



Full wwPDB EM Validation Report ⓘ

Nov 11, 2025 – 09:10 PM JST

PDB ID : 8ZSO / pdb_00008zso
EMDB ID : EMD-60422
Title : Respirasome close state 2 in presence of metformin (SC-MetC2)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-06-05
Resolution : 3.11 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

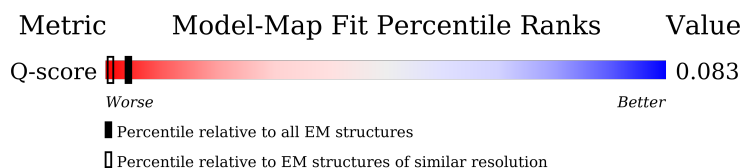
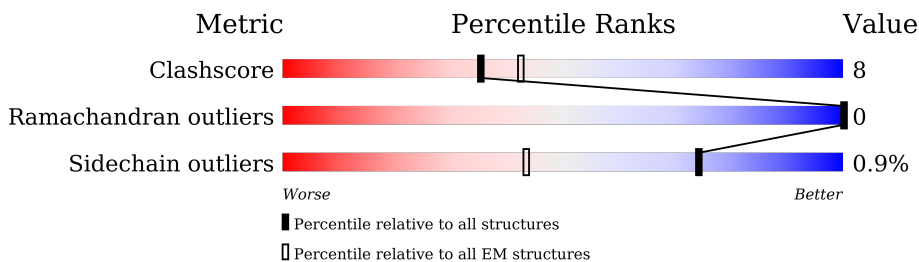
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14465 (2.61 - 3.61)

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	4L	98	<div> <div>11%</div> <div> <div></div> <div>77%</div> <div>23%</div> </div> </div>
2	5A	102	<div> <div>78%</div> <div> <div></div> <div>50%</div> <div>47%</div> <div>.</div> </div> </div>
3	5B	95	<div> <div>54%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div>.</div> </div> </div>
4	6A	73	<div> <div>53%</div> <div> <div></div> <div>73%</div> <div>26%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	6B	82	
6	6C	70	
7	7A	57	
8	7B	50	
9	7C	47	
10	8B	43	
11	A1	70	
12	A2	85	
13	A3	83	
14	A5	112	
15	A6	114	
16	A7	112	
17	A8	171	
18	A9	341	
19	AB	87	
19	AC	87	
20	AK	321	
21	AL	140	
22	AM	144	
23	AN	142	
24	B1	56	
25	B2	67	
26	B3	80	
27	B4	128	
28	B5	138	

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Mol	Chain	Length	Quality of chain
29	B6	126	
30	B7	125	
31	B8	156	
32	B9	178	
33	BK	176	
34	BL	102	
35	C1	514	
36	C2	228	
37	C3	260	
38	C4	138	
39	CA	49	
40	CB	121	
41	N1	318	
42	N2	347	
43	N3	115	
44	N4	459	
45	N5	603	
46	N6	174	
47	QA	419	
47	Qa	419	
48	QB	446	
48	Qb	446	
49	QC	379	
49	Qc	379	
50	QD	241	

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Mol	Chain	Length	Quality of chain
50	Qd	241	82% 90% 9%
51	QE	196	90% 74% 26%
51	Qe	196	93% 79% 21%
52	QF	67	88% 88% 12%
52	Qf	67	88% 81% 15%
53	QG	101	81% 87% 13%
53	Qg	101	79% 85% 15%
54	QH	79	82% 80% 19%
54	Qh	79	80% 86% 14%
55	QI	62	81% 89% 11%
55	Qi	62	77% 89% 8%
56	QJ	49	92% 92% 8%
57	QK	78	86% 79% 13% 6%
58	Qj	51	76% 92% 8%
59	S1	689	60% 83% 17%
60	S2	430	21% 77% 21% ..
61	S3	208	58% 86% 14%
62	S4	125	65% 86% 14%
63	S5	105	19% 82% 18%
64	S6	96	46% 84% 16%
65	S7	156	19% 71% 27% .
66	S8	176	7% 75% 24% .
67	V1	431	15% 76% 23% .
68	V2	217	17% 79% 21%
69	V3	42	36% 62% 38%

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
84	FES	Qe	301	-	-	X	-

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 116635 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 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4L	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	102	Total	C	N	O	S	0	0
			825	528	139	156	2		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5B	95	Total	C	N	O	S	0	0
			724	449	128	141	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6A	73	Total	C	N	O	S	0	0
			609	395	116	97	1		

- Molecule 5 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6B	82	Total	C	N	O	S	0	0
			684	431	125	123	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6C	70	Total	C	N	O	S	0	0
			574	375	101	95	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7A	57	Total	C	N	O	S	0	0
			447	287	76	81	3		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7B	50	Total	C	N	O	S	0	0
			392	254	66	71	1		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7C	47	Total	C	N	O	S	0	0
			387	257	65	63	2		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	8B	43	Total	C	N	O	0	0
			338	222	57	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A1	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	85	Total	C	N	O	S	0	0
			686	431	128	125	2		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A3	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A5	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A6	114	Total	C	N	O	S	0	0
			967	617	178	167	5		

- Molecule 16 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A7	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A8	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A9	341	Total	C	N	O	S	0	0
			2743	1777	480	477	9		

- Molecule 19 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AB	77	Total	C	N	O	S	0	0
			624	402	93	124	5		
19	AC	87	Total	C	N	O	S	0	0
			702	452	103	142	5		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AK	321	Total	C	N	O	S	0	0
			2601	1655	444	492	10		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AL	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AM	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AN	142	Total	C	N	O	S	0	0
			1173	755	203	206	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B1	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B2	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B3	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B4	128	Total	C	N	O	S	0	0
			1062	691	182	189			

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B5	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	101	Total	C	N	O	S	0	0
			861	562	153	145	1		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B7	125	Total	C	N	O	S	0	0
			1068	663	204	190	11		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B8	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B9	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	174	Total	C	N	O	S	0	0
			1456	913	264	271	8		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	99	Total	C	N	O	S	0	0
			828	531	137	156	4		

- Molecule 35 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C1	514	Total	C	N	O	S	0	0
			4024	2692	625	675	32		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C2	228	Total	C	N	O	S	0	0
			1833	1193	282	340	18		

- Molecule 37 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C3	260	Total	C	N	O	S	0	0
			2103	1403	337	353	10		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	C4	138	Total	C	N	O	S	0	0
			1153	751	188	210	4		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	CA	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	CB	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	N1	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N2	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	N3	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	N4	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	N5	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	N6	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	QA	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		
47	Qa	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	QB	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		
48	Qb	433	Total	C	N	O	S	0	0
			3367	2103	592	653	19		

- Molecule 49 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	QC	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
49	Qc	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

- Molecule 50 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	QD	241	Total	C	N	O	S	0	0
			1921	1225	330	350	16		
50	Qd	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	QE	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		
51	Qe	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	QF	67	Total	C	N	O	S	0	0
			552	336	100	111	5		
52	Qf	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	QG	101	Total	C	N	O	S	0	0
			893	572	157	162	2		
53	Qg	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	QH	78	Total	C	N	O	S	0	0
			662	432	121	107	2		
54	Qh	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 55 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	QI	62	Total	C	N	O	0	0
			507	331	90	86		
55	Qi	60	Total	C	N	O	0	0
			493	322	87	84		

- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	QJ	49	Total	C	N	O	S	0	0
			405	269	71	63	2		

- Molecule 57 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	QK	73	Total	C	N	O	S	0	0
			520	328	98	92	2		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Qj	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 59 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	S1	689	Total	C	N	O	S	0	0
			5290	3317	922	1012	39		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	S2	427	Total	C	N	O	S	0	0
			3436	2198	591	623	24		

- Molecule 61 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	S3	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	S4	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	S5	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	S6	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	S7	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	S8	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	V1	431	Total	C	N	O	S	0	0
			3316	2092	592	612	20		

- Molecule 68 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	V2	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 69 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	V3	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 70 is ZINC ION (CCD ID: ZN) (formula: Zn).

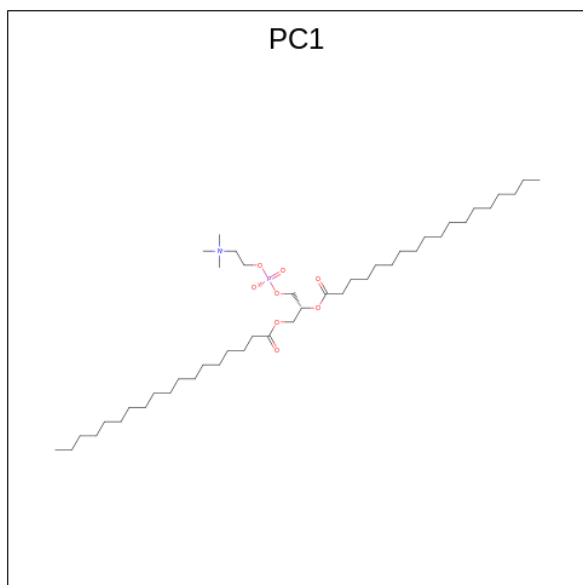
Mol	Chain	Residues	Atoms		AltConf
70	5B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
70	S6	1	Total	Zn	0
			1	1	

- Molecule 71 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



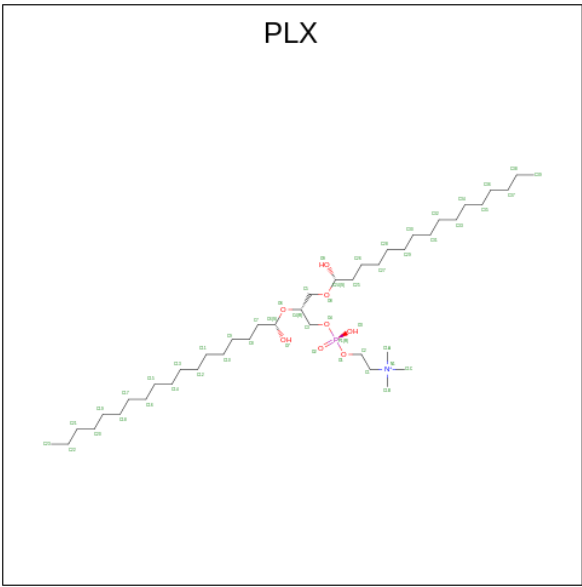
Mol	Chain	Residues	Atoms					AltConf
71	6A	1	Total	C	N	O	P	0
			45	35	1	8	1	
71	B4	1	Total	C	N	O	P	0
			50	40	1	8	1	
71	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
71	C3	1	Total	C	N	O	P	0
			50	40	1	8	1	
71	CB	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	N1	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	N4	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	N4	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	QB	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
71	QB	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qb	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qh	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qj	1	Total	C	N	O	P	0
			43	33	1	8	1	
71	S7	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 72 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



