THR:HG22	2.13	0.48
61:8G:32:THR:OG1	87:8G:101:PGV:C30	2.61	0.48
2:1B:65:PRO:HA	8:1H:34:ARG:HG2	1.94	0.48
2:1B:68:ASP:OD2	8:1H:34:ARG:HB3	2.13	0.48
5:1E:160:TYR:O	5:1E:185:GLY:N	2.44	0.48
6:1F:93:LEU:O	6:1F:134:ALA:HA	2.14	0.48
7:1G:218:ARG:HD2	7:1G:220:TRP:CH2	2.48	0.48
7:1G:241:SER:HB2	7:1G:249:ARG:HG3	1.95	0.48
8:1H:316:PRO:HG3	25:1Z:57:ARG:HB3	1.94	0.48
20:1T:52:MET:SD	22:1W:37:ARG:HD3	2.54	0.48
22:1W:89:GLU:O	22:1W:93:THR:HG22	2.13	0.48
38:1m:32:GLN:HA	38:1m:35:ARG:HD2	1.95	0.48
39:1n:10:THR:O	39:1n:14:LYS:HG3	2.12	0.48
39:1n:89:SER:O	39:1n:89:SER:OG	2.31	0.48
45:3A:142:ASP:OD2	49:3E:79:SER:OG	2.27	0.48
45:3A:324:PHE:CG	45:3A:334:MET:HE3	2.48	0.48
45:3A:358:LYS:O	45:3A:362:ARG:HG3	2.13	0.48
69:3C:504:3PE:H322	70:3X:101:PC1:H252	1.95	0.48
51:3G:21:SER:O	51:3G:25:GLN:HG2	2.12	0.48
45:3N:444:LEU:HB3	75:3N:502:CDL:H712	1.95	0.48
49:3R:191:GLU:HG3	49:3R:194:GLN:H	1.78	0.48
50:3S:82:LYS:HB2	50:3S:85:GLU:HG3	1.94	0.48
55:8A:69:MET:HG2	55:8A:70:VAL:N	2.28	0.48
55:8A:313:ALA:HB2	55:8A:356:ILE:HD11	1.95	0.48
75:8D:201:CDL:H171	75:8D:201:CDL:H721	1.95	0.48
59:8E:72:LYS:HB2	59:8E:82:TYR:HE2	0.81	0.48
65:8K:17:ILE:HD12	65:8K:17:ILE:H	1.78	0.48
68:8N:35:ARG:HE	68:8N:65:PHE:HE1	1.61	0.48
2:1B:57:VAL:HA	2:1B:60:MET:HG2	1.95	0.48
4:1D:62:LEU:HD11	4:1D:78:PRO:HB3	1.95	0.48
12:1L:127:THR:HG21	12:1L:146:GLY:HA3	1.94	0.48
12:1L:237:MET:HB3	12:1L:299:LYS:HE2	1.95	0.48
13:1M:41:LEU:HD13	13:1M:66:LEU:HD13	1.96	0.48
16:1P:63:GLY:HA3	16:1P:68:ILE:HD13	1.94	0.48
19:1S:43:LEU:HD12	19:1S:47:ASN:ND2	2.27	0.48
25:1Z:87:LEU:HD11	25:1Z:119:PRO:HG3	1.94	0.48
45:3A:240:GLU:OE1	45:3A:242:ARG:NH1	2.45	0.48
45:3N:29:GLN:NE2	45:3N:204:GLU:OE1	2.45	0.48
46:3O:276:GLN:HB2	46:3O:322:PHE:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:4D:60:TYR:CD1	58:4D:60:TYR:C	2.91	0.48
58:4D:61:ARG:NH1	58:4D:65:ASN:O	2.47	0.48
66:8L:19:TRP:CH2	67:8M:14:GLU:OE1	2.66	0.48
68:8N:11:LYS:HD3	68:8N:11:LYS:H	1.78	0.48
2:1B:71:ARG:HA	8:1H:37:PRO:HA	1.95	0.48
8:1H:197:PRO:HB2	8:1H:280:PHE:HD2	1.78	0.48
12:1L:367:PRO:O	12:1L:371:THR:HG23	2.13	0.48
13:1M:6:ILE:HD12	31:1f:23:GLY:HA2	1.94	0.48
13:1M:220:HIS:HD2	13:1M:232:ALA:HB2	1.77	0.48
14:1N:107:GLY:O	14:1N:187:MET:CE	2.60	0.48
15:1O:9:VAL:HG12	15:1O:10:LEU:HD23	1.96	0.48
15:1O:306:PRO:HB2	28:1c:7:PRO:HB3	1.96	0.48
15:1O:318:TRP:CD1	15:1O:318:TRP:H	2.31	0.48
16:1P:317:VAL:HG23	16:1P:318:LEU:HD22	1.94	0.48
24:1Y:80:ARG:HB3	24:1Y:82:LYS:HE2	1.95	0.48
33:1h:41:THR:HG22	75:1h:202:CDL:H711	1.94	0.48
46:3B:37:SER:HB3	46:3B:216:LEU:HD12	1.94	0.48
47:3C:119:LEU:HD22	85:3C:502:HEM:HBB2	1.95	0.48
49:3E:155:LYS:NZ	49:3E:274:GLY:OXT	2.39	0.48
49:3R:243:TYR:HB3	49:3R:247:GLY:HA2	1.94	0.48
57:4C:25:LEU:HD23	64:4J:43:THR:HG22	1.96	0.48
57:4C:47:LEU:HD13	87:4C:302:PGV:H12	1.96	0.48
55:8A:244:TYR:O	55:8A:248:LEU:HD12	2.14	0.48
58:8D:23:PRO:O	59:8E:66:ARG:NH1	2.46	0.48
59:8E:53:ARG:HH12	59:8E:92:THR:HG23	1.78	0.48
2:1B:150:PRO:HD3	4:1D:190:HIS:CD2	2.49	0.48
5:1E:78:MET:HE3	7:1G:173:GLY:CA	2.44	0.48
6:1F:21:ILE:CG2	6:1F:117:LYS:HZ1	2.27	0.48
6:1F:32:ARG:HH12	44:1s:42:GLN:NE2	2.11	0.48
6:1F:308:PRO:HD2	6:1F:311:VAL:HB	1.94	0.48
9:1I:144:HIS:CE1	16:1P:65:LEU:HD21	2.48	0.48
11:1K:22:TYR:CD2	11:1K:90:VAL:HG21	2.48	0.48
12:1L:156:GLY:HA3	13:1M:416:ARG:HH12	1.78	0.48
12:1L:419:THR:HA	12:1L:422:TYR:CE2	2.48	0.48
13:1M:237:LYS:HD2	13:1M:316:MET:HB3	1.95	0.48
69:1M:502:3PE:H2B2	69:1M:504:3PE:H252	1.94	0.48
24:1Y:72:THR:HB	24:1Y:92:GLY:HA2	1.95	0.48
25:1Z:140:PHE:HB2	26:1a:45:TRP:CD1	2.49	0.48
31:1f:2:ASN:O	31:1f:6:ILE:HG13	2.13	0.48
46:3B:222:ARG:HD2	46:3B:223:PHE:CE1	2.49	0.48
47:3C:100:ARG:HA	69:3C:503:3PE:H252	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4B:49:LYS:NZ	59:4E:76:GLY:C	2.71	0.48
55:8A:21:LEU:HB3	87:8L:101:PGV:H271	1.95	0.48
55:8A:181:THR:O	55:8A:270:TYR:OH	2.24	0.48
55:8A:266:GLU:HB3	60:8F:68:THR:HG21	1.95	0.48
56:8B:112:ASP:OD1	62:8H:62:SER:OG	2.31	0.48
56:8B:132:GLU:HB3	56:8B:137:GLU:HG3	1.95	0.48
58:8D:52:SER:N	58:8D:55:GLU:OE2	2.45	0.48
2:1B:50:PHE:HE2	2:1B:96:MET:CE	2.26	0.48
2:1B:69:MET:HG3	2:1B:74:VAL:O	2.14	0.48
6:1F:90:PRO:O	6:1F:218:CYS:HB2	2.14	0.48
8:1H:9:LEU:O	8:1H:13:ILE:HG12	2.13	0.48
10:1J:10:SER:O	10:1J:14:VAL:HG23	2.14	0.48
12:1L:154:LEU:HD13	12:1L:243:VAL:HG22	1.95	0.48
17:1Q:89:LYS:NZ	17:1Q:107:GLU:OE2	2.47	0.48
22:1W:62:LYS:HD3	22:1W:62:LYS:HA	1.74	0.48
32:1g:48:ASP:C	32:1g:48:ASP:OD1	2.57	0.48
75:1h:202:CDL:HA4	75:1h:202:CDL:H722	1.95	0.48
37:1l:3:HIS:ND1	37:1l:4:VAL:HG23	2.28	0.48
41:1p:98:ASP:HA	41:1p:101:ILE:HD12	1.95	0.48
47:3C:307:LEU:HD11	47:3C:363:LEU:HD23	1.95	0.48
55:4A:54:TYR:O	55:4A:58:VAL:HG23	2.13	0.48
55:4A:127:THR:HA	55:4A:235:PHE:CE2	2.48	0.48
57:4C:109:THR:HG21	57:4C:111:GLU:OE2	2.14	0.48
58:4D:141:ASP:O	58:4D:143:ASN:N	2.47	0.48
60:4F:43:LYS:HG3	60:4F:44:GLU:OE2	2.13	0.48
62:4H:4:ILE:HG21	62:4H:52:VAL:HG13	1.95	0.48
62:4H:5:GLN:CD	62:4H:5:GLN:H	2.20	0.48
66:4L:37:PHE:HB3	67:4M:33:VAL:HG21	1.95	0.48
55:8A:413:HIS:CE1	55:8A:468:MET:HE3	2.49	0.48
6:1F:369:VAL:HA	6:1F:372:MET:HE2	1.95	0.48
7:1G:168:GLY:HA3	7:1G:416:THR:HB	1.95	0.48
8:1H:152:SER:HA	8:1H:155:LEU:HD12	1.96	0.48
9:1I:65:HIS:ND1	9:1I:113:MET:HE1	2.28	0.48
12:1L:273:VAL:O	12:1L:277:THR:HG23	2.13	0.48
12:1L:349:SER:HB2	12:1L:366:MET:CE	2.43	0.48
13:1M:287:ALA:O	13:1M:291:VAL:HG23	2.13	0.48
14:1N:102:LEU:HD13	14:1N:142:LEU:HG	1.96	0.48
14:1N:270:MET:HE1	14:1N:282:MET:HE1	1.95	0.48
16:1P:45:VAL:HG12	16:1P:47:VAL:HG23	1.95	0.48
20:1T:31:SER:OG	20:1T:34:SER:OG	2.27	0.48
20:1T:60:PHE:CZ	20:1T:80:ILE:HG23	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:44:SER:O	20:1U:48:VAL:HG23	2.13	0.48
23:1X:8:THR:O	23:1X:12:LEU:HG	2.14	0.48
69:1d:201:3PE:H2A2	70:1d:202:PC1:H332	1.96	0.48
34:1i:69:PHE:O	34:1i:73:HIS:HB2	2.13	0.48
45:3A:40:TRP:HB3	45:3A:384:LEU:HD11	1.95	0.48
46:3O:70:ARG:HD3	46:3O:100:SER:OG	2.13	0.48
48:3Q:224:ARG:NH1	75:3T:101:CDL:OB3	2.46	0.48
52:3U:68:CYS:O	52:3U:72:LYS:HG2	2.13	0.48
55:4A:345:ILE:O	55:4A:349:THR:OG1	2.26	0.48
88:4A:604:HEA:H132	88:4A:604:HEA:HHC	1.96	0.48
57:4C:22:LEU:HD22	64:4J:43:THR:HG21	1.94	0.48
87:4L:101:PGV:H131	87:4L:101:PGV:H311	1.96	0.48
59:8E:24:ILE:HD12	59:8E:25:ASP:N	2.27	0.48
68:8N:52:GLU:HB2	68:8N:54:TRP:CE2	2.48	0.48
2:1B:162:GLN:HE21	9:1I:142:GLU:HG2	1.77	0.48
3:1C:79:THR:HB	4:1D:390:LYS:HG2	1.96	0.48
6:1F:164:LYS:CA	44:1s:63:MET:HE1	2.42	0.48
6:1F:275:PRO:HB2	6:1F:278:GLU:HG2	1.95	0.48
7:1G:426:PRO:HB2	7:1G:656:LEU:HD23	1.96	0.48
9:1I:169:ILE:O	9:1I:173:TYR:HB3	2.13	0.48
11:1K:44:SER:HB2	11:1K:59:MET:HE1	1.96	0.48
12:1L:140:LEU:HD22	12:1L:182:PHE:CE2	2.44	0.48
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.47	0.48
14:1N:65:THR:O	14:1N:69:MET:HG3	2.14	0.48
15:1O:70:ASP:OD2	15:1O:72:GLN:NE2	2.46	0.48
16:1P:89:ASN:OD1	16:1P:89:ASN:C	2.57	0.48
16:1P:94:LEU:HD13	16:1P:132:ILE:HG13	1.95	0.48
20:1T:65:ILE:H	20:1T:65:ILE:HD12	1.78	0.48
75:1X:201:CDL:H273	75:1X:201:CDL:H322	1.96	0.48
34:1i:44:GLN:HA	34:1i:47:ASN:ND2	2.29	0.48
46:3B:226:MET:HG3	46:3B:227:ARG:N	2.29	0.48
47:3C:120:LEU:O	47:3C:124:MET:HG3	2.14	0.48
46:3O:395:PRO:O	46:3O:399:LEU:HG	2.14	0.48
55:4A:3:VAL:HA	55:4A:7:LEU:HB2	1.94	0.48
55:4A:254:ILE:HG13	55:4A:344:PHE:CD2	2.48	0.48
58:4D:28:ALA:HB1	58:4D:63:LYS:HA	1.95	0.48
62:4H:57:ARG:HA	62:4H:60:TYR:HD1	1.78	0.48
87:4K:101:PGV:H21	87:4K:101:PGV:H62	1.96	0.48
68:4N:3:ARG:HG3	68:4N:4:GLN:N	2.28	0.48
57:8C:103:HIS:HA	87:8C:304:PGV:O02	2.14	0.48
59:8E:81:ILE:HG23	63:8I:9:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:8G:101:PGV:H02	87:8G:101:PGV:H21	1.52	0.48
1:1A:51:PHE:O	1:1A:52:SER:HB3	2.14	0.48
4:1D:62:LEU:HD22	4:1D:425:PHE:HZ	1.79	0.48
4:1D:148:LEU:HD23	4:1D:174:ARG:HG2	1.95	0.48
4:1D:284:ASP:O	4:1D:306:GLN:HG3	2.14	0.48
12:1L:574:SER:OG	14:1N:171:ASN:HB2	2.14	0.48
14:1N:118:VAL:O	14:1N:122:ILE:HG23	2.14	0.48
16:1P:112:LYS:HD3	16:1P:112:LYS:N	2.29	0.48
37:1l:10:PRO:HD3	38:1m:66:ARG:HG2	1.96	0.48
49:3E:204:ARG:NH2	49:3E:246:SER:OG	2.40	0.48
50:3F:61:ARG:NH2	50:3F:112:GLU:OE1	2.36	0.48
45:3N:224:VAL:CG1	45:3N:225:GLU:OE1	2.61	0.48
75:3P:504:CDL:OB4	51:3T:40:ARG:NE	2.38	0.48
49:3R:169:TRP:CD1	49:3R:174:LEU:HD22	2.48	0.48
56:4B:165:VAL:HG11	56:4B:168:LEU:HD12	1.96	0.48
59:4E:42:VAL:HG21	59:4E:81:ILE:HG21	1.95	0.48
55:8A:86:MET:HE1	55:8A:184:PHE:HD2	1.78	0.48
57:8C:175:LEU:HD22	87:8C:305:PGV:H221	1.96	0.48
4:1D:94:LYS:HD2	4:1D:102:TYR:HE2	1.79	0.48
4:1D:121:ALA:HA	4:1D:365:THR:HG21	1.95	0.48
4:1D:424:VAL:O	4:1D:428:VAL:HG23	2.13	0.48
6:1F:261:HIS:ND1	6:1F:338:ASP:OD1	2.37	0.48
6:1F:279:LEU:HD12	6:1F:317:MET:HG3	1.95	0.48
7:1G:522:LEU:HD22	7:1G:537:LEU:HD11	1.96	0.48
7:1G:534:ARG:HH22	42:1q:145:LYS:HE3	1.79	0.48
69:1M:504:3PE:H272	14:1N:246:VAL:HG21	1.96	0.48
15:1O:49:ARG:HD3	15:1O:114:HIS:CD2	2.48	0.48
16:1P:118:ALA:HA	16:1P:129:LEU:HD21	1.95	0.48
16:1P:258:LEU:HD23	16:1P:263:TYR:CE1	2.49	0.48
17:1Q:49:VAL:O	17:1Q:49:VAL:HG22	2.13	0.48
23:1X:56:LEU:O	23:1X:60:LYS:HG2	2.14	0.48
29:1d:14:LEU:HD11	29:1d:77:LYS:HB3	1.95	0.48
39:1n:126:ARG:O	39:1n:130:GLU:HG2	2.14	0.48
41:1p:98:ASP:O	41:1p:102:VAL:HG23	2.14	0.48
46:3B:36:ALA:HB3	46:3B:207:ILE:HG13	1.95	0.48
48:3D:135:ALA:HA	48:3D:178:TYR:HA	1.95	0.48
48:3Q:212:MET:SD	69:3R:302:3PE:H352	2.54	0.48
49:3R:211:VAL:HG11	49:3R:245:ALA:O	2.13	0.48
55:4A:3:VAL:HG11	87:4A:601:PGV:H31	1.95	0.48
55:4A:62:ALA:HB2	88:4A:604:HEA:HBD1	1.95	0.48
56:4B:125:THR:HG22	56:4B:134:ARG:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:4J:51:GLY:O	64:4J:54:SER:OG	2.31	0.48
55:8A:455:SER:O	55:8A:458:SER:OG	2.29	0.48
75:8B:303:CDL:H182	75:8B:303:CDL:H442	1.96	0.48
64:8J:46:SER:O	64:8J:50:LEU:HG	2.14	0.48
2:1B:179:ARG:HH12	78:1P:402:NDP:P2B	2.37	0.47
5:1E:78:MET:HA	5:1E:81:TYR:CD2	2.49	0.47
6:1F:154:ARG:HD2	44:1s:57:GLU:OE1	2.14	0.47
6:1F:404:ILE:HG22	7:1G:53:ARG:NH1	2.29	0.47
12:1L:245:ALA:HB2	12:1L:340:PHE:HB3	1.96	0.47
13:1M:250:LEU:O	13:1M:254:THR:OG1	2.26	0.47
32:1g:114:ASP:HB3	32:1g:117:LYS:HD2	1.95	0.47
34:1i:99:ARG:HA	41:1p:115:ARG:HA	1.96	0.47
45:3A:349:ALA:O	45:3A:350:THR:HB	2.14	0.47
47:3C:63:PHE:O	47:3C:67:THR:HG23	2.14	0.47
47:3C:181:PHE:CZ	47:3P:53:MET:HE2	2.49	0.47
49:3E:159:ILE:HG12	49:3E:165:MET:CG	2.42	0.47
45:3N:272:VAL:O	45:3N:276:ILE:HG13	2.14	0.47
55:4A:282:PHE:HA	87:4A:603:PGV:H292	1.95	0.47
63:4I:23:GLY:O	63:4I:26:ILE:HG13	2.14	0.47
55:8A:44:PRO:HG3	58:8D:111:PHE:CZ	2.49	0.47
57:8C:176:LEU:O	57:8C:180:GLU:OE1	2.31	0.47
58:8D:86:LEU:HA	58:8D:89:ILE:CD1	2.44	0.47
7:1G:144:PRO:HD2	7:1G:192:MET:HE1	1.96	0.47
7:1G:344:CYS:HB3	7:1G:510:GLY:O	2.14	0.47
7:1G:511:VAL:HG22	7:1G:514:ILE:HB	1.96	0.47
8:1H:63:PRO:HG2	8:1H:66:SER:HB3	1.96	0.47
8:1H:85:MET:CE	8:1H:233:MET:HG3	2.44	0.47
12:1L:178:GLY:HA2	12:1L:218:LEU:HG	1.96	0.47
12:1L:593:ILE:O	12:1L:597:ILE:HG13	2.14	0.47
13:1M:243:MET:HE3	13:1M:301:ILE:CG2	2.44	0.47
15:1O:75:GLY:HA2	15:1O:99:TRP:CD2	2.49	0.47
15:1O:180:GLN:O	15:1O:183:ILE:HG13	2.14	0.47
21:1V:17:GLU:HG2	21:1V:18:THR:HG23	1.96	0.47
23:1X:165:ARG:O	33:1h:104:ARG:NH1	2.44	0.47
29:1d:113:LEU:HD22	32:1g:121:PRO:HG3	1.96	0.47
39:1n:12:GLN:O	39:1n:16:LEU:HG	2.14	0.47
39:1n:153:LEU:HD13	39:1n:165:LEU:HB2	1.96	0.47
45:3A:121:SER:O	45:3A:179:ARG:NH1	2.47	0.47
48:3D:304:LEU:HD21	49:3E:124:GLY:HA3	1.97	0.47
49:3R:128:ALA:HB1	69:3R:302:3PE:H361	1.96	0.47
55:4A:129:TYR:OH	55:4A:236:TRP:NE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:217:THR:HB	57:8C:195:SER:HB3	1.96	0.47
57:8C:77:LYS:CD	57:8C:80:ARG:HD3	2.43	0.47
59:8E:73:ASP:C	59:8E:73:ASP:OD1	2.57	0.47
61:8G:15:THR:O	61:8G:19:LEU:CD1	2.53	0.47
1:1A:22:PHE:CD1	8:1H:60:PRO:HG2	2.49	0.47
1:1A:54:LYS:NZ	4:1D:71:GLU:HB2	2.29	0.47
4:1D:115:GLU:HG3	4:1D:194:ILE:HB	1.96	0.47
6:1F:15:LEU:HD13	6:1F:271:GLU:HB2	1.95	0.47
6:1F:115:PRO:O	6:1F:119:VAL:HG23	2.14	0.47
6:1F:261:HIS:CD2	6:1F:261:HIS:N	2.78	0.47
7:1G:386:PHE:CE1	7:1G:668:ILE:HD13	2.49	0.47
8:1H:92:PRO:HD3	8:1H:255:TYR:HD1	1.80	0.47
9:1I:54:LYS:HD3	42:1q:91:HIS:CE1	2.49	0.47
12:1L:63:ILE:O	12:1L:79:SER:HA	2.14	0.47
16:1P:153:GLU:OE2	16:1P:167:LYS:NZ	2.46	0.47
18:1R:20:ASP:OD1	18:1R:21:GLY:N	2.46	0.47
41:1p:139:GLN:O	41:1p:143:SER:HB2	2.13	0.47
41:1p:141:ARG:HG3	41:1p:142:TYR:CD1	2.50	0.47
45:3A:280:TYR:HA	45:3A:284:TYR:CE2	2.49	0.47
48:3D:313:ARG:HD3	51:3G:28:PHE:CE2	2.50	0.47
48:3Q:47:ALA:HA	48:3Q:90:TYR:HA	1.95	0.47
75:4D:201:CDL:OB4	75:4D:201:CDL:HA4	2.14	0.47
55:8A:499:PRO:HG3	66:8L:10:ASN:ND2	2.29	0.47
56:8B:221:LYS:HD2	56:8B:221:LYS:O	2.14	0.47
58:8D:94:LEU:HD23	58:8D:97:ILE:HD11	1.96	0.47
1:1A:23:TRP:HZ2	70:1A:202:PC1:H222	1.79	0.47
70:1B:203:PC1:H2	70:1B:203:PC1:H221	1.36	0.47
4:1D:52:GLY:H	4:1D:53:PRO:CD	2.24	0.47
10:1J:39:VAL:O	10:1J:43:ILE:HG13	2.14	0.47
12:1L:297:ASP:O	12:1L:301:ILE:HG13	2.14	0.47
21:1V:48:GLU:O	21:1V:52:ASN:ND2	2.47	0.47
75:1X:201:CDL:HA21	75:1X:201:CDL:H541	1.96	0.47
34:1i:79:TRP:HD1	41:1p:40:VAL:HG13	1.79	0.47
49:3I:32:ALA:N	49:3I:71:ASN:OD1	2.47	0.47
45:3N:279:HIS:HD1	45:3N:284:TYR:HH	1.54	0.47
75:3N:502:CDL:OA9	47:3P:221:HIS:NE2	2.47	0.47
47:3P:116:GLY:C	85:3P:502:HEM:HBC2	2.38	0.47
47:3P:119:LEU:HD22	85:3P:502:HEM:HBB2	1.97	0.47
57:4C:156:ARG:NH2	57:4C:222:GLN:O	2.46	0.47
63:4I:41:GLU:O	63:4I:41:GLU:CD	2.56	0.47
55:8A:378:HIS:O	55:8A:382:SER:OG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:412:ILE:HG13	58:8D:81:ILE:HG23	1.97	0.47
56:8B:68:LEU:O	56:8B:72:ILE:HG13	2.14	0.47
1:1A:53:MET:HE1	11:1K:79:VAL:HG13	1.95	0.47
4:1D:241:ASP:OD1	4:1D:290:ARG:NH1	2.47	0.47
6:1F:308:PRO:HD3	6:1F:421:HIS:CD2	2.50	0.47
7:1G:453:LEU:HD21	7:1G:458:LEU:HD21	1.96	0.47
34:1i:94:TYR:OH	41:1p:10:PRO:O	2.26	0.47
45:3A:6:GLN:HA	45:3A:9:GLN:HG2	1.96	0.47
46:3B:370:MET:HA	46:3B:373:GLU:HG3	1.95	0.47
47:3C:316:MET:HG2	47:3C:317:PHE:CE1	2.49	0.47
49:3R:187:GLU:OE2	49:3R:244:ASP:HB2	2.15	0.47
55:4A:469:ILE:HD13	67:4M:26:PHE:CE1	2.50	0.47
56:4B:12:ALA:N	63:4I:47:TYR:OH	2.39	0.47
60:4F:79:THR:HG21	60:4F:88:HIS:HB3	1.97	0.47
55:8A:243:VAL:HG13	88:8A:605:HEA:C3C	2.44	0.47
55:8A:251:PHE:HB3	55:8A:319:LYS:NZ	2.30	0.47
57:8C:51:THR:HG22	87:8C:303:PGV:H172	1.95	0.47
1:1A:37:TYR:HB2	2:1B:81:ARG:HH11	1.79	0.47
6:1F:154:ARG:HB2	44:1s:58:LEU:HD11	1.95	0.47
14:1N:69:MET:HE3	14:1N:97:MET:HE3	1.95	0.47
49:3E:264:GLU:H	49:3E:272:ILE:HG12	1.78	0.47
55:4A:117:MET:O	66:4L:46:LYS:NZ	2.47	0.47
55:4A:334:TRP:CZ3	75:4D:201:CDL:H121	2.50	0.47
56:4B:60:GLU:H	56:4B:60:GLU:CD	2.22	0.47
57:4C:83:MET:HG2	57:4C:237:ALA:HB1	1.97	0.47
58:4D:78:TRP:HB3	75:4D:201:CDL:H182	1.95	0.47
63:4I:57:MET:O	63:4I:61:GLU:HG2	2.15	0.47
55:8A:31:THR:HG21	55:8A:465:VAL:HG11	1.96	0.47
55:8A:277:MET:O	55:8A:280:ILE:HG13	2.15	0.47
55:8A:342:LEU:HD22	56:8B:46:LEU:HD11	1.97	0.47
75:8C:306:CDL:O1	75:8C:306:CDL:OA7	2.31	0.47
1:1A:4:MET:HE2	70:1H:403:PC1:H261	1.96	0.47
2:1B:30:VAL:HG13	2:1B:173:LEU:HB3	1.97	0.47
2:1B:36:LEU:HD22	70:1B:203:PC1:H2C2	1.97	0.47
2:1B:179:ARG:NH2	70:1B:202:PC1:H111	2.29	0.47
4:1D:312:SER:O	4:1D:316:ASN:ND2	2.48	0.47
5:1E:78:MET:O	5:1E:82:GLU:HG3	2.14	0.47
6:1F:92:TYR:CD1	6:1F:133:ALA:HB3	2.50	0.47
7:1G:16:GLN:OE1	7:1G:17:SER:N	2.48	0.47
7:1G:110:GLN:NE2	17:1Q:45:MET:HB3	2.25	0.47
7:1G:655:GLN:OE1	7:1G:655:GLN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:62:ILE:HG21	14:1N:31:ILE:HD11	1.97	0.47
12:1L:11:THR:O	12:1L:15:LEU:HD13	2.14	0.47
12:1L:83:ASP:OD1	12:1L:85:PHE:N	2.47	0.47
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	1.97	0.47
13:1M:237:LYS:NZ	13:1M:316:MET:O	2.41	0.47
13:1M:328:CYS:HB3	13:1M:437:MET:HE1	1.96	0.47
16:1P:109:VAL:HA	16:1P:113:ILE:HD12	1.97	0.47
20:1U:55:GLU:OE1	39:1n:24:ARG:NH1	2.31	0.47
20:1U:72:CYS:N	20:1U:75:GLU:OE1	2.47	0.47
26:1a:59:ARG:NH2	26:1a:61:HIS:NE2	2.63	0.47
26:1a:61:HIS:HD1	26:1a:62:VAL:N	2.13	0.47
31:1f:8:ARG:HA	31:1f:8:ARG:HD2	1.77	0.47
36:1k:62:PHE:O	36:1k:66:LEU:HD23	2.15	0.47
42:1q:94:THR:OG1	42:1q:96:ASP:OD1	2.30	0.47
44:1s:74:ARG:NH1	44:1s:74:ARG:HB2	2.30	0.47
45:3A:329:MET:HE3	45:3A:430:GLN:HE22	1.80	0.47
46:3B:100:SER:OG	46:3B:105:MET:HG2	2.15	0.47
69:3C:503:3PE:H281	69:3C:503:3PE:H242	1.97	0.47
48:3D:253:ILE:HD11	86:3D:501:HEC:HBB2	1.96	0.47
52:3H:60:GLU:OE1	52:3H:60:GLU:N	2.41	0.47
45:3N:40:TRP:HB3	45:3N:384:LEU:HD11	1.96	0.47
49:3R:210:TRP:CD1	49:3R:268:ASP:HB3	2.50	0.47
55:4A:93:ALA:HA	55:4A:171:MET:HE3	1.83	0.47
55:4A:147:ILE:HG23	55:4A:206:ILE:HB	1.95	0.47
55:4A:449:ALA:O	55:4A:453:ILE:HG12	2.15	0.47
56:4B:40:TYR:CD2	63:4I:24:ALA:HA	2.50	0.47
57:4C:132:LEU:HD22	57:4C:176:LEU:CD2	2.44	0.47
64:4J:16:ASN:O	64:4J:18:LEU:HD12	2.14	0.47
64:4J:37:THR:HG23	87:4J:101:PGV:H152	1.96	0.47
66:4L:41:ARG:CB	67:4M:40:TYR:HE2	2.26	0.47
67:4M:14:GLU:HA	67:4M:17:ILE:HG22	1.95	0.47
55:8A:104:LEU:HB2	55:8A:156:SER:HB3	1.97	0.47
55:8A:155:VAL:HG12	55:8A:159:LEU:HD11	1.96	0.47
57:8C:165:ILE:HD13	87:8C:302:PGV:H11	1.97	0.47
57:8C:251:PHE:HA	57:8C:254:VAL:HG22	1.96	0.47
62:8H:20:PHE:CG	62:8H:28:ASN:ND2	2.83	0.47
62:8H:36:PHE:CE1	62:8H:40:GLU:OE2	2.68	0.47
68:8N:41:PRO:O	68:8N:54:TRP:HE3	1.98	0.47
7:1G:199:ILE:HD13	7:1G:202:ILE:HD11	1.96	0.47
10:1J:86:ASN:ND2	10:1J:88:THR:HB	2.30	0.47
13:1M:183:SER:O	41:1p:152:ARG:NH2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:131:LEU:HA	14:1N:135:LYS:HE2	1.96	0.47
15:1O:40:ARG:NH2	15:1O:50:HIS:HE1	2.12	0.47
20:1U:69:LYS:NZ	34:1i:7:GLU:OE1	2.45	0.47
29:1d:11:LEU:O	30:1e:8:ARG:NH2	2.47	0.47
40:1o:40:ALA:HB3	40:1o:45:MET:HE2	1.97	0.47
45:3A:238:GLY:O	51:3G:21:SER:OG	2.27	0.47
69:3A:503:3PE:C35	47:3C:11:MET:HE2	2.37	0.47
48:3Q:203:ARG:HH22	53:3W:53:LYS:HZ2	1.62	0.47
55:4A:22:PHE:HE2	55:4A:105:LEU:HB3	1.77	0.47
55:4A:172:LYS:HG3	55:4A:176:MET:HE2	1.96	0.47
55:4A:405:LEU:HD22	55:4A:471:ILE:HD12	1.97	0.47
56:4B:198:GLU:O	56:4B:204:HIS:CE1	2.68	0.47
68:4N:53:PRO:HD2	68:4N:54:TRP:CE3	2.49	0.47
55:8A:202:LEU:O	55:8A:206:ILE:HG12	2.14	0.47
55:8A:209:LEU:HA	55:8A:212:ASP:OD2	2.15	0.47
87:8A:601:PGV:H341	87:8L:101:PGV:H152	1.96	0.47
4:1D:302:GLU:HG2	9:1I:3:LYS:HD3	1.97	0.47
5:1E:27:ASN:ND2	5:1E:57:GLN:OE1	2.48	0.47
5:1E:73:LEU:HB2	5:1E:75:VAL:HG12	1.97	0.47
6:1F:84:LYS:HB2	6:1F:84:LYS:HE3	1.63	0.47
6:1F:395:ILE:O	6:1F:399:ILE:HG23	2.14	0.47
7:1G:627:SER:HB3	7:1G:630:LEU:HD13	1.96	0.47
10:1J:86:ASN:HD22	11:1K:23:ARG:NH2	2.13	0.47
11:1K:27:MET:HE2	11:1K:78:LEU:CD1	2.45	0.47
14:1N:317:PHE:HZ	15:1O:106:LEU:HD21	1.80	0.47
19:1S:21:HIS:O	19:1S:62:PRO:HA	2.14	0.47
32:1g:50:ASP:HB3	32:1g:53:VAL:HG22	1.97	0.47
32:1g:111:ASN:OD1	41:1p:161:ARG:NH1	2.47	0.47
42:1q:2:GLU:O	42:1q:6:VAL:HG23	2.14	0.47
47:3C:11:MET:CE	47:3C:11:MET:HA	2.45	0.47
46:3O:101:THR:HG22	49:3V:65:VAL:HG12	1.97	0.47
48:3Q:27:ARG:HB2	48:3Q:55:CYS:HB2	1.96	0.47
49:3R:198:PRO:O	49:3R:199:GLN:HG2	2.15	0.47
49:3R:224:PRO:HA	49:3R:237:PRO:HD3	1.97	0.47
55:4A:271:MET:CA	55:4A:271:MET:CE	2.90	0.47
57:4C:151:LEU:HD21	57:4C:159:MET:HE1	1.97	0.47
63:4I:41:GLU:OE1	63:4I:41:GLU:O	2.33	0.47
64:4J:36:MET:HG2	87:4J:101:PGV:H182	1.97	0.47
57:8C:58:TRP:HD1	57:8C:61:ILE:HD12	1.80	0.47
60:8F:13:ALA:O	60:8F:18:ARG:NH2	2.47	0.47
61:8G:13:ALA:O	61:8G:17:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:8G:101:PGV:H261	87:8G:101:PGV:H92	1.96	0.47
68:8N:41:PRO:HA	68:8N:53:PRO:O	2.14	0.47
4:1D:110:SER:HA	4:1D:145:THR:HG22	1.97	0.47
5:1E:172:ILE:HG12	5:1E:187:ARG:HH21	1.80	0.47
5:1E:191:PHE:N	5:1E:194:GLU:OE1	2.47	0.47
7:1G:455:SER:O	7:1G:459:GLN:HG2	2.15	0.47
12:1L:486:MET:HA	12:1L:489:THR:OG1	2.15	0.47
75:1L:702:CDL:H562	75:1L:702:CDL:H601	1.97	0.47
20:1U:31:SER:OG	20:1U:32:VAL:N	2.48	0.47
39:1n:34:ASP:OD1	39:1n:35:LYS:N	2.46	0.47
43:1r:53:TYR:CE2	43:1r:57:ASP:HB2	2.50	0.47
46:3B:109:VAL:HG22	46:3B:123:LEU:HD22	1.97	0.47
47:3C:215:MET:HB2	51:3G:12:MET:HE2	1.97	0.47
45:3N:100:LYS:O	46:3O:370:MET:HE1	2.15	0.47
47:3P:344:GLU:HA	47:3P:344:GLU:OE2	2.15	0.47
49:3R:239:HIS:HE1	49:3R:253:PRO:HD2	1.80	0.47
55:4A:243:VAL:HG13	88:4A:605:HEA:C3C	2.44	0.47
58:4D:60:TYR:OH	58:4D:67:SER:HA	2.15	0.47
75:4D:201:CDL:H512	75:4D:201:CDL:HB4	1.39	0.47
63:4I:55:ASP:OD1	63:4I:55:ASP:O	2.33	0.47
55:8A:349:THR:HG23	88:8A:605:HEA:H272	1.97	0.47
62:8H:17:ASP:OD1	62:8H:17:ASP:C	2.57	0.47
1:1A:1:FME:O1	1:1A:2:ASN:N	2.47	0.46
2:1B:134:ARG:HE	3:1C:173:GLU:CD	2.23	0.46
4:1D:306:GLN:O	4:1D:310:ILE:HG13	2.15	0.46
7:1G:242:THR:HG21	7:1G:586:ALA:HB1	1.96	0.46
7:1G:703:ILE:HB	18:1R:83:THR:OG1	2.14	0.46
8:1H:165:LEU:HD13	8:1H:241:LEU:HA	1.98	0.46
10:1J:173:ARG:HH12	15:1O:254:ARG:HD3	1.80	0.46
14:1N:187:MET:HB2	14:1N:187:MET:HE2	1.55	0.46
15:1O:236:GLU:HG3	21:1V:29:LYS:NZ	2.30	0.46
16:1P:111:VAL:HB	16:1P:112:LYS:HD3	1.97	0.46
20:1T:49:GLU:OE2	22:1W:40:TYR:OH	2.32	0.46
22:1W:43:VAL:HG11	22:1W:60:ARG:HG3	1.96	0.46
30:1e:88:GLU:HB2	30:1e:90:LYS:NZ	2.30	0.46
45:3A:329:MET:HE3	45:3A:430:GLN:NE2	2.30	0.46
46:3B:274:VAL:O	46:3B:278:VAL:HG23	2.15	0.46
47:3C:272:TRP:HA	47:3C:275:LEU:HG	1.98	0.46
48:3D:297:MET:HE3	48:3D:297:MET:HB3	1.88	0.46
46:3O:56:ARG:HD2	46:3O:103:GLU:HG2	1.96	0.46
56:4B:102:HIS:O	56:4B:207:MET:HE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:8B:28:LEU:HD21	75:8B:303:CDL:H561	1.97	0.46
57:8C:221:ARG:HH21	57:8C:226:HIS:HB3	1.80	0.46
75:8D:201:CDL:H581	75:8D:201:CDL:H621	1.98	0.46
7:1G:190:MET:SD	7:1G:690:ALA:HB1	2.54	0.46
11:1K:95:LEU:HD23	11:1K:95:LEU:H	1.80	0.46
13:1M:114:GLU:HG2	13:1M:117:LEU:H	1.79	0.46
69:1M:501:3PE:H332	69:1M:501:3PE:H291	1.96	0.46
16:1P:191:VAL:O	16:1P:255:PRO:HA	2.14	0.46
19:1S:23:CYS:HA	19:1S:57:CYS:O	2.15	0.46
23:1X:84:TYR:CE2	23:1X:88:ILE:HD11	2.50	0.46
32:1g:66:PHE:O	32:1g:71:VAL:HG23	2.14	0.46
37:1l:82:ASP:OD1	37:1l:82:ASP:N	2.46	0.46
37:1l:111:PHE:O	37:1l:115:MET:HG2	2.15	0.46
37:1l:128:VAL:HG22	37:1l:129:GLY:O	2.15	0.46
45:3N:156:THR:O	45:3N:239:SER:OG	2.32	0.46
69:3N:501:3PE:H332	75:3N:502:CDL:H111	1.96	0.46
46:3O:342:ASP:O	46:3O:346:THR:HG23	2.16	0.46
49:3R:162:GLY:N	49:3R:178:HIS:HB3	2.29	0.46
49:3R:248:ARG:NH1	49:3R:257:ASN:HD22	2.13	0.46
67:4M:33:VAL:O	67:4M:37:LEU:HG	2.15	0.46
55:8A:340:TRP:HZ2	55:8A:413:HIS:CE1	2.33	0.46
56:8B:24:HIS:HE1	56:8B:28:LEU:HD22	1.80	0.46
57:8C:94:PHE:HB3	57:8C:98:PHE:CE2	2.50	0.46
3:1C:53:HIS:HD1	3:1C:55:ASP:H	1.61	0.46
4:1D:342:MET:HE2	4:1D:346:ILE:HG13	1.97	0.46
9:1I:44:GLU:HG3	26:1a:1:MET:CE	2.39	0.46
9:1I:160:LYS:HD2	9:1I:161:TRP:NE1	2.30	0.46
12:1L:434:LYS:HG3	36:1k:52:TYR:CD2	2.50	0.46
13:1M:24:TRP:CD2	13:1M:81:GLN:HB3	2.51	0.46
14:1N:112:HIS:CE1	14:1N:164:ILE:HG21	2.50	0.46
14:1N:278:MET:O	14:1N:282:MET:HG3	2.16	0.46
14:1N:326:LEU:O	14:1N:330:ILE:HG12	2.15	0.46
23:1X:137:PRO:HB2	23:1X:140:PRO:HG3	1.98	0.46
25:1Z:89:GLU:OE1	30:1e:96:HIS:ND1	2.46	0.46
31:1f:5:GLN:O	31:1f:9:ASP:CB	2.60	0.46
45:3A:80:GLU:HG2	46:3B:284:HIS:HB2	1.97	0.46
45:3A:191:LYS:O	45:3A:195:MET:HG3	2.16	0.46
48:3D:121:TYR:HA	48:3D:125:CYS:SG	2.56	0.46
49:3E:201:ASP:HB2	49:3E:248:ARG:NH2	2.30	0.46
55:4A:470:PHE:CG	67:4M:19:LEU:HD13	2.50	0.46
56:4B:138:VAL:HG12	56:4B:140:ASN:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:8D:56:LYS:HB2	59:8E:104:LEU:HD21	1.98	0.46
63:8I:14:ALA:O	63:8I:18:ARG:HG2	2.15	0.46
66:8L:18:LYS:HZ3	67:8M:14:GLU:CD	2.10	0.46
3:1C:133:GLU:OE2	4:1D:430:ARG:NH2	2.49	0.46
5:1E:214:GLN:CD	5:1E:214:GLN:N	2.73	0.46
6:1F:133:ALA:HB1	6:1F:176:PHE:HE1	1.81	0.46
8:1H:312:ALA:HB3	25:1Z:55:ARG:HH21	1.80	0.46
10:1J:41:CYS:HA	10:1J:44:VAL:HG22	1.98	0.46
11:1K:76:SER:HA	11:1K:79:VAL:HG12	1.96	0.46
12:1L:205:ASN:O	12:1L:207:GLU:N	2.49	0.46
12:1L:291:CYS:O	12:1L:295:GLN:HG2	2.15	0.46
15:1O:310:GLU:HA	15:1O:314:ASP:HB2	1.96	0.46
17:1Q:11:ILE:O	22:1W:16:SER:OG	2.29	0.46
75:1X:201:CDL:H512	31:1f:26:LEU:HD21	1.96	0.46
28:1c:46:ASN:C	28:1c:46:ASN:OD1	2.57	0.46
30:1e:50:ARG:O	30:1e:54:GLU:HG3	2.15	0.46
39:1n:107:HIS:CD2	39:1n:108:PRO:HD2	2.50	0.46
43:1r:5:ARG:HA	43:1r:8:GLN:HB2	1.97	0.46
50:3F:79:ASP:OD1	50:3F:82:MET:CE	2.63	0.46
46:3O:306:PRO:HA	49:3V:52:ARG:HD3	1.96	0.46
47:3P:300:ILE:HA	47:3P:303:LEU:HD23	1.97	0.46
47:3P:310:SER:HB2	47:3P:370:SER:HB2	1.96	0.46
55:4A:96:ARG:HB3	57:4C:57:TRP:CZ2	2.49	0.46
55:4A:189:LEU:HD21	87:4A:603:PGV:H212	1.98	0.46
57:4C:43:LEU:HD21	87:4C:302:PGV:H262	1.97	0.46
58:4D:93:ALA:HB2	65:4K:29:TRP:CE2	2.50	0.46
55:8A:32:ALA:HB3	66:8L:36:PRO:HG2	1.97	0.46
58:8D:48:TRP:CZ3	59:8E:61:PHE:HD2	2.26	0.46
65:8K:42:LEU:HD11	87:8K:101:PGV:H012	1.96	0.46
8:1H:47:GLN:NE2	8:1H:51:ASP:OD1	2.48	0.46
8:1H:179:TRP:N	8:1H:180:PRO:HD2	2.31	0.46
9:1I:121:PHE:HA	9:1I:124:GLU:HG2	1.98	0.46
10:1J:23:LYS:HE2	11:1K:23:ARG:HG3	1.96	0.46
12:1L:207:GLU:C	12:1L:209:PRO:HD3	2.40	0.46
14:1N:172:GLN:HB2	14:1N:178:ILE:HG13	1.97	0.46
14:1N:266:ILE:O	14:1N:270:MET:HG3	2.16	0.46
14:1N:270:MET:CE	14:1N:282:MET:CE	2.90	0.46
15:1O:53:GLU:HG2	15:1O:104:ARG:HH12	1.80	0.46
20:1U:4:PRO:O	20:1U:4:PRO:CD	2.63	0.46
31:1f:1:MET:SD	31:1f:2:ASN:HB2	2.56	0.46
32:1g:63:PHE:O	32:1g:67:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:78:GLU:HG2	41:1p:79:LYS:HG2	1.96	0.46
47:3C:278:TYR:CZ	47:3C:282:ARG:HD3	2.50	0.46
49:3E:226:ALA:HA	49:3E:234:TYR:HD1	1.80	0.46
47:3P:24:PRO:HB2	47:3P:27:ILE:HG23	1.98	0.46
55:4A:251:PHE:HB3	55:4A:319:LYS:NZ	2.30	0.46
64:4J:52:TRP:O	64:4J:57:HIS:ND1	2.48	0.46
55:8A:62:ALA:O	55:8A:66:ILE:HG22	2.16	0.46
57:8C:6:HIS:CD2	57:8C:8:TYR:CD2	3.02	0.46
57:8C:121:ILE:HG21	57:8C:193:TYR:CD2	2.50	0.46
59:8E:24:ILE:CG2	59:8E:57:ARG:HH12	2.29	0.46
64:8J:29:ASN:O	64:8J:33:ARG:HG2	2.16	0.46
67:8M:32:TRP:CE3	67:8M:36:HIS:CE1	3.03	0.46
68:8N:17:PRO:HA	68:8N:20:VAL:HG23	1.96	0.46
1:1A:85:LYS:HG3	1:1A:86:THR:N	2.31	0.46
4:1D:141:PHE:O	4:1D:145:THR:OG1	2.34	0.46
6:1F:301:GLY:H	6:1F:333:ALA:HB3	1.80	0.46
7:1G:281:GLN:HG2	7:1G:592:LEU:HD12	1.98	0.46
8:1H:312:ALA:HA	27:1b:41:ALA:HB2	1.96	0.46
9:1I:81:LYS:HE2	9:1I:94:ILE:HG22	1.98	0.46
12:1L:136:ASN:OD1	12:1L:139:GLN:HB2	2.15	0.46
13:1M:91:ARG:HH22	15:1O:290:ASP:CG	2.24	0.46
13:1M:186:LEU:HD23	13:1M:253:LEU:HD22	1.96	0.46
69:1M:502:3PE:H3E2	75:1X:201:CDL:H442	1.98	0.46
69:1M:504:3PE:H3B1	14:1N:245:MET:HE1	1.97	0.46
14:1N:187:MET:HA	14:1N:190:MET:HE3	1.98	0.46
14:1N:270:MET:CE	14:1N:282:MET:HE2	2.39	0.46
20:1U:73:PRO:O	20:1U:77:VAL:HG13	2.16	0.46
22:1W:70:ASN:N	22:1W:70:ASN:ND2	2.63	0.46
40:1o:2:ALA:O	40:1o:6:ARG:HG3	2.14	0.46
49:3E:159:ILE:HD11	49:3E:167:PHE:HE2	1.80	0.46
49:3R:265:PHE:O	49:3R:265:PHE:CG	2.69	0.46
55:4A:275:TRP:HE3	87:4A:603:PGV:H12	1.80	0.46
87:8A:602:PGV:H301	67:8M:19:LEU:HD12	1.98	0.46
57:8C:148:HIS:CE1	57:8C:152:MET:HE2	2.47	0.46
58:8D:59:LEU:HA	58:8D:59:LEU:HD23	1.64	0.46
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.98	0.46
7:1G:469:ALA:O	7:1G:473:ILE:HG13	2.15	0.46
12:1L:144:TRP:CE2	12:1L:223:LYS:HG3	2.51	0.46
13:1M:243:MET:HB3	13:1M:301:ILE:HG21	1.98	0.46
14:1N:26:TRP:CH2	14:1N:86:ILE:HD12	2.51	0.46
15:1O:49:ARG:HB3	15:1O:122:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:134:PHE:O	15:1O:138:MET:HG3	2.15	0.46
15:1O:287:HIS:HB2	32:1g:28:GLU:OE1	2.15	0.46
17:1Q:70:MET:SD	42:1q:126:PRO:HB2	2.56	0.46
25:1Z:122:GLY:C	30:1e:75:LEU:HD11	2.41	0.46
29:1d:108:THR:HA	41:1p:77:GLU:HA	1.97	0.46
33:1h:108:LEU:HD23	33:1h:108:LEU:HA	1.81	0.46
40:1o:83:GLN:NE2	40:1o:87:ASP:OD1	2.49	0.46
41:1p:35:ILE:O	41:1p:39:LEU:HG	2.16	0.46
47:3C:377:LEU:HG	50:3F:32:TYR:HE2	1.81	0.46
51:3G:40:LEU:O	51:3G:44:ARG:HG3	2.16	0.46
50:3S:75:LEU:O	50:3S:80:TRP:NE1	2.39	0.46
55:4A:211:THR:HG22	55:4A:215:LEU:HD22	1.98	0.46
56:4B:82:ARG:HA	56:4B:82:ARG:HD3	1.82	0.46
56:8B:100:MET:HE1	56:8B:156:SER:C	2.41	0.46
64:8J:28:ASP:HA	64:8J:31:LEU:HD12	1.97	0.46
4:1D:78:PRO:HG3	4:1D:402:LEU:HD23	1.98	0.46
4:1D:116:GLN:NE2	4:1D:276:ASP:OD2	2.42	0.46
7:1G:611:LEU:HD13	7:1G:613:TYR:OH	2.15	0.46
11:1K:8:ILE:HG21	11:1K:43:MET:HB2	1.97	0.46
15:1O:18:LEU:HD21	15:1O:256:PHE:CE2	2.50	0.46
20:1U:17:TYR:O	20:1U:20:LYS:HG2	2.15	0.46
32:1g:55:LEU:HD21	32:1g:59:ARG:NH1	2.31	0.46
34:1i:13:GLN:HE22	39:1n:156:ALA:HB3	1.81	0.46
34:1i:78:VAL:HG22	41:1p:40:VAL:HG11	1.98	0.46
36:1k:61:SER:OG	36:1k:62:PHE:N	2.49	0.46
38:1m:82:THR:HG23	38:1m:84:LYS:H	1.81	0.46
39:1n:30:CYS:O	39:1n:32:HIS:N	2.48	0.46
47:3C:29:SER:HA	47:3C:32:ASN:HD22	1.81	0.46
47:3C:361:ILE:HG12	47:3C:365:LEU:HD12	1.97	0.46
48:3D:102:HIS:O	48:3D:291:LYS:NZ	2.49	0.46
49:3E:174:LEU:HD13	49:3E:214:ILE:HD13	1.96	0.46
45:3N:356:ARG:O	45:3N:360:ILE:HG13	2.15	0.46
69:3N:501:3PE:H31	75:3N:502:CDL:H512	1.98	0.46
48:3Q:33:TYR:CD1	48:3Q:37:CYS:HB2	2.51	0.46
49:3R:145:ASP:O	49:3R:149:MET:HB2	2.16	0.46
52:3U:22:GLU:O	52:3U:26:GLN:HG2	2.16	0.46
55:4A:35:LEU:HG	55:4A:462:LEU:HD22	1.98	0.46
55:4A:239:GLY:O	55:4A:243:VAL:HG23	2.16	0.46
55:4A:469:ILE:CD1	67:4M:26:PHE:CE1	2.98	0.46
57:4C:122:HIS:CE1	61:4G:45:PRO:HB3	2.50	0.46
75:4C:305:CDL:H512	75:4C:305:CDL:HB4	1.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:4E:78:HIS:CD2	59:4E:78:HIS:N	2.83	0.46
87:4M:101:PGV:H81	87:4M:101:PGV:H242	1.97	0.46
55:8A:155:VAL:O	55:8A:159:LEU:CD1	2.54	0.46
56:8B:11:ASP:HB2	58:8D:129:ALA:HA	1.97	0.46
56:8B:37:LEU:O	56:8B:41:ILE:HG13	2.15	0.46
57:8C:72:THR:O	57:8C:76:GLN:HG3	2.16	0.46
57:8C:221:ARG:HB3	57:8C:226:HIS:HB2	1.97	0.46
1:1A:37:TYR:HB2	2:1B:81:ARG:NH1	2.30	0.46
4:1D:352:TYR:HD1	9:1I:86:VAL:HG21	1.81	0.46
6:1F:208:PRO:HG2	6:1F:213:VAL:HG22	1.98	0.46
7:1G:237:ASN:HB3	7:1G:253:ARG:HE	1.79	0.46
8:1H:257:ILE:HG13	26:1a:17:PHE:HE2	1.81	0.46
10:1J:170:GLU:OE2	10:1J:173:ARG:NH2	2.49	0.46
13:1M:367:LEU:HD12	13:1M:407:SER:HB2	1.96	0.46
21:1V:54:LYS:O	21:1V:58:VAL:HG23	2.16	0.46
32:1g:80:LEU:HA	32:1g:80:LEU:HD23	1.79	0.46
75:1h:202:CDL:H712	75:1h:202:CDL:HB62	1.52	0.46
69:3A:502:3PE:H32	69:3A:502:3PE:H322	1.66	0.46
48:3D:314:HIS:NE2	51:3G:22:PRO:HB2	2.31	0.46
49:3E:195:LEU:HD22	49:3E:250:ARG:HA	1.97	0.46
49:3E:207:LYS:HB3	49:3E:209:GLU:OE2	2.16	0.46
45:3N:284:TYR:CD2	49:3V:71:ASN:HA	2.50	0.46
75:4B:303:CDL:C32	63:4I:34:PHE:HE1	2.29	0.46
58:4D:112:GLU:O	58:4D:116:VAL:HG23	2.16	0.46
55:8A:128:VAL:O	55:8A:128:VAL:HG12	2.15	0.46
56:8B:165:VAL:HG11	56:8B:168:LEU:HD12	1.98	0.46
60:8F:62:CYS:HB3	60:8F:85:CYS:HB3	1.98	0.46
62:8H:41:LYS:HE3	62:8H:85:ILE:OXT	2.15	0.46
1:1A:1:FME:HA	1:1A:1:FME:HE3	1.97	0.46
6:1F:96:ASN:O	6:1F:225:VAL:HG23	2.16	0.46
7:1G:596:ASP:OD1	7:1G:596:ASP:N	2.48	0.46
8:1H:296:LEU:HD13	70:1H:402:PC1:H351	1.98	0.46
10:1J:99:MET:SD	10:1J:103:MET:HG2	2.56	0.46
12:1L:137:LEU:HD12	12:1L:137:LEU:HA	1.75	0.46
13:1M:59:ASP:OD2	13:1M:245:ARG:NH1	2.42	0.46
13:1M:203:PHE:HB2	13:1M:243:MET:HG3	1.98	0.46
15:1O:129:TYR:CE2	15:1O:166:PRO:HD3	2.51	0.46
17:1Q:16:LYS:HA	17:1Q:16:LYS:HD2	1.80	0.46
20:1T:25:ILE:HD11	20:1T:42:LEU:HD11	1.98	0.46
24:1Y:13:GLU:HA	24:1Y:20:LYS:NZ	2.30	0.46
38:1m:82:THR:HG23	38:1m:84:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1s:40:ASN:O	44:1s:43:HIS:ND1	2.39	0.46
45:3A:117:VAL:HG23	45:3A:118:GLN:HG3	1.98	0.46
46:3B:163:LEU:HD11	46:3B:258:VAL:HG22	1.97	0.46
45:3N:87:ASN:ND2	45:3N:98:TYR:OH	2.34	0.46
45:3N:145:MET:SD	45:3N:248:LEU:HD13	2.56	0.46
75:3P:504:CDL:H312	75:3T:101:CDL:H731	1.98	0.46
48:3Q:230:LEU:O	48:3Q:233:ARG:HG2	2.16	0.46
49:3R:179:ARG:HB2	49:3R:183:GLU:HB2	1.98	0.46
54:3X:48:ILE:O	54:3X:51:LYS:HG2	2.16	0.46
55:4A:71:MET:HB2	55:4A:72:PRO:HD3	1.97	0.46
55:4A:361:SER:HB3	56:4B:84:LEU:HD22	1.98	0.46
55:4A:478:SER:OG	55:4A:480:ARG:NH2	2.49	0.46
64:4J:40:LEU:HD12	87:4J:101:PGV:H142	1.98	0.46
55:8A:3:VAL:HG11	87:8A:601:PGV:H02	1.98	0.46
55:8A:346:PHE:HD2	55:8A:347:LEU:HD13	1.80	0.46
57:8C:182:TYR:HD2	87:8C:305:PGV:O11	1.99	0.46
57:8C:217:VAL:O	57:8C:221:ARG:HG3	2.15	0.46
60:8F:76:LYS:HG3	60:8F:91:LEU:HD23	1.97	0.46
2:1B:48:MET:CE	2:1B:80:PRO:HB3	2.46	0.45
3:1C:204:GLU:OE2	3:1C:210:ARG:NE	2.49	0.45
4:1D:143:GLU:HG3	4:1D:310:ILE:HB	1.98	0.45
4:1D:171:PHE:HA	4:1D:174:ARG:HB2	1.98	0.45
12:1L:419:THR:HA	12:1L:422:TYR:CZ	2.51	0.45
19:1S:24:GLN:NE2	19:1S:56:GLU:HG3	2.29	0.45
22:1W:64:ARG:O	22:1W:68:MET:HG2	2.16	0.45
30:1e:31:ARG:NH2	30:1e:66:LEU:O	2.49	0.45
75:1h:202:CDL:H511	75:1h:202:CDL:HB4	1.56	0.45
34:1i:9:LEU:O	34:1i:13:GLN:HG3	2.16	0.45
34:1i:31:GLU:HG2	39:1n:115:PRO:HD2	1.97	0.45
37:1l:7:ASP:OD1	37:1l:8:MET:N	2.49	0.45
37:1l:34:TYR:OH	37:1l:46:ASP:O	2.24	0.45
37:1l:136:ASN:ND2	37:1l:150:PRO:HG2	2.30	0.45
46:3B:46:ARG:HG2	46:3B:379:LEU:HD22	1.99	0.45
48:3D:121:TYR:CD1	48:3D:125:CYS:HB2	2.51	0.45
46:3O:257:LEU:HD11	46:3O:422:LYS:HB3	1.99	0.45
48:3Q:3:LEU:HD23	48:3Q:3:LEU:H	1.81	0.45
56:4B:100:MET:HE1	56:4B:155:SER:OG	2.16	0.45
56:4B:145:PRO:HA	56:4B:214:VAL:O	2.17	0.45
66:4L:42:HIS:NE2	66:4L:46:LYS:HD3	2.31	0.45
55:8A:462:LEU:O	55:8A:465:VAL:HG12	2.15	0.45
56:8B:28:LEU:HG	63:8I:35:TYR:CE2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:8C:306:CDL:H371	75:8C:306:CDL:H251	1.98	0.45
58:8D:78:TRP:CE2	58:8D:79:LYS:HG2	2.51	0.45
5:1E:6:LEU:HD21	18:1R:76:ASP:OD2	2.16	0.45
6:1F:121:GLY:HA2	6:1F:124:VAL:HG22	1.98	0.45
9:1I:175:TYR:CZ	43:1r:38:PRO:HG3	2.50	0.45
12:1L:36:VAL:HG21	12:1L:118:PHE:HB3	1.97	0.45
13:1M:453:MET:HE1	32:1g:80:LEU:CD1	2.36	0.45
14:1N:95:MET:CE	14:1N:149:ILE:HG23	2.46	0.45
19:1S:34:ASP:O	19:1S:38:LYS:HG2	2.16	0.45
20:1T:69:LYS:O	20:1T:71:MET:HG2	2.17	0.45
20:1U:68:GLU:C	20:1U:68:GLU:OE1	2.59	0.45
23:1X:131:LYS:HD2	23:1X:131:LYS:HA	1.76	0.45
37:1l:134:PRO:HD3	40:1o:56:ASP:HA	1.97	0.45
46:3B:56:ARG:NH1	46:3B:103:GLU:OE2	2.48	0.45
46:3B:227:ARG:HG3	46:3B:229:GLY:N	2.29	0.45
48:3D:226:PRO:HG3	52:3H:84:LEU:HD22	1.97	0.45
49:3E:130:LYS:NZ	54:3Y:34:TRP:O	2.46	0.45
45:3N:224:VAL:HG13	45:3N:225:GLU:CD	2.40	0.45
49:3R:172:LYS:HB2	49:3R:214:ILE:HD12	1.99	0.45
55:4A:266:GLU:HB3	60:4F:68:THR:HG21	1.98	0.45
56:4B:110:TYR:CE2	56:4B:222:TRP:HH2	2.34	0.45
55:8A:165:ILE:HG23	55:8A:169:ILE:HD11	1.97	0.45
56:8B:188:ARG:HG3	56:8B:188:ARG:HH11	1.81	0.45
58:8D:48:TRP:CZ3	59:8E:61:PHE:CG	2.99	0.45
58:8D:82:VAL:O	58:8D:86:LEU:HG	2.16	0.45
58:8D:89:ILE:HD12	58:8D:89:ILE:H	1.81	0.45
58:8D:144:GLU:HG2	58:8D:145:TRP:O	2.16	0.45
68:8N:50:ASN:OD1	68:8N:50:ASN:C	2.59	0.45
12:1L:13:ILE:N	12:1L:13:ILE:HD13	2.32	0.45
12:1L:362:LEU:HA	12:1L:365:ALA:HB3	1.98	0.45
12:1L:435:PRO:HB3	12:1L:437:PHE:CZ	2.51	0.45
69:1M:502:3PE:H111	15:1O:304:TYR:HE1	1.81	0.45
69:1M:502:3PE:H2G2	69:1M:504:3PE:H3G2	1.98	0.45
14:1N:122:ILE:HD12	14:1N:126:ALA:CB	2.46	0.45
21:1V:75:GLN:O	21:1V:79:VAL:HG23	2.17	0.45
39:1n:97:LYS:HD2	39:1n:173:PRO:HB2	1.98	0.45
40:1o:62:LEU:HD23	40:1o:66:LEU:HD13	1.97	0.45
45:3N:244:ARG:NH1	51:3T:10:MET:HE3	2.31	0.45
55:4A:119:GLU:CD	55:4A:141:ALA:H	2.24	0.45
56:4B:105:TYR:HE2	56:4B:119:ASP:OD1	1.99	0.45
75:4B:303:CDL:H861	75:4B:303:CDL:H202	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:4D:122:ARG:HG3	65:4K:53:TRP:CE2	2.52	0.45
56:8B:98:LYS:HB2	56:8B:98:LYS:HE3	1.67	0.45
57:8C:130:PRO:HB2	57:8C:253:TYR:CE1	2.51	0.45
1:1A:49:LEU:H	8:1H:126:LYS:HE2	1.81	0.45
5:1E:51:LEU:HD22	5:1E:61:LEU:HD11	1.98	0.45
5:1E:168:ASP:HB3	5:1E:187:ARG:HG2	1.98	0.45
6:1F:92:TYR:HB2	6:1F:220:THR:HG22	1.97	0.45
8:1H:31:MET:HG3	9:1I:41:LEU:HB2	1.97	0.45
12:1L:97:THR:O	12:1L:101:MET:HG3	2.15	0.45
13:1M:30:HIS:CD2	31:1f:16:VAL:HB	2.52	0.45
13:1M:126:LEU:HD21	13:1M:153:THR:OG1	2.16	0.45
13:1M:187:SER:O	13:1M:192:ASN:ND2	2.44	0.45
15:1O:308:TYR:CE1	15:1O:320:LYS:HG2	2.51	0.45
16:1P:244:TYR:O	16:1P:248:VAL:HG23	2.15	0.45
20:1T:37:MET:HE1	20:1T:71:MET:CE	2.47	0.45
25:1Z:59:ARG:CA	25:1Z:62:ILE:HG22	2.47	0.45
44:1s:46:TYR:CD2	44:1s:50:THR:HG21	2.51	0.45
46:3B:97:SER:HA	49:3I:69:GLY:HA2	1.99	0.45
49:3R:173:PRO:O	49:3R:215:GLY:N	2.40	0.45
55:4A:229:ILE:HD11	56:4B:175:ILE:HD12	1.98	0.45
75:4D:201:CDL:H171	75:4D:201:CDL:H721	1.97	0.45
63:4I:21:ILE:CG2	63:4I:25:PHE:CE2	3.00	0.45
55:8A:279:SER:HB3	68:8N:22:ILE:HG12	1.99	0.45
62:8H:6:THR:HA	62:8H:9:LYS:HZ2	1.78	0.45
62:8H:17:ASP:OD1	62:8H:18:SER:N	2.50	0.45
62:8H:75:ARG:HG3	62:8H:75:ARG:NH1	2.32	0.45
7:1G:215:PHE:HD1	9:1I:104:ARG:HH11	1.63	0.45
7:1G:427:LYS:HA	7:1G:427:LYS:HD2	1.81	0.45
8:1H:173:TRP:HB3	8:1H:175:ILE:HG22	1.98	0.45
13:1M:76:MET:SD	13:1M:230:VAL:HB	2.57	0.45
17:1Q:27:GLU:CD	17:1Q:28:GLU:OE1	2.60	0.45
19:1S:43:LEU:HD12	19:1S:43:LEU:C	2.42	0.45
19:1S:44:LYS:HE2	19:1S:52:ILE:HD13	1.97	0.45
20:1T:35:HIS:ND1	20:1T:38:LYS:HE3	2.32	0.45
20:1U:18:VAL:O	20:1U:21:LEU:HB2	2.16	0.45
75:1X:201:CDL:H612	75:1X:201:CDL:H241	1.97	0.45
24:1Y:105:ARG:NE	24:1Y:105:ARG:HA	2.31	0.45
24:1Y:124:VAL:HA	69:1Y:204:3PE:H222	1.98	0.45
27:1b:68:HIS:CD2	27:1b:70:GLN:HB2	2.52	0.45
32:1g:73:GLY:O	32:1g:77:VAL:HG23	2.17	0.45
35:1j:38:TRP:CZ3	35:1j:42:HIS:CE1	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1r:24:GLN:H	43:1r:24:GLN:HG2	1.62	0.45
45:3A:155:ALA:HA	45:3A:164:ALA:HB1	1.99	0.45
49:3E:155:LYS:HZ1	49:3E:176:VAL:HG21	1.80	0.45
49:3R:149:MET:HA	49:3R:149:MET:HE2	1.99	0.45
55:4A:25:TRP:HB2	87:4L:101:PGV:H281	1.97	0.45
57:4C:91:VAL:O	57:4C:95:THR:HG23	2.16	0.45
58:4D:84:THR:HG21	87:4M:101:PGV:H71	1.98	0.45
58:4D:134:PHE:HE1	65:4K:44:PRO:HD2	1.82	0.45
61:4G:47:PHE:CE1	61:4G:81:GLY:HA2	2.50	0.45
55:8A:118:VAL:HA	64:8J:54:SER:HA	1.99	0.45
75:8B:303:CDL:HA61	75:8B:303:CDL:H311	1.74	0.45
58:8D:111:PHE:HE2	65:8K:41:ASN:HB2	1.82	0.45
87:8K:101:PGV:H62	87:8K:101:PGV:H21	1.99	0.45
68:8N:81:ASP:N	68:8N:81:ASP:OD1	2.50	0.45
70:1A:202:PC1:H222	70:1A:202:PC1:H261	1.97	0.45
70:1B:203:PC1:H321	8:1H:46:LEU:HD13	1.98	0.45
4:1D:334:LYS:HB2	4:1D:337:GLU:CD	2.41	0.45
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.37	0.45
6:1F:21:ILE:CG2	6:1F:117:LYS:NZ	2.80	0.45
6:1F:257:ASN:OD1	6:1F:267:THR:OG1	2.16	0.45
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.57	0.45
8:1H:55:LEU:HD13	8:1H:221:ALA:HB2	1.98	0.45
12:1L:19:ILE:HD12	12:1L:123:LEU:HG	1.98	0.45
13:1M:159:PRO:HB3	69:1M:501:3PE:H2A1	1.99	0.45
69:1M:501:3PE:O12	69:1M:501:3PE:N	2.35	0.45
14:1N:230:LEU:HD21	14:1N:244:MET:SD	2.56	0.45
16:1P:275:PHE:HE2	70:1P:401:PC1:C21	2.29	0.45
17:1Q:23:THR:HG23	17:1Q:25:VAL:HG13	1.99	0.45
28:1c:6:GLU:OE1	28:1c:7:PRO:HD2	2.16	0.45
36:1k:33:GLU:OE1	36:1k:33:GLU:HA	2.17	0.45
39:1n:12:GLN:NE2	39:1n:13:GLN:HG3	2.30	0.45
39:1n:58:LYS:O	39:1n:62:LEU:HG	2.17	0.45
48:3D:185:ASN:HD21	48:3Q:78:GLY:HA2	1.81	0.45
49:3E:199:GLN:O	49:3E:248:ARG:HD3	2.17	0.45
49:3V:65:VAL:HG22	49:3V:77:ARG:C	2.41	0.45
54:3Y:14:ALA:O	54:3Y:18:ILE:HG12	2.17	0.45
55:4A:131:PRO:HD3	56:4B:160:LEU:HD13	1.98	0.45
55:4A:440:TYR:OH	56:4B:195:GLN:HB3	2.15	0.45
56:4B:49:LYS:HE3	59:4E:76:GLY:HA2	1.98	0.45
57:4C:33:MET:HE1	64:4J:49:CYS:O	2.16	0.45
59:4E:96:LEU:HB3	59:4E:98:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:4F:50:PRO:O	60:4F:56:ARG:NH1	2.40	0.45
67:4M:37:LEU:HA	67:4M:40:TYR:HB2	1.98	0.45
55:8A:1:FME:SD	87:8A:601:PGV:H211	2.57	0.45
55:8A:221:ASP:C	55:8A:221:ASP:OD1	2.59	0.45
55:8A:282:PHE:HA	87:8A:603:PGV:H292	1.98	0.45
56:8B:23:PHE:CZ	56:8B:80:SER:HB2	2.51	0.45
56:8B:28:LEU:HD12	56:8B:28:LEU:O	2.16	0.45
57:8C:31:LEU:HD12	87:8C:301:PGV:H181	1.98	0.45
57:8C:182:TYR:CD2	87:8C:305:PGV:O11	2.69	0.45
58:8D:77:GLU:C	58:8D:81:ILE:CD1	2.88	0.45
58:8D:77:GLU:CG	58:8D:81:ILE:HD11	2.44	0.45
62:8H:33:TYR:HD1	62:8H:60:TYR:CD2	2.35	0.45
3:1C:45:PHE:HD1	3:1C:47:GLU:HG3	1.81	0.45
3:1C:51:PHE:HB3	21:1V:111:TRP:CE2	2.52	0.45
4:1D:62:LEU:HB2	4:1D:425:PHE:CZ	2.51	0.45
10:1J:7:PHE:CD1	11:1K:3:LEU:HD13	2.51	0.45
12:1L:49:VAL:HB	12:1L:50:PRO:HD3	1.99	0.45
13:1M:71:TRP:CH2	13:1M:439:LEU:HD22	2.51	0.45
69:1M:504:3PE:H2H2	14:1N:256:PRO:HG2	1.97	0.45
16:1P:192:PRO:HB3	16:1P:256:TYR:CZ	2.52	0.45
19:1S:33:ARG:O	19:1S:37:GLU:OE2	2.35	0.45
23:1X:20:SER:HB3	26:1a:51:ASP:OD1	2.17	0.45
23:1X:21:SER:OG	26:1a:51:ASP:OD2	2.28	0.45
38:1m:82:THR:CG2	38:1m:85:THR:H	2.29	0.45
39:1n:142:GLU:OE2	39:1n:157:ARG:NH1	2.49	0.45
41:1p:73:ILE:HG23	41:1p:155:LEU:HD22	1.99	0.45
46:3B:51:ILE:HG23	46:3B:204:MET:HG2	1.99	0.45
51:3G:73:ARG:HA	52:3H:82:GLU:OE1	2.16	0.45
45:3N:106:LEU:HD22	45:3N:203:VAL:HG12	1.98	0.45
46:3O:223:PHE:O	46:3O:226:MET:HE2	2.17	0.45
48:3Q:11:PRO:HG2	52:3U:74:PHE:HB2	1.97	0.45
55:4A:192:ALA:HA	55:4A:195:LEU:HD12	1.99	0.45
57:4C:221:ARG:NH1	87:4C:306:PGV:O13	2.49	0.45
55:8A:151:HIS:CD2	55:8A:206:ILE:CD1	3.00	0.45
55:8A:462:LEU:O	55:8A:462:LEU:HD12	2.17	0.45
56:8B:26:HIS:HA	56:8B:29:MET:SD	2.56	0.45
68:8N:32:TYR:CZ	68:8N:36:LEU:HD21	2.51	0.45
3:1C:148:LEU:O	22:1W:88:MET:HE2	2.17	0.45
4:1D:326:ASP:HB2	43:1r:44:PRO:HD2	1.97	0.45
4:1D:350:LYS:HD2	7:1G:117:GLN:HB3	1.99	0.45
7:1G:338:VAL:HG13	7:1G:609:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:66:TRP:HB2	69:1L:703:3PE:H351	1.97	0.45
14:1N:315:TRP:HZ3	15:1O:292:VAL:HG12	1.82	0.45
24:1Y:14:GLY:O	24:1Y:78:GLN:HG2	2.17	0.45
46:3B:276:GLN:HB2	46:3B:322:PHE:HE1	1.82	0.45
48:3D:314:HIS:CD2	51:3G:22:PRO:HB2	2.51	0.45
46:3O:51:ILE:HG23	46:3O:204:MET:HG3	1.99	0.45
49:3R:149:MET:O	49:3R:151:LYS:N	2.50	0.45
53:3W:52:TRP:O	53:3W:56:LYS:HB2	2.16	0.45
55:4A:283:LEU:HD11	68:4N:22:ILE:HD12	1.99	0.45
56:4B:161:HIS:CE1	56:4B:200:CYS:HB2	2.52	0.45
57:4C:45:LEU:CD1	64:4J:38:LEU:HD22	2.39	0.45
87:4C:301:PGV:H132	87:4C:301:PGV:H322	1.99	0.45
62:4H:30:TRP:CE2	62:4H:34:LEU:HD11	2.52	0.45
55:8A:276:ALA:O	55:8A:280:ILE:HG12	2.17	0.45
55:8A:316:THR:HG21	88:8A:605:HEA:H131	1.98	0.45
55:8A:512:ASN:HD21	60:8F:38:ALA:HA	1.81	0.45
57:8C:50:ASN:OD1	57:8C:50:ASN:C	2.60	0.45
57:8C:86:PHE:O	57:8C:89:SER:OG	2.28	0.45
75:8C:306:CDL:HB4	75:8C:306:CDL:H512	1.42	0.45
58:8D:53:MET:N	58:8D:53:MET:SD	2.89	0.45
60:8F:42:THR:OG1	60:8F:43:LYS:N	2.49	0.45
4:1D:147:LEU:HD22	4:1D:218:PHE:HE2	1.82	0.45
9:1I:17:VAL:HG21	27:1b:9:LYS:HE3	1.98	0.45
10:1J:86:ASN:HD21	10:1J:88:THR:HB	1.82	0.45
12:1L:207:GLU:HG2	12:1L:269:THR:HG21	1.98	0.45
13:1M:311:GLY:HA2	13:1M:377:GLY:HA2	1.99	0.45
15:1O:140:ARG:HB2	15:1O:201:ASP:OD2	2.16	0.45
40:1o:61:TYR:HA	40:1o:64:GLN:HG2	1.98	0.45
41:1p:7:ASP:OD1	41:1p:7:ASP:N	2.50	0.45
45:3A:140:GLU:HG2	49:3I:48:SER:O	2.17	0.45
45:3A:172:GLU:C	45:3A:172:GLU:CD	2.85	0.45
47:3C:111:GLU:H	47:3C:111:GLU:CD	2.25	0.45
49:3E:110:ARG:HD2	51:3G:23:PHE:O	2.17	0.45
52:3H:52:ILE:O	52:3H:56:ILE:HG12	2.17	0.45
49:3V:55:LEU:O	49:3V:58:GLN:HB2	2.17	0.45
55:4A:32:ALA:HB3	66:4L:36:PRO:HG2	1.99	0.45
55:4A:354:THR:HG22	55:4A:376:HIS:HB2	1.99	0.45
55:8A:229:ILE:HD11	56:8B:175:ILE:HD12	1.98	0.45
55:8A:283:LEU:O	55:8A:287:VAL:HG22	2.16	0.45
55:8A:367:LEU:HD23	55:8A:367:LEU:HA	1.76	0.45
57:8C:91:VAL:O	57:8C:95:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8C:240:TRP:CZ2	75:8C:306:CDL:H721	2.52	0.45
58:8D:33:LEU:HB3	58:8D:38:LYS:HG3	1.98	0.45
58:8D:86:LEU:HA	58:8D:89:ILE:HD13	1.97	0.45
67:8M:39:HIS:HA	67:8M:42:ARG:HE	1.82	0.45
2:1B:77:ARG:HG3	2:1B:78:ALA:H	1.82	0.45
3:1C:51:PHE:CE2	3:1C:108:LYS:HD3	2.52	0.45
4:1D:335:ARG:NH2	9:1I:129:ASP:OD1	2.50	0.45
5:1E:67:ASN:OD1	5:1E:81:TYR:OH	2.25	0.45
5:1E:206:PRO:HB3	6:1F:23:THR:HB	1.99	0.45
6:1F:68:ARG:HD2	6:1F:254:LYS:HG3	1.99	0.45
7:1G:13:VAL:HB	7:1G:33:VAL:HG21	1.98	0.45
12:1L:400:ASN:HB3	12:1L:486:MET:HE3	1.99	0.45
13:1M:207:MET:O	13:1M:294:MET:HG3	2.16	0.45
13:1M:227:GLY:O	13:1M:231:LEU:HD12	2.17	0.45
16:1P:157:ARG:HD3	16:1P:157:ARG:HA	1.80	0.45
20:1T:6:LEU:O	20:1T:86:VAL:HG11	2.17	0.45
22:1W:22:SER:N	22:1W:80:ASP:OD2	2.50	0.45
23:1X:129:LYS:HD3	27:1b:65:VAL:HG13	1.98	0.45
33:1h:56:PRO:HD3	41:1p:63:TYR:CE2	2.51	0.45
38:1m:43:LYS:HD3	38:1m:47:LEU:HG	1.98	0.45
45:3N:41:ILE:HG12	45:3N:195:MET:HG2	1.98	0.45
46:3O:370:MET:HA	46:3O:373:GLU:HG3	1.99	0.45
49:3R:136:PHE:O	49:3R:139:SER:OG	2.27	0.45
55:4A:22:PHE:HE1	55:4A:109:PHE:HD2	1.65	0.45
56:4B:123:ILE:HD11	56:4B:139:ASP:HB3	1.98	0.45
57:4C:27:MET:CE	57:4C:50:ASN:ND2	2.80	0.45
58:4D:63:LYS:CG	58:4D:64:PHE:CE1	2.98	0.45
59:4E:41:LEU:C	59:4E:41:LEU:CD1	2.90	0.45
62:4H:27:ARG:NH1	68:4N:54:TRP:CZ3	2.85	0.45
65:4K:9:PHE:HA	65:4K:12:LYS:HE3	1.97	0.45
87:8C:304:PGV:H171	75:8C:306:CDL:H872	1.99	0.45
58:8D:80:THR:HG21	65:8K:10:HIS:ND1	2.32	0.45
58:8D:97:ILE:HG22	65:8K:36:ILE:CD1	2.38	0.45
59:8E:43:PRO:CB	59:8E:48:ILE:HD11	2.46	0.45
66:8L:36:PRO:HA	66:8L:39:ILE:CD1	2.47	0.45
1:1A:30:TYR:OH	2:1B:111:ARG:NH2	2.49	0.44
8:1H:287:HIS:O	8:1H:291:LYS:HB2	2.17	0.44
11:1K:70:GLU:HG2	14:1N:60:PHE:HE1	1.82	0.44
13:1M:197:LEU:HB3	69:1M:501:3PE:H2D1	1.97	0.44
14:1N:287:LEU:HB3	69:1N:901:3PE:H291	1.97	0.44
15:1O:135:LEU:HD13	15:1O:152:TYR:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1R:19:ASP:OD1	18:1R:19:ASP:N	2.50	0.44
28:1c:41:GLU:HA	28:1c:41:GLU:OE1	2.16	0.44
34:1i:79:TRP:HE1	41:1p:40:VAL:HA	1.81	0.44
42:1q:17:HIS:CD2	42:1q:26:VAL:HG21	2.53	0.44
45:3A:244:ARG:NH2	45:3A:429:GLU:OE1	2.50	0.44
46:3B:340:ALA:O	46:3B:344:VAL:HG23	2.17	0.44
51:3G:38:ASN:O	51:3G:42:ARG:HG3	2.17	0.44
47:3P:30:TRP:HB3	47:3P:100:ARG:HG3	1.99	0.44
49:3R:179:ARG:NH1	49:3R:246:SER:OG	2.50	0.44
53:3W:51:LEU:HB2	53:3W:54:HIS:ND1	2.32	0.44
58:4D:24:LEU:HD11	59:4E:67:ILE:HG22	1.99	0.44
61:4G:72:ASN:OD1	61:4G:75:VAL:HG12	2.17	0.44
57:8C:59:ARG:O	57:8C:63:ARG:HG2	2.17	0.44
2:1B:90:GLY:HA2	71:1B:201:SF4:S2	2.57	0.44
3:1C:32:ILE:HG23	21:1V:43:TYR:HB2	1.99	0.44
4:1D:406:SER:HB2	4:1D:414:VAL:HG22	1.98	0.44
7:1G:43:HIS:NE2	7:1G:261:GLU:OE2	2.42	0.44
7:1G:575:ASN:ND2	7:1G:577:GLU:OE2	2.51	0.44
10:1J:99:MET:HE3	10:1J:100:GLU:H	1.81	0.44
11:1K:59:MET:HE2	14:1N:84:TRP:HH2	1.81	0.44
12:1L:375:ILE:HG12	35:1j:32:MET:SD	2.57	0.44
69:1M:504:3PE:H241	69:1M:504:3PE:H3C1	2.00	0.44
14:1N:197:ASN:OD1	14:1N:200:MET:HG2	2.17	0.44
16:1P:188:PHE:CG	69:1P:403:3PE:H3B2	2.52	0.44
21:1V:105:GLU:OE1	21:1V:106:PRO:HD2	2.17	0.44
25:1Z:98:MET:HE3	25:1Z:104:TRP:CZ2	2.52	0.44
26:1a:59:ARG:HE	26:1a:61:HIS:HE1	1.59	0.44
31:1f:53:GLU:HG2	31:1f:54:VAL:HG22	1.99	0.44
45:3A:431:LEU:HD12	45:3A:432:PRO:HD2	2.00	0.44
47:3C:181:PHE:HA	47:3C:184:ILE:HG22	1.99	0.44
50:3F:119:TRP:CZ2	46:3O:87:ARG:HB3	2.53	0.44
49:3R:164:ASN:HB3	49:3R:227:ASN:ND2	2.32	0.44
55:4A:5:ARG:NH2	66:4L:10:ASN:OD1	2.47	0.44
55:4A:22:PHE:CE1	55:4A:109:PHE:HD2	2.35	0.44
56:4B:218:TYR:HA	56:4B:221:LYS:HG2	1.98	0.44
57:4C:240:TRP:CZ2	75:4C:305:CDL:H721	2.52	0.44
58:4D:20:ARG:HD2	59:4E:73:ASP:OD2	2.16	0.44
58:4D:64:PHE:CD1	58:4D:64:PHE:N	2.85	0.44
59:4E:52:LEU:CD1	59:4E:98:ILE:CD1	2.94	0.44
68:4N:9:ALA:HB1	68:4N:16:ILE:HD13	1.99	0.44
55:8A:251:PHE:HB3	55:8A:319:LYS:HZ3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:345:ILE:O	55:8A:349:THR:OG1	2.26	0.44
55:8A:466:MET:HE2	67:8M:23:PHE:CD1	2.52	0.44
57:8C:171:VAL:O	57:8C:175:LEU:HG	2.17	0.44
59:8E:43:PRO:HB3	59:8E:47:ILE:HD11	1.98	0.44
66:8L:20:ARG:CZ	66:8L:24:MET:CE	2.93	0.44
9:1I:50:TYR:OH	9:1I:138:GLU:OE2	2.24	0.44
11:1K:94:ASN:ND2	12:1L:581:LYS:O	2.42	0.44
12:1L:264:TYR:CD2	12:1L:265:PRO:HD3	2.53	0.44
12:1L:331:MET:SD	12:1L:465:GLY:HA2	2.58	0.44
12:1L:600:THR:HB	12:1L:601:LEU:H	1.65	0.44
13:1M:30:HIS:HB3	31:1f:16:VAL:HG21	2.00	0.44
14:1N:281:LEU:O	14:1N:285:THR:OG1	2.28	0.44
42:1q:10:GLY:O	42:1q:14:VAL:HG23	2.18	0.44
42:1q:78:ASP:C	42:1q:78:ASP:OD1	2.60	0.44
48:3D:115:ARG:O	48:3D:119:GLN:HG3	2.16	0.44
48:3D:306:PRO:HB3	69:3G:101:3PE:H362	1.98	0.44
45:3N:371:GLY:C	45:3N:374:PRO:HD2	2.43	0.44
47:3P:234:PHE:CE2	75:3P:504:CDL:H141	2.53	0.44
48:3Q:143:LEU:HD23	48:3Q:147:LEU:HB3	2.00	0.44
49:3R:230:ASP:OD1	49:3R:231:PHE:N	2.48	0.44
60:4F:25:ARG:HG2	60:4F:25:ARG:NH1	2.31	0.44
64:4J:33:ARG:HH11	87:4J:101:PGV:H171	1.82	0.44
64:4J:36:MET:CB	87:4J:101:PGV:H182	2.47	0.44
68:4N:58:GLY:HA3	68:4N:61:ASP:OD1	2.17	0.44
55:8A:21:LEU:HD22	87:8L:101:PGV:H242	1.98	0.44
55:8A:168:ILE:HD13	55:8A:189:LEU:HB2	1.99	0.44
55:8A:229:ILE:HD13	56:8B:178:ARG:NH1	2.32	0.44
55:8A:343:GLY:O	55:8A:347:LEU:HD23	2.18	0.44
87:8A:602:PGV:H271	87:8A:602:PGV:H132	1.99	0.44
57:8C:248:VAL:O	57:8C:252:LEU:HG	2.17	0.44
61:8G:32:THR:OG1	87:8G:101:PGV:H302	2.17	0.44
64:8J:28:ASP:OD1	64:8J:28:ASP:C	2.60	0.44
4:1D:242:ILE:HD12	4:1D:413:ASP:OD2	2.18	0.44
6:1F:299:PRO:HG3	6:1F:327:THR:HG21	1.98	0.44
7:1G:7:ASN:OD1	7:1G:7:ASN:N	2.46	0.44
8:1H:228:TYR:HA	8:1H:231:ILE:HD12	1.99	0.44
11:1K:10:MET:HE2	11:1K:10:MET:HB2	1.90	0.44
12:1L:203:MET:HB2	41:1p:113:GLN:HG3	1.98	0.44
12:1L:575:ILE:HD13	14:1N:171:ASN:ND2	2.32	0.44
13:1M:74:PRO:HA	13:1M:77:LEU:HD12	1.99	0.44
69:1M:502:3PE:H362	29:1d:44:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:43:ASP:OD1	35:1j:43:ASP:C	2.60	0.44
35:1j:64:LEU:HD23	35:1j:64:LEU:HA	1.81	0.44
37:1l:12:PRO:O	37:1l:46:ASP:HB3	2.17	0.44
45:3A:248:LEU:HD12	45:3A:426:GLY:HA2	1.99	0.44
46:3B:179:PRO:O	46:3B:183:ILE:HG13	2.17	0.44
47:3C:168:PHE:HZ	49:3R:147:LEU:HD23	1.81	0.44
49:3I:53:GLU:HA	49:3I:56:ARG:NH1	2.32	0.44
47:3P:197:LEU:HD11	85:3P:502:HEM:HMA3	1.98	0.44
48:3Q:158:ILE:HG12	48:3Q:160:MET:HB2	1.99	0.44
49:3R:160:PRO:HD2	49:3R:163:LYS:HB3	1.99	0.44
57:4C:144:ILE:HD13	57:4C:239:ALA:HA	1.99	0.44
62:4H:4:ILE:HD11	68:4N:79:GLY:HA2	2.00	0.44
56:8B:32:PHE:CZ	75:8B:303:CDL:H132	2.52	0.44
58:8D:143:ASN:HB2	58:8D:144:GLU:OE1	2.17	0.44
61:8G:68:THR:HG22	61:8G:69:LEU:N	2.29	0.44
9:1I:44:GLU:OE1	81:1q:202:AYA:CT	2.66	0.44
9:1I:50:TYR:CD1	9:1I:51:PRO:HA	2.53	0.44
17:1Q:88:THR:OG1	17:1Q:91:ASP:OD2	2.30	0.44
31:1f:1:MET:SD	31:1f:1:MET:C	3.00	0.44
31:1f:29:ARG:HD3	31:1f:29:ARG:HA	1.60	0.44
34:1i:92:LYS:HG2	34:1i:93:PRO:HD2	2.00	0.44
45:3A:301:ARG:HB2	45:3A:303:LEU:HG	2.00	0.44
47:3C:318:ARG:O	47:3C:322:GLN:HG3	2.16	0.44
50:3F:79:ASP:OD1	50:3F:82:MET:HE1	2.18	0.44
52:3H:63:GLU:O	52:3H:67:GLN:HG3	2.18	0.44
52:3H:76:GLU:HA	52:3H:76:GLU:OE2	2.17	0.44
45:3N:270:LEU:HD22	45:3N:320:LEU:HD21	1.99	0.44
46:3O:28:ARG:NH2	46:3O:390:GLY:CA	2.79	0.44
92:4B:305:PSC:H21	92:4B:305:PSC:H02	1.58	0.44
57:4C:79:LEU:HB3	57:4C:233:PHE:CE2	2.52	0.44
59:4E:33:MET:CE	59:4E:67:ILE:HD12	2.47	0.44
57:8C:57:TRP:NE1	87:8C:301:PGV:O14	2.45	0.44
59:8E:61:PHE:HE1	59:8E:65:VAL:HG21	1.82	0.44
68:8N:40:ASN:OD1	68:8N:40:ASN:N	2.50	0.44
1:1A:55:PHE:HE1	8:1H:134:ARG:HD3	1.82	0.44
6:1F:423:ARG:N	6:1F:424:PRO:HD2	2.33	0.44
7:1G:366:THR:HB	7:1G:450:MET:HE2	1.99	0.44
12:1L:83:ASP:OD1	12:1L:83:ASP:C	2.59	0.44
13:1M:425:ASN:HB2	38:1m:57:GLY:HA2	2.00	0.44
14:1N:36:ASN:OD1	14:1N:134:GLN:NE2	2.50	0.44
14:1N:179:MET:HE3	14:1N:179:MET:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:193:VAL:HB	14:1N:266:ILE:HG23	2.00	0.44
16:1P:147:ARG:HH12	59:8E:9:GLU:N	2.02	0.44
24:1Y:91:ILE:HD13	24:1Y:91:ILE:HA	1.89	0.44
25:1Z:36:PHE:O	25:1Z:40:ILE:HG12	2.17	0.44
49:3E:155:LYS:O	49:3E:270:LEU:HA	2.18	0.44
49:3E:263:TYR:CD1	49:3E:271:VAL:HG12	2.52	0.44
51:3G:38:ASN:ND2	75:3G:103:CDL:OA3	2.36	0.44
45:3N:50:GLU:HG2	45:3N:51:LYS:HD3	2.00	0.44
48:3Q:8:PRO:HG3	52:3U:66:ASP:HB3	2.00	0.44
49:3R:222:CYS:HB3	49:3R:238:CYS:HB3	1.49	0.44
49:3R:234:TYR:HB2	49:3R:243:TYR:HB2	2.00	0.44
50:3S:18:LYS:HB2	50:3S:18:LYS:HE3	1.69	0.44
56:4B:45:MET:CE	92:4B:305:PSC:H62	2.47	0.44
56:4B:148:MET:C	56:4B:185:MET:HE1	2.43	0.44
87:4J:101:PGV:H302	87:4J:101:PGV:H343	2.00	0.44
67:4M:24:LEU:HD23	67:4M:24:LEU:HA	1.85	0.44
55:8A:308:ALA:C	55:8A:311:ILE:HD12	2.42	0.44
55:8A:427:PRO:HB3	55:8A:450:TRP:HE3	1.83	0.44
55:8A:452:THR:O	55:8A:456:MET:HG3	2.16	0.44
57:8C:62:ILE:HG13	87:8C:307:PGV:H21	2.00	0.44
57:8C:141:GLY:O	57:8C:145:THR:HG23	2.17	0.44
58:8D:48:TRP:HH2	59:8E:61:PHE:CA	2.30	0.44
58:8D:99:GLU:OE1	58:8D:103:VAL:CG2	2.65	0.44
59:8E:25:ASP:C	59:8E:28:GLU:OE2	2.60	0.44
59:8E:33:MET:CE	59:8E:67:ILE:CG2	2.87	0.44
62:8H:37:HIS:HB2	62:8H:85:ILE:HB	1.99	0.44
63:8I:54:TYR:CD1	63:8I:54:TYR:C	2.94	0.44
2:1B:46:TRP:HB3	2:1B:77:ARG:HG2	1.99	0.44
5:1E:63:ILE:HD12	5:1E:63:ILE:HA	1.82	0.44
7:1G:105:CYS:N	71:1G:801:SF4:S4	2.91	0.44
7:1G:376:VAL:HG12	7:1G:405:LYS:HB3	2.00	0.44
8:1H:277:TYR:CZ	9:1I:30:LEU:HB3	2.53	0.44
10:1J:25:SER:HB2	10:1J:81:GLU:C	2.43	0.44
19:1S:17:GLU:HG2	19:1S:67:ARG:HH21	1.83	0.44
23:1X:168:PHE:CE1	75:1X:201:CDL:H172	2.53	0.44
34:1i:92:LYS:HB3	34:1i:95:THR:HG21	1.98	0.44
39:1n:122:GLU:O	39:1n:126:ARG:HG3	2.17	0.44
41:1p:5:ASP:HB3	41:1p:8:VAL:CG1	2.47	0.44
48:3D:268:MET:N	52:3H:40:ASP:OD2	2.51	0.44
45:3N:248:LEU:HD12	45:3N:426:GLY:HA2	1.99	0.44
49:3R:170:ARG:C	49:3R:172:LYS:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:3U:49:GLN:OE1	52:3U:49:GLN:C	2.61	0.44
56:4B:1:FME:HE3	58:4D:128:VAL:HG22	1.99	0.44
55:8A:305:PHE:O	55:8A:309:THR:HG22	2.18	0.44
57:8C:33:MET:HE2	64:8J:49:CYS:SG	2.58	0.44
8:1H:84:THR:O	8:1H:87:VAL:HG22	2.18	0.44
8:1H:186:PHE:CD2	70:1H:402:PC1:H2D2	2.52	0.44
9:1I:13:ASP:O	9:1I:17:VAL:HG22	2.18	0.44
11:1K:40:LEU:HD23	14:1N:72:MET:HE2	1.99	0.44
13:1M:19:LYS:HE2	13:1M:19:LYS:HB3	1.81	0.44
13:1M:206:LYS:HE3	13:1M:206:LYS:HB3	1.75	0.44
75:1N:902:CDL:H392	75:1N:902:CDL:H232	2.00	0.44
16:1P:187:TRP:CE2	69:1P:403:3PE:H262	2.53	0.44
21:1V:49:GLN:HA	21:1V:52:ASN:HD21	1.83	0.44
24:1Y:109:ILE:HG23	70:1Y:207:PC1:H342	2.00	0.44
25:1Z:20:ASP:N	25:1Z:20:ASP:OD1	2.49	0.44
39:1n:166:TRP:CE3	39:1n:170:VAL:HG11	2.53	0.44
42:1q:66:THR:HG23	42:1q:74:PHE:HD1	1.83	0.44
47:3C:376:LEU:O	50:3F:29:ARG:HD3	2.17	0.44
45:3N:268:VAL:HB	45:3N:269:PRO:HD3	2.00	0.44
52:3U:28:GLU:OE1	52:3U:29:LYS:N	2.50	0.44
53:3W:51:LEU:HD12	53:3W:54:HIS:HE1	1.82	0.44
55:4A:187:SER:HB3	55:4A:277:MET:HE3	1.99	0.44
58:4D:129:ALA:HB1	58:4D:133:GLY:HA3	1.98	0.44
66:4L:28:TYR:HE2	87:4L:101:PGV:H302	1.80	0.44
55:8A:46:THR:O	55:8A:46:THR:OG1	2.35	0.44
55:8A:88:GLY:HA2	55:8A:505:PHE:CZ	2.53	0.44
58:8D:122:ARG:HG3	65:8K:53:TRP:CD1	2.52	0.44
59:8E:18:TYR:CE2	59:8E:32:GLY:HA3	2.53	0.44
69:1A:201:3PE:H362	27:1b:11:ALA:HB1	1.99	0.44
8:1H:58:LYS:HG2	8:1H:217:ALA:HB2	1.99	0.44
69:1L:703:3PE:H2A1	34:1i:80:ILE:HG12	1.99	0.44
13:1M:95:TYR:CE1	13:1M:132:ILE:HD12	2.53	0.44
69:1M:502:3PE:H271	69:1M:502:3PE:H222	2.00	0.44
20:1T:6:LEU:HD23	20:1T:6:LEU:H	1.82	0.44
21:1V:43:TYR:CE2	21:1V:93:MET:HG3	2.53	0.44
22:1W:49:LEU:HD23	22:1W:49:LEU:C	2.42	0.44
22:1W:70:ASN:N	22:1W:70:ASN:HD22	2.14	0.44
23:1X:165:ARG:HH12	29:1d:87:ASP:CG	2.26	0.44
69:1Y:203:3PE:H2	69:1Y:203:3PE:H221	1.43	0.44
47:3C:8:HIS:O	47:3C:12:LYS:N	2.45	0.44
48:3D:120:VAL:HG21	48:3D:271:VAL:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3E:234:TYR:HB2	49:3E:243:TYR:HB3	1.99	0.44
45:3N:4:TYR:CZ	45:3N:8:LEU:HD11	2.52	0.44
69:3N:501:3PE:H351	47:3P:11:MET:SD	2.57	0.44
47:3P:28:SER:HB2	75:3P:504:CDL:HA22	2.00	0.44
49:3R:217:CYS:HB2	49:3R:224:PRO:HD3	2.00	0.44
55:4A:129:TYR:CZ	55:4A:232:GLN:HG2	2.53	0.44
56:4B:11:ASP:OD1	58:4D:129:ALA:HA	2.18	0.44
56:4B:62:GLU:HG3	68:4N:14:SER:CB	2.48	0.44
56:4B:115:ASP:OD1	56:4B:115:ASP:C	2.61	0.44
56:4B:161:HIS:HB2	56:4B:174:ALA:HB3	2.00	0.44
87:4B:301:PGV:H281	75:4D:201:CDL:H261	2.00	0.44
57:4C:109:THR:CG2	57:4C:111:GLU:OE2	2.66	0.44
58:4D:77:GLU:O	58:4D:81:ILE:HD12	2.18	0.44
87:4G:101:PGV:H202	87:4G:101:PGV:H012	1.23	0.44
66:4L:37:PHE:O	66:4L:40:VAL:HG22	2.17	0.44
55:8A:275:TRP:O	55:8A:279:SER:OG	2.29	0.44
57:8C:90:GLU:HB2	57:8C:244:PHE:HE2	1.81	0.44
58:8D:78:TRP:CA	58:8D:81:ILE:CD1	2.90	0.44
75:8D:201:CDL:HB61	75:8D:201:CDL:H711	1.49	0.44
59:8E:72:LYS:HD2	59:8E:82:TYR:CE2	2.52	0.44
62:8H:49:ASP:O	62:8H:52:VAL:HG12	2.18	0.44
2:1B:175:ILE:O	2:1B:179:ARG:HG3	2.18	0.43
4:1D:165:THR:HG22	4:1D:169:TRP:CE2	2.53	0.43
4:1D:373:GLU:OE1	4:1D:392:LYS:NZ	2.51	0.43
8:1H:98:MET:HE2	70:1H:403:PC1:H2	2.01	0.43
10:1J:115:ILE:O	10:1J:117:PHE:N	2.49	0.43
16:1P:206:TYR:O	16:1P:210:VAL:HG23	2.18	0.43
16:1P:215:ILE:O	16:1P:218:ILE:HB	2.18	0.43
20:1U:17:TYR:C	20:1U:21:LEU:HD23	2.40	0.43
28:1c:19:LEU:C	75:1d:203:CDL:H122	2.43	0.43
51:3G:73:ARG:CZ	52:3H:82:GLU:HG2	2.48	0.43
49:3I:65:VAL:HG22	49:3I:77:ARG:HB3	2.00	0.43
55:4A:383:MET:CE	55:4A:421:VAL:HG13	2.45	0.43
59:4E:61:PHE:O	59:4E:65:VAL:HG13	2.18	0.43
55:8A:104:LEU:HD12	55:8A:152:LEU:HD13	1.99	0.43
57:8C:160:ILE:HG23	57:8C:219:LEU:HD11	2.00	0.43
62:8H:4:ILE:HB	62:8H:52:VAL:HG23	1.99	0.43
63:8I:45:LYS:HD2	63:8I:45:LYS:O	2.17	0.43
68:8N:8:GLN:CA	68:8N:11:LYS:HZ1	2.24	0.43
2:1B:162:GLN:NE2	9:1I:142:GLU:HG2	2.33	0.43
4:1D:71:GLU:OE2	4:1D:410:MET:HE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:68:LYS:HE3	5:1E:68:LYS:HB2	1.84	0.43
6:1F:263:ASN:HB2	6:1F:264:HIS:CD2	2.53	0.43
7:1G:433:ALA:HB2	7:1G:473:ILE:HG12	2.01	0.43
8:1H:124:ASN:C	8:1H:126:LYS:H	2.25	0.43
8:1H:264:LEU:HD22	26:1a:12:MET:HE2	1.99	0.43
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	1.99	0.43
15:1O:37:ARG:NH2	15:1O:40:ARG:HH11	2.15	0.43
16:1P:279:THR:OG1	69:1P:403:3PE:H352	2.18	0.43
21:1V:6:LYS:HE3	21:1V:6:LYS:HB2	1.83	0.43
23:1X:17:VAL:HG22	23:1X:19:VAL:HG22	1.99	0.43
29:1d:120:ARG:O	38:1m:108:ARG:NH2	2.34	0.43
47:3P:183:PHE:CZ	85:3P:501:HEM:HBC1	2.53	0.43
55:4A:21:LEU:HB3	87:4L:101:PGV:H271	1.99	0.43
55:4A:508:PRO:HG3	57:4C:6:HIS:HB3	2.00	0.43
56:4B:214:VAL:HG12	63:4I:60:PHE:HE1	1.83	0.43
58:4D:145:TRP:CZ3	65:4K:45:VAL:HA	2.53	0.43
55:8A:66:ILE:HG23	55:8A:67:PHE:CD2	2.53	0.43
57:8C:222:GLN:HE21	57:8C:222:GLN:C	2.24	0.43
75:8D:201:CDL:HB4	75:8D:201:CDL:H512	1.39	0.43
59:8E:27:TRP:CH2	59:8E:31:LYS:HD3	2.54	0.43
59:8E:69:GLU:O	59:8E:72:LYS:HB3	2.18	0.43
61:8G:15:THR:HG22	61:8G:19:LEU:HD11	2.00	0.43
3:1C:78:LEU:HB3	3:1C:130:TYR:HB3	2.01	0.43
4:1D:291:GLY:O	4:1D:296:ARG:NH2	2.52	0.43
6:1F:97:ALA:HB3	6:1F:138:ILE:HA	1.99	0.43
6:1F:277:LYS:HE2	6:1F:277:LYS:HB2	1.69	0.43
7:1G:343:LEU:HB3	7:1G:507:TYR:CE2	2.52	0.43
7:1G:444:LYS:HA	7:1G:444:LYS:HD2	1.85	0.43
8:1H:102:VAL:HG21	8:1H:154:LEU:CD1	2.48	0.43
75:1H:401:CDL:H511	75:1H:401:CDL:HB4	1.41	0.43
12:1L:213:LEU:HD21	12:1L:266:LEU:HG	2.00	0.43
13:1M:150:LEU:HG	13:1M:154:LEU:HD12	2.00	0.43
14:1N:55:ALA:HB1	14:1N:118:VAL:HA	1.99	0.43
14:1N:158:ALA:HB1	14:1N:188:GLY:O	2.18	0.43
15:1O:73:LEU:HD23	15:1O:292:VAL:HG13	2.00	0.43
15:1O:174:VAL:HG22	15:1O:225:ALA:HB2	2.00	0.43
16:1P:145:TYR:CE1	16:1P:149:LYS:HD2	2.53	0.43
22:1W:23:ARG:N	22:1W:27:GLU:OE2	2.45	0.43
32:1g:95:ARG:HH21	41:1p:64:HIS:CE1	2.36	0.43
33:1h:134:ASP:C	33:1h:134:ASP:OD1	2.61	0.43
40:1o:30:PHE:HB2	40:1o:33:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3A:388:ARG:HH22	45:3A:394:GLU:CD	2.25	0.43
46:3B:54:GLY:O	46:3B:194:TYR:OH	2.37	0.43
49:3E:112:GLY:CA	53:3J:14:TYR:HB2	2.48	0.43
46:3O:276:GLN:HG2	46:3O:281:ALA:HB2	1.98	0.43
55:4A:471:ILE:HG13	55:4A:472:ILE:N	2.33	0.43
56:4B:62:GLU:CA	56:4B:65:TRP:CZ2	3.00	0.43
65:4K:44:PRO:HB3	65:4K:48:VAL:CG2	2.47	0.43
55:8A:440:TYR:CZ	56:8B:205:SER:HA	2.54	0.43
87:8B:301:PGV:O14	87:8B:301:PGV:O05	2.27	0.43
57:8C:90:GLU:HB2	57:8C:244:PHE:CZ	2.53	0.43
58:8D:40:LEU:HD21	58:8D:59:LEU:CD2	2.48	0.43
58:8D:42:GLU:O	58:8D:45:LYS:HG2	2.17	0.43
58:8D:64:PHE:CE2	59:8E:66:ARG:HD3	2.53	0.43
66:8L:39:ILE:HD12	66:8L:39:ILE:H	1.83	0.43
1:1A:70:ALA:HB2	10:1J:59:ILE:HG13	1.99	0.43
2:1B:34:ASP:OD2	2:1B:171:LYS:HA	2.18	0.43
70:1B:202:PC1:H3D1	8:1H:53:LEU:HG	2.00	0.43
6:1F:147:SER:O	6:1F:151:VAL:HG12	2.19	0.43
7:1G:190:MET:HE1	7:1G:690:ALA:O	2.19	0.43
7:1G:314:ASP:O	7:1G:520:LYS:N	2.49	0.43
8:1H:103:LEU:HD23	8:1H:103:LEU:HA	1.88	0.43