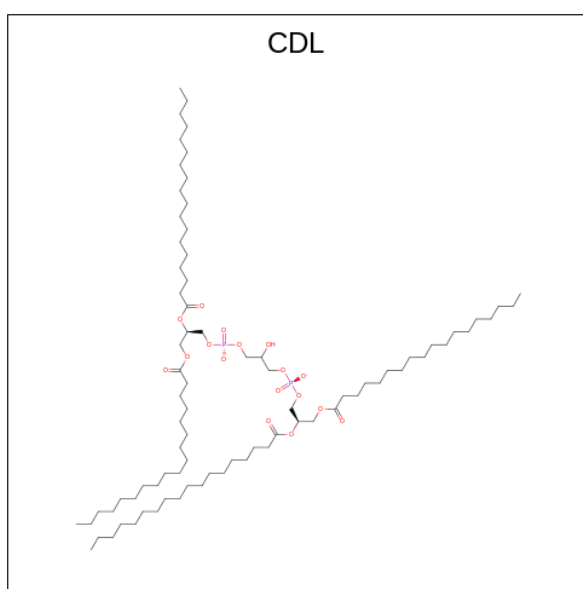
Mol	Chain	Residues	Atoms					AltConf
72	6C	1	Total	C	N	O	P	0
			31	21	1	8	1	
72	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	B5	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
72	N2	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	N4	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	QE	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	QI	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 73 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



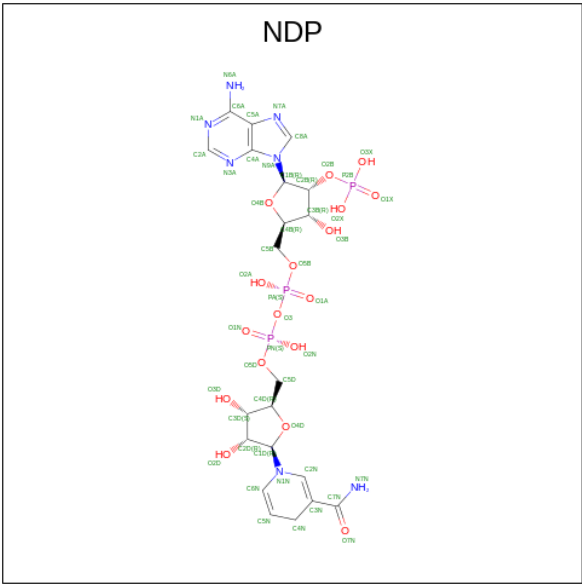
Mol	Chain	Residues	Atoms				AltConf
73	A8	1	Total	C	O	P	0
			83	64	17	2	
73	AL	1	Total	C	O	P	0
			91	72	17	2	
73	AL	1	Total	C	O	P	0
			89	70	17	2	
73	B4	1	Total	C	O	P	0
			80	61	17	2	
73	B5	1	Total	C	O	P	0
			100	81	17	2	
73	CB	1	Total	C	O	P	0
			100	81	17	2	
73	N1	1	Total	C	O	P	0
			78	59	17	2	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
73	N2	1	Total 68	49	17	2	0
73	N5	1	Total 89	70	17	2	0
73	N5	1	Total 100	81	17	2	0
73	QB	1	Total 62	43	17	2	0
73	QD	1	Total 64	45	17	2	0
73	QH	1	Total 61	42	17	2	0
73	QH	1	Total 64	45	17	2	0
73	Qb	1	Total 64	45	17	2	0
73	Qh	1	Total 55	36	17	2	0

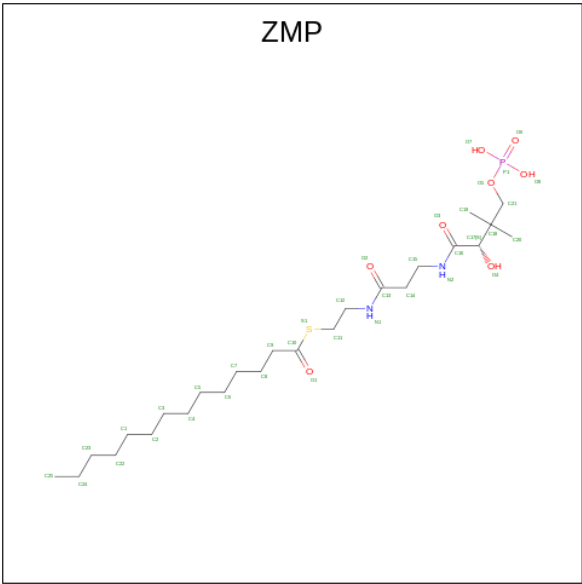
- Molecule 74 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
74	A9	1	Total 48	21	7	17	3	0

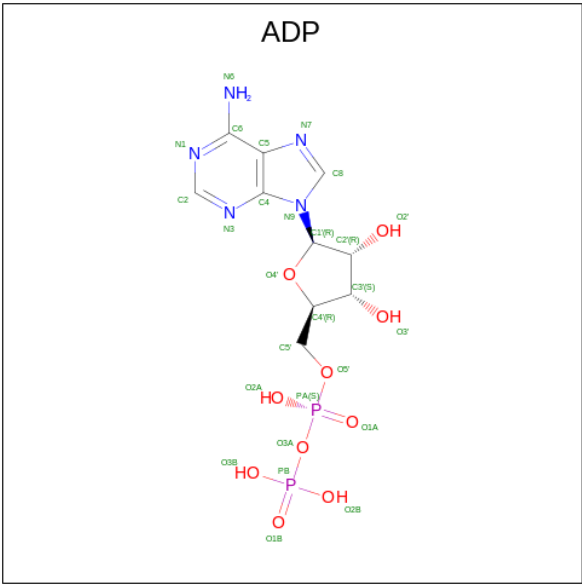
- Molecule 75 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alan

yl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



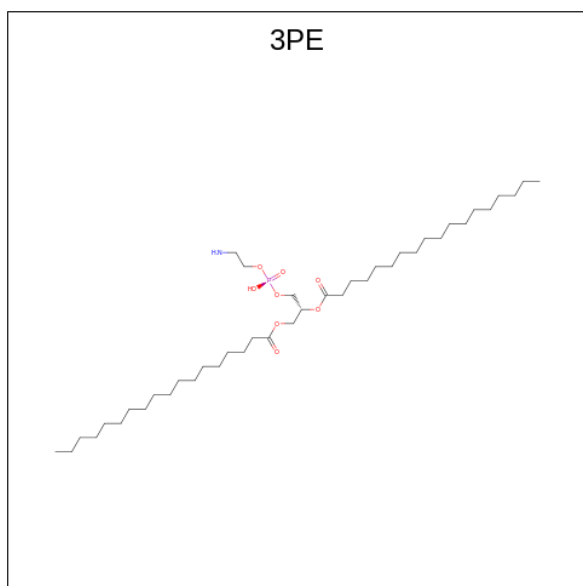
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
75	AB	1	36	25	2	7	1	1	0
75	AC	1	36	25	2	7	1	1	0

- Molecule 76 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



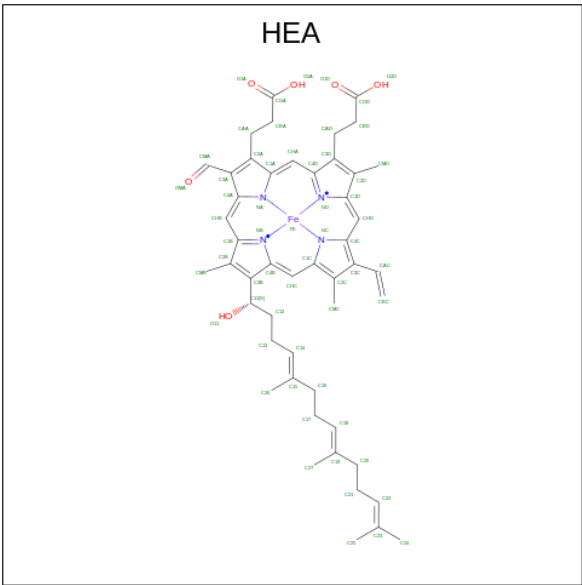
Mol	Chain	Residues	Atoms					AltConf
76	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 77 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
77	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
77	C1	1	Total	C	N	O	P	0
			51	41	1	8	1	
77	CB	1	Total	C	N	O	P	0
			51	41	1	8	1	
77	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
77	QC	1	Total	C	N	O	P	0
			34	24	1	8	1	
77	QE	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 78 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
78	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0
78	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0

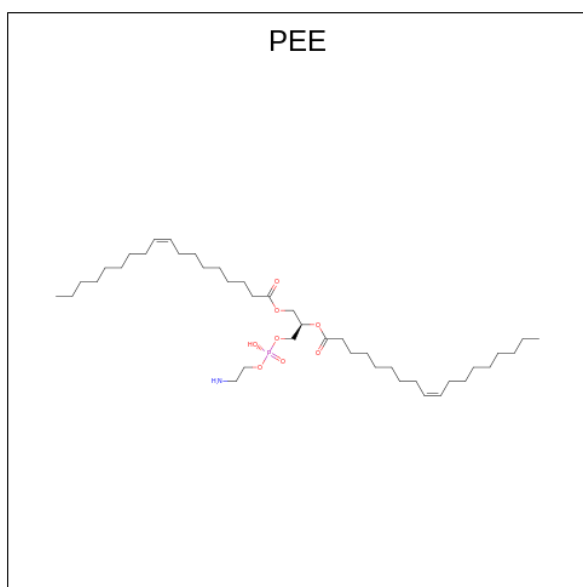
- Molecule 79 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
79	C1	1	Total	Cu	0
			1	1	
79	C2	2	Total	Cu	0
			2	2	

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

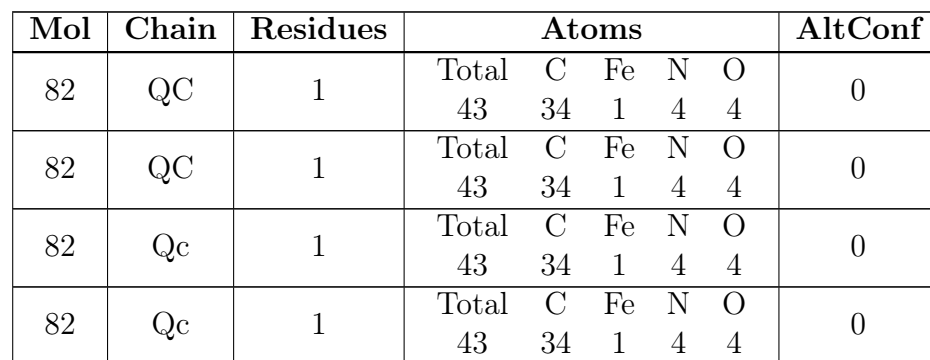
Mol	Chain	Residues	Atoms		AltConf
80	C1	1	Total	Mg	0
			1	1	
80	S1	1	Total	Mg	0
			1	1	

- Molecule 81 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).

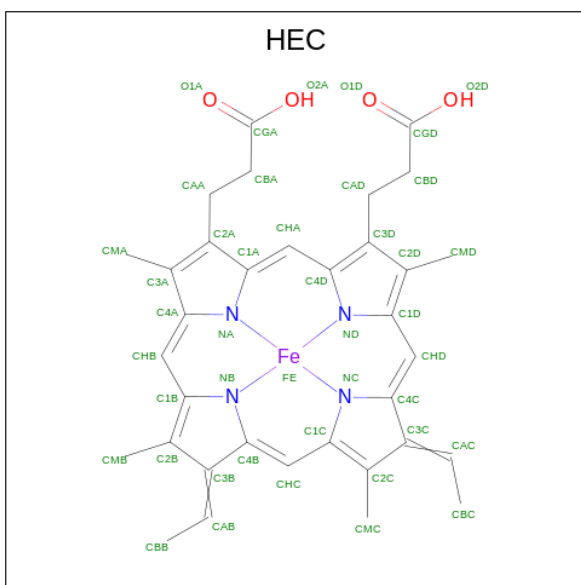


Mol	Chain	Residues	Atoms					AltConf
81	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
81	N4	1	Total	C	N	O	P	0
			46	36	1	8	1	
81	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
81	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
81	N6	1	Total	C	N	O	P	0
			51	41	1	8	1	
81	QC	1	Total	C	N	O	P	0
			40	30	1	8	1	
81	QE	1	Total	C	N	O	P	0
			47	37	1	8	1	
81	Qc	1	Total	C	N	O	P	0
			42	32	1	8	1	
81	Qe	1	Total	C	N	O	P	0
			44	34	1	8	1	
81	S2	1	Total	C	N	O	P	0
			48	38	1	8	1	
81	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 82 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

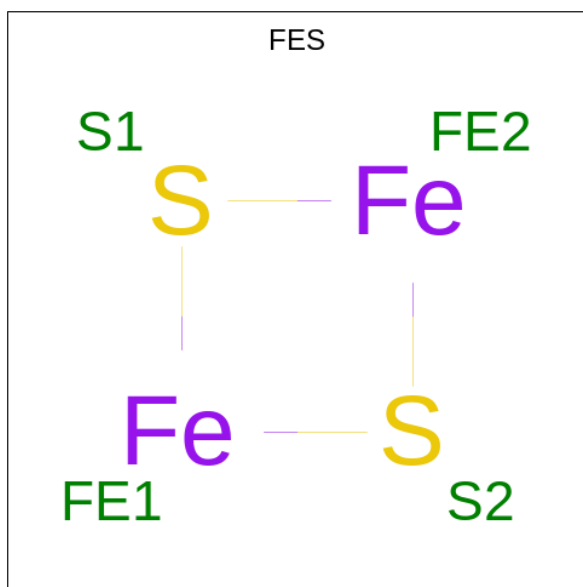


- Molecule 83 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



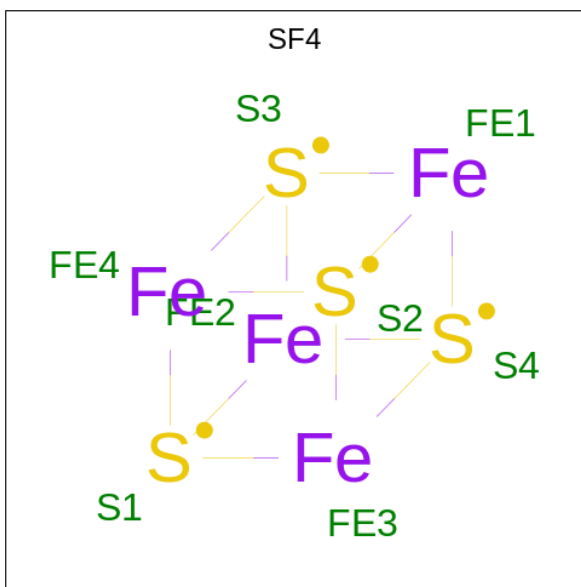
Mol	Chain	Residues	Atoms					AltConf
83	QD	1	Total 43	C 34	Fe 1	N 4	O 4	0
83	Qd	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 84 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



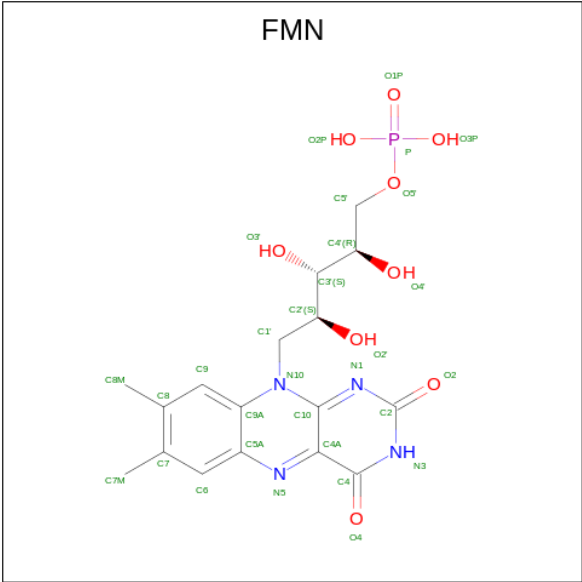
Mol	Chain	Residues	Atoms			AltConf
84	QE	1	Total	Fe	S	0
			4	2	2	
84	Qe	1	Total	Fe	S	0
			4	2	2	
84	S1	1	Total	Fe	S	0
			4	2	2	
84	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 85 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
85	S1	1	Total	Fe	S	0
			8	4	4	
85	S1	1	Total	Fe	S	0
			8	4	4	
85	S7	1	Total	Fe	S	0
			8	4	4	
85	S8	1	Total	Fe	S	0
			8	4	4	
85	S8	1	Total	Fe	S	0
			8	4	4	
85	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 86 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

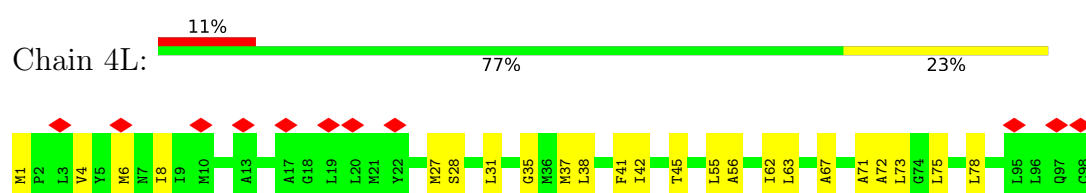


Mol	Chain	Residues	Atoms					AltConf
86	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

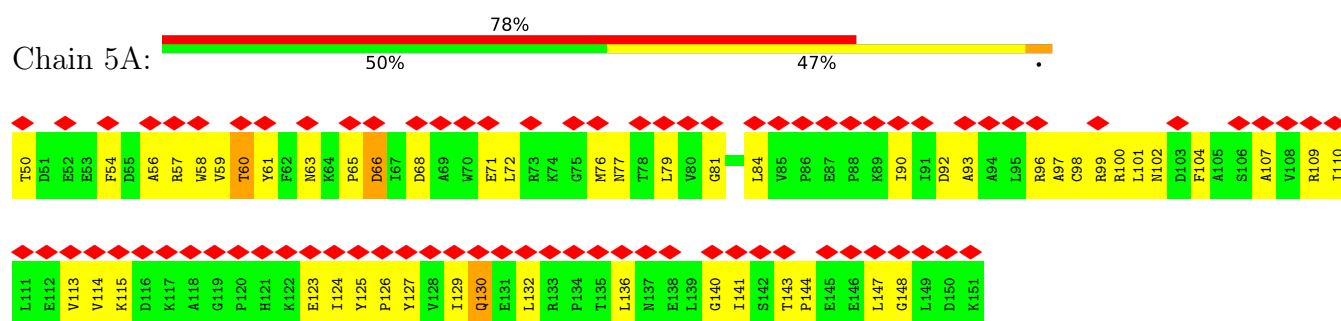
3 Residue-property plots [i](#)

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.

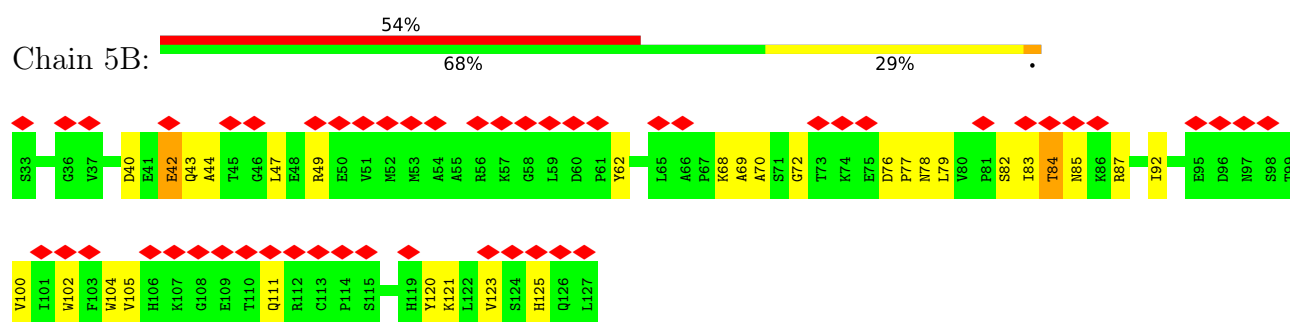
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



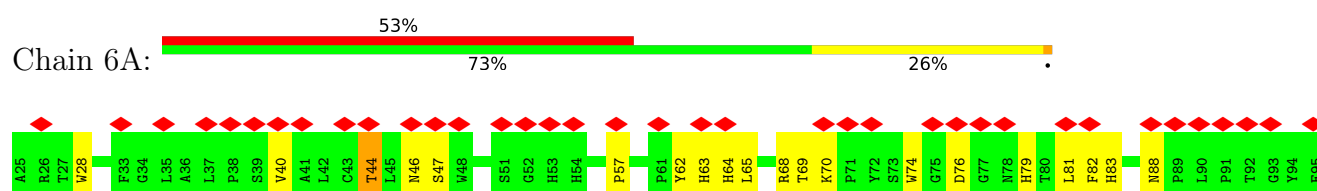
- Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial



- Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial

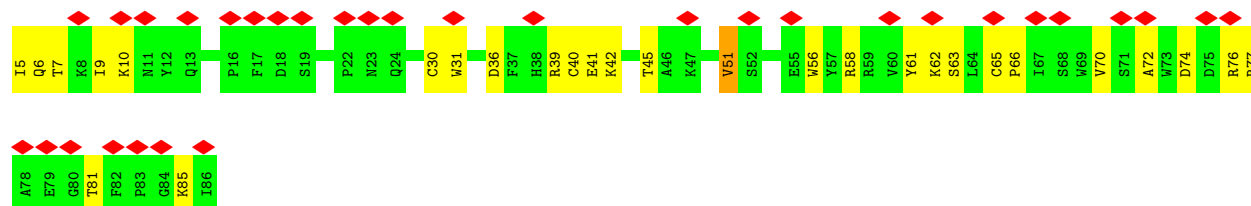
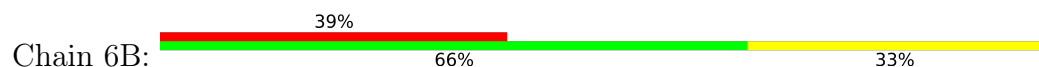


- Molecule 4: Cytochrome c oxidase subunit

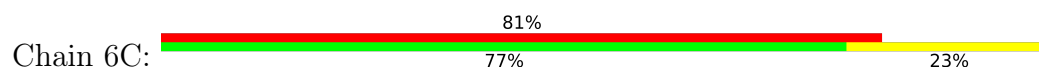




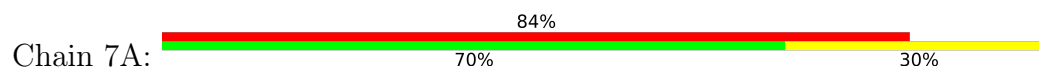
• Molecule 5: Cytochrome c oxidase subunit



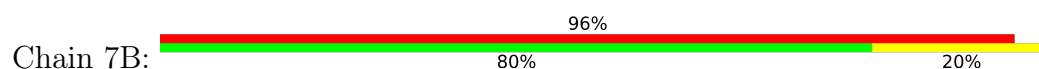
• Molecule 6: Cytochrome c oxidase subunit 6C



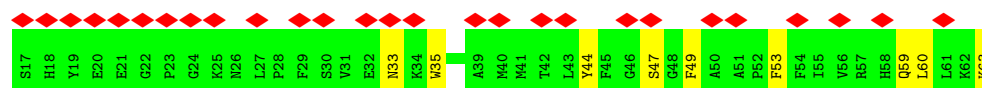
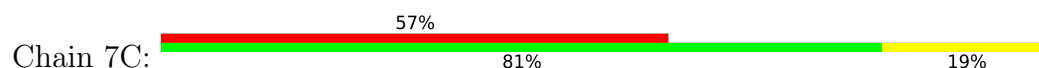
• Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial



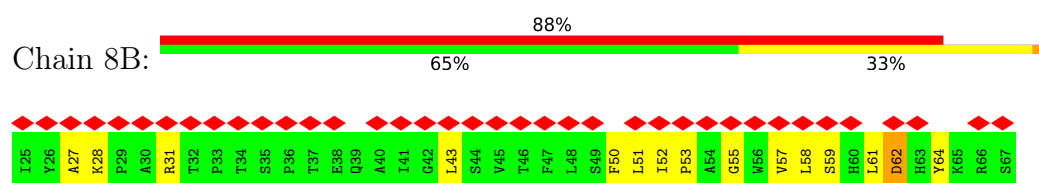
• Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial



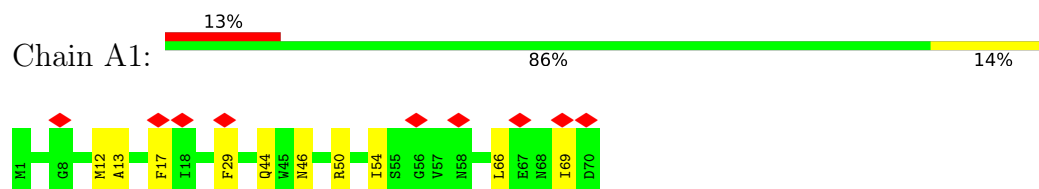
• Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial



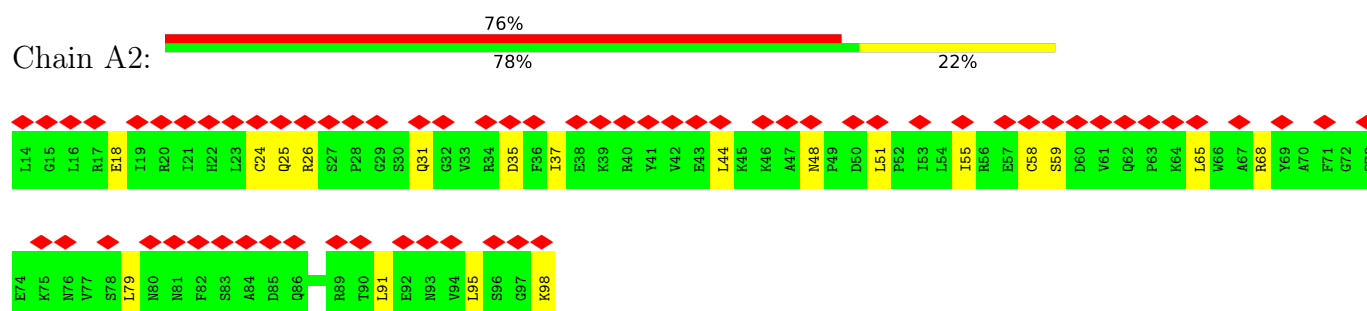
• Molecule 10: Cytochrome c oxidase subunit 8



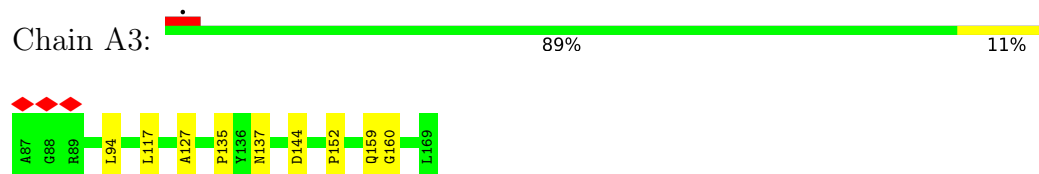
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



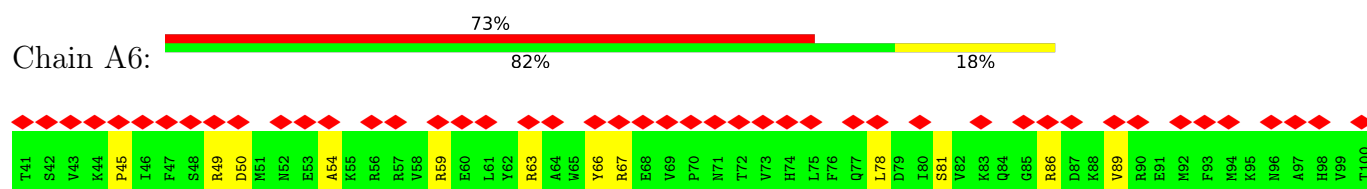
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

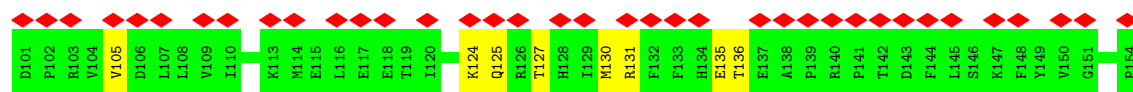


- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

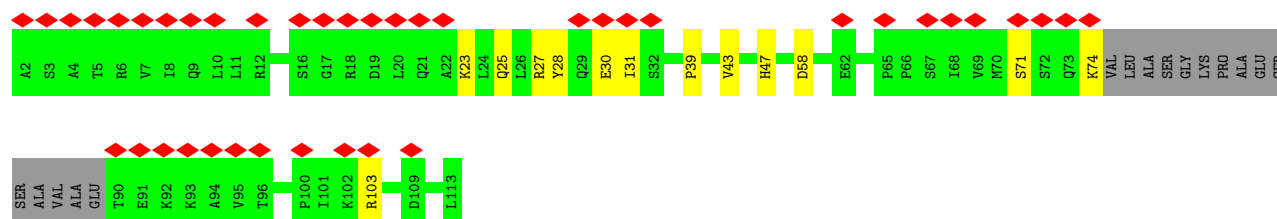
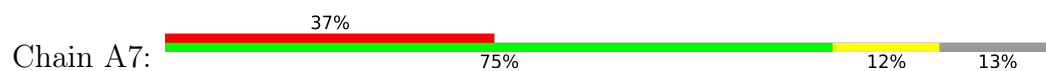


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

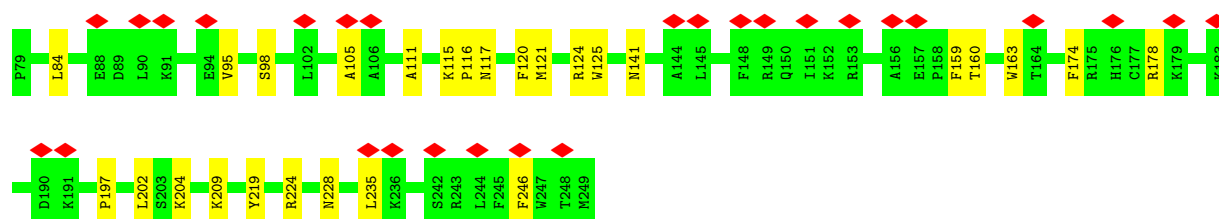
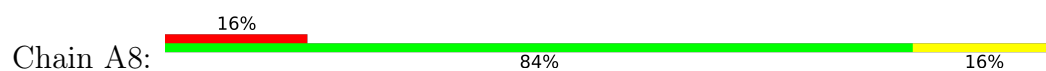