10:1J:21:SER:O	10:1J:23:LYS:NZ	2.51	0.43
12:1L:152:PHE:CD1	12:1L:168:ALA:HB1	2.53	0.43
12:1L:558:LEU:HB3	13:1M:214:LEU:HD21	2.00	0.43
13:1M:269:MET:SD	13:1M:399:ASN:ND2	2.91	0.43
13:1M:318:ALA:HB2	13:1M:373:ILE:HG13	2.00	0.43
14:1N:143:CYS:HB3	14:1N:198:THR:CG2	2.48	0.43
14:1N:170:LEU:O	14:1N:295:ARG:NH2	2.49	0.43
20:1T:30:LEU:HA	20:1T:40:LEU:HD21	2.00	0.43
22:1W:29:LYS:HB3	22:1W:29:LYS:NZ	2.27	0.43
29:1d:11:LEU:HA	70:1d:202:PC1:H12	1.99	0.43
32:1g:26:LEU:HD12	32:1g:26:LEU:HA	1.75	0.43
35:1j:35:TRP:CH2	35:1j:39:ARG:HD3	2.54	0.43
46:3B:137:VAL:HG12	46:3B:141:GLN:HE21	1.84	0.43
47:3C:152:ALA:HB2	47:3C:287:LYS:HE3	2.00	0.43
49:3E:150:SER:HB3	49:3E:170:ARG:HG3	1.99	0.43
49:3E:181:LYS:HA	49:3E:184:ILE:HB	1.99	0.43
49:3E:263:TYR:HB3	49:3E:273:VAL:HG22	1.99	0.43
47:3P:215:MET:O	51:3T:10:MET:HE1	2.19	0.43
47:3P:223:TYR:HB3	48:3Q:227:TRP:CZ2	2.53	0.43
55:4A:86:MET:HE3	55:4A:185:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:219:PHE:HE2	57:4C:199:VAL:HG21	1.83	0.43
56:4B:28:LEU:HG	56:4B:32:PHE:CE2	2.52	0.43
58:4D:23:PRO:HG3	59:4E:37:VAL:HG21	2.00	0.43
64:4J:36:MET:HG2	87:4J:101:PGV:C18	2.49	0.43
55:8A:100:MET:N	57:8C:17:PRO:HB3	2.34	0.43
56:8B:146:MET:HE1	56:8B:189:PRO:HD3	1.99	0.43
92:8B:305:PSC:H02	92:8B:305:PSC:H21	1.45	0.43
75:8D:201:CDL:H562	75:8D:201:CDL:H191	2.00	0.43
68:8N:57:LEU:HD23	68:8N:57:LEU:HA	1.85	0.43
4:1D:379:VAL:HB	4:1D:388:ARG:HB3	1.99	0.43
6:1F:56:ILE:HG23	6:1F:235:CYS:SG	2.58	0.43
6:1F:133:ALA:HA	6:1F:174:ASP:O	2.17	0.43
7:1G:174:THR:HG22	7:1G:183:VAL:HG22	1.99	0.43
7:1G:668:ILE:HD12	7:1G:668:ILE:HA	1.89	0.43
12:1L:51:LEU:HD22	12:1L:91:PRO:HG2	2.00	0.43
12:1L:510:TYR:HE2	64:4J:29:ASN:HD21	1.66	0.43
12:1L:548:SER:HA	12:1L:552:LEU:HB3	1.99	0.43
14:1N:1:FME:CN	15:1O:258:ARG:NH1	2.76	0.43
15:1O:83:TYR:HB2	15:1O:190:HIS:HB3	1.99	0.43
15:1O:145:ARG:O	15:1O:149:VAL:HG13	2.19	0.43
20:1T:64:ASP:CG	22:1W:37:ARG:HH22	2.26	0.43
28:1c:43:LYS:NZ	28:1c:49:GLU:OE2	2.52	0.43
30:1e:4:ASP:OD1	30:1e:4:ASP:O	2.37	0.43
34:1i:83:TYR:CD1	34:1i:87:TYR:HD2	2.36	0.43
35:1j:35:TRP:O	35:1j:39:ARG:HG2	2.17	0.43
39:1n:54:LYS:HD3	39:1n:54:LYS:HA	1.63	0.43
46:3B:33:LEU:HD12	46:3B:204:MET:O	2.18	0.43
50:3F:84:GLN:HB2	75:3G:103:CDL:HA22	2.00	0.43
45:3N:283:THR:HA	46:3O:143:GLN:NE2	2.32	0.43
46:3O:163:LEU:HD11	46:3O:258:VAL:HG22	1.99	0.43
48:3Q:27:ARG:NH2	48:3Q:60:GLU:OE1	2.48	0.43
49:3R:143:SER:OG	49:3R:145:ASP:OD1	2.35	0.43
49:3R:207:LYS:NZ	49:3R:209:GLU:OE1	2.50	0.43
55:4A:53:ILE:O	55:4A:56:VAL:HG22	2.18	0.43
55:4A:319:LYS:HE2	55:4A:319:LYS:HB3	1.81	0.43
56:4B:62:GLU:CB	56:4B:65:TRP:CE2	3.02	0.43
75:4B:303:CDL:H811	75:4B:303:CDL:H262	2.01	0.43
59:4E:31:LYS:CE	60:4F:83:PRO:O	2.65	0.43
55:8A:115:SER:HB2	55:8A:145:LEU:HB2	2.00	0.43
55:8A:354:THR:HG22	55:8A:376:HIS:HB2	1.99	0.43
87:8A:602:PGV:H31	65:8K:9:PHE:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:8B:105:TYR:HB2	56:8B:120:SER:O	2.18	0.43
57:8C:15:PRO:O	57:8C:19:THR:OG1	2.32	0.43
59:8E:104:LEU:HB3	59:8E:106:LEU:CD2	2.48	0.43
63:8I:35:TYR:O	63:8I:35:TYR:HD1	2.02	0.43
3:1C:114:LEU:HD12	22:1W:77:ARG:HB2	1.99	0.43
5:1E:104:THR:O	5:1E:104:THR:OG1	2.37	0.43
7:1G:324:ASP:CB	7:1G:571:ALA:HB1	2.48	0.43
8:1H:96:ILE:CG2	8:1H:98:MET:HE3	2.49	0.43
8:1H:169:GLN:CG	8:1H:174:MET:HG3	2.46	0.43
16:1P:145:TYR:O	16:1P:149:LYS:HG3	2.19	0.43
20:1T:52:MET:CE	22:1W:40:TYR:CD2	3.01	0.43
20:1U:49:GLU:HB3	36:1k:44:TRP:HE1	1.83	0.43
41:1p:76:CYS:SG	41:1p:84:MET:HG2	2.58	0.43
42:1q:32:ASP:OD1	42:1q:32:ASP:C	2.62	0.43
45:3A:411:CYS:O	45:3A:415:PHE:HB2	2.18	0.43
45:3N:436:ARG:HD3	47:3P:222:PRO:HD3	2.01	0.43
69:3N:503:3PE:H2	69:3N:503:3PE:H221	1.37	0.43
55:4A:279:SER:HB3	68:4N:22:ILE:HG13	1.99	0.43
55:4A:356:ILE:HD12	56:4B:73:LEU:HD11	1.99	0.43
55:4A:377:PHE:O	55:4A:381:LEU:HB2	2.18	0.43
55:4A:425:PHE:HA	55:4A:428:GLN:HG3	2.01	0.43
57:4C:62:ILE:HG13	87:4C:306:PGV:H21	2.00	0.43
59:4E:29:LEU:HD23	59:4E:29:LEU:C	2.44	0.43
62:4H:14:ALA:HB3	62:4H:63:PHE:CE1	2.53	0.43
63:4I:59:ASP:OD1	63:4I:59:ASP:C	2.61	0.43
64:4J:21:HIS:O	64:4J:22:LEU:HD12	2.18	0.43
55:8A:66:ILE:HD13	55:8A:126:TRP:CZ2	2.54	0.43
55:8A:254:ILE:HD11	55:8A:388:ALA:CB	2.48	0.43
56:8B:61:VAL:HG12	56:8B:65:TRP:CZ3	2.54	0.43
56:8B:110:TYR:HB2	56:8B:116:LEU:HB3	2.00	0.43
59:8E:33:MET:HE1	59:8E:67:ILE:CB	2.48	0.43
60:8F:55:LYS:HG3	60:8F:73:TRP:CZ3	2.53	0.43
4:1D:50:ASN:HB2	4:1D:65:VAL:HG22	2.00	0.43
4:1D:247:ALA:HA	4:1D:265:ILE:HD11	2.01	0.43
7:1G:196:SER:OG	7:1G:265:ASP:OD2	2.29	0.43
8:1H:230:ASN:O	8:1H:234:MET:HG2	2.18	0.43
10:1J:20:PHE:CE1	11:1K:32:CYS:HA	2.45	0.43
10:1J:173:ARG:NH1	15:1O:254:ARG:NH1	2.66	0.43
11:1K:3:LEU:CD2	11:1K:6:MET:SD	3.06	0.43
12:1L:161:ARG:NH1	12:1L:238:GLU:OE1	2.51	0.43
13:1M:401:MET:O	13:1M:405:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:226:THR:HG23	14:1N:229:SER:H	1.83	0.43
20:1T:22:TYR:CE2	20:1T:24:LYS:HB2	2.53	0.43
25:1Z:141:ILE:H	25:1Z:141:ILE:HG12	1.63	0.43
30:1e:29:PRO:HB3	33:1h:138:LYS:HG3	2.00	0.43
32:1g:93:ALA:O	32:1g:97:VAL:HG22	2.18	0.43
37:1l:32:GLU:OE1	37:1l:32:GLU:N	2.51	0.43
45:3N:50:GLU:H	45:3N:50:GLU:CD	2.26	0.43
46:3O:350:GLY:HA2	46:3O:411:ILE:HD13	2.00	0.43
57:4C:206:LEU:HD23	57:4C:206:LEU:HA	1.85	0.43
60:4F:29:ASP:OD1	60:4F:32:ASN:N	2.52	0.43
66:4L:21:LEU:HD12	66:4L:21:LEU:O	2.18	0.43
66:4L:36:PRO:O	66:4L:40:VAL:HG13	2.19	0.43
55:8A:340:TRP:HH2	55:8A:417:MET:HG2	1.84	0.43
57:8C:156:ARG:HB3	60:8F:5:GLY:HA3	1.99	0.43
57:8C:187:THR:HA	93:8C:308:PEK:O12	2.19	0.43
58:8D:37:GLN:HG3	58:8D:37:GLN:H	1.61	0.43
64:8J:38:LEU:HD12	64:8J:38:LEU:HA	1.90	0.43
65:8K:24:PHE:CD1	65:8K:24:PHE:C	2.96	0.43
1:1A:41:PHE:CZ	2:1B:99:ALA:HB2	2.54	0.43
6:1F:112:ARG:HB3	6:1F:145:GLU:HG3	2.01	0.43
7:1G:40:PHE:HB2	7:1G:52:CYS:SG	2.58	0.43
7:1G:299:ALA:O	7:1G:303:VAL:HG23	2.18	0.43
10:1J:61:LEU:HA	10:1J:61:LEU:HD12	1.80	0.43
12:1L:15:LEU:HB3	12:1L:126:ILE:HG12	2.01	0.43
12:1L:361:GLY:HA2	36:1k:59:ASN:HD21	1.84	0.43
15:1O:52:PRO:O	15:1O:107:GLN:NE2	2.43	0.43
16:1P:315:ILE:HG13	16:1P:322:ARG:HH12	1.84	0.43
70:1P:401:PC1:H222	70:1P:401:PC1:H152	2.01	0.43
20:1U:18:VAL:HG21	20:1U:57:GLU:OE1	2.18	0.43
21:1V:25:ILE:HG13	21:1V:26:LEU:N	2.33	0.43
24:1Y:34:ILE:HD12	69:1Y:205:3PE:H372	2.01	0.43
70:1d:202:PC1:H2	70:1d:202:PC1:H222	1.50	0.43
30:1e:68:ARG:O	30:1e:72:MET:HG2	2.18	0.43
35:1j:69:ASP:HB3	40:1o:117:ARG:NH2	2.33	0.43
38:1m:3:PRO:HD2	39:1n:72:TYR:CE1	2.54	0.43
39:1n:156:ALA:HB1	39:1n:161:ASP:OD1	2.18	0.43
46:3B:309:VAL:HG23	46:3B:326:THR:HG22	2.01	0.43
50:3F:114:LYS:O	50:3F:118:GLU:HG2	2.18	0.43
87:4G:101:PGV:H21	87:4G:101:PGV:H02	1.52	0.43
55:8A:233:HIS:HB3	57:8C:99:TRP:CZ2	2.54	0.43
55:8A:347:LEU:HD21	55:8A:418:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:406:ASN:HB3	55:8A:471:ILE:HD11	2.01	0.43
57:8C:98:PHE:CE2	87:8C:304:PGV:H182	2.54	0.43
57:8C:165:ILE:HD12	93:8G:102:PEK:H11	1.99	0.43
65:8K:8:ASP:O	65:8K:12:LYS:HD2	2.19	0.43
4:1D:111:MET:SD	4:1D:111:MET:N	2.92	0.43
7:1G:150:MET:HE2	7:1G:183:VAL:O	2.19	0.43
10:1J:124:ASP:OD1	11:1K:4:VAL:HG22	2.19	0.43
12:1L:73:THR:HG22	12:1L:194:ASN:ND2	2.13	0.43
12:1L:140:LEU:HD23	12:1L:140:LEU:C	2.43	0.43
12:1L:172:ILE:HG21	13:1M:408:LEU:HD12	1.99	0.43
12:1L:331:MET:HG3	12:1L:391:SER:HB3	2.01	0.43
13:1M:167:ILE:HG12	13:1M:195:MET:HE3	2.01	0.43
14:1N:249:LEU:HD23	14:1N:294:MET:HE1	2.00	0.43
17:1Q:60:ASP:OD2	17:1Q:62:ARG:NH1	2.51	0.43
19:1S:91:GLU:O	19:1S:95:SER:HB3	2.18	0.43
22:1W:54:ILE:HD13	22:1W:107:PHE:CE2	2.54	0.43
25:1Z:98:MET:HE3	25:1Z:104:TRP:CH2	2.54	0.43
25:1Z:113:THR:HG21	30:1e:35:PHE:HE1	1.84	0.43
40:1o:47:ASP:OD1	40:1o:47:ASP:C	2.62	0.43
40:1o:55:ARG:NH2	41:1p:119:SER:HB3	2.30	0.43
41:1p:158:GLN:C	41:1p:162:MET:HE3	2.44	0.43
44:1s:33:PHE:O	44:1s:33:PHE:CD1	2.72	0.43
45:3A:328:ASN:HB3	45:3A:427:PRO:HB2	2.00	0.43
48:3D:222:TYR:HH	48:3D:249:MET:HB3	1.84	0.43
45:3N:142:ASP:OD2	49:3R:79:SER:N	2.52	0.43
47:3P:229:ILE:CG2	70:3R:303:PC1:H371	2.49	0.43
50:3S:35:ASP:OD2	50:3S:61:ARG:NH1	2.51	0.43
56:4B:28:LEU:HD11	75:4B:303:CDL:H592	2.01	0.43
56:4B:68:LEU:HG	92:4B:305:PSC:H183	2.00	0.43
65:4K:41:ASN:OD1	65:4K:41:ASN:O	2.37	0.43
56:8B:83:ILE:O	56:8B:87:MET:HG3	2.19	0.43
57:8C:157:LYS:NZ	87:8C:302:PGV:H02	2.34	0.43
64:8J:31:LEU:O	64:8J:35:THR:OG1	2.37	0.43
64:8J:36:MET:O	64:8J:39:CYS:SG	2.68	0.43
1:1A:39:CYS:O	4:1D:53:PRO:HD2	2.19	0.43
1:1A:53:MET:HE3	10:1J:172:THR:HG23	2.01	0.43
4:1D:208:LEU:HD22	4:1D:315:LEU:HD23	1.99	0.43
6:1F:16:LYS:HB2	6:1F:16:LYS:HE2	1.79	0.43
6:1F:110:ILE:CD1	6:1F:114:ASP:HB2	2.48	0.43
6:1F:137:TYR:HB3	6:1F:192:LEU:HD11	2.00	0.43
7:1G:9:ILE:HG13	7:1G:75:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:394:ARG:HD3	7:1G:394:ARG:HA	1.89	0.43
12:1L:90:ILE:HB	12:1L:91:PRO:HD3	2.01	0.43
13:1M:318:ALA:HB1	13:1M:374:ASN:CG	2.43	0.43
33:1h:110:VAL:HG12	33:1h:114:MET:HE2	1.99	0.43
35:1j:61:ASP:N	35:1j:61:ASP:OD1	2.52	0.43
36:1k:27:PRO:HG2	36:1k:52:TYR:CE2	2.54	0.43
47:3P:63:PHE:O	47:3P:67:THR:HG23	2.19	0.43
48:3Q:203:ARG:NH2	53:3W:53:LYS:HZ2	2.16	0.43
55:4A:3:VAL:HG22	55:4A:7:LEU:HD22	2.00	0.43
55:4A:69:MET:HG2	55:4A:70:VAL:N	2.34	0.43
57:4C:148:HIS:HA	57:4C:235:PHE:HE2	1.84	0.43
57:4C:151:LEU:CG	57:4C:159:MET:SD	3.06	0.43
93:4C:307:PEK:H42	93:4C:307:PEK:H72	1.89	0.43
58:4D:141:ASP:OD1	58:4D:141:ASP:C	2.61	0.43
55:8A:96:ARG:NH2	57:8C:61:ILE:HG13	2.34	0.43
55:8A:309:THR:HG23	55:8A:359:ALA:HB1	2.01	0.43
75:8B:303:CDL:H141	75:8B:303:CDL:H631	2.00	0.43
57:8C:150:SER:HB3	57:8C:155:ASP:HB3	2.01	0.43
57:8C:172:TYR:CE2	93:8G:102:PEK:H181	2.53	0.43
59:8E:52:LEU:HD21	59:8E:68:LEU:CD1	2.48	0.43
60:8F:13:ALA:O	60:8F:18:ARG:CZ	2.67	0.43
64:8J:36:MET:HE2	64:8J:39:CYS:SG	2.59	0.43
1:1A:90:MET:HA	1:1A:90:MET:CE	2.41	0.42
4:1D:170:MET:HE2	4:1D:225:LEU:HD22	2.00	0.42
6:1F:194:GLU:OE2	17:1Q:133:LYS:HD3	2.19	0.42
6:1F:394:GLU:OE2	43:1r:50:ASN:N	2.39	0.42
8:1H:66:SER:HA	8:1H:122:ALA:O	2.19	0.42
8:1H:96:ILE:HG23	25:1Z:144:THR:HB	2.01	0.42
10:1J:126:VAL:O	25:1Z:120:MET:HE3	2.19	0.42
13:1M:122:PHE:HE1	13:1M:206:LYS:HD3	1.84	0.42
13:1M:270:ILE:HD11	13:1M:395:LEU:O	2.19	0.42
30:1e:85:LEU:HB3	30:1e:91:TYR:HB2	2.01	0.42
32:1g:83:TYR:CE2	32:1g:84:ARG:HG3	2.54	0.42
34:1i:83:TYR:CE1	41:1p:48:ARG:HD3	2.54	0.42
48:3D:115:ARG:HB2	48:3D:143:CYS:HB2	2.01	0.42
46:3O:307:PHE:CD2	49:3V:52:ARG:HD2	2.53	0.42
54:3Y:23:MET:O	54:3Y:27:VAL:HG23	2.18	0.42
55:4A:110:LEU:HB2	87:4A:601:PGV:H181	2.01	0.42
55:4A:168:ILE:HD13	55:4A:189:LEU:HB2	2.01	0.42
55:4A:278:MET:HB3	87:4A:603:PGV:H11	2.01	0.42
56:4B:40:TYR:O	56:4B:40:TYR:CD1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4B:102:HIS:O	56:4B:207:MET:CE	2.67	0.42
59:4E:18:TYR:HD1	59:4E:19:PHE:CD1	2.36	0.42
62:4H:4:ILE:HD13	62:4H:7:LYS:HE2	2.00	0.42
55:8A:124:THR:OG1	55:8A:132:LEU:HD23	2.19	0.42
55:8A:246:LEU:HD13	55:8A:381:LEU:HD21	2.01	0.42
56:8B:103:GLN:HA	56:8B:104:TRP:HA	1.80	0.42
56:8B:162:SER:HB2	56:8B:198:GLU:HB2	2.00	0.42
58:8D:52:SER:O	58:8D:56:LYS:HG3	2.18	0.42
58:8D:99:GLU:OE2	58:8D:104:TYR:CZ	2.68	0.42
59:8E:37:VAL:HG11	59:8E:70:VAL:HG21	2.00	0.42
1:1A:38:GLU:O	4:1D:51:PHE:HD2	2.02	0.42
2:1B:94:ASN:HB3	3:1C:174:LEU:HD22	2.01	0.42
6:1F:96:ASN:HD22	73:1F:501:FMN:C2	2.31	0.42
6:1F:418:LEU:HD12	6:1F:422:PHE:HB2	2.01	0.42
7:1G:328:LEU:O	7:1G:507:TYR:OH	2.35	0.42
7:1G:364:LEU:HB3	7:1G:577:GLU:HA	2.02	0.42
7:1G:377:ILE:HG12	7:1G:450:MET:HB3	2.01	0.42
7:1G:510:GLY:HA3	7:1G:512:GLU:OE2	2.18	0.42
10:1J:33:LEU:HD23	10:1J:65:LEU:HD21	2.00	0.42
10:1J:60:TYR:CD1	11:1K:64:LEU:HD11	2.54	0.42
12:1L:243:VAL:HG13	12:1L:247:LEU:HD13	2.01	0.42
15:1O:37:ARG:NE	15:1O:37:ARG:HA	2.34	0.42
16:1P:172:PHE:HB2	16:1P:179:LEU:HD21	2.00	0.42
23:1X:36:ASP:OD1	23:1X:36:ASP:C	2.62	0.42
35:1j:61:ASP:HB3	35:1j:66:ILE:HB	2.01	0.42
38:1m:29:ARG:HB3	39:1n:8:TYR:OH	2.19	0.42
39:1n:43:MET:HE2	39:1n:43:MET:HB2	1.93	0.42
46:3B:74:SER:O	46:3B:74:SER:OG	2.32	0.42
47:3C:10:LEU:O	47:3C:14:ILE:HG12	2.19	0.42
48:3D:297:MET:HA	69:3D:502:3PE:H321	2.00	0.42
47:3P:124:MET:HE1	47:3P:298:ILE:HD11	2.01	0.42
55:4A:485:VAL:HG12	67:4M:1:ILE:HD12	2.01	0.42
56:4B:16:ILE:HG12	56:4B:87:MET:HG2	1.99	0.42
55:8A:69:MET:HE1	88:8A:604:HEA:C18	2.49	0.42
55:8A:271:MET:HA	55:8A:274:VAL:HG22	2.01	0.42
60:8F:93:SER:O	60:8F:94:HIS:HB3	2.19	0.42
3:1C:168:LEU:HD21	4:1D:90:LEU:HD23	2.00	0.42
5:1E:22:ASP:OD1	5:1E:68:LYS:NZ	2.42	0.42
5:1E:76:PRO:HA	5:1E:77:PRO:HD3	1.93	0.42
6:1F:184:TYR:CE1	73:1F:501:FMN:H6	2.53	0.42
8:1H:180:PRO:HB3	70:1H:402:PC1:H381	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:29:GLU:HG2	9:1I:30:LEU:N	2.33	0.42
12:1L:291:CYS:SG	12:1L:526:LEU:HA	2.59	0.42
12:1L:555:LEU:HD13	38:1m:75:ILE:HD13	2.01	0.42
13:1M:54:LEU:HD11	33:1h:96:ILE:HD11	2.01	0.42
13:1M:71:TRP:CD1	70:1M:505:PC1:H2C2	2.54	0.42
69:1M:506:3PE:H271	69:1M:506:3PE:H2B2	2.00	0.42
14:1N:78:LEU:HD12	14:1N:82:GLY:HA2	2.01	0.42
16:1P:196:LEU:O	16:1P:239:PHE:HB2	2.20	0.42
19:1S:52:ILE:HD12	19:1S:52:ILE:N	2.32	0.42
29:1d:12:GLN:HG2	69:1d:201:3PE:H111	2.01	0.42
30:1e:68:ARG:HB3	30:1e:71:THR:HB	2.00	0.42
32:1g:55:LEU:HD12	32:1g:58:MET:HE3	2.01	0.42
43:1r:100:ILE:HD12	43:1r:100:ILE:HA	1.92	0.42
45:3A:30:SER:HB2	45:3A:32:GLN:HG3	2.00	0.42
45:3A:78:GLU:OE1	45:3A:108:LYS:NZ	2.53	0.42
49:3E:225:ILE:HG12	49:3E:237:PRO:HD3	2.00	0.42
53:3J:8:THR:HG23	53:3J:11:ALA:H	1.85	0.42
45:3N:270:LEU:HD13	45:3N:320:LEU:HD22	2.00	0.42
69:3N:503:3PE:H322	70:3R:303:PC1:H31	2.02	0.42
46:3O:109:VAL:HG22	46:3O:123:LEU:HD22	2.02	0.42
49:3R:150:SER:CB	49:3R:170:ARG:H	2.27	0.42
55:4A:271:MET:HG3	68:4N:12:HIS:CD2	2.53	0.42
56:4B:61:VAL:HG13	92:4B:305:PSC:H271	2.01	0.42
92:4B:305:PSC:H252	92:4B:305:PSC:H302	2.00	0.42
87:4C:302:PGV:H011	87:4C:302:PGV:H202	1.24	0.42
60:4F:10:GLU:OE1	60:4F:11:GLU:OE2	2.37	0.42
55:8A:5:ARG:HD2	66:8L:3:TYR:CE2	2.54	0.42
55:8A:65:MET:HB3	88:8A:604:HEA:HBC1	2.01	0.42
55:8A:509:THR:HG22	60:8F:57:ILE:HB	2.02	0.42
87:8C:305:PGV:H21	87:8C:305:PGV:H222	2.00	0.42
58:8D:103:VAL:HG13	67:8M:34:LEU:O	2.19	0.42
75:8D:201:CDL:H402	75:8D:201:CDL:H592	2.02	0.42
61:8G:32:THR:OG1	87:8G:101:PGV:H301	2.19	0.42
2:1B:77:ARG:HA	2:1B:77:ARG:HD2	1.66	0.42
70:1B:203:PC1:O14	70:1B:203:PC1:H121	2.20	0.42
4:1D:100:LEU:HD13	4:1D:196:PRO:HD3	2.00	0.42
4:1D:342:MET:HB2	7:1G:134:LYS:NZ	2.34	0.42
7:1G:186:TYR:CD2	7:1G:187:ILE:HG23	2.54	0.42
7:1G:643:GLN:O	7:1G:647:GLU:HG2	2.19	0.42
8:1H:19:PHE:CZ	70:1q:201:PC1:H2D1	2.54	0.42
8:1H:87:VAL:HG12	8:1H:95:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:74:GLU:HG2	18:1R:87:CYS:O	2.19	0.42
12:1L:294:THR:O	12:1L:294:THR:OG1	2.36	0.42
12:1L:575:ILE:HD13	14:1N:171:ASN:HD21	1.83	0.42
13:1M:42:LEU:CB	13:1M:453:MET:HE3	2.49	0.42
13:1M:71:TRP:HH2	13:1M:439:LEU:HD22	1.85	0.42
14:1N:3:PRO:O	14:1N:7:THR:HG23	2.19	0.42
15:1O:27:VAL:HG21	15:1O:39:ALA:HB2	2.02	0.42
15:1O:138:MET:CE	76:1O:401:GTP:HN21	2.32	0.42
16:1P:151:VAL:HG23	59:8E:9:GLU:OE1	2.18	0.42
16:1P:315:ILE:HD12	16:1P:331:MET:HB3	2.01	0.42
20:1U:40:LEU:HB3	20:1U:42:LEU:HD13	2.00	0.42
22:1W:68:MET:HA	22:1W:68:MET:HE3	2.01	0.42
27:1b:78:GLU:OE2	27:1b:82:ASN:OD1	2.38	0.42
37:1l:134:PRO:HD2	37:1l:138:LEU:HD21	2.02	0.42
38:1m:17:LEU:HD11	39:1n:71:TRP:HB2	2.01	0.42
38:1m:82:THR:HG22	38:1m:85:THR:H	1.84	0.42
45:3N:191:LYS:HE3	45:3N:191:LYS:HB3	1.87	0.42
46:3O:54:GLY:O	46:3O:194:TYR:OH	2.37	0.42
47:3P:185:LEU:HA	47:3P:185:LEU:HD23	1.82	0.42
49:3R:152:ILE:O	49:3R:153:GLU:HG2	2.20	0.42
55:4A:467:LEU:O	55:4A:471:ILE:HG23	2.19	0.42
56:4B:56:MET:HE3	56:4B:56:MET:HB2	1.92	0.42
57:4C:189:SER:O	61:4G:55:ILE:HD12	2.19	0.42
55:8A:93:ALA:HA	55:8A:171:MET:SD	2.60	0.42
55:8A:129:TYR:OH	55:8A:236:TRP:NE1	2.46	0.42
55:8A:377:PHE:CD1	55:8A:377:PHE:C	2.98	0.42
55:8A:415:VAL:HG22	75:8D:201:CDL:HB32	2.01	0.42
55:8A:473:TRP:CG	66:8L:22:LEU:HD13	2.54	0.42
56:8B:30:ILE:HG21	56:8B:76:ILE:HD11	2.02	0.42
57:8C:146:TRP:CE2	61:8G:17:ARG:HB3	2.54	0.42
57:8C:206:LEU:HD11	93:8C:308:PEK:H11	2.00	0.42
93:8C:308:PEK:H42	93:8C:308:PEK:H72	1.88	0.42
1:1A:53:MET:HE1	11:1K:79:VAL:CG1	2.50	0.42
2:1B:129:SER:HB2	4:1D:90:LEU:HD11	2.01	0.42
4:1D:47:LEU:O	4:1D:67:GLU:HA	2.20	0.42
4:1D:112:MET:HG3	4:1D:181:TYR:CZ	2.54	0.42
8:1H:107:ALA:HB1	10:1J:57:PHE:HB3	2.01	0.42
11:1K:11:ALA:O	11:1K:14:ILE:HG13	2.18	0.42
12:1L:295:GLN:O	12:1L:425:ARG:NH1	2.51	0.42
12:1L:315:VAL:HG11	12:1L:412:THR:HG21	2.01	0.42
12:1L:425:ARG:HA	12:1L:505:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:572:LYS:NZ	69:1Y:203:3PE:H351	2.34	0.42
13:1M:164:LEU:O	13:1M:174:LEU:HD11	2.19	0.42
13:1M:341:THR:HG22	13:1M:343:ILE:H	1.84	0.42
20:1T:24:LYS:HA	20:1T:24:LYS:HD3	1.81	0.42
70:1Y:207:PC1:H231	70:1Y:207:PC1:H122	2.02	0.42
37:1I:117:TRP:O	37:1I:121:ILE:HG23	2.20	0.42
48:3D:198:PRO:HA	48:3D:199:PRO:HD3	1.94	0.42
46:3O:195:VAL:O	46:3O:199:PHE:HB2	2.19	0.42
57:4C:121:ILE:HD11	61:4G:53:LEU:HD21	2.00	0.42
57:4C:128:GLU:OE1	57:4C:128:GLU:N	2.53	0.42
87:4C:303:PGV:H171	75:4C:305:CDL:H872	2.01	0.42
59:4E:72:LYS:HA	59:4E:82:TYR:HD2	1.85	0.42
59:4E:85:VAL:HG13	59:4E:86:ILE:HD13	2.00	0.42
59:4E:91:PRO:O	59:4E:95:GLU:HG2	2.19	0.42
55:8A:399:LEU:HB2	55:8A:494:TRP:CZ3	2.55	0.42
56:8B:116:LEU:CD2	56:8B:226:MET:HE2	2.49	0.42
87:8B:302:PGV:C20	87:8C:304:PGV:H62	2.49	0.42
92:8B:305:PSC:H302	92:8B:305:PSC:H252	2.01	0.42
87:8C:302:PGV:H012	87:8C:302:PGV:H21	2.01	0.42
60:8F:21:MET:HB3	60:8F:22:MET:HE2	2.00	0.42
62:8H:56:TYR:O	62:8H:60:TYR:HD1	2.02	0.42
64:8J:34:VAL:O	64:8J:38:LEU:HB2	2.19	0.42
6:1F:193:ILE:HG23	6:1F:215:VAL:HA	2.02	0.42
10:1J:33:LEU:HD23	10:1J:65:LEU:HD11	2.01	0.42
12:1L:142:ILE:HA	13:1M:370:PRO:HG2	2.01	0.42
12:1L:197:ASP:OD2	41:1p:110:LYS:HD3	2.19	0.42
12:1L:565:THR:HG23	70:1Y:207:PC1:H32	2.02	0.42
13:1M:24:TRP:CE3	13:1M:81:GLN:HB3	2.54	0.42
17:1Q:57:MET:HE3	17:1Q:86:PHE:CE1	2.54	0.42
18:1R:39:PHE:O	18:1R:43:LEU:HG	2.20	0.42
23:1X:53:ARG:HG3	23:1X:54:ARG:HG2	2.01	0.42
24:1Y:103:ARG:HD2	24:1Y:103:ARG:HA	1.84	0.42
29:1d:94:VAL:HG21	33:1h:106:LYS:HD2	2.02	0.42
32:1g:114:ASP:OD1	32:1g:114:ASP:C	2.61	0.42
35:1j:60:THR:C	35:1j:62:GLU:H	2.28	0.42
45:3A:41:ILE:HG12	45:3A:195:MET:HG2	2.01	0.42
45:3A:41:ILE:HG23	45:3A:195:MET:HG2	2.01	0.42
49:3E:159:ILE:HD11	49:3E:165:MET:HB2	2.01	0.42
49:3E:195:LEU:HD13	49:3E:249:ILE:O	2.20	0.42
45:3N:303:LEU:HD23	45:3N:303:LEU:HA	1.84	0.42
47:3P:128:PHE:CE1	47:3P:146:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3P:307:LEU:HD11	47:3P:363:LEU:HD23	2.01	0.42
51:3T:51:PRO:O	51:3T:54:VAL:HG22	2.20	0.42
55:4A:73:ILE:HD13	88:4A:604:HEA:H242	2.01	0.42
55:4A:243:VAL:HG13	88:4A:605:HEA:C4C	2.50	0.42
55:4A:462:LEU:O	55:4A:465:VAL:HG12	2.20	0.42
57:4C:60:ASP:OD1	57:4C:60:ASP:N	2.53	0.42
58:4D:68:PHE:CD1	59:4E:69:GLU:HB3	2.54	0.42
62:4H:28:ASN:ND2	62:4H:63:PHE:HE2	2.18	0.42
68:4N:35:ARG:NH2	68:4N:63:TYR:CE1	2.88	0.42
55:8A:273:MET:HE3	55:8A:322:SER:HB2	2.00	0.42
56:8B:59:GLN:HG2	68:8N:13:PRO:HD2	2.01	0.42
56:8B:122:MET:SD	56:8B:135:LEU:HA	2.59	0.42
57:8C:58:TRP:CD1	57:8C:61:ILE:HD12	2.54	0.42
75:8D:201:CDL:HA4	75:8D:201:CDL:OB4	2.20	0.42
59:8E:26:ALA:O	59:8E:30:ARG:HD3	2.19	0.42
64:8J:33:ARG:HD2	87:8J:101:PGV:H181	2.02	0.42
1:1A:54:LYS:HE3	1:1A:113:TRP:HB3	2.01	0.42
2:1B:86:MET:HE1	2:1B:104:TYR:HB2	2.01	0.42
70:1B:203:PC1:O14	42:1q:75:TRP:HB3	2.20	0.42
6:1F:92:TYR:CE1	6:1F:133:ALA:HB3	2.54	0.42
6:1F:197:GLU:OE2	17:1Q:129:ARG:NH2	2.47	0.42
6:1F:292:ASP:OD1	6:1F:292:ASP:N	2.52	0.42
7:1G:53:ARG:N	72:1G:803:FES:S1	2.81	0.42
8:1H:2:PHE:CE2	8:1H:6:ILE:HD11	2.55	0.42
8:1H:24:GLU:OE1	8:1H:228:TYR:OH	2.23	0.42
8:1H:65:THR:HA	16:1P:324:TYR:HB2	2.01	0.42
11:1K:4:VAL:O	11:1K:8:ILE:HG12	2.20	0.42
12:1L:175:ASN:C	12:1L:179:ASP:OD2	2.63	0.42
16:1P:115:HIS:CE1	16:1P:119:GLN:OE1	2.70	0.42
16:1P:169:SER:HB3	16:1P:231:VAL:HG23	2.01	0.42
20:1T:64:ASP:HA	20:1T:67:ALA:HB3	2.02	0.42
25:1Z:108:GLU:O	30:1e:74:ARG:NH1	2.53	0.42
29:1d:11:LEU:HD21	30:1e:3:PHE:HB3	2.01	0.42
30:1e:75:LEU:HA	30:1e:78:ILE:HG22	2.02	0.42
45:3A:195:MET:HE1	45:3A:219:LEU:HD12	2.01	0.42
46:3B:86:THR:O	46:3B:90:GLU:HG3	2.19	0.42
48:3D:320:LYS:HA	48:3D:320:LYS:HD2	1.95	0.42
49:3E:112:GLY:HA2	53:3J:14:TYR:HB2	2.01	0.42
49:3E:143:SER:OG	49:3E:145:ASP:OD1	2.36	0.42
46:3O:369:LEU:HD11	46:3O:399:LEU:HD11	2.02	0.42
57:4C:132:LEU:HD22	57:4C:176:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:4C:303:PGV:H032	87:4C:303:PGV:H042	2.02	0.42
55:8A:403:TYR:CZ	55:8A:479:LYS:HG2	2.54	0.42
55:8A:409:TRP:HB2	55:8A:471:ILE:HD11	1.98	0.42
56:8B:7:LEU:O	75:8B:303:CDL:H552	2.19	0.42
56:8B:43:SER:OG	87:8B:301:PGV:O02	2.33	0.42
58:8D:78:TRP:HB3	75:8D:201:CDL:H182	2.01	0.42
61:8G:72:ASN:HB3	61:8G:75:VAL:HG12	2.02	0.42
1:1A:92:LEU:HD13	27:1b:29:ILE:HG12	2.01	0.42
2:1B:65:PRO:HD3	4:1D:168:PHE:HB3	2.02	0.42
2:1B:114:VAL:HG22	2:1B:144:ILE:HB	2.00	0.42
4:1D:126:LEU:HD23	4:1D:359:PRO:HD3	2.02	0.42
4:1D:193:TYR:OH	4:1D:201:GLN:O	2.34	0.42
5:1E:12:THR:O	5:1E:16:ASN:ND2	2.52	0.42
5:1E:55:GLN:NE2	5:1E:90:TYR:HD1	2.18	0.42
6:1F:129:MET:CE	6:1F:221:THR:HB	2.49	0.42
6:1F:150:GLN:HB3	44:1s:54:LEU:HD12	2.02	0.42
7:1G:616:LEU:HA	7:1G:619:VAL:HG12	2.02	0.42
10:1J:130:THR:HG22	25:1Z:121:MET:SD	2.60	0.42
12:1L:73:THR:HG21	12:1L:194:ASN:HD21	1.77	0.42
13:1M:61:LEU:HB2	13:1M:457:PRO:HD3	2.01	0.42
15:1O:3:TYR:CZ	15:1O:260:ARG:HD3	2.55	0.42
17:1Q:9:GLN:CB	22:1W:23:ARG:NH2	2.80	0.42
32:1g:112:CYS:N	41:1p:158:GLN:OE1	2.53	0.42
33:1h:94:LEU:HD23	33:1h:94:LEU:HA	1.92	0.42
45:3A:146:ARG:HA	45:3A:149:VAL:HG12	2.02	0.42
46:3B:31:ASN:OD1	46:3B:228:GLY:HA2	2.19	0.42
46:3O:118:ILE:H	46:3O:118:ILE:HG13	1.60	0.42
47:3P:105:GLY:O	47:3P:108:MET:HG2	2.20	0.42
47:3P:141:TRP:HB3	47:3P:268:ILE:HD13	2.02	0.42
75:3P:504:CDL:H721	51:3T:41:THR:OG1	2.19	0.42
49:3R:225:ILE:HG22	49:3R:228:ALA:HB3	2.02	0.42
54:3Y:39:ARG:O	54:3Y:43:ASP:OD1	2.36	0.42
55:4A:65:MET:HE3	88:4A:604:HEA:H131	2.02	0.42
87:4A:603:PGV:H141	87:4A:603:PGV:H182	2.01	0.42
56:4B:1:FME:HG2	56:4B:10:GLN:OE1	2.20	0.42
56:4B:122:MET:HE2	56:4B:122:MET:HB3	1.99	0.42
57:4C:15:PRO:HB2	64:4J:36:MET:CE	2.49	0.42
57:4C:112:LEU:HG	57:4C:118:PRO:HB3	2.00	0.42
58:4D:96:LEU:C	58:4D:96:LEU:CD2	2.89	0.42
60:4F:70:ILE:HG21	60:4F:83:PRO:HD2	2.01	0.42
68:4N:44:CYS:HB2	68:4N:53:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:8:TYR:O	57:8C:13:PRO:HB3	2.20	0.42
55:8A:92:MET:HB3	55:8A:163:ASN:HD21	1.85	0.42
55:8A:114:ALA:O	55:8A:118:VAL:HG13	2.20	0.42
55:8A:232:GLN:HB3	55:8A:292:MET:HE1	1.99	0.42
55:8A:239:GLY:O	55:8A:243:VAL:N	2.45	0.42
55:8A:318:VAL:HG13	56:8B:65:TRP:HE1	1.85	0.42
55:8A:364:ASP:O	55:8A:368:HIS:HB2	2.20	0.42
55:8A:427:PRO:HB3	55:8A:450:TRP:CE3	2.55	0.42
55:8A:439:ARG:NH2	88:8A:604:HEA:O1D	2.52	0.42
64:8J:36:MET:CA	64:8J:39:CYS:SG	3.06	0.42
2:1B:50:PHE:CZ	2:1B:103:VAL:HG21	2.55	0.42
70:1B:202:PC1:H3D2	8:1H:56:VAL:HG21	2.02	0.42
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.27	0.42
6:1F:36:ALA:HB1	6:1F:41:ASP:HB2	2.02	0.42
6:1F:46:LYS:HB2	6:1F:46:LYS:HE2	1.77	0.42
7:1G:216:THR:HG22	7:1G:248:MET:CE	2.49	0.42
8:1H:183:MET:HB3	9:1I:27:TRP:CH2	2.54	0.42
9:1I:153:LYS:HA	9:1I:153:LYS:HD2	1.73	0.42
10:1J:7:PHE:CZ	11:1K:3:LEU:HD13	2.55	0.42
70:1M:505:PC1:H332	75:1h:202:CDL:OA8	2.20	0.42
14:1N:322:GLN:HE22	29:1d:49:ARG:HG2	1.84	0.42
16:1P:46:ILE:HD12	18:1R:26:VAL:HG21	2.02	0.42
16:1P:81:ILE:HD13	16:1P:117:ILE:HD13	2.00	0.42
16:1P:136:ASN:HB3	16:1P:146:LEU:HD13	2.02	0.42
16:1P:319:ARG:HA	16:1P:322:ARG:HD3	2.00	0.42
19:1S:87:THR:O	19:1S:91:GLU:OE2	2.38	0.42
20:1T:70:LEU:HD11	20:1T:79:TYR:CG	2.54	0.42
27:1b:58:ASP:HA	27:1b:62:MET:SD	2.59	0.42
28:1c:31:LEU:HD13	29:1d:70:PHE:HA	2.02	0.42
31:1f:48:LEU:H	31:1f:48:LEU:HD12	1.85	0.42
32:1g:68:ILE:O	32:1g:72:LEU:HB2	2.20	0.42
33:1h:40:ILE:HG22	75:1h:202:CDL:OB9	2.19	0.42
34:1i:74:VAL:C	34:1i:77:PRO:HD2	2.45	0.42
40:1o:33:ARG:HA	40:1o:33:ARG:HD2	1.83	0.42
41:1p:35:ILE:N	41:1p:35:ILE:HD13	2.35	0.42
45:3A:356:ARG:HG3	46:3B:91:ALA:HA	2.02	0.42
69:3A:503:3PE:H2	69:3A:503:3PE:O14	2.19	0.42
47:3C:322:GLN:NE2	69:3C:503:3PE:H111	2.35	0.42
48:3Q:126:TYR:OH	86:3Q:501:HEC:O2A	2.22	0.42
52:3U:77:LEU:HD23	52:3U:77:LEU:HA	1.86	0.42
54:3Y:40:LEU:HB2	69:3Y:101:3PE:H122	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:142:SER:O	55:4A:146:THR:HG23	2.20	0.42
55:4A:202:LEU:HB2	55:4A:238:PHE:CG	2.54	0.42
56:4B:62:GLU:HA	56:4B:65:TRP:CE3	2.52	0.42
56:4B:142:VAL:HG12	56:4B:144:LEU:HG	2.02	0.42
75:4B:303:CDL:H442	75:4B:303:CDL:H182	2.01	0.42
57:4C:158:HIS:HE2	93:4G:102:PEK:H041	1.85	0.42
55:8A:200:PRO:HB2	57:8C:92:LEU:HB3	2.01	0.42
87:8A:601:PGV:H92	87:8A:601:PGV:H241	2.01	0.42
56:8B:1:FME:HE2	56:8B:192:TYR:HA	2.01	0.42
56:8B:103:GLN:OE1	56:8B:104:TRP:CE2	2.73	0.42
56:8B:108:TYR:HB2	56:8B:118:PHE:CE1	2.53	0.42
56:8B:193:TYR:HD1	56:8B:210:VAL:HG22	1.84	0.42
67:8M:42:ARG:H	67:8M:42:ARG:HG3	1.67	0.42
1:1A:24:LEU:HD21	70:1B:202:PC1:H3C2	2.02	0.42
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.55	0.42
7:1G:528:ASP:OD1	7:1G:545:TYR:OH	2.36	0.42
9:1I:155:LEU:HD23	9:1I:155:LEU:HA	1.88	0.42
10:1J:64:MET:HE3	10:1J:64:MET:HB2	1.60	0.42
11:1K:37:MET:HG3	11:1K:67:ALA:CB	2.50	0.42
12:1L:538:THR:HB	69:1L:701:3PE:H271	2.01	0.42
14:1N:137:ALA:HB3	14:1N:138:PRO:HD3	2.02	0.42
16:1P:289:MET:HE3	16:1P:289:MET:HB2	1.82	0.42
20:1T:76:ILE:O	20:1T:80:ILE:HG13	2.19	0.42
20:1U:37:MET:HA	20:1U:42:LEU:O	2.20	0.42
39:1n:132:TRP:O	39:1n:135:GLU:HG2	2.19	0.42
45:3A:206:ARG:HG3	45:3A:207:GLN:N	2.35	0.42
47:3C:111:GLU:OE2	47:3C:111:GLU:N	2.45	0.42
47:3C:186:PRO:HA	47:3C:189:ILE:HD12	2.02	0.42
48:3D:232:ARG:HG3	49:3R:235:TYR:HE1	1.84	0.42
49:3E:145:ASP:OD1	49:3E:145:ASP:N	2.53	0.42
53:3J:57:LYS:N	53:3J:60:LYS:HG3	2.35	0.42
45:3N:155:ALA:HA	45:3N:164:ALA:HB1	2.02	0.42
47:3P:5:ARG:HG2	47:3P:15:ASN:HB2	2.02	0.42
49:3R:263:TYR:HB2	49:3R:271:VAL:HG22	2.01	0.42
87:4B:302:PGV:H102	87:4B:302:PGV:H271	2.02	0.42
57:4C:103:HIS:HA	87:4C:303:PGV:O02	2.19	0.42
57:4C:137:LEU:HD23	57:4C:137:LEU:HA	1.72	0.42
66:4L:45:LEU:CD2	67:4M:40:TYR:CD2	3.03	0.42
55:8A:25:TRP:CD1	87:8L:101:PGV:H291	2.55	0.42
59:8E:42:VAL:CG2	63:8I:9:MET:SD	3.08	0.42
59:8E:102:GLU:HA	59:8E:107:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:8G:26:PRO:HB2	93:8G:102:PEK:H383	2.01	0.42
68:8N:52:GLU:HG3	68:8N:55:ASN:OD1	2.19	0.42
1:1A:84:LEU:HD23	1:1A:84:LEU:HA	1.90	0.41
2:1B:99:ALA:O	2:1B:103:VAL:HG13	2.19	0.41
2:1B:154:GLU:HB3	9:1I:137:PHE:HE2	1.84	0.41
6:1F:189:GLU:HG2	6:1F:190:THR:N	2.34	0.41
6:1F:319:PHE:CZ	6:1F:329:LEU:HD23	2.55	0.41
7:1G:74:MET:HE2	7:1G:77:TRP:CZ2	2.54	0.41
8:1H:30:TYR:HE1	9:1I:45:PRO:HG3	1.85	0.41
12:1L:63:ILE:HG13	34:1i:96:VAL:HG22	2.02	0.41
12:1L:386:LEU:HD23	12:1L:386:LEU:HA	1.89	0.41
13:1M:196:TRP:HZ2	13:1M:254:THR:HG23	1.85	0.41
14:1N:339:MET:HE3	14:1N:339:MET:HB3	1.88	0.41
15:1O:211:LEU:HD13	15:1O:222:GLN:HE21	1.85	0.41
16:1P:200:THR:OG1	16:1P:288:HIS:O	2.22	0.41
25:1Z:105:LYS:HD3	25:1Z:105:LYS:N	2.35	0.41
33:1h:111:ARG:NH1	82:1h:201:AME:O	2.49	0.41
47:3C:326:TRP:NE1	51:3G:50:VAL:HG22	2.34	0.41
48:3D:145:THR:HG22	53:3J:56:TRP:HZ2	1.85	0.41
52:3H:53:GLU:HG3	52:3H:57:LYS:HE3	2.02	0.41
56:4B:104:TRP:CG	56:4B:203:ASN:HB2	2.55	0.41
62:4H:24:ASN:OD1	62:4H:26:THR:HG22	2.20	0.41
63:4I:21:ILE:HG22	63:4I:25:PHE:CE2	2.55	0.41
55:8A:157:SER:HB2	55:8A:199:LEU:CD1	2.49	0.41
56:8B:105:TYR:CE2	56:8B:119:ASP:OD2	2.71	0.41
57:8C:176:LEU:O	57:8C:180:GLU:HG2	2.19	0.41
59:8E:10:GLU:O	59:8E:14:ARG:HG2	2.19	0.41
59:8E:23:ASP:OD1	59:8E:23:ASP:C	2.63	0.41
1:1A:46:SER:HB3	1:1A:49:LEU:HD11	2.02	0.41
3:1C:192:GLN:HB2	17:1Q:72:TRP:CD1	2.55	0.41
6:1F:94:VAL:HB	6:1F:222:VAL:HG22	2.01	0.41
6:1F:355:LYS:HE3	6:1F:355:LYS:HB3	1.97	0.41
7:1G:139:ASP:HB3	7:1G:148:THR:O	2.20	0.41
7:1G:209:THR:HG22	7:1G:210:SER:H	1.85	0.41
12:1L:203:MET:HE2	41:1p:113:GLN:HG2	2.02	0.41
12:1L:257:VAL:HG23	12:1L:329:ILE:HD11	2.02	0.41
12:1L:416:THR:O	12:1L:419:THR:OG1	2.37	0.41
12:1L:499:MET:HE1	64:4J:37:THR:CG2	2.49	0.41
13:1M:393:ILE:HD12	13:1M:393:ILE:HA	1.85	0.41
15:1O:72:GLN:H	15:1O:72:GLN:HG3	1.63	0.41
16:1P:194:ILE:HG13	16:1P:263:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:87:TYR:C	20:1T:88:GLU:HG2	2.45	0.41
24:1Y:51:GLY:HA3	69:1Y:206:3PE:H232	2.01	0.41
34:1i:43:GLU:O	34:1i:47:ASN:ND2	2.53	0.41
45:3A:50:GLU:O	45:3A:173:ASN:ND2	2.37	0.41
47:3C:240:LEU:HD21	69:3D:502:3PE:H242	2.02	0.41
47:3C:326:TRP:CH2	69:3C:503:3PE:H231	2.55	0.41
46:3O:100:SER:OG	46:3O:105:MET:HG2	2.20	0.41
47:3P:138:MET:HG2	47:3P:254:ASP:HB3	2.02	0.41
48:3Q:225:HIS:CD2	51:3T:20:PRO:HB2	2.55	0.41
49:3R:169:TRP:HD1	49:3R:174:LEU:HD22	1.84	0.41
64:4J:55:PHE:HB2	64:4J:57:HIS:CE1	2.55	0.41
55:8A:331:ASN:OD1	58:8D:20:ARG:NE	2.53	0.41
55:8A:404:THR:HG21	67:8M:3:ALA:HB2	2.03	0.41
56:8B:63:THR:HG22	56:8B:67:ILE:CD1	2.40	0.41
58:8D:44:GLU:OE1	59:8E:59:ASN:C	2.63	0.41
66:8L:18:LYS:NZ	66:8L:19:TRP:CE2	2.71	0.41
67:8M:2:TYR:HD1	67:8M:2:TYR:H	1.68	0.41
1:1A:3:ILE:HG21	70:1H:403:PC1:H252	2.01	0.41
2:1B:60:MET:HG3	4:1D:171:PHE:HE2	1.84	0.41
3:1C:138:PHE:O	3:1C:163:ARG:NE	2.53	0.41
4:1D:107:ASP:OD2	4:1D:371:LYS:HE2	2.20	0.41
4:1D:152:MET:HE2	4:1D:152:MET:HB2	1.98	0.41
6:1F:250:ASN:HB2	6:1F:319:PHE:HD2	1.85	0.41
7:1G:157:THR:HG22	7:1G:161:ARG:HG3	2.02	0.41
7:1G:210:SER:HB2	7:1G:269:PHE:HE1	1.86	0.41
7:1G:510:GLY:C	7:1G:512:GLU:OE2	2.64	0.41
7:1G:625:GLU:O	19:1S:21:HIS:HE1	2.03	0.41
8:1H:260:VAL:O	8:1H:264:LEU:HG	2.19	0.41
12:1L:281:GLY:HA3	12:1L:314:MET:HB3	2.02	0.41
13:1M:244:MET:HG3	13:1M:301:ILE:HD13	2.02	0.41
14:1N:323:MET:HE3	14:1N:323:MET:HB3	1.94	0.41
14:1N:337:LEU:O	14:1N:340:THR:OG1	2.24	0.41
15:1O:154:GLU:O	15:1O:158:VAL:HG23	2.20	0.41
17:1Q:116:LYS:HD3	17:1Q:116:LYS:HA	1.92	0.41
28:1c:39:VAL:O	28:1c:43:LYS:HG3	2.20	0.41
39:1n:144:PRO:HD3	39:1n:147:GLY:O	2.20	0.41
46:3B:257:LEU:HD11	46:3B:422:LYS:HB3	2.02	0.41
48:3D:160:ASP:HB3	48:3D:169:PHE:CZ	2.56	0.41
50:3F:110:ILE:O	50:3F:114:LYS:HG2	2.21	0.41
47:3P:291:VAL:O	47:3P:295:VAL:HG22	2.21	0.41
47:3P:377:LEU:HD23	47:3P:377:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:219:HIS:CE1	49:3R:239:HIS:ND1	2.89	0.41
49:3R:226:ALA:HA	49:3R:234:TYR:HD1	1.86	0.41
55:4A:489:SER:OG	60:4F:70:ILE:HG23	2.20	0.41
62:4H:54:GLU:O	62:4H:54:GLU:HG3	2.20	0.41
56:8B:29:MET:HE3	63:8I:36:LYS:HG3	2.02	0.41
57:8C:61:ILE:HD11	87:8C:301:PGV:H031	2.02	0.41
57:8C:247:VAL:CG1	57:8C:251:PHE:HE1	2.28	0.41
59:8E:49:ASP:O	59:8E:53:ARG:HG3	2.20	0.41
65:8K:52:GLU:OE2	65:8K:54:ARG:N	2.53	0.41
4:1D:148:LEU:HG	4:1D:177:MET:SD	2.61	0.41
4:1D:164:MET:O	4:1D:167:PHE:HB3	2.20	0.41
5:1E:15:ASN:OD1	5:1E:60:TRP:CH2	2.73	0.41
5:1E:159:ASN:OD1	5:1E:159:ASN:N	2.51	0.41
5:1E:205:PRO:HA	5:1E:206:PRO:HD2	1.97	0.41
6:1F:293:ASN:OD1	6:1F:339:ARG:HB2	2.20	0.41
7:1G:441:GLN:OE1	7:1G:441:GLN:HA	2.21	0.41
10:1J:17:PHE:HA	10:1J:20:PHE:CE2	2.56	0.41
12:1L:558:LEU:HD23	12:1L:558:LEU:HA	1.83	0.41
69:1N:901:3PE:H2	69:1N:901:3PE:H111	2.02	0.41
15:1O:19:THR:HG22	15:1O:20:GLU:H	1.85	0.41
16:1P:29:PHE:HZ	16:1P:173:GLY:HA3	1.86	0.41
16:1P:110:PHE:HB2	16:1P:148:SER:OG	2.20	0.41
19:1S:19:ARG:HG3	19:1S:53:LEU:HB2	2.03	0.41
22:1W:82:LEU:HD12	22:1W:82:LEU:HA	1.95	0.41
23:1X:47:TRP:CG	27:1b:54:VAL:HG21	2.54	0.41
23:1X:84:TYR:CE1	23:1X:103:GLN:HB2	2.56	0.41
69:1Y:203:3PE:H282	70:1Y:207:PC1:H3D1	2.03	0.41
34:1i:44:GLN:O	34:1i:48:LYS:HG3	2.21	0.41
45:3A:93:GLU:HG3	45:3A:94:HIS:CD2	2.56	0.41
48:3D:225:PRO:HA	48:3D:226:PRO:HD3	1.91	0.41
48:3D:326:TYR:HB2	50:3F:72:PHE:CE1	2.56	0.41
49:3E:213:LEU:HD13	49:3E:247:GLY:HA3	2.01	0.41
49:3E:231:PHE:CE1	49:3E:242:HIS:HB3	2.47	0.41
46:3O:181:TYR:CZ	46:3O:182:ARG:HG2	2.55	0.41
47:3P:138:MET:HE1	47:3P:268:ILE:HA	2.02	0.41
48:3Q:124:GLU:HG2	48:3Q:191:ARG:HB2	2.02	0.41
55:4A:291:HIS:CE1	88:4A:605:HEA:HBD1	2.55	0.41
55:4A:420:GLY:O	55:4A:424:THR:OG1	2.33	0.41
56:4B:152:MET:HA	56:4B:152:MET:HE3	2.02	0.41
58:4D:63:LYS:HB3	58:4D:64:PHE:CE1	2.54	0.41
60:4F:33:ILE:HG22	60:4F:34:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:155:VAL:CG1	55:8A:159:LEU:HD11	2.51	0.41
75:8C:306:CDL:H111	75:8C:306:CDL:H152	2.01	0.41
87:8J:101:PGV:H302	87:8J:101:PGV:H343	2.02	0.41
1:1A:54:LYS:HZ3	4:1D:71:GLU:HB2	1.86	0.41
3:1C:137:MET:HB3	3:1C:162:PHE:HB2	2.02	0.41
7:1G:41:CYS:O	7:1G:161:ARG:NH2	2.51	0.41
8:1H:161:THR:HG22	8:1H:163:SER:H	1.85	0.41
9:1I:47:THR:O	42:1q:58:ARG:HD2	2.21	0.41
9:1I:143:THR:OG1	9:1I:146:GLU:HG3	2.21	0.41
12:1L:295:GLN:HB2	12:1L:301:ILE:HG12	2.02	0.41
13:1M:343:ILE:HG13	13:1M:346:ARG:HD3	2.02	0.41
15:1O:163:TYR:OH	15:1O:269:VAL:HG13	2.20	0.41
16:1P:136:ASN:HA	16:1P:292:MET:HG3	2.01	0.41
17:1Q:34:LYS:HE2	17:1Q:34:LYS:HB2	1.81	0.41
18:1R:22:ASP:OD2	18:1R:24:ARG:NH1	2.53	0.41
24:1Y:72:THR:HG22	24:1Y:91:ILE:HG22	2.02	0.41
40:1o:93:ASP:O	40:1o:97:ARG:HG3	2.21	0.41
44:1s:58:LEU:HA	44:1s:61:PHE:CE1	2.55	0.41
46:3B:122:PHE:O	46:3B:126:VAL:HG13	2.20	0.41
46:3B:160:LEU:HD12	49:3I:64:LEU:HD13	2.02	0.41
47:3C:111:GLU:CD	47:3C:111:GLU:N	2.78	0.41
47:3C:185:LEU:HD23	47:3C:188:ILE:HD12	2.01	0.41
47:3C:326:TRP:CZ2	69:3C:503:3PE:H231	2.55	0.41
49:3E:101:LYS:HE2	49:3E:101:LYS:HB2	1.88	0.41
49:3E:196:ARG:HD2	49:3E:196:ARG:HA	1.78	0.41
49:3I:62:ARG:HB3	49:3I:63:PRO:HD2	2.03	0.41
45:3N:87:ASN:HB3	45:3N:98:TYR:CZ	2.56	0.41
45:3N:344:ARG:HH12	45:3N:353:GLU:CD	2.27	0.41
47:3P:309:THR:HG1	47:3P:370:SER:HG	1.59	0.41
51:3T:71:ARG:HD2	52:3U:56:GLU:OE1	2.21	0.41
56:4B:40:TYR:CD2	63:4I:27:VAL:HG11	2.55	0.41
57:4C:27:MET:CE	57:4C:50:ASN:HD22	2.33	0.41
57:4C:203:PHE:O	57:4C:207:HIS:ND1	2.38	0.41
58:4D:76:ASN:HD22	58:4D:79:LYS:NZ	2.18	0.41
58:4D:93:ALA:O	58:4D:97:ILE:HG13	2.20	0.41
55:8A:51:ASP:HB2	56:8B:202:SER:O	2.20	0.41
56:8B:129:LYS:N	56:8B:132:GLU:OE2	2.53	0.41
87:8C:303:PGV:H202	87:8C:303:PGV:H011	1.24	0.41
1:1A:18:VAL:HG21	8:1H:76:ILE:HG13	2.03	0.41
2:1B:68:ASP:O	2:1B:71:ARG:HG2	2.21	0.41
4:1D:100:LEU:HD12	4:1D:118:TYR:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:275:TYR:CZ	4:1D:367:ILE:HB	2.55	0.41
4:1D:423:ILE:HG23	4:1D:428:VAL:HG21	2.01	0.41
5:1E:55:GLN:NE2	5:1E:90:TYR:HA	2.30	0.41
7:1G:237:ASN:H	7:1G:259:ASN:HD22	1.66	0.41
8:1H:100:LEU:HB3	8:1H:103:LEU:HB2	2.03	0.41
8:1H:310:MET:O	27:1b:37:TYR:HB2	2.21	0.41
12:1L:161:ARG:NH2	39:1n:87:GLY:O	2.41	0.41
12:1L:169:LEU:HD12	12:1L:169:LEU:HA	1.91	0.41
12:1L:313:MET:HA	12:1L:316:THR:HG22	2.01	0.41
12:1L:401:MET:HE3	12:1L:401:MET:HB3	1.88	0.41
12:1L:560:THR:O	12:1L:565:THR:OG1	2.37	0.41
13:1M:56:PHE:CZ	13:1M:108:MET:HG2	2.56	0.41
13:1M:71:TRP:O	13:1M:74:PRO:HD2	2.20	0.41
13:1M:88:THR:OG1	13:1M:91:ARG:HG3	2.20	0.41
15:1O:6:LEU:HD12	15:1O:6:LEU:HA	1.81	0.41
18:1R:27:ARG:HE	18:1R:27:ARG:HB3	1.67	0.41
25:1Z:56:GLU:OE1	25:1Z:59:ARG:NH2	2.40	0.41
37:1l:118:VAL:O	37:1l:121:ILE:HG12	2.21	0.41
41:1p:42:ARG:O	41:1p:46:LEU:HG	2.20	0.41
45:3A:156:THR:O	45:3A:239:SER:OG	2.39	0.41
46:3B:35:ILE:HG22	46:3B:213:HIS:CE1	2.56	0.41
47:3C:113:TRP:O	47:3C:117:VAL:HG23	2.21	0.41
47:3C:223:TYR:O	47:3C:226:ILE:HG22	2.20	0.41
69:3C:504:3PE:H281	54:3X:35:ALA:HB1	2.03	0.41
49:3E:130:LYS:NZ	54:3Y:37:ASP:OD1	2.54	0.41
49:3E:242:HIS:CG	49:3E:251:LYS:HB3	2.56	0.41
46:3O:102:ARG:NH2	46:3O:161:GLU:OE1	2.46	0.41
49:3R:152:ILE:HD12	49:3R:152:ILE:HA	1.66	0.41
49:3R:207:LYS:HB2	49:3R:265:PHE:HD2	1.85	0.41
51:3T:71:ARG:HD3	51:3T:71:ARG:HA	1.80	0.41
55:4A:28:MET:HE2	67:4M:26:PHE:CZ	2.55	0.41
88:4A:604:HEA:H171	88:4A:604:HEA:H202	1.80	0.41
56:4B:134:ARG:HD3	58:4D:110:THR:OG1	2.21	0.41
57:4C:15:PRO:O	57:4C:19:THR:OG1	2.36	0.41
66:4L:41:ARG:HG3	67:4M:40:TYR:OH	2.21	0.41
67:4M:11:SER:OG	67:4M:14:GLU:HG3	2.20	0.41
68:4N:57:LEU:HD23	68:4N:57:LEU:HA	1.91	0.41
55:8A:177:SER:HB3	55:8A:180:GLN:HG3	2.02	0.41
55:8A:489:SER:OG	60:8F:70:ILE:HG23	2.21	0.41
57:8C:140:SER:CB	57:8C:242:TRP:HE1	2.34	0.41
58:8D:48:TRP:NE1	59:8E:56:ARG:CD	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:8D:57:VAL:O	58:8D:61:ARG:HG2	2.20	0.41
68:8N:46:ASP:OD1	68:8N:48:LYS:HG3	2.20	0.41
2:1B:71:ARG:HB2	8:1H:38:ASN:OD1	2.21	0.41
4:1D:230:THR:HG23	4:1D:298:LEU:HD21	2.01	0.41
5:1E:143:GLU:HB3	6:1F:353:PHE:HD1	1.86	0.41
6:1F:45:THR:O	6:1F:49:LEU:HD23	2.20	0.41
6:1F:256:PHE:CD1	6:1F:317:MET:HE2	2.56	0.41
12:1L:161:ARG:HH21	39:1n:90:TYR:N	2.18	0.41
69:1L:703:3PE:H282	75:1h:202:CDL:OA9	2.21	0.41
13:1M:86:LYS:HB2	13:1M:86:LYS:HE2	1.71	0.41
13:1M:281:ASP:HB3	13:1M:284:SER:HB3	2.02	0.41
15:1O:318:TRP:CD2	15:1O:319:LEU:HD12	2.55	0.41
16:1P:64:ASP:HB3	16:1P:67:GLN:HG2	2.02	0.41
16:1P:113:ILE:HB	16:1P:114:PRO:HD3	2.03	0.41
20:1U:60:PHE:CE1	20:1U:80:ILE:HG13	2.55	0.41
21:1V:13:LEU:HD23	21:1V:13:LEU:HA	1.79	0.41
26:1a:59:ARG:NE	26:1a:61:HIS:NE2	2.69	0.41
32:1g:113:PHE:HB2	41:1p:158:GLN:HE22	1.86	0.41
34:1i:89:VAL:O	34:1i:95:THR:OG1	2.37	0.41
37:1l:72:ASN:HB3	37:1l:75:GLU:HG2	2.03	0.41
40:1o:83:GLN:C	40:1o:83:GLN:OE1	2.63	0.41
70:1q:201:PC1:H3B2	70:1q:201:PC1:H2E1	2.01	0.41
45:3A:77:LYS:HE3	45:3A:77:LYS:HB2	1.77	0.41
45:3A:316:GLU:OE1	45:3A:316:GLU:N	2.54	0.41
45:3A:439:SER:HA	45:3A:442:PHE:CE2	2.55	0.41
46:3B:70:ARG:HD3	46:3B:100:SER:OG	2.20	0.41
47:3C:33:PHE:HA	47:3C:36:LEU:HB2	2.03	0.41
69:3N:501:3PE:H262	75:3N:502:CDL:HB62	2.02	0.41
47:3P:50:PHE:HZ	69:3R:302:3PE:H2I3	1.86	0.41
47:3P:150:LEU:HD23	47:3P:150:LEU:HA	1.89	0.41
55:4A:94:PHE:N	55:4A:163:ASN:OD1	2.49	0.41
55:4A:113:LEU:HD22	66:4L:39:ILE:HD11	2.02	0.41
55:4A:362:SER:O	56:4B:87:MET:HE1	2.20	0.41
55:8A:467:LEU:HD13	58:8D:88:PHE:CE2	2.56	0.41
55:8A:508:PRO:HD2	57:8C:5:THR:HG22	2.01	0.41
2:1B:32:LYS:HA	2:1B:32:LYS:HD2	1.75	0.41
4:1D:283:PHE:CG	4:1D:310:ILE:HD11	2.55	0.41
5:1E:14:GLU:N	5:1E:14:GLU:CD	2.79	0.41
5:1E:31:ILE:HG13	5:1E:53:LEU:HD23	2.03	0.41
6:1F:95:VAL:HB	6:1F:136:ILE:HA	2.02	0.41
7:1G:210:SER:HB2	7:1G:269:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:153:VAL:O	8:1H:156:MET:HG2	2.21	0.41
9:1I:64:GLU:OE2	9:1I:149:TYR:OH	2.35	0.41
10:1J:125:TRP:HH2	25:1Z:126:GLY:HA2	1.84	0.41
11:1K:44:SER:CB	11:1K:59:MET:HE1	2.51	0.41
12:1L:316:THR:HG23	12:1L:325:ALA:HB2	2.02	0.41
13:1M:88:THR:O	13:1M:92:LYS:HG3	2.20	0.41
14:1N:74:ILE:HG13	14:1N:98:MET:HE1	2.03	0.41
14:1N:231:SER:O	14:1N:234:TRP:HD1	2.04	0.41
14:1N:276:ILE:C	14:1N:279:PRO:HD2	2.45	0.41
15:1O:133:VAL:HG21	15:1O:206:TYR:CE2	2.56	0.41
15:1O:135:LEU:HD21	15:1O:149:VAL:HB	2.02	0.41
23:1X:73:ILE:HD13	23:1X:73:ILE:HA	1.97	0.41
24:1Y:31:THR:O	24:1Y:35:VAL:HG12	2.21	0.41
25:1Z:53:TRP:NE1	25:1Z:57:ARG:HD2	2.35	0.41
41:1p:27:ASN:OD1	41:1p:29:VAL:HG22	2.20	0.41
41:1p:140:ASP:O	41:1p:161:ARG:NH2	2.52	0.41
42:1q:22:GLY:O	42:1q:26:VAL:HG22	2.21	0.41
45:3A:27:SER:HA	45:3A:199:ALA:O	2.20	0.41
45:3A:36:THR:HG21	45:3A:373:THR:HA	2.01	0.41
45:3A:172:GLU:O	45:3A:176:LYS:HD3	2.21	0.41
49:3E:236:CYS:HB2	49:3E:241:SER:O	2.20	0.41
49:3E:249:ILE:H	49:3E:257:ASN:HB3	1.86	0.41
45:3N:223:TYR:O	45:3N:224:VAL:C	2.63	0.41
45:3N:242:ARG:NH2	45:3N:432:PRO:O	2.53	0.41
55:4A:383:MET:HE1	55:4A:422:ASN:HA	2.03	0.41
61:4G:73:PRO:CA	61:4G:83:GLU:OE2	2.66	0.41
55:8A:53:ILE:HA	55:8A:56:VAL:HG22	2.03	0.41
55:8A:282:PHE:CD1	55:8A:282:PHE:C	2.97	0.41
55:8A:442:ASP:HB3	56:8B:135:LEU:HD21	2.02	0.41
57:8C:51:THR:HA	57:8C:54:MET:HE3	2.03	0.41
1:1A:49:LEU:N	1:1A:50:PRO:HD2	2.35	0.41
4:1D:49:LEU:HD12	4:1D:49:LEU:HA	1.97	0.41
6:1F:230:VAL:O	6:1F:234:ILE:HG12	2.21	0.41
6:1F:405:CYS:HB2	71:1F:502:SF4:S1	2.59	0.41
7:1G:24:THR:O	7:1G:73:VAL:HG22	2.21	0.41
7:1G:118:ASP:O	7:1G:122:MET:HG2	2.20	0.41
7:1G:190:MET:HG2	7:1G:192:MET:HE3	1.99	0.41
7:1G:549:HIS:NE2	7:1G:677:ILE:HG22	2.35	0.41
8:1H:26:LYS:NZ	8:1H:35:LYS:O	2.47	0.41
8:1H:130:ILE:HD13	8:1H:130:ILE:HA	1.95	0.41
9:1I:54:LYS:HZ2	9:1I:54:LYS:HG2	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:1I:203:PC1:H362	70:1I:203:PC1:H3A1	2.02	0.41
10:1J:86:ASN:ND2	11:1K:23:ARG:NH1	2.67	0.41
11:1K:3:LEU:HD23	11:1K:6:MET:SD	2.60	0.41
11:1K:26:LEU:HB3	11:1K:78:LEU:HD12	2.02	0.41
12:1L:27:TYR:O	12:1L:115:ASN:ND2	2.49	0.41
12:1L:371:THR:HG21	35:1j:25:ALA:HB1	2.02	0.41
13:1M:207:MET:HE1	13:1M:240:GLY:HA2	2.03	0.41
15:1O:180:GLN:OE1	15:1O:196:ALA:HB2	2.21	0.41
16:1P:268:ARG:O	16:1P:272:VAL:HG23	2.21	0.41
19:1S:13:LEU:HD22	19:1S:69:ALA:HB3	2.02	0.41
25:1Z:59:ARG:HA	25:1Z:62:ILE:CG2	2.50	0.41
25:1Z:97:ILE:HD13	30:1e:82:ARG:HB2	2.03	0.41
27:1b:56:LEU:HD13	27:1b:62:MET:HE1	2.02	0.41
28:1c:41:GLU:OE2	28:1c:45:ARG:NH2	2.48	0.41
29:1d:30:ARG:O	29:1d:34:MET:HG2	2.21	0.41
70:1d:202:PC1:H112	70:1d:202:PC1:H321	2.02	0.41
30:1e:75:LEU:HA	30:1e:75:LEU:HD23	1.79	0.41
31:1f:11:TRP:O	31:1f:14:ILE:HG12	2.20	0.41
35:1j:65:GLY:HA3	40:1o:30:PHE:CD1	2.54	0.41
37:1l:6:LYS:HA	37:1l:9:PHE:HD1	1.86	0.41
37:1l:156:TYR:CD1	40:1o:33:ARG:HB3	2.56	0.41
40:1o:16:PRO:HG2	40:1o:101:PHE:CE2	2.56	0.41
40:1o:92:LEU:O	40:1o:96:LYS:HG3	2.20	0.41
40:1o:96:LYS:O	40:1o:100:GLU:HG2	2.21	0.41
41:1p:8:VAL:HG13	41:1p:9:TYR:CD1	2.56	0.41
42:1q:25:ARG:HD2	42:1q:74:PHE:CZ	2.54	0.41
46:3B:306:PRO:HA	49:3I:52:ARG:HB2	2.02	0.41
47:3C:223:TYR:HB3	48:3D:316:TRP:CZ2	2.56	0.41
50:3F:87:LEU:O	50:3F:92:TRP:NE1	2.43	0.41
46:3O:340:ALA:O	46:3O:344:VAL:HG23	2.21	0.41
49:3R:110:ARG:HD2	51:3T:21:PHE:O	2.21	0.41
56:4B:49:LYS:O	56:4B:49:LYS:HG2	2.21	0.41
56:4B:105:TYR:HB2	56:4B:120:SER:O	2.20	0.41
57:4C:92:LEU:HD13	57:4C:92:LEU:HA	1.95	0.41
57:4C:132:LEU:HD12	61:4G:31:CYS:C	2.45	0.41
57:4C:141:GLY:O	57:4C:144:ILE:HG22	2.21	0.41
58:4D:33:LEU:HB3	58:4D:38:LYS:HG3	2.03	0.41
58:4D:82:VAL:HG22	75:4D:201:CDL:OB7	2.21	0.41
75:4D:201:CDL:HB61	75:4D:201:CDL:H711	1.48	0.41
60:4F:51:SER:HB3	60:4F:91:LEU:HD22	2.02	0.41
60:4F:90:LYS:NZ	60:4F:90:LYS:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:244:TYR:HB3	55:8A:248:LEU:HD11	2.02	0.41
55:8A:351:GLY:HA3	55:8A:380:VAL:HG13	2.02	0.41
55:8A:376:HIS:O	55:8A:380:VAL:HG22	2.20	0.41
55:8A:377:PHE:HB2	88:8A:605:HEA:C2D	2.51	0.41
57:8C:63:ARG:CD	64:8J:12:PHE:HE2	2.33	0.41
57:8C:101:PHE:CZ	57:8C:256:ILE:HA	2.56	0.41
58:8D:100:LYS:HG2	65:8K:36:ILE:HG21	2.03	0.41
59:8E:44:GLU:CD	59:8E:46:LYS:HB2	2.46	0.41
63:8I:28:SER:O	63:8I:31:VAL:HG22	2.20	0.41
63:8I:43:ARG:O	63:8I:47:TYR:CD1	2.71	0.41
1:1A:37:TYR:CD1	1:1A:37:TYR:C	2.99	0.41
1:1A:73:LEU:HD13	8:1H:103:LEU:HD21	2.03	0.41
2:1B:45:LEU:O	2:1B:47:PRO:HD3	2.21	0.41
2:1B:144:ILE:HD12	2:1B:162:GLN:HG2	2.02	0.41
3:1C:35:LYS:HD3	3:1C:36:TYR:CZ	2.55	0.41
6:1F:429:ARG:HE	6:1F:429:ARG:HB2	1.65	0.41
7:1G:113:GLU:HA	17:1Q:46:GLN:NE2	2.35	0.41
7:1G:366:THR:CB	7:1G:450:MET:HE2	2.51	0.41
9:1I:43:ARG:HG2	43:1r:11:ARG:HH21	1.86	0.41
12:1L:556:ILE:HD13	12:1L:556:ILE:HA	1.91	0.41
69:1M:502:3PE:H321	69:1M:502:3PE:H31	1.21	0.41
14:1N:131:LEU:HD12	14:1N:216:PHE:HE2	1.86	0.41
14:1N:310:ASN:HB2	15:1O:274:THR:HG22	2.02	0.41
19:1S:87:THR:O	19:1S:91:GLU:CD	2.64	0.41
20:1T:52:MET:HA	20:1T:55:GLU:CG	2.51	0.41
20:1U:60:PHE:HE1	20:1U:80:ILE:HG13	1.86	0.41
20:1U:61:GLU:OE2	39:1n:84:SER:OG	2.25	0.41
27:1b:38:THR:O	27:1b:42:ILE:HG13	2.21	0.41
29:1d:63:LEU:HD23	75:1d:203:CDL:HA62	2.02	0.41
36:1k:29:GLU:O	36:1k:33:GLU:HG2	2.20	0.41
38:1m:106:THR:O	38:1m:110:LYS:HG3	2.21	0.41
45:3A:87:ASN:ND2	45:3A:98:TYR:OH	2.41	0.41
46:3B:232:LEU:HD12	46:3B:232:LEU:HA	1.81	0.41
47:3C:50:PHE:CE2	49:3E:140:MET:HE2	2.56	0.41
49:3E:195:LEU:HD11	49:3E:248:ARG:HD2	2.03	0.41
45:3N:21:ASN:ND2	45:3N:216:PHE:O	2.54	0.41
45:3N:214:LYS:HE2	45:3N:214:LYS:HB2	1.86	0.41
49:3R:177:ARG:HH21	49:3R:245:ALA:HA	1.86	0.41
51:3T:50:PRO:O	51:3T:54:VAL:HG13	2.21	0.41
55:4A:127:THR:HB	55:4A:129:TYR:CE1	2.56	0.41
56:4B:4:PRO:HB3	65:4K:41:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:4D:201:CDL:H581	75:4D:201:CDL:H621	2.02	0.41
59:4E:49:ASP:C	59:4E:49:ASP:OD1	2.62	0.41
59:4E:72:LYS:HB2	59:4E:82:TYR:CE2	2.56	0.41
55:8A:53:ILE:O	55:8A:56:VAL:HG22	2.20	0.41
56:8B:102:HIS:HB2	56:8B:105:TYR:CE1	2.56	0.41
56:8B:147:GLU:C	56:8B:185:MET:HE1	2.46	0.41
58:8D:34:SER:CB	58:8D:37:GLN:OE1	2.69	0.41
63:8I:34:PHE:CD1	63:8I:34:PHE:C	2.99	0.41
5:1E:23:PHE:HA	5:1E:57:GLN:HE22	1.87	0.40
5:1E:192:SER:OG	5:1E:193:CYS:N	2.53	0.40
6:1F:15:LEU:HB2	6:1F:271:GLU:HB2	2.03	0.40
6:1F:47:GLU:O	6:1F:51:LYS:HG2	2.21	0.40
6:1F:126:GLY:HA3	6:1F:173:PHE:CE1	2.56	0.40
7:1G:94:MET:HE3	7:1G:120:SER:N	2.35	0.40
8:1H:74:ALA:HB3	8:1H:75:PRO:HD3	2.03	0.40
8:1H:144:VAL:O	8:1H:148:ILE:HG13	2.21	0.40
10:1J:171:ILE:HG23	14:1N:45:MET:SD	2.61	0.40
11:1K:41:PHE:HD1	11:1K:42:ILE:HD13	1.85	0.40
12:1L:355:ASP:OD2	12:1L:357:ARG:NH2	2.54	0.40
14:1N:155:LEU:HD22	14:1N:278:MET:HE2	2.02	0.40
15:1O:146:LYS:O	15:1O:149:VAL:HG22	2.22	0.40
17:1Q:85:THR:HG23	21:1V:115:ILE:HD11	2.03	0.40
26:1a:26:ILE:HD13	26:1a:26:ILE:N	2.36	0.40
36:1k:15:LEU:H	36:1k:15:LEU:HD12	1.86	0.40
37:1l:62:TYR:HD1	37:1l:63:ASP:N	2.19	0.40
44:1s:33:PHE:CD1	44:1s:33:PHE:C	2.99	0.40
45:3A:260:PRO:HB2	45:3A:264:ASN:HB3	2.03	0.40
45:3A:342:TRP:CZ3	45:3A:441:MET:HE1	2.56	0.40
45:3N:145:MET:HE1	45:3N:250:LEU:O	2.22	0.40
45:3N:316:GLU:OE1	45:3N:316:GLU:N	2.54	0.40
49:3R:267:SER:O	49:3R:271:VAL:HB	2.21	0.40
69:3R:302:3PE:H3B1	70:3R:303:PC1:H3F1	2.03	0.40
52:3U:49:GLN:C	52:3U:49:GLN:CD	2.89	0.40
55:4A:8:TYR:O	57:4C:13:PRO:HB3	2.21	0.40
55:4A:202:LEU:HD22	55:4A:238:PHE:CE2	2.56	0.40
56:4B:62:GLU:HG3	68:4N:14:SER:OG	2.21	0.40
75:4B:303:CDL:HA61	75:4B:303:CDL:H311	1.69	0.40
57:4C:129:VAL:HB	57:4C:130:PRO:HD3	2.03	0.40
58:4D:122:ARG:HG3	65:4K:53:TRP:CD2	2.56	0.40
55:8A:25:TRP:HB2	87:8L:101:PGV:H281	2.03	0.40
87:8A:601:PGV:H321	87:8A:601:PGV:H292	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:8B:148:MET:N	56:8B:148:MET:SD	2.94	0.40
57:8C:23:SER:O	57:8C:27:MET:HG3	2.21	0.40
57:8C:175:LEU:HD13	87:8C:305:PGV:H221	2.03	0.40
58:8D:77:GLU:O	58:8D:80:THR:OG1	2.33	0.40
59:8E:24:ILE:CD1	59:8E:28:GLU:HB2	2.51	0.40
2:1B:47:PRO:HD2	2:1B:75:VAL:O	2.21	0.40
2:1B:53:ALA:HB3	71:1B:201:SF4:S2	2.61	0.40
3:1C:58:ILE:HD12	3:1C:118:GLU:HG2	2.03	0.40
3:1C:147:ASP:OD1	3:1C:147:ASP:N	2.54	0.40
4:1D:237:ASN:CB	8:1H:284:GLN:OE1	2.68	0.40
6:1F:397:LYS:HA	6:1F:397:LYS:HD2	1.87	0.40
7:1G:195:LEU:HD11	7:1G:393:ALA:HB2	2.02	0.40
7:1G:349:PHE:H	7:1G:509:PRO:HB2	1.86	0.40
12:1L:116:ARG:HD3	75:1L:702:CDL:OB3	2.20	0.40
12:1L:341:MET:CE	12:1L:457:LEU:HD12	2.50	0.40
12:1L:545:SER:OG	13:1M:274:SER:HB3	2.22	0.40
69:1L:703:3PE:H281	75:1h:202:CDL:HB62	2.04	0.40
13:1M:325:MET:CE	13:1M:441:ILE:HB	2.51	0.40
14:1N:122:ILE:HD12	14:1N:126:ALA:HB1	2.03	0.40
15:1O:101:TYR:CE1	15:1O:128:ILE:HG23	2.48	0.40
17:1Q:27:GLU:HG2	17:1Q:28:GLU:OE1	2.21	0.40
19:1S:17:GLU:HB2	19:1S:51:PRO:HB2	2.03	0.40
25:1Z:131:GLU:HG3	25:1Z:132:GLU:N	2.35	0.40
28:1c:45:ARG:HE	28:1c:45:ARG:HB2	1.69	0.40
33:1h:11:ILE:HG22	39:1n:98:VAL:HG12	2.03	0.40
33:1h:56:PRO:HD3	41:1p:63:TYR:HE2	1.84	0.40
35:1j:69:ASP:CG	40:1o:117:ARG:HH22	2.28	0.40
42:1q:44:TYR:OH	42:1q:113:HIS:N	2.55	0.40
45:3A:40:TRP:CZ2	45:3A:377:GLU:HA	2.57	0.40
46:3B:181:TYR:CZ	46:3B:182:ARG:HG2	2.56	0.40
47:3C:226:ILE:HD12	47:3C:226:ILE:HA	1.98	0.40
51:3G:36:ILE:HB	51:3G:37:PRO:HD3	2.02	0.40
53:3J:23:THR:N	54:3Y:23:MET:SD	2.95	0.40
53:3J:56:TRP:HA	53:3J:59:ILE:HG12	2.03	0.40
45:3N:445:ARG:NH2	69:3N:501:3PE:O22	2.54	0.40
47:3P:72:ASP:CG	48:3Q:49:ARG:HH22	2.29	0.40
75:3P:504:CDL:OA9	75:3P:504:CDL:H341	2.21	0.40
55:4A:233:HIS:HB3	57:4C:99:TRP:CZ2	2.56	0.40
57:4C:22:LEU:O	57:4C:26:LEU:HG	2.21	0.40
57:4C:151:LEU:HD12	57:4C:151:LEU:HA	1.91	0.40
75:4C:305:CDL:H651	75:4C:305:CDL:H261	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:4H:75:ARG:HB3	62:4H:80:THR:O	2.21	0.40
65:4K:42:LEU:HD12	87:4K:101:PGV:H221	2.02	0.40
68:4N:14:SER:O	68:4N:17:PRO:HD2	2.22	0.40
55:8A:28:MET:HG3	66:8L:29:PHE:CD1	2.54	0.40
55:8A:253:MET:O	55:8A:257:ILE:HG12	2.20	0.40
55:8A:289:ALA:HB1	55:8A:297:MET:HE1	2.03	0.40
56:8B:41:ILE:CG2	56:8B:45:MET:CE	2.98	0.40
56:8B:136:LEU:HD22	56:8B:193:TYR:HB3	2.03	0.40
56:8B:145:PRO:HA	56:8B:214:VAL:O	2.20	0.40
4:1D:237:ASN:HB3	8:1H:284:GLN:OE1	2.21	0.40
6:1F:29:HIS:HA	44:1s:39:ARG:HH11	1.87	0.40
6:1F:57:LEU:HD23	6:1F:57:LEU:HA	1.96	0.40
7:1G:255:HIS:CE1	7:1G:257:ASP:HB2	2.57	0.40
8:1H:90:PRO:HG3	8:1H:162:LEU:HB3	2.04	0.40
8:1H:149:ILE:HG12	8:1H:181:LEU:HD22	2.04	0.40
9:1I:135:PRO:HB2	42:1q:93:MET:HE1	2.03	0.40
10:1J:127:ILE:HG21	11:1K:2:PRO:HG3	2.03	0.40
12:1L:127:THR:HA	12:1L:130:ILE:HD12	2.04	0.40
12:1L:292:ALA:HB2	12:1L:304:PHE:CB	2.51	0.40
12:1L:516:PRO:HB3	39:1n:29:TRP:CH2	2.57	0.40
13:1M:410:MET:HA	13:1M:413:THR:HG22	2.03	0.40
14:1N:149:ILE:CD1	14:1N:154:MET:CE	2.99	0.40
14:1N:284:MET:HE3	14:1N:284:MET:HB3	1.92	0.40
16:1P:81:ILE:O	16:1P:85:VAL:HB	2.22	0.40
16:1P:116:ALA:O	16:1P:120:VAL:HG23	2.21	0.40
17:1Q:69:LEU:HA	18:1R:27:ARG:HH12	1.87	0.40
20:1U:52:MET:HE1	39:1n:23:LEU:HD12	2.02	0.40
21:1V:93:MET:CE	21:1V:98:PRO:HG2	2.51	0.40
26:1a:55:SER:HB2	26:1a:62:VAL:HG13	2.03	0.40
32:1g:90:ARG:HA	32:1g:90:ARG:HD3	1.91	0.40
41:1p:10:PRO:HD2	41:1p:108:ARG:HG2	2.03	0.40
45:3A:270:LEU:HD22	45:3A:320:LEU:HD21	2.03	0.40
69:3A:503:3PE:N	47:3C:3:ASN:OD1	2.34	0.40
47:3C:152:ALA:HB2	47:3C:287:LYS:HG2	2.03	0.40
45:3N:444:LEU:HA	53:3W:17:THR:HG21	2.03	0.40
46:3O:109:VAL:HB	46:3O:119:LEU:HD12	2.04	0.40
47:3P:318:ARG:O	47:3P:322:GLN:HG3	2.22	0.40
51:3T:10:MET:HE2	51:3T:10:MET:HB2	1.90	0.40
75:3T:101:CDL:HB61	75:3T:101:CDL:H711	1.49	0.40
52:3U:47:ARG:HG3	52:3U:49:GLN:H	1.86	0.40
55:4A:191:THR:CG2	55:4A:245:ILE:HG23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:508:PRO:HG2	60:4F:32:ASN:ND2	2.36	0.40
87:4A:602:PGV:H181	57:4C:31:LEU:HD12	2.02	0.40
56:4B:7:LEU:HD11	75:4B:303:CDL:H761	2.02	0.40
56:4B:155:SER:OG	56:4B:156:SER:N	2.55	0.40
57:4C:109:THR:OG1	87:4C:303:PGV:H062	2.21	0.40
60:4F:62:CYS:HB3	60:4F:85:CYS:HB3	2.02	0.40
60:4F:76:LYS:HD3	60:4F:76:LYS:C	2.47	0.40
66:4L:38:PHE:HD1	66:4L:41:ARG:HD2	1.85	0.40
55:8A:52:GLN:OE1	55:8A:56:VAL:CG1	2.69	0.40
59:8E:61:PHE:CE1	59:8E:65:VAL:CG2	3.05	0.40
62:8H:6:THR:CA	62:8H:9:LYS:HZ2	2.29	0.40
3:1C:49:GLU:HG2	3:1C:106:ARG:NE	2.36	0.40
3:1C:177:ASP:OD1	3:1C:180:VAL:HG22	2.20	0.40
4:1D:128:ILE:CG1	4:1D:325:VAL:HG21	2.51	0.40
5:1E:120:ILE:HG22	5:1E:139:LEU:HD22	2.02	0.40
7:1G:521:VAL:HG22	7:1G:542:PHE:HB3	2.03	0.40
9:1I:95:GLU:HG3	9:1I:108:ARG:HD2	2.04	0.40
10:1J:162:LEU:O	10:1J:166:VAL:HG23	2.22	0.40
14:1N:21:MET:HE1	70:1d:202:PC1:H3B2	2.03	0.40
14:1N:49:ASN:O	14:1N:53:THR:HG23	2.22	0.40
14:1N:258:SER:HB3	14:1N:333:SER:O	2.22	0.40
15:1O:100:LEU:HD23	15:1O:100:LEU:HA	1.90	0.40
15:1O:136:GLU:O	15:1O:140:ARG:HG2	2.22	0.40
17:1Q:82:LEU:HD12	17:1Q:82:LEU:HA	1.87	0.40
20:1U:45:LEU:O	20:1U:49:GLU:HG3	2.21	0.40
24:1Y:11:ILE:H	24:1Y:11:ILE:HG12	1.75	0.40
29:1d:85:LEU:HD23	29:1d:85:LEU:HA	1.92	0.40
32:1g:33:GLU:H	32:1g:33:GLU:CD	2.30	0.40
35:1j:69:ASP:CB	40:1o:117:ARG:HH12	2.34	0.40
37:1l:54:SER:OG	37:1l:55:GLN:N	2.54	0.40
40:1o:73:PHE:CG	40:1o:74:PRO:HA	2.56	0.40
41:1p:49:GLU:O	41:1p:53:GLN:HG2	2.21	0.40
45:3A:154:HIS:NE2	45:3A:314:TYR:OH	2.39	0.40
45:3A:436:ARG:HD3	47:3C:222:PRO:HD3	2.03	0.40
46:3B:36:ALA:O	46:3B:207:ILE:HA	2.20	0.40
48:3D:108:SER:HB2	48:3D:288:ASP:CG	2.46	0.40
49:3E:175:PHE:CZ	49:3E:215:GLY:HA3	2.56	0.40
49:3E:235:TYR:HA	49:3E:243:TYR:H	1.87	0.40
47:3P:344:GLU:HG3	51:3T:66:PHE:HE1	1.85	0.40
48:3Q:33:TYR:HA	48:3Q:37:CYS:SG	2.61	0.40
48:3Q:41:HIS:CE1	86:3Q:501:HEC:NA	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:195:LEU:HD23	49:3R:195:LEU:HA	1.83	0.40
52:3U:19:THR:O	52:3U:23:GLN:OE1	2.39	0.40
55:4A:217:THR:HB	57:4C:195:SER:HB3	2.03	0.40
56:4B:40:TYR:HD2	63:4I:24:ALA:HA	1.85	0.40
87:4B:302:PGV:C20	87:4C:303:PGV:H62	2.52	0.40
57:4C:181:TYR:HE2	93:4C:307:PEK:H22	1.87	0.40
75:4C:305:CDL:H462	68:4N:1:MET:HG3	2.04	0.40
58:4D:67:SER:CB	59:4E:106:LEU:HB3	2.50	0.40
58:4D:110:THR:HG22	58:4D:115:TRP:NE1	2.37	0.40
58:4D:120:THR:O	58:4D:124:LEU:HD22	2.22	0.40
66:4L:45:LEU:HD21	67:4M:40:TYR:CD2	2.56	0.40
55:8A:119:GLU:OE1	55:8A:119:GLU:HA	2.22	0.40
55:8A:220:PHE:CE1	55:8A:231:TYR:HB2	2.57	0.40
55:8A:334:TRP:HB2	75:8D:201:CDL:H752	2.04	0.40
75:8B:303:CDL:H861	75:8B:303:CDL:H202	2.04	0.40
57:8C:76:GLN:NE2	57:8C:231:HIS:CE1	2.89	0.40
68:8N:44:CYS:HB2	68:8N:53:PRO:HG3	2.02	0.40
2:1B:116:MET:SD	2:1B:156:LEU:HD22	2.61	0.40
4:1D:417:ILE:O	4:1D:420:THR:HG22	2.22	0.40
5:1E:187:ARG:HA	5:1E:187:ARG:HD3	1.82	0.40
6:1F:52:GLY:O	6:1F:56:ILE:HG13	2.21	0.40
6:1F:270:GLU:HG3	6:1F:271:GLU:N	2.36	0.40
6:1F:391:SER:OG	43:1r:48:LEU:HB3	2.21	0.40
7:1G:53:ARG:CZ	7:1G:56:LEU:HD11	2.51	0.40
7:1G:201:ASP:OD2	7:1G:268:ARG:NH1	2.54	0.40
7:1G:508:LYS:H	7:1G:508:LYS:HG2	1.69	0.40
70:1H:402:PC1:O12	9:1I:24:THR:HG23	2.22	0.40
12:1L:364:LYS:O	35:1j:17:LEU:HD21	2.22	0.40
12:1L:483:PRO:HB2	12:1L:485:TYR:CD1	2.56	0.40
13:1M:133:ILE:HG12	13:1M:223:ALA:HB2	2.02	0.40
13:1M:225:ILE:HD13	13:1M:331:ASN:HB2	2.02	0.40
14:1N:73:ALA:HB3	14:1N:98:MET:HE3	2.04	0.40
14:1N:198:THR:O	14:1N:202:ILE:HG13	2.22	0.40
14:1N:323:MET:H	14:1N:323:MET:HG2	1.71	0.40
16:1P:57:MET:HA	16:1P:60:ARG:HE	1.85	0.40
16:1P:253:PHE:O	16:1P:254:LEU:HD23	2.22	0.40
17:1Q:69:LEU:HD11	42:1q:126:PRO:HG2	2.03	0.40
19:1S:32:VAL:O	19:1S:36:ILE:HG12	2.21	0.40
20:1T:37:MET:HE2	20:1T:37:MET:HB2	1.70	0.40
75:1X:201:CDL:H382	29:1d:32:VAL:HG12	2.04	0.40
25:1Z:57:ARG:HA	25:1Z:60:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1d:34:MET:HE1	75:1d:203:CDL:H441	2.04	0.40
40:1o:93:ASP:C	40:1o:93:ASP:OD1	2.64	0.40
42:1q:8:ARG:HG2	42:1q:12:GLN:HE21	1.86	0.40
45:3A:64:PHE:CD1	45:3A:86:LEU:HD21	2.56	0.40
49:3E:174:LEU:HD12	49:3E:213:LEU:O	2.21	0.40
49:3E:195:LEU:O	49:3E:195:LEU:HD12	2.22	0.40
49:3E:226:ALA:HA	49:3E:234:TYR:CD1	2.56	0.40
70:3J:101:PC1:H2C1	54:3Y:31:GLY:HA3	2.02	0.40
45:3N:373:THR:HB	45:3N:374:PRO:HD3	2.03	0.40
48:3Q:98:PRO:O	48:3Q:102:ARG:HG3	2.20	0.40
49:3R:150:SER:HB3	49:3R:170:ARG:N	2.30	0.40
49:3R:184:ILE:H	49:3R:184:ILE:HG13	1.68	0.40
51:3T:32:LYS:HB2	51:3T:32:LYS:HE2	1.75	0.40
55:4A:495:LEU:HD22	60:4F:73:TRP:CD1	2.57	0.40
56:4B:89:GLU:OE2	68:4N:68:VAL:CB	2.67	0.40
60:4F:82:CYS:SG	60:4F:83:PRO:CD	3.10	0.40
87:8B:301:PGV:H342	87:8B:301:PGV:H302	2.04	0.40
57:8C:6:HIS:CD2	57:8C:8:TYR:HB2	2.56	0.40
57:8C:63:ARG:CD	64:8J:12:PHE:CE2	3.04	0.40
87:8G:101:PGV:H202	87:8G:101:PGV:H012	1.18	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	103 (91%)	8 (7%)	2 (2%)	6	6
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
3	1C	207/264 (78%)	199 (96%)	8 (4%)	0	100	100
4	1D	427/476 (90%)	412 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1E	212/249 (85%)	200 (94%)	11 (5%)	1 (0%)	24	31
6	1F	430/464 (93%)	402 (94%)	25 (6%)	3 (1%)	18	23
7	1G	697/727 (96%)	668 (96%)	28 (4%)	1 (0%)	48	60
8	1H	316/318 (99%)	294 (93%)	20 (6%)	2 (1%)	21	27
9	1I	174/239 (73%)	167 (96%)	7 (4%)	0	100	100
10	1J	172/175 (98%)	161 (94%)	10 (6%)	1 (1%)	21	27
11	1K	96/98 (98%)	93 (97%)	2 (2%)	1 (1%)	12	15
12	1L	604/606 (100%)	563 (93%)	41 (7%)	0	100	100
13	1M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
14	1N	345/347 (99%)	335 (97%)	9 (3%)	1 (0%)	36	46
15	1O	318/357 (89%)	305 (96%)	13 (4%)	0	100	100
16	1P	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
17	1Q	127/175 (73%)	118 (93%)	9 (7%)	0	100	100
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
19	1S	85/99 (86%)	80 (94%)	5 (6%)	0	100	100
20	1T	83/156 (53%)	82 (99%)	1 (1%)	0	100	100
20	1U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
22	1W	113/128 (88%)	106 (94%)	7 (6%)	0	100	100
23	1X	169/172 (98%)	163 (96%)	5 (3%)	1 (1%)	21	27
24	1Y	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
25	1Z	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
26	1a	68/70 (97%)	68 (100%)	0	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	1d	117/122 (96%)	113 (97%)	4 (3%)	0	100	100
30	1e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/135 (41%)	50 (91%)	5 (9%)	0	100	100
32	1g	98/154 (64%)	90 (92%)	8 (8%)	0	100	100
33	1h	136/189 (72%)	136 (100%)	0	0	100	100
34	1i	126/128 (98%)	118 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	1j	69/105 (66%)	67 (97%)	2 (3%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	146 (95%)	8 (5%)	0	100	100
38	1m	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
39	1n	170/179 (95%)	161 (95%)	9 (5%)	0	100	100
40	1o	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
42	1q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
43	1r	90/113 (80%)	87 (97%)	3 (3%)	0	100	100
44	1s	43/471 (9%)	42 (98%)	1 (2%)	0	100	100
45	3A	436/480 (91%)	428 (98%)	6 (1%)	2 (0%)	24	31
45	3N	444/480 (92%)	427 (96%)	16 (4%)	1 (0%)	43	55
46	3B	414/453 (91%)	403 (97%)	11 (3%)	0	100	100
46	3O	413/453 (91%)	404 (98%)	8 (2%)	1 (0%)	43	55
47	3C	377/379 (100%)	366 (97%)	11 (3%)	0	100	100
47	3P	377/379 (100%)	369 (98%)	8 (2%)	0	100	100
48	3D	235/326 (72%)	229 (97%)	6 (3%)	0	100	100
48	3Q	237/326 (73%)	231 (98%)	6 (2%)	0	100	100
49	3E	194/274 (71%)	177 (91%)	16 (8%)	1 (0%)	24	31
49	3I	45/274 (16%)	43 (96%)	2 (4%)	0	100	100
49	3R	194/274 (71%)	172 (89%)	18 (9%)	4 (2%)	5	4
49	3V	29/274 (11%)	29 (100%)	0	0	100	100
50	3F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
50	3S	96/111 (86%)	96 (100%)	0	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%)	62 (98%)	0	1 (2%)	7	7
52	3U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
53	3J	54/60 (90%)	52 (96%)	1 (2%)	1 (2%)	6	5
53	3W	54/60 (90%)	53 (98%)	1 (2%)	0	100	100
54	3X	50/56 (89%)	47 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	3Y	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
55	4A	512/514 (100%)	497 (97%)	14 (3%)	1 (0%)	43	55
55	8A	512/514 (100%)	497 (97%)	13 (2%)	2 (0%)	30	38
56	4B	225/229 (98%)	215 (96%)	10 (4%)	0	100	100
56	8B	225/229 (98%)	216 (96%)	9 (4%)	0	100	100
57	4C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
57	8C	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
58	4D	137/169 (81%)	126 (92%)	11 (8%)	0	100	100
58	8D	137/169 (81%)	132 (96%)	5 (4%)	0	100	100
59	4E	103/152 (68%)	101 (98%)	2 (2%)	0	100	100
59	8E	103/152 (68%)	101 (98%)	2 (2%)	0	100	100
60	4F	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
60	8F	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
61	4G	73/97 (75%)	70 (96%)	3 (4%)	0	100	100
61	8G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
62	4H	80/86 (93%)	75 (94%)	5 (6%)	0	100	100
62	8H	80/86 (93%)	74 (92%)	6 (8%)	0	100	100
63	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
63	8I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
64	4J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
64	8J	56/80 (70%)	54 (96%)	2 (4%)	0	100	100
65	4K	47/80 (59%)	44 (94%)	3 (6%)	0	100	100
65	8K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
66	4L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
66	8L	44/63 (70%)	44 (100%)	0	0	100	100
67	4M	41/70 (59%)	41 (100%)	0	0	100	100
67	8M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	9	10
68	8N	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	10
All	All	15889/19086 (83%)	15257 (96%)	603 (4%)	29 (0%)	44	55