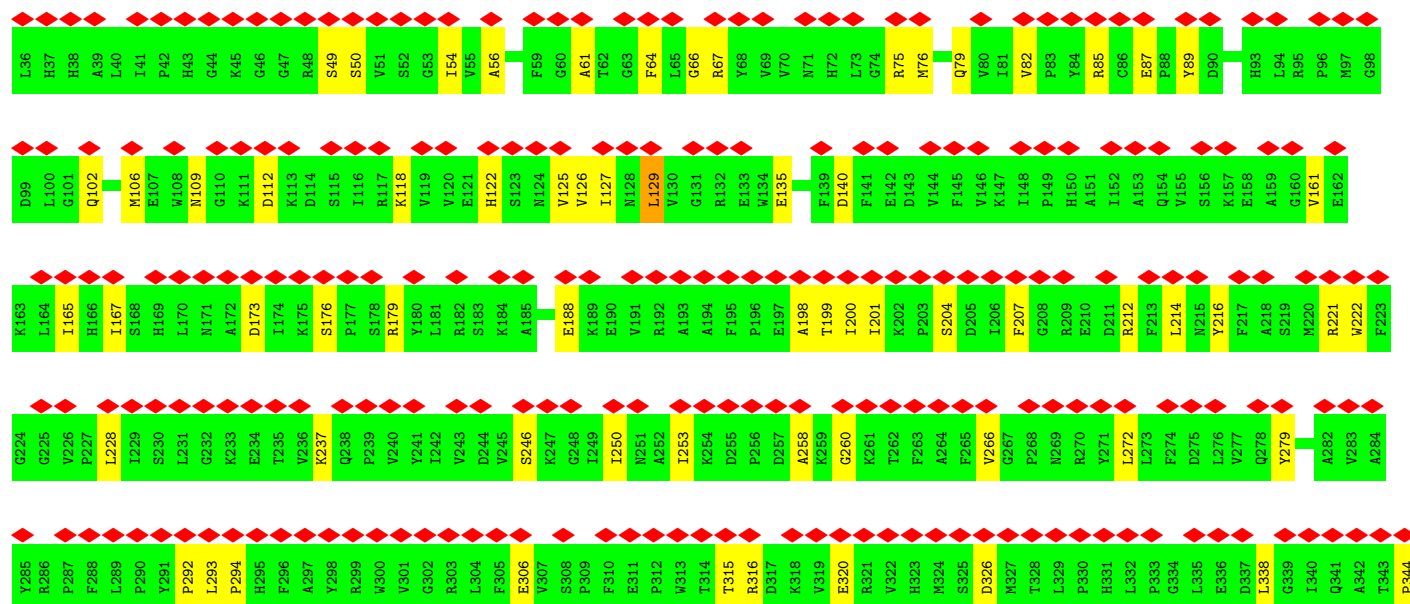
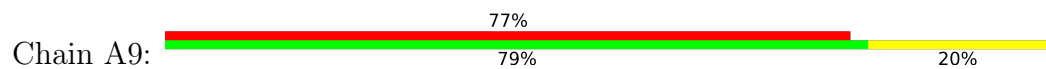
• Molecule 16: Complex I-B14.5a

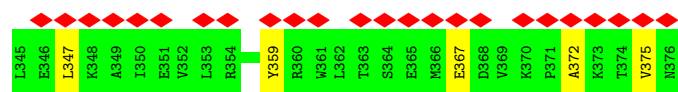


• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

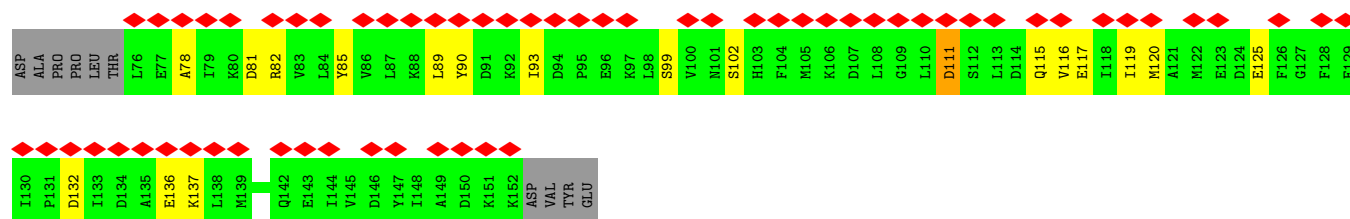
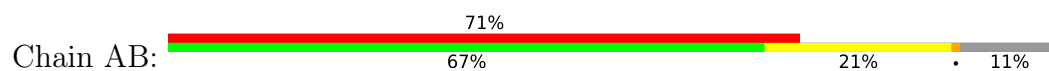


• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

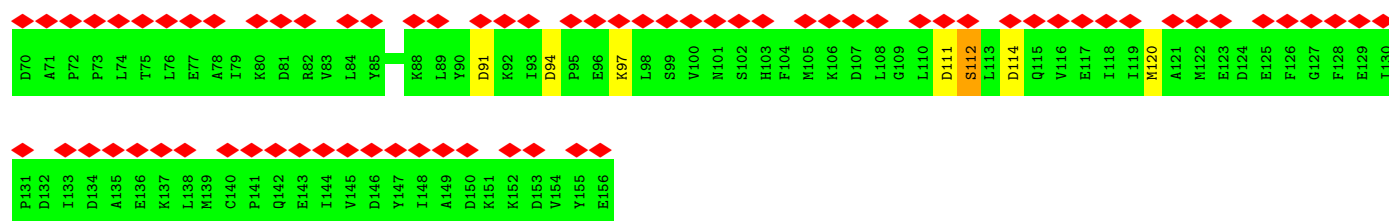
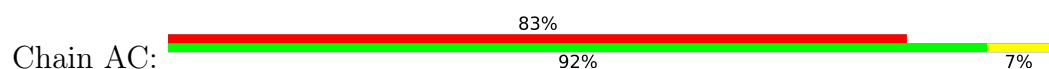




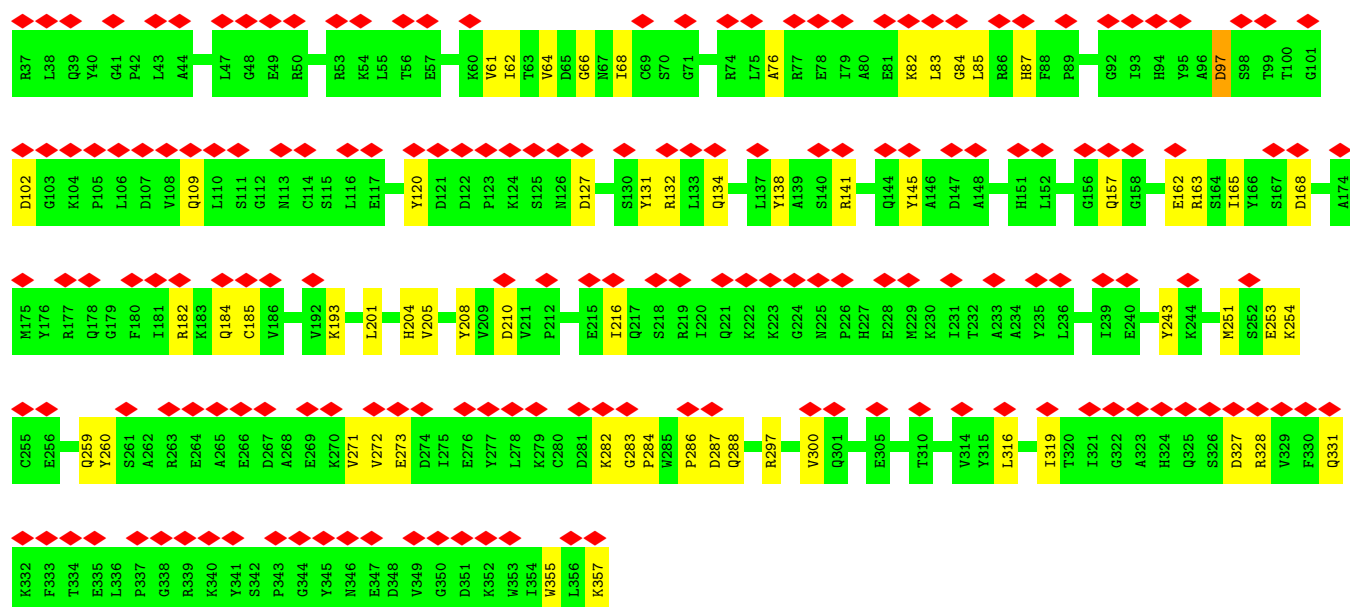
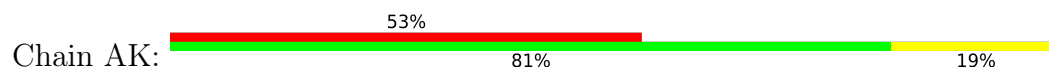
- Molecule 19: Acyl carrier protein



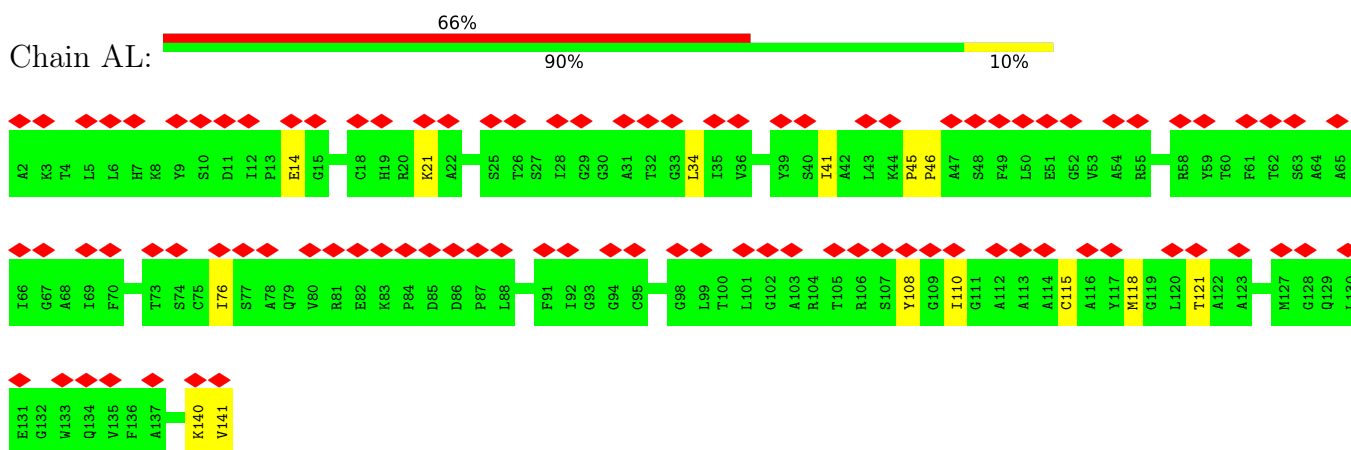
- Molecule 19: Acyl carrier protein



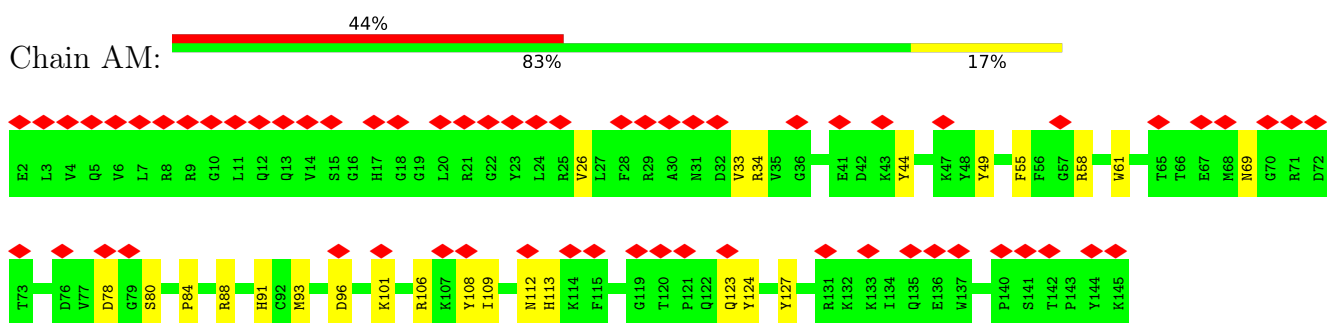
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



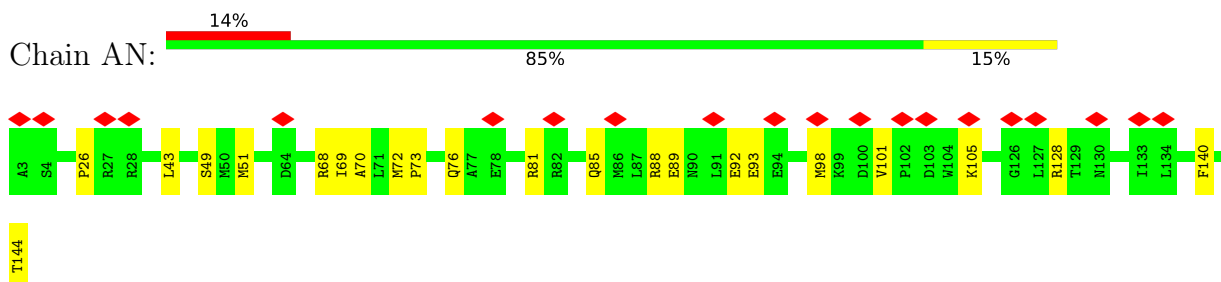
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



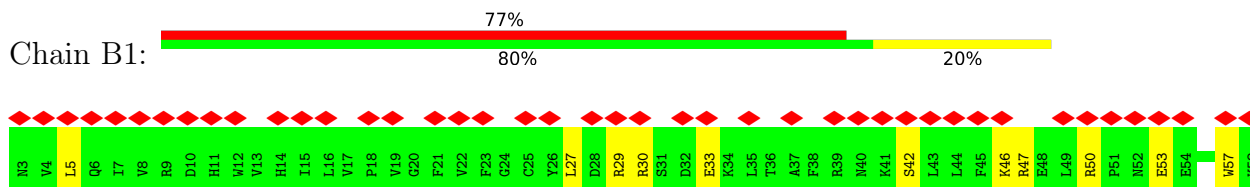
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



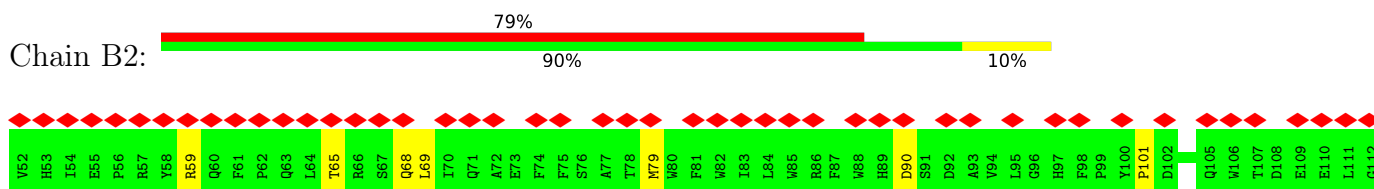
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

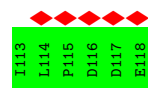


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

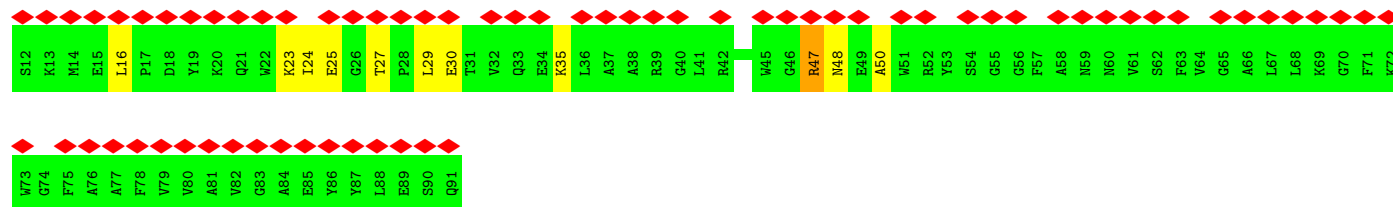
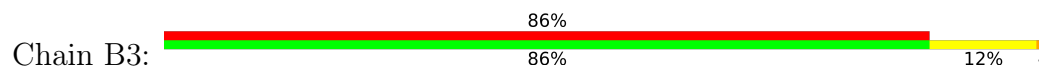


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

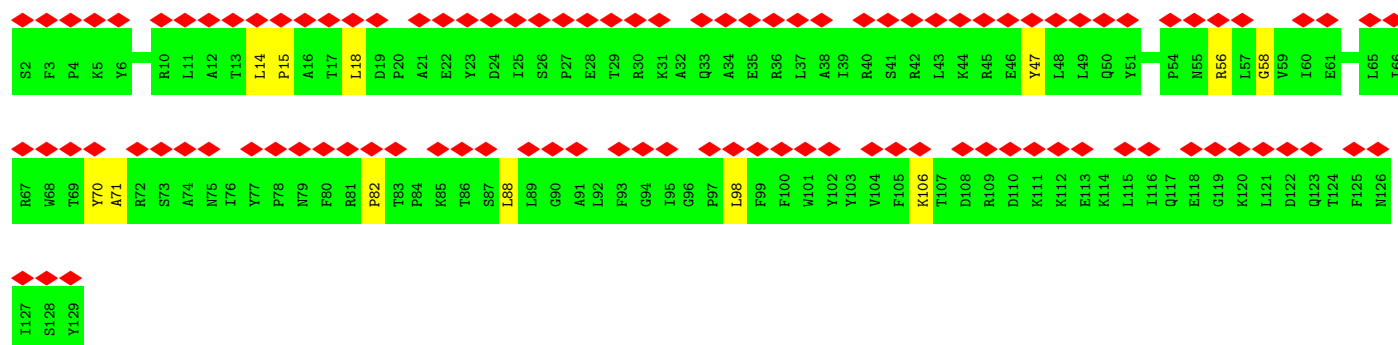
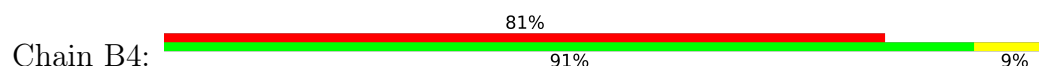




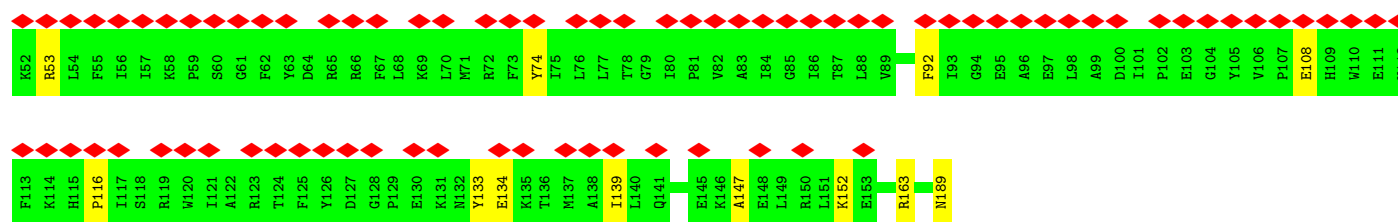
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

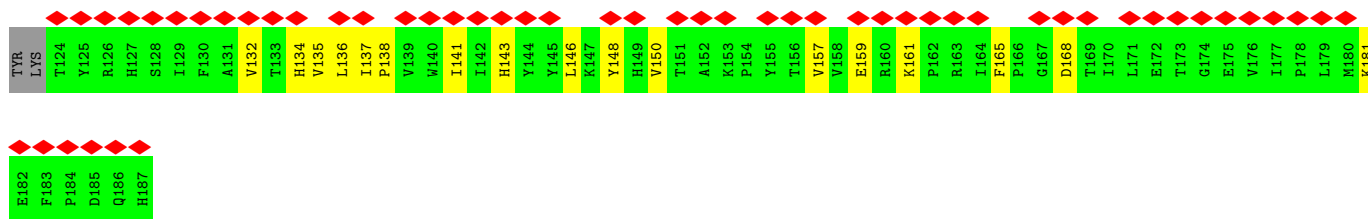


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

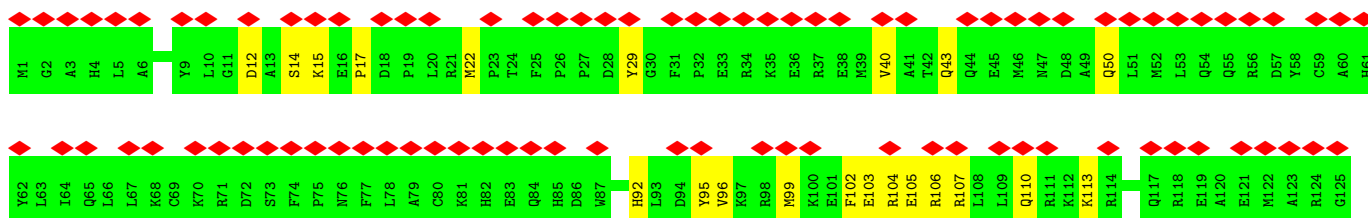
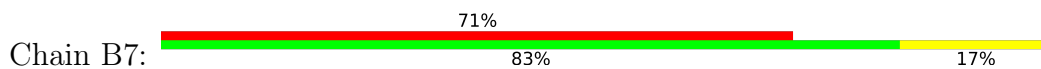


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

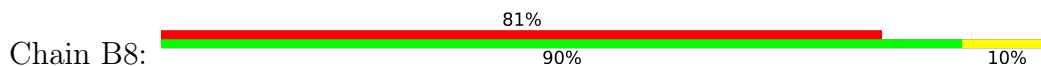




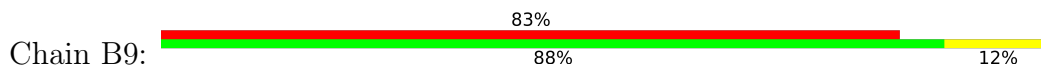
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