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1H	92	PRO
10	1J	66	VAL
23	1X	28	ALA
49	3E	271	VAL
53	3J	57	LYS
45	3N	224	VAL
1	1A	52	SER
8	1H	208	VAL
49	3R	181	LYS
49	3R	228	ALA
68	8N	33	VAL
1	1A	109	LYS
6	1F	249	ARG
6	1F	297	VAL
49	3R	273	VAL
68	4N	33	VAL
46	3O	171	ALA
49	3R	150	SER
7	1G	654	GLN
11	1K	2	PRO
45	3A	231	PHE
5	1E	215	ALA
6	1F	207	PRO
45	3A	350	THR
52	3H	79	ASP
55	8A	128	VAL
55	4A	128	VAL
55	8A	3	VAL
14	1N	110	PRO

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%)	99 (100%)	0	100	100
2	1B	131/212 (62%)	130 (99%)	1 (1%)	73	86
3	1C	190/227 (84%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	1D	371/405 (92%)	370 (100%)	1 (0%)	86	93
5	1E	183/207 (88%)	183 (100%)	0	100	100
6	1F	346/368 (94%)	344 (99%)	2 (1%)	78	89
7	1G	588/610 (96%)	587 (100%)	1 (0%)	87	94
8	1H	274/274 (100%)	273 (100%)	1 (0%)	84	92
9	1I	151/201 (75%)	151 (100%)	0	100	100
10	1J	140/141 (99%)	139 (99%)	1 (1%)	76	87
11	1K	84/84 (100%)	84 (100%)	0	100	100
12	1L	539/539 (100%)	539 (100%)	0	100	100
13	1M	408/408 (100%)	407 (100%)	1 (0%)	87	94
14	1N	310/310 (100%)	310 (100%)	0	100	100
15	1O	283/307 (92%)	283 (100%)	0	100	100
16	1P	296/323 (92%)	296 (100%)	0	100	100
17	1Q	117/152 (77%)	117 (100%)	0	100	100
18	1R	79/97 (81%)	78 (99%)	1 (1%)	61	77
19	1S	77/82 (94%)	77 (100%)	0	100	100
20	1T	79/133 (59%)	79 (100%)	0	100	100
20	1U	79/133 (59%)	79 (100%)	0	100	100
21	1V	100/101 (99%)	100 (100%)	0	100	100
22	1W	107/112 (96%)	107 (100%)	0	100	100
23	1X	153/154 (99%)	153 (100%)	0	100	100
24	1Y	101/102 (99%)	101 (100%)	0	100	100
25	1Z	123/124 (99%)	123 (100%)	0	100	100
26	1a	58/58 (100%)	58 (100%)	0	100	100
27	1b	69/70 (99%)	69 (100%)	0	100	100
28	1c	45/66 (68%)	45 (100%)	0	100	100
29	1d	106/109 (97%)	105 (99%)	1 (1%)	70	84
30	1e	87/94 (93%)	87 (100%)	0	100	100
31	1f	54/113 (48%)	54 (100%)	0	100	100
32	1g	92/129 (71%)	91 (99%)	1 (1%)	65	81
33	1h	121/158 (77%)	120 (99%)	1 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1i	120/120 (100%)	119 (99%)	1 (1%)	73	86
35	1j	62/84 (74%)	62 (100%)	0	100	100
36	1k	63/76 (83%)	63 (100%)	0	100	100
37	1l	141/161 (88%)	141 (100%)	0	100	100
38	1m	113/114 (99%)	112 (99%)	1 (1%)	70	84
39	1n	156/160 (98%)	156 (100%)	0	100	100
40	1o	110/119 (92%)	110 (100%)	0	100	100
41	1p	154/156 (99%)	153 (99%)	1 (1%)	78	89
42	1q	131/131 (100%)	131 (100%)	0	100	100
43	1r	85/98 (87%)	85 (100%)	0	100	100
44	1s	44/351 (12%)	44 (100%)	0	100	100
45	3A	367/397 (92%)	366 (100%)	1 (0%)	86	93
45	3N	372/397 (94%)	370 (100%)	2 (0%)	81	90
46	3B	328/355 (92%)	327 (100%)	1 (0%)	86	93
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%)	330 (99%)	2 (1%)	78	89
48	3D	202/259 (78%)	202 (100%)	0	100	100
48	3Q	204/259 (79%)	203 (100%)	1 (0%)	81	90
49	3E	166/226 (74%)	165 (99%)	1 (1%)	78	89
49	3I	37/226 (16%)	37 (100%)	0	100	100
49	3R	166/226 (74%)	165 (99%)	1 (1%)	78	89
49	3V	24/226 (11%)	23 (96%)	1 (4%)	26	40
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%)	67 (100%)	0	100	100
52	3H	62/85 (73%)	62 (100%)	0	100	100
52	3U	62/85 (73%)	62 (100%)	0	100	100
53	3J	46/48 (96%)	46 (100%)	0	100	100
53	3W	46/48 (96%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	423 (100%)	1 (0%)	87	94
55	8A	424/424 (100%)	423 (100%)	1 (0%)	87	94
56	4B	210/211 (100%)	208 (99%)	2 (1%)	68	82
56	8B	210/211 (100%)	208 (99%)	2 (1%)	68	82
57	4C	223/225 (99%)	223 (100%)	0	100	100
57	8C	223/225 (99%)	222 (100%)	1 (0%)	84	92
58	4D	124/149 (83%)	124 (100%)	0	100	100
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%)	91 (99%)	1 (1%)	65	81
60	4F	80/100 (80%)	79 (99%)	1 (1%)	61	77
60	8F	80/100 (80%)	80 (100%)	0	100	100
61	4G	65/80 (81%)	65 (100%)	0	100	100
61	8G	65/80 (81%)	65 (100%)	0	100	100
62	4H	73/76 (96%)	72 (99%)	1 (1%)	59	76
62	8H	73/76 (96%)	73 (100%)	0	100	100
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%)	47 (96%)	2 (4%)	27	41
64	8J	49/68 (72%)	48 (98%)	1 (2%)	48	67
65	4K	38/66 (58%)	38 (100%)	0	100	100
65	8K	38/66 (58%)	36 (95%)	2 (5%)	20	30
66	4L	39/55 (71%)	38 (97%)	1 (3%)	40	59
66	8L	39/55 (71%)	39 (100%)	0	100	100
67	4M	37/57 (65%)	36 (97%)	1 (3%)	39	58
67	8M	37/57 (65%)	36 (97%)	1 (3%)	39	58
68	4N	70/70 (100%)	70 (100%)	0	100	100
68	8N	70/70 (100%)	70 (100%)	0	100	100
All	All	13845/16096 (86%)	13802 (100%)	43 (0%)	84	93

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1B	134	ARG
4	1D	337	GLU
6	1F	21	ILE
6	1F	247	ARG
7	1G	651	LEU
8	1H	127	TYR
10	1J	66	VAL
13	1M	114	GLU
18	1R	89	LEU
29	1d	64	TYR
32	1g	54	ASP
33	1h	79	PHE
34	1i	16	GLU
38	1m	117	GLU
41	1p	34	LYS
45	3A	146	ARG
46	3B	400	GLN
49	3E	218	THR
45	3N	112	LEU
45	3N	117	VAL
47	3P	254	ASP
47	3P	345	HIS
48	3Q	97	ASN
49	3R	152	ILE
49	3V	76	VAL
55	4A	101	SER
56	4B	45	MET
56	4B	55	THR
60	4F	51	SER
62	4H	31	GLN
64	4J	15	ASP
64	4J	49	CYS
66	4L	46	LYS
67	4M	25	SER
55	8A	69	MET
56	8B	158	ASP
56	8B	181	GLN
57	8C	92	LEU
59	8E	33	MET
64	8J	57	HIS
65	8K	15	ASN
65	8K	52	GLU

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Mol	Chain	Res	Type
67	8M	4	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	106	GLN
2	1B	162	GLN
2	1B	164	GLN
3	1C	39	GLN
3	1C	41	GLN
3	1C	144	ASN
4	1D	129	GLN
4	1D	201	GLN
4	1D	316	ASN
5	1E	15	ASN
5	1E	27	ASN
5	1E	37	ASN
6	1F	250	ASN
7	1G	51	ASN
7	1G	101	HIS
7	1G	259	ASN
7	1G	476	ASN
7	1G	646	ASN
8	1H	157	ASN
8	1H	304	HIS
9	1I	144	HIS
9	1I	150	ASN
11	1K	92	ASN
12	1L	23	ASN
12	1L	30	ASN
12	1L	194	ASN
12	1L	351	ASN
12	1L	506	ASN
12	1L	603	ASN
13	1M	51	ASN
13	1M	168	GLN
13	1M	220	HIS
13	1M	331	ASN
14	1N	174	GLN
14	1N	204	ASN
14	1N	322	GLN
14	1N	347	ASN

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Mol	Chain	Res	Type
15	1O	114	HIS
15	1O	120	GLN
15	1O	251	GLN
15	1O	288	GLN
16	1P	136	ASN
16	1P	321	HIS
19	1S	47	ASN
19	1S	72	GLN
19	1S	85	GLN
20	1U	33	ASN
21	1V	75	GLN
22	1W	51	GLN
22	1W	70	ASN
22	1W	99	GLN
23	1X	98	HIS
24	1Y	78	GLN
24	1Y	88	ASN
26	1a	25	HIS
29	1d	46	ASN
30	1e	44	HIS
32	1g	103	ASN
34	1i	47	ASN
34	1i	51	GLN
34	1i	127	HIS
38	1m	51	ASN
39	1n	12	GLN
39	1n	13	GLN
40	1o	81	HIS
40	1o	116	GLN
41	1p	106	GLN
41	1p	123	ASN
42	1q	123	GLN
43	1r	35	GLN
44	1s	44	HIS
44	1s	65	GLN
44	1s	71	GLN
44	1s	75	HIS
45	3A	94	HIS
45	3A	159	GLN
46	3B	305	GLN
46	3B	354	ASN
46	3B	358	GLN

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Mol	Chain	Res	Type
47	3C	54	HIS
47	3C	85	ASN
47	3C	341	GLN
48	3D	102	HIS
48	3D	193	ASN
49	3E	131	ASN
49	3E	164	ASN
49	3E	199	GLN
50	3F	34	ASN
51	3G	25	GLN
51	3G	75	ASN
45	3N	9	GLN
45	3N	69	ASN
45	3N	159	GLN
46	3O	143	GLN
46	3O	351	ASN
46	3O	354	ASN
47	3P	54	HIS
47	3P	85	ASN
47	3P	341	GLN
49	3R	257	ASN
55	4A	214	ASN
55	4A	491	ASN
57	4C	50	ASN
57	4C	76	GLN
57	4C	231	HIS
58	4D	29	HIS
58	4D	72	ASN
58	4D	76	ASN
59	4E	78	HIS
60	4F	32	ASN
60	4F	94	HIS
61	4G	41	HIS
61	4G	43	HIS
62	4H	22	ASN
62	4H	28	ASN
66	4L	17	ASN
66	4L	42	HIS
68	4N	8	GLN
68	4N	55	ASN
55	8A	328	HIS
55	8A	406	ASN

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Mol	Chain	Res	Type
55	8A	413	HIS
55	8A	422	ASN
56	8B	6	GLN
56	8B	24	HIS
57	8C	6	HIS
57	8C	38	ASN
57	8C	50	ASN
57	8C	76	GLN
57	8C	122	HIS
59	8E	78	HIS
59	8E	94	ASN
60	8F	66	ASN
62	8H	12	GLN
62	8H	25	GLN
62	8H	28	ASN
64	8J	29	ASN
65	8K	41	ASN
68	8N	12	HIS
68	8N	50	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	$\# Z > 2$
12	FME	1L	1	12	8,9,10	0.57	0	8,9,11	0.90	1 (12%)
55	FME	4A	1	55	8,9,10	0.55	0	8,9,11	1.01	1 (12%)
1	FME	1A	1	1	8,9,10	0.54	0	8,9,11	1.07	1 (12%)
8	FME	1H	1	8	8,9,10	0.56	0	8,9,11	1.01	1 (12%)

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	0.56	0	8,9,11	1.04	1 (12%)
11	FME	1K	1	11	8,9,10	0.55	0	8,9,11	0.98	1 (12%)
55	FME	8A	1	55	8,9,10	0.55	0	8,9,11	1.16	1 (12%)
14	FME	1N	1	14	8,9,10	0.56	0	8,9,11	1.02	1 (12%)
56	FME	8B	1	56	8,9,10	0.56	0	8,9,11	0.83	1 (12%)
56	FME	4B	1	56	8,9,10	0.56	0	8,9,11	0.99	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
12	FME	1L	1	12	-	1/7/9/11	-
55	FME	4A	1	55	-	1/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
13	FME	1M	1	13	-	0/7/9/11	-
11	FME	1K	1	11	-	3/7/9/11	-
55	FME	8A	1	55	-	1/7/9/11	-
14	FME	1N	1	14	-	1/7/9/11	-
56	FME	8B	1	56	-	1/7/9/11	-
56	FME	4B	1	56	-	3/7/9/11	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1M	1	FME	O-C-CA	-2.63	118.01	124.77
11	1K	1	FME	O-C-CA	-2.61	118.07	124.77
1	1A	1	FME	O-C-CA	-2.60	118.08	124.77
8	1H	1	FME	O-C-CA	-2.57	118.17	124.77
55	8A	1	FME	O-C-CA	-2.48	118.38	124.77
14	1N	1	FME	O-C-CA	-2.46	118.44	124.77
55	4A	1	FME	O-C-CA	-2.44	118.50	124.77
56	4B	1	FME	O-C-CA	-2.38	118.65	124.77
12	1L	1	FME	O-C-CA	-2.38	118.66	124.77
56	8B	1	FME	O-C-CA	-2.29	118.87	124.77

There are no chirality outliers.

All (12) 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	8B	1	FME	O1-CN-N-CA
55	4A	1	FME	CA-CB-CG-SD
11	1K	1	FME	N-CA-CB-CG
55	8A	1	FME	CA-CB-CG-SD
11	1K	1	FME	C-CA-CB-CG
11	1K	1	FME	CB-CG-SD-CE
12	1L	1	FME	CB-CA-N-CN
56	4B	1	FME	CA-CB-CG-SD

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	4A	1	FME	1	0
1	1A	1	FME	3	0
13	1M	1	FME	1	0
11	1K	1	FME	3	0
55	8A	1	FME	1	0
14	1N	1	FME	2	0
56	8B	1	FME	1	0
56	4B	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 11 are monoatomic - leaving 135 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
69	3PE	1m	201	-	40,40,50	0.29	0	43,45,55	0.40	0
70	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.30	0
87	PGV	8A	601	-	50,50,50	0.29	0	53,56,56	0.41	0
87	PGV	8C	303	-	50,50,50	0.29	0	53,56,56	0.32	0
70	PC1	1P	401	-	32,32,53	0.33	0	38,40,61	0.37	0
87	PGV	4A	603	-	50,50,50	0.28	0	53,56,56	0.35	0
70	PC1	1H	402	-	53,53,53	0.28	0	59,61,61	0.35	0
76	GTP	1O	401	77	33,34,34	0.56	0	50,54,54	0.57	0
69	3PE	1Y	203	-	39,39,50	0.31	0	42,44,55	0.50	0
75	CDL	4D	201	-	99,99,99	0.27	0	105,111,111	0.43	0
91	CUA	4B	304	56	0,1,1	-	-	-		
70	PC1	3X	101	-	28,28,53	0.36	0	34,36,61	0.48	0
81	AYA	1q	202	-	6,7,8	0.62	0	6,8,10	0.89	0
87	PGV	8A	602	-	50,50,50	0.28	0	53,56,56	0.30	0
71	SF4	1B	201	2	0,12,12	-	-	-		
75	CDL	3G	103	-	55,55,99	0.34	0	61,67,111	0.48	0
86	HEC	3Q	501	48	50,50,50	2.89	28 (56%)	68,82,82	2.48	26 (38%)
93	PEK	8G	102	-	52,52,52	0.26	0	55,57,57	0.40	0
93	PEK	4G	102	-	52,52,52	0.26	0	55,57,57	0.40	0
87	PGV	4C	304	-	50,50,50	0.29	0	53,56,56	0.47	1 (1%)
80	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.05	1 (2%)
69	3PE	1Y	202	-	30,30,50	0.32	0	33,35,55	0.53	0
75	CDL	3N	502	-	42,42,99	0.37	0	48,54,111	0.52	0
75	CDL	1X	201	-	85,85,99	0.29	0	91,97,111	0.39	0
70	PC1	1M	503	-	34,34,53	0.32	0	40,42,61	0.52	0
70	PC1	3J	101	-	46,46,53	0.28	0	52,54,61	0.32	0
69	3PE	3N	501	-	31,31,50	0.33	0	34,36,55	0.49	0
70	PC1	1q	201	-	48,48,53	0.28	0	54,56,61	0.33	0
72	FES	1E	301	5	0,4,4	-	-	-		
94	PO4	8H	101	-	4,4,4	0.97	0	6,6,6	0.44	0
75	CDL	1N	902	-	61,61,99	0.31	0	67,73,111	0.69	1 (1%)
71	SF4	1I	202	9	0,12,12	-	-	-		
69	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.36	0
72	FES	3E	301	49	0,4,4	-	-	-		
87	PGV	4G	101	-	50,50,50	0.28	0	53,56,56	0.45	1 (1%)
80	EHZ	1T	101	20	31,36,37	0.20	0	36,44,47	1.12	1 (2%)
69	3PE	1j	101	-	43,43,50	0.29	0	46,48,55	0.44	0
70	PC1	1H	403	-	47,47,53	0.29	0	53,55,61	0.36	0
69	3PE	3Y	101	-	29,29,50	0.34	0	32,34,55	0.42	0
93	PEK	8C	308	-	51,51,52	0.26	0	54,56,57	0.41	0
85	HEM	3P	502	47	50,50,50	1.56	8 (16%)	67,82,82	1.59	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
70	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.35	0
88	HEA	8A	604	55	67,67,67	2.45	26 (38%)	81,103,103	2.54	33 (40%)
69	3PE	1M	504	-	50,50,50	0.28	0	53,55,55	0.46	0
69	3PE	3A	503	45	31,31,50	0.41	0	34,36,55	0.48	0
69	3PE	3P	503	-	32,32,50	0.33	0	35,37,55	0.37	0
70	PC1	1d	202	-	38,38,53	0.31	0	44,46,61	0.47	0
75	CDL	8C	306	-	99,99,99	0.27	0	105,111,111	0.40	0
87	PGV	8C	307	-	50,50,50	0.29	0	53,56,56	0.35	0
93	PEK	4C	307	-	51,51,52	0.26	0	54,56,57	0.42	0
71	SF4	1F	502	6	0,12,12	-	-	-		
87	PGV	4M	101	-	50,50,50	0.29	0	53,56,56	0.30	0
87	PGV	4B	302	56	50,50,50	0.29	0	53,56,56	0.36	0
70	PC1	1Y	207	-	45,45,53	0.29	0	51,53,61	0.34	0
87	PGV	8B	302	56	50,50,50	0.28	0	53,56,56	0.37	0
88	HEA	8A	605	55	67,67,67	2.45	26 (38%)	81,103,103	2.53	34 (41%)
85	HEM	3P	501	47	50,50,50	1.57	8 (16%)	67,82,82	1.61	11 (16%)
81	AYA	1Y	201	-	6,7,8	0.64	0	6,8,10	0.86	0
87	PGV	4C	303	-	50,50,50	0.28	0	53,56,56	0.39	0
75	CDL	1q	203	-	60,60,99	0.34	0	66,72,111	0.42	0
88	HEA	4A	605	55	67,67,67	2.45	26 (38%)	81,103,103	2.55	34 (41%)
75	CDL	3P	504	-	55,55,99	0.35	0	61,67,111	0.52	0
91	CUA	8B	304	56	0,1,1	-	-	-		
70	PC1	1M	505	-	43,43,53	0.31	0	49,51,61	0.40	0
87	PGV	8J	101	-	50,50,50	0.28	0	53,56,56	0.40	0
69	3PE	3G	101	-	28,28,50	0.33	0	31,33,55	0.37	0
69	3PE	1Y	204	-	29,29,50	0.34	0	32,34,55	0.80	1 (3%)
85	HEM	3C	502	-	50,50,50	1.56	9 (18%)	67,82,82	1.58	12 (17%)
82	AME	1h	201	-	9,10,11	0.51	0	9,11,13	0.99	1 (11%)
72	FES	1G	803	7	0,4,4	-	-	-		
69	3PE	3C	503	-	34,34,50	0.32	0	37,39,55	0.45	0
69	3PE	3N	503	-	24,24,50	0.37	0	27,29,55	0.56	0
69	3PE	3C	504	-	33,33,50	0.33	0	36,38,55	0.41	0
71	SF4	1G	802	7	0,12,12	-	-	-		
69	3PE	1P	403	-	34,34,50	0.31	0	37,39,55	0.43	0
87	PGV	8L	101	-	50,50,50	0.28	0	53,56,56	0.41	0
75	CDL	3T	101	-	56,56,99	0.35	0	62,68,111	0.48	0
87	PGV	4J	101	-	50,50,50	0.30	0	53,56,56	0.38	0
75	CDL	1h	202	-	79,79,99	0.31	0	85,91,111	0.42	0
87	PGV	8C	301	-	50,50,50	0.27	0	53,56,56	0.35	0
69	3PE	3A	502	-	26,26,50	0.36	0	29,31,55	0.64	1 (3%)
75	CDL	8D	201	-	99,99,99	0.27	0	105,111,111	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	CDL	4B	303	-	99,99,99	0.27	0	105,111,111	0.30	0
70	PC1	1I	203	-	43,43,53	0.29	0	49,51,61	0.32	0
94	PO4	4H	101	-	4,4,4	0.97	0	6,6,6	0.47	0
87	PGV	4C	306	-	50,50,50	0.29	0	53,56,56	0.36	0
72	FES	3R	301	49	0,4,4	-	-	-		
88	HEA	4A	604	55	67,67,67	2.45	25 (37%)	81,103,103	2.55	35 (43%)
78	NDP	1P	402	-	51,52,52	0.50	0	71,80,80	0.83	2 (2%)
86	HEC	3D	501	48	48,49,50	2.96	28 (58%)	66,80,82	2.50	25 (37%)
87	PGV	4A	602	-	50,50,50	0.28	0	53,56,56	0.32	0
75	CDL	1H	401	-	50,50,99	0.36	0	56,62,111	0.60	1 (1%)
87	PGV	8K	101	-	50,50,50	0.29	0	53,56,56	0.32	0
75	CDL	3A	501	-	57,57,99	0.33	0	63,69,111	0.42	0
84	MYR	1I	201	-	13,14,15	0.31	0	12,13,15	0.29	0
87	PGV	4C	302	-	50,50,50	0.29	0	53,56,56	0.31	0
75	CDL	1d	203	-	64,64,99	0.32	0	70,76,111	0.41	0
70	PC1	1A	202	-	34,34,53	0.37	0	40,42,61	0.44	0
87	PGV	8C	302	-	50,50,50	0.29	0	53,56,56	0.72	1 (1%)
70	PC1	1A	203	-	34,34,53	0.33	0	40,42,61	0.39	0
69	3PE	1L	703	-	44,44,50	0.29	0	47,49,55	0.34	0
70	PC1	3R	303	-	44,44,53	0.29	0	50,52,61	0.36	0
87	PGV	8C	305	-	50,50,50	0.29	0	53,56,56	0.46	1 (1%)
75	CDL	1L	702	-	75,75,99	0.29	0	81,87,111	0.37	0
83	CHD	1i	201	-	32,32,32	0.51	0	51,51,51	0.57	0
87	PGV	8A	603	-	50,50,50	0.28	0	53,56,56	0.33	0
87	PGV	4B	301	-	50,50,50	0.27	0	53,56,56	0.31	0
92	PSC	8B	305	-	51,51,51	0.29	0	57,59,59	0.42	0
69	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.33	0
87	PGV	8B	301	-	50,50,50	0.28	0	53,56,56	0.32	0
87	PGV	8C	304	-	50,50,50	0.28	0	53,56,56	0.38	0
75	CDL	8B	303	-	99,99,99	0.27	0	105,111,111	0.30	0
87	PGV	4C	301	-	50,50,50	0.29	0	53,56,56	0.74	1 (1%)
87	PGV	8G	101	-	50,50,50	0.29	0	53,56,56	0.45	1 (1%)
69	3PE	1N	901	-	48,48,50	0.28	0	51,53,55	0.36	0
75	CDL	4C	305	-	99,99,99	0.27	0	105,111,111	0.39	0
75	CDL	3G	102	-	51,51,99	0.35	0	57,63,111	0.56	0
69	3PE	1M	501	-	44,44,50	0.29	0	47,49,55	0.34	0
71	SF4	1I	201	9	0,12,12	-	-	-		
71	SF4	1G	801	7	0,12,12	-	-	-		
70	PC1	1B	203	-	47,47,53	0.29	0	53,55,61	0.42	0
69	3PE	1M	506	-	49,49,50	0.28	0	52,54,55	0.33	0
69	3PE	3R	302	-	46,46,50	0.28	0	49,51,55	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	1d	201	-	48,48,50	0.27	0	51,53,55	0.36	0
87	PGV	4L	101	-	50,50,50	0.28	0	53,56,56	0.38	0
69	3PE	1Y	205	-	32,32,50	0.32	0	35,37,55	0.52	0
73	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.67	1 (2%)
87	PGV	4A	601	-	50,50,50	0.28	0	53,56,56	0.40	0
69	3PE	1M	502	-	47,47,50	0.27	0	50,52,55	0.33	0
85	HEM	3C	501	47	50,50,50	1.56	8 (16%)	67,82,82	1.62	11 (16%)
69	3PE	3D	502	-	32,32,50	0.33	0	35,37,55	0.49	0
92	PSC	4B	305	-	51,51,51	0.29	0	57,59,59	0.47	1 (1%)
69	3PE	1K	101	-	43,43,50	0.30	0	46,48,55	0.34	0
87	PGV	4K	101	-	50,50,50	0.28	0	53,56,56	0.31	0
69	3PE	1Y	206	-	26,26,50	0.35	0	29,31,55	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1m	201	-	-	9/44/44/54	-
70	PC1	1h	203	-	-	12/50/50/57	-
87	PGV	8A	601	-	-	11/55/55/55	-
87	PGV	8C	303	-	-	10/55/55/55	-
70	PC1	1P	401	-	-	5/36/36/57	-
87	PGV	4A	603	-	-	3/55/55/55	-
70	PC1	1H	402	-	-	6/57/57/57	-
76	GTP	1O	401	77	-	4/22/38/38	0/3/3/3
69	3PE	1Y	203	-	-	14/43/43/54	-
75	CDL	4D	201	-	-	15/110/110/110	-
70	PC1	3X	101	-	-	2/32/32/57	-
81	AYA	1q	202	-	-	0/5/6/8	-
87	PGV	8A	602	-	-	8/55/55/55	-
75	CDL	3G	103	-	-	8/66/66/110	-
71	SF4	1B	201	2	-	-	0/6/5/5
86	HEC	3Q	501	48	1/1/3/7	7/14/54/54	-
93	PEK	8G	102	-	-	6/56/56/56	-
93	PEK	4G	102	-	-	6/56/56/56	-
87	PGV	4C	304	-	-	4/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	EHZ	1n	201	-	-	4/42/44/45	-
69	3PE	1Y	202	-	-	9/34/34/54	-
75	CDL	3N	502	-	-	8/53/53/110	-
75	CDL	1X	201	-	-	17/96/96/110	-
70	PC1	1M	503	-	-	6/38/38/57	-
70	PC1	3J	101	-	-	1/50/50/57	-
69	3PE	3N	501	-	-	10/35/35/54	-
70	PC1	1q	201	-	-	3/52/52/57	-
72	FES	1E	301	5	-	-	0/1/1/1
75	CDL	1N	902	-	-	15/71/71/110	-
71	SF4	1I	202	9	-	-	0/6/5/5
69	3PE	1A	201	-	-	7/50/50/54	-
87	PGV	4G	101	-	-	10/55/55/55	-
72	FES	3E	301	49	-	-	0/1/1/1
80	EHZ	1T	101	20	-	10/42/44/45	-
69	3PE	1j	101	-	-	3/47/47/54	-
70	PC1	1H	403	-	-	4/51/51/57	-
69	3PE	3Y	101	-	-	5/33/33/54	-
93	PEK	8C	308	-	-	2/55/55/56	-
85	HEM	3P	502	47	-	8/14/54/54	-
70	PC1	1B	202	-	-	3/49/49/57	-
88	HEA	8A	604	55	-	6/36/76/76	-
69	3PE	1M	504	-	-	10/54/54/54	-
69	3PE	3A	503	45	-	6/35/35/54	-
69	3PE	3P	503	-	-	6/36/36/54	-
70	PC1	1d	202	-	-	7/42/42/57	-
75	CDL	8C	306	-	-	18/110/110/110	-
87	PGV	8C	307	-	-	3/55/55/55	-
93	PEK	4C	307	-	-	3/55/55/56	-
87	PGV	4M	101	-	-	7/55/55/55	-
71	SF4	1F	502	6	-	-	0/6/5/5
87	PGV	4B	302	56	-	5/55/55/55	-
70	PC1	1Y	207	-	-	8/49/49/57	-
87	PGV	8B	302	56	-	5/55/55/55	-
88	HEA	8A	605	55	-	6/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	HEM	3P	501	47	-	9/14/54/54	-
81	AYA	1Y	201	-	-	0/5/6/8	-
87	PGV	4C	303	-	-	9/55/55/55	-
75	CDL	1q	203	-	-	6/71/71/110	-
88	HEA	4A	605	55	-	5/36/76/76	-
75	CDL	3P	504	-	-	17/66/66/110	-
70	PC1	1M	505	-	-	13/47/47/57	-
87	PGV	8J	101	-	-	9/55/55/55	-
69	3PE	3G	101	-	-	3/32/32/54	-
69	3PE	1Y	204	-	-	9/33/33/54	-
85	HEM	3C	502	-	-	6/14/54/54	-
82	AME	1h	201	-	-	2/9/10/12	-
72	FES	1G	803	7	-	-	0/1/1/1
69	3PE	3C	503	-	-	11/38/38/54	-
69	3PE	3N	503	-	-	5/28/28/54	-
69	3PE	3C	504	-	-	8/37/37/54	-
71	SF4	1G	802	7	-	-	0/6/5/5
69	3PE	1P	403	-	-	5/38/38/54	-
87	PGV	8L	101	-	-	5/55/55/55	-
75	CDL	3T	101	-	-	9/67/67/110	-
87	PGV	4J	101	-	-	7/55/55/55	-
75	CDL	1h	202	-	-	19/90/90/110	-
87	PGV	8C	301	-	-	3/55/55/55	-
69	3PE	3A	502	-	-	7/30/30/54	-
75	CDL	8D	201	-	-	14/110/110/110	-
75	CDL	4B	303	-	-	14/110/110/110	-
70	PC1	1I	203	-	-	5/47/47/57	-
87	PGV	4C	306	-	-	2/55/55/55	-
72	FES	3R	301	49	-	-	0/1/1/1
88	HEA	4A	604	55	-	10/36/76/76	-
78	NDP	1P	402	-	-	3/34/77/77	0/5/5/5
86	HEC	3D	501	48	1/1/2/7	7/13/53/54	-
87	PGV	4A	602	-	-	1/55/55/55	-
75	CDL	1H	401	-	-	4/61/61/110	-
87	PGV	8K	101	-	-	13/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	3A	501	-	-	1/68/68/110	-
84	MYR	1l	201	-	-	1/12/12/13	-
87	PGV	4C	302	-	-	9/55/55/55	-
75	CDL	1d	203	-	-	11/75/75/110	-
70	PC1	1A	202	-	-	4/38/38/57	-
87	PGV	8C	302	-	-	15/55/55/55	-
70	PC1	1A	203	-	-	2/38/38/57	-
69	3PE	1L	703	-	-	6/48/48/54	-
70	PC1	3R	303	-	-	3/48/48/57	-
87	PGV	8C	305	-	-	6/55/55/55	-
75	CDL	1L	702	-	-	13/86/86/110	-
83	CHD	1i	201	-	-	2/9/74/74	0/4/4/4
87	PGV	8A	603	-	-	4/55/55/55	-
87	PGV	4B	301	-	-	2/55/55/55	-
92	PSC	8B	305	-	-	16/55/55/55	-
69	3PE	1L	701	-	-	4/49/49/54	-
87	PGV	8B	301	-	-	7/55/55/55	-
87	PGV	8C	304	-	-	13/55/55/55	-
75	CDL	8B	303	-	-	15/110/110/110	-
87	PGV	4C	301	-	-	11/55/55/55	-
87	PGV	8G	101	-	-	8/55/55/55	-
69	3PE	1N	901	-	-	11/52/52/54	-
75	CDL	4C	305	-	-	18/110/110/110	-
75	CDL	3G	102	-	-	8/62/62/110	-
69	3PE	1M	501	-	-	6/48/48/54	-
71	SF4	1I	201	9	-	-	0/6/5/5
71	SF4	1G	801	7	-	-	0/6/5/5
70	PC1	1B	203	-	-	10/51/51/57	-
69	3PE	1M	506	-	-	7/53/53/54	-
69	3PE	3R	302	-	-	4/50/50/54	-
69	3PE	1d	201	-	-	7/52/52/54	-
87	PGV	4L	101	-	-	5/55/55/55	-
69	3PE	1Y	205	-	-	2/36/36/54	-
73	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
87	PGV	4A	601	-	-	14/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1M	502	-	-	13/51/51/54	-
85	HEM	3C	501	47	-	7/14/54/54	-
69	3PE	3D	502	-	-	1/36/36/54	-
92	PSC	4B	305	-	-	14/55/55/55	-
69	3PE	1K	101	-	-	9/47/47/54	-
87	PGV	4K	101	-	-	14/55/55/55	-
69	3PE	1Y	206	-	-	5/30/30/54	-

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	8A	604	HEA	FE-NB	5.66	2.12	1.94
88	4A	604	HEA	FE-ND	5.65	2.12	1.94
88	4A	604	HEA	FE-NB	5.64	2.12	1.94
88	8A	604	HEA	FE-ND	5.62	2.12	1.94
88	4A	605	HEA	FE-ND	5.61	2.12	1.94
88	8A	605	HEA	FE-ND	5.58	2.12	1.94
88	4A	605	HEA	FE-NB	5.54	2.12	1.94
88	8A	605	HEA	FE-NB	5.51	2.11	1.94
88	8A	604	HEA	C3B-C2B	5.50	1.47	1.34
88	8A	605	HEA	C3B-C2B	5.47	1.47	1.34
88	4A	604	HEA	C3B-C2B	5.45	1.47	1.34
88	4A	605	HEA	C3B-C2B	5.43	1.47	1.34
85	3C	501	HEM	FE-NB	5.33	2.11	1.94
85	3P	501	HEM	FE-NB	5.32	2.11	1.94
86	3D	501	HEC	C3B-C2B	5.22	1.48	1.36
86	3Q	501	HEC	C3B-C2B	5.21	1.48	1.36
85	3C	502	HEM	FE-NB	5.20	2.10	1.94
85	3P	502	HEM	FE-NB	5.17	2.10	1.94
86	3Q	501	HEC	FE-ND	5.14	2.10	1.94
86	3D	501	HEC	FE-ND	5.13	2.10	1.94
86	3D	501	HEC	C2A-C3A	5.07	1.47	1.36
86	3D	501	HEC	FE-NB	5.06	2.10	1.94
86	3D	501	HEC	C3D-C2D	5.05	1.47	1.36
86	3Q	501	HEC	FE-NB	5.04	2.10	1.94
88	8A	604	HEA	FE-NC	4.97	2.11	1.95
88	8A	605	HEA	C3D-C2D	4.97	1.47	1.36
86	3Q	501	HEC	C2A-C3A	4.96	1.47	1.36
88	4A	604	HEA	FE-NC	4.92	2.11	1.95
88	4A	605	HEA	FE-NC	4.91	2.11	1.95
88	4A	605	HEA	C3D-C2D	4.89	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	8A	605	HEA	FE-NC	4.88	2.11	1.95
86	3D	501	HEC	CHB-C4A	4.84	1.47	1.38
86	3Q	501	HEC	CHB-C4A	4.84	1.47	1.38
88	8A	604	HEA	C3D-C2D	4.83	1.47	1.36
86	3Q	501	HEC	C3D-C2D	4.83	1.47	1.36
86	3Q	501	HEC	CHA-C1A	4.80	1.47	1.38
88	4A	604	HEA	C3D-C2D	4.78	1.47	1.36
86	3D	501	HEC	CHA-C1A	4.76	1.47	1.38
86	3D	501	HEC	CHD-C1D	4.75	1.48	1.38
86	3Q	501	HEC	FE-NA	4.73	2.10	1.95
86	3Q	501	HEC	CHD-C1D	4.73	1.48	1.38
88	8A	604	HEA	C3A-C2A	4.69	1.47	1.37
86	3Q	501	HEC	FE-NC	4.67	2.10	1.95
86	3D	501	HEC	FE-NA	4.67	2.10	1.95
86	3D	501	HEC	FE-NC	4.65	2.10	1.95
88	4A	604	HEA	C3A-C2A	4.63	1.47	1.37
88	8A	605	HEA	C3A-C2A	4.59	1.47	1.37
86	3Q	501	HEC	CHC-C4B	4.57	1.47	1.38
86	3D	501	HEC	CHC-C4B	4.55	1.47	1.38
88	4A	605	HEA	C3A-C2A	4.54	1.47	1.37
88	8A	605	HEA	CHC-C4B	4.46	1.47	1.38
88	4A	605	HEA	CHD-C1D	4.45	1.47	1.38
88	4A	604	HEA	CHC-C4B	4.42	1.47	1.38
88	8A	605	HEA	CHD-C1D	4.42	1.47	1.38
88	4A	605	HEA	CHC-C4B	4.41	1.47	1.38
88	4A	604	HEA	CHB-C4A	4.38	1.47	1.38
88	4A	604	HEA	CHD-C1D	4.36	1.47	1.38
88	8A	604	HEA	CHD-C1D	4.32	1.47	1.38
88	4A	605	HEA	C1A-NA	4.31	1.47	1.39
88	8A	604	HEA	CHC-C4B	4.30	1.47	1.38
88	8A	605	HEA	CHB-C4A	4.29	1.46	1.38
88	4A	605	HEA	CHB-C4A	4.26	1.46	1.38
88	4A	604	HEA	CHA-C1A	4.26	1.46	1.38
88	8A	604	HEA	CHB-C4A	4.26	1.46	1.38
88	8A	604	HEA	C1A-NA	4.25	1.47	1.39
88	8A	604	HEA	CHA-C1A	4.25	1.46	1.38
85	3P	501	HEM	FE-NC	4.22	2.09	1.95
85	3C	501	HEM	FE-NC	4.22	2.09	1.95
88	4A	604	HEA	C1A-NA	4.18	1.47	1.39
85	3P	502	HEM	FE-NC	4.17	2.08	1.95
88	8A	605	HEA	C1A-NA	4.16	1.47	1.39
85	3C	502	HEM	FE-NC	4.16	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	8A	605	HEA	CHA-C1A	4.06	1.46	1.38
88	4A	605	HEA	CHA-C1A	4.05	1.46	1.38
88	8A	605	HEA	C4A-NA	4.00	1.47	1.39
88	4A	605	HEA	C4A-NA	4.00	1.47	1.39
88	8A	604	HEA	C4A-NA	4.00	1.47	1.39
88	4A	604	HEA	C4A-NA	3.99	1.47	1.39
86	3D	501	HEC	CHA-C4D	3.86	1.48	1.39
86	3D	501	HEC	CHD-C4C	3.83	1.48	1.39
86	3Q	501	HEC	CHD-C4C	3.82	1.48	1.39
86	3Q	501	HEC	CHA-C4D	3.80	1.47	1.39
86	3Q	501	HEC	CHB-C1B	3.77	1.47	1.39
86	3D	501	HEC	CHB-C1B	3.77	1.47	1.39
86	3Q	501	HEC	CHC-C1C	3.73	1.47	1.39
86	3D	501	HEC	CHC-C1C	3.66	1.47	1.39
88	4A	605	HEA	CHD-C4C	3.57	1.47	1.39
88	8A	605	HEA	CHC-C1C	3.52	1.47	1.39
88	8A	605	HEA	CHD-C4C	3.52	1.47	1.39
86	3D	501	HEC	C3C-C2C	3.49	1.48	1.38
88	4A	604	HEA	CHC-C1C	3.49	1.47	1.39
88	4A	605	HEA	CHC-C1C	3.47	1.47	1.39
86	3Q	501	HEC	C3C-C2C	3.47	1.48	1.38
88	4A	604	HEA	CHD-C4C	3.44	1.47	1.39
88	8A	604	HEA	CHC-C1C	3.38	1.47	1.39
88	8A	604	HEA	CHD-C4C	3.37	1.47	1.39
85	3C	502	HEM	C1B-NB	-3.35	1.34	1.40
85	3P	502	HEM	C1B-NB	-3.35	1.34	1.40
88	8A	604	HEA	CHA-C4D	3.31	1.46	1.39
88	4A	604	HEA	CHA-C4D	3.31	1.46	1.39
88	8A	605	HEA	CHB-C1B	3.28	1.46	1.39
88	4A	605	HEA	CHB-C1B	3.25	1.46	1.39
85	3C	502	HEM	C4D-ND	-3.25	1.34	1.40
88	4A	604	HEA	CHB-C1B	3.24	1.46	1.39
88	4A	605	HEA	CHA-C4D	3.23	1.46	1.39
85	3P	502	HEM	C4D-ND	-3.22	1.34	1.40
88	8A	605	HEA	CHA-C4D	3.22	1.46	1.39
85	3P	501	HEM	C1B-NB	-3.21	1.34	1.40
88	8A	604	HEA	CHB-C1B	3.19	1.46	1.39
85	3C	501	HEM	C1B-NB	-3.17	1.34	1.40
85	3C	501	HEM	C4D-ND	-3.16	1.34	1.40
85	3P	501	HEM	C4D-ND	-3.15	1.34	1.40
86	3D	501	HEC	C4B-NB	-3.01	1.35	1.40
86	3Q	501	HEC	C4B-NB	-2.97	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	3D	501	HEC	C1D-ND	-2.82	1.35	1.40
88	4A	604	HEA	C4B-C3B	2.80	1.49	1.44
86	3Q	501	HEC	C1D-ND	-2.79	1.35	1.40
88	8A	604	HEA	C4B-C3B	2.73	1.49	1.44
88	8A	605	HEA	C1D-ND	-2.69	1.35	1.40
88	4A	604	HEA	C1D-ND	-2.68	1.35	1.40
88	8A	605	HEA	C4B-C3B	2.66	1.49	1.44
88	4A	605	HEA	C1D-ND	-2.62	1.35	1.40
88	4A	605	HEA	C4B-C3B	2.62	1.49	1.44
86	3Q	501	HEC	C1C-C2C	2.61	1.49	1.43
88	8A	605	HEA	C4B-NB	-2.60	1.35	1.40
88	8A	604	HEA	C1D-ND	-2.59	1.35	1.40
88	4A	604	HEA	C4D-C3D	2.57	1.49	1.45
88	4A	605	HEA	C4B-NB	-2.56	1.35	1.40
86	3D	501	HEC	C1C-C2C	2.54	1.49	1.43
88	4A	604	HEA	C4B-NB	-2.53	1.35	1.40
88	8A	605	HEA	C1C-C2C	2.53	1.49	1.43
88	4A	604	HEA	C1C-C2C	2.52	1.49	1.43
88	8A	604	HEA	C1C-C2C	2.52	1.49	1.43
88	8A	604	HEA	C4B-NB	-2.52	1.35	1.40
88	4A	605	HEA	C1C-C2C	2.51	1.49	1.43
85	3P	502	HEM	FE-ND	-2.47	1.87	1.94
85	3C	502	HEM	FE-ND	-2.47	1.87	1.94
85	3C	501	HEM	FE-ND	-2.45	1.87	1.94
88	8A	604	HEA	C4D-C3D	2.43	1.49	1.45
85	3P	501	HEM	FE-ND	-2.42	1.87	1.94
86	3D	501	HEC	C1A-NA	-2.37	1.35	1.39
86	3D	501	HEC	C4A-NA	-2.36	1.35	1.39
86	3D	501	HEC	C1B-C2B	2.36	1.49	1.44
85	3P	501	HEM	C1C-C2C	-2.35	1.40	1.45
85	3P	502	HEM	C1C-C2C	-2.35	1.40	1.45
86	3Q	501	HEC	C1B-C2B	2.34	1.49	1.44
85	3C	502	HEM	C1C-C2C	-2.34	1.40	1.45
86	3D	501	HEC	C4D-C3D	2.32	1.49	1.45
86	3Q	501	HEC	C4A-NA	-2.32	1.35	1.39
85	3C	501	HEM	C1C-C2C	-2.31	1.40	1.45
88	4A	605	HEA	C1D-C2D	2.31	1.49	1.44
86	3D	501	HEC	C4C-NC	-2.30	1.35	1.39
86	3Q	501	HEC	C4C-NC	-2.30	1.35	1.39
88	8A	605	HEA	C11-C3B	-2.27	1.48	1.51
88	8A	605	HEA	C4D-C3D	2.27	1.48	1.45
86	3Q	501	HEC	C1A-NA	-2.26	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	8A	604	HEA	C1A-C2A	2.23	1.49	1.45
88	4A	605	HEA	C11-C3B	-2.23	1.48	1.51
88	8A	605	HEA	C1D-C2D	2.22	1.49	1.44
88	4A	605	HEA	C4D-C3D	2.20	1.48	1.45
86	3D	501	HEC	C1D-C2D	2.19	1.49	1.44
88	4A	605	HEA	C1A-C2A	2.18	1.49	1.45
88	8A	604	HEA	C1D-C2D	2.17	1.48	1.44
85	3P	502	HEM	C1D-ND	-2.17	1.34	1.38
86	3Q	501	HEC	C1D-C2D	2.17	1.48	1.44
86	3D	501	HEC	C1C-NC	-2.17	1.35	1.39
88	4A	604	HEA	C4C-NC	-2.15	1.35	1.39
88	8A	605	HEA	C4C-NC	-2.15	1.35	1.39
88	4A	604	HEA	C1A-C2A	2.15	1.49	1.45
85	3P	501	HEM	C1D-ND	-2.14	1.34	1.38
88	4A	605	HEA	C4C-NC	-2.13	1.35	1.39
88	8A	605	HEA	C1A-C2A	2.13	1.48	1.45
86	3Q	501	HEC	C4D-C3D	2.12	1.48	1.45
88	8A	604	HEA	C4C-NC	-2.12	1.35	1.39
86	3Q	501	HEC	C1C-NC	-2.11	1.35	1.39
85	3C	502	HEM	C1D-ND	-2.11	1.34	1.38
85	3P	501	HEM	C3C-C4C	-2.10	1.42	1.46
86	3D	501	HEC	C1A-C2A	2.09	1.48	1.45
88	8A	604	HEA	C1B-C2B	2.08	1.48	1.44
88	4A	604	HEA	C1D-C2D	2.06	1.48	1.44
86	3Q	501	HEC	C1A-C2A	2.06	1.48	1.45
85	3C	501	HEM	C1D-ND	-2.05	1.34	1.38
85	3P	502	HEM	C3C-C4C	-2.05	1.42	1.46
88	4A	605	HEA	C3C-C4C	2.04	1.48	1.42
88	4A	604	HEA	C1B-C2B	2.04	1.48	1.44
85	3C	502	HEM	C3C-C4C	-2.03	1.42	1.46
85	3C	501	HEM	C3C-C4C	-2.03	1.42	1.46
88	8A	605	HEA	C1B-C2B	2.03	1.48	1.44
86	3D	501	HEC	C4C-C3C	2.02	1.48	1.44
85	3C	502	HEM	C4B-NB	-2.01	1.34	1.38
86	3Q	501	HEC	C4C-C3C	2.01	1.48	1.44
88	8A	604	HEA	C11-C3B	-2.01	1.48	1.51

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	4A	605	HEA	C3D-C4D-ND	6.64	116.77	110.35
88	8A	605	HEA	C3D-C4D-ND	6.63	116.76	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	4A	604	HEA	C3D-C4D-ND	6.54	116.67	110.35
88	8A	604	HEA	C3D-C4D-ND	6.47	116.60	110.35
80	1T	101	EHZ	C10-S1-C9	6.20	120.16	101.84
88	8A	604	HEA	C2B-C1B-NB	6.02	116.86	109.90
80	1n	201	EHZ	C10-S1-C9	5.93	119.36	101.84
86	3D	501	HEC	C1B-C2B-C3B	-5.90	100.78	106.98
86	3Q	501	HEC	C1B-C2B-C3B	-5.89	100.79	106.98
88	4A	605	HEA	C2B-C1B-NB	5.89	116.71	109.90
88	4A	604	HEA	C2B-C1B-NB	5.83	116.64	109.90
88	8A	604	HEA	C3B-C4B-NB	5.79	116.50	109.84
88	8A	604	HEA	C3C-C4C-NC	5.79	114.67	109.80
88	8A	605	HEA	C2A-C1A-NA	5.73	115.85	110.32
88	8A	605	HEA	C2B-C1B-NB	5.70	116.49	109.90
88	4A	605	HEA	C2A-C1A-NA	5.66	115.79	110.32
88	4A	604	HEA	C2D-C1D-ND	5.66	116.34	109.84
88	8A	604	HEA	C2D-C1D-ND	5.64	116.32	109.84
88	8A	605	HEA	C2D-C1D-ND	5.63	116.31	109.84
88	4A	604	HEA	C3B-C4B-NB	5.59	116.26	109.84
88	4A	605	HEA	C3C-C2C-C1C	-5.56	100.61	107.17
88	8A	605	HEA	C3C-C2C-C1C	-5.54	100.64	107.17
88	4A	605	HEA	C3B-C4B-NB	5.52	116.19	109.84
88	4A	605	HEA	C2D-C1D-ND	5.52	116.19	109.84
88	4A	604	HEA	C3C-C2C-C1C	-5.48	100.71	107.17
86	3D	501	HEC	C2B-C1B-NB	5.45	116.20	109.90
88	8A	604	HEA	C3C-C2C-C1C	-5.43	100.77	107.17
88	4A	604	HEA	C3C-C4C-NC	5.42	114.37	109.80
86	3Q	501	HEC	C2B-C1B-NB	5.41	116.16	109.90
88	8A	605	HEA	C3B-C4B-NB	5.38	116.03	109.84
88	4A	604	HEA	C2A-C1A-NA	5.35	115.49	110.32
86	3D	501	HEC	C2A-C1A-NA	5.32	115.46	110.32
86	3Q	501	HEC	C1C-C2C-C3C	-5.30	100.75	106.82
86	3D	501	HEC	C1C-C2C-C3C	-5.23	100.82	106.82
86	3Q	501	HEC	C2A-C1A-NA	5.21	115.35	110.32
88	8A	604	HEA	C2A-C1A-NA	5.21	115.35	110.32
86	3D	501	HEC	C3D-C4D-ND	5.16	115.34	110.35
88	8A	605	HEA	C3C-C4C-NC	5.15	114.13	109.80
88	4A	605	HEA	C3C-C4C-NC	5.14	114.12	109.80
85	3C	501	HEM	CHC-C4B-NB	5.09	129.90	124.42
86	3Q	501	HEC	C3D-C4D-ND	5.00	115.18	110.35
78	1P	402	NDP	P2B-O2B-C2B	-4.98	110.14	123.43
85	3P	501	HEM	CHC-C4B-NB	4.93	129.72	124.42
85	3P	502	HEM	CHC-C4B-NB	4.92	129.71	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	3C	502	HEM	CHC-C4B-NB	4.91	129.71	124.42
86	3D	501	HEC	C2D-C1D-ND	4.67	115.20	109.84
86	3Q	501	HEC	CBB-CAB-C3B	4.60	124.89	112.42
86	3D	501	HEC	CBB-CAB-C3B	4.58	124.84	112.42
86	3Q	501	HEC	CBC-CAC-C3C	4.54	124.72	112.42
86	3Q	501	HEC	C2D-C1D-ND	4.51	115.03	109.84
86	3D	501	HEC	CBC-CAC-C3C	4.45	124.48	112.42
85	3C	501	HEM	CHD-C1D-ND	4.39	129.15	124.42
88	4A	604	HEA	CHA-C4D-ND	-4.35	119.74	124.42
85	3P	501	HEM	CHD-C1D-ND	4.35	129.10	124.42
85	3P	502	HEM	CHD-C1D-ND	4.29	129.04	124.42
88	4A	605	HEA	C1D-C2D-C3D	-4.23	102.53	106.98
88	8A	604	HEA	C2C-C1C-NC	4.22	116.91	110.14
88	8A	605	HEA	C1D-C2D-C3D	-4.22	102.54	106.98
88	4A	605	HEA	C2C-C1C-NC	4.21	116.89	110.14
88	8A	605	HEA	C3A-C2A-C1A	-4.18	103.09	107.05
88	4A	605	HEA	C3A-C2A-C1A	-4.16	103.11	107.05
88	4A	604	HEA	C2C-C1C-NC	4.12	116.74	110.14
88	8A	605	HEA	C2C-C1C-NC	4.10	116.71	110.14
88	8A	604	HEA	C1D-C2D-C3D	-4.07	102.70	106.98
75	1N	902	CDL	OB6-CB5-C51	4.02	118.25	111.09
85	3C	502	HEM	CHD-C1D-ND	4.00	128.72	124.42
86	3D	501	HEC	C1D-C2D-C3D	-3.95	102.83	106.98
88	4A	604	HEA	C1D-C2D-C3D	-3.89	102.89	106.98
86	3Q	501	HEC	C1D-C2D-C3D	-3.88	102.89	106.98
86	3Q	501	HEC	C2C-C1C-NC	3.87	116.34	110.14
86	3D	501	HEC	C2C-C1C-NC	3.84	116.30	110.14
88	8A	604	HEA	C3A-C2A-C1A	-3.83	103.42	107.05
88	4A	604	HEA	C3A-C2A-C1A	-3.83	103.42	107.05
87	4C	301	PGV	O01-C1-C2	3.82	119.74	111.48
88	8A	605	HEA	CHA-C4D-ND	-3.80	120.33	124.42
88	4A	605	HEA	C1B-C2B-C3B	-3.73	102.47	106.80
88	8A	604	HEA	C1B-C2B-C3B	-3.72	102.49	106.80
88	8A	605	HEA	C1B-C2B-C3B	-3.70	102.51	106.80
86	3D	501	HEC	C3B-C4B-NB	3.70	114.23	110.17
86	3Q	501	HEC	C3B-C4B-NB	3.69	114.22	110.17
87	8C	302	PGV	O01-C1-C2	3.58	119.23	111.48
88	4A	604	HEA	C1B-C2B-C3B	-3.58	102.65	106.80
85	3C	501	HEM	CHA-C4D-ND	3.53	128.73	124.37
86	3Q	501	HEC	C3C-C4C-NC	3.49	114.03	110.15
86	3D	501	HEC	C1A-C2A-C3A	-3.49	102.51	107.11
88	4A	604	HEA	CAD-C3D-C4D	3.47	130.75	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	4A	605	HEA	C4A-NA-C1A	-3.46	100.17	105.82
85	3P	502	HEM	C1B-NB-C4B	3.45	109.30	105.21
85	3P	501	HEM	CHB-C1B-NB	3.44	128.62	124.37
88	4A	604	HEA	C4D-C3D-C2D	-3.44	101.89	106.89
85	3C	502	HEM	C1B-NB-C4B	3.44	109.28	105.21
88	8A	604	HEA	CHA-C4D-ND	-3.44	120.73	124.42
85	3P	501	HEM	CHA-C4D-ND	3.43	128.62	124.37
86	3D	501	HEC	C3C-C4C-NC	3.42	113.95	110.15
88	8A	605	HEA	C4A-NA-C1A	-3.40	100.27	105.82
86	3Q	501	HEC	C1A-C2A-C3A	-3.38	102.66	107.11
85	3C	502	HEM	CHA-C4D-ND	3.37	128.53	124.37
88	8A	605	HEA	C13-C12-C11	-3.36	109.03	114.39
88	4A	605	HEA	CHA-C4D-ND	-3.34	120.83	124.42
88	4A	605	HEA	C13-C12-C11	-3.33	109.07	114.39
88	8A	604	HEA	C13-C14-C15	-3.30	120.06	127.62
88	8A	605	HEA	C4D-C3D-C2D	-3.30	102.08	106.89
88	4A	604	HEA	C13-C14-C15	-3.28	120.11	127.62
85	3C	501	HEM	CHB-C1B-NB	3.27	128.41	124.37
88	8A	604	HEA	C4D-C3D-C2D	-3.27	102.13	106.89
88	4A	604	HEA	C4A-NA-C1A	-3.25	100.52	105.82
88	4A	605	HEA	C4D-C3D-C2D	-3.23	102.19	106.89
85	3P	502	HEM	CHA-C4D-ND	3.22	128.35	124.37
85	3C	501	HEM	C1B-NB-C4B	3.19	108.99	105.21
85	3P	501	HEM	C1B-NB-C4B	3.19	108.98	105.21
88	8A	604	HEA	C4B-C3B-C2B	-3.18	102.09	107.44
88	8A	605	HEA	C13-C14-C15	-3.17	120.36	127.62
88	8A	604	HEA	C4A-NA-C1A	-3.17	100.65	105.82
88	4A	604	HEA	C4B-C3B-C2B	-3.16	102.12	107.44
88	4A	605	HEA	C13-C14-C15	-3.15	120.41	127.62
88	8A	604	HEA	CHB-C1B-NB	-3.12	121.07	124.42
86	3D	501	HEC	C3A-C4A-NA	3.10	115.37	109.64
85	3P	502	HEM	CHB-C1B-NB	3.10	128.20	124.37
69	1Y	204	3PE	O21-C21-C22	3.07	118.13	111.48
86	3Q	501	HEC	C3A-C4A-NA	3.06	115.31	109.64
85	3C	502	HEM	CHB-C1B-NB	3.05	128.14	124.37
86	3D	501	HEC	CMC-C2C-C3C	3.04	132.08	125.62
88	4A	605	HEA	C4B-C3B-C2B	-3.03	102.34	107.44
86	3Q	501	HEC	CMC-C2C-C3C	3.01	132.00	125.62
88	4A	604	HEA	C26-C15-C16	3.00	120.44	115.23
88	8A	604	HEA	C26-C15-C16	3.00	120.44	115.23
88	8A	604	HEA	CAD-C3D-C4D	3.00	129.92	124.70
88	8A	605	HEA	C4B-C3B-C2B	-2.99	102.41	107.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	3D	501	HEC	C4D-C3D-C2D	-2.94	102.62	106.89
86	3Q	501	HEC	CMD-C2D-C1D	2.90	129.56	125.03
88	4A	604	HEA	CHB-C1B-NB	-2.86	121.34	124.42
88	8A	605	HEA	CHA-C1A-NA	-2.85	121.35	124.45
86	3D	501	HEC	C4A-C3A-C2A	-2.83	102.77	106.97
88	4A	604	HEA	CHA-C1A-NA	-2.83	121.37	124.45
85	3P	502	HEM	C3B-C4B-NB	-2.83	107.44	109.47
86	3Q	501	HEC	C4A-C3A-C2A	-2.82	102.79	106.97
82	1h	201	AME	O-C-CA	-2.80	117.58	124.77
85	3C	502	HEM	C3B-C4B-NB	-2.78	107.47	109.47
86	3Q	501	HEC	C4D-C3D-C2D	-2.78	102.85	106.89
88	4A	605	HEA	C26-C15-C16	2.78	120.05	115.23
88	4A	605	HEA	CHA-C1A-NA	-2.71	121.50	124.45
88	4A	605	HEA	C17-C18-C19	-2.69	121.46	127.62
88	8A	605	HEA	C26-C15-C16	2.68	119.88	115.23
78	1P	402	NDP	O4D-C1D-C2D	-2.66	100.92	106.62
85	3P	501	HEM	CHD-C4C-NC	2.66	127.35	124.45
88	8A	604	HEA	C4B-NB-C1B	-2.66	102.06	105.21
88	4A	605	HEA	CHB-C1B-NB	-2.66	121.56	124.42
88	8A	605	HEA	C27-C19-C20	2.65	119.82	115.23
85	3P	501	HEM	CHD-C1D-C2D	-2.61	120.90	125.03
85	3C	501	HEM	CHD-C1D-C2D	-2.59	120.93	125.03
88	4A	605	HEA	C27-C19-C20	2.59	119.72	115.23
88	8A	605	HEA	CHB-C1B-NB	-2.59	121.64	124.42
86	3Q	501	HEC	CAD-C3D-C4D	2.57	129.18	124.70
88	4A	604	HEA	CMC-C2C-C1C	2.56	129.32	125.42
85	3C	501	HEM	CHD-C4C-NC	2.56	127.24	124.45
85	3P	501	HEM	C3B-C4B-NB	-2.55	107.64	109.47
88	8A	604	HEA	CHC-C1C-C2C	-2.55	120.04	127.43
88	8A	605	HEA	C17-C18-C19	-2.54	121.81	127.62
88	4A	605	HEA	CHC-C1C-C2C	-2.53	120.08	127.43
85	3C	501	HEM	C3B-C4B-NB	-2.53	107.65	109.47
88	4A	604	HEA	C1D-ND-C4D	-2.53	102.21	105.21
88	8A	604	HEA	C17-C18-C19	-2.52	121.86	127.62
88	8A	604	HEA	C1D-ND-C4D	-2.50	102.24	105.21
85	3P	502	HEM	CHD-C1D-C2D	-2.49	121.10	125.03
88	4A	605	HEA	C4B-NB-C1B	-2.47	102.28	105.21
88	8A	605	HEA	C1D-ND-C4D	-2.45	102.31	105.21
88	8A	605	HEA	C1A-CHA-C4D	-2.45	120.82	126.02
88	4A	604	HEA	CHC-C1C-C2C	-2.44	120.33	127.43
88	4A	604	HEA	C4B-NB-C1B	-2.44	102.32	105.21
88	4A	605	HEA	C1D-ND-C4D	-2.43	102.33	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	4A	605	HEA	C25-C23-C24	2.43	120.18	114.59
88	8A	605	HEA	CHC-C1C-C2C	-2.43	120.38	127.43
88	8A	604	HEA	CBA-CAA-C2A	-2.40	105.89	112.53
86	3D	501	HEC	CAD-C3D-C4D	2.40	128.88	124.70
85	3C	502	HEM	C4C-CHD-C1D	-2.40	120.92	126.02
88	4A	604	HEA	C17-C18-C19	-2.39	122.15	127.62
86	3Q	501	HEC	CAC-C3C-C2C	2.38	130.66	126.89
88	8A	604	HEA	CMC-C2C-C1C	2.38	129.04	125.42
88	4A	605	HEA	CMB-C2B-C1B	2.37	128.74	125.03
86	3Q	501	HEC	CAA-CBA-CGA	-2.37	107.37	113.67
88	4A	604	HEA	CMB-C2B-C1B	2.37	128.74	125.03
88	8A	604	HEA	CMB-C2B-C1B	2.37	128.73	125.03
88	4A	605	HEA	CMC-C2C-C1C	2.36	129.01	125.42
88	8A	605	HEA	CMC-C2C-C1C	2.35	129.00	125.42
88	8A	604	HEA	CHD-C1D-C2D	-2.35	120.28	126.95
88	4A	604	HEA	CHD-C1D-C2D	-2.34	120.28	126.95
85	3P	502	HEM	C4C-CHD-C1D	-2.34	121.04	126.02
86	3D	501	HEC	CAC-C3C-C2C	2.34	130.59	126.89
88	4A	604	HEA	C1A-CHA-C4D	-2.33	121.06	126.02
88	4A	604	HEA	C27-C19-C20	2.33	119.26	115.23
92	4B	305	PSC	O01-C1-C2	2.30	116.46	111.48
88	8A	605	HEA	CAD-C3D-C4D	2.29	128.69	124.70
88	4A	604	HEA	C13-C12-C11	-2.29	110.73	114.39
88	8A	605	HEA	CMB-C2B-C1B	2.28	128.59	125.03
69	3A	502	3PE	O21-C21-C22	2.27	116.40	111.48
88	8A	604	HEA	C25-C23-C24	2.27	119.81	114.59
88	8A	604	HEA	CHA-C1A-NA	-2.27	121.99	124.45
85	3C	502	HEM	CHD-C1D-C2D	-2.26	121.45	125.03
85	3P	501	HEM	C1A-CHA-C4D	-2.26	120.94	126.25
88	8A	605	HEA	C25-C23-C24	2.26	119.78	114.59
88	4A	605	HEA	CAD-C3D-C4D	2.26	128.63	124.70
88	4A	605	HEA	C1A-CHA-C4D	-2.26	121.22	126.02
85	3P	502	HEM	C1A-CHA-C4D	-2.25	120.95	126.25
88	8A	604	HEA	CMD-C2D-C1D	2.25	128.54	125.03
85	3C	502	HEM	C1A-CHA-C4D	-2.24	120.97	126.25
88	8A	605	HEA	C4B-NB-C1B	-2.24	102.55	105.21
88	4A	605	HEA	CMD-C2D-C1D	2.24	128.53	125.03
85	3P	502	HEM	CHD-C4C-NC	2.23	126.88	124.45
86	3D	501	HEC	CMD-C2D-C1D	2.22	128.50	125.03
88	8A	605	HEA	CHD-C1D-C2D	-2.21	120.67	126.95
88	4A	604	HEA	C25-C23-C24	2.20	119.65	114.59
88	4A	604	HEA	CMD-C2D-C1D	2.19	128.46	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	3C	502	HEM	C4A-CHB-C1B	-2.19	121.09	126.25
88	4A	605	HEA	CHD-C1D-C2D	-2.18	120.75	126.95
88	8A	604	HEA	CHB-C4A-NA	-2.18	122.08	124.45
86	3D	501	HEC	CHB-C1B-NB	-2.17	122.09	124.42
85	3P	502	HEM	C4D-ND-C1D	2.17	107.77	105.21
88	4A	604	HEA	CBA-CAA-C2A	-2.16	106.55	112.53
85	3C	501	HEM	C1A-CHA-C4D	-2.15	121.19	126.25
86	3D	501	HEC	CHC-C1C-C2C	-2.14	121.21	127.43
85	3C	501	HEM	CHA-C4D-C3D	-2.14	121.28	125.23
86	3Q	501	HEC	CHC-C1C-C2C	-2.14	121.22	127.43
86	3Q	501	HEC	CMB-C2B-C3B	2.13	131.90	126.15
86	3Q	501	HEC	CHB-C1B-NB	-2.12	122.14	124.42
87	8G	101	PGV	O01-C1-C2	2.12	116.06	111.48
86	3Q	501	HEC	CHA-C4D-C3D	-2.12	121.69	124.77
88	8A	604	HEA	C21-C22-C23	-2.11	120.59	127.64
86	3D	501	HEC	CMB-C2B-C3B	2.11	131.87	126.15
86	3Q	501	HEC	CHB-C1B-C2B	-2.11	121.69	125.03
87	4G	101	PGV	O01-C1-C2	2.11	116.04	111.48
86	3D	501	HEC	CHB-C1B-C2B	-2.11	121.70	125.03
88	4A	604	HEA	CHB-C4A-NA	-2.10	122.16	124.45
85	3C	502	HEM	C4D-ND-C1D	2.10	107.70	105.21
73	1F	501	FMN	C4-N3-C2	-2.10	121.92	125.64
85	3P	502	HEM	C4A-CHB-C1B	-2.10	121.31	126.25
88	4A	605	HEA	CHB-C1B-C2B	-2.09	121.72	125.03
75	1H	401	CDL	OB6-CB5-C51	2.09	116.00	111.48
87	4C	304	PGV	O01-C1-C2	2.09	116.00	111.48
86	3D	501	HEC	CAA-CBA-CGA	-2.08	108.14	113.67
85	3P	501	HEM	CHA-C4D-C3D	-2.08	121.39	125.23
88	8A	605	HEA	CMD-C2D-C1D	2.06	128.26	125.03
88	8A	604	HEA	C4C-C3C-C2C	-2.05	104.75	107.30
87	8C	305	PGV	O01-C1-C2	2.05	115.92	111.48
88	8A	605	HEA	C21-C22-C23	-2.05	120.82	127.64
85	3C	502	HEM	CHD-C4C-NC	2.04	126.67	124.45
88	4A	605	HEA	C21-C22-C23	-2.03	120.86	127.64
85	3C	501	HEM	CHA-C1A-NA	2.03	127.54	123.86
85	3P	501	HEM	CHB-C1B-C2B	-2.03	121.18	126.95
88	4A	604	HEA	C21-C22-C23	-2.03	120.88	127.64
88	8A	605	HEA	CHB-C1B-C2B	-2.00	121.86	125.03

All (2) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
86	3D	501	HEC	NA
86	3Q	501	HEC	NA

All (895) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C11-O13-P-O12
69	1K	101	3PE	C1-O11-P-O13
69	1K	101	3PE	C1-O11-P-O14
69	1L	701	3PE	O32-C31-O31-C3
69	1L	701	3PE	C32-C31-O31-C3
69	1L	703	3PE	C2-C1-O11-P
69	1M	501	3PE	C11-O13-P-O14
69	1M	502	3PE	C1-O11-P-O12
69	1M	502	3PE	C2-C1-O11-P
69	1M	502	3PE	O32-C31-O31-C3
69	1M	502	3PE	C32-C31-O31-C3
69	1M	504	3PE	C2-C1-O11-P
69	1M	506	3PE	C1-O11-P-O14
69	1N	901	3PE	C1-O11-P-O12
69	1N	901	3PE	C1-O11-P-O13
69	1N	901	3PE	C1-O11-P-O14
69	1P	403	3PE	C1-O11-P-O12
69	1Y	202	3PE	C1-O11-P-O13
69	1Y	202	3PE	C2-C1-O11-P
69	1Y	203	3PE	C1-O11-P-O13
69	1Y	203	3PE	C1-O11-P-O14
69	1Y	203	3PE	C2-C1-O11-P
69	1Y	203	3PE	O22-C21-O21-C2
69	1Y	203	3PE	C22-C21-O21-C2
69	1Y	204	3PE	O22-C21-O21-C2
69	1Y	204	3PE	C22-C21-O21-C2
69	1Y	206	3PE	C11-O13-P-O14
69	1Y	206	3PE	C12-C11-O13-P
69	1j	101	3PE	O22-C21-O21-C2
69	1j	101	3PE	C22-C21-O21-C2
69	1m	201	3PE	O32-C31-O31-C3
69	1m	201	3PE	C32-C31-O31-C3
69	3A	502	3PE	O32-C31-O31-C3
69	3A	502	3PE	C32-C31-O31-C3
69	3A	502	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
69	3A	502	3PE	C22-C21-O21-C2
69	3A	503	3PE	C1-O11-P-O14
69	3A	503	3PE	C2-C1-O11-P
69	3C	503	3PE	C11-O13-P-O11
69	3C	503	3PE	C11-O13-P-O12
69	3C	503	3PE	C11-O13-P-O14
69	3C	504	3PE	O21-C2-C3-O31
69	3G	101	3PE	O32-C31-O31-C3
69	3G	101	3PE	C32-C31-O31-C3
69	3N	501	3PE	C1-O11-P-O13
69	3N	501	3PE	C1-O11-P-O14
69	3N	501	3PE	C2-C1-O11-P
69	3N	503	3PE	O22-C21-O21-C2
69	3N	503	3PE	C22-C21-O21-C2
69	3P	503	3PE	C11-O13-P-O11
69	3P	503	3PE	C11-O13-P-O12
69	3P	503	3PE	C11-O13-P-O14
69	3Y	101	3PE	C2-C1-O11-P
70	1B	203	PC1	O22-C21-O21-C2
70	1B	203	PC1	C22-C21-O21-C2
70	1I	203	PC1	C1-O11-P-O14
70	1M	503	PC1	C11-O13-P-O11
70	1M	503	PC1	O22-C21-O21-C2
70	1M	503	PC1	C22-C21-O21-C2
70	1M	505	PC1	C1-O11-P-O12
70	1d	202	PC1	O22-C21-O21-C2
70	1d	202	PC1	C22-C21-O21-C2
70	1h	203	PC1	C11-O13-P-O14
70	1h	203	PC1	O32-C31-O31-C3
70	1h	203	PC1	C32-C31-O31-C3
70	3R	303	PC1	O32-C31-O31-C3
70	3R	303	PC1	C32-C31-O31-C3
70	3X	101	PC1	C1-O11-P-O14
75	1H	401	CDL	CA4-CA3-OA5-PA1
75	1H	401	CDL	OB7-CB5-OB6-CB4
75	1H	401	CDL	C51-CB5-OB6-CB4
75	1L	702	CDL	OA6-CA4-CA6-OA8
75	1L	702	CDL	CB3-OB5-PB2-OB4
75	1N	902	CDL	OA6-CA4-CA6-OA8
75	1N	902	CDL	CB3-OB5-PB2-OB3
75	1X	201	CDL	C1-CA2-OA2-PA1
75	1X	201	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
75	1X	201	CDL	C1-CB2-OB2-PB2
75	1h	202	CDL	CA2-OA2-PA1-OA4
75	1h	202	CDL	CA2-OA2-PA1-OA5
75	1h	202	CDL	C1-CB2-OB2-PB2
75	1h	202	CDL	CB2-OB2-PB2-OB3
75	1h	202	CDL	OB7-CB5-OB6-CB4
75	1h	202	CDL	C51-CB5-OB6-CB4
75	1h	202	CDL	OB9-CB7-OB8-CB6
75	1h	202	CDL	C71-CB7-OB8-CB6
75	3G	102	CDL	CB2-OB2-PB2-OB3
75	3G	102	CDL	CB2-OB2-PB2-OB4
75	3G	102	CDL	CB2-OB2-PB2-OB5
75	3G	103	CDL	CB2-OB2-PB2-OB4
75	3G	103	CDL	CB2-OB2-PB2-OB5
75	3P	504	CDL	OB9-CB7-OB8-CB6
75	3P	504	CDL	C71-CB7-OB8-CB6
75	3T	101	CDL	CA3-OA5-PA1-OA3
75	3T	101	CDL	CA3-OA5-PA1-OA4
75	3T	101	CDL	OB9-CB7-OB8-CB6
75	3T	101	CDL	C71-CB7-OB8-CB6
75	4B	303	CDL	OA9-CA7-OA8-CA6
75	4B	303	CDL	C31-CA7-OA8-CA6
75	4B	303	CDL	CB3-OB5-PB2-OB2
75	4B	303	CDL	CB3-OB5-PB2-OB3
75	4C	305	CDL	C1-CA2-OA2-PA1
75	4C	305	CDL	OB7-CB5-OB6-CB4
75	4C	305	CDL	C51-CB5-OB6-CB4
75	4C	305	CDL	OB9-CB7-OB8-CB6
75	4C	305	CDL	C71-CB7-OB8-CB6
75	4D	201	CDL	C1-CA2-OA2-PA1
75	4D	201	CDL	CA3-OA5-PA1-OA3
75	4D	201	CDL	CB3-OB5-PB2-OB3
75	4D	201	CDL	OB7-CB5-OB6-CB4
75	4D	201	CDL	C51-CB5-OB6-CB4
75	4D	201	CDL	OB9-CB7-OB8-CB6
75	4D	201	CDL	C71-CB7-OB8-CB6
75	8B	303	CDL	OA9-CA7-OA8-CA6
75	8B	303	CDL	C31-CA7-OA8-CA6
75	8B	303	CDL	CB3-OB5-PB2-OB3
75	8C	306	CDL	C1-CA2-OA2-PA1
75	8C	306	CDL	OB7-CB5-OB6-CB4
75	8C	306	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
75	8C	306	CDL	OB9-CB7-OB8-CB6
75	8C	306	CDL	C71-CB7-OB8-CB6
75	8D	201	CDL	C1-CA2-OA2-PA1
75	8D	201	CDL	CA3-OA5-PA1-OA3
75	8D	201	CDL	CB3-OB5-PB2-OB3
75	8D	201	CDL	OB7-CB5-OB6-CB4
75	8D	201	CDL	C51-CB5-OB6-CB4
75	8D	201	CDL	OB9-CB7-OB8-CB6
75	8D	201	CDL	C71-CB7-OB8-CB6
76	1O	401	GTP	C5'-O5'-PA-O1A
80	1T	101	EHZ	N2-C15-C16-O5
84	1I	201	MYR	O1-C1-C2-C3
85	3C	501	HEM	C2B-C3B-CAB-CBB
85	3C	501	HEM	C4B-C3B-CAB-CBB
85	3C	502	HEM	C2B-C3B-CAB-CBB
85	3C	502	HEM	C2C-C3C-CAC-CBC
85	3P	501	HEM	C2B-C3B-CAB-CBB
85	3P	501	HEM	C4B-C3B-CAB-CBB
85	3P	502	HEM	C2B-C3B-CAB-CBB
85	3P	502	HEM	C2C-C3C-CAC-CBC
87	4A	601	PGV	O04-C19-O03-C01
87	4A	601	PGV	C20-C19-O03-C01
87	4A	603	PGV	C02-C03-O11-P
87	4C	301	PGV	C05-C04-O12-P
87	4C	301	PGV	O02-C1-O01-C02
87	4C	301	PGV	C2-C1-O01-C02
87	4C	302	PGV	C03-O11-P-O14
87	4C	302	PGV	O04-C19-O03-C01
87	4C	302	PGV	C20-C19-O03-C01
87	4C	303	PGV	C03-O11-P-O13
87	4C	304	PGV	O02-C1-O01-C02
87	4C	304	PGV	C2-C1-O01-C02
87	4G	101	PGV	O02-C1-O01-C02
87	4G	101	PGV	C2-C1-O01-C02
87	4G	101	PGV	O04-C19-O03-C01
87	4G	101	PGV	C20-C19-O03-C01
87	4K	101	PGV	C03-O11-P-O12
87	4K	101	PGV	C03-O11-P-O14
87	4K	101	PGV	O04-C19-O03-C01
87	4K	101	PGV	C20-C19-O03-C01
87	8A	601	PGV	O04-C19-O03-C01
87	8A	601	PGV	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
87	8A	603	PGV	C02-C03-O11-P
87	8B	301	PGV	C03-O11-P-O12
87	8B	301	PGV	C03-O11-P-O13
87	8B	301	PGV	C04-O12-P-O11
87	8C	302	PGV	C04-O12-P-O11
87	8C	302	PGV	C04-O12-P-O13
87	8C	302	PGV	C05-C04-O12-P
87	8C	302	PGV	O02-C1-O01-C02
87	8C	302	PGV	C2-C1-O01-C02
87	8C	303	PGV	C03-O11-P-O14
87	8C	303	PGV	O04-C19-O03-C01
87	8C	303	PGV	C20-C19-O03-C01
87	8C	304	PGV	C03-O11-P-O12
87	8C	304	PGV	C03-O11-P-O13
87	8C	305	PGV	O02-C1-O01-C02
87	8C	305	PGV	C2-C1-O01-C02
87	8G	101	PGV	O02-C1-O01-C02
87	8G	101	PGV	C2-C1-O01-C02
87	8G	101	PGV	O04-C19-O03-C01
87	8G	101	PGV	C20-C19-O03-C01
87	8K	101	PGV	C03-O11-P-O12
87	8K	101	PGV	C03-O11-P-O14
87	8K	101	PGV	O04-C19-O03-C01
87	8K	101	PGV	C20-C19-O03-C01
92	4B	305	PSC	C03-O11-P-O12
92	4B	305	PSC	C03-O11-P-O13
92	4B	305	PSC	C02-C03-O11-P
92	4B	305	PSC	O02-C1-O01-C02
92	4B	305	PSC	C2-C1-O01-C02
92	8B	305	PSC	C03-O11-P-O12
92	8B	305	PSC	C03-O11-P-O13
92	8B	305	PSC	O02-C1-O01-C02
92	8B	305	PSC	C2-C1-O01-C02
86	3D	501	HEC	C4B-C3B-CAB-CBB
86	3Q	501	HEC	C4B-C3B-CAB-CBB
86	3D	501	HEC	C4C-C3C-CAC-CBC
86	3Q	501	HEC	C4C-C3C-CAC-CBC
86	3D	501	HEC	C2B-C3B-CAB-CBB
86	3Q	501	HEC	C2B-C3B-CAB-CBB
86	3D	501	HEC	C2C-C3C-CAC-CBC
86	3Q	501	HEC	C2C-C3C-CAC-CBC
80	1T	101	EHZ	C13-C12-N1-C11

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Mol	Chain	Res	Type	Atoms
75	4C	305	CDL	O1-C1-CA2-OA2
75	4D	201	CDL	O1-C1-CB2-OB2
75	8C	306	CDL	O1-C1-CA2-OA2
75	8D	201	CDL	O1-C1-CB2-OB2
75	1N	902	CDL	C51-CB5-OB6-CB4
75	1N	902	CDL	OB7-CB5-OB6-CB4
86	3D	501	HEC	C3D-CAD-CBD-CGD
88	4A	604	HEA	C19-C20-C21-C22
88	8A	604	HEA	C19-C20-C21-C22
75	1N	902	CDL	C1-CA2-OA2-PA1
92	8B	305	PSC	C02-C03-O11-P
80	1T	101	EHZ	O3-C12-N1-C11
75	4C	305	CDL	CB2-C1-CA2-OA2
75	8C	306	CDL	CB2-C1-CA2-OA2
78	1P	402	NDP	O4D-C1D-N1N-C6N
69	3C	503	3PE	C21-C22-C23-C24
70	1q	201	PC1	C31-C32-C33-C34
87	4B	302	PGV	C1-C2-C3-C4
70	1Y	207	PC1	C2-C1-O11-P
70	1H	403	PC1	C31-C32-C33-C34
87	8B	302	PGV	C1-C2-C3-C4
69	1m	201	3PE	C31-C32-C33-C34
87	4J	101	PGV	C21-C22-C23-C24
87	8J	101	PGV	C21-C22-C23-C24
75	3G	102	CDL	O1-C1-CB2-OB2
70	1h	203	PC1	C2-C1-O11-P
73	1F	501	FMN	C4'-C5'-O5'-P
69	1N	901	3PE	C32-C33-C34-C35
87	4C	302	PGV	C5-C6-C7-C8
87	8C	303	PGV	C5-C6-C7-C8
75	1d	203	CDL	CA5-C11-C12-C13
87	8C	302	PGV	C26-C27-C28-C29
69	1L	703	3PE	C39-C3A-C3B-C3C
69	1M	501	3PE	C26-C27-C28-C29
75	1q	203	CDL	C16-C17-C18-C19
69	3P	503	3PE	C1-C2-C3-O31
75	1N	902	CDL	CB3-CB4-CB6-OB8
93	8C	308	PEK	C21-C22-C23-C24
69	1d	201	3PE	C3C-C3D-C3E-C3F
70	1Y	207	PC1	C23-C24-C25-C26
69	3A	503	3PE	C36-C37-C38-C39
75	8B	303	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
69	1Y	204	3PE	C23-C24-C25-C26
70	1M	505	PC1	C23-C24-C25-C26
75	4B	303	CDL	C59-C60-C61-C62
87	4B	301	PGV	C22-C23-C24-C25
69	3C	504	3PE	C2-C1-O11-P
87	4C	306	PGV	C02-C03-O11-P
69	1M	504	3PE	C38-C39-C3A-C3B
85	3C	501	HEM	C3D-CAD-CBD-CGD
69	3A	503	3PE	C32-C33-C34-C35
69	3R	302	3PE	C35-C36-C37-C38
69	1M	501	3PE	C21-C22-C23-C24
87	8B	301	PGV	C22-C23-C24-C25
80	1T	101	EHZ	C21-C22-C23-C24
92	8B	305	PSC	C25-C26-C27-C28
92	4B	305	PSC	C25-C26-C27-C28
75	1d	203	CDL	C32-C33-C34-C35
75	1L	702	CDL	CA7-C31-C32-C33
87	8C	302	PGV	C7-C8-C9-C10
69	1d	201	3PE	C31-C32-C33-C34
75	3T	101	CDL	OA5-CA3-CA4-OA6
69	3R	302	3PE	C27-C28-C29-C2A
87	8L	101	PGV	C21-C22-C23-C24
85	3C	502	HEM	C4B-C3B-CAB-CBB
85	3C	502	HEM	C4C-C3C-CAC-CBC
85	3P	502	HEM	C4B-C3B-CAB-CBB
85	3P	502	HEM	C4C-C3C-CAC-CBC
69	1M	502	3PE	C22-C23-C24-C25
69	1A	201	3PE	C36-C37-C38-C39
75	1h	202	CDL	C60-C61-C62-C63
87	4K	101	PGV	C02-C03-O11-P
87	8C	304	PGV	C02-C03-O11-P
87	8C	307	PGV	C02-C03-O11-P
75	8D	201	CDL	C71-C72-C73-C74
70	1B	203	PC1	C28-C29-C2A-C2B
87	4L	101	PGV	C6-C7-C8-C9
87	4L	101	PGV	C21-C22-C23-C24
87	8A	602	PGV	C22-C23-C24-C25
69	1L	703	3PE	C33-C34-C35-C36
80	1T	101	EHZ	O4-C15-C16-O5
69	1M	502	3PE	C3B-C3C-C3D-C3E
75	3T	101	CDL	OA5-CA3-CA4-CA6
75	4C	305	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
93	4C	307	PEK	C21-C22-C23-C24
69	1N	901	3PE	C2E-C2F-C2G-C2H
75	3T	101	CDL	C52-C53-C54-C55
87	8L	101	PGV	C6-C7-C8-C9
75	1X	201	CDL	C23-C24-C25-C26
69	1Y	203	3PE	C31-C32-C33-C34
75	3G	103	CDL	CA5-C11-C12-C13
69	1L	703	3PE	C1-C2-C3-O31
69	1M	502	3PE	C1-C2-C3-O31
69	3C	504	3PE	C1-C2-C3-O31
70	1B	203	PC1	C1-C2-C3-O31
70	1h	203	PC1	C1-C2-C3-O31
75	1N	902	CDL	CA3-CA4-CA6-OA8
75	8C	306	CDL	C36-C37-C38-C39
75	1L	702	CDL	C57-C58-C59-C60
70	1I	203	PC1	C24-C25-C26-C27
70	1h	203	PC1	C32-C33-C34-C35
75	8D	201	CDL	C62-C63-C64-C65
87	4C	304	PGV	C02-C03-O11-P
87	8K	101	PGV	C02-C03-O11-P
93	8G	102	PEK	C21-C22-C23-C24
70	1h	203	PC1	C2A-C2B-C2C-C2D
70	1H	402	PC1	O11-C1-C2-O21
87	8B	302	PGV	C24-C25-C26-C27
87	8K	101	PGV	C22-C23-C24-C25
87	4B	302	PGV	C24-C25-C26-C27
69	1N	901	3PE	O21-C2-C3-O31
87	8C	304	PGV	O03-C01-C02-O01
75	1N	902	CDL	C32-C31-CA7-OA8
87	8C	302	PGV	C3-C4-C5-C6
88	8A	605	HEA	C3B-C11-C12-C13
75	1L	702	CDL	C11-C12-C13-C14
75	4B	303	CDL	C38-C39-C40-C41
75	1X	201	CDL	C61-C62-C63-C64
87	4C	301	PGV	C7-C8-C9-C10
75	1N	902	CDL	C12-C13-C14-C15
75	8C	306	CDL	C59-C60-C61-C62
87	8C	302	PGV	C27-C28-C29-C30
69	1N	901	3PE	C2-C1-O11-P
75	3N	502	CDL	CB4-CB3-OB5-PB2
87	4K	101	PGV	C05-C04-O12-P
87	8B	301	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
87	8C	305	PGV	C02-C03-O11-P
87	8K	101	PGV	C05-C04-O12-P
70	1M	505	PC1	C32-C33-C34-C35
75	4D	201	CDL	C71-C72-C73-C74
69	1M	506	3PE	C21-C22-C23-C24
69	1M	506	3PE	C27-C28-C29-C2A
87	4A	601	PGV	C21-C22-C23-C24
69	1N	901	3PE	O11-C1-C2-C3
69	3A	503	3PE	O11-C1-C2-C3
69	3C	504	3PE	O11-C1-C2-C3
75	1d	203	CDL	OA5-CA3-CA4-CA6
75	3P	504	CDL	OB5-CB3-CB4-CB6
87	8A	602	PGV	C01-C02-C03-O11
75	3G	102	CDL	C72-C71-CB7-OB8
93	4G	102	PEK	O03-C21-C22-C23
93	8G	102	PEK	O03-C21-C22-C23
69	3Y	101	3PE	C31-C32-C33-C34
70	1q	201	PC1	C2A-C2B-C2C-C2D
75	4D	201	CDL	CA2-C1-CB2-OB2
75	1h	202	CDL	C76-C77-C78-C79
69	1Y	202	3PE	C1-C2-C3-O31
69	1Y	204	3PE	C1-C2-C3-O31
69	3N	501	3PE	C1-C2-C3-O31
75	1L	702	CDL	CA3-CA4-CA6-OA8
75	4B	303	CDL	CB3-CB4-CB6-OB8
75	8B	303	CDL	CB3-CB4-CB6-OB8
87	4J	101	PGV	O03-C01-C02-C03
75	1h	202	CDL	C34-C35-C36-C37
69	1d	201	3PE	C28-C29-C2A-C2B
70	1B	203	PC1	C35-C36-C37-C38
69	3G	101	3PE	C31-C32-C33-C34
75	4C	305	CDL	C59-C60-C61-C62
93	4G	102	PEK	C21-C22-C23-C24
69	1M	504	3PE	O11-C1-C2-O21
69	1m	201	3PE	O11-C1-C2-O21
69	3A	502	3PE	O11-C1-C2-O21
87	4C	302	PGV	O01-C02-C03-O11
87	8C	303	PGV	O01-C02-C03-O11
69	1M	502	3PE	C34-C35-C36-C37
69	1Y	204	3PE	C2-C1-O11-P
75	3T	101	CDL	CA4-CA3-OA5-PA1
75	4B	303	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
87	4G	101	PGV	C02-C03-O11-P
87	8G	101	PGV	C02-C03-O11-P
70	1M	505	PC1	C2A-C2B-C2C-C2D
82	1h	201	AME	C-CA-N-CT1
70	1I	203	PC1	C37-C38-C39-C3A
88	4A	605	HEA	C2A-CAA-CBA-CGA
69	1Y	203	3PE	C22-C23-C24-C25
75	1L	702	CDL	C33-C34-C35-C36
75	1q	203	CDL	C52-C51-CB5-OB6
69	1Y	204	3PE	O21-C2-C3-O31
69	3N	501	3PE	O21-C2-C3-O31
69	3N	503	3PE	O21-C2-C3-O31
75	3N	502	CDL	OA6-CA4-CA6-OA8
75	4B	303	CDL	OB6-CB4-CB6-OB8
87	4C	303	PGV	O03-C01-C02-O01
87	8J	101	PGV	O03-C01-C02-O01
75	8B	303	CDL	C38-C39-C40-C41
92	4B	305	PSC	C9-C10-C11-C12
92	4B	305	PSC	C10-C11-C12-C13
92	8B	305	PSC	C9-C10-C11-C12
92	8B	305	PSC	C10-C11-C12-C13
93	4G	102	PEK	C5-C6-C7-C8
93	4G	102	PEK	C9-C10-C11-C12
93	8G	102	PEK	C5-C6-C7-C8
93	8G	102	PEK	C9-C10-C11-C12
69	1M	504	3PE	C31-C32-C33-C34
87	4J	101	PGV	C19-C20-C21-C22
70	1A	202	PC1	C22-C23-C24-C25
75	3P	504	CDL	CA5-C11-C12-C13
75	1L	702	CDL	C37-C38-C39-C40
87	4L	101	PGV	C3-C4-C5-C6
75	1X	201	CDL	C36-C37-C38-C39
76	1O	401	GTP	PB-O3A-PA-O5'
75	1h	202	CDL	CB7-C71-C72-C73
75	4D	201	CDL	C59-C60-C61-C62
87	8J	101	PGV	C19-C20-C21-C22
75	4C	305	CDL	C52-C53-C54-C55
70	1H	402	PC1	O11-C1-C2-C3
75	4B	303	CDL	OA5-CA3-CA4-CA6
75	1X	201	CDL	C58-C59-C60-C61
87	4C	303	PGV	C02-C03-O11-P
87	8C	304	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
87	4C	303	PGV	C24-C25-C26-C27
69	1A	201	3PE	O21-C21-C22-C23
70	1Y	207	PC1	O31-C31-C32-C33
85	3C	501	HEM	C2C-C3C-CAC-CBC
85	3P	501	HEM	C2C-C3C-CAC-CBC
75	4D	201	CDL	C62-C63-C64-C65
69	1Y	204	3PE	O31-C31-C32-C33
69	1N	901	3PE	O11-C1-C2-O21
75	1d	203	CDL	OA5-CA3-CA4-OA6
75	4B	303	CDL	OA5-CA3-CA4-OA6
87	8A	601	PGV	O01-C02-C03-O11
69	1M	501	3PE	C1-C2-C3-O31
69	1N	901	3PE	C1-C2-C3-O31
69	3N	503	3PE	C1-C2-C3-O31
75	3P	504	CDL	CB3-CB4-CB6-OB8
87	8J	101	PGV	O03-C01-C02-C03
88	4A	604	HEA	O11-C11-C12-C13
88	8A	604	HEA	O11-C11-C12-C13
75	3G	103	CDL	C52-C53-C54-C55
87	4C	301	PGV	C26-C27-C28-C29
75	1h	202	CDL	C38-C39-C40-C41
69	1K	101	3PE	C12-C11-O13-P
69	1L	701	3PE	C12-C11-O13-P
69	1M	504	3PE	C12-C11-O13-P
69	1Y	203	3PE	C12-C11-O13-P
69	1m	201	3PE	C12-C11-O13-P
69	3C	503	3PE	C12-C11-O13-P
69	3C	504	3PE	C12-C11-O13-P
69	3P	503	3PE	C12-C11-O13-P
70	1A	203	PC1	C12-C11-O13-P
70	1B	203	PC1	C12-C11-O13-P
70	1P	401	PC1	C12-C11-O13-P
93	4C	307	PEK	C05-C04-O12-P
93	4G	102	PEK	C05-C04-O12-P
93	8C	308	PEK	C05-C04-O12-P
93	8G	102	PEK	C05-C04-O12-P
75	8C	306	CDL	C52-C53-C54-C55
69	1L	703	3PE	O21-C2-C3-O31
69	3P	503	3PE	O21-C2-C3-O31
70	1H	403	PC1	O21-C2-C3-O31
70	1h	203	PC1	O21-C2-C3-O31
75	3P	504	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
75	8B	303	CDL	OB6-CB4-CB6-OB8
87	4J	101	PGV	O03-C01-C02-O01
75	1d	203	CDL	C71-C72-C73-C74
75	3P	504	CDL	C31-C32-C33-C34
87	4K	101	PGV	C22-C23-C24-C25
75	1X	201	CDL	C35-C36-C37-C38
87	8L	101	PGV	C3-C4-C5-C6
70	1A	202	PC1	O13-C11-C12-N
70	1B	203	PC1	O13-C11-C12-N
70	1P	401	PC1	O13-C11-C12-N
70	1Y	207	PC1	O13-C11-C12-N
70	1h	203	PC1	O13-C11-C12-N
76	1O	401	GTP	PA-O3A-PB-O1B
85	3P	501	HEM	C3D-CAD-CBD-CGD
75	8D	201	CDL	CA2-C1-CB2-OB2
75	8D	201	CDL	C59-C60-C61-C62
87	8B	302	PGV	C20-C21-C22-C23
70	1I	203	PC1	C23-C24-C25-C26
87	4B	302	PGV	C27-C28-C29-C30
87	4A	601	PGV	C11-C10-C9-C8
69	1M	504	3PE	O11-C1-C2-C3
69	1m	201	3PE	O11-C1-C2-C3
75	8B	303	CDL	OA5-CA3-CA4-CA6
87	4A	601	PGV	C01-C02-C03-O11
87	4M	101	PGV	C01-C02-C03-O11
75	1d	203	CDL	C1-CA2-OA2-PA1
75	1h	202	CDL	CB4-CB3-OB5-PB2
87	4A	601	PGV	C02-C03-O11-P
87	8A	601	PGV	C29-C30-C31-C32
80	1n	201	EHZ	C11-C10-S1-C9
87	4C	301	PGV	C3-C4-C5-C6
87	8B	302	PGV	C27-C28-C29-C30
69	3A	503	3PE	O11-C1-C2-O21
70	1M	505	PC1	O11-C1-C2-O21
75	8B	303	CDL	OA5-CA3-CA4-OA6
87	4A	601	PGV	O01-C02-C03-O11
87	4M	101	PGV	O01-C02-C03-O11
87	8A	602	PGV	O01-C02-C03-O11
75	4C	305	CDL	C11-C12-C13-C14
75	4C	305	CDL	C16-C17-C18-C19
69	1Y	202	3PE	O21-C2-C3-O31
70	1B	203	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
75	1N	902	CDL	OB6-CB4-CB6-OB8
70	1Y	207	PC1	C36-C37-C38-C39
87	4G	101	PGV	C22-C23-C24-C25
69	1M	502	3PE	C24-C25-C26-C27
70	1H	402	PC1	C1-C2-C3-O31
80	1T	101	EHZ	C10-C11-N1-C12
80	1n	201	EHZ	C10-C11-N1-C12
70	1H	403	PC1	C39-C3A-C3B-C3C
69	1A	201	3PE	C11-O13-P-O11
69	1A	201	3PE	C11-O13-P-O14
69	1K	101	3PE	C1-O11-P-O12
69	1K	101	3PE	C11-O13-P-O14
69	1M	502	3PE	C1-O11-P-O13
69	1M	504	3PE	C11-O13-P-O14
69	1M	506	3PE	C11-O13-P-O14
69	1P	403	3PE	C1-O11-P-O13
69	1P	403	3PE	C1-O11-P-O14
69	1Y	202	3PE	C11-O13-P-O14
69	1Y	203	3PE	C11-O13-P-O14
69	1d	201	3PE	C11-O13-P-O14
69	1j	101	3PE	C1-O11-P-O14
69	1m	201	3PE	C11-O13-P-O14
69	3C	503	3PE	C1-O11-P-O14
69	3N	501	3PE	C1-O11-P-O12
69	3N	501	3PE	C11-O13-P-O14
69	3N	503	3PE	C11-O13-P-O14
70	1A	203	PC1	C1-O11-P-O14
70	1M	503	PC1	C1-O11-P-O14
70	1M	505	PC1	C1-O11-P-O14
70	1M	505	PC1	C1-O11-P-O13
70	1d	202	PC1	C1-O11-P-O14
75	1N	902	CDL	CA3-OA5-PA1-OA3
75	1X	201	CDL	CA2-OA2-PA1-OA5
75	1X	201	CDL	CB2-OB2-PB2-OB3
75	1d	203	CDL	CB2-OB2-PB2-OB3
75	1h	202	CDL	CB2-OB2-PB2-OB4
75	1h	202	CDL	CB2-OB2-PB2-OB5
75	3G	103	CDL	CA2-OA2-PA1-OA3
75	3G	103	CDL	CB3-OB5-PB2-OB3
75	3N	502	CDL	CB3-OB5-PB2-OB3
75	3P	504	CDL	CA3-OA5-PA1-OA3
75	3P	504	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
75	3T	101	CDL	CA3-OA5-PA1-OA2
75	4B	303	CDL	CB3-OB5-PB2-OB4
75	4D	201	CDL	CB2-OB2-PB2-OB3
75	8B	303	CDL	CB3-OB5-PB2-OB2
75	8B	303	CDL	CB3-OB5-PB2-OB4
75	8D	201	CDL	CB2-OB2-PB2-OB3
87	4A	601	PGV	C04-O12-P-O13
87	4C	302	PGV	C03-O11-P-O12
87	4K	101	PGV	C04-O12-P-O13
87	8A	601	PGV	C04-O12-P-O13
87	8B	301	PGV	C04-O12-P-O13
87	8C	302	PGV	C04-O12-P-O14
87	8C	304	PGV	C03-O11-P-O14
87	8C	305	PGV	C03-O11-P-O14
87	8K	101	PGV	C04-O12-P-O13
92	4B	305	PSC	C04-O12-P-O14
92	8B	305	PSC	C04-O12-P-O14
69	1M	506	3PE	C28-C29-C2A-C2B
70	1H	402	PC1	C2-C1-O11-P
70	1M	505	PC1	C2-C1-O11-P
75	1d	203	CDL	C1-CB2-OB2-PB2
75	3P	504	CDL	CB4-CB3-OB5-PB2
75	8B	303	CDL	C1-CA2-OA2-PA1
87	8A	601	PGV	C02-C03-O11-P
69	1Y	203	3PE	C33-C34-C35-C36
70	1d	202	PC1	C37-C38-C39-C3A
87	8C	301	PGV	C11-C12-C13-C14
92	8B	305	PSC	C12-C13-C14-C15
92	8B	305	PSC	C19-C20-C21-C22
75	1H	401	CDL	CA3-CA4-OA6-CA5
88	4A	604	HEA	C15-C16-C17-C18
69	3Y	101	3PE	O11-C1-C2-C3
70	1M	505	PC1	O11-C1-C2-C3
75	8C	306	CDL	OB5-CB3-CB4-CB6
87	8K	101	PGV	C2-C3-C4-C5
87	8C	304	PGV	C9-C10-C11-C12
87	8C	305	PGV	C9-C10-C11-C12
87	8K	101	PGV	C9-C10-C11-C12
69	1Y	203	3PE	O11-C1-C2-O21
69	3C	504	3PE	O11-C1-C2-O21
75	1L	702	CDL	OA5-CA3-CA4-OA6
75	3P	504	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
69	1m	201	3PE	C23-C24-C25-C26
69	1M	504	3PE	C24-C25-C26-C27
69	1Y	205	3PE	C33-C34-C35-C36
87	4K	101	PGV	C2-C3-C4-C5
69	1M	502	3PE	O21-C2-C3-O31
87	4B	301	PGV	C30-C31-C32-C33
69	1m	201	3PE	O21-C21-C22-C23
69	3C	504	3PE	O31-C31-C32-C33
70	3X	101	PC1	O21-C21-C22-C23
69	3C	503	3PE	C29-C2A-C2B-C2C
87	8C	301	PGV	C11-C10-C9-C8
88	4A	605	HEA	C3B-C11-C12-C13
87	8C	302	PGV	C1-C2-C3-C4
87	4C	303	PGV	C5-C6-C7-C8
87	4C	301	PGV	C1-C2-C3-C4
80	1n	201	EHZ	C7-C8-C9-O2
87	4K	101	PGV	C9-C10-C11-C12
87	4L	101	PGV	C9-C10-C11-C12
69	3C	504	3PE	C23-C24-C25-C26
75	8C	306	CDL	C11-C12-C13-C14
75	8C	306	CDL	C16-C17-C18-C19
75	8C	306	CDL	C51-C52-C53-C54
70	1B	202	PC1	C36-C37-C38-C39
80	1T	101	EHZ	C1-C21-C22-C23
75	1L	702	CDL	C38-C39-C40-C41
70	1Y	207	PC1	C25-C26-C27-C28
87	4M	101	PGV	C3-C4-C5-C6
69	1d	201	3PE	C2-C1-O11-P
69	3R	302	3PE	C21-C22-C23-C24
87	4J	101	PGV	C2-C3-C4-C5
75	1X	201	CDL	OB5-CB3-CB4-OB6
92	8B	305	PSC	O01-C02-C03-O11
87	4A	602	PGV	C11-C12-C13-C14
87	4C	301	PGV	C9-C10-C11-C12
87	4C	304	PGV	C9-C10-C11-C12
87	4M	101	PGV	C9-C10-C11-C12
87	8L	101	PGV	C9-C10-C11-C12
92	4B	305	PSC	C12-C13-C14-C15
85	3C	501	HEM	C4C-C3C-CAC-CBC
69	1Y	202	3PE	C31-C32-C33-C34
75	4C	305	CDL	C51-C52-C53-C54
69	1P	403	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
87	8A	602	PGV	C9-C10-C11-C12
87	8C	303	PGV	C9-C10-C11-C12
87	8J	101	PGV	C9-C10-C11-C12
75	1X	201	CDL	C55-C56-C57-C58
69	3Y	101	3PE	O21-C2-C3-O31
70	1M	505	PC1	O21-C2-C3-O31
87	8B	302	PGV	C11-C10-C9-C8
75	1L	702	CDL	C58-C59-C60-C61
75	8B	303	CDL	C11-C12-C13-C14
87	8C	304	PGV	C13-C14-C15-C16
87	4A	601	PGV	C29-C30-C31-C32
87	4B	302	PGV	C20-C21-C22-C23
75	1L	702	CDL	CA4-CA3-OA5-PA1
87	8C	304	PGV	C5-C6-C7-C8
69	1M	502	3PE	C2A-C2B-C2C-C2D
88	8A	605	HEA	C2A-CAA-CBA-CGA
75	1N	902	CDL	O1-C1-CB2-OB2
69	3N	501	3PE	C33-C34-C35-C36
87	4C	303	PGV	C9-C10-C11-C12
87	8A	603	PGV	C11-C12-C13-C14
87	8C	302	PGV	C11-C12-C13-C14
87	8C	307	PGV	C11-C12-C13-C14
87	8A	601	PGV	C24-C25-C26-C27
85	3C	501	HEM	CAA-CBA-CGA-O1A
85	3C	501	HEM	CAA-CBA-CGA-O2A
85	3P	501	HEM	CAA-CBA-CGA-O2A
85	3P	502	HEM	CAA-CBA-CGA-O1A
88	8A	604	HEA	CAD-CBD-CGD-O1D
69	1Y	202	3PE	O31-C31-C32-C33
69	1M	504	3PE	C1-C2-O21-C21
69	1Y	202	3PE	C1-C2-O21-C21
69	1Y	205	3PE	C1-C2-O21-C21
87	8C	304	PGV	C01-C02-O01-C1
88	8A	604	HEA	CAD-CBD-CGD-O2D
70	1B	202	PC1	C3D-C3E-C3F-C3G
75	1X	201	CDL	C31-C32-C33-C34
87	4A	603	PGV	C11-C12-C13-C14
88	4A	604	HEA	CAD-CBD-CGD-O1D
88	8A	605	HEA	CAD-CBD-CGD-O1D
75	1N	902	CDL	C32-C31-CA7-OA9
69	1N	901	3PE	C23-C24-C25-C26
70	1h	203	PC1	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
69	3C	503	3PE	O11-C1-C2-O21
92	4B	305	PSC	O01-C02-C03-O11
87	8G	101	PGV	C7-C8-C9-C10
87	8A	603	PGV	C15-C16-C17-C18
69	1M	506	3PE	C25-C26-C27-C28
88	4A	604	HEA	C2C-C3C-CAC-CBC
87	8G	101	PGV	C9-C10-C11-C12
75	1N	902	CDL	C1-CB2-OB2-PB2
75	3N	502	CDL	C1-CB2-OB2-PB2
85	3C	502	HEM	CAA-CBA-CGA-O1A
88	8A	605	HEA	C26-C15-C16-C17
75	4C	305	CDL	OB5-CB3-CB4-CB6
92	4B	305	PSC	C2-C3-C4-C5
69	3A	502	3PE	O21-C2-C3-O31
75	1q	203	CDL	OB6-CB4-CB6-OB8
75	3G	103	CDL	OB6-CB4-CB6-OB8
75	4D	201	CDL	OA6-CA4-CA6-OA8
85	3P	501	HEM	CAD-CBD-CGD-O1D
85	3P	502	HEM	CAD-CBD-CGD-O1D
87	4K	101	PGV	C3-C4-C5-C6
87	8K	101	PGV	C3-C4-C5-C6
93	4G	102	PEK	O04-C21-C22-C23
78	1P	402	NDP	O4D-C4D-C5D-O5D
78	1P	402	NDP	C2N-C3N-C7N-N7N
87	4M	101	PGV	C22-C23-C24-C25
88	4A	605	HEA	CAD-CBD-CGD-O2D
75	1d	203	CDL	C72-C73-C74-C75
93	8G	102	PEK	O04-C21-C22-C23
87	4C	301	PGV	C11-C12-C13-C14
87	4M	101	PGV	C11-C12-C13-C14
87	8L	101	PGV	C11-C12-C13-C14
70	1P	401	PC1	C33-C34-C35-C36
69	3C	503	3PE	C25-C26-C27-C28
75	3A	501	CDL	O1-C1-CA2-OA2
87	4C	301	PGV	C6-C7-C8-C9
85	3P	501	HEM	CAA-CBA-CGA-O1A
88	4A	604	HEA	CAD-CBD-CGD-O2D
88	8A	605	HEA	CAD-CBD-CGD-O2D
87	8J	101	PGV	C5-C6-C7-C8
75	3N	502	CDL	CA4-CA6-OA8-CA7
69	3N	501	3PE	C22-C23-C24-C25
69	3Y	101	3PE	C2-C3-O31-C31

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Mol	Chain	Res	Type	Atoms
85	3P	502	HEM	CAD-CBD-CGD-O2D
87	8C	304	PGV	O03-C01-C02-C03
85	3C	502	HEM	CAA-CBA-CGA-O2A
86	3Q	501	HEC	CAA-CBA-CGA-O2A
87	8C	307	PGV	C5-C6-C7-C8
87	4G	101	PGV	C9-C10-C11-C12
87	4J	101	PGV	C9-C10-C11-C12
87	4B	302	PGV	C11-C10-C9-C8
87	8A	603	PGV	C2-C3-C4-C5
75	1h	202	CDL	OB5-CB3-CB4-OB6
85	3P	502	HEM	CAA-CBA-CGA-O2A
92	8B	305	PSC	C15-C16-C17-C18
87	8C	302	PGV	C6-C7-C8-C9
88	4A	604	HEA	C4C-C3C-CAC-CBC
85	3P	501	HEM	CAD-CBD-CGD-O2D
87	4A	601	PGV	C11-C12-C13-C14
87	4C	302	PGV	C9-C10-C11-C12
87	4C	306	PGV	C11-C12-C13-C14
87	8A	602	PGV	C11-C12-C13-C14
87	8C	302	PGV	C9-C10-C11-C12
69	1K	101	3PE	O21-C21-C22-C23
70	1B	202	PC1	C3C-C3D-C3E-C3F
88	4A	605	HEA	CAD-CBD-CGD-O1D
70	1P	401	PC1	C24-C25-C26-C27
69	1Y	203	3PE	O11-C1-C2-C3
75	1L	702	CDL	OA5-CA3-CA4-CA6
75	1h	202	CDL	OB5-CB3-CB4-CB6
88	4A	604	HEA	C27-C19-C20-C21
88	4A	605	HEA	C26-C15-C16-C17
69	3R	302	3PE	C22-C23-C24-C25
69	1d	201	3PE	O21-C2-C3-O31
92	4B	305	PSC	C19-C20-C21-C22
86	3D	501	HEC	CAA-CBA-CGA-O2A
75	4B	303	CDL	C12-C11-CA5-OA6
87	4C	303	PGV	C13-C14-C15-C16
87	8J	101	PGV	C2-C3-C4-C5
75	4C	305	CDL	C81-C82-C83-C84
69	1M	506	3PE	C2B-C2C-C2D-C2E
70	1M	505	PC1	C28-C29-C2A-C2B
69	1K	101	3PE	C24-C25-C26-C27
87	4K	101	PGV	C11-C12-C13-C14
87	8A	601	PGV	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
87	8K	101	PGV	C11-C12-C13-C14
87	8B	301	PGV	C30-C31-C32-C33
83	1i	201	CHD	C22-C23-C24-O26
69	3C	503	3PE	C2C-C2D-C2E-C2F
75	3G	102	CDL	C72-C71-CB7-OB9
86	3Q	501	HEC	CAA-CBA-CGA-O1A
69	1L	703	3PE	C29-C2A-C2B-C2C
69	1Y	206	3PE	C3-C2-O21-C21
69	3C	503	3PE	C1-C2-O21-C21
87	4C	303	PGV	C01-C02-O01-C1
75	1X	201	CDL	C34-C35-C36-C37
69	3N	501	3PE	C26-C27-C28-C29
69	1K	101	3PE	C26-C27-C28-C29
75	3G	102	CDL	C12-C13-C14-C15
82	1h	201	AME	CB-CA-N-CT1
87	8C	304	PGV	C05-C04-O12-P
75	3G	102	CDL	CA2-C1-CB2-OB2
70	1M	503	PC1	C11-C12-N-C15
75	4C	305	CDL	C75-C76-C77-C78
70	1M	505	PC1	C1-C2-C3-O31
75	3N	502	CDL	CA3-CA4-CA6-OA8
85	3P	501	HEM	C4C-C3C-CAC-CBC
70	3R	303	PC1	C27-C28-C29-C2A
88	8A	605	HEA	O11-C11-C12-C13
69	3D	502	3PE	C24-C25-C26-C27
87	4A	601	PGV	C9-C10-C11-C12
83	1i	201	CHD	C22-C23-C24-O25
80	1T	101	EHZ	C15-C16-C17-C19
70	1h	203	PC1	C22-C23-C24-C25
69	1A	201	3PE	C2A-C2B-C2C-C2D
87	8A	602	PGV	C3-C4-C5-C6
86	3D	501	HEC	CAA-CBA-CGA-O1A
87	4C	303	PGV	C3-C4-C5-C6
93	4C	307	PEK	O03-C01-C02-O01
69	3A	502	3PE	O11-C1-C2-C3
70	1B	203	PC1	O11-C1-C2-C3
87	4C	302	PGV	C01-C02-C03-O11
87	8C	303	PGV	C01-C02-C03-O11
92	4B	305	PSC	C01-C02-C03-O11
92	8B	305	PSC	C01-C02-C03-O11
87	4K	101	PGV	C1-C2-C3-C4
75	8C	306	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
87	4G	101	PGV	C7-C8-C9-C10
69	1Y	203	3PE	C2D-C2E-C2F-C2G
70	1M	505	PC1	C2D-C2E-C2F-C2G
87	8C	303	PGV	C14-C15-C16-C17
76	1O	401	GTP	PA-O3A-PB-O2B
70	1A	202	PC1	C23-C24-C25-C26
80	1n	201	EHZ	C21-C1-C2-C3
87	8C	303	PGV	C26-C27-C28-C29
75	3G	103	CDL	C11-C12-C13-C14
75	8C	306	CDL	C71-C72-C73-C74
87	8K	101	PGV	C5-C6-C7-C8
92	8B	305	PSC	C4-C5-C6-C7
75	8C	306	CDL	C18-C19-C20-C21
87	4A	601	PGV	C24-C25-C26-C27
75	1d	203	CDL	C32-C31-CA7-OA8
87	8C	303	PGV	C6-C7-C8-C9
69	1Y	206	3PE	O21-C21-C22-C23
87	8A	601	PGV	O03-C19-C20-C21
70	1I	203	PC1	C22-C23-C24-C25
70	1H	402	PC1	C31-C32-C33-C34
75	3P	504	CDL	C32-C31-CA7-OA8
87	8A	602	PGV	C21-C22-C23-C24
80	1T	101	EHZ	C4-C5-C6-C7
88	8A	604	HEA	CAA-CBA-CGA-O1A
69	1d	201	3PE	C35-C36-C37-C38
87	4C	301	PGV	C28-C29-C30-C31
70	1d	202	PC1	O21-C21-C22-C23
88	4A	604	HEA	CAA-CBA-CGA-O1A
88	8A	604	HEA	CAA-CBA-CGA-O2A
69	1P	403	3PE	O21-C21-C22-C23
87	4A	601	PGV	O03-C19-C20-C21
75	4C	305	CDL	C18-C19-C20-C21
75	1q	203	CDL	C52-C51-CB5-OB7
88	4A	604	HEA	CAA-CBA-CGA-O2A
69	1M	504	3PE	C32-C33-C34-C35
75	1X	201	CDL	OB5-CB3-CB4-CB6
73	1F	501	FMN	N10-C1'-C2'-O2'
75	1X	201	CDL	CB2-C1-CA2-OA2
70	1H	402	PC1	C36-C37-C38-C39
75	8C	306	CDL	C75-C76-C77-C78
69	1M	502	3PE	C29-C2A-C2B-C2C
69	1Y	202	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
75	3N	502	CDL	CB3-CB4-OB6-CB5
75	3N	502	CDL	CB6-CB4-OB6-CB5
75	1X	201	CDL	C63-C64-C65-C66
87	8J	101	PGV	C30-C31-C32-C33
87	8C	304	PGV	C3-C4-C5-C6
69	1K	101	3PE	C34-C35-C36-C37
70	1P	401	PC1	C32-C33-C34-C35
75	3P	504	CDL	C72-C71-CB7-OB8
75	3P	504	CDL	C13-C14-C15-C16
87	8A	602	PGV	C05-C04-O12-P
70	1Y	207	PC1	O32-C31-C32-C33
70	1q	201	PC1	C32-C33-C34-C35
75	4C	305	CDL	C71-C72-C73-C74
69	1Y	203	3PE	C27-C28-C29-C2A
87	8G	101	PGV	C22-C23-C24-C25
75	1q	203	CDL	CA5-C11-C12-C13
75	8B	303	CDL	CB5-C51-C52-C53
75	1h	202	CDL	C74-C75-C76-C77
75	1N	902	CDL	CA7-C31-C32-C33
70	3J	101	PC1	C22-C23-C24-C25
70	1M	503	PC1	C11-C12-N-C14
75	4B	303	CDL	C13-C14-C15-C16
87	4G	101	PGV	C23-C24-C25-C26
87	4L	101	PGV	C11-C12-C13-C14
70	1d	202	PC1	O22-C21-C22-C23
69	1L	701	3PE	C28-C29-C2A-C2B
87	4A	603	PGV	C6-C7-C8-C9
69	1M	501	3PE	C23-C24-C25-C26
87	8A	601	PGV	O04-C19-C20-C21
69	1M	501	3PE	O21-C2-C3-O31
75	8D	201	CDL	OA6-CA4-CA6-OA8
87	8J	101	PGV	C27-C28-C29-C30
86	3Q	501	HEC	CAD-CBD-CGD-O2D
75	1d	203	CDL	C32-C31-CA7-OA9
87	4J	101	PGV	C27-C28-C29-C30
87	8C	301	PGV	C26-C27-C28-C29
69	1A	201	3PE	C27-C28-C29-C2A
70	1A	202	PC1	O31-C31-C32-C33
87	8C	305	PGV	C7-C8-C9-C10
69	1Y	206	3PE	O22-C21-C22-C23
75	3P	504	CDL	C32-C31-CA7-OA9
87	4A	601	PGV	O04-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
75	8B	303	CDL	C12-C11-CA5-OA6
70	1Y	207	PC1	C3A-C3B-C3C-C3D
70	1H	403	PC1	O11-C1-C2-C3
87	8A	601	PGV	C01-C02-C03-O11
75	1q	203	CDL	C12-C11-CA5-OA6
80	1T	101	EHZ	C2-C3-C4-C5
87	4M	101	PGV	C20-C21-C22-C23
92	8B	305	PSC	C2-C3-C4-C5
75	3P	504	CDL	C72-C71-CB7-OB9
75	3P	504	CDL	CB5-C51-C52-C53
70	1B	203	PC1	O31-C31-C32-C33
70	1h	203	PC1	O31-C31-C32-C33
75	4D	201	CDL	C32-C31-CA7-OA8
87	4G	101	PGV	O03-C19-C20-C21
87	8C	302	PGV	O03-C19-C20-C21
87	4K	101	PGV	C5-C6-C7-C8
69	1Y	204	3PE	O22-C21-C22-C23
69	1Y	204	3PE	O21-C21-C22-C23
70	1d	202	PC1	O31-C31-C32-C33
87	4C	302	PGV	C26-C27-C28-C29

There are no ring outliers.