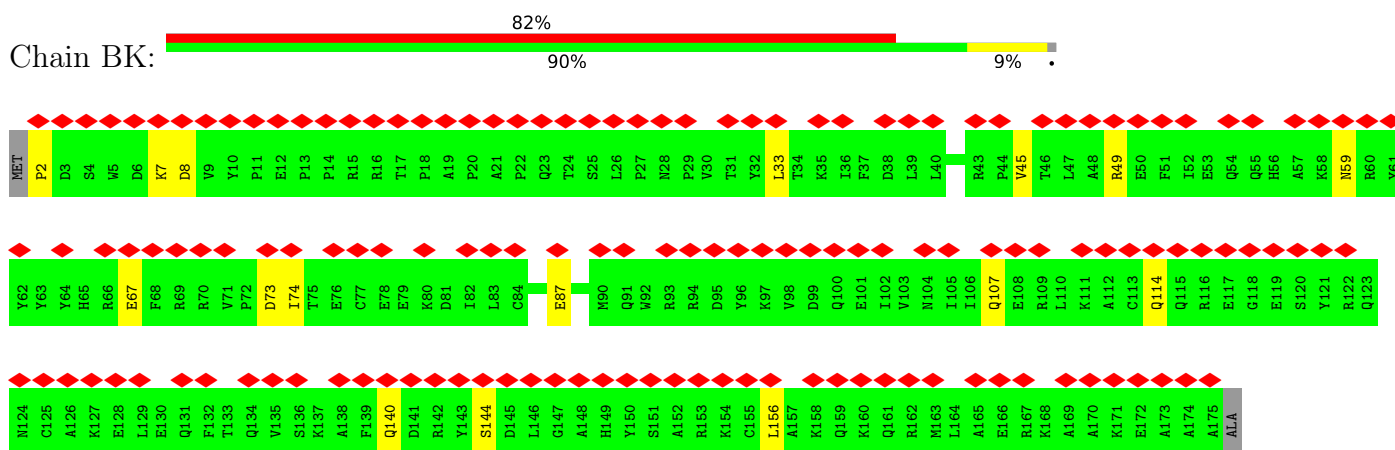
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



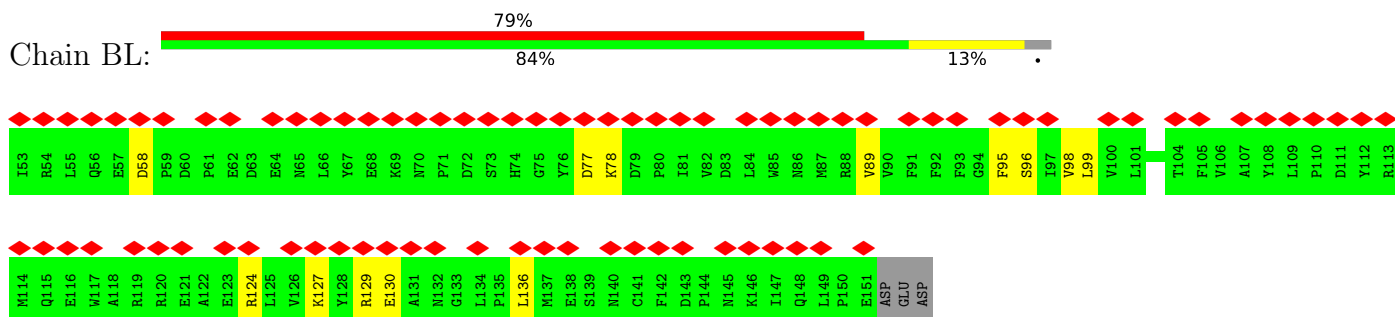
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



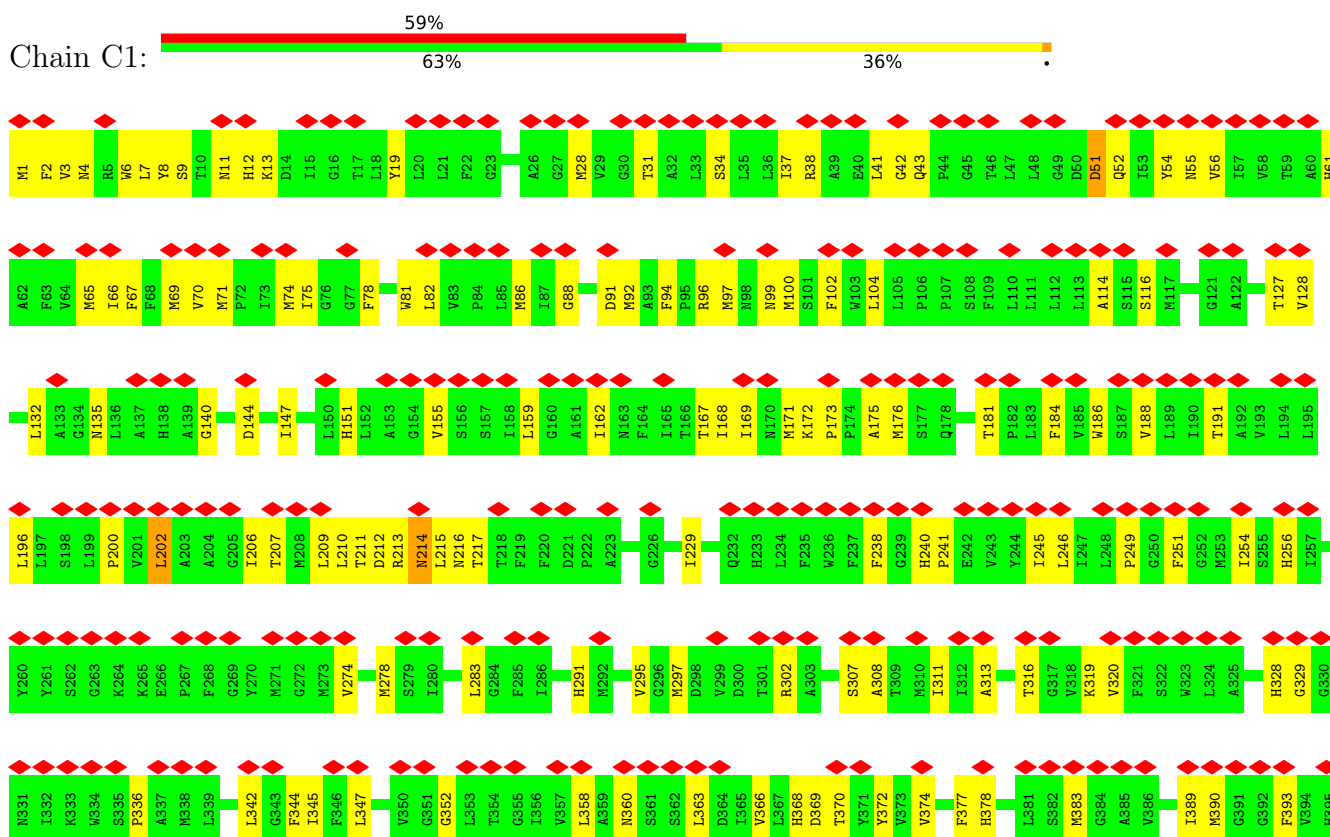
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

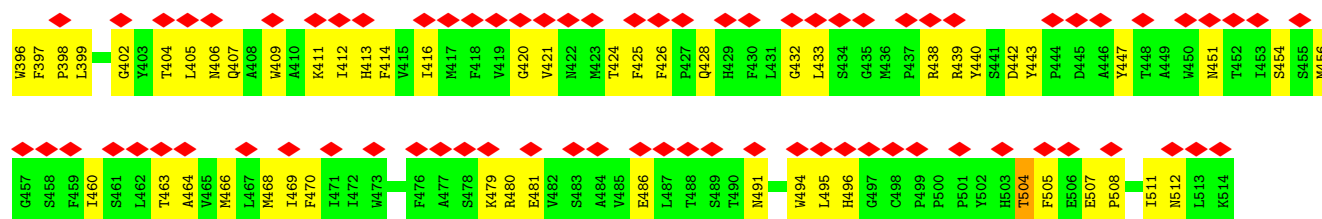


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

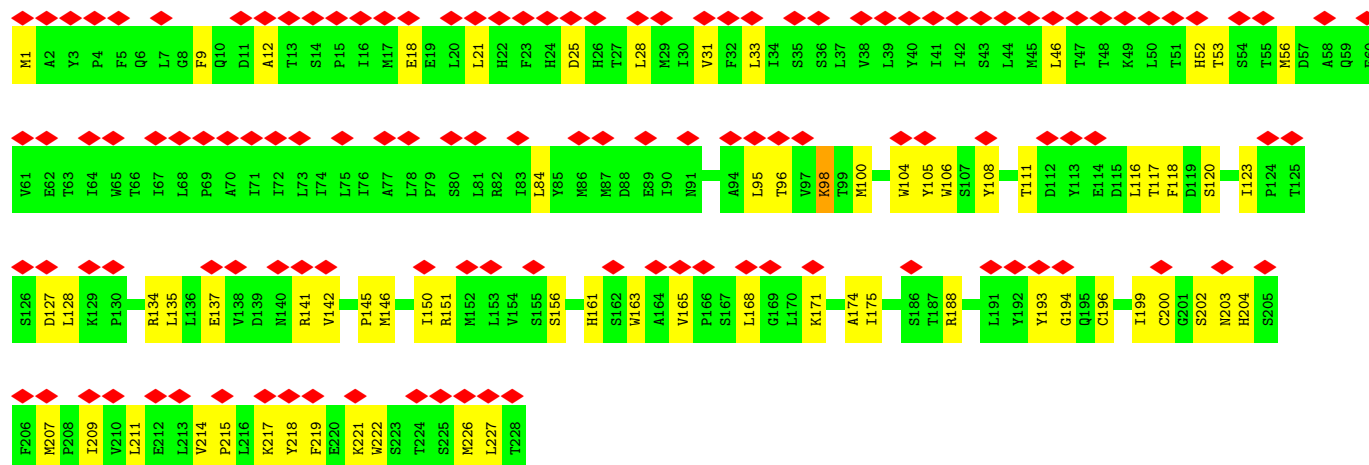
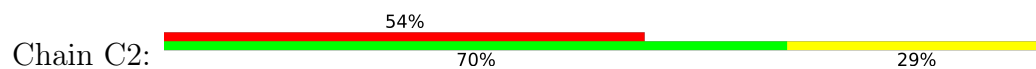