121 monomers are involved in 593 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	1h	203	PC1	1	0
87	8A	601	PGV	10	0
87	8C	303	PGV	8	0
70	1P	401	PC1	2	0
87	4A	603	PGV	10	0
70	1H	402	PC1	5	0
76	1O	401	GTP	3	0
69	1Y	203	3PE	9	0
75	4D	201	CDL	17	0
91	4B	304	CUA	1	0
70	3X	101	PC1	2	0
81	1q	202	AYA	2	0
87	8A	602	PGV	8	0
71	1B	201	SF4	2	0
75	3G	103	CDL	6	0
86	3Q	501	HEC	3	0
93	8G	102	PEK	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
93	4G	102	PEK	2	0
87	4C	304	PGV	1	0
80	1n	201	EHZ	1	0
69	1Y	202	3PE	7	0
75	3N	502	CDL	7	0
75	1X	201	CDL	12	0
70	1M	503	PC1	3	0
70	3J	101	PC1	4	0
69	3N	501	3PE	5	0
70	1q	201	PC1	4	0
94	8H	101	PO4	1	0
75	1N	902	CDL	3	0
69	1A	201	3PE	3	0
72	3E	301	FES	2	0
87	4G	101	PGV	5	0
70	1H	403	PC1	7	0
69	3Y	101	3PE	2	0
93	8C	308	PEK	5	0
85	3P	502	HEM	3	0
70	1B	202	PC1	7	0
88	8A	604	HEA	8	0
69	1M	504	3PE	11	0
69	3A	503	3PE	8	0
70	1d	202	PC1	8	0
75	8C	306	CDL	16	0
87	8C	307	PGV	8	0
93	4C	307	PEK	5	0
71	1F	502	SF4	2	0
87	4M	101	PGV	3	0
87	4B	302	PGV	4	0
70	1Y	207	PC1	7	0
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88	8A	605	HEA	4	0
85	3P	501	HEM	1	0
87	4C	303	PGV	7	0
75	1q	203	CDL	2	0
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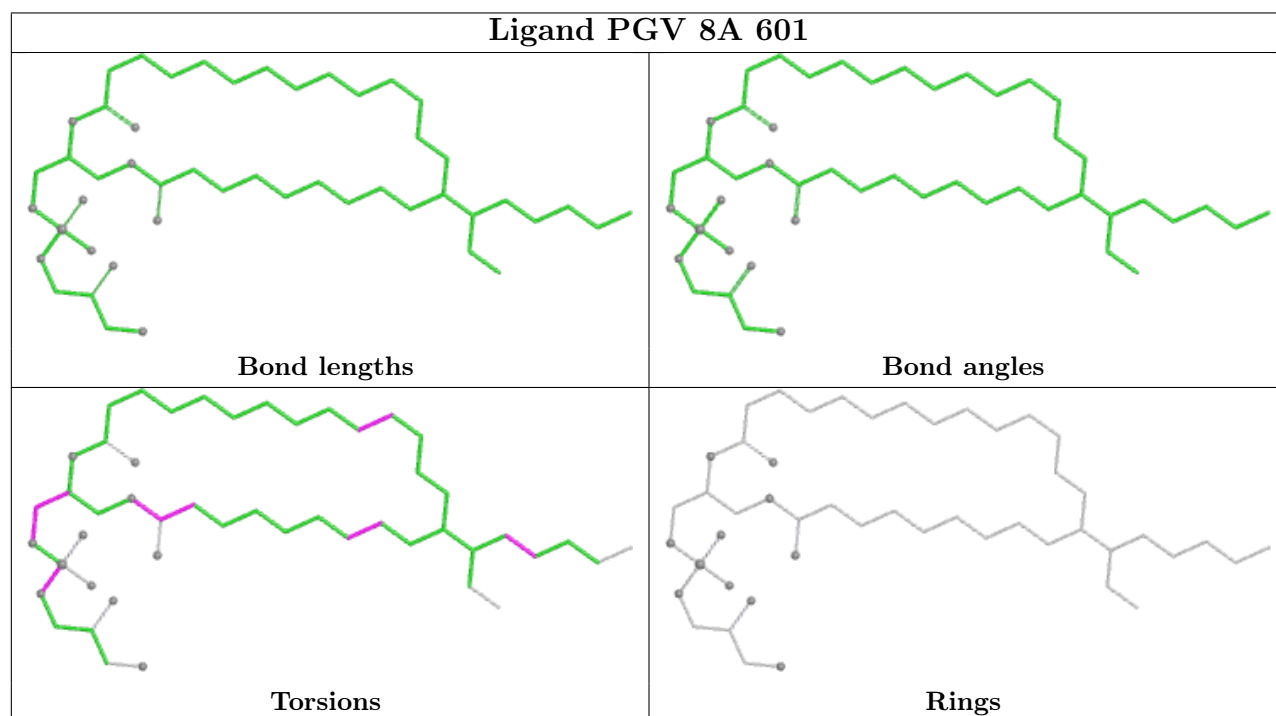
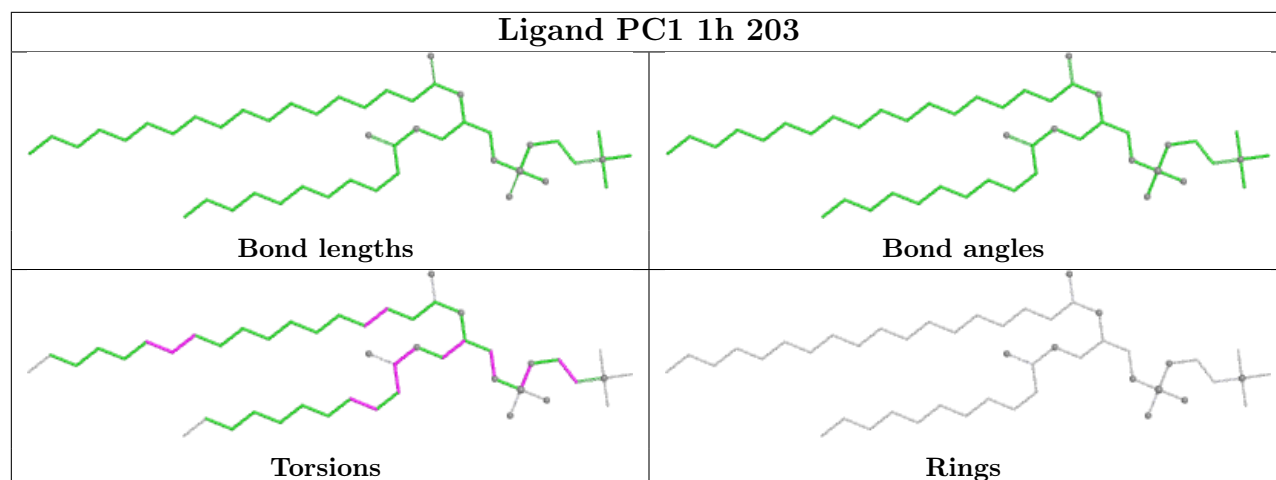
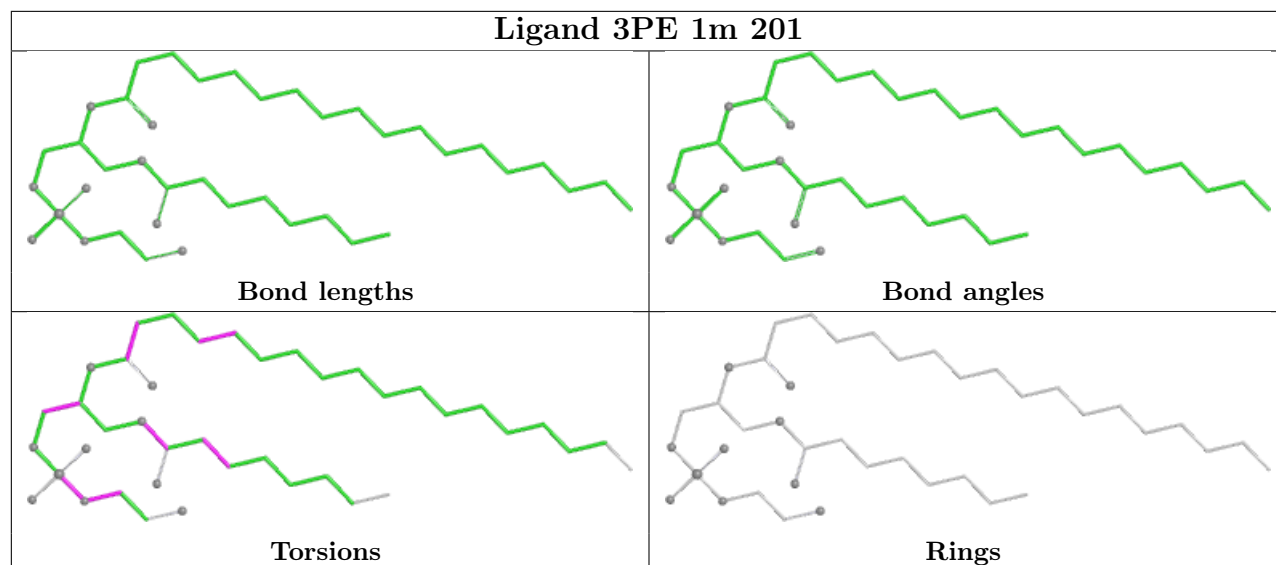
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72	1G	803	FES	2	0
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69	3N	503	3PE	3	0
69	3C	504	3PE	4	0
69	1P	403	3PE	3	0
87	8L	101	PGV	7	0
75	3T	101	CDL	9	0
87	4J	101	PGV	10	0
75	1h	202	CDL	14	0
87	8C	301	PGV	5	0
69	3A	502	3PE	1	0
75	8D	201	CDL	15	0
75	4B	303	CDL	14	0
70	1I	203	PC1	3	0
87	4C	306	PGV	8	0
72	3R	301	FES	2	0
88	4A	604	HEA	6	0
78	1P	402	NDP	2	0
86	3D	501	HEC	2	0
87	4A	602	PGV	4	0
75	1H	401	CDL	1	0
87	8K	101	PGV	3	0
75	3A	501	CDL	3	0
87	4C	302	PGV	5	0
75	1d	203	CDL	6	0
70	1A	202	PC1	7	0
87	8C	302	PGV	5	0
69	1L	703	3PE	5	0
70	3R	303	PC1	4	0
87	8C	305	PGV	10	0
75	1L	702	CDL	6	0
87	8A	603	PGV	5	0
87	4B	301	PGV	4	0
92	8B	305	PSC	8	0
69	1L	701	3PE	3	0
87	8B	301	PGV	8	0
87	8C	304	PGV	7	0
75	8B	303	CDL	10	0
87	4C	301	PGV	2	0

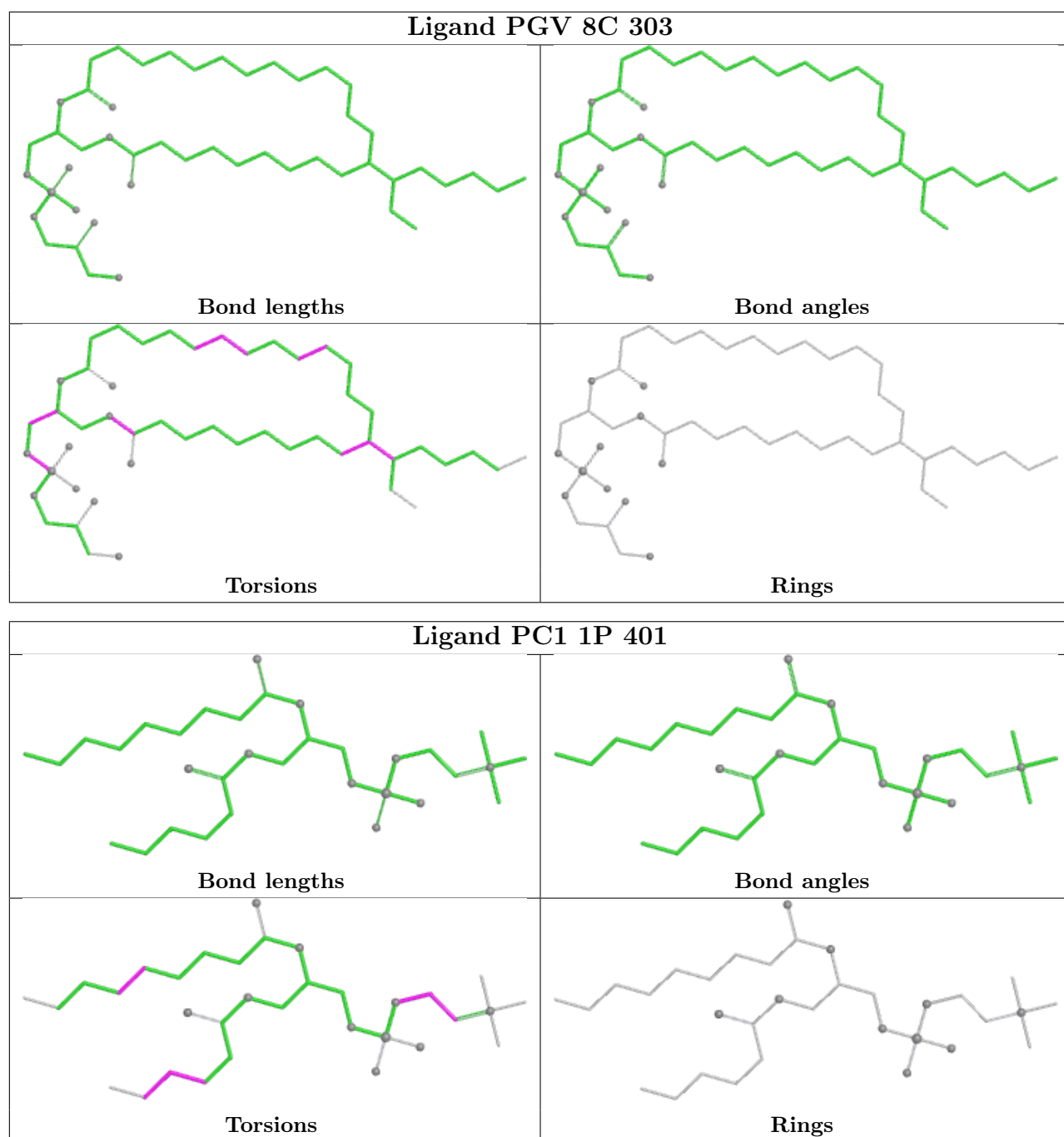
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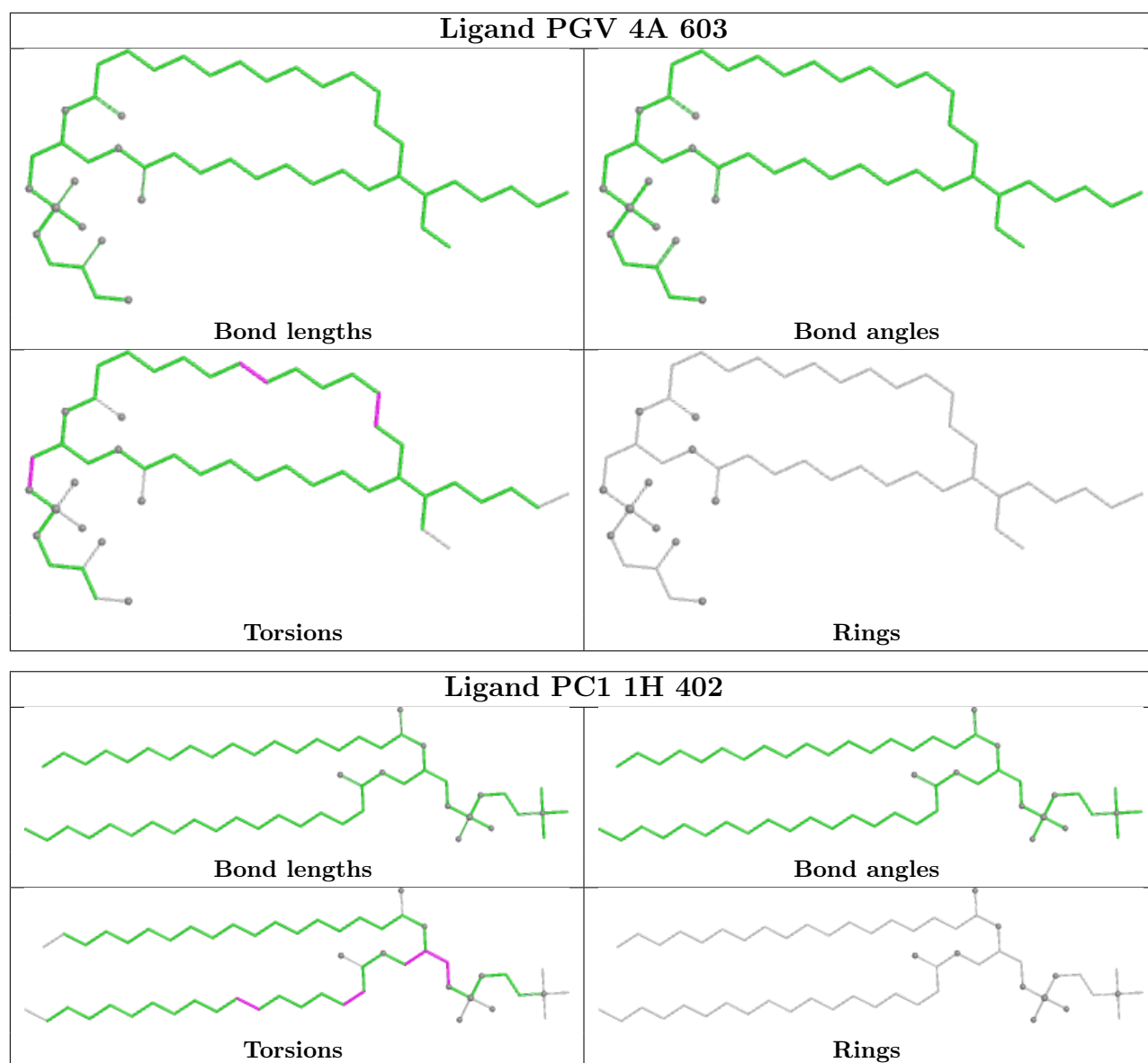
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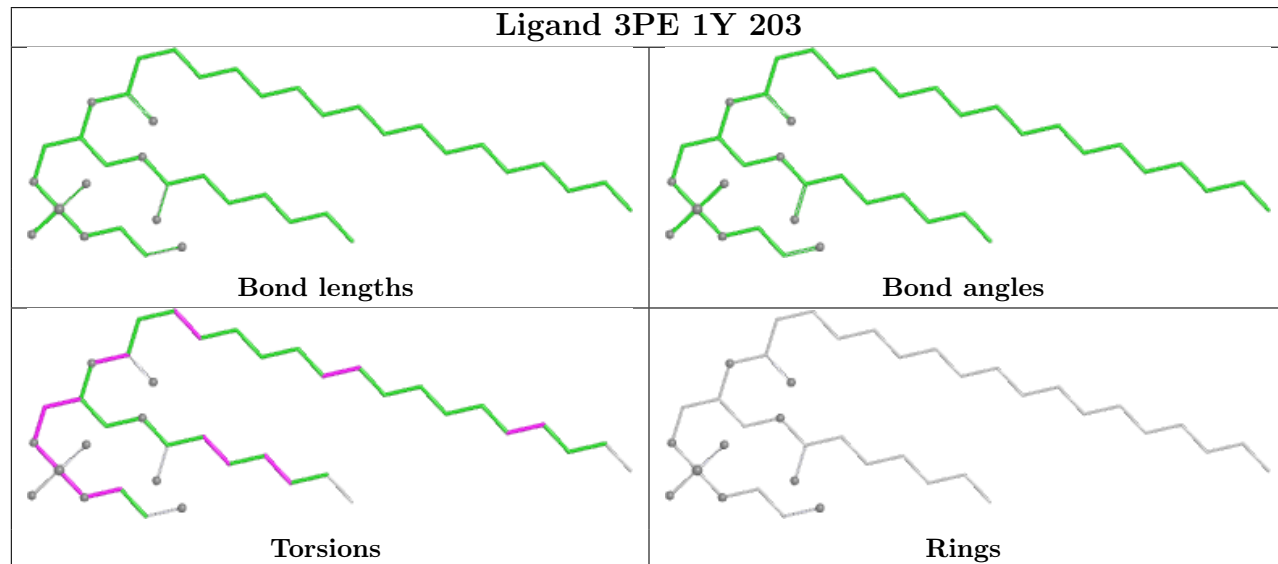
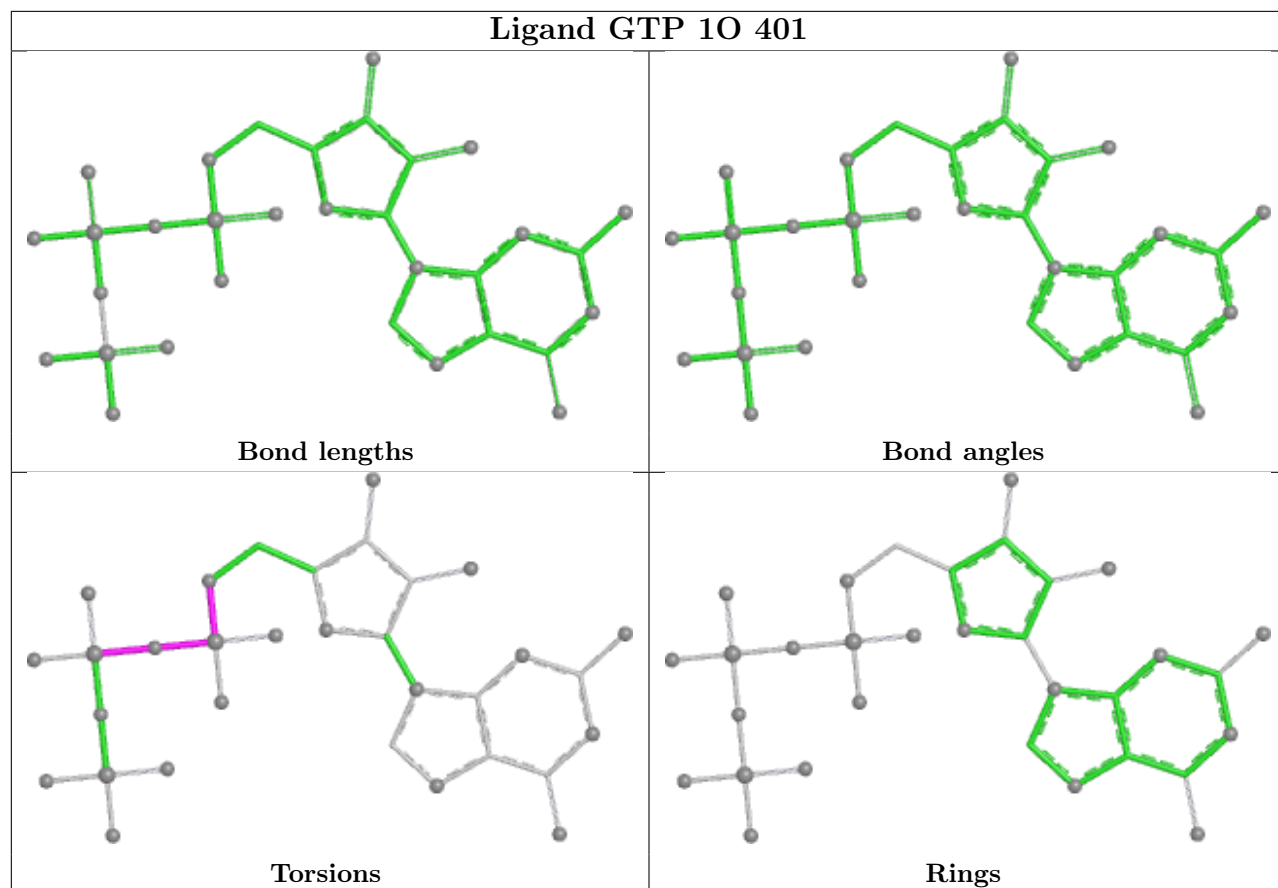
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	8G	101	PGV	8	0
69	1N	901	3PE	5	0
75	4C	305	CDL	15	0
75	3G	102	CDL	2	0
69	1M	501	3PE	7	0
71	1G	801	SF4	3	0
70	1B	203	PC1	9	0
69	1M	506	3PE	3	0
69	3R	302	3PE	5	0
69	1d	201	3PE	5	0
87	4L	101	PGV	7	0
69	1Y	205	3PE	3	0
73	1F	501	FMN	4	0
87	4A	601	PGV	6	0
69	1M	502	3PE	12	0
69	3D	502	3PE	2	0
92	4B	305	PSC	8	0
69	1K	101	3PE	2	0
87	4K	101	PGV	2	0
69	1Y	206	3PE	2	0

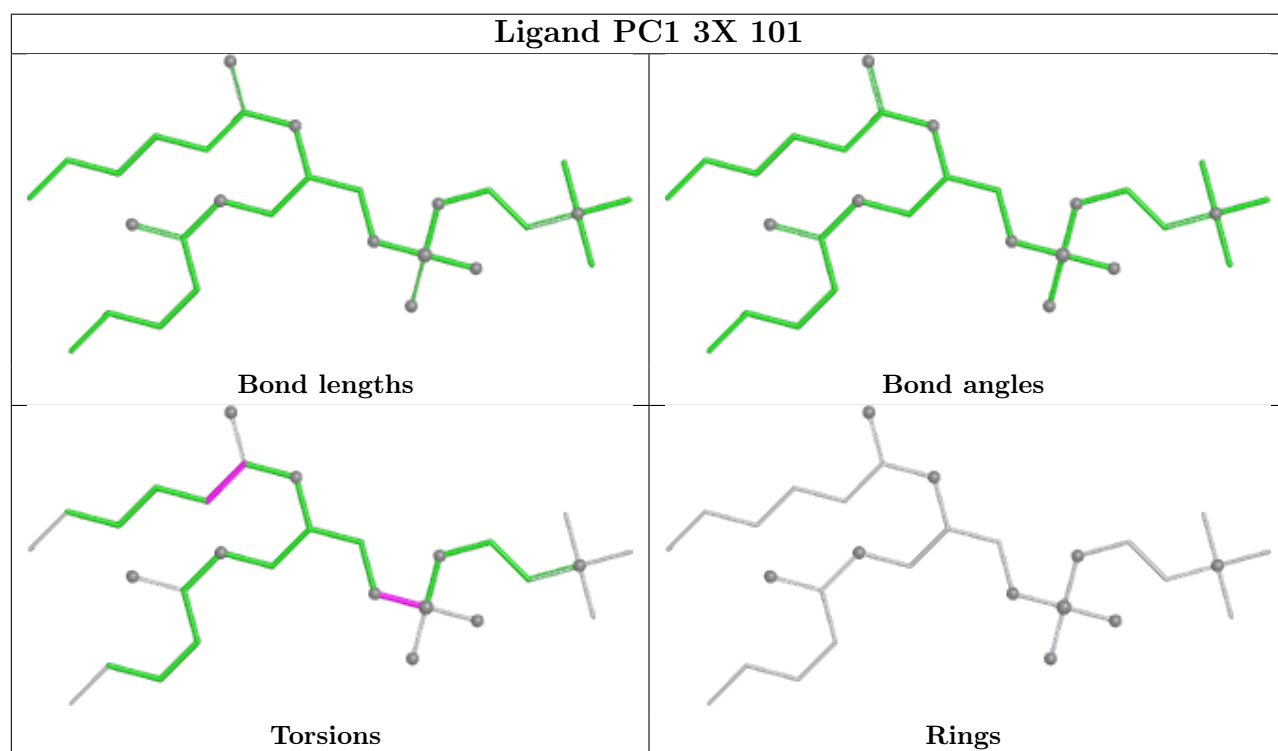
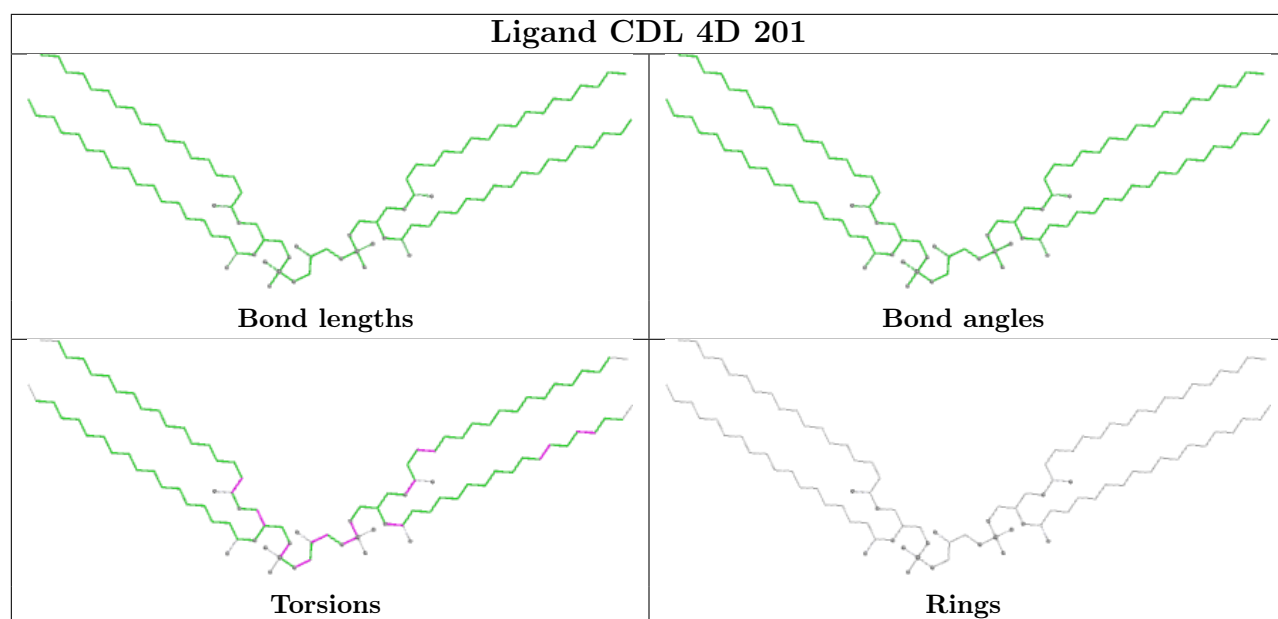
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

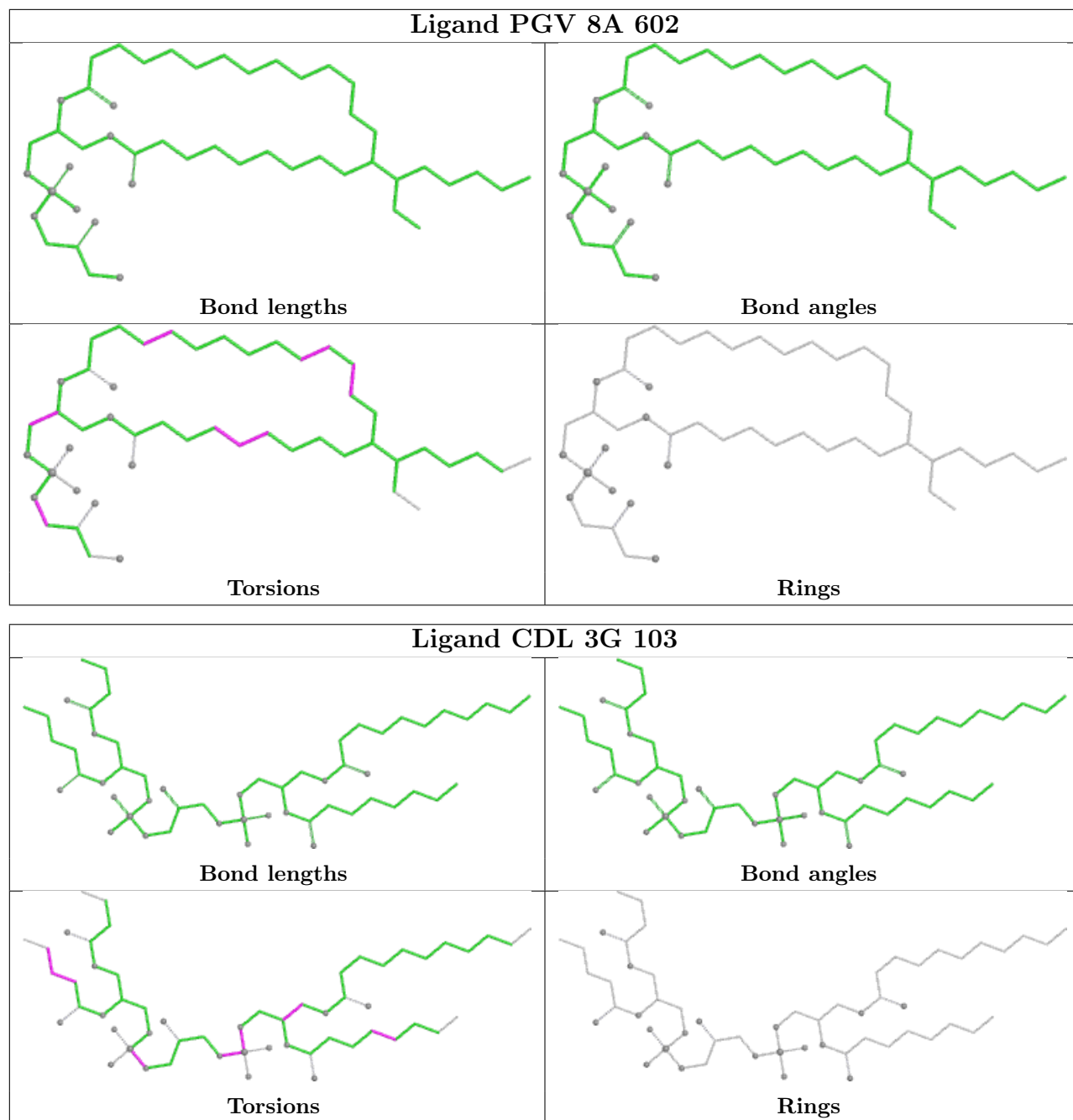




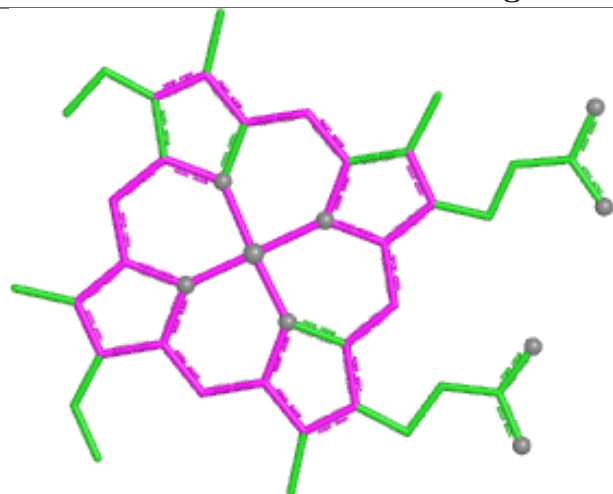




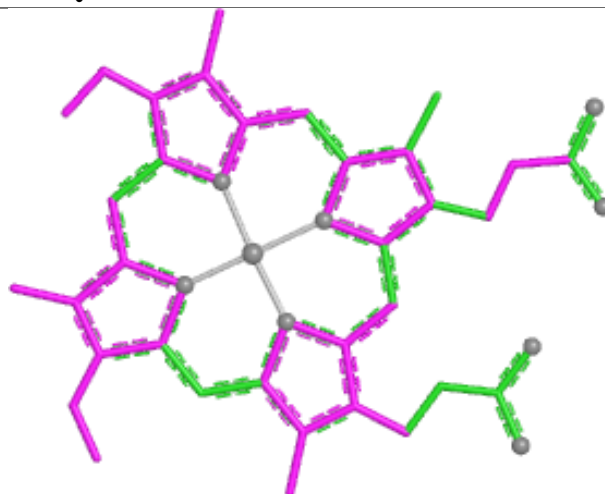




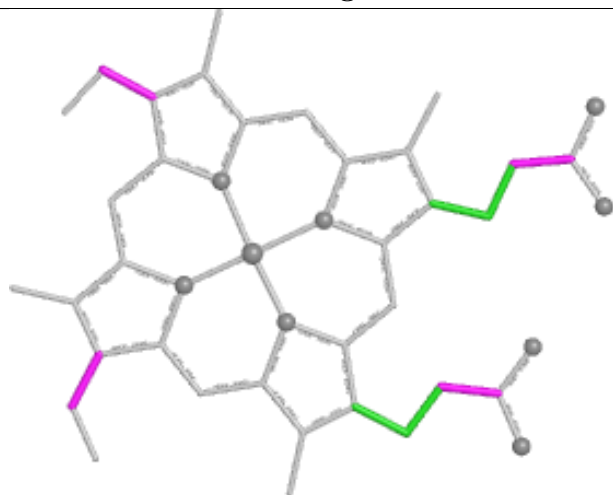
Ligand HEC 3Q 501



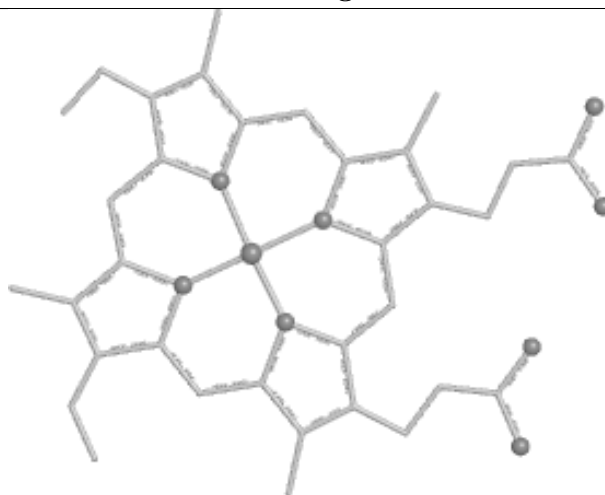
Bond lengths



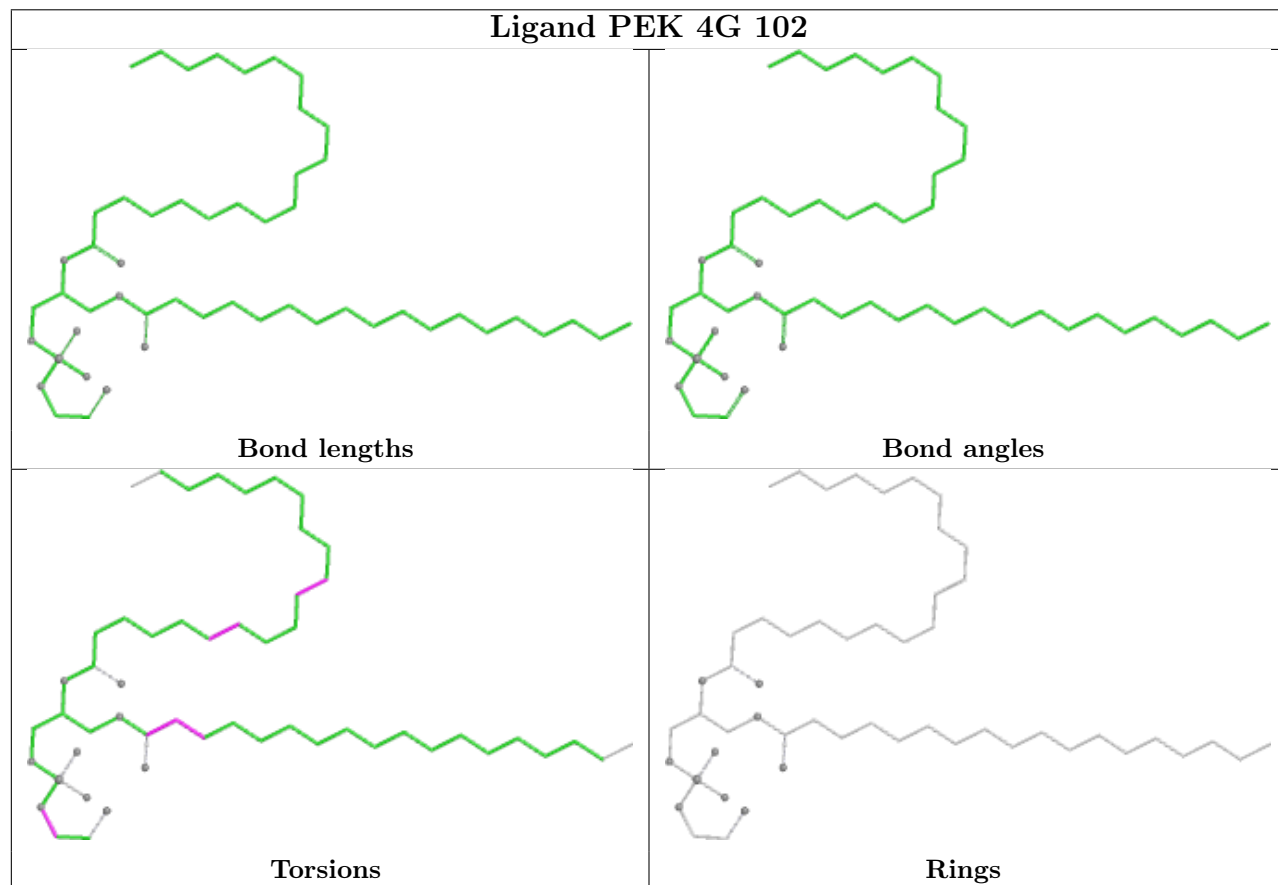
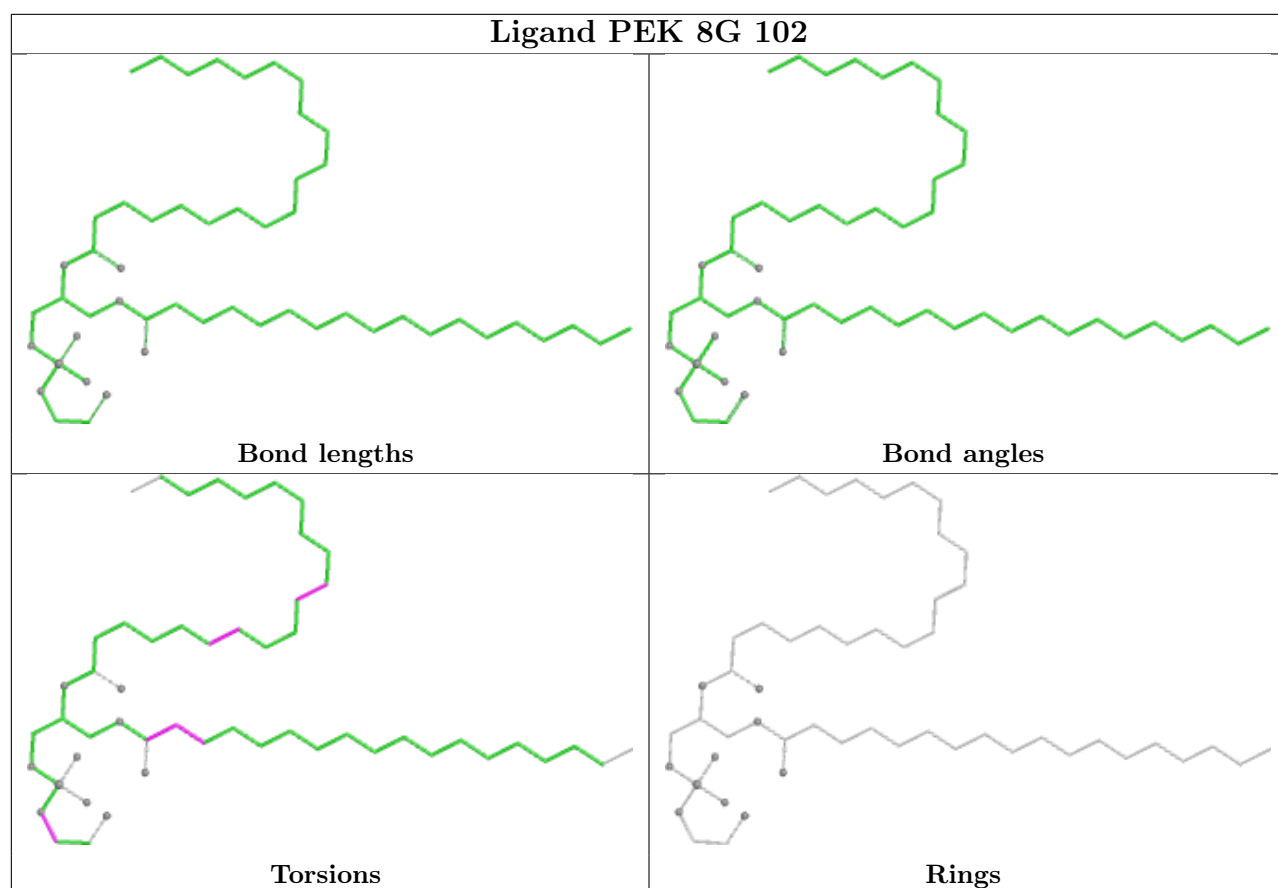
Bond angles

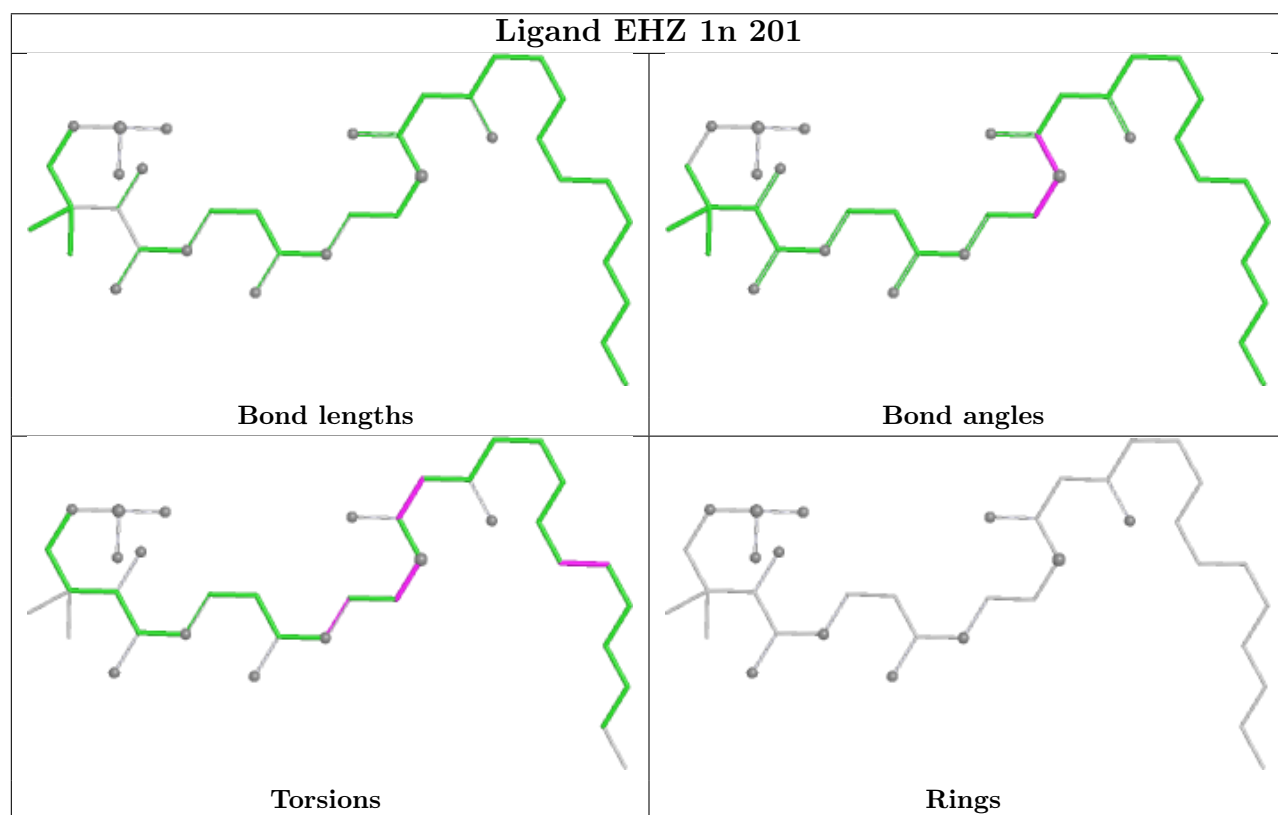
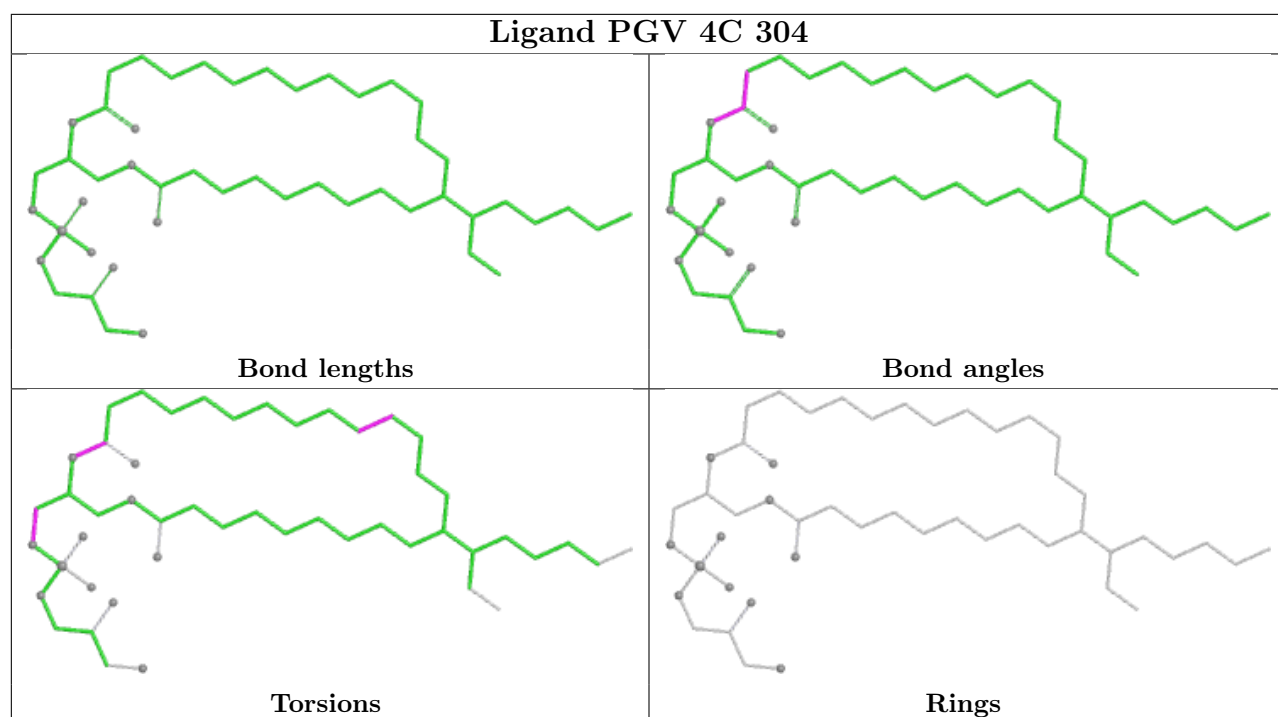


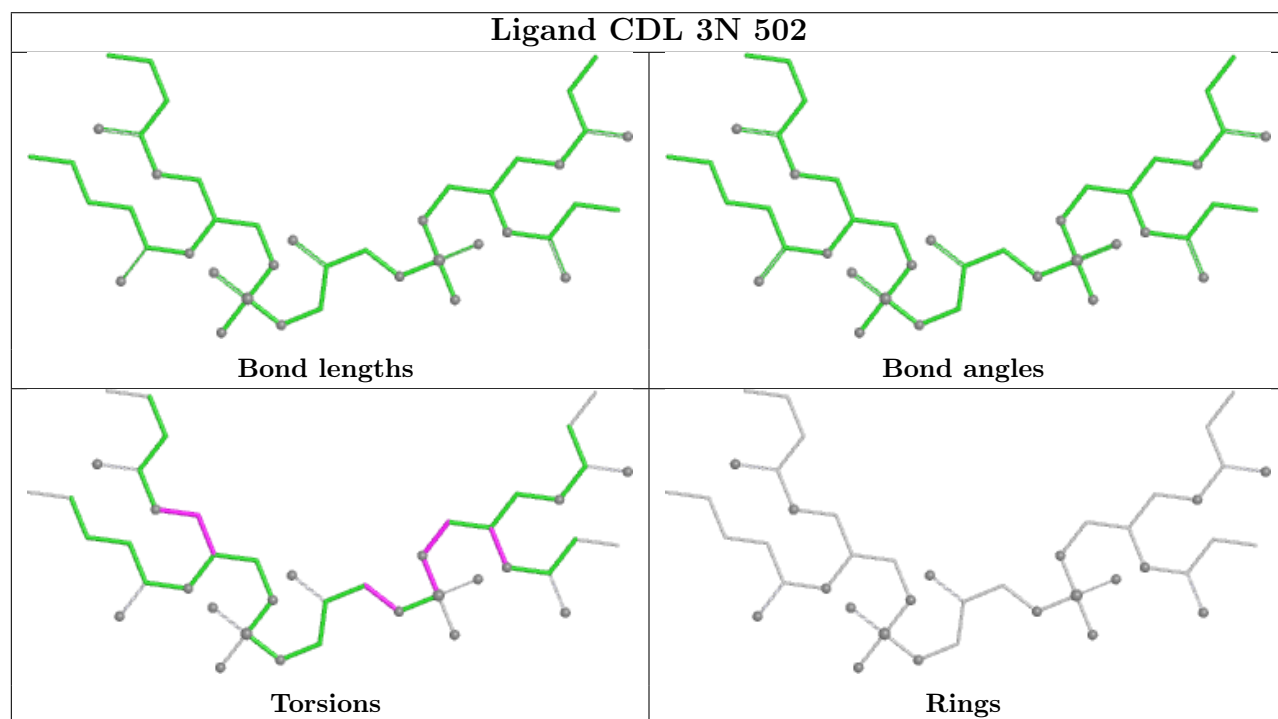
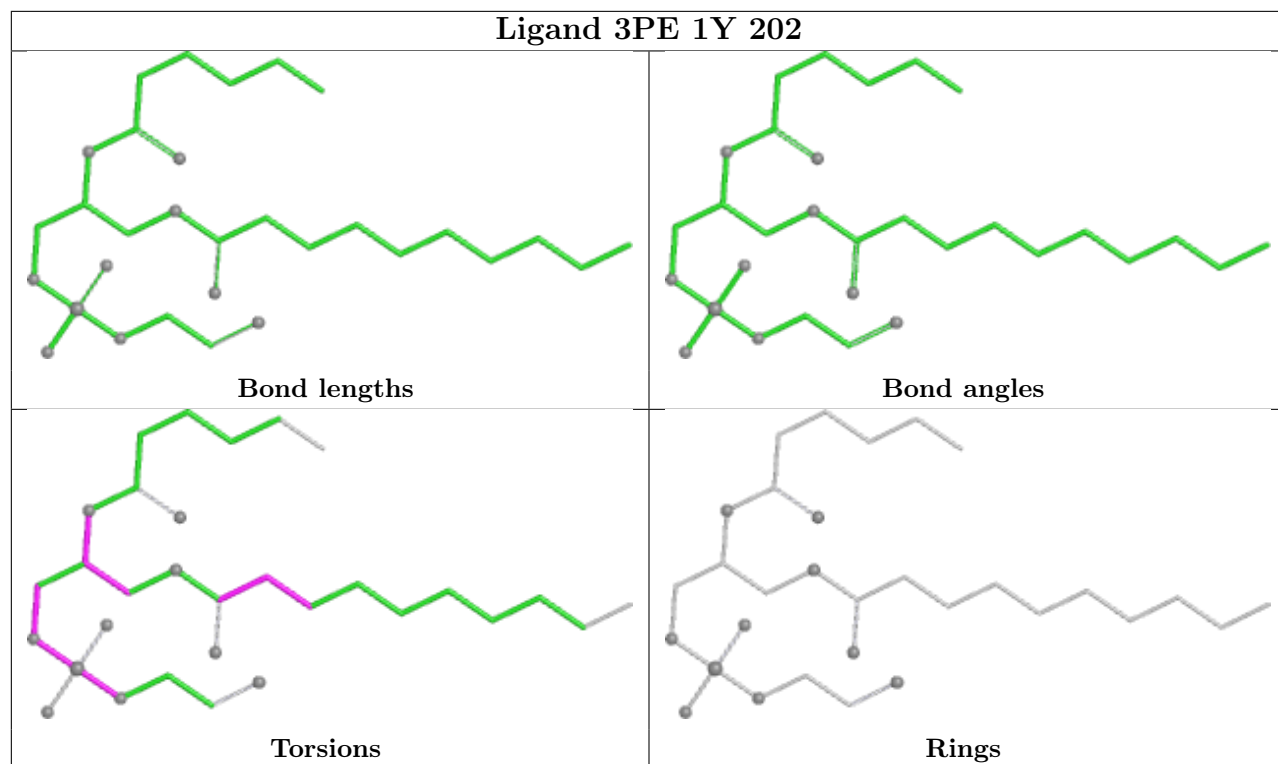
Torsions

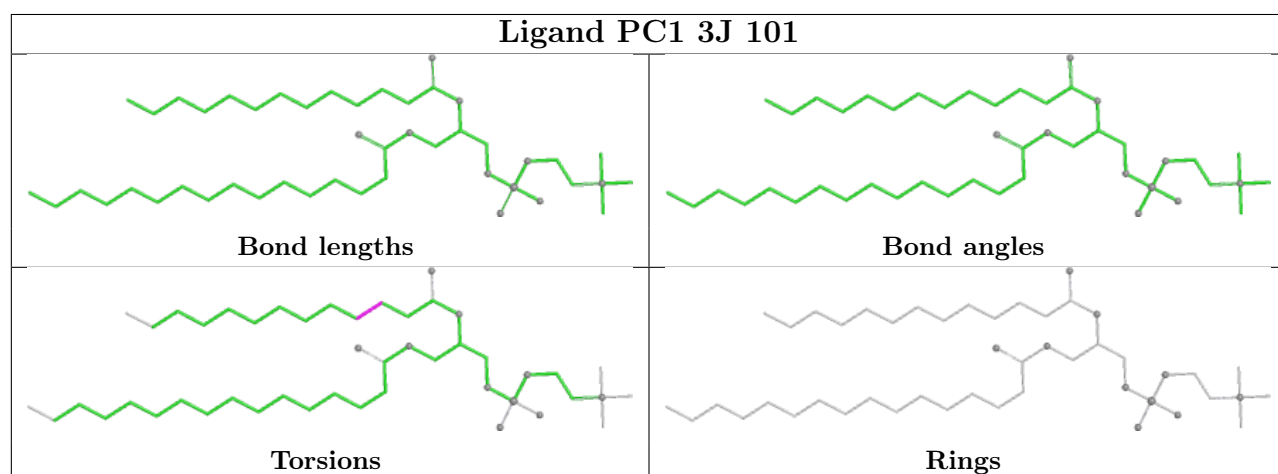
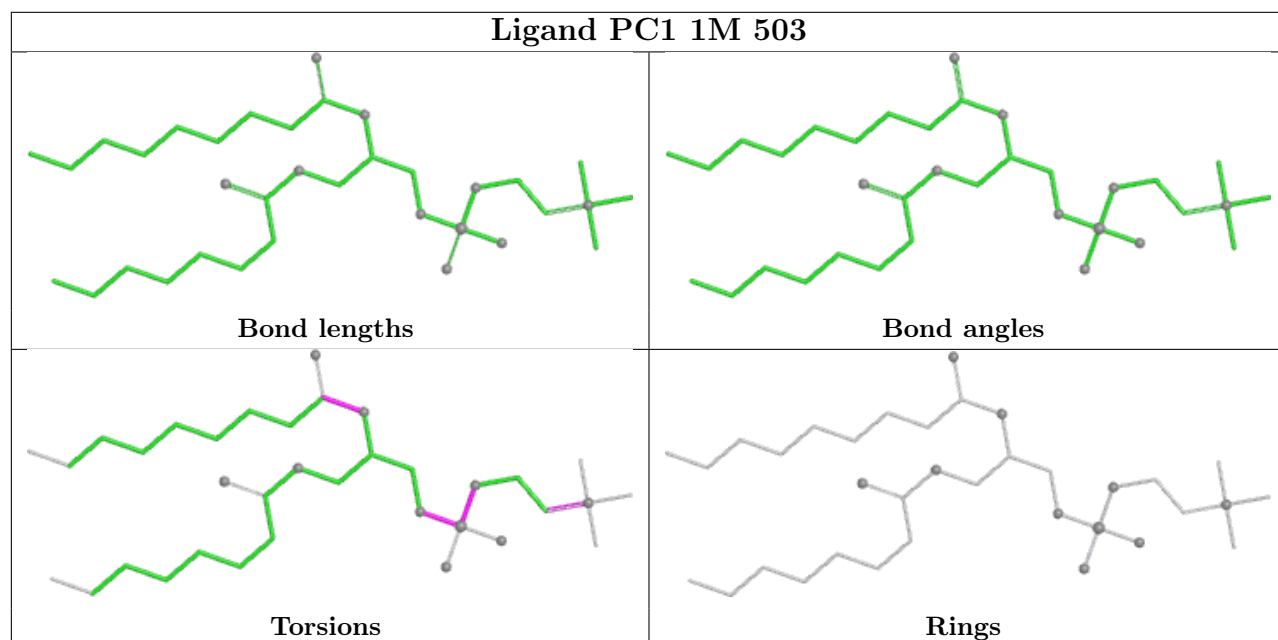
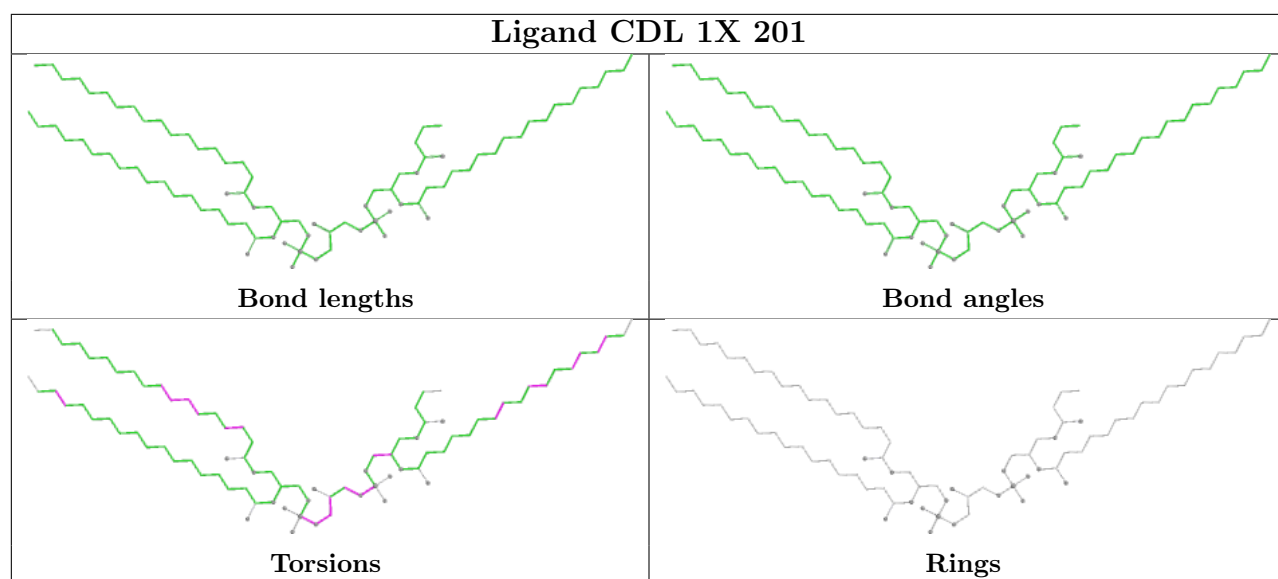


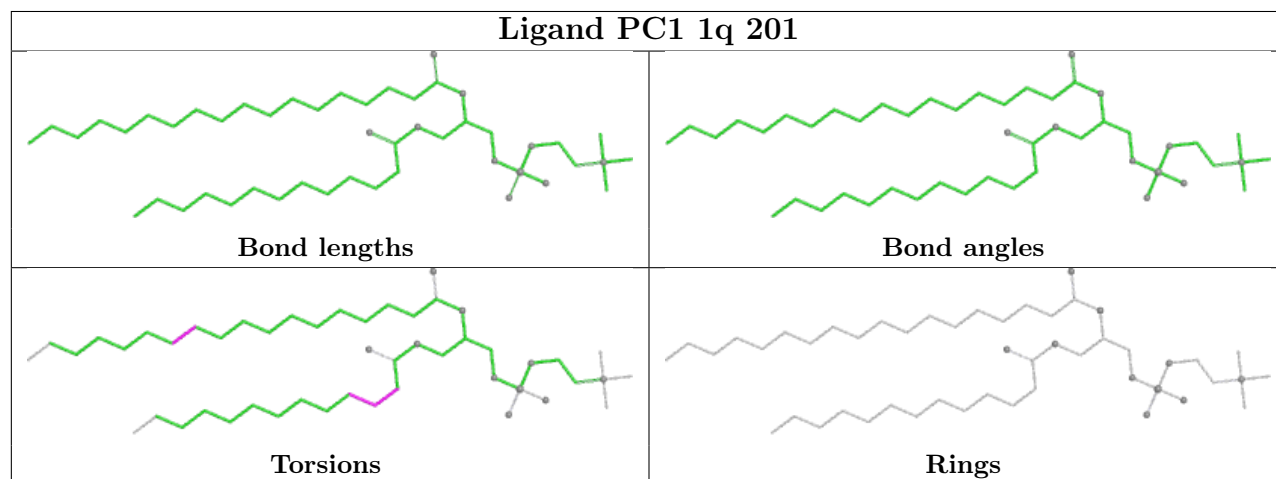
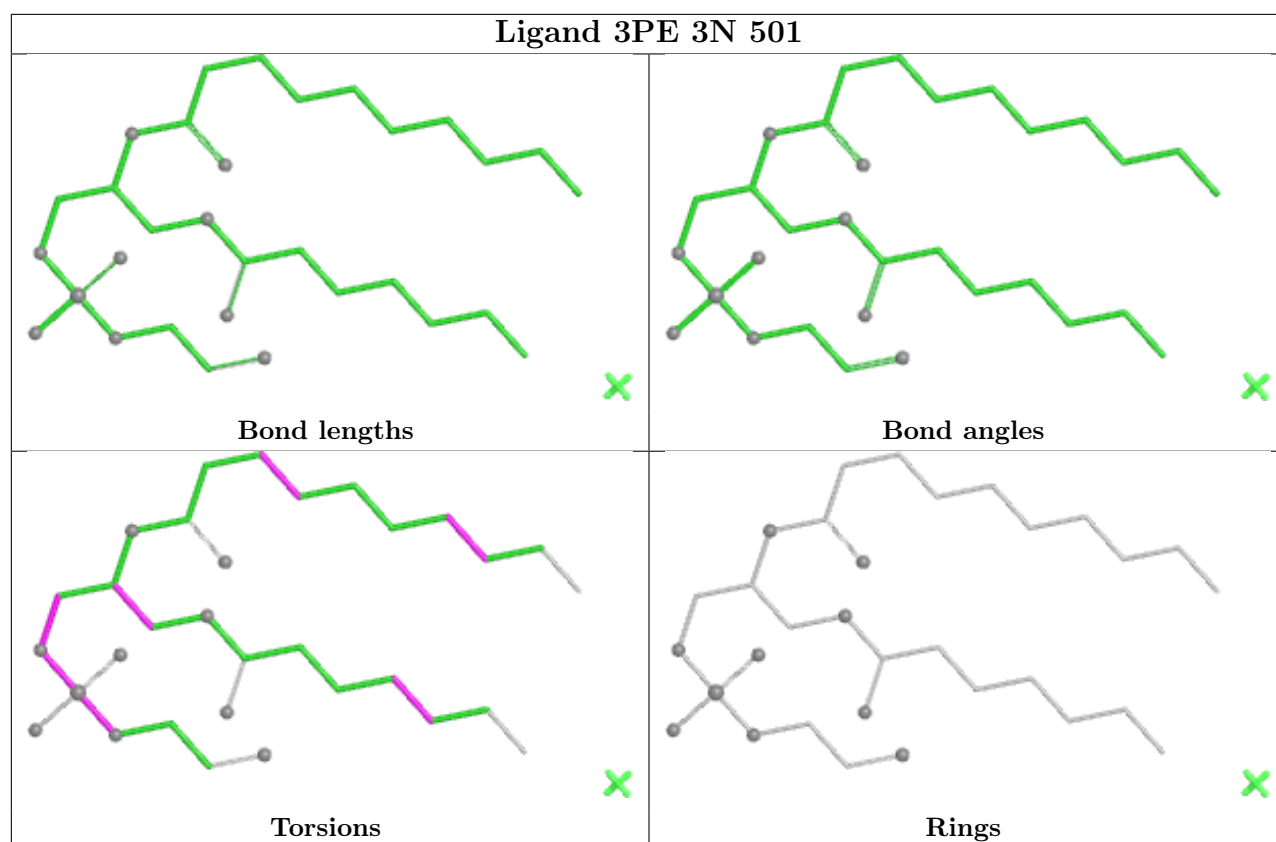
Rings

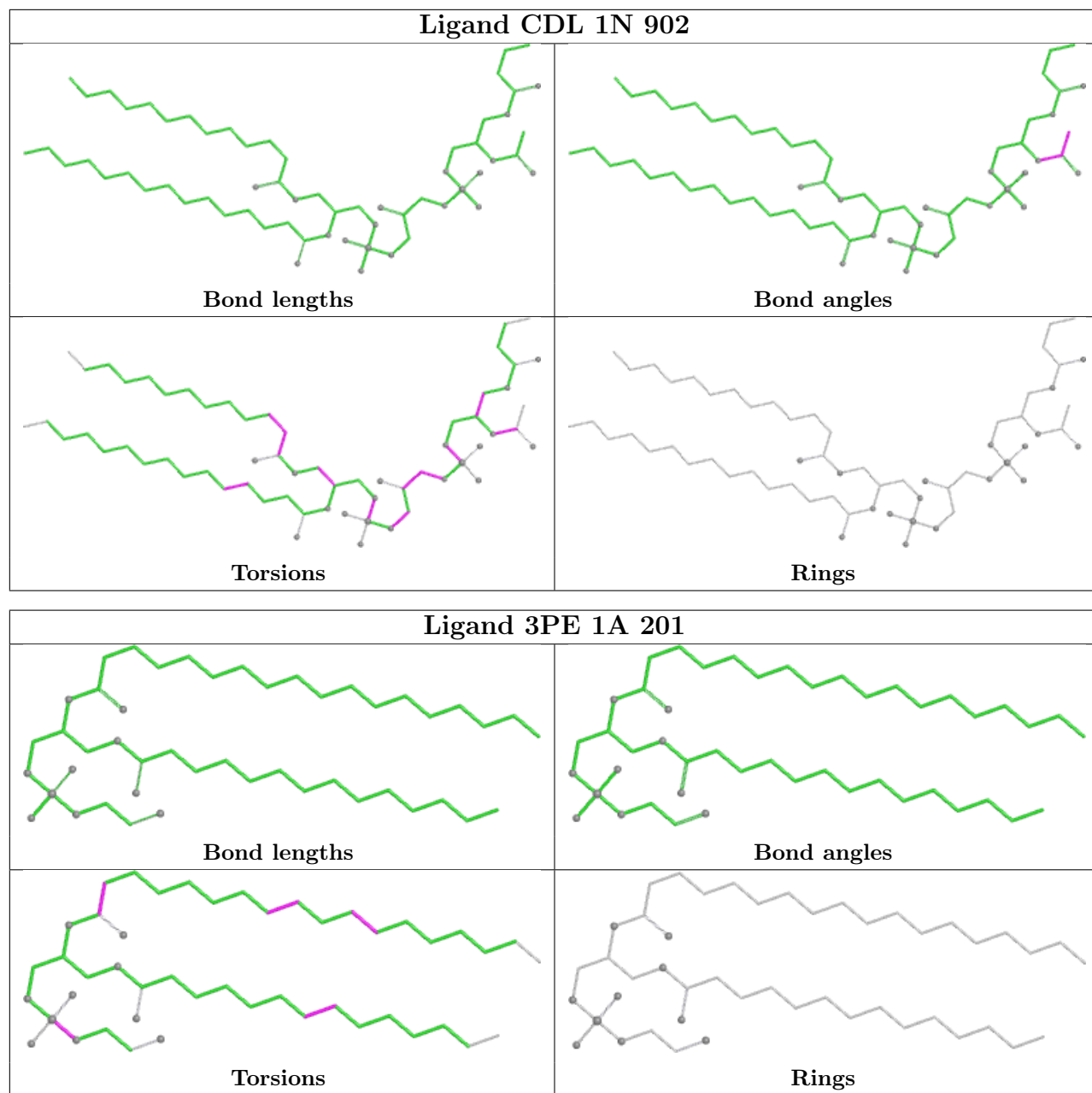


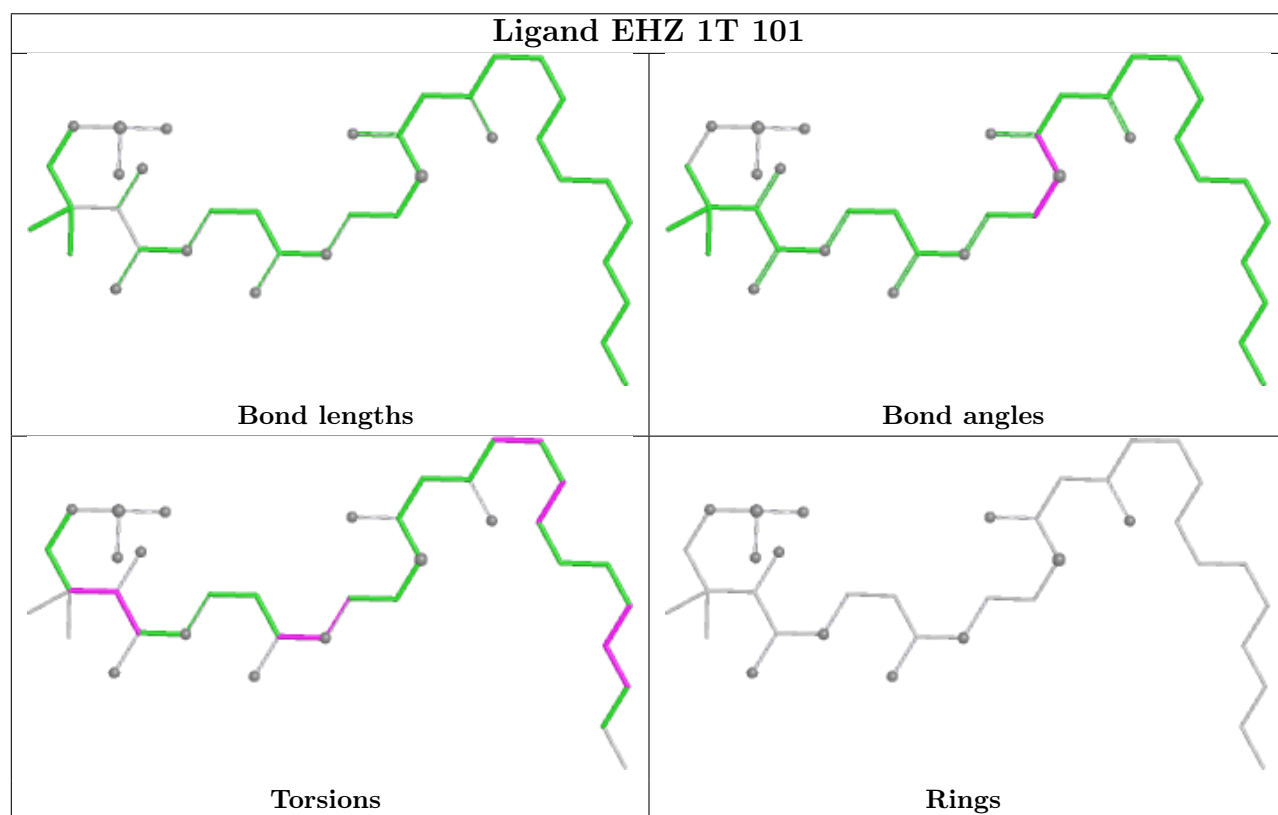
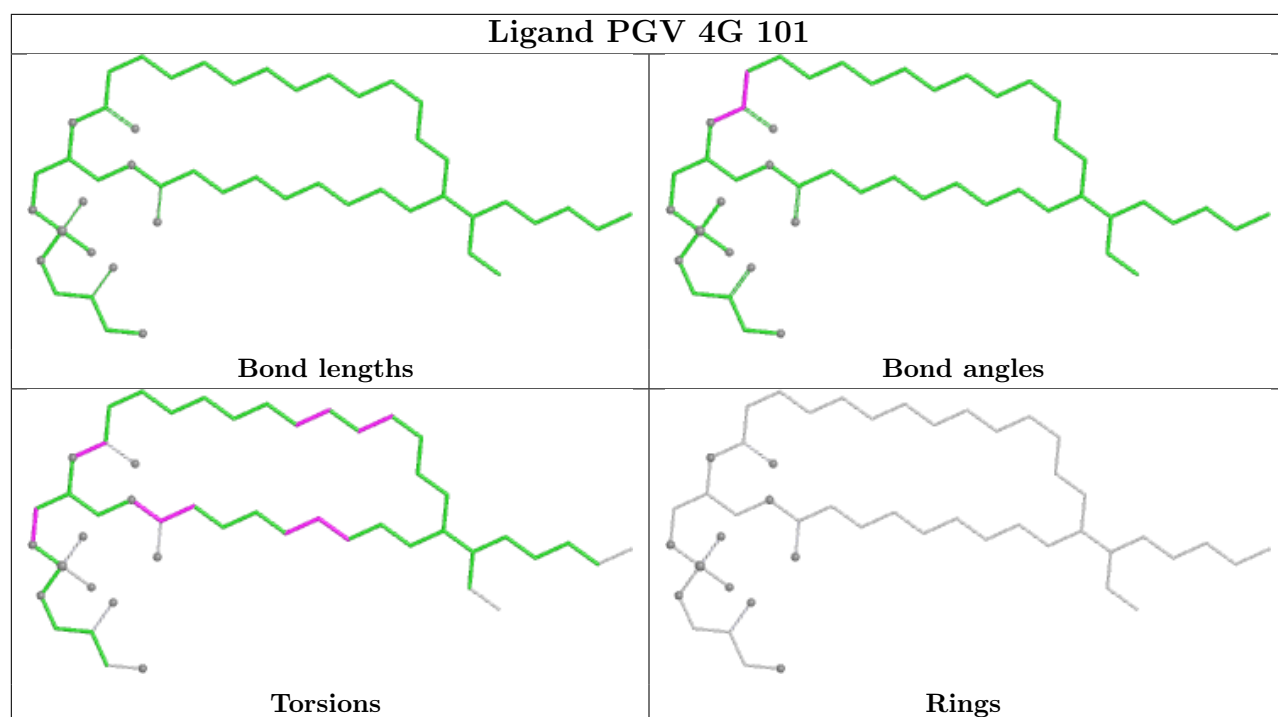


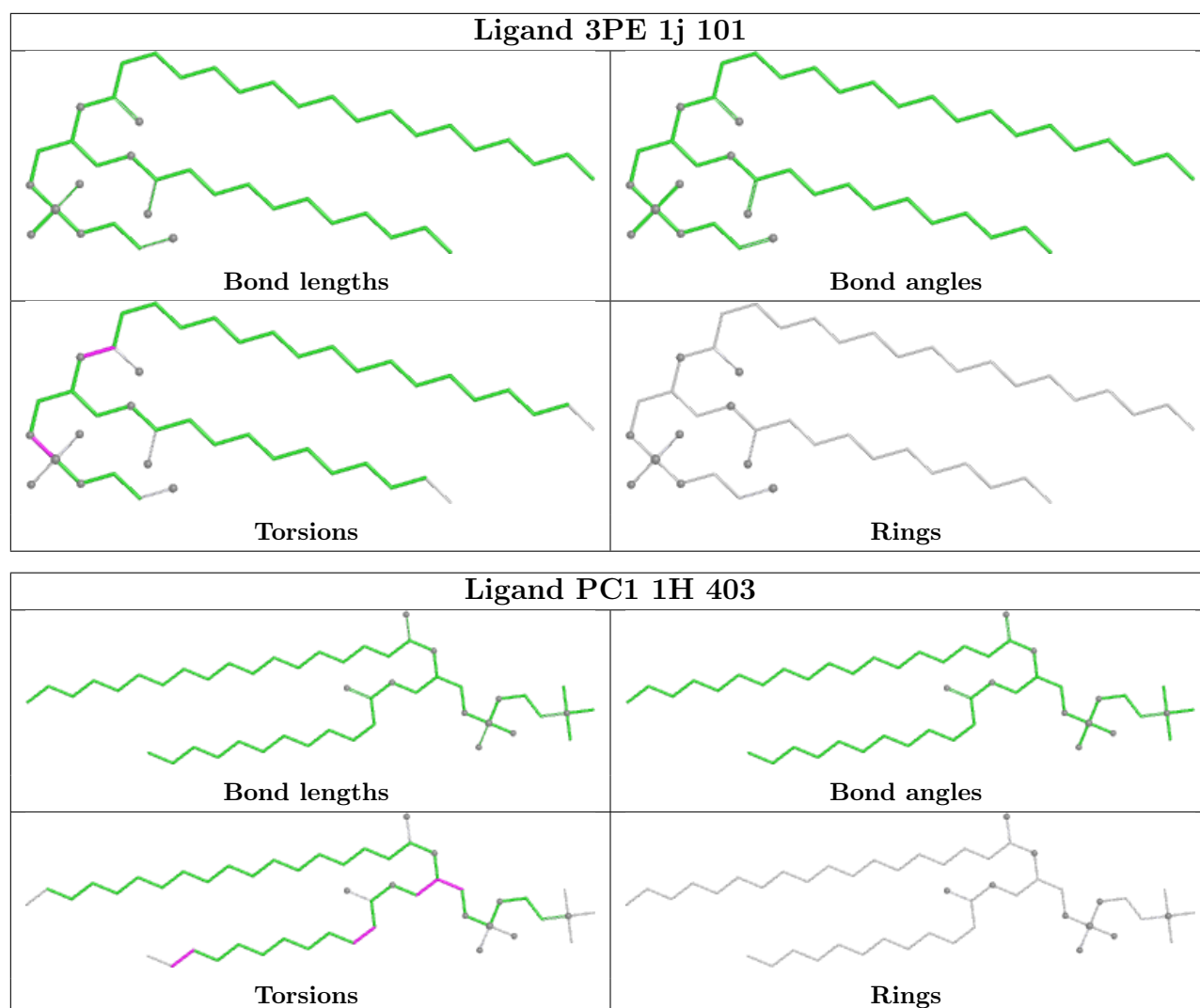


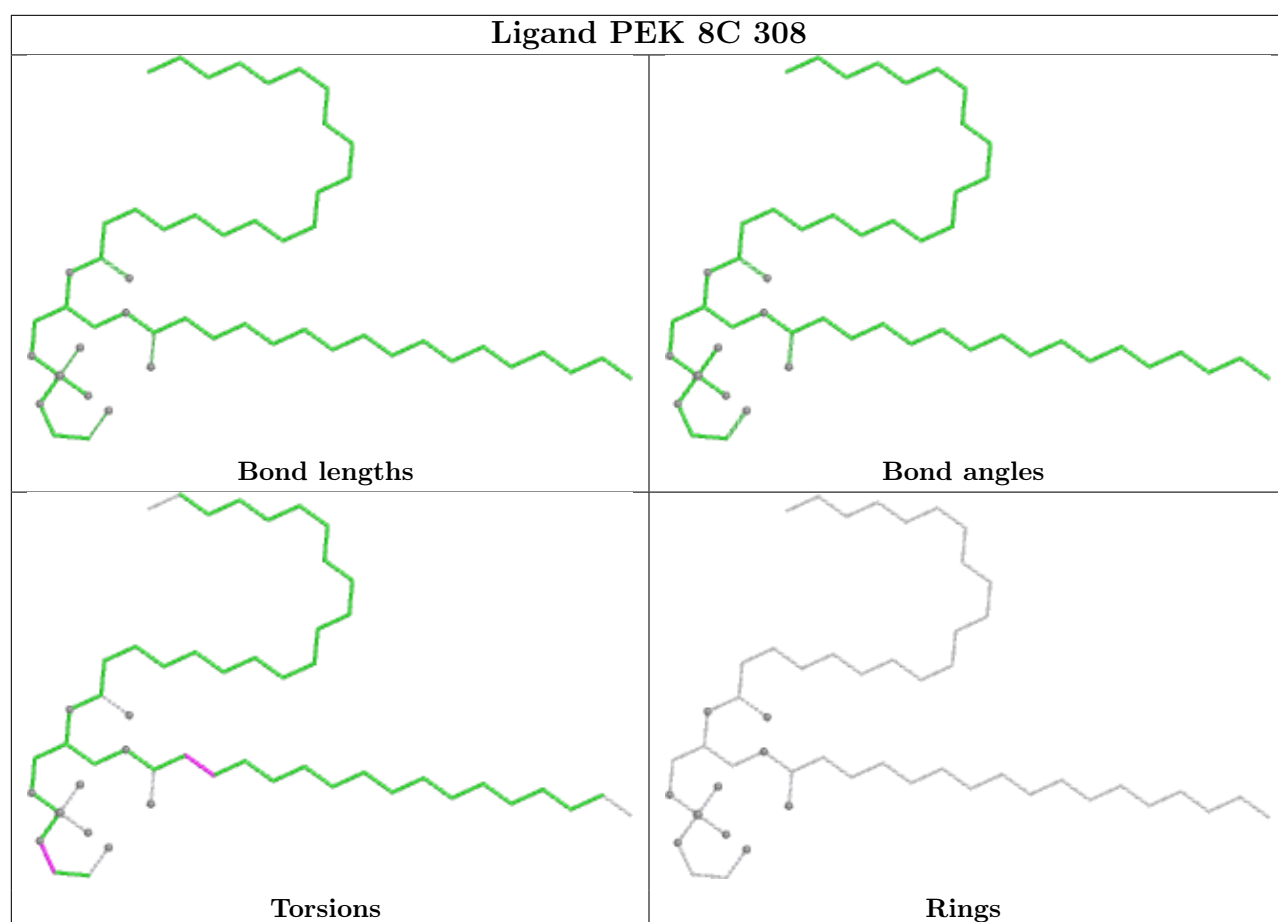
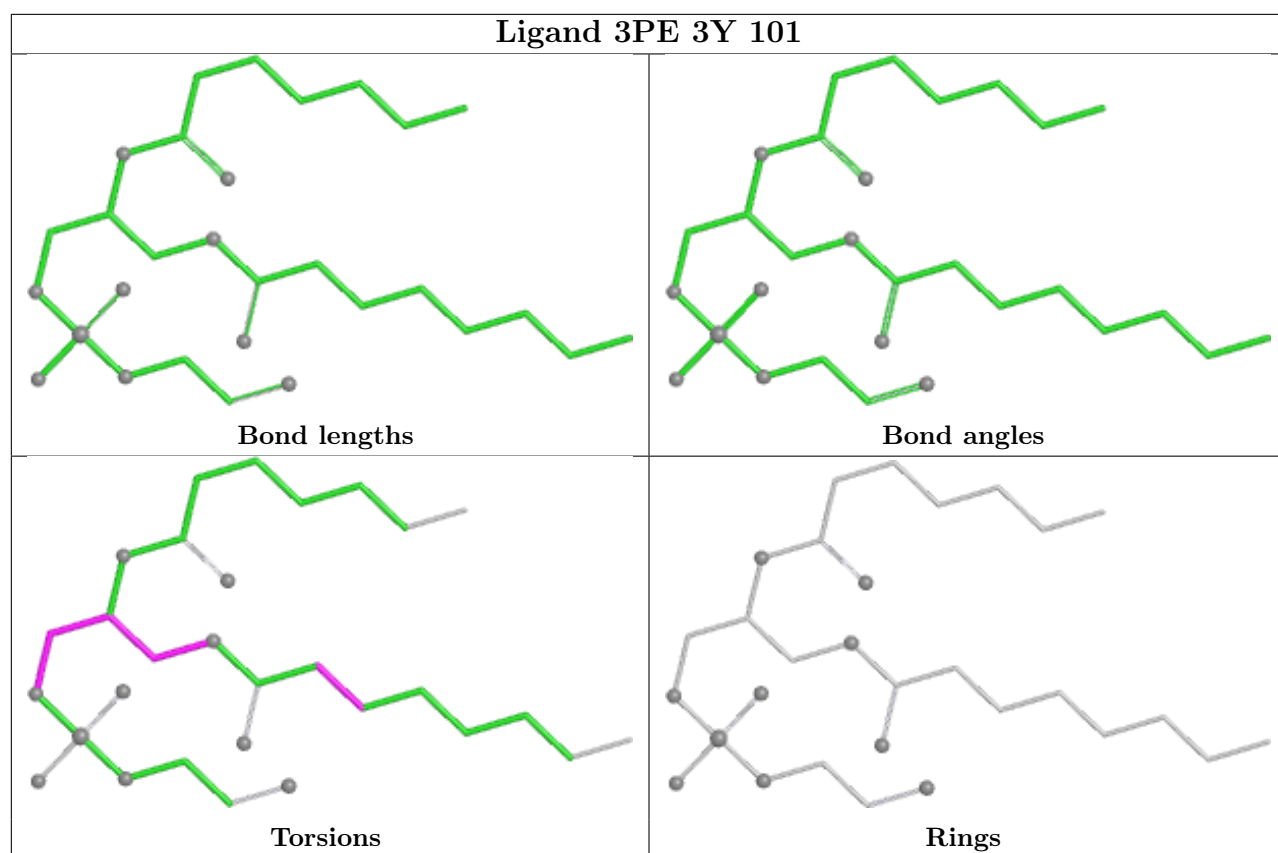




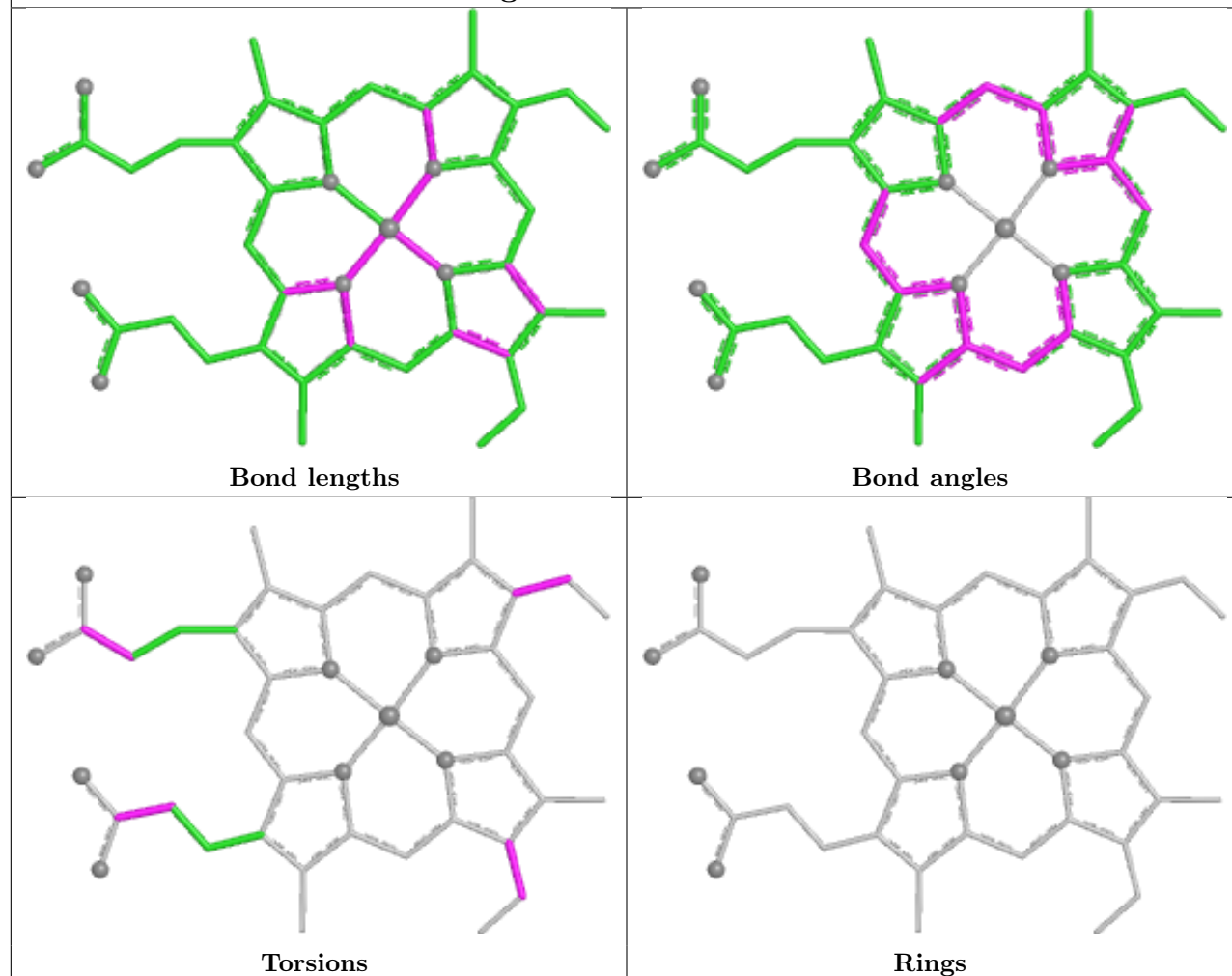




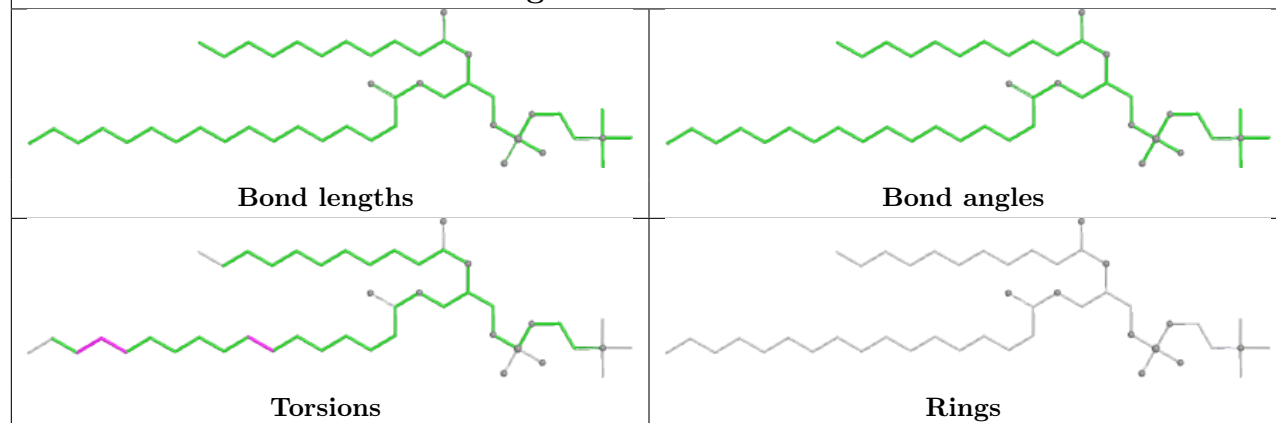


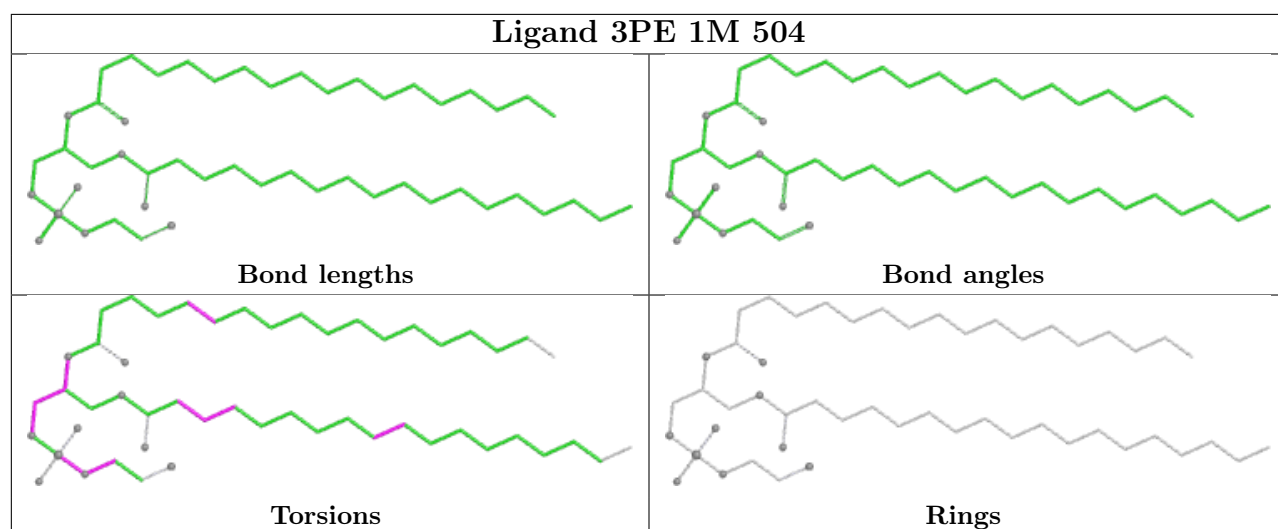
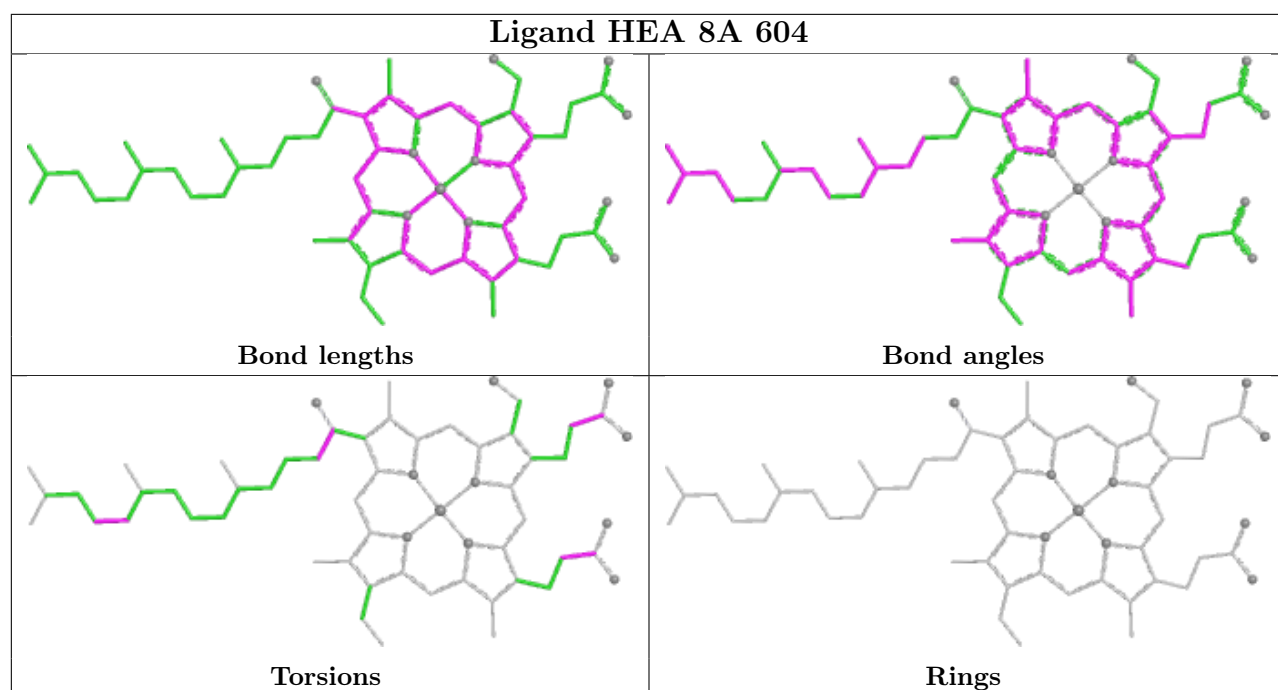


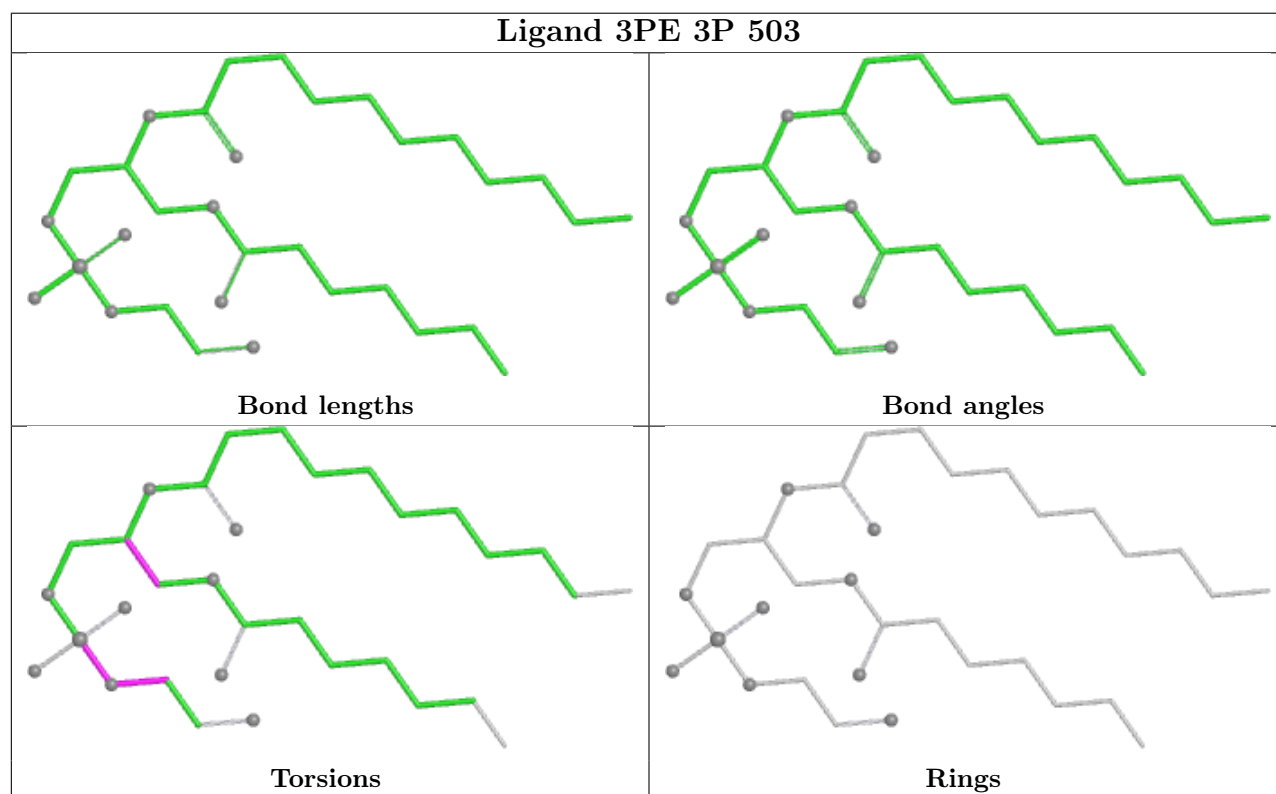
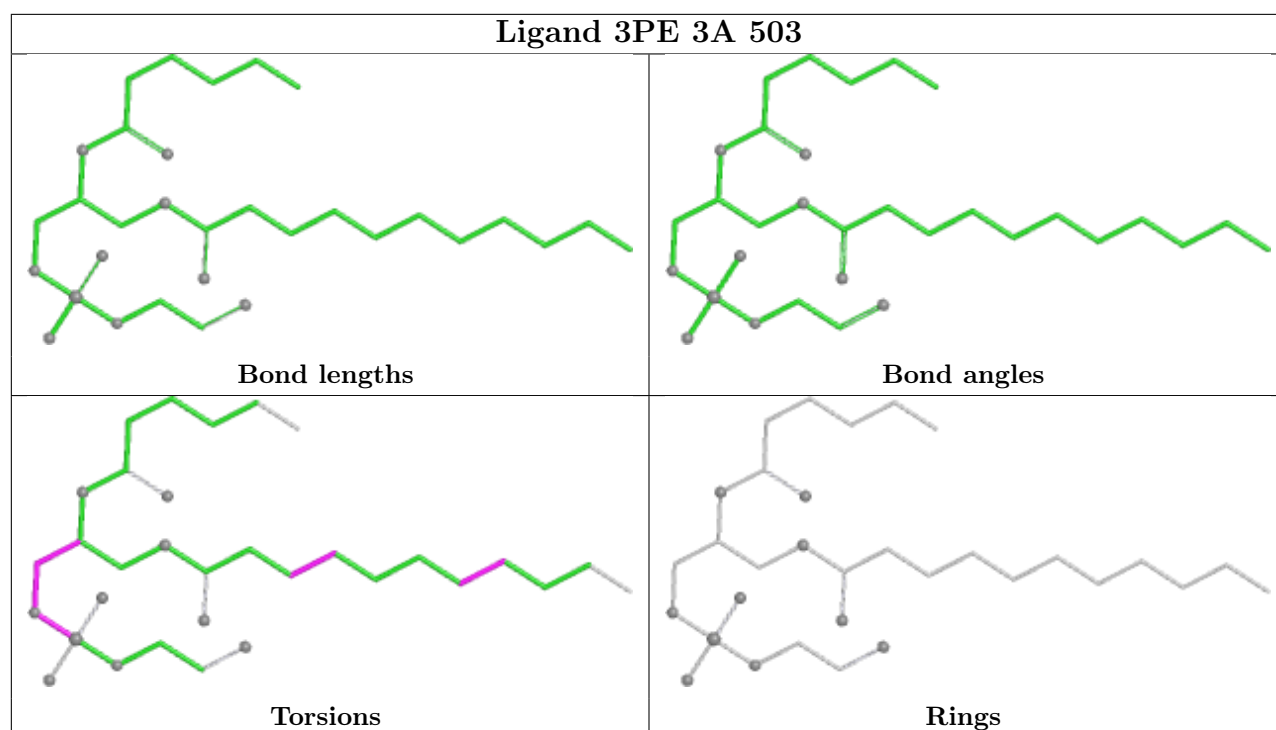
Ligand HEM 3P 502

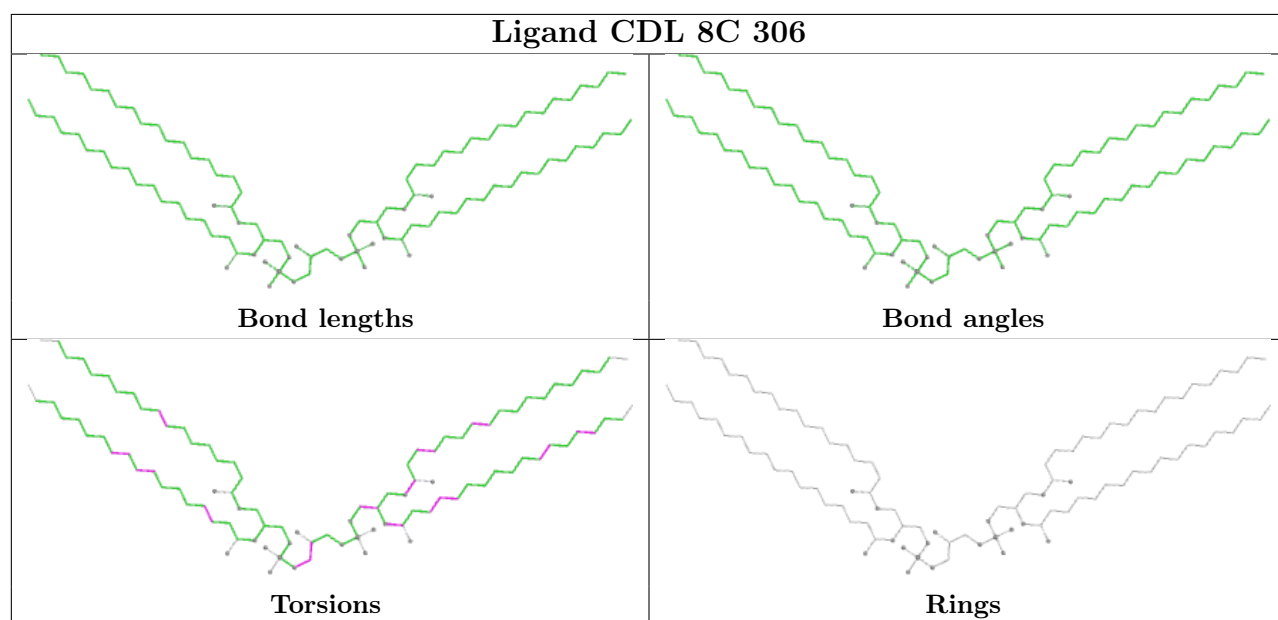
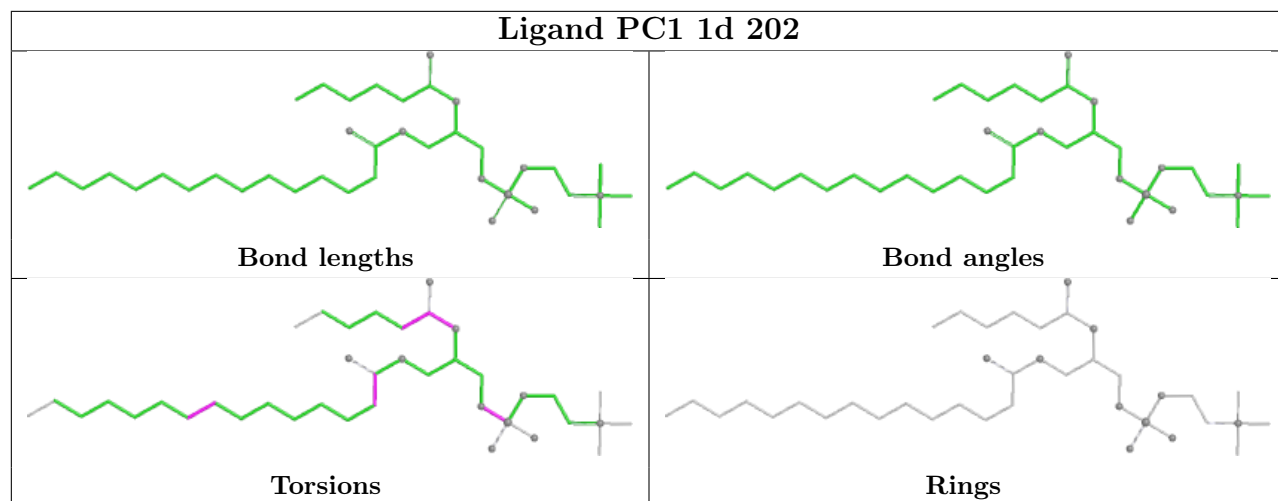


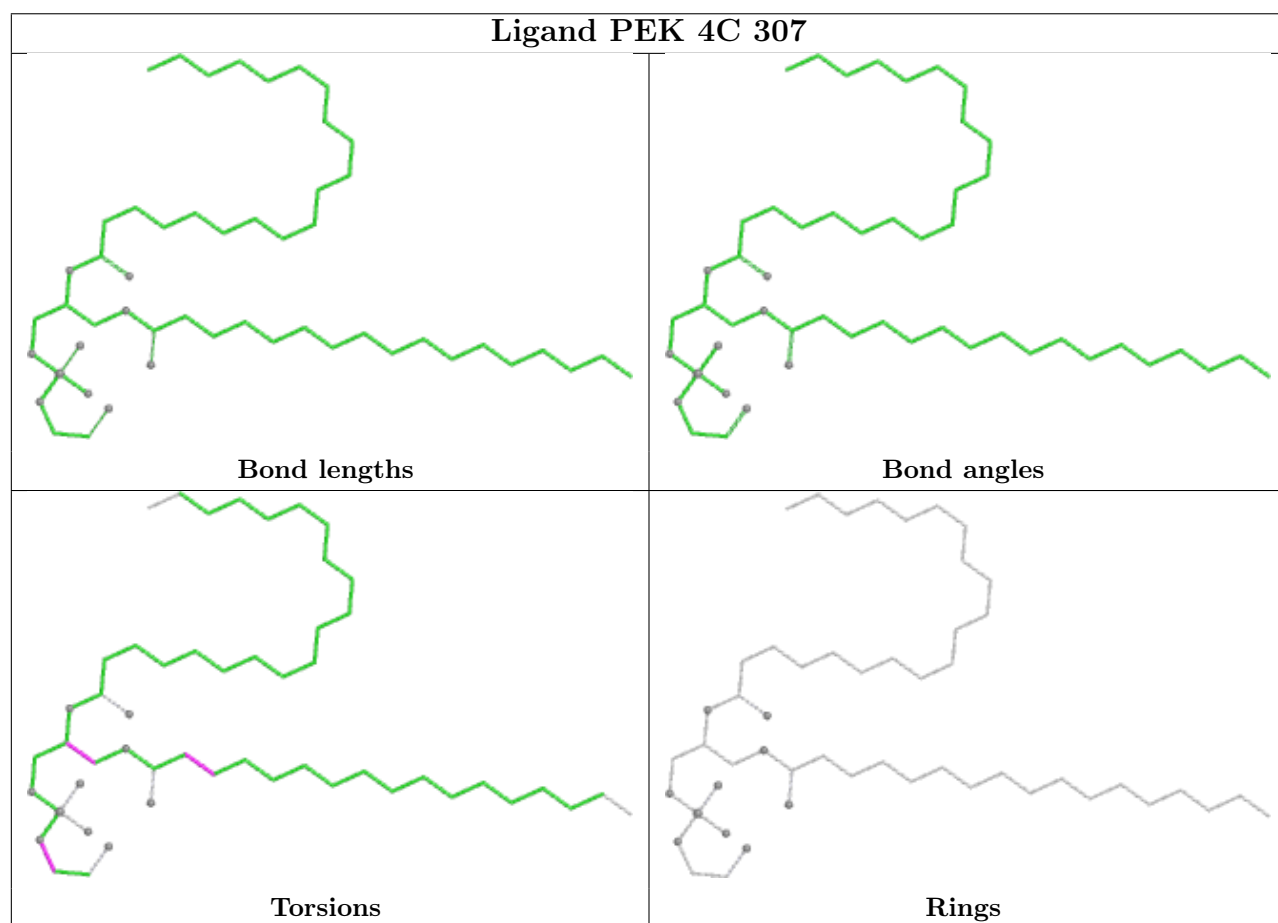
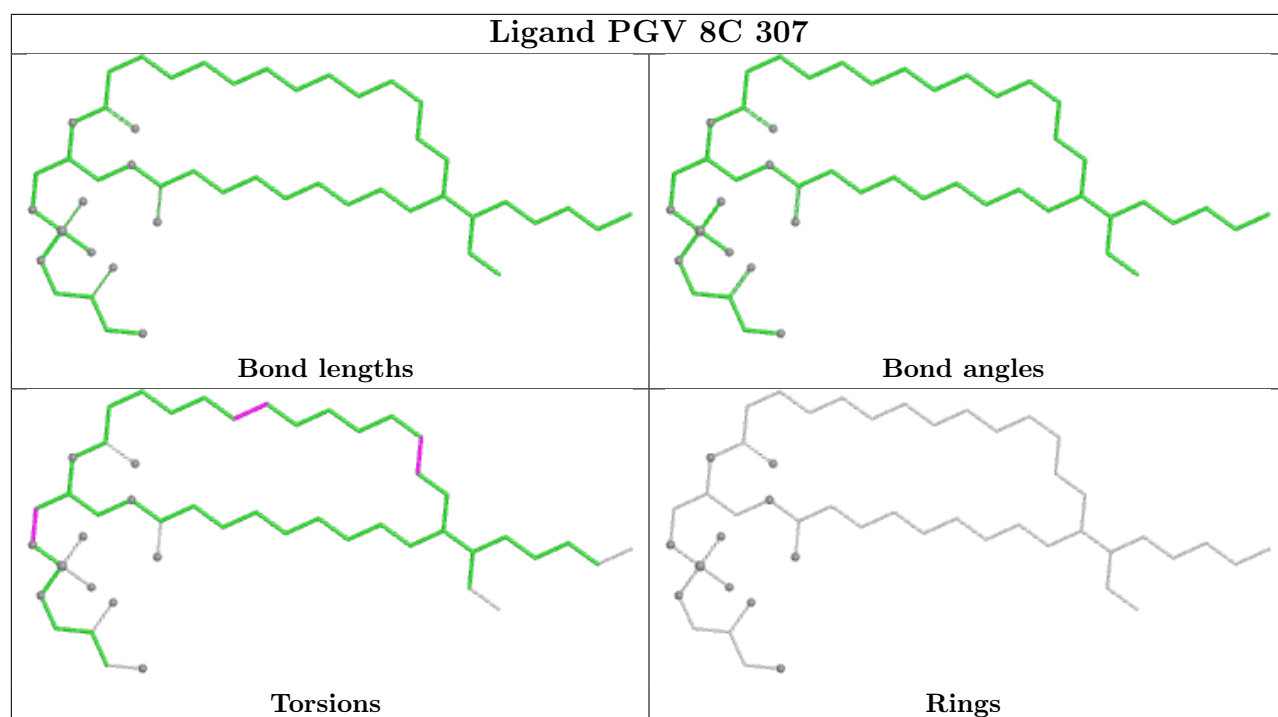
Ligand PC1 1B 202

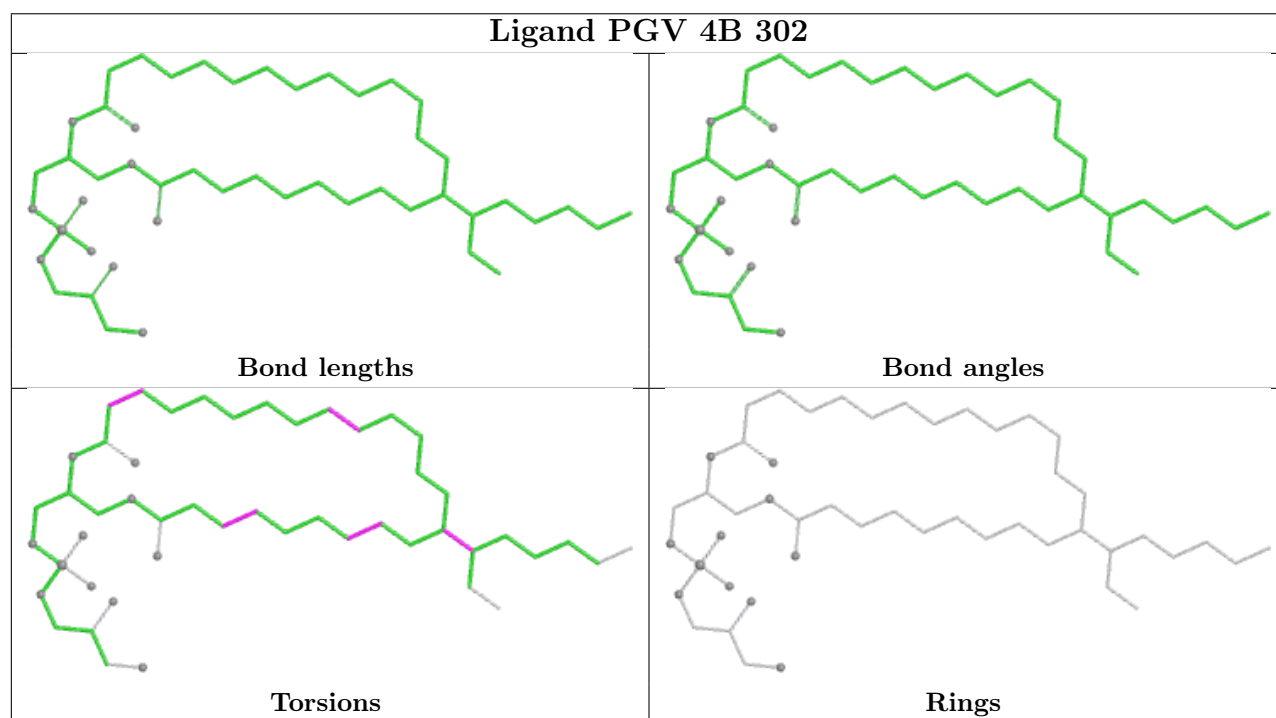
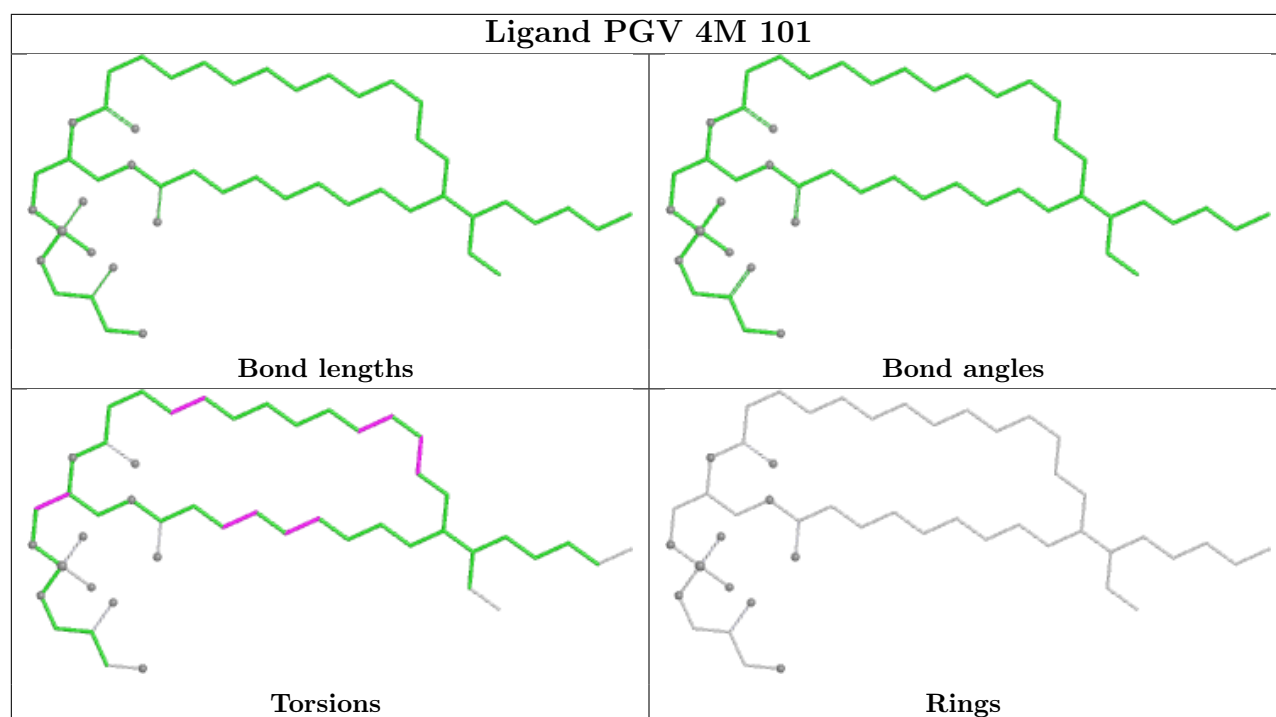


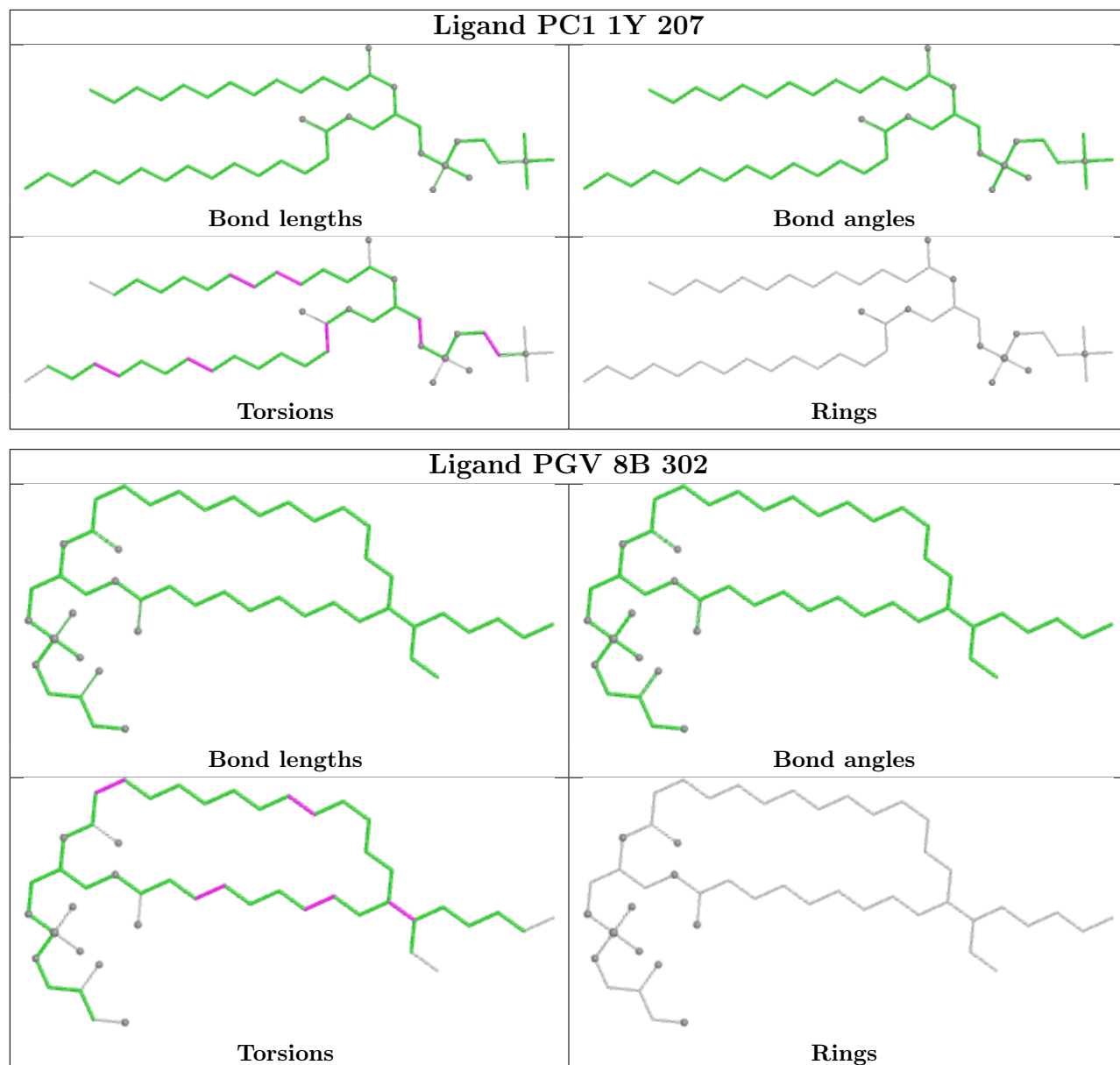




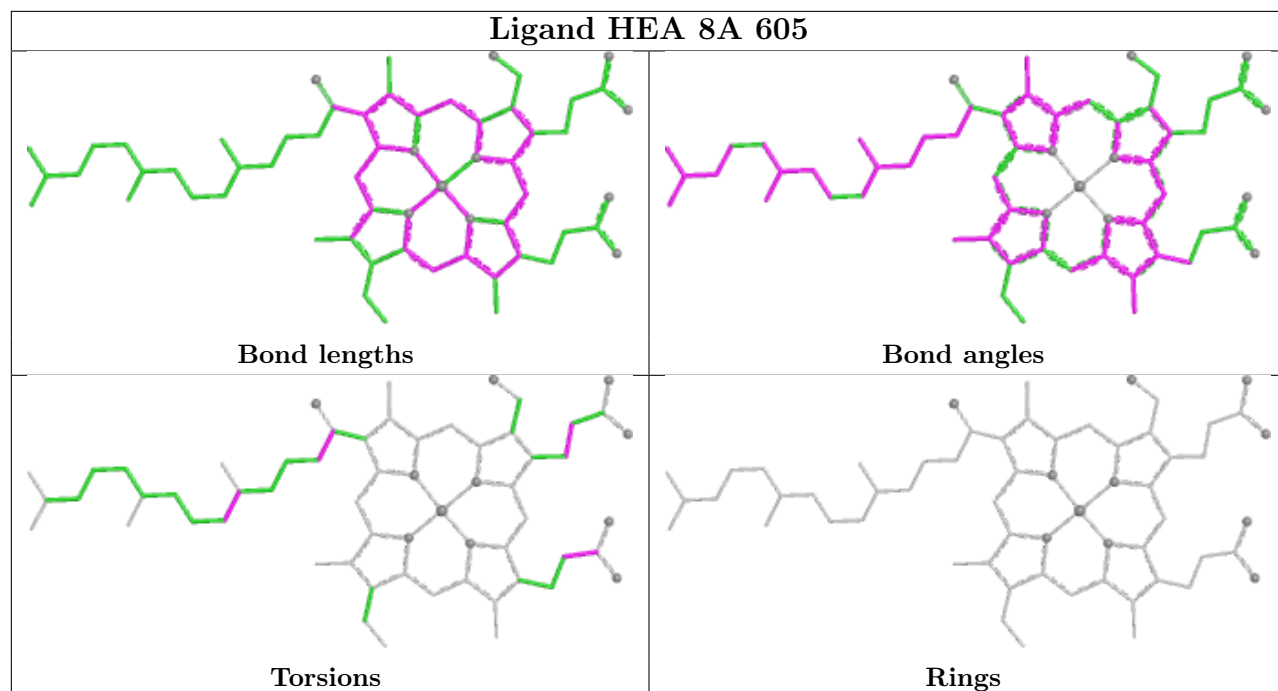




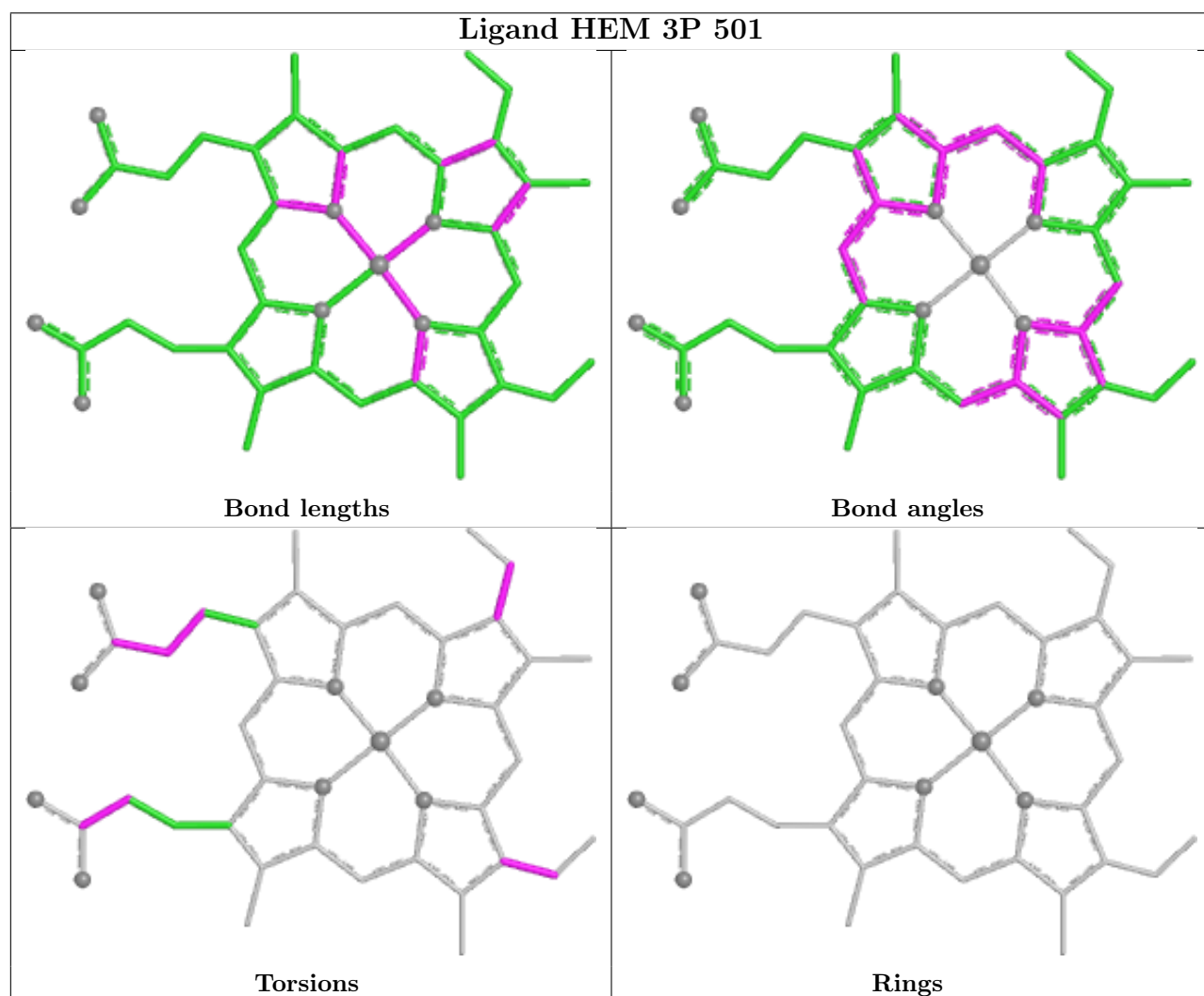


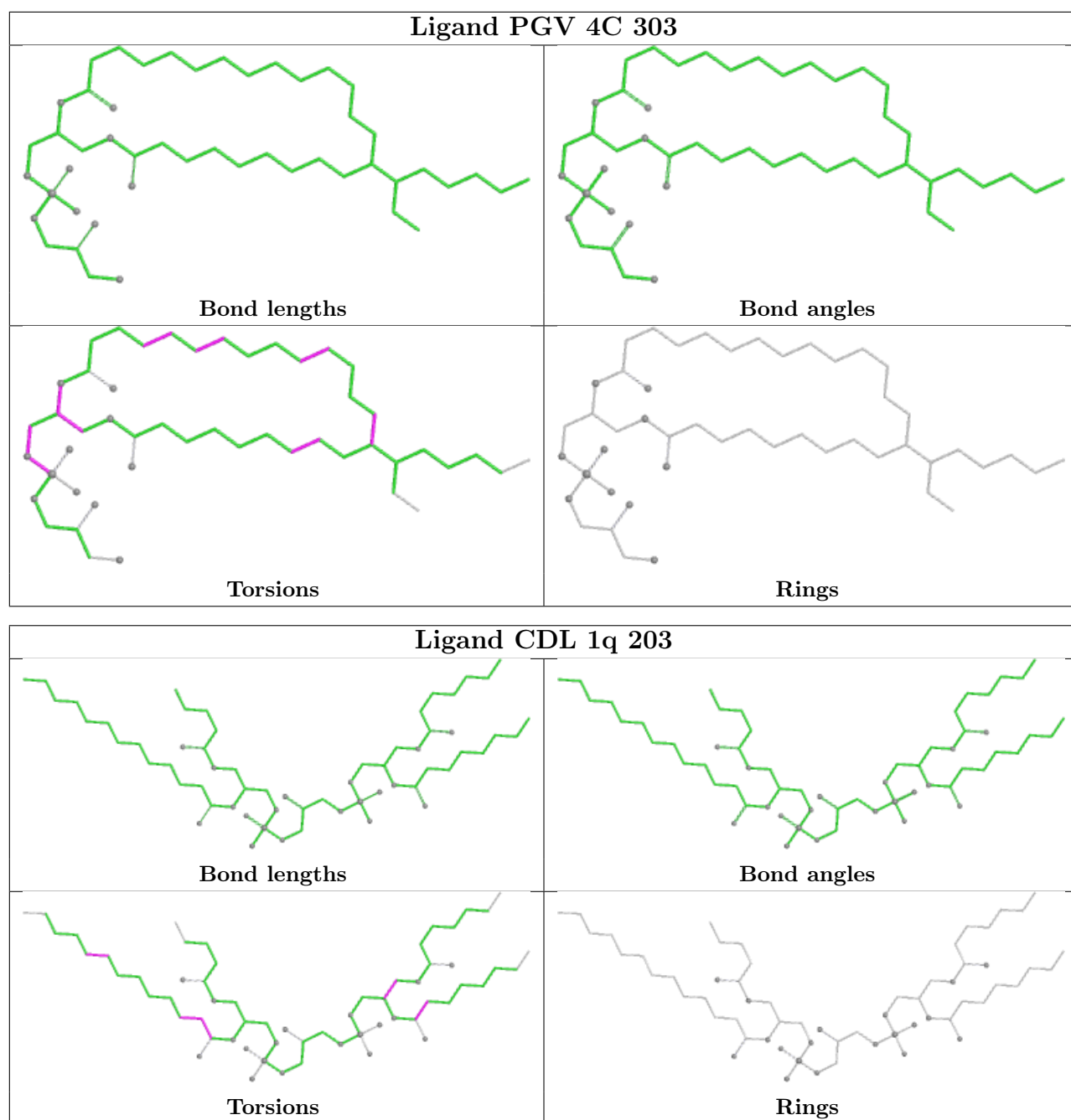


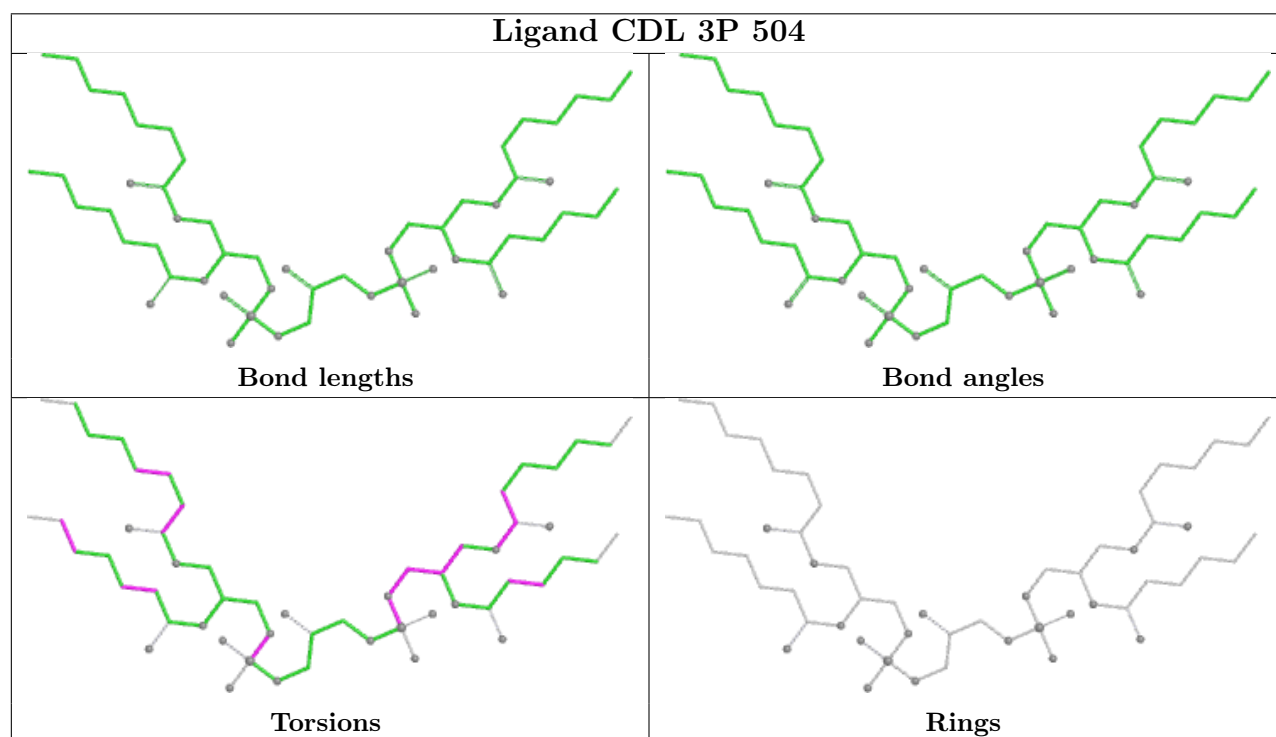
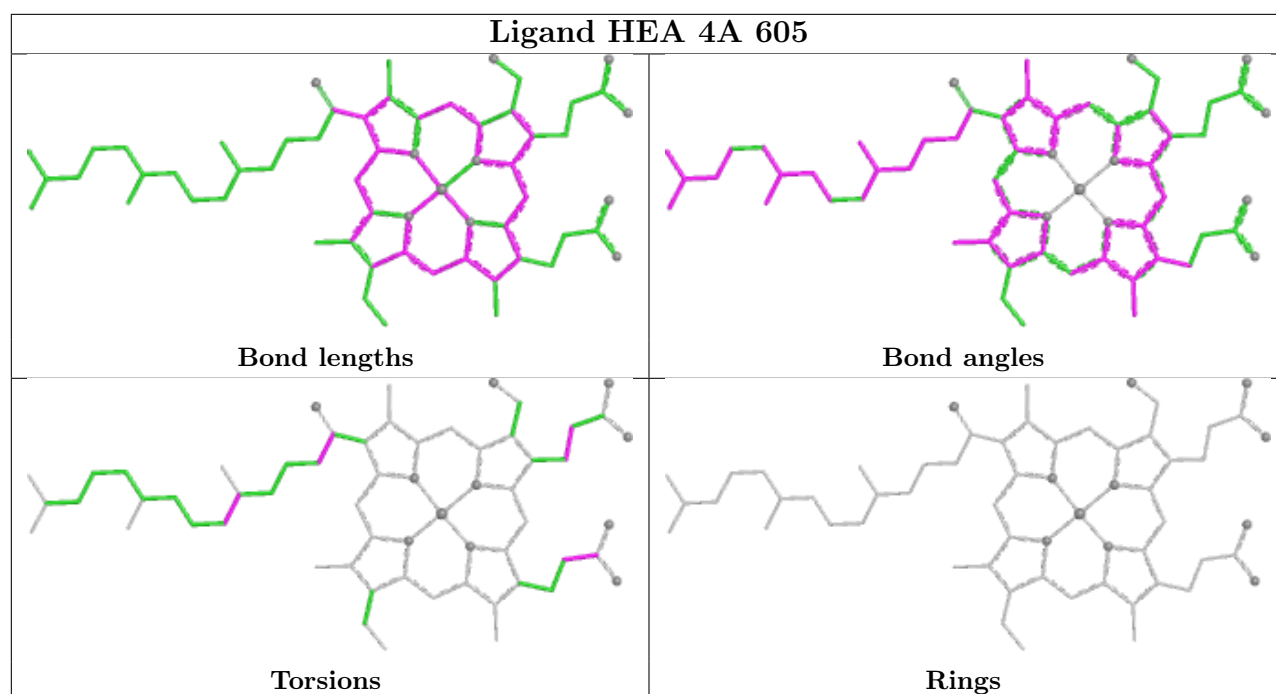
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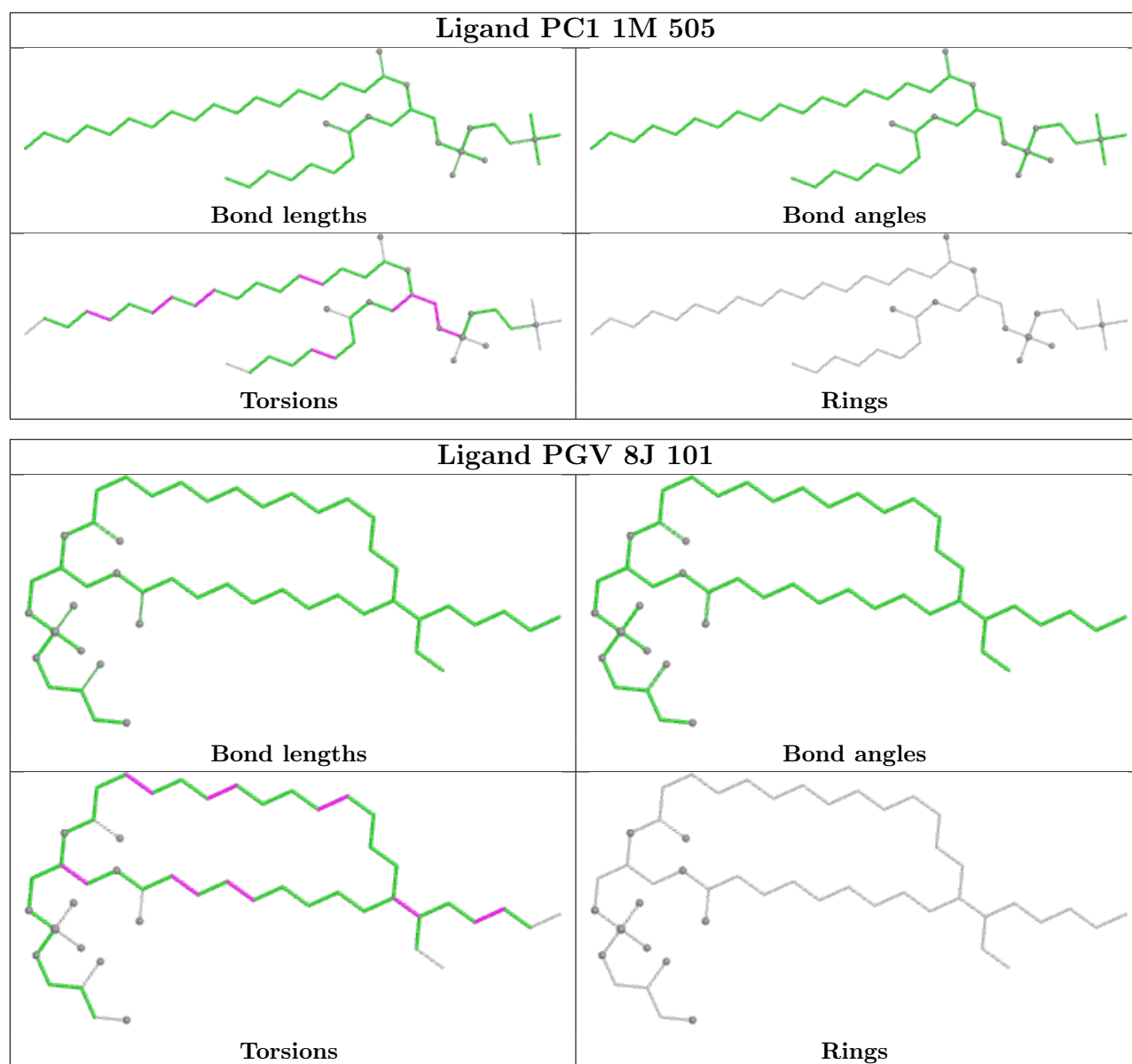


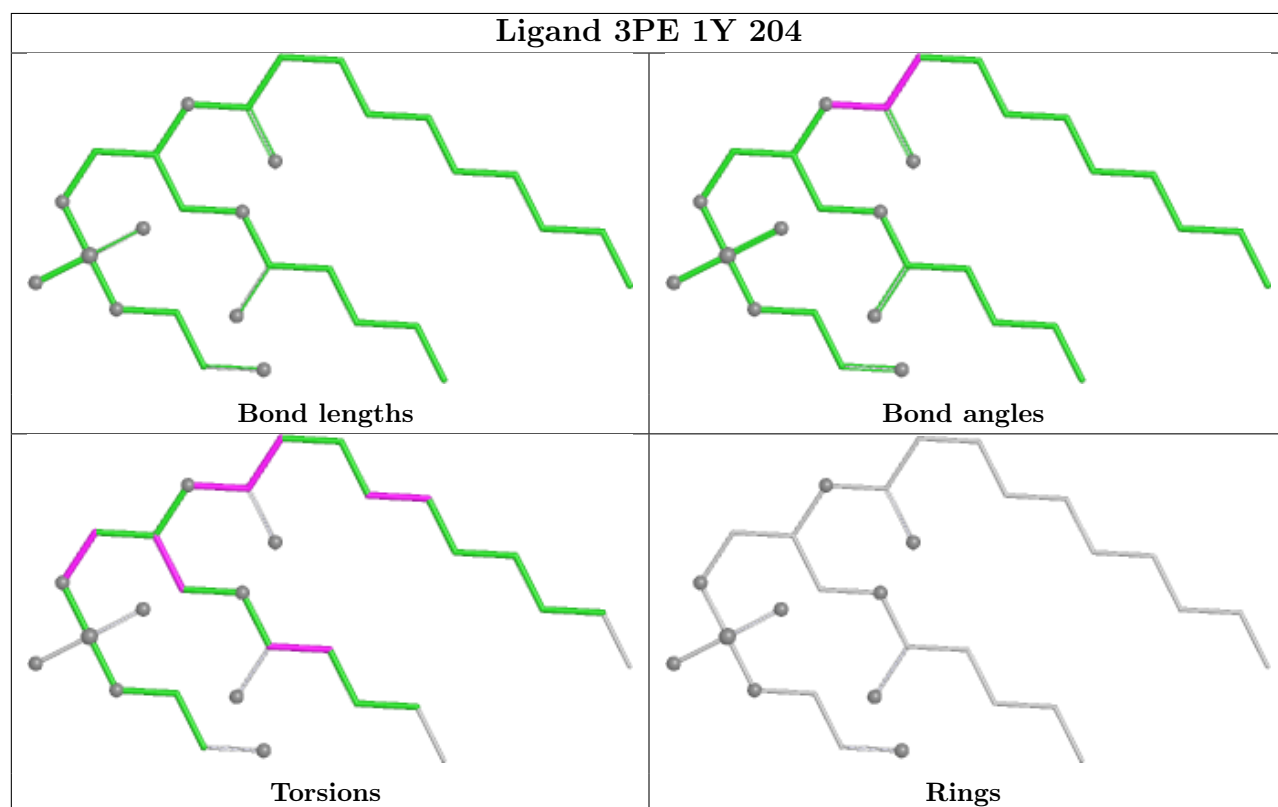
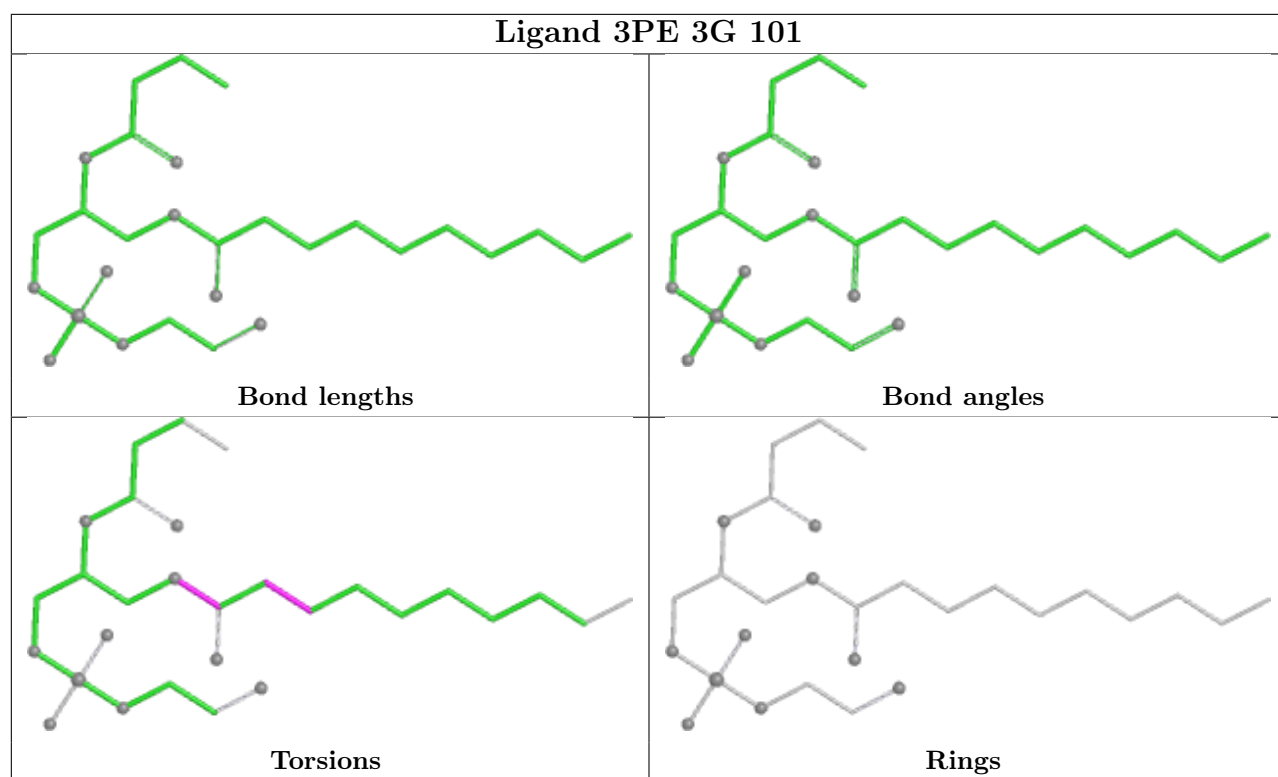
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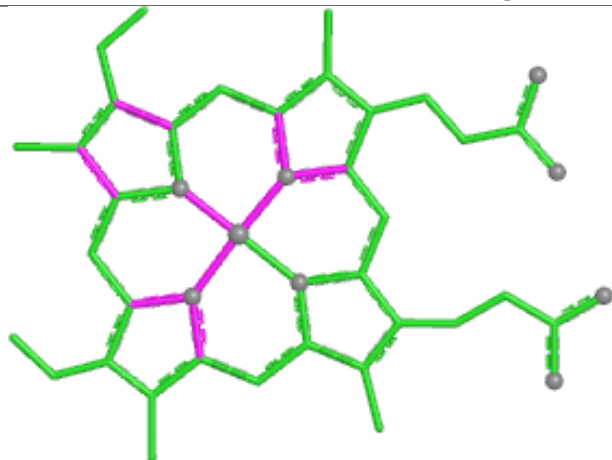




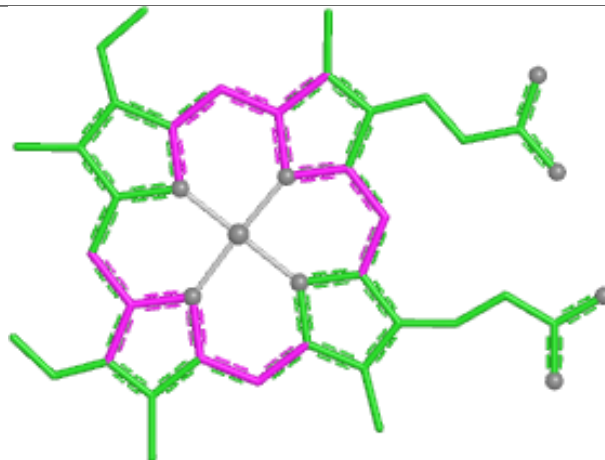




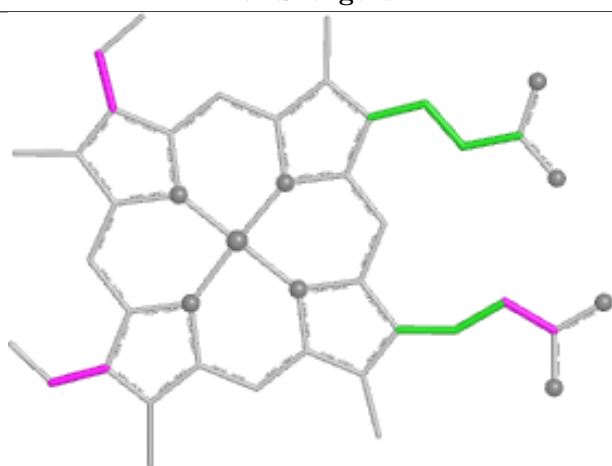
Ligand HEM 3C 502



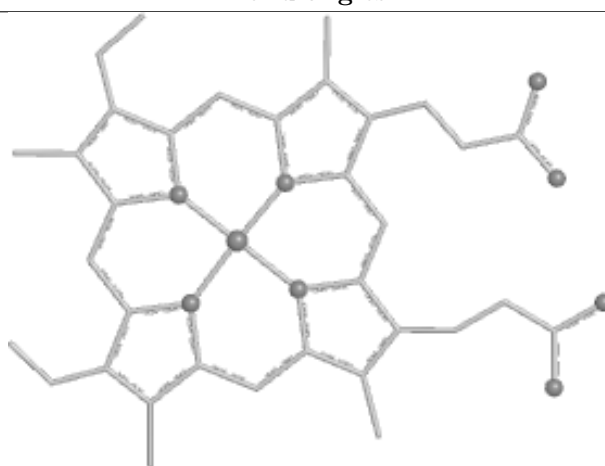
Bond lengths



Bond angles

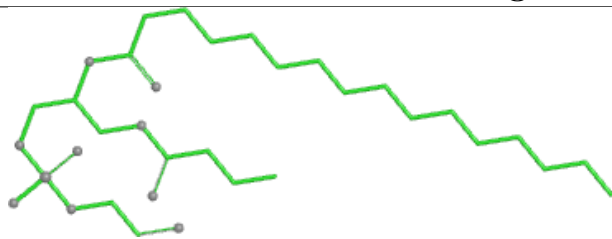


Torsions

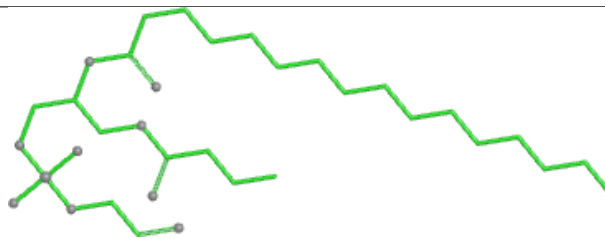


Rings

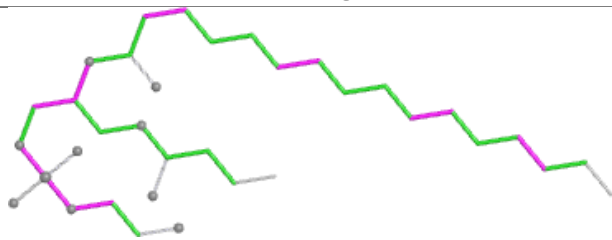
Ligand 3PE 3C 503



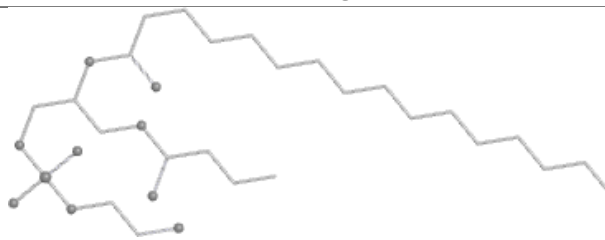
Bond lengths



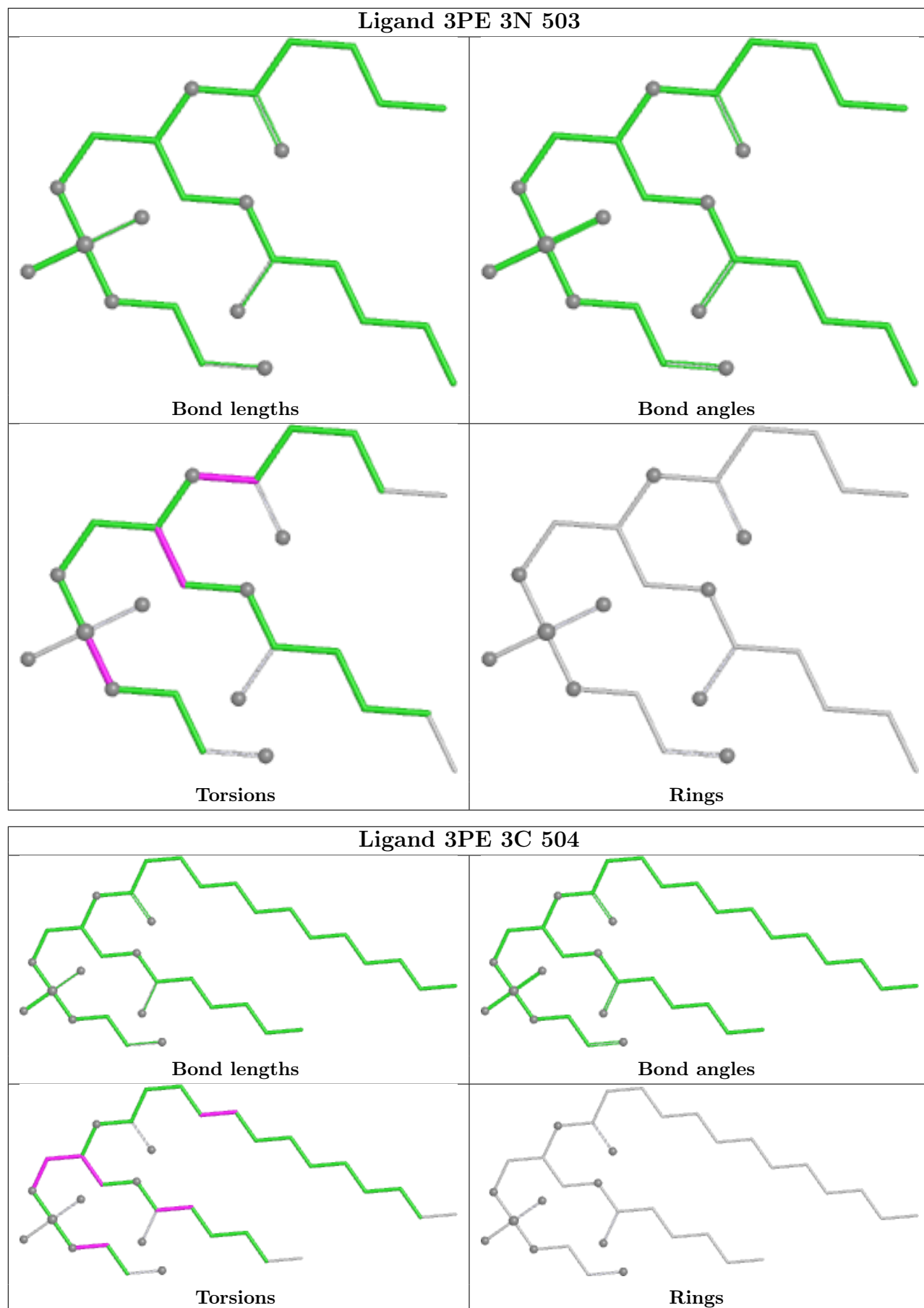
Bond angles

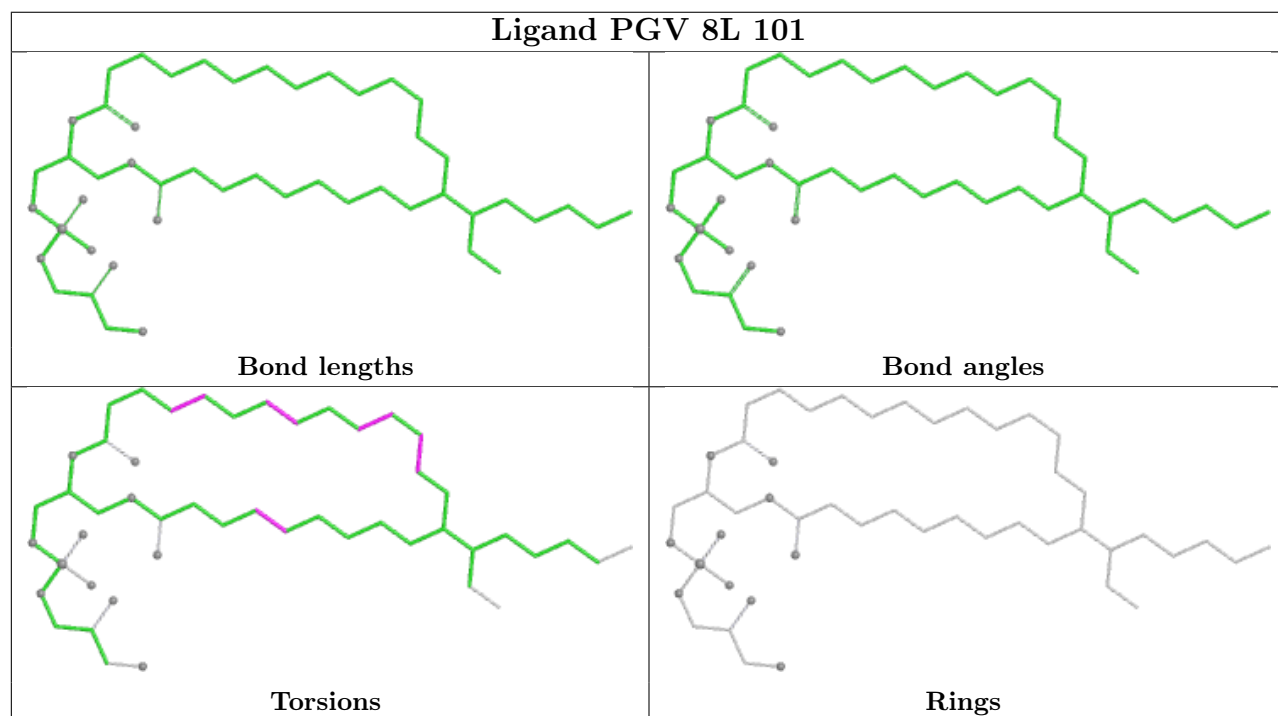
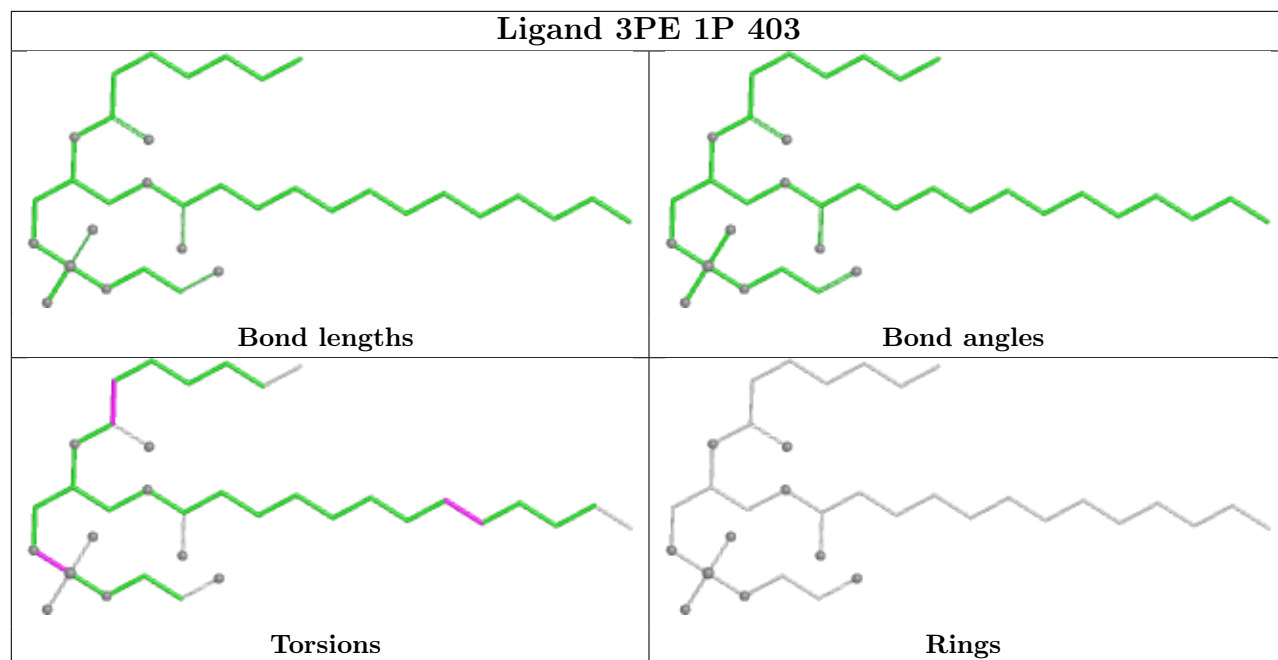


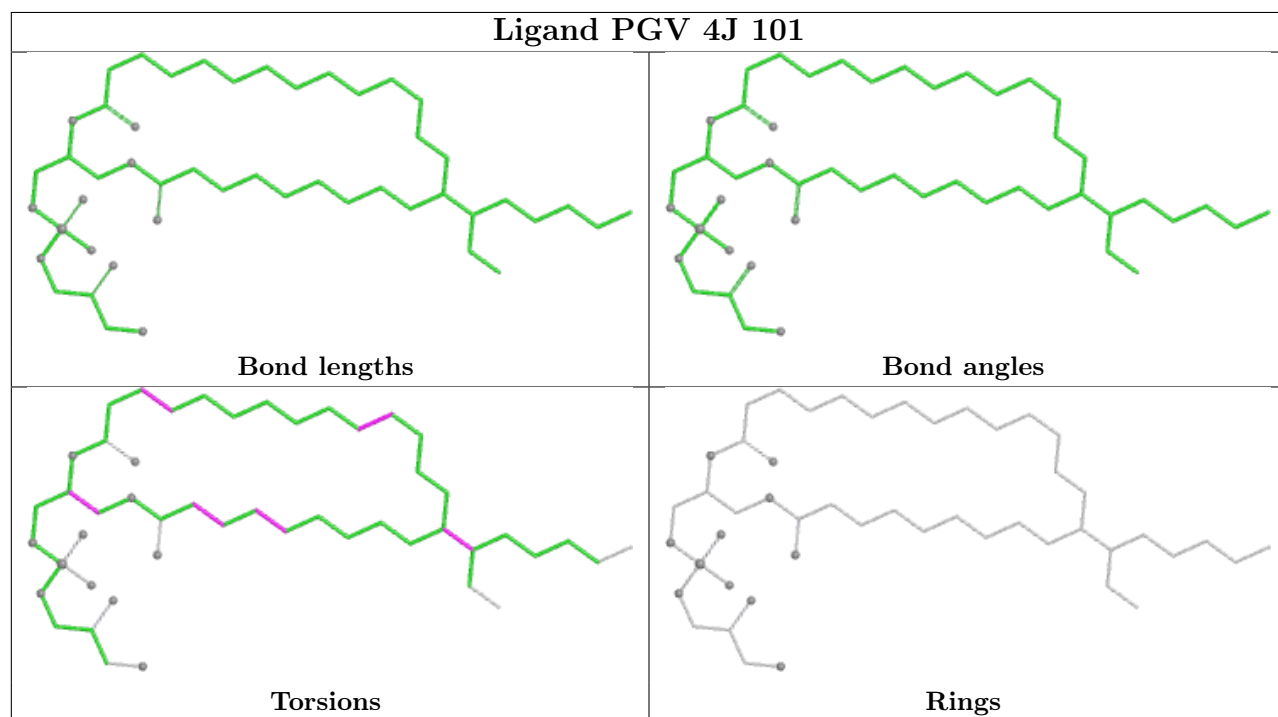
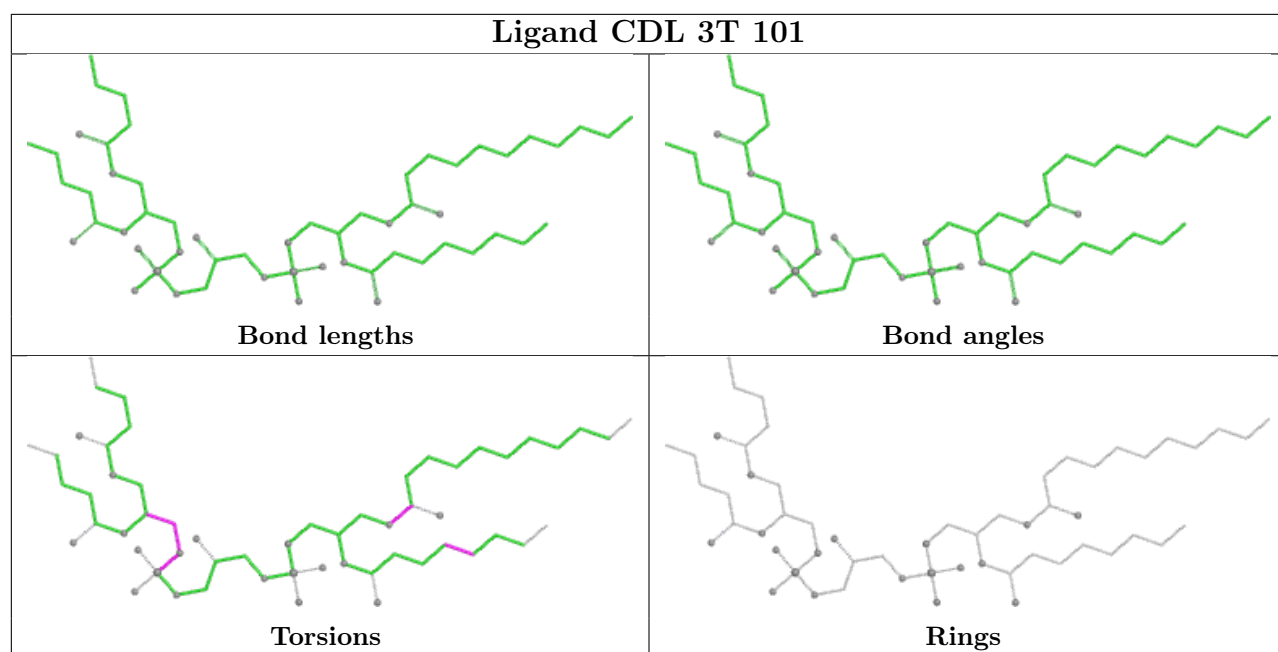
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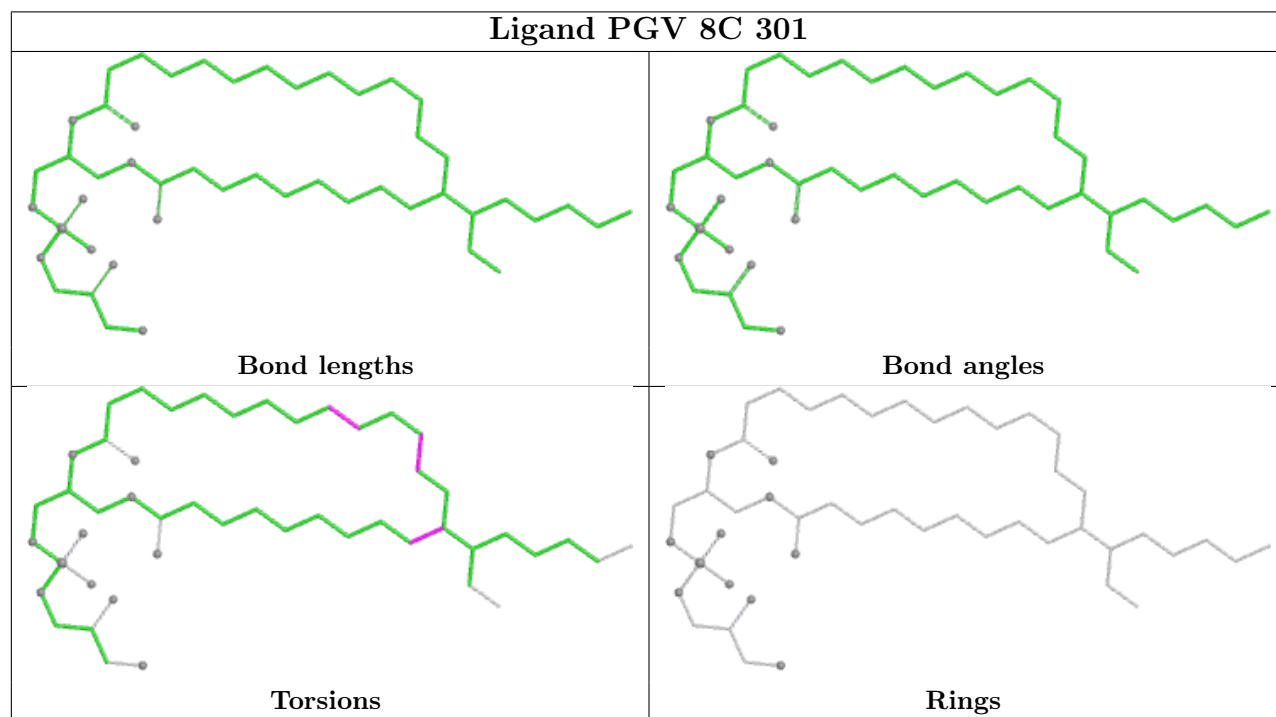
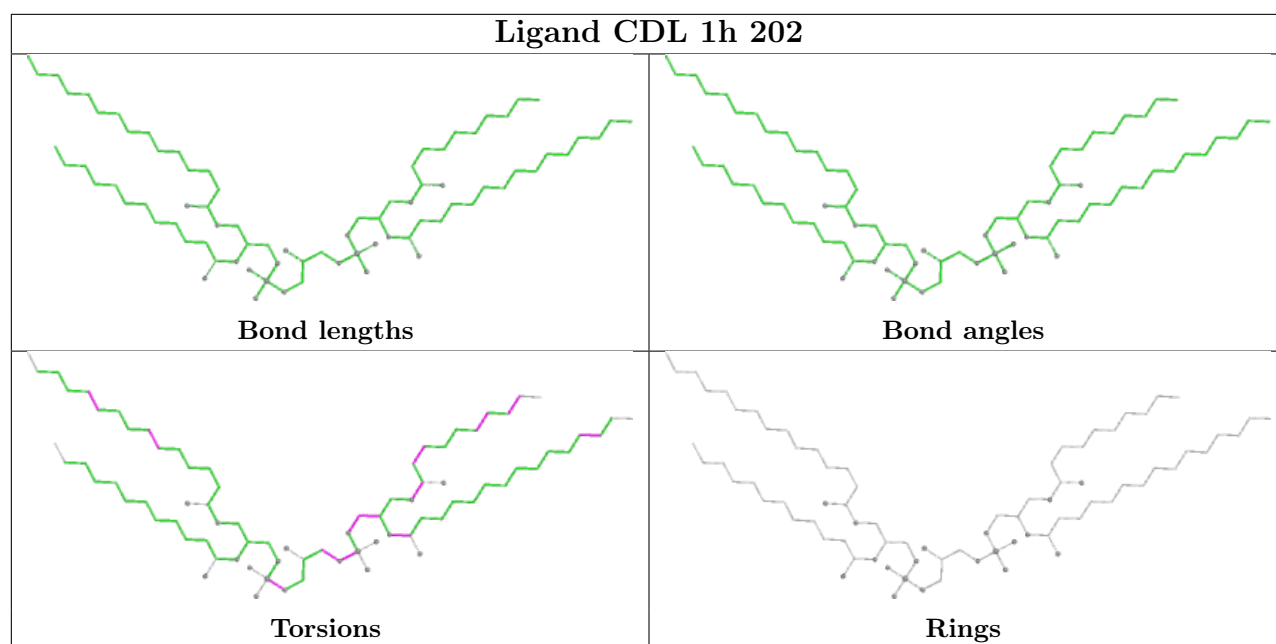


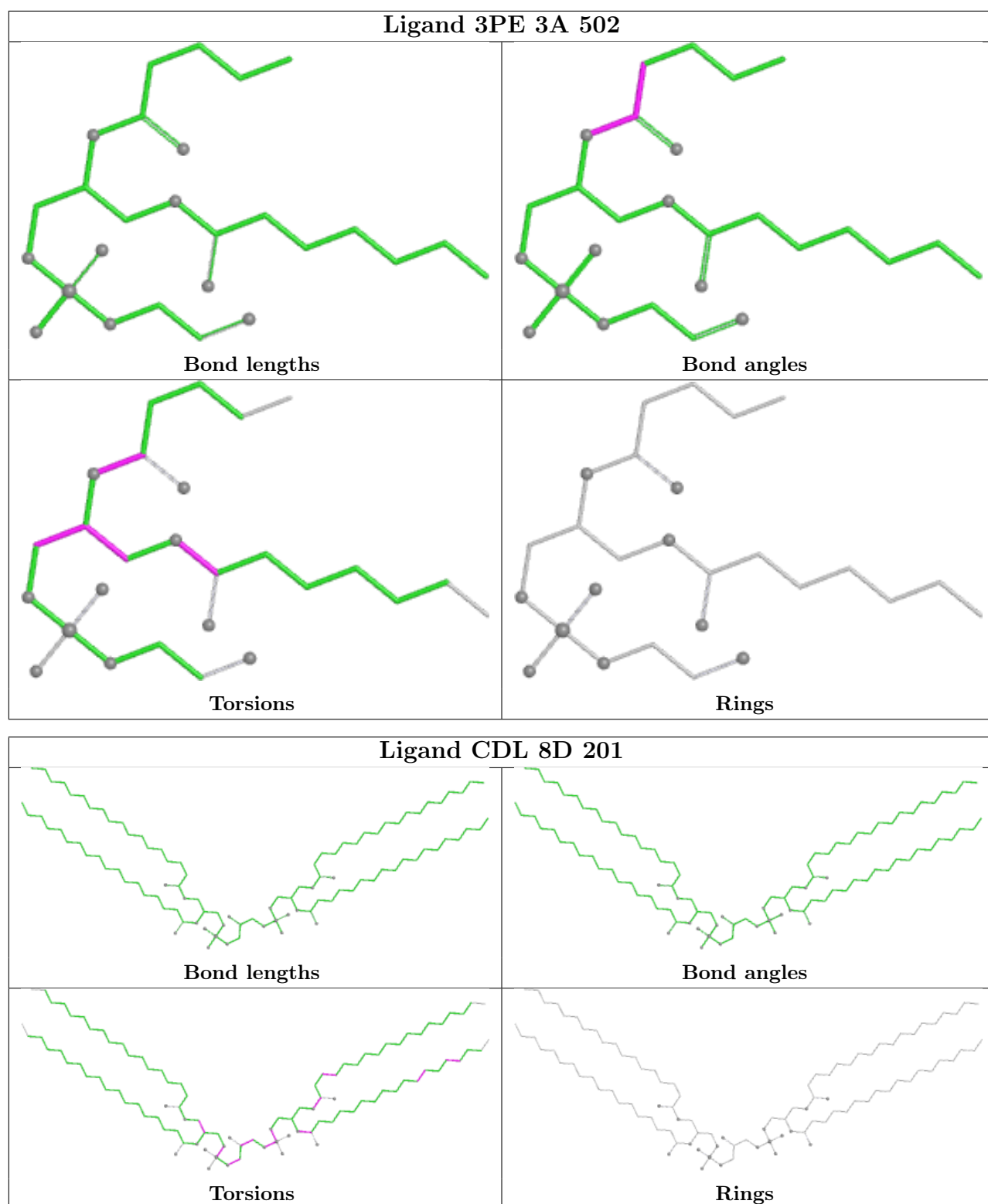
Rings

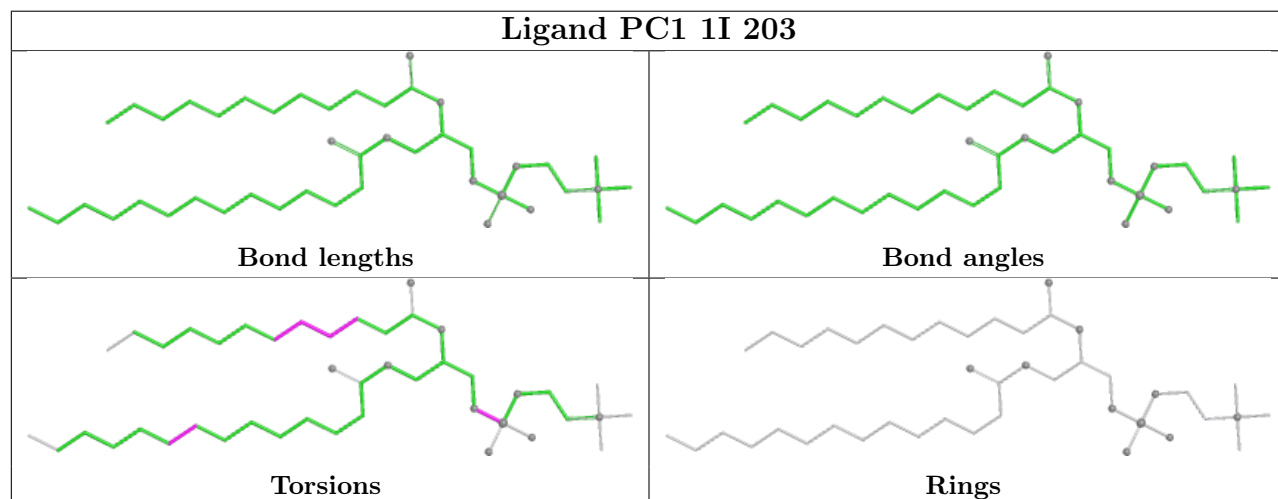
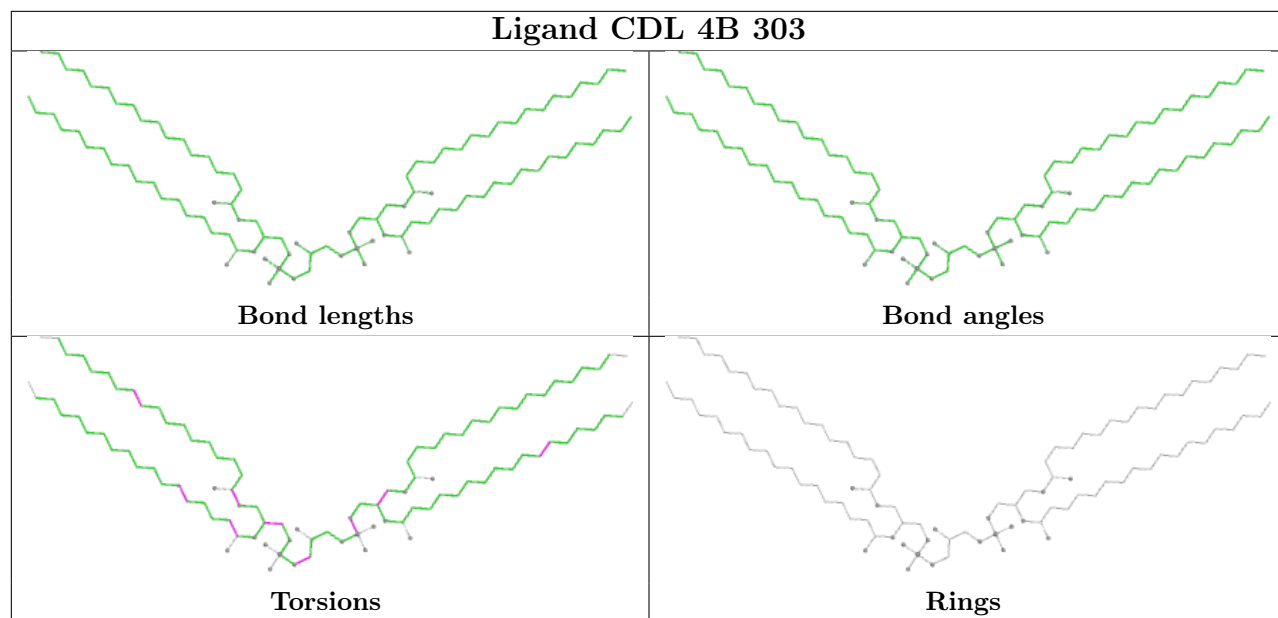


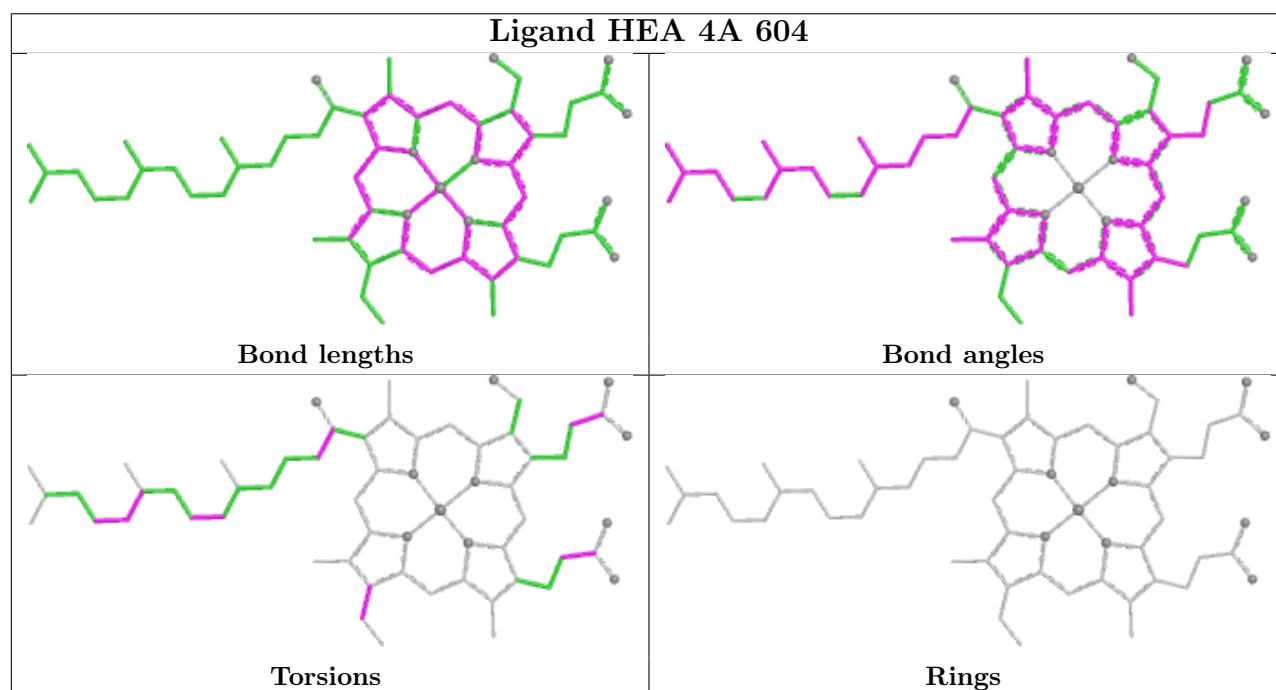
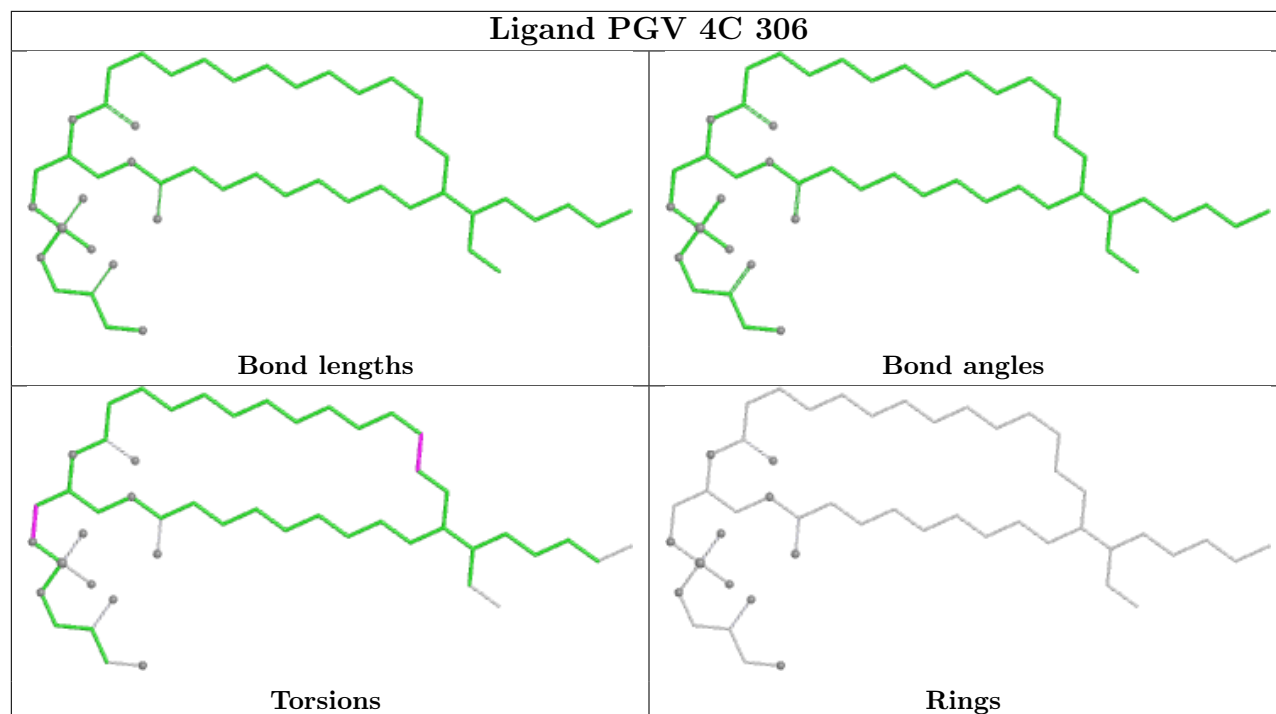


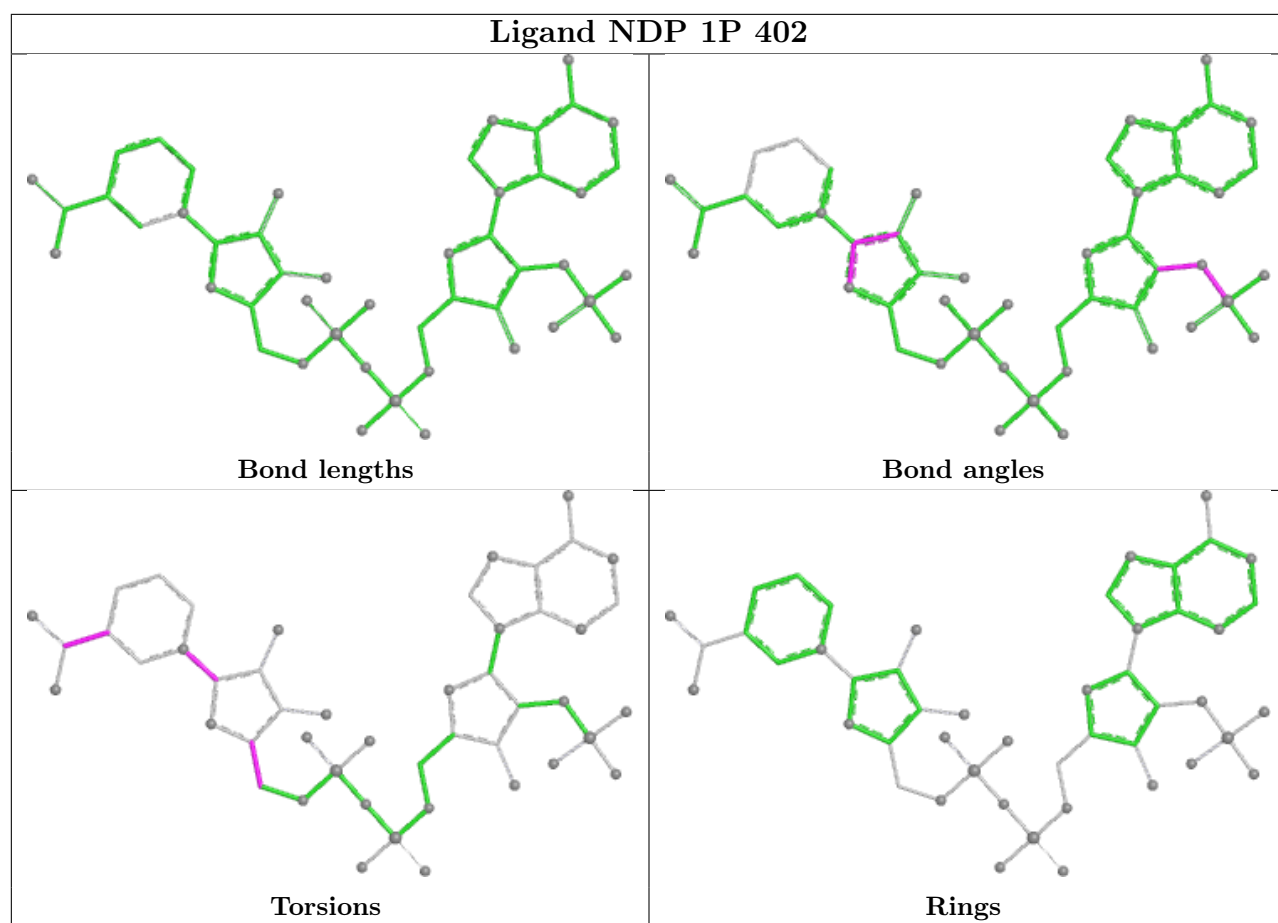




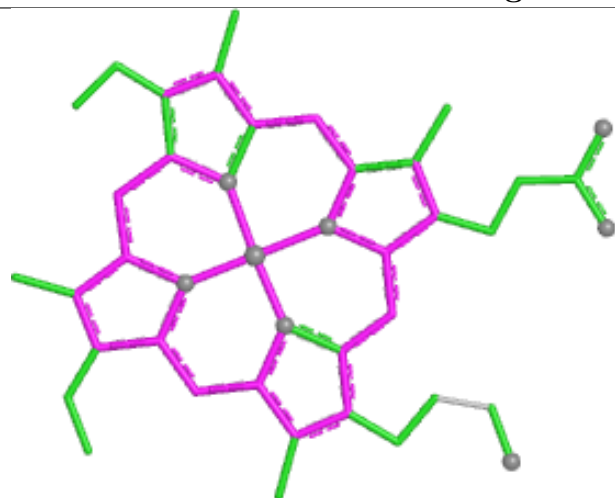




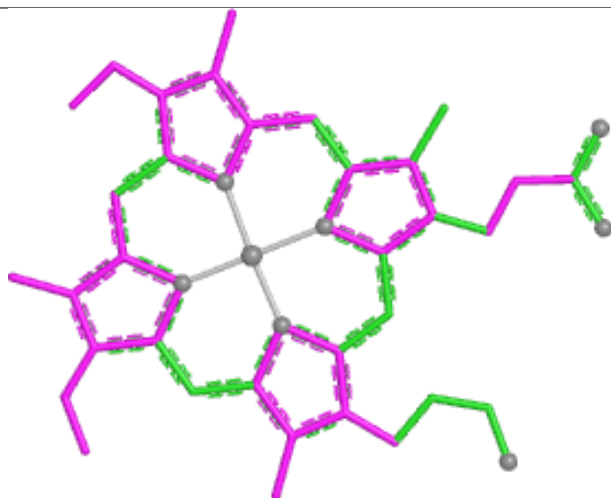




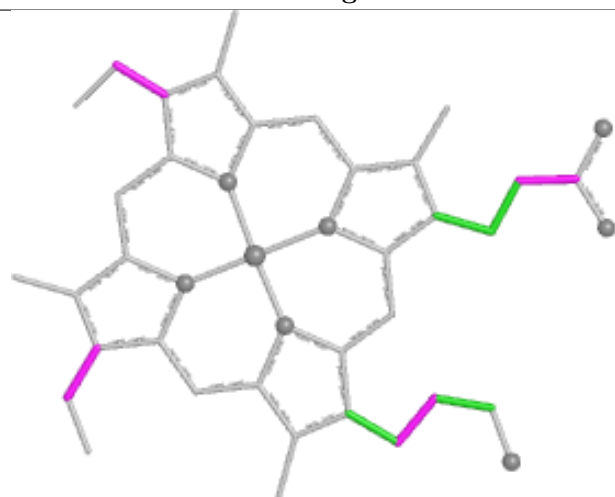
Ligand HEC 3D 501



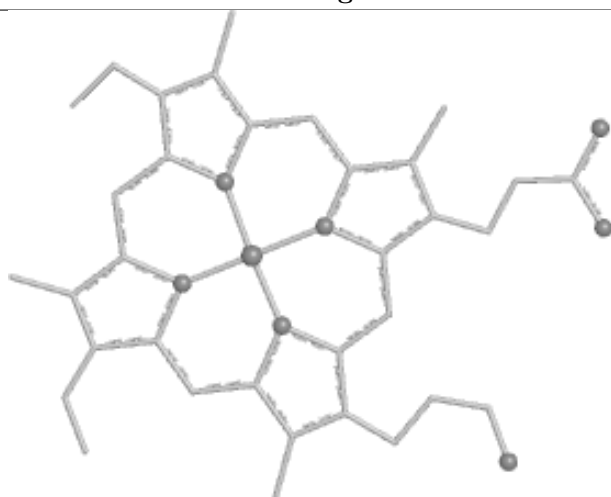
Bond lengths



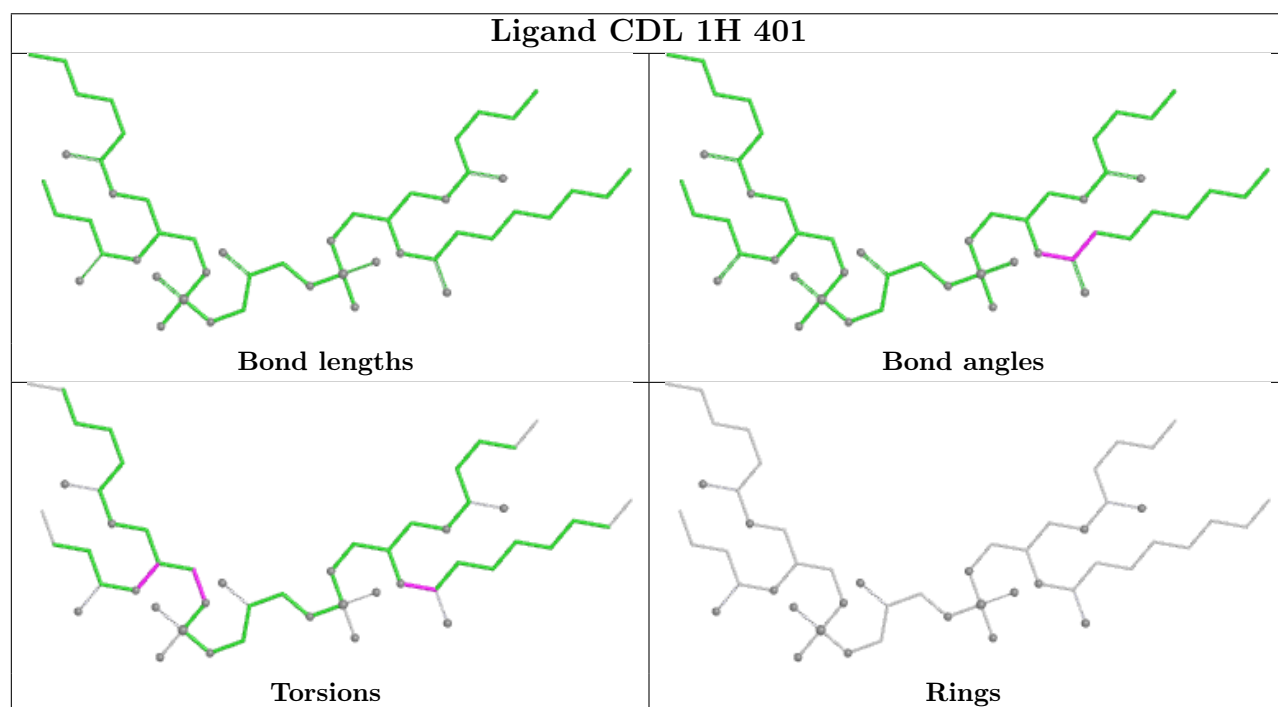
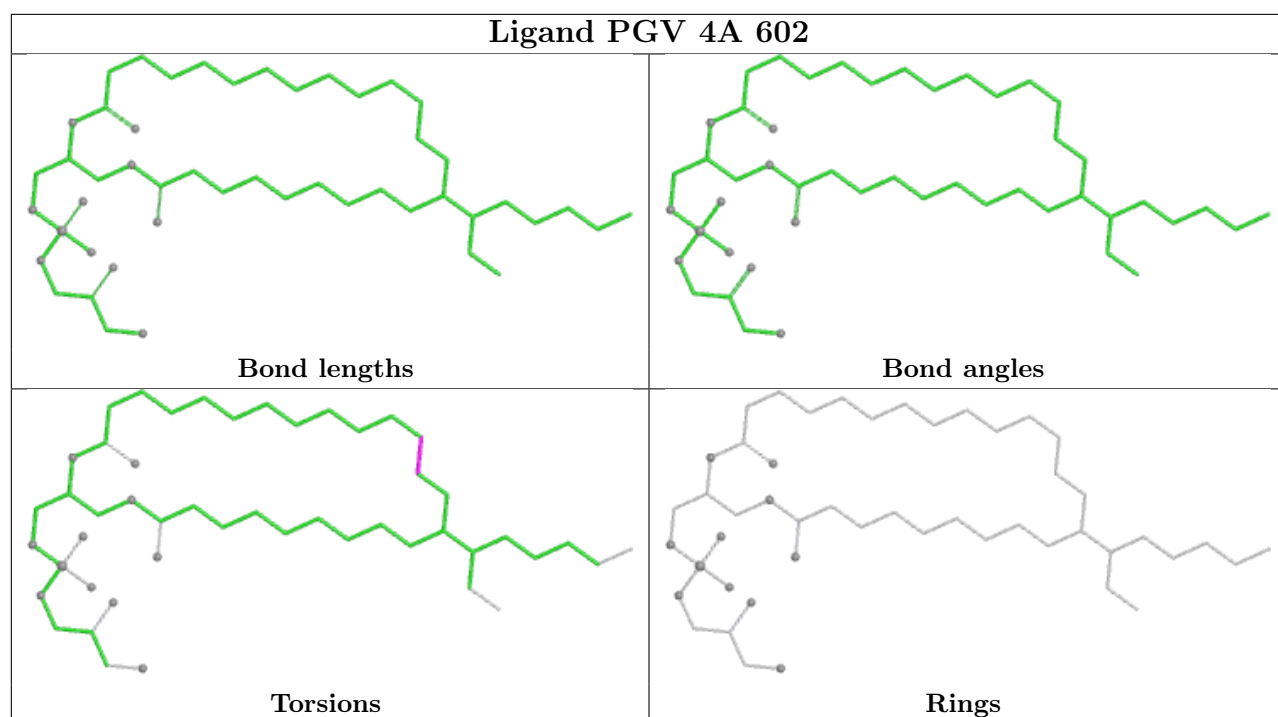
Bond angles

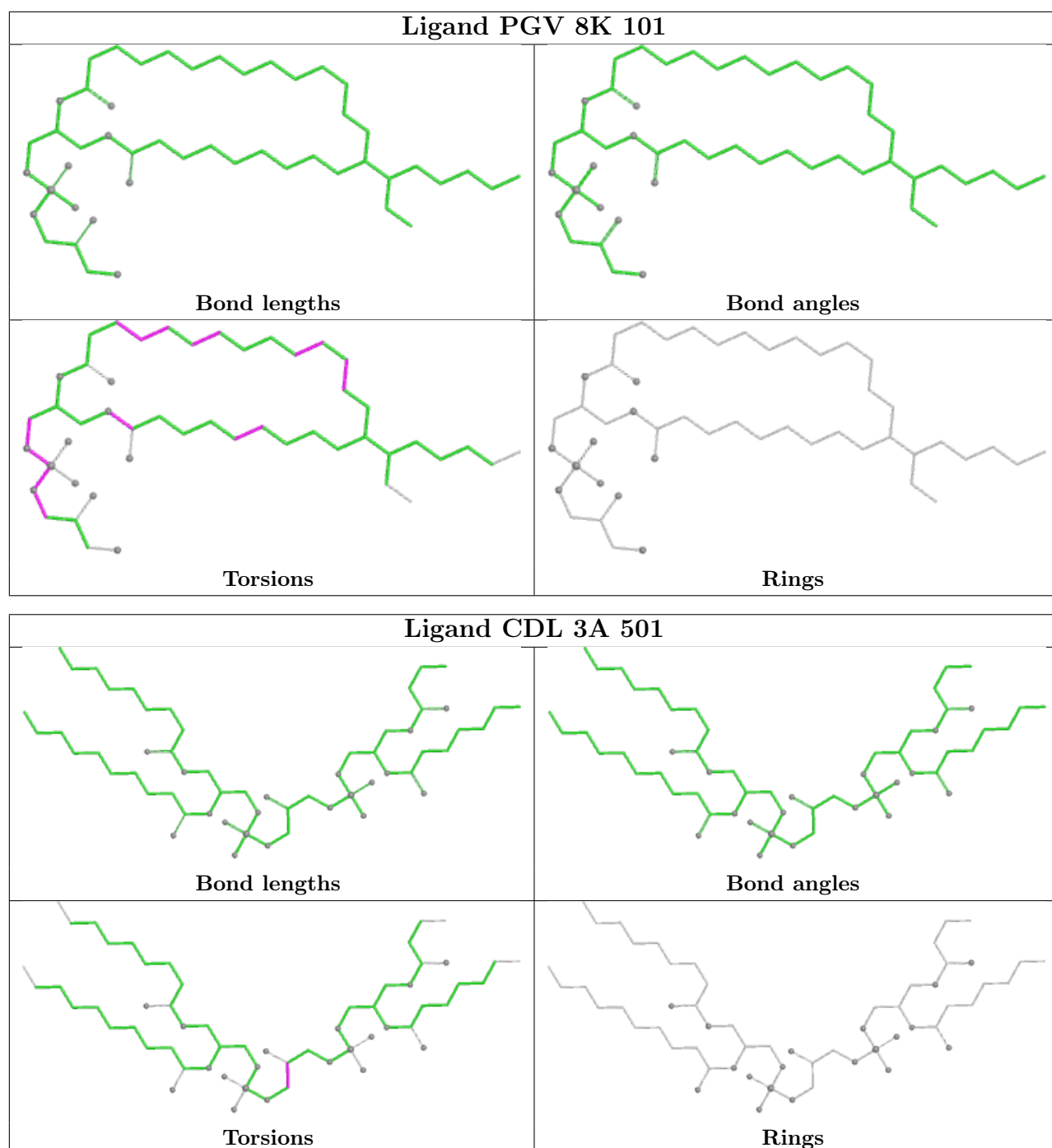


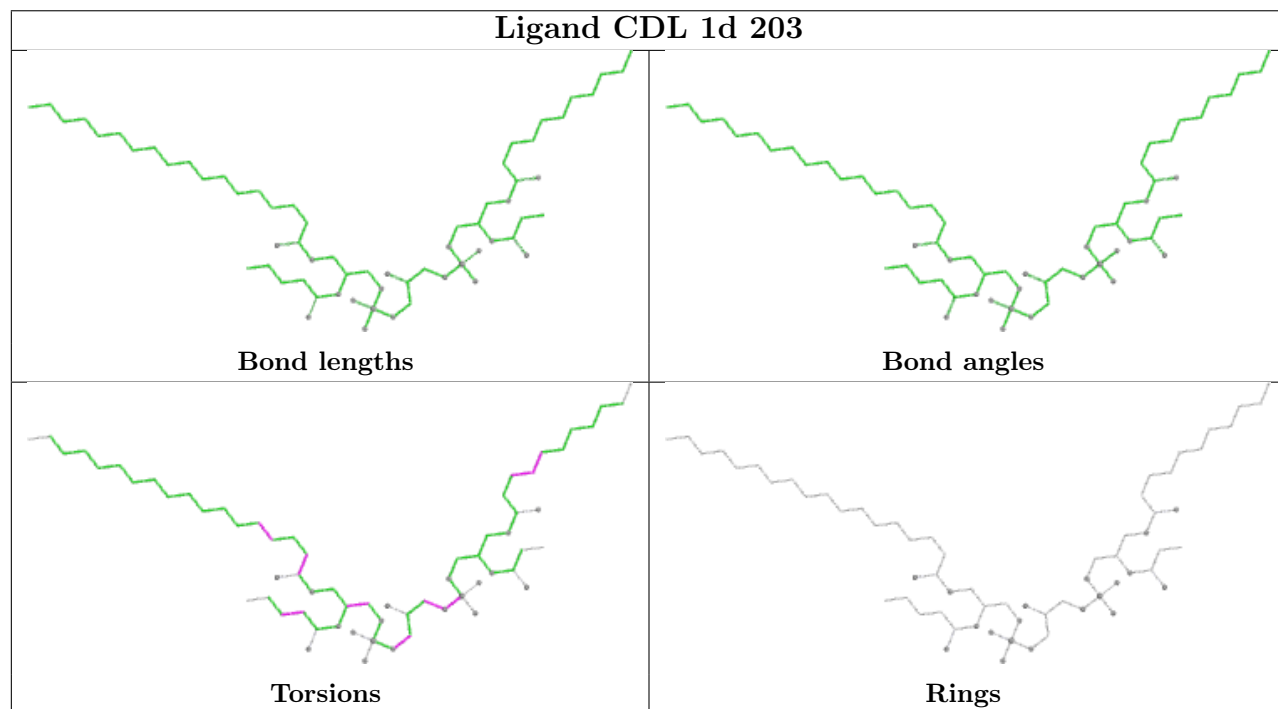
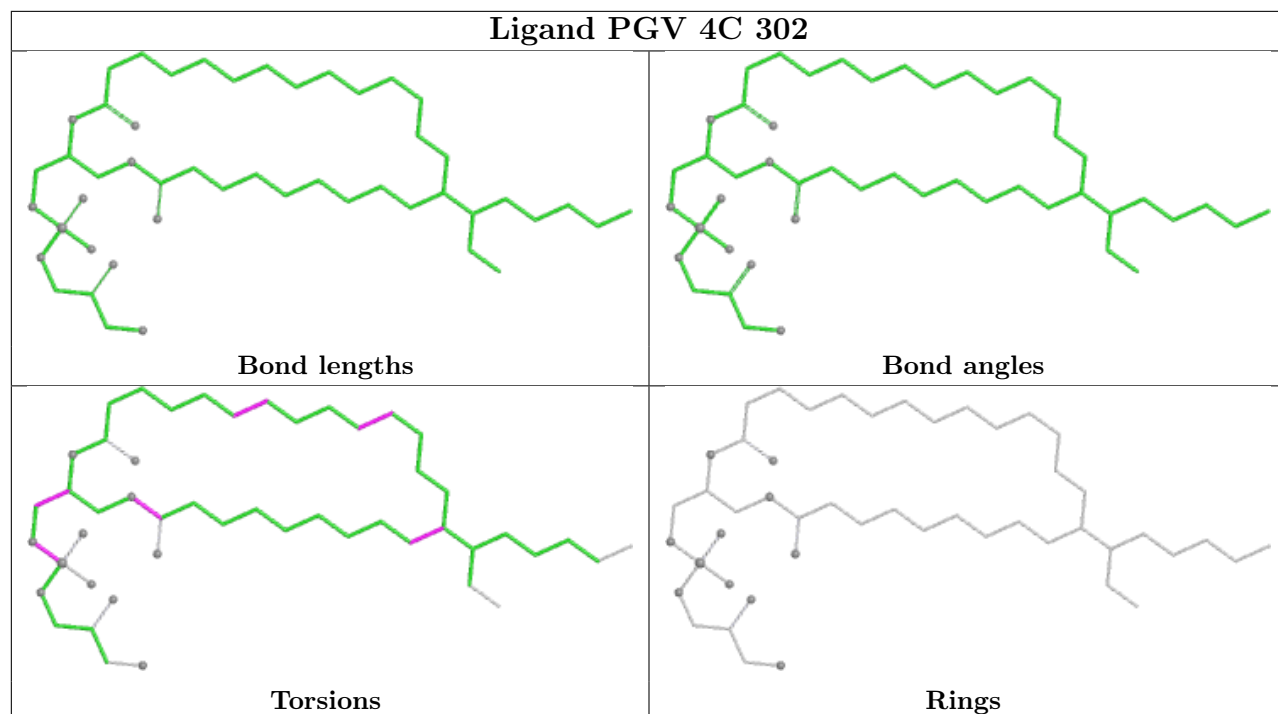
Torsions

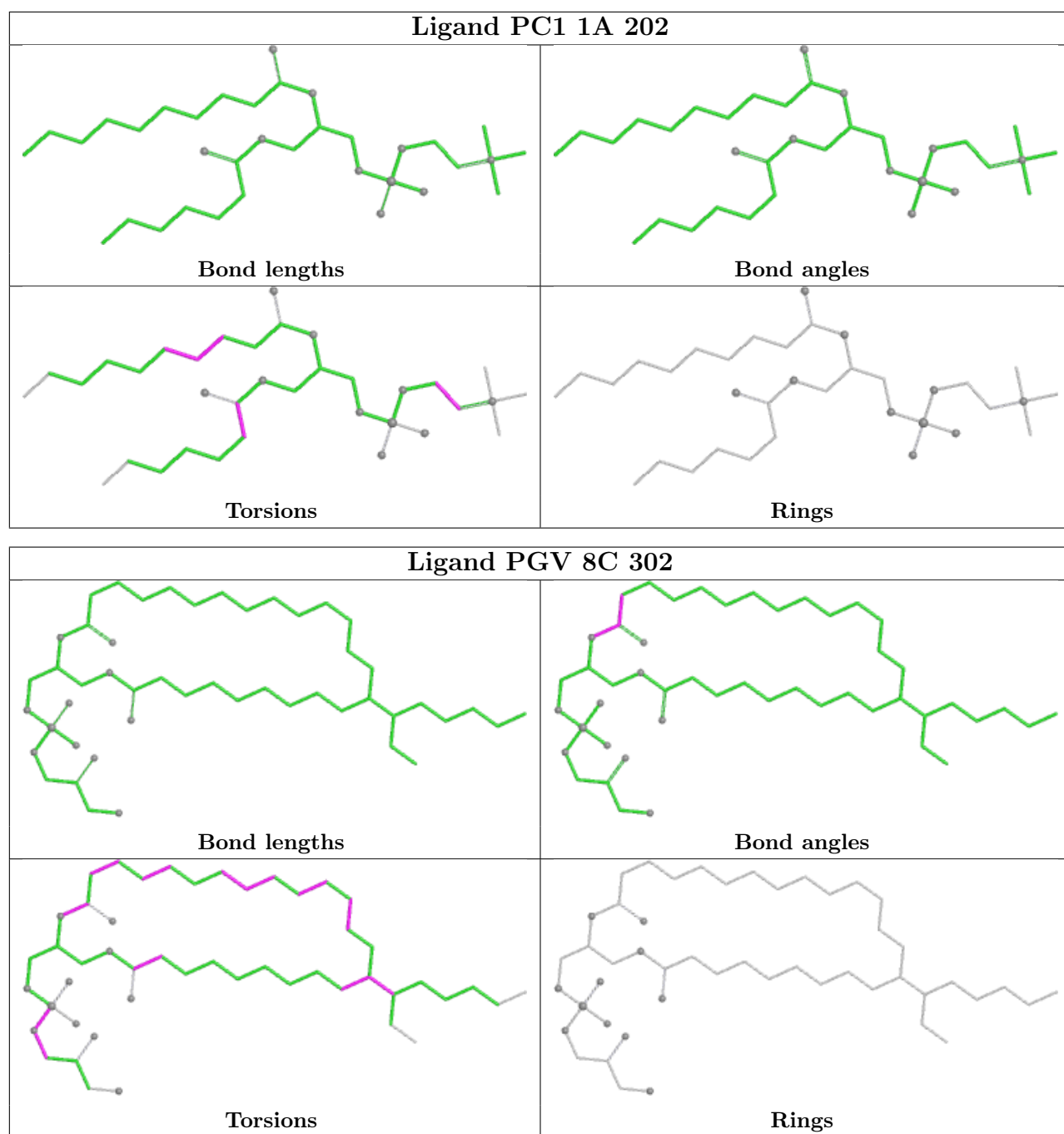


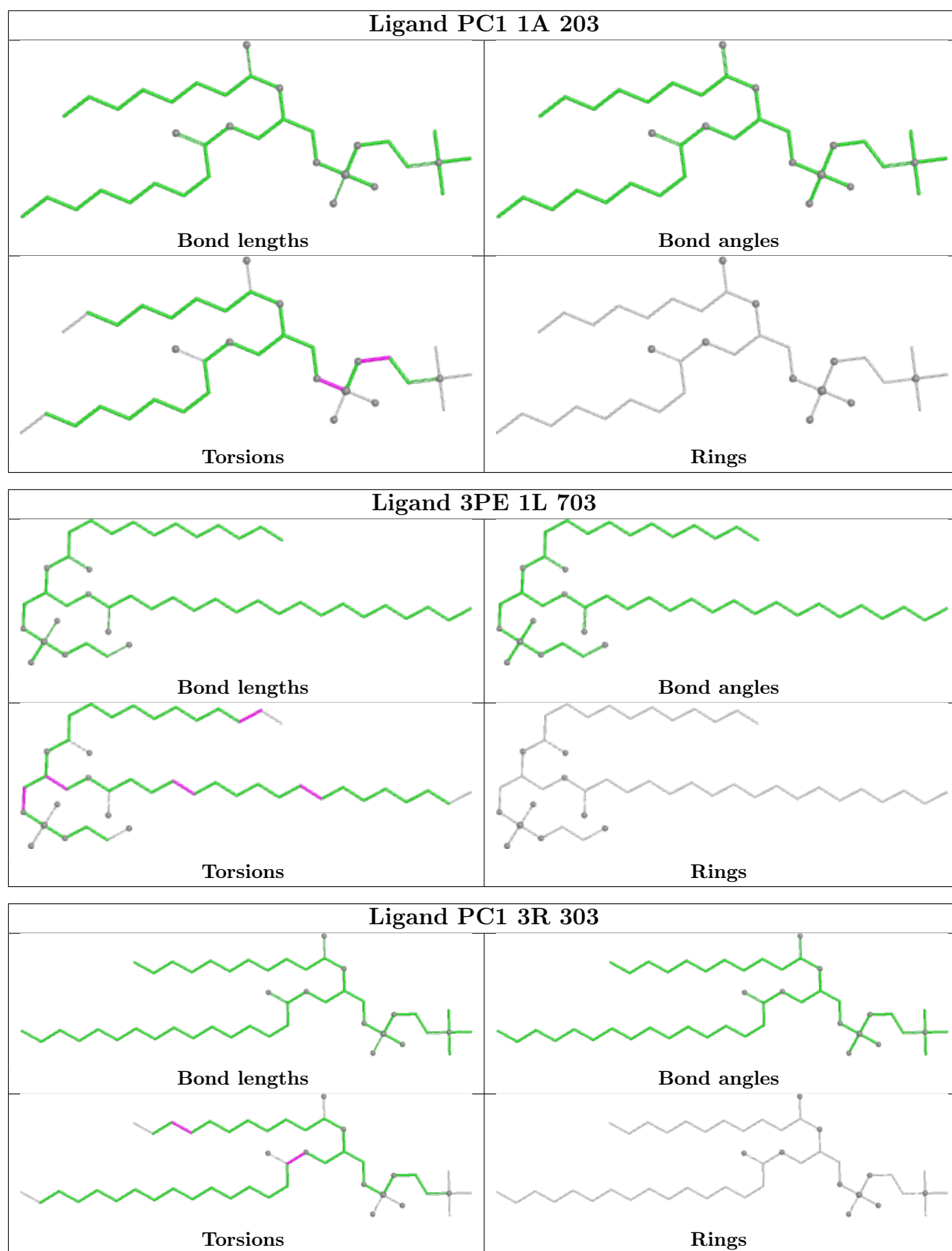
Rings

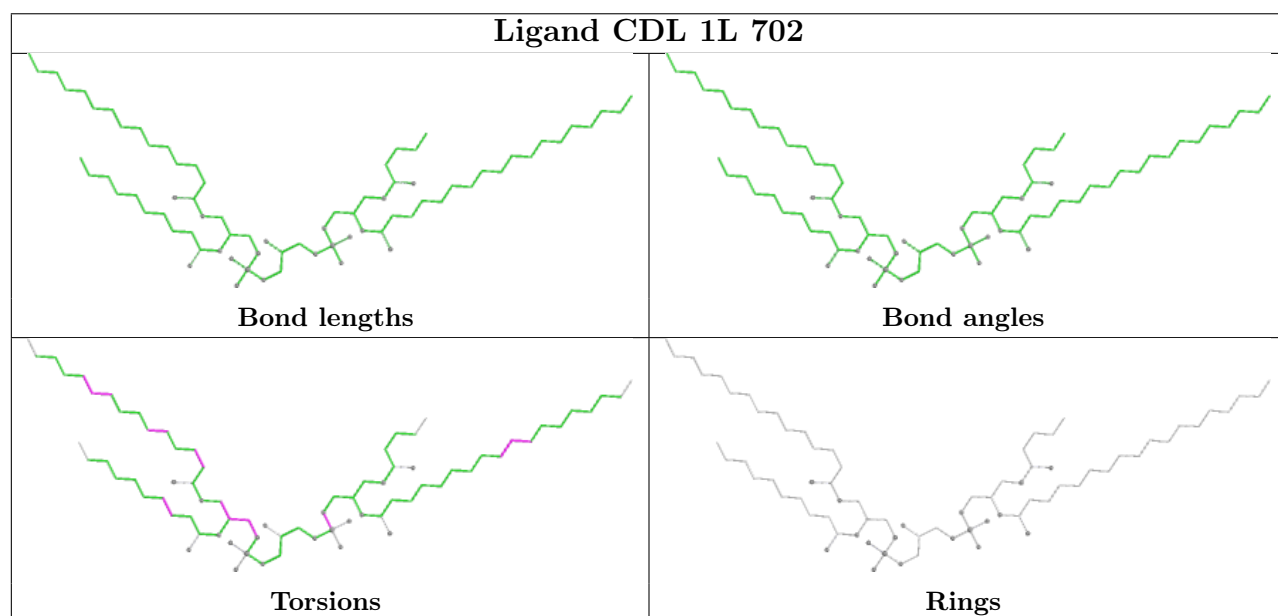
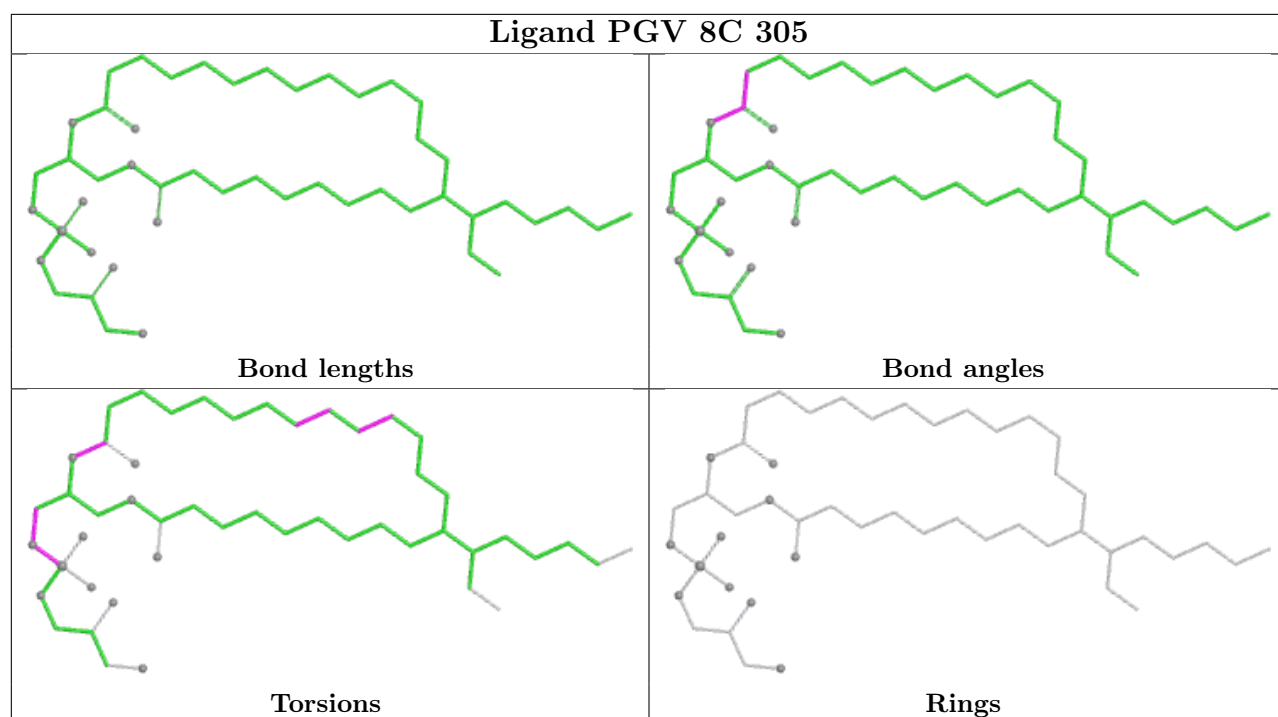


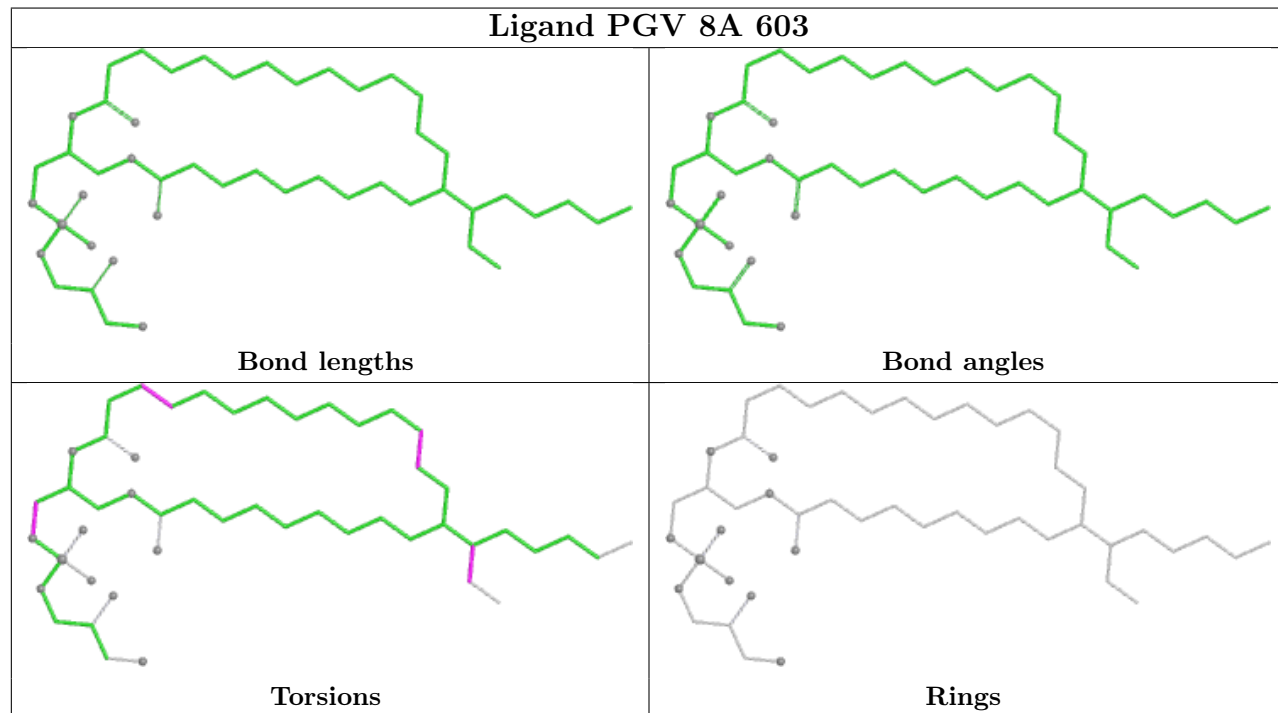
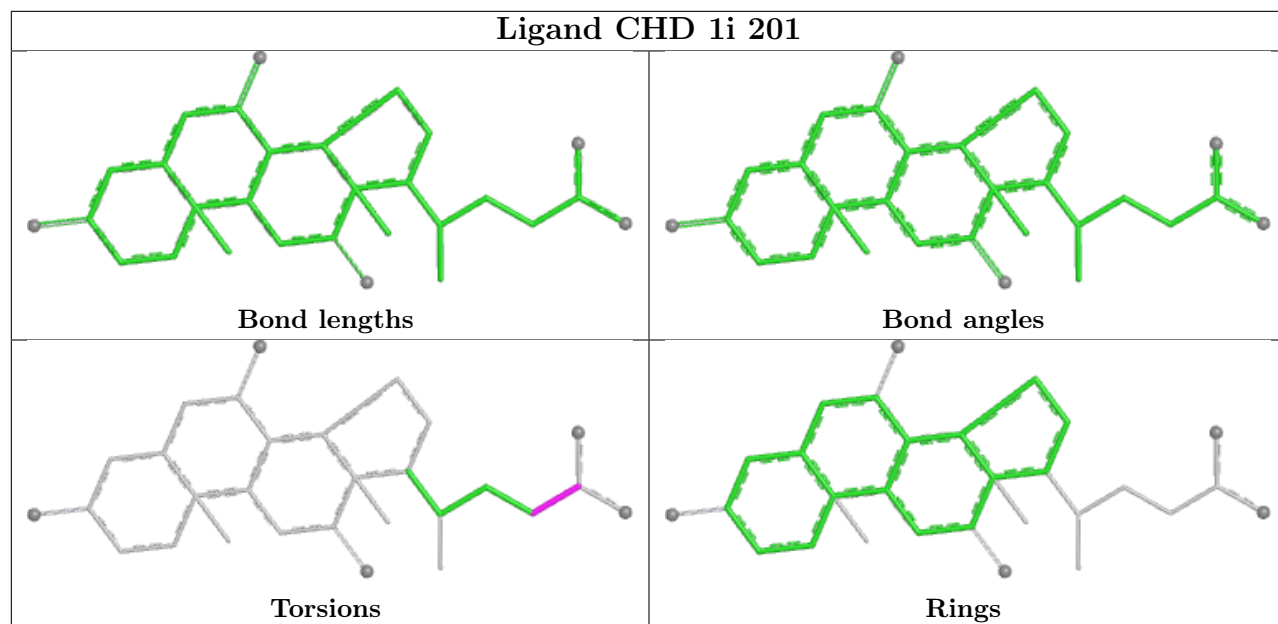


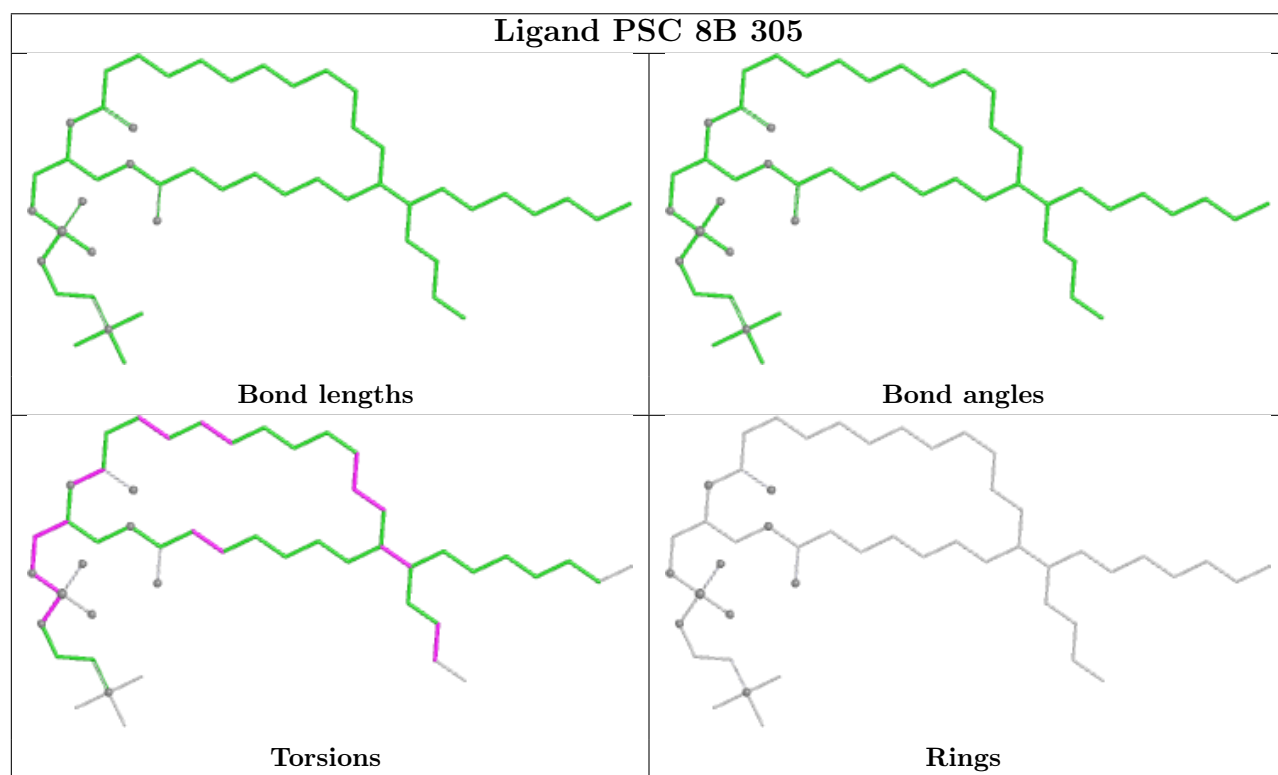
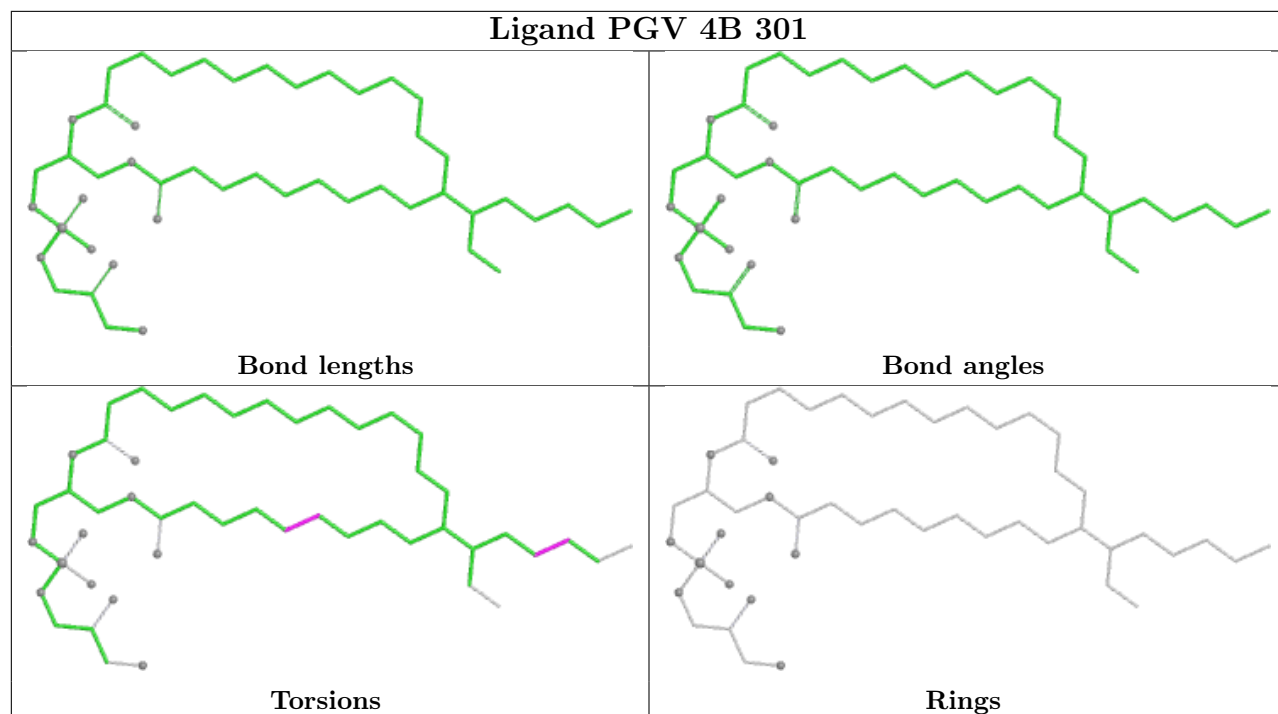


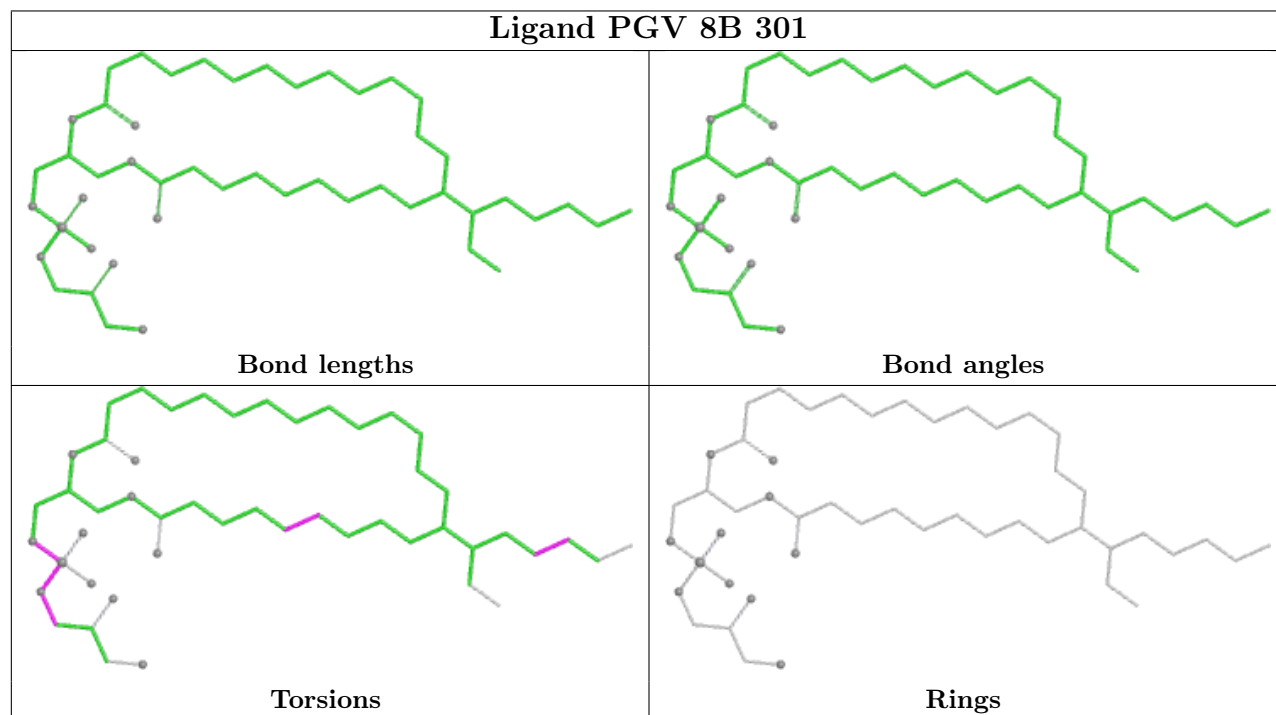
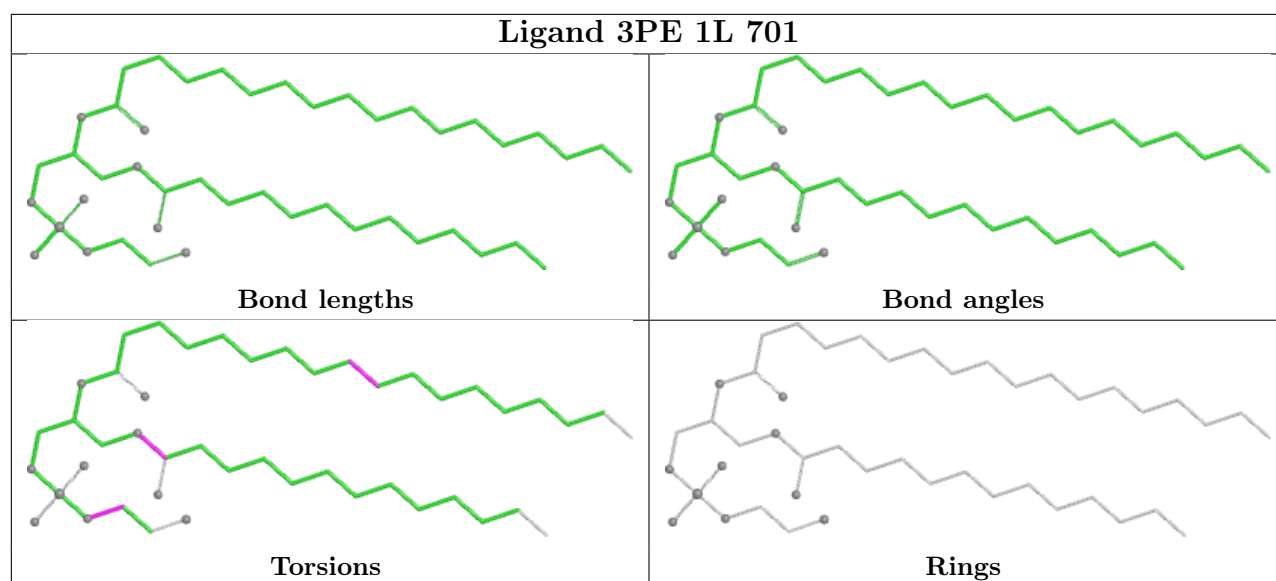


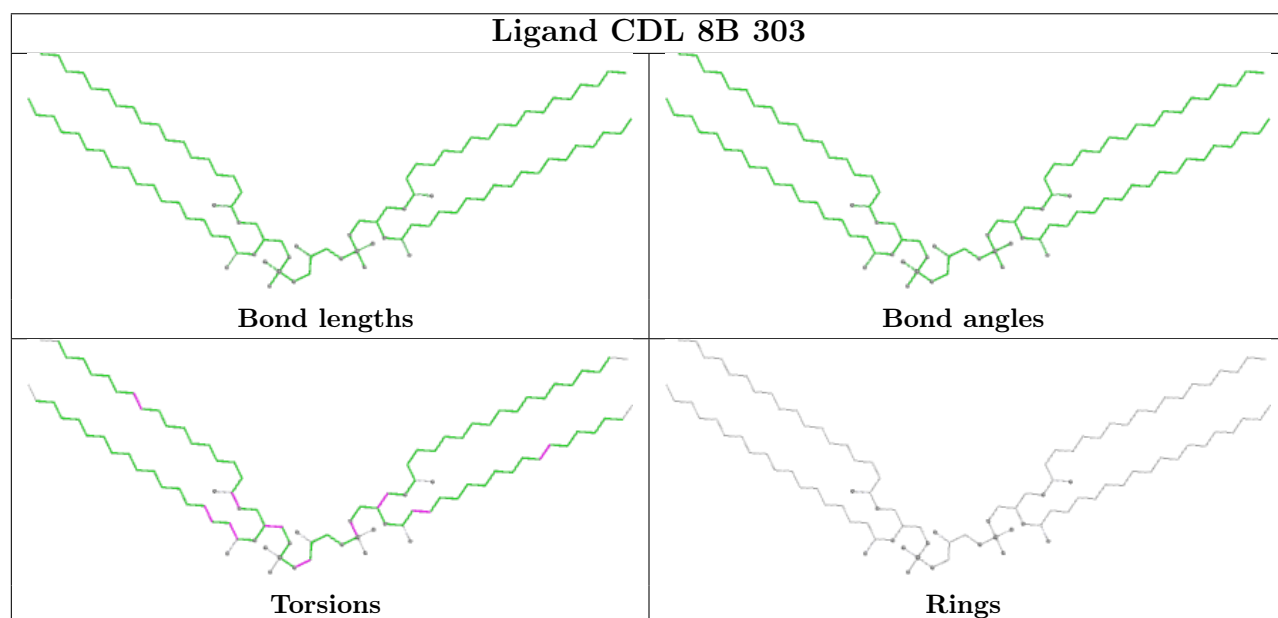
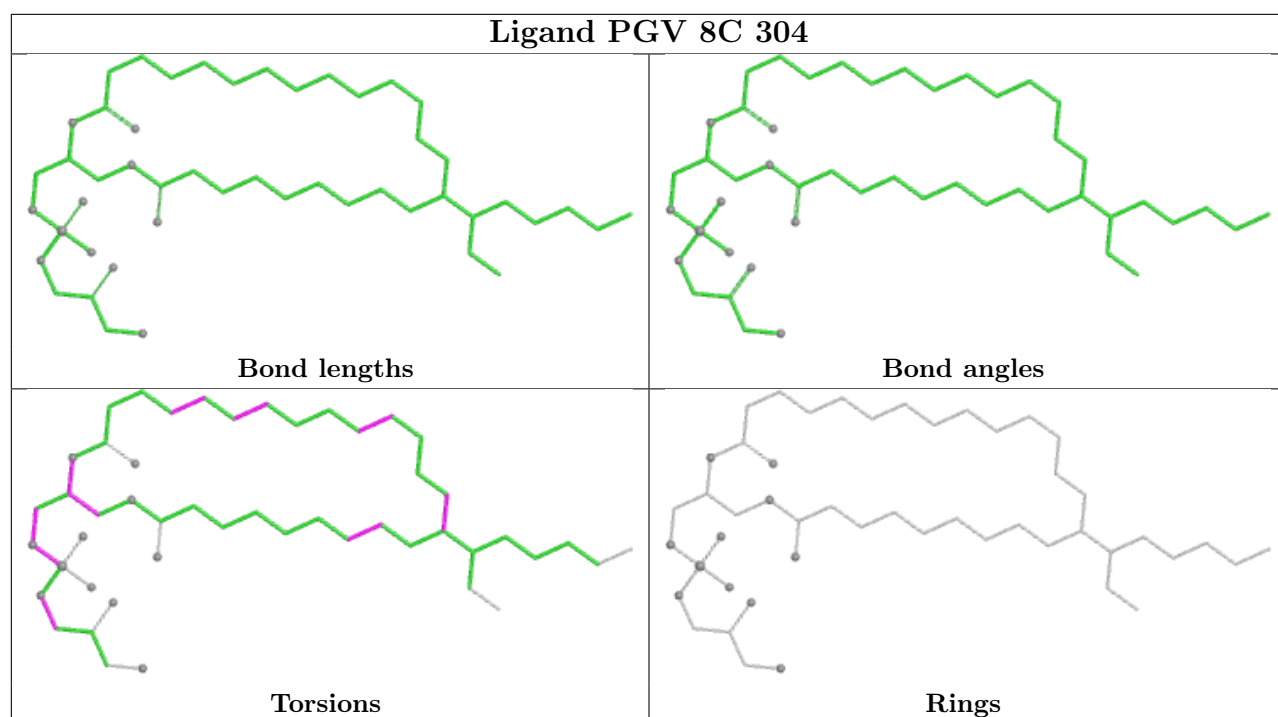


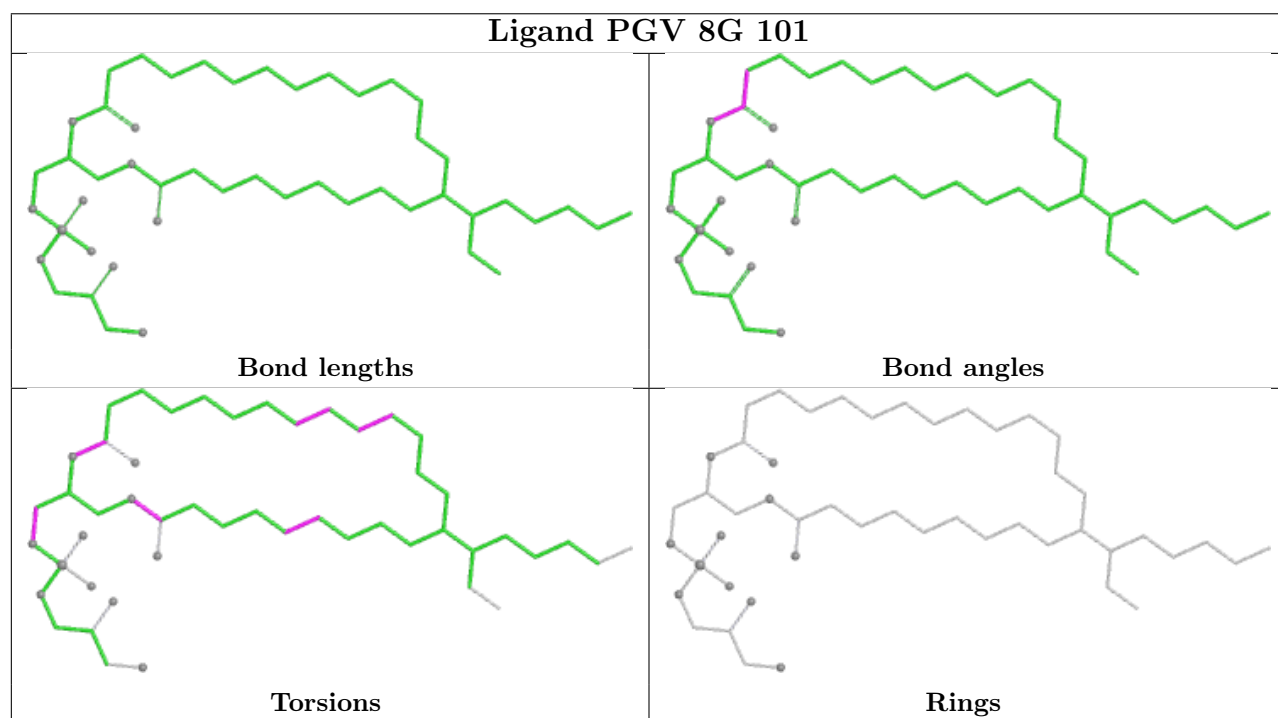
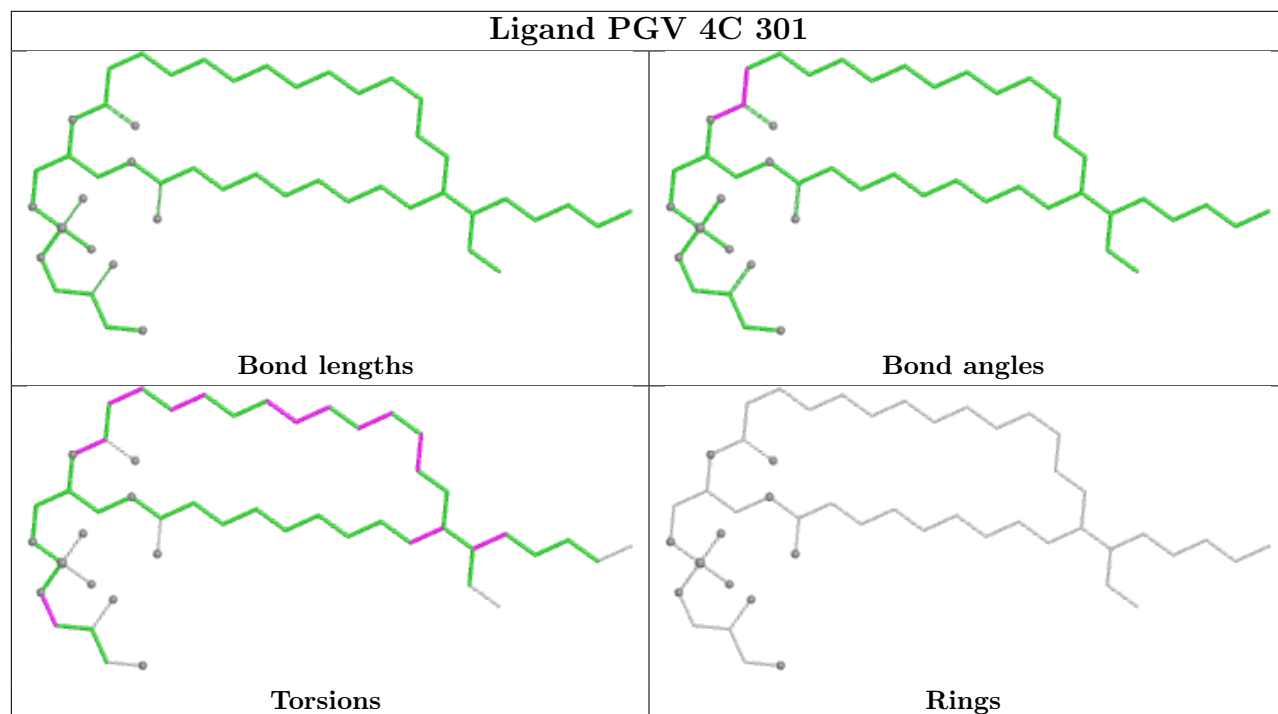


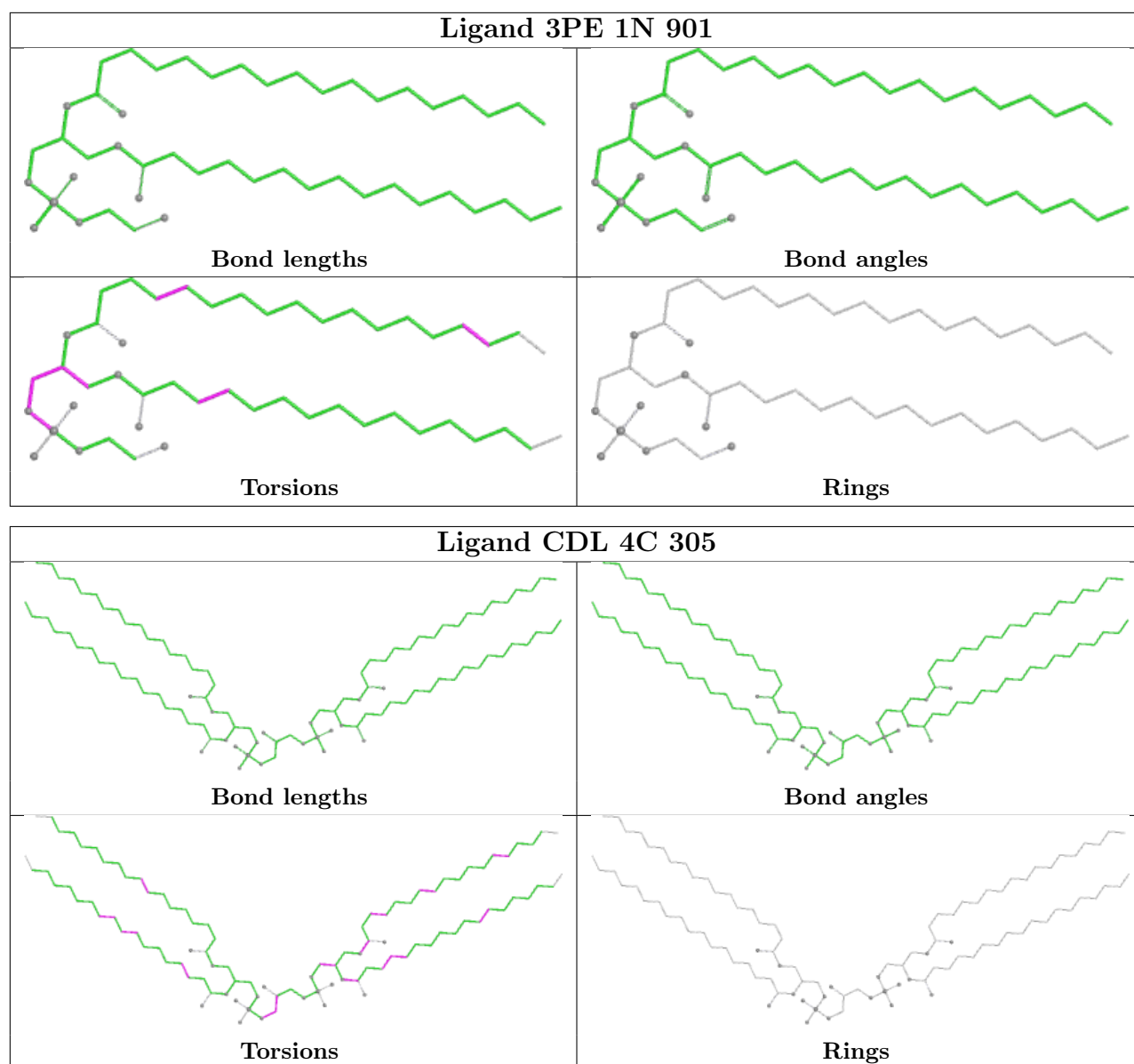


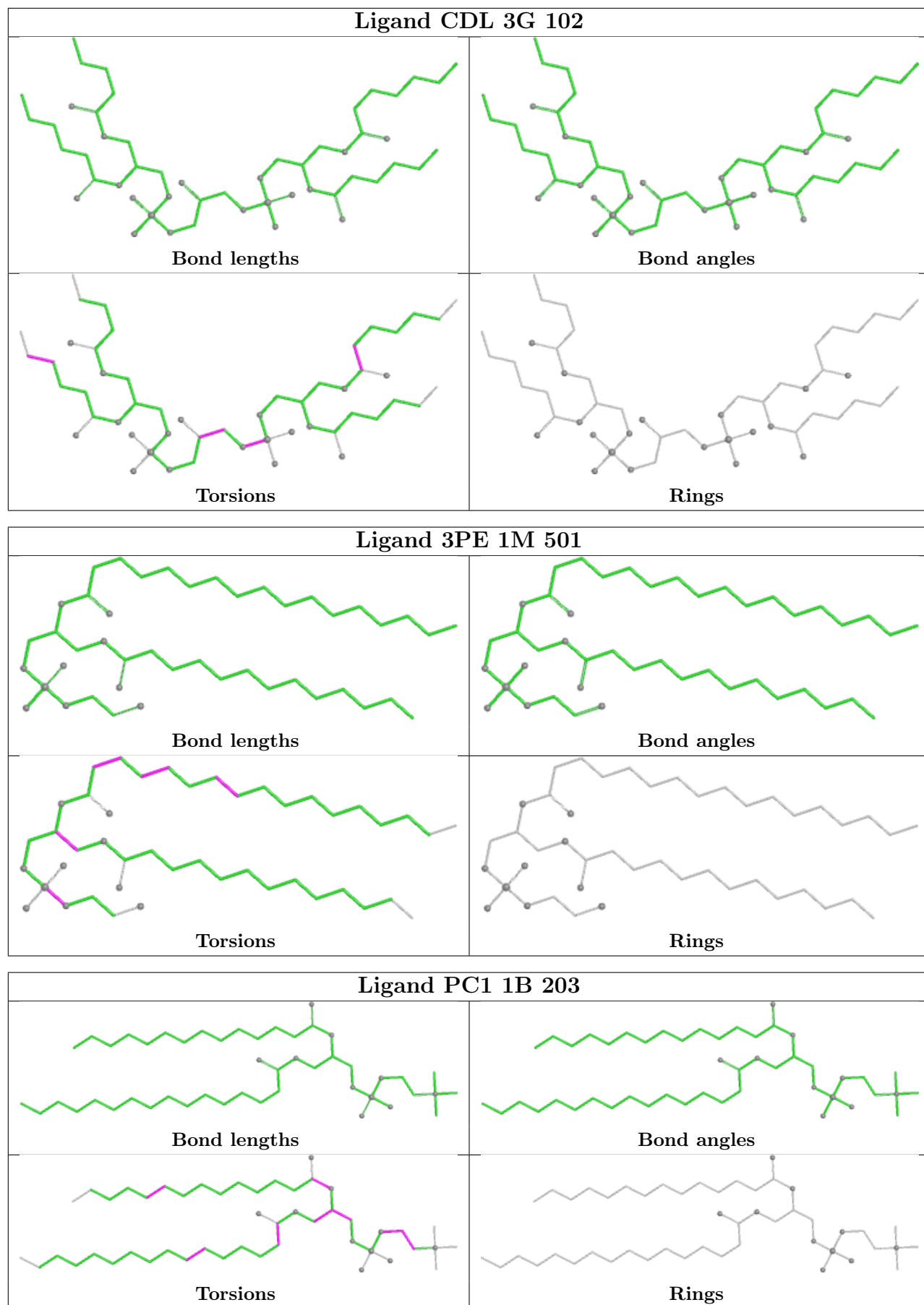


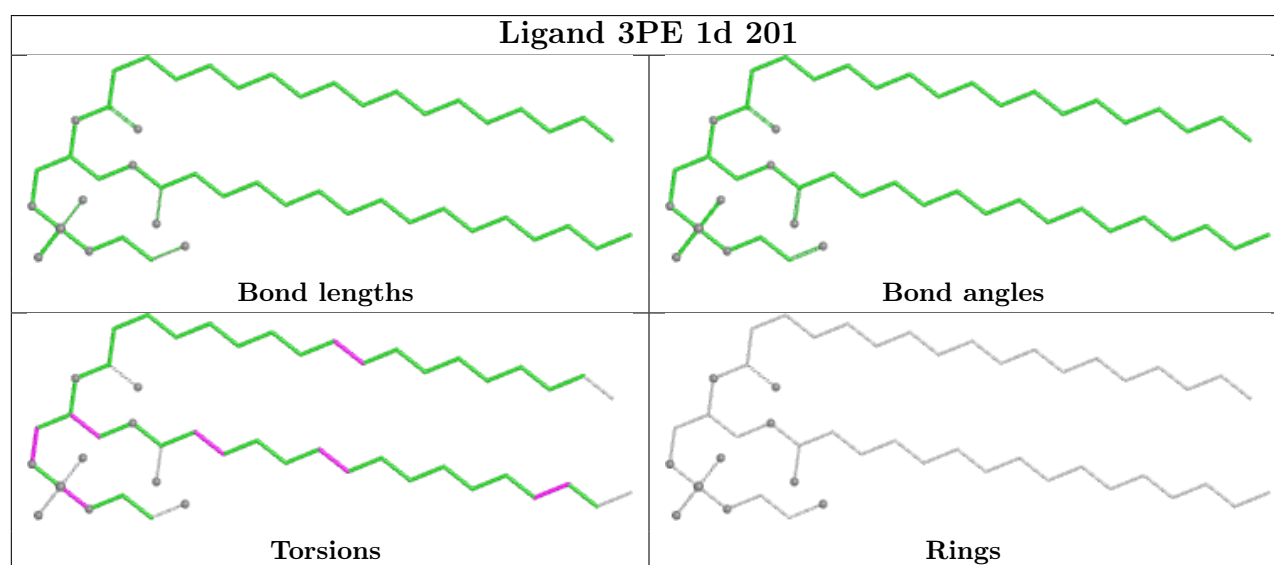
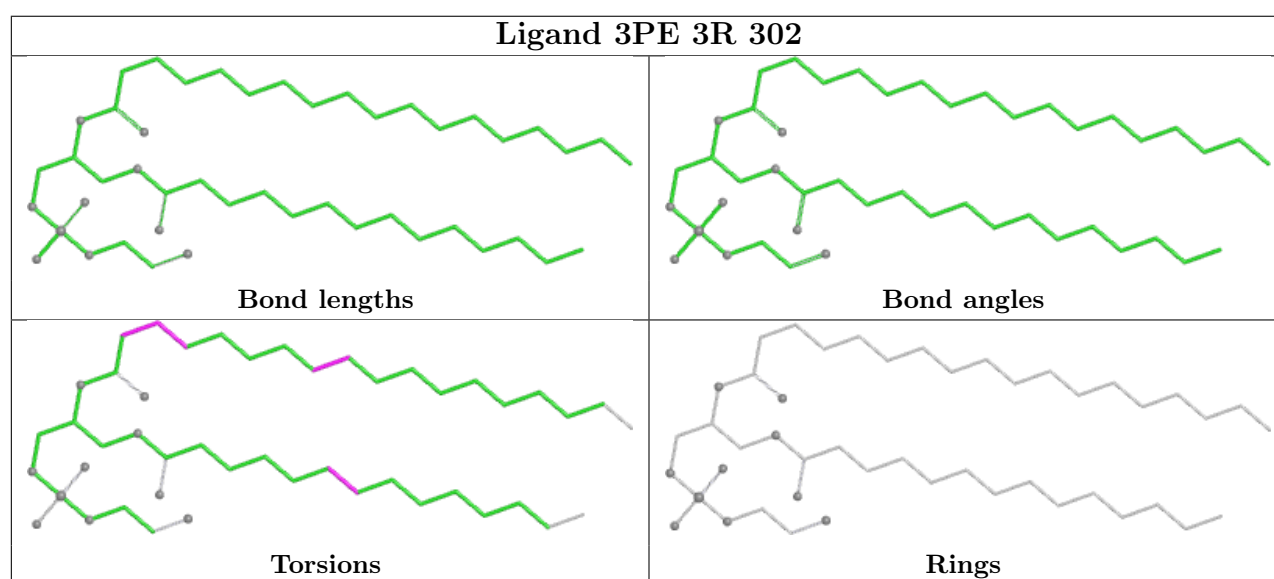
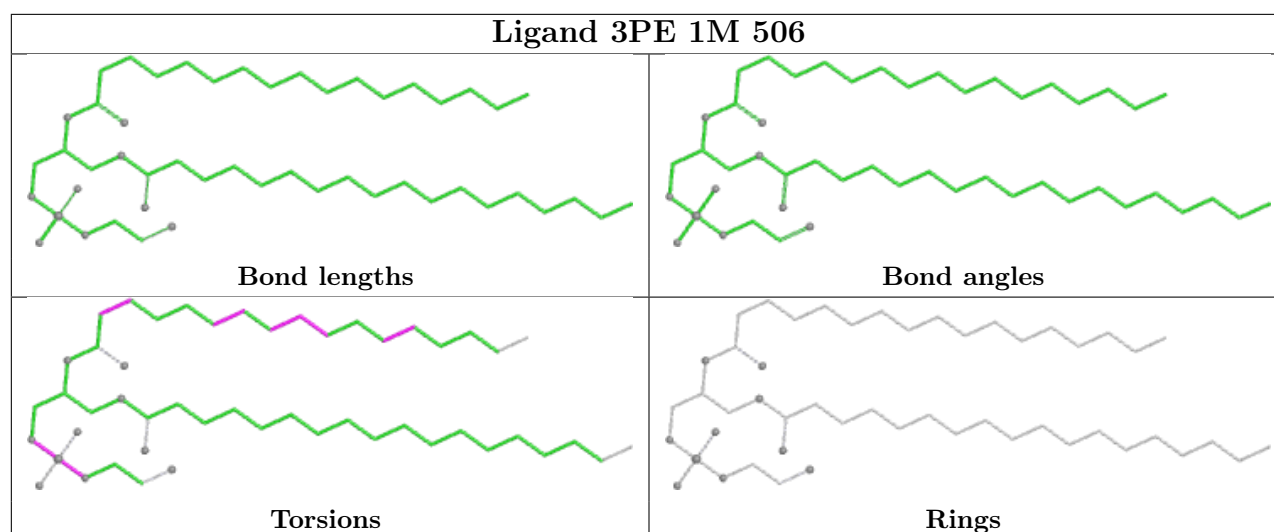


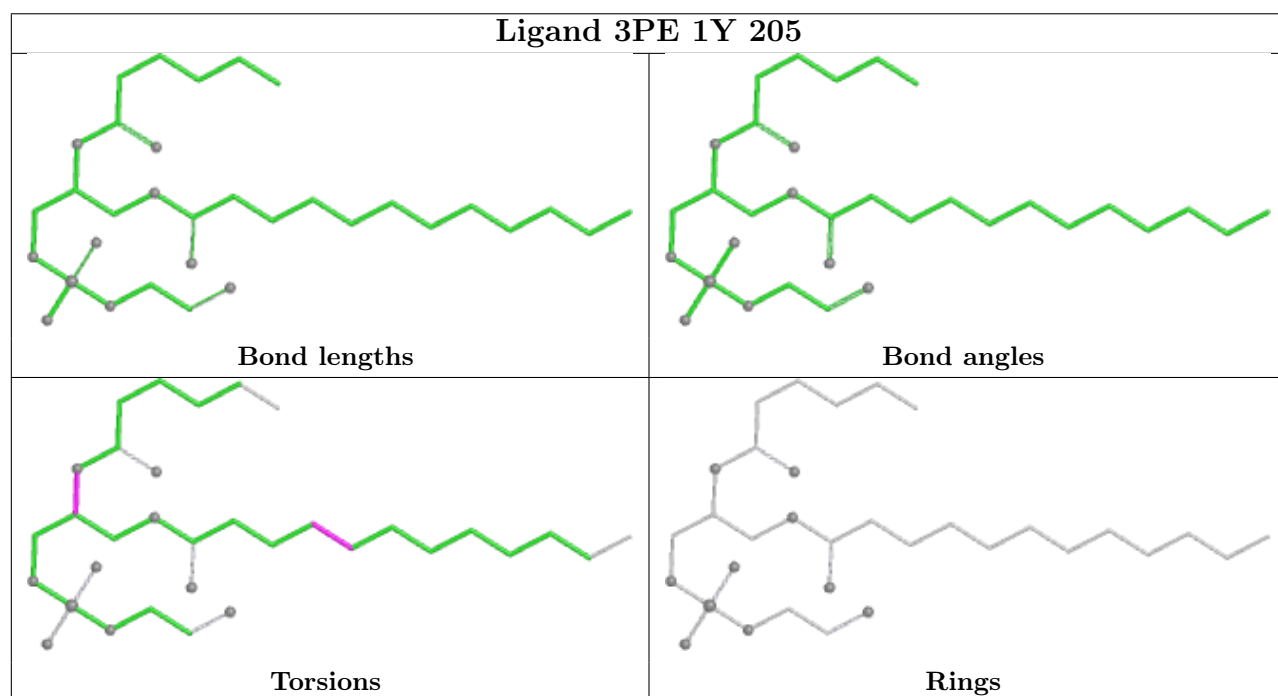
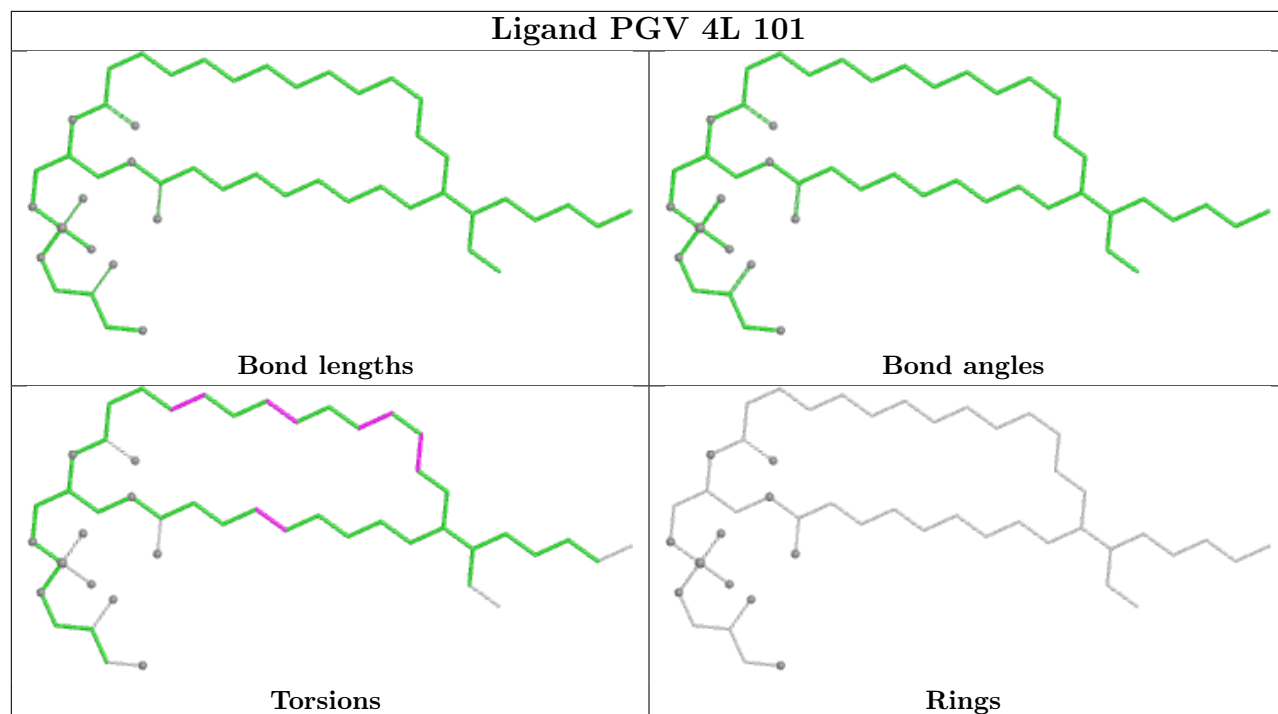




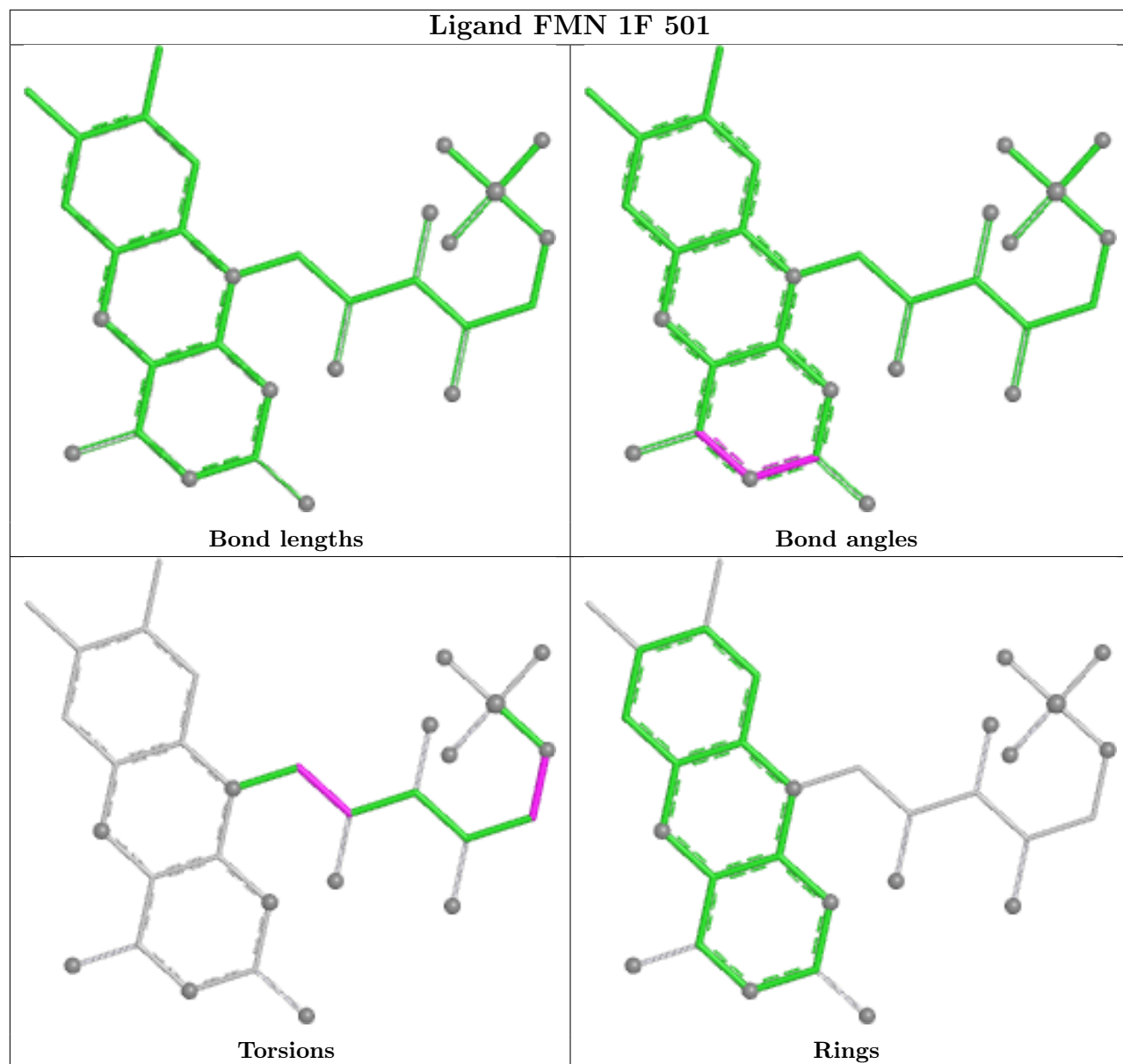


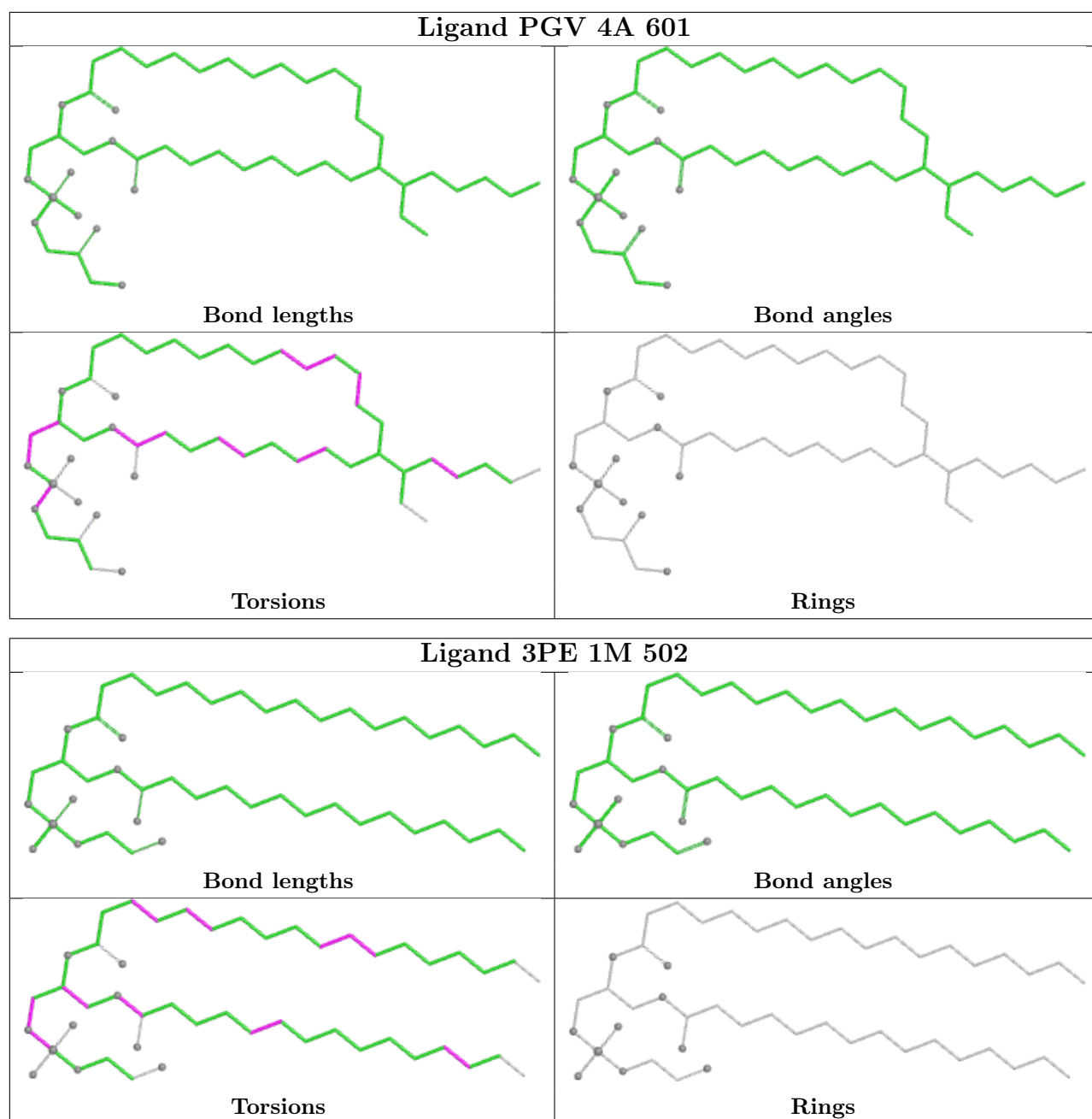




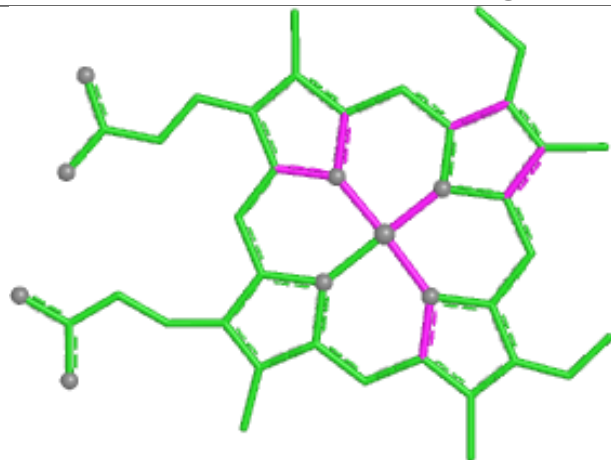


Ligand FMN 1F 501

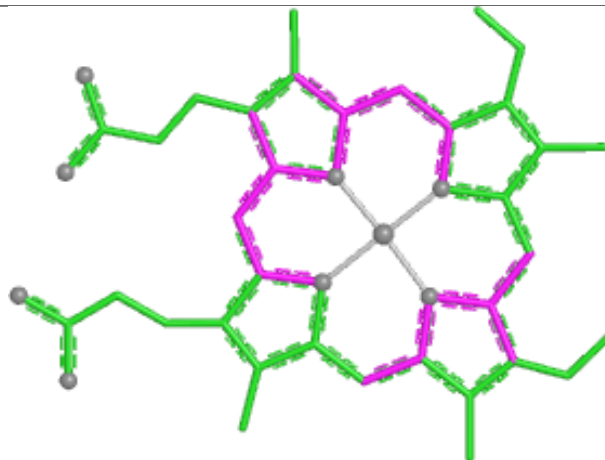




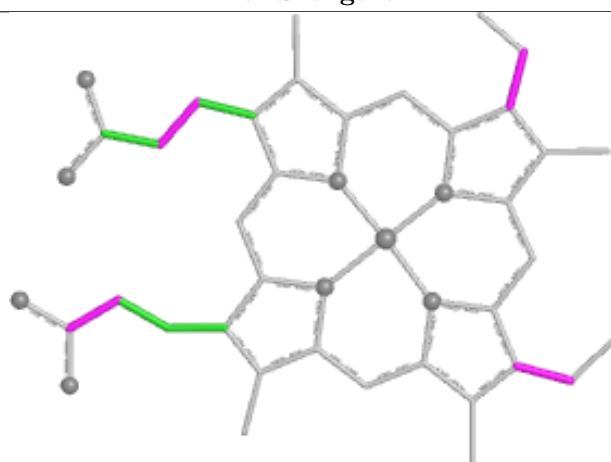
Ligand HEM 3C 501



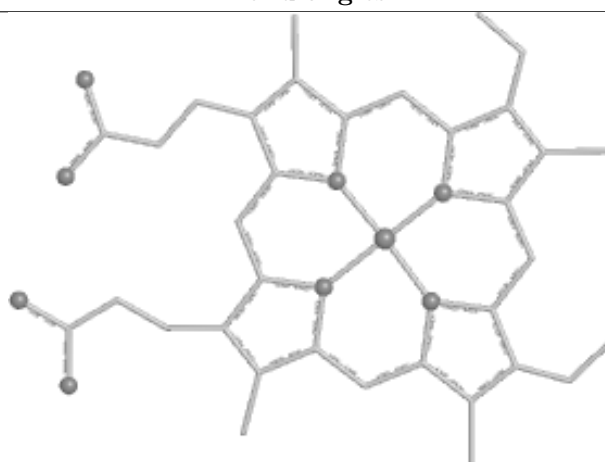
Bond lengths



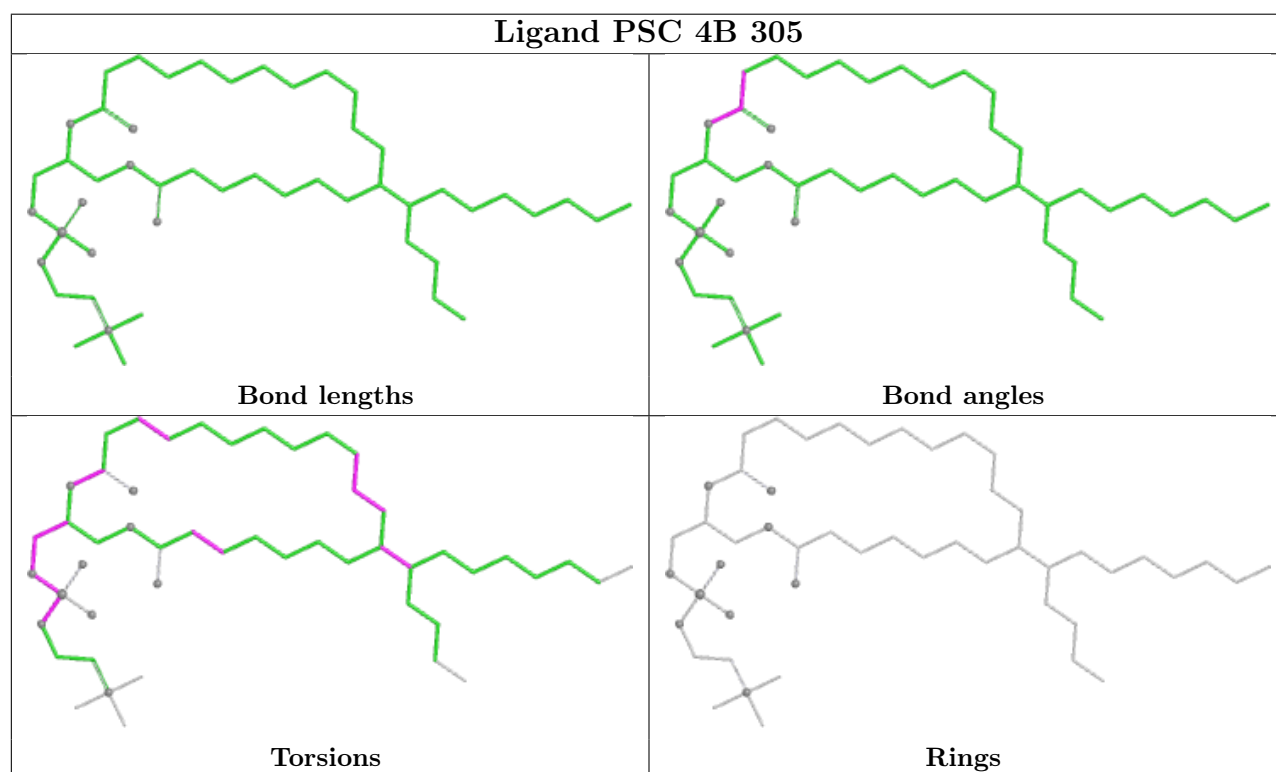
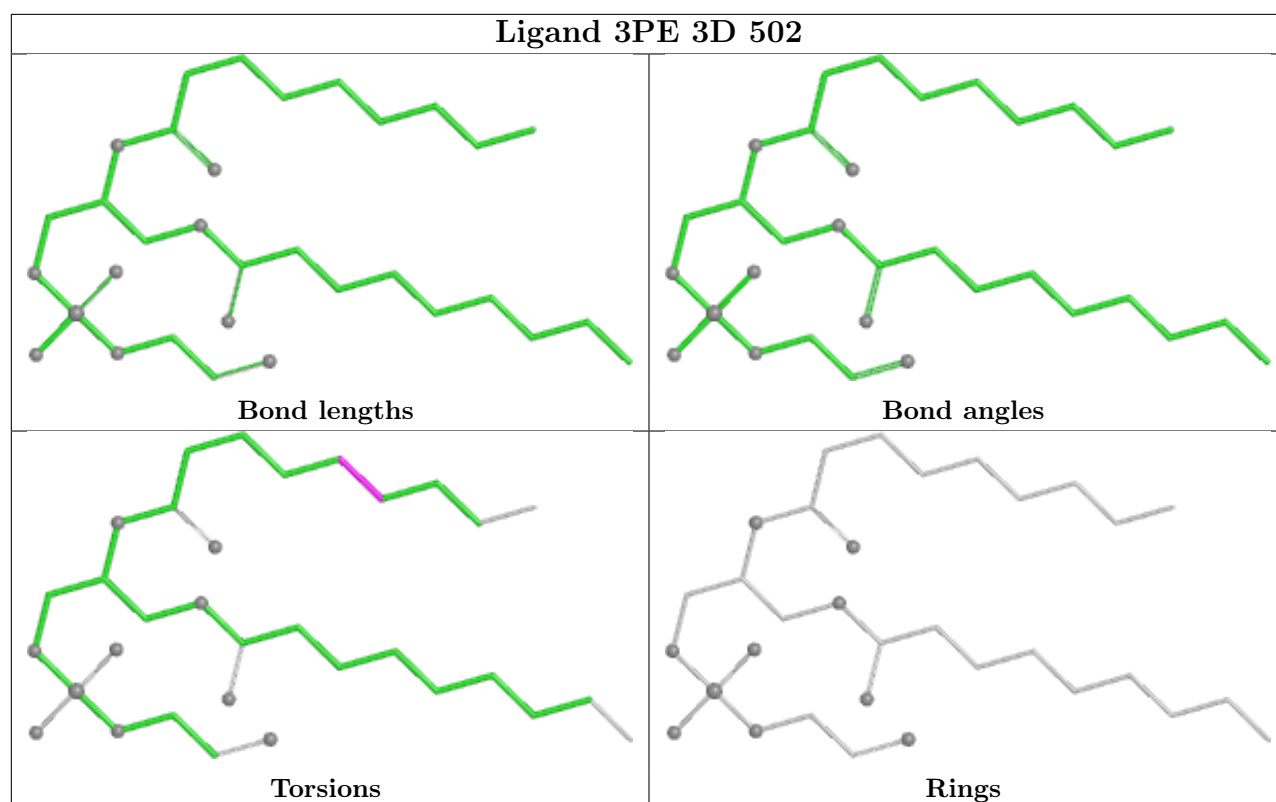
Bond angles

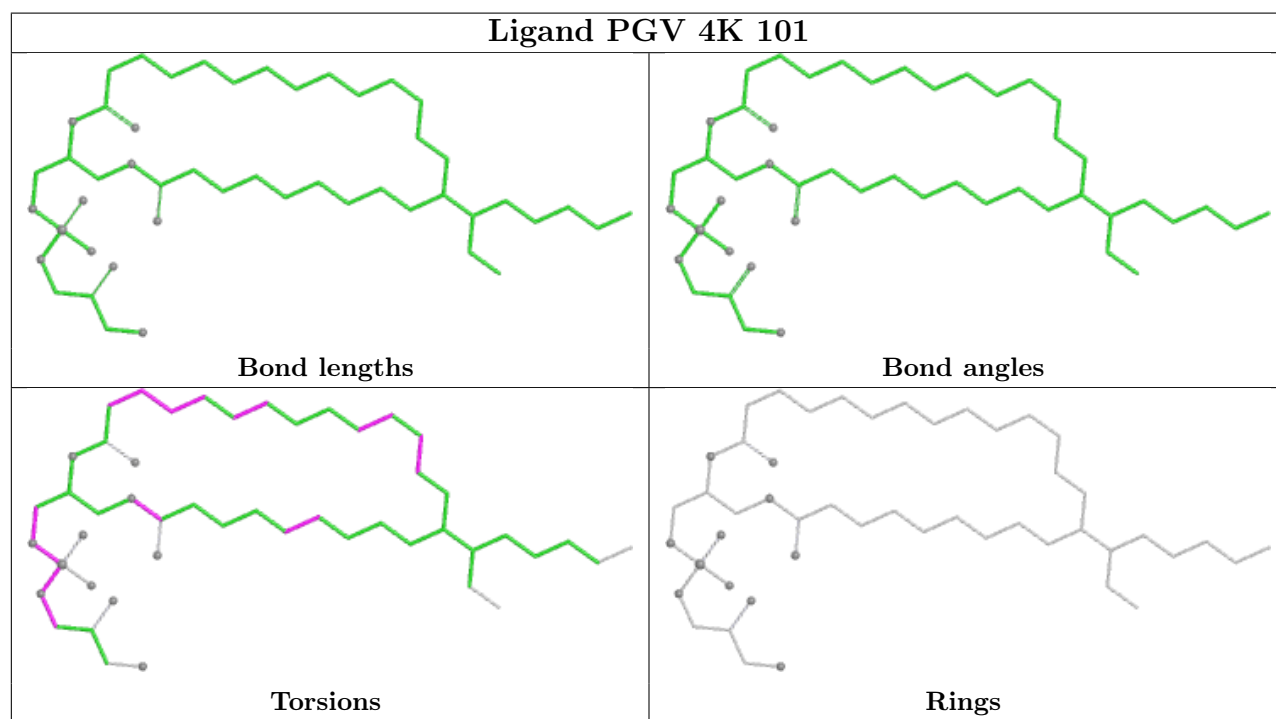
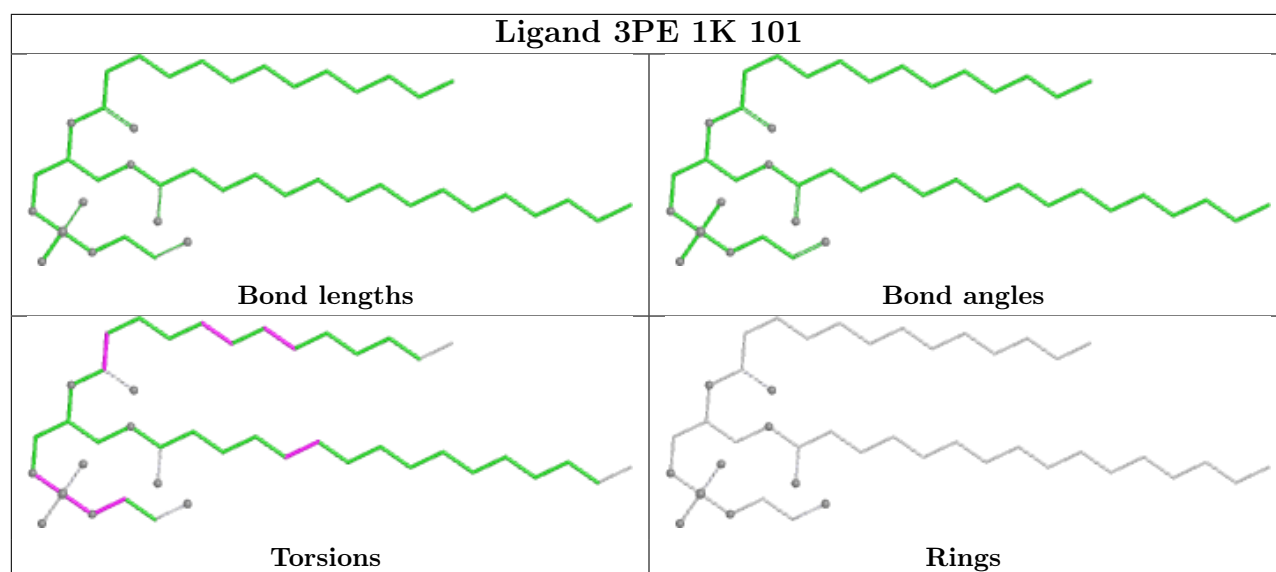


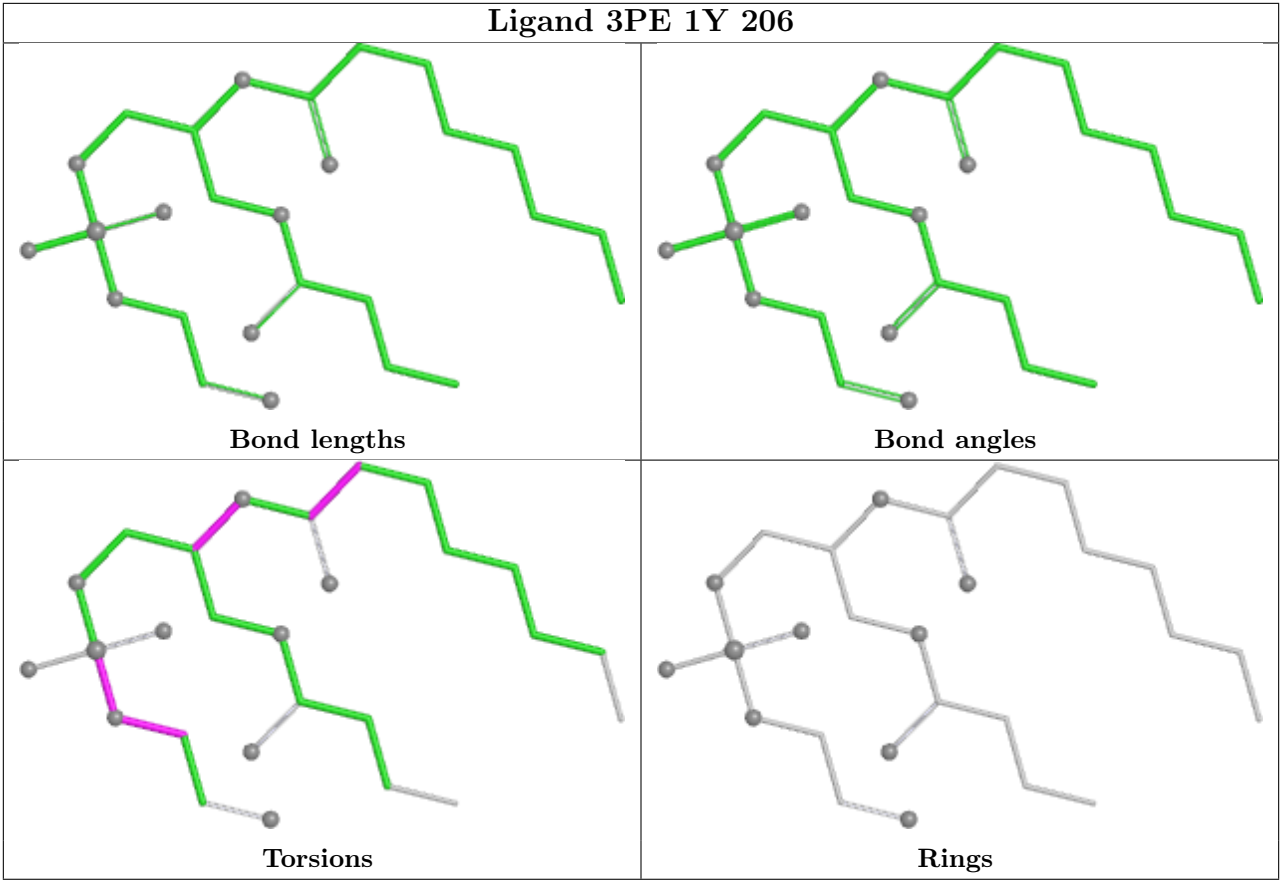
Torsions



Rings







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
49	3V	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3V	49:VAL	C	50:LEU	N	1.69
1	3V	48:SER	C	49:VAL	N	1.19

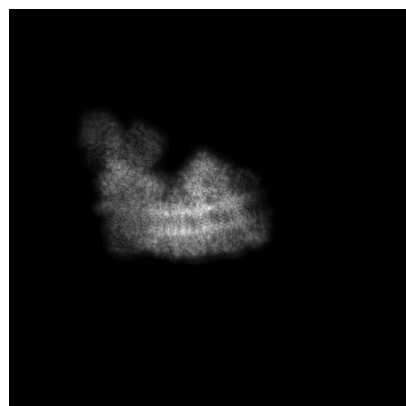
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42227. These allow visual inspection of the internal detail of the map and identification of artifacts.

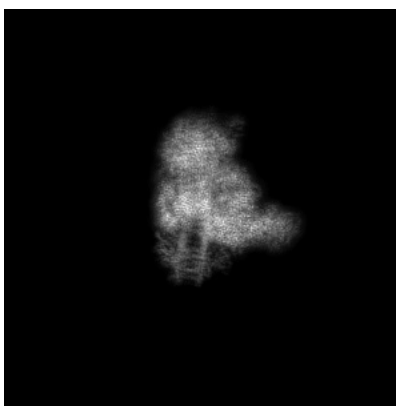
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

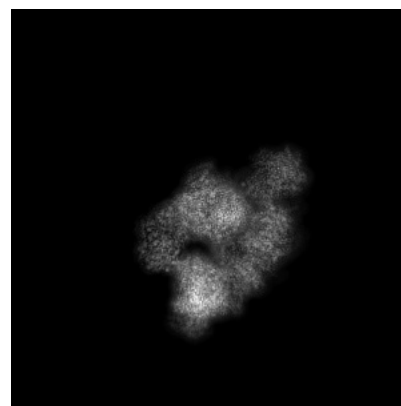
6.1.1 Primary map



X

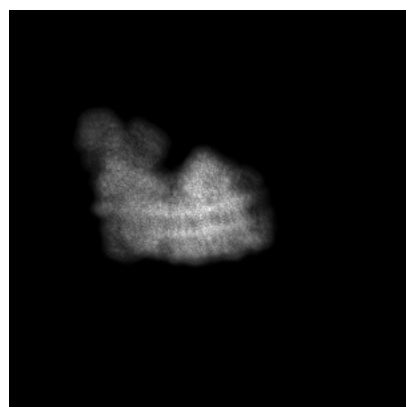


Y

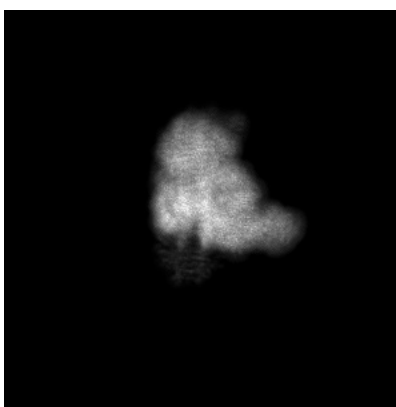


Z

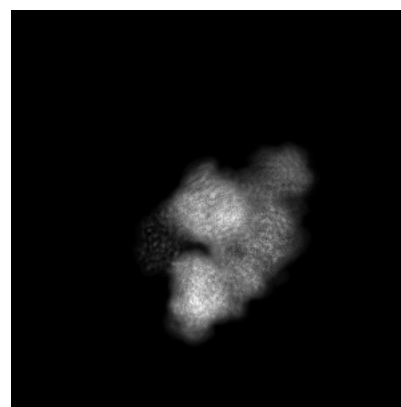
6.1.2 Raw map



X



Y

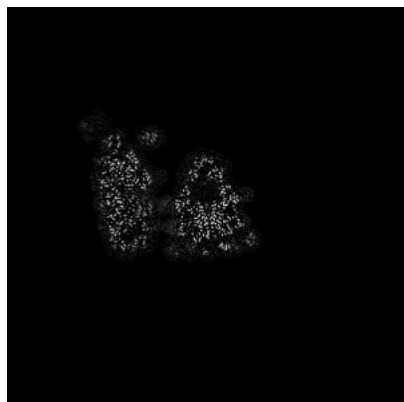


Z

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

6.2 Central slices [i](#)

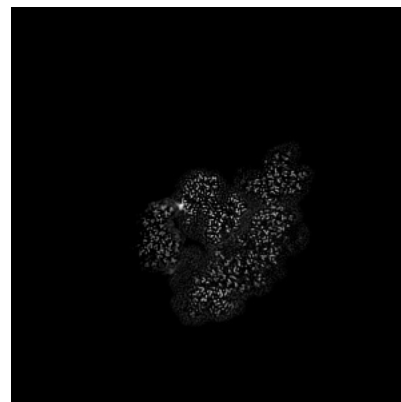
6.2.1 Primary map



X Index: 275

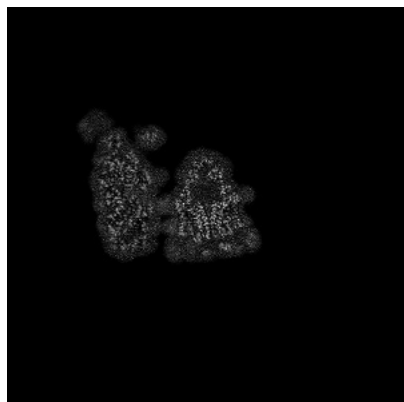


Y Index: 275

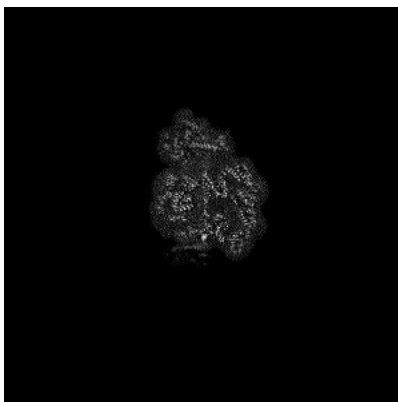


Z Index: 275

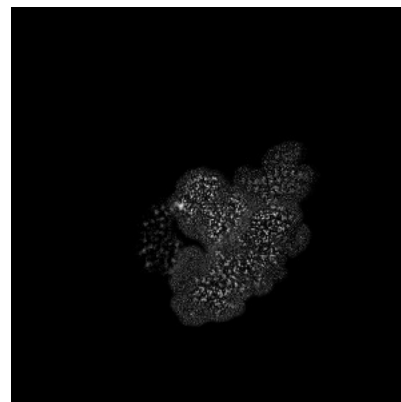
6.2.2 Raw map



X Index: 275



Y Index: 275

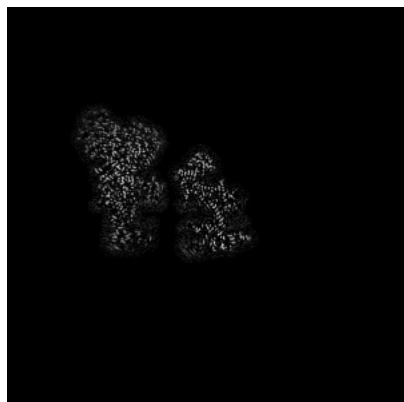


Z Index: 275

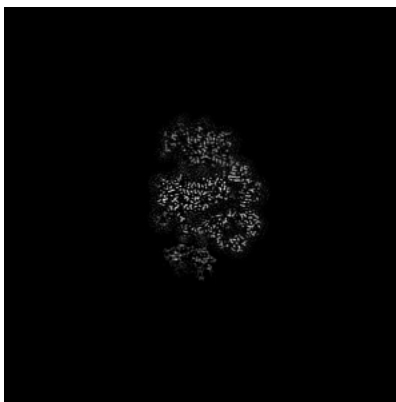
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

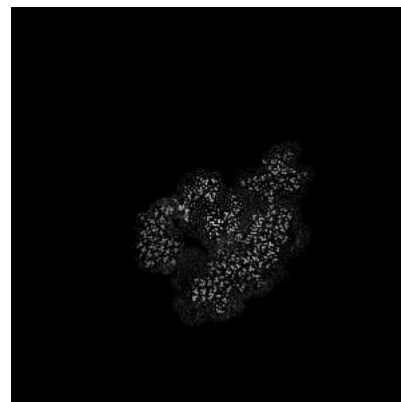
6.3.1 Primary map



X Index: 256

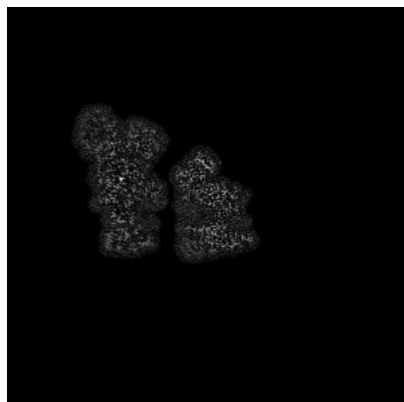


Y Index: 264

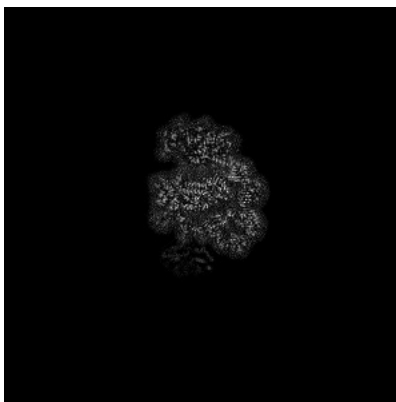


Z Index: 272

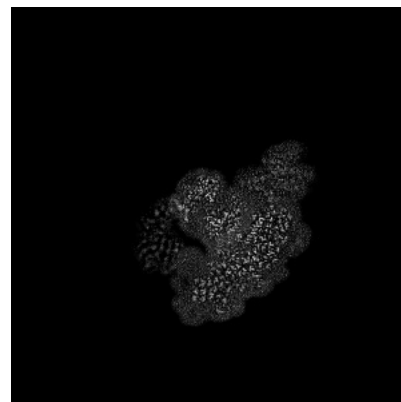
6.3.2 Raw map



X Index: 260



Y Index: 264

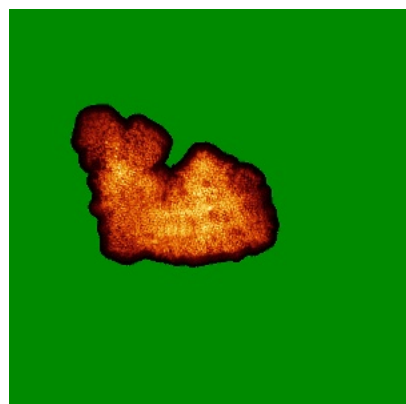


Z Index: 272

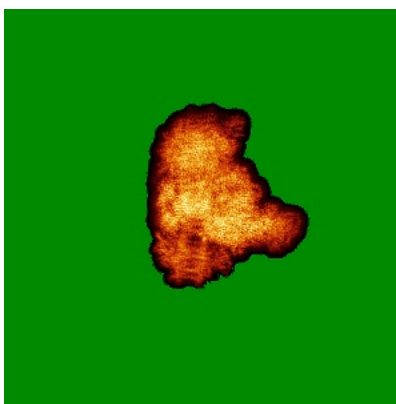
The images above show the largest variance slices of the map in three orthogonal directions.

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

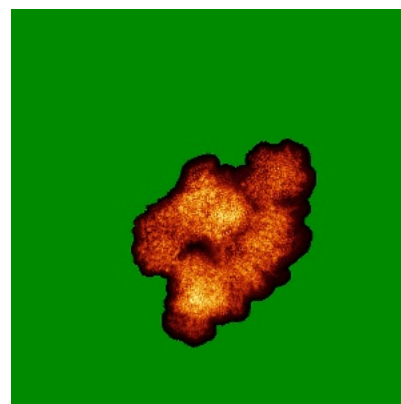
6.4.1 Primary map



X

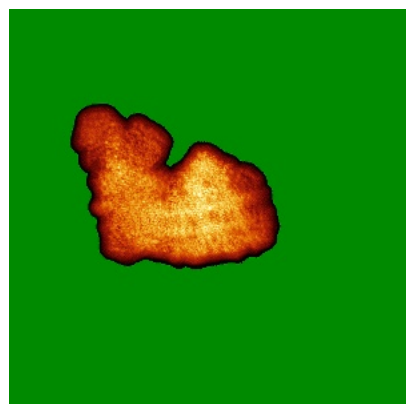


Y

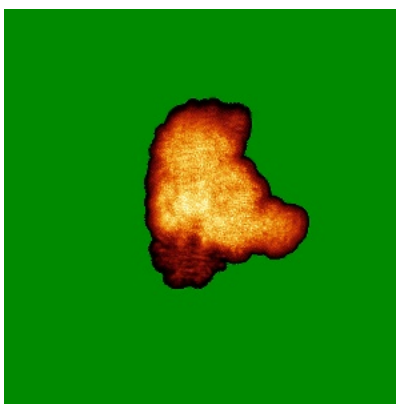


Z

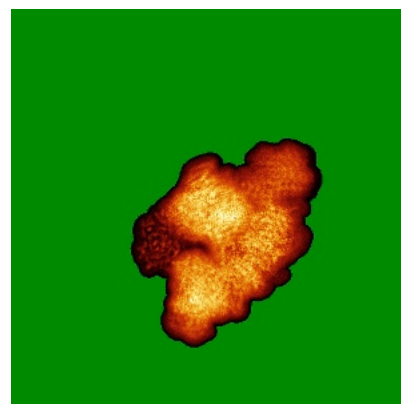
6.4.2 Raw map



X



Y

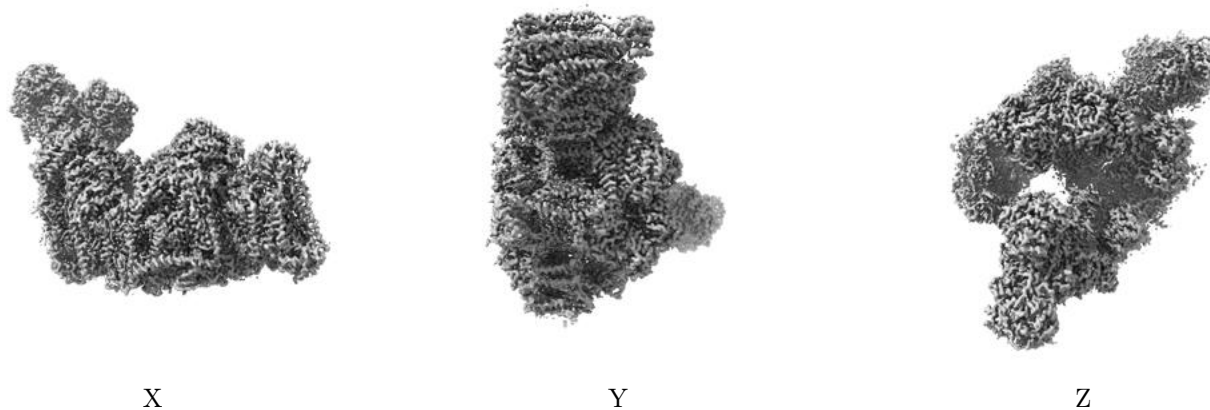


Z

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

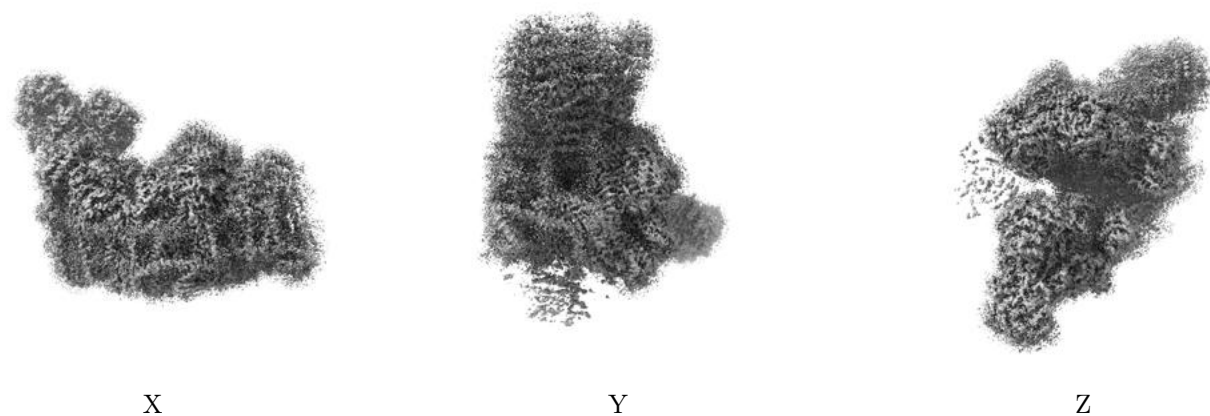
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

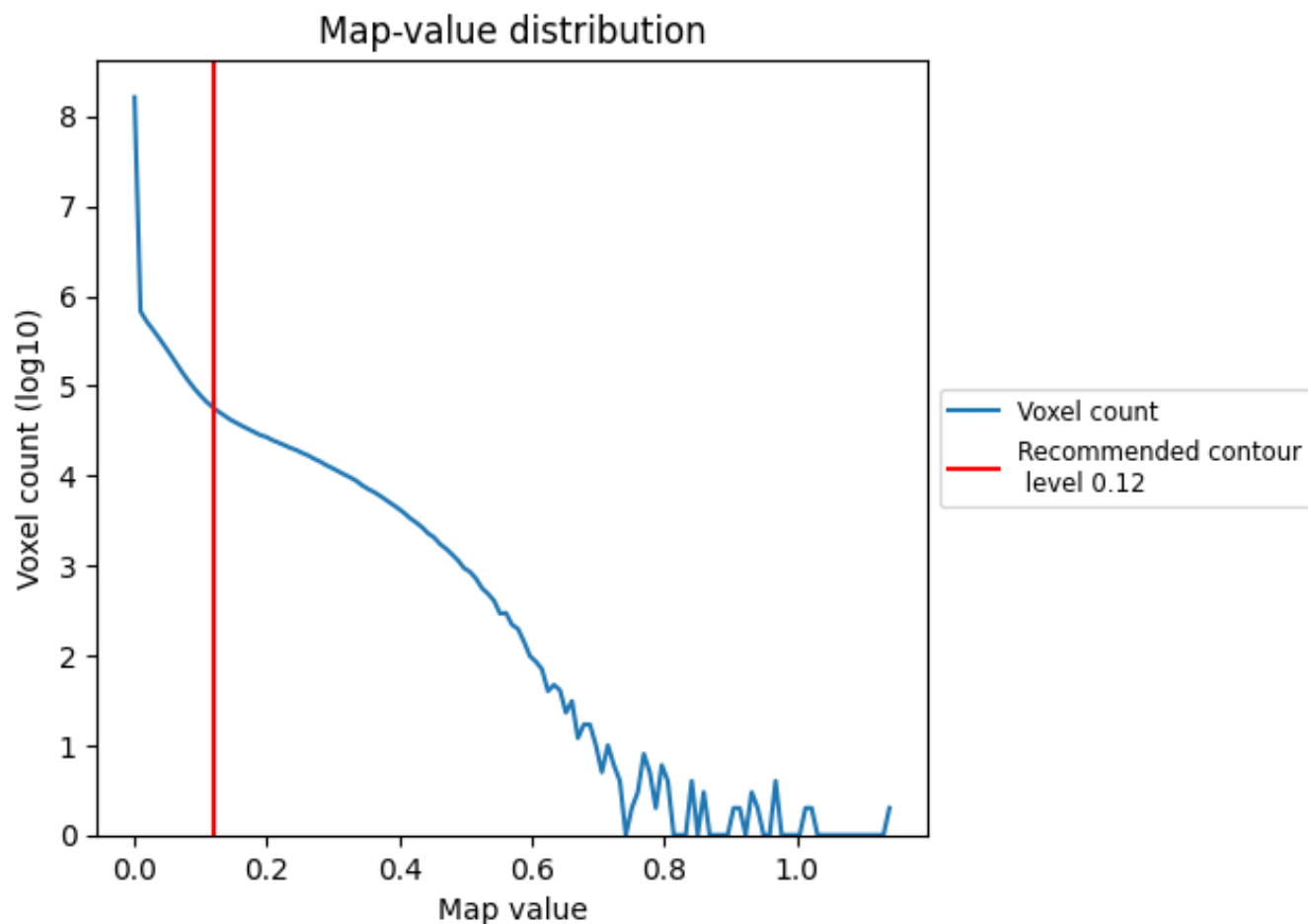
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

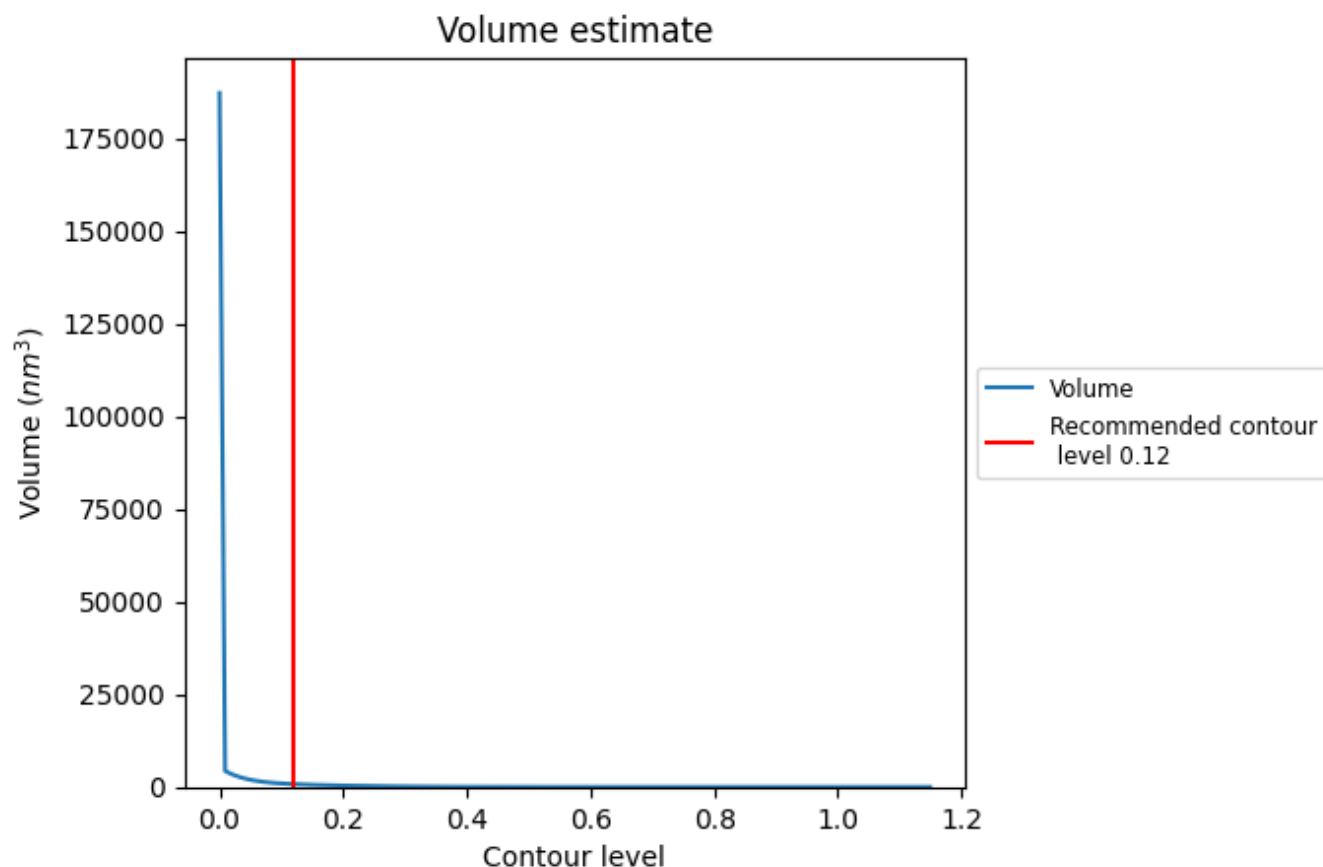
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

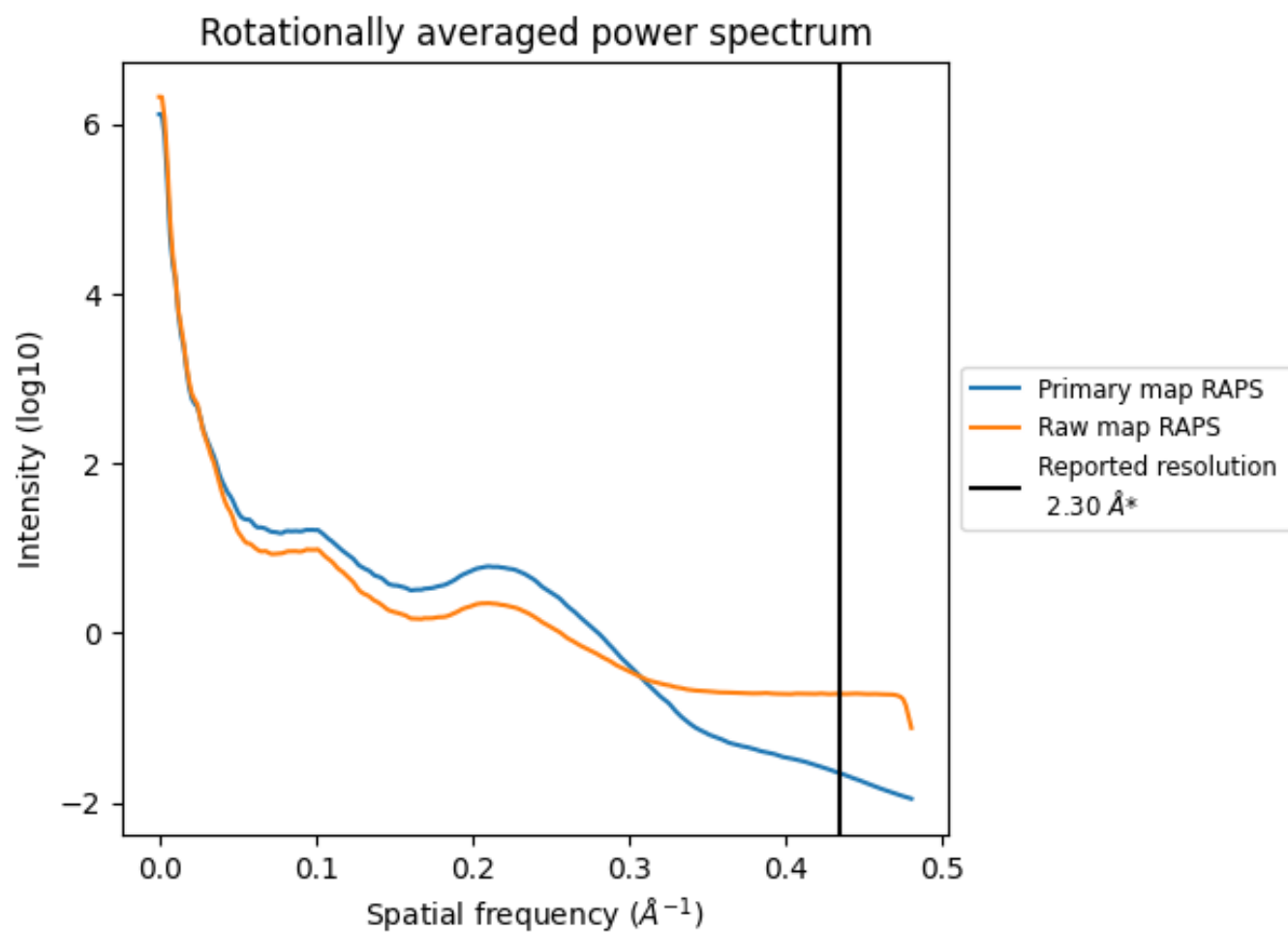
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 771 nm^3 ; this corresponds to an approximate mass of 696 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 ⓘ

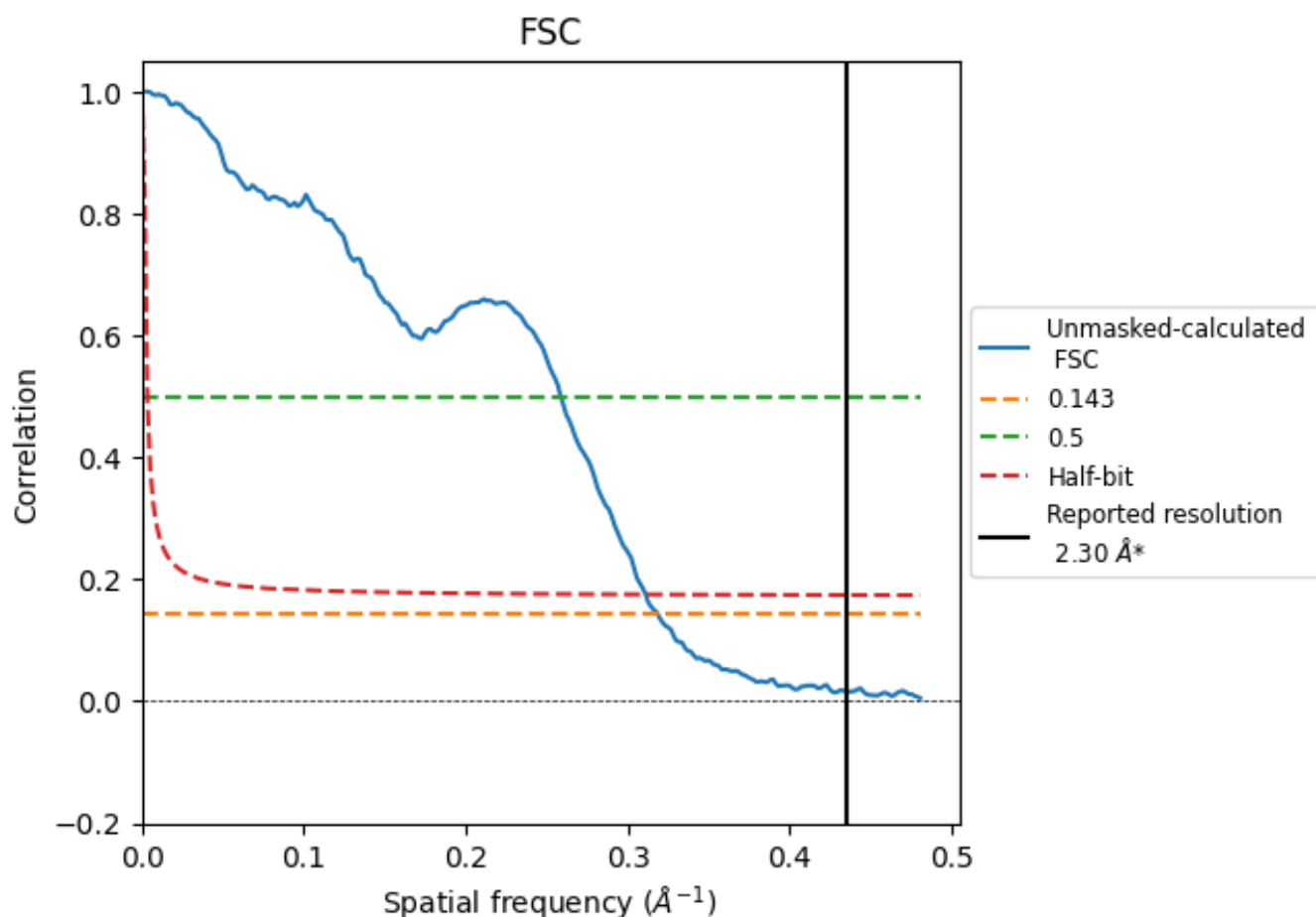


*Reported resolution corresponds to spatial frequency of 0.435 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

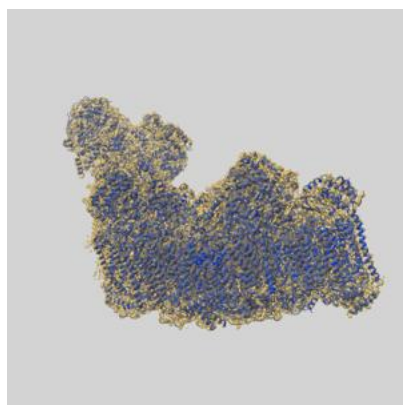
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.86	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.3 by more than 10 %

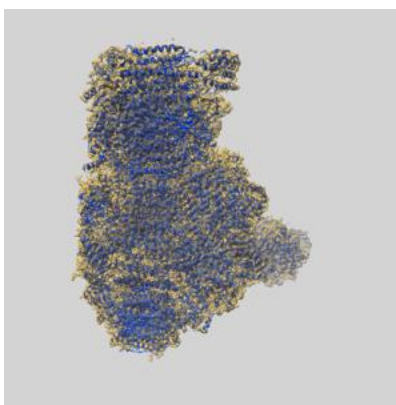
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42227 and PDB model 8UGJ. Per-residue inclusion information can be found in section 3 on page 38.

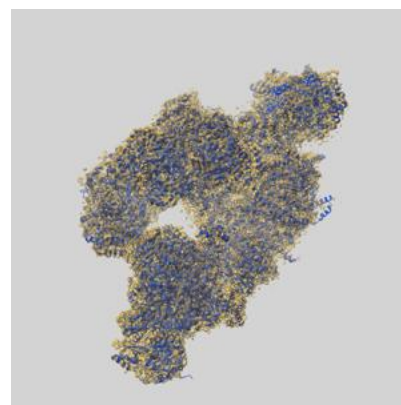
9.1 Map-model overlay [i](#)



X



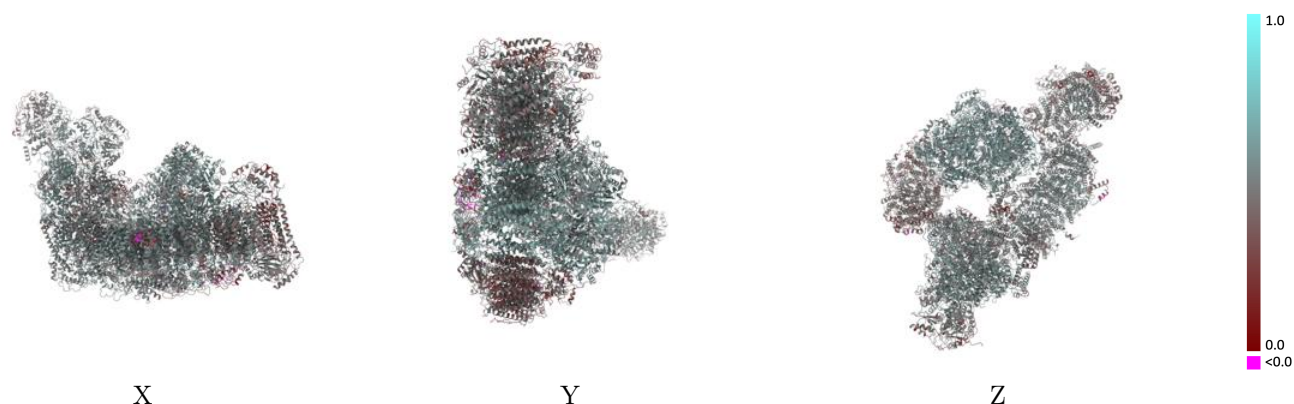
Y



Z

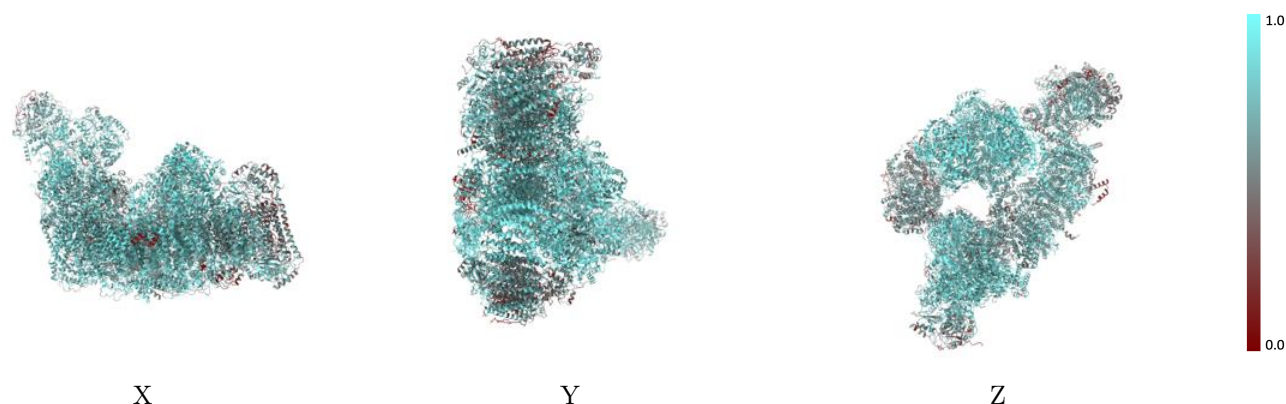
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



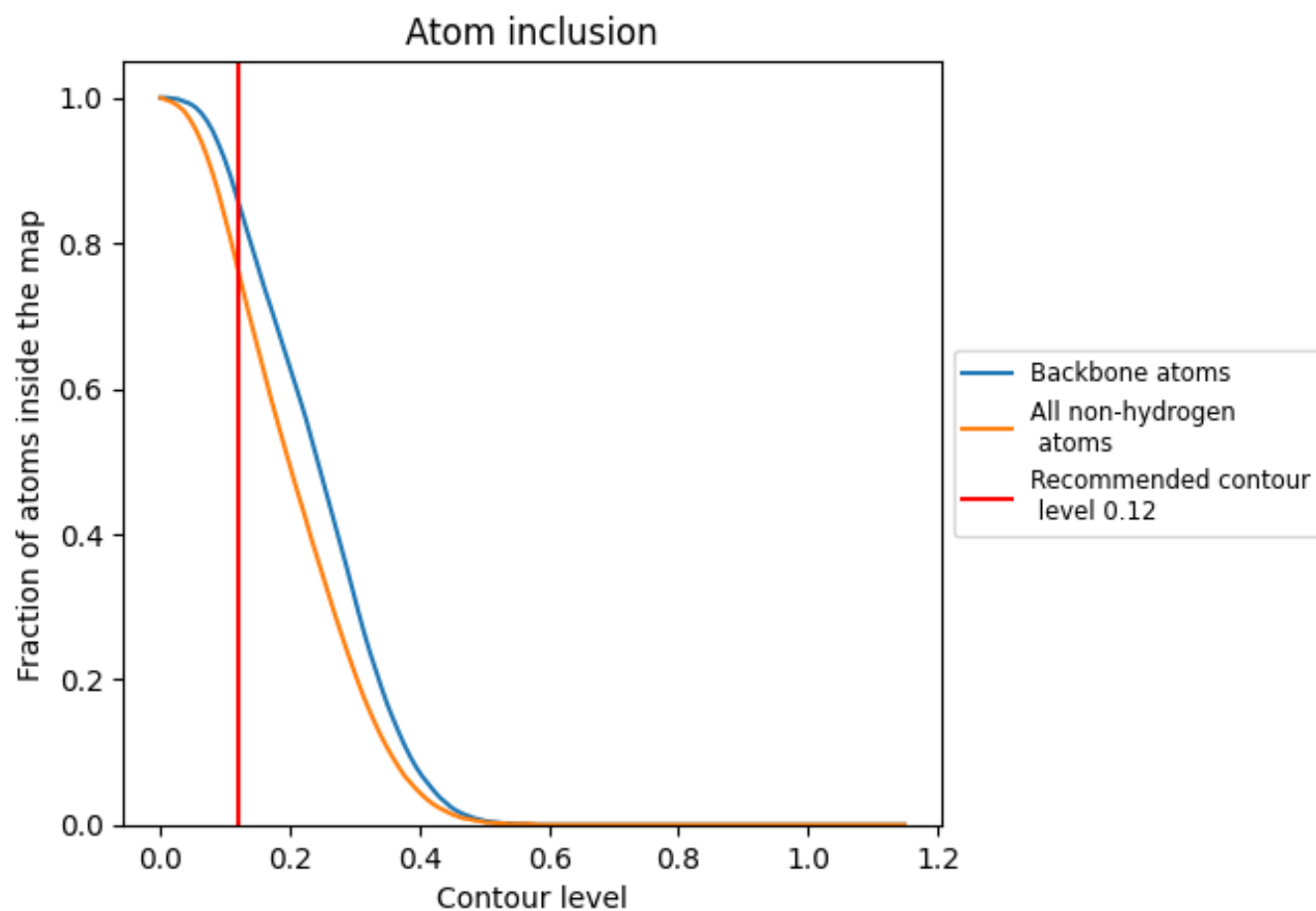
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7620	 0.4950
1A	 0.6590	 0.4580
1B	 0.8660	 0.5350
1C	 0.8720	 0.5560
1D	 0.8450	 0.5410
1E	 0.6430	 0.4590
1F	 0.6550	 0.4660
1G	 0.8050	 0.5150
1H	 0.8060	 0.5140
1I	 0.8950	 0.5560
1J	 0.6710	 0.4620
1K	 0.7730	 0.5060
1L	 0.8300	 0.5200
1M	 0.8490	 0.5390
1N	 0.8340	 0.5390
1O	 0.7540	 0.4680
1P	 0.7610	 0.4890
1Q	 0.7830	 0.5130
1R	 0.8030	 0.5350
1S	 0.7300	 0.4740
1T	 0.5330	 0.3490
1U	 0.7690	 0.4940
1V	 0.7410	 0.4990
1W	 0.8070	 0.5110
1X	 0.7450	 0.5010
1Y	 0.7760	 0.4830
1Z	 0.7800	 0.5210
1a	 0.8400	 0.5270
1b	 0.7490	 0.4940
1c	 0.7170	 0.4900
1d	 0.7770	 0.5180
1e	 0.7480	 0.5190
1f	 0.6950	 0.4990
1g	 0.7700	 0.5060
1h	 0.7590	 0.5160



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Chain	Atom inclusion	Q-score
1i	 0.5600	 0.4240
1j	 0.6760	 0.4540
1k	 0.6750	 0.4500
1l	 0.8060	 0.5080
1m	 0.8060	 0.5160
1n	 0.8200	 0.5110
1o	 0.7010	 0.4450
1p	 0.7580	 0.5020
1q	 0.7880	 0.5240
1r	 0.8190	 0.5450
1s	 0.6280	 0.4670
3A	 0.8560	 0.5540
3B	 0.8650	 0.5550
3C	 0.9140	 0.5770
3D	 0.9080	 0.5710
3E	 0.5160	 0.3660
3F	 0.8710	 0.5680
3G	 0.8490	 0.5510
3H	 0.7930	 0.5240
3I	 0.4830	 0.4250
3J	 0.8800	 0.5130
3N	 0.9010	 0.5680
3O	 0.8710	 0.5560
3P	 0.9170	 0.5790
3Q	 0.9170	 0.5760
3R	 0.5040	 0.3410
3S	 0.8830	 0.5740
3T	 0.9110	 0.5600
3U	 0.8120	 0.5130
3V	 0.7290	 0.5270
3W	 0.9180	 0.5770
3X	 0.8590	 0.5500
3Y	 0.8180	 0.5350
4A	 0.7670	 0.4960
4B	 0.6290	 0.4440
4C	 0.6810	 0.4580
4D	 0.5470	 0.4050
4E	 0.5240	 0.3980
4F	 0.6500	 0.4690
4G	 0.5720	 0.4200
4H	 0.7020	 0.4510
4I	 0.5490	 0.4430

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Chain	Atom inclusion	Q-score
4J	 0.6570	 0.4500
4K	 0.4960	 0.4260
4L	 0.6710	 0.4540
4M	 0.5840	 0.4440
4N	 0.4840	 0.4220
8A	 0.7010	 0.4270
8B	 0.6480	 0.3960
8C	 0.6210	 0.3890
8D	 0.5890	 0.3680
8E	 0.5910	 0.3680
8F	 0.4800	 0.3690
8G	 0.5780	 0.3700
8H	 0.7180	 0.4000
8I	 0.7430	 0.4120
8J	 0.5710	 0.3790
8K	 0.6140	 0.3890
8L	 0.5740	 0.3870
8M	 0.6250	 0.3910
8N	 0.6560	 0.3990