- Molecule 35: Cytochrome c oxidase subunit 1

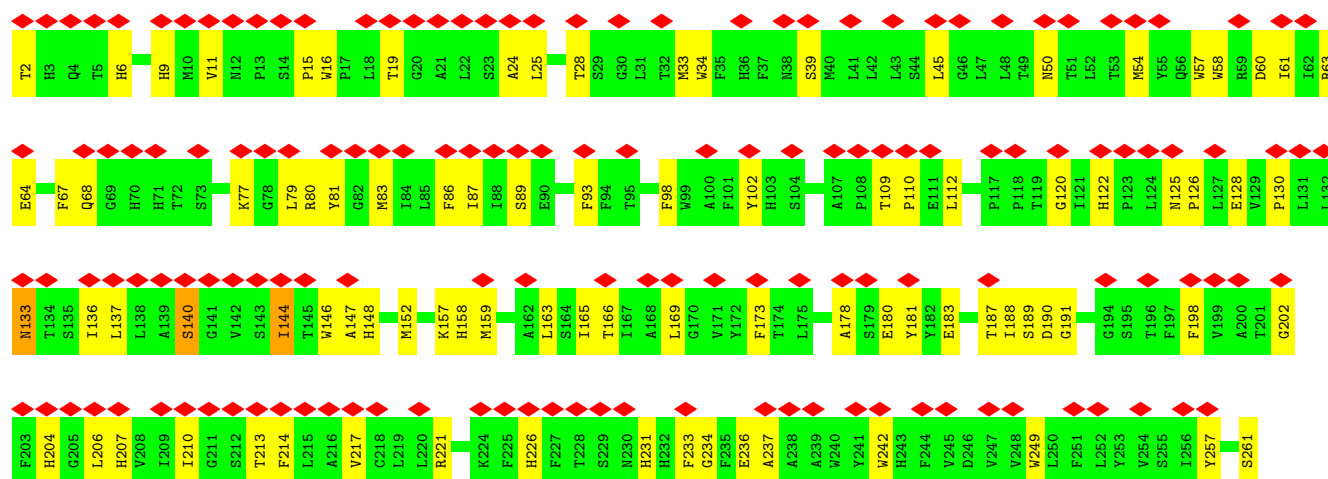




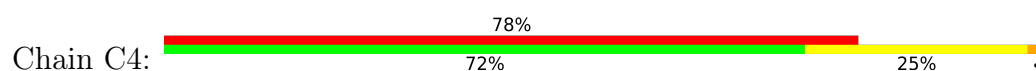
• Molecule 36: Cytochrome c oxidase subunit 2

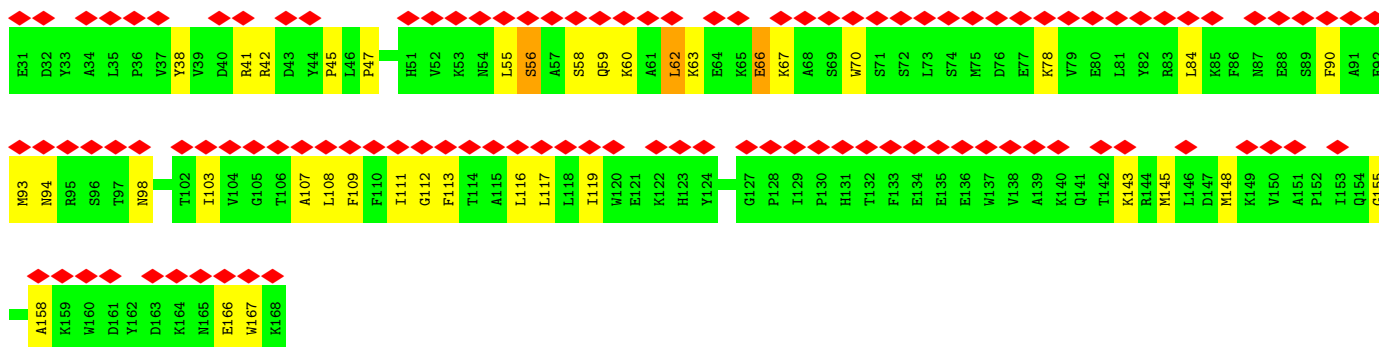


• Molecule 37: Cytochrome c oxidase subunit 3

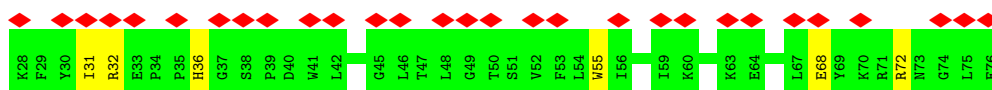


• Molecule 38: Cytochrome c oxidase subunit 4

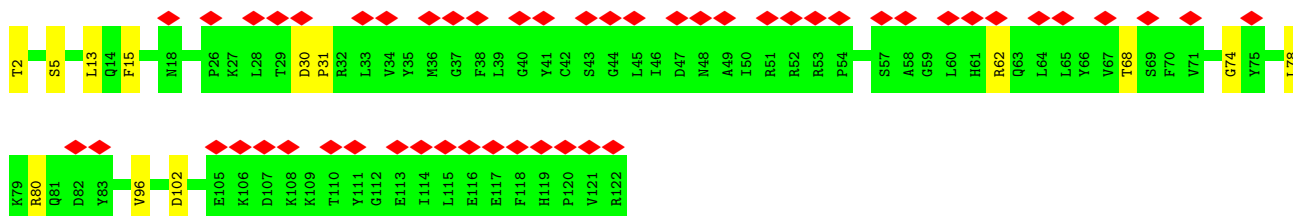
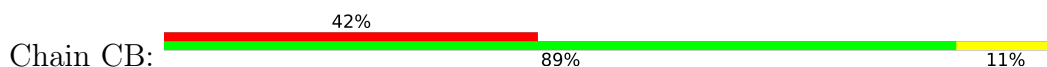




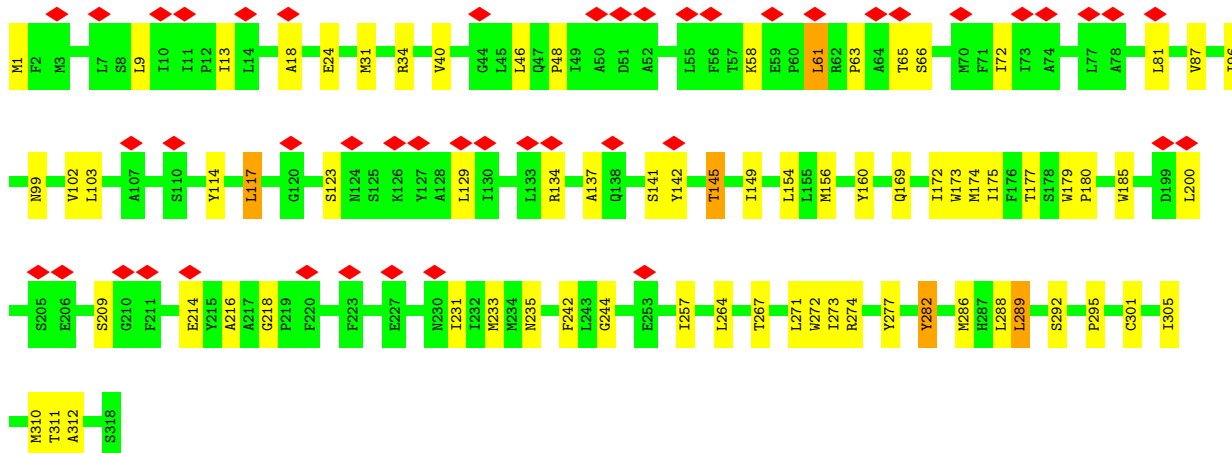
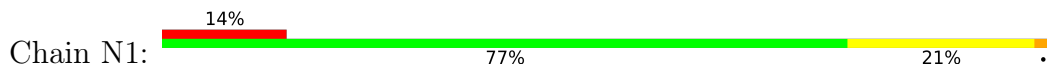
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



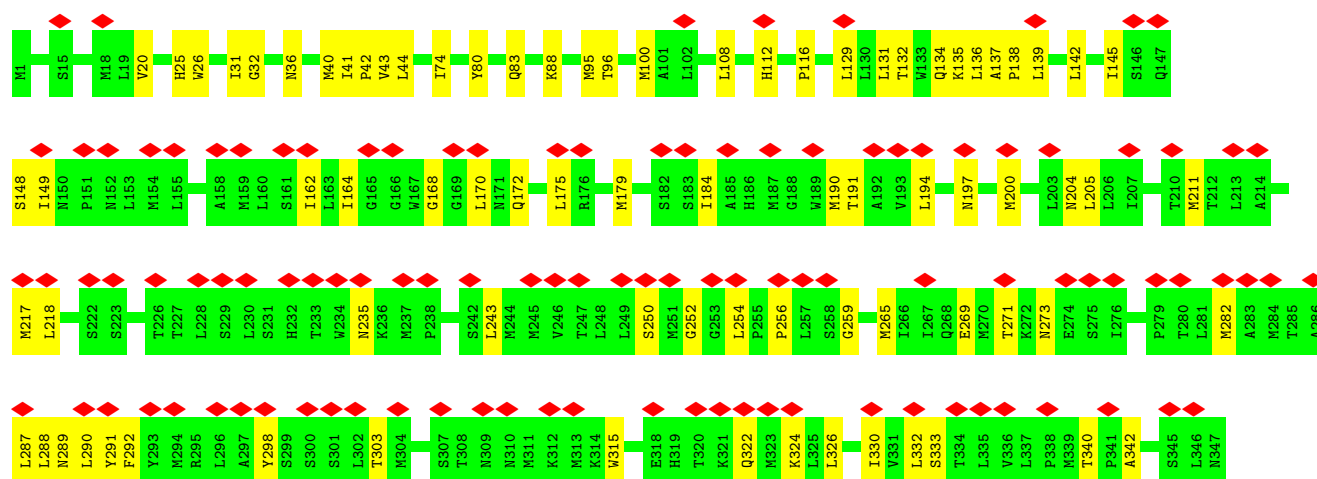
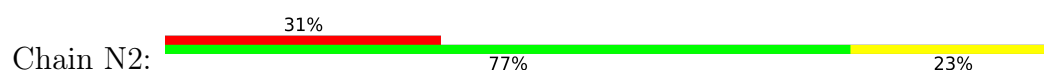
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2



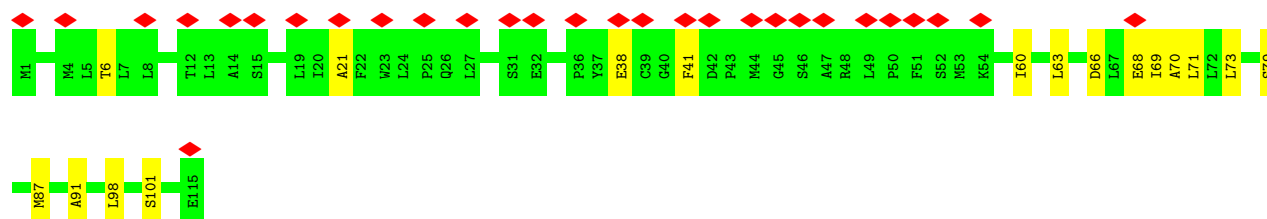
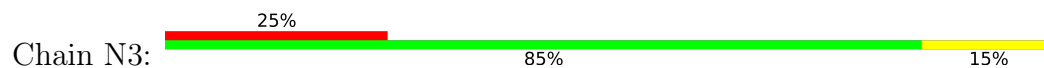
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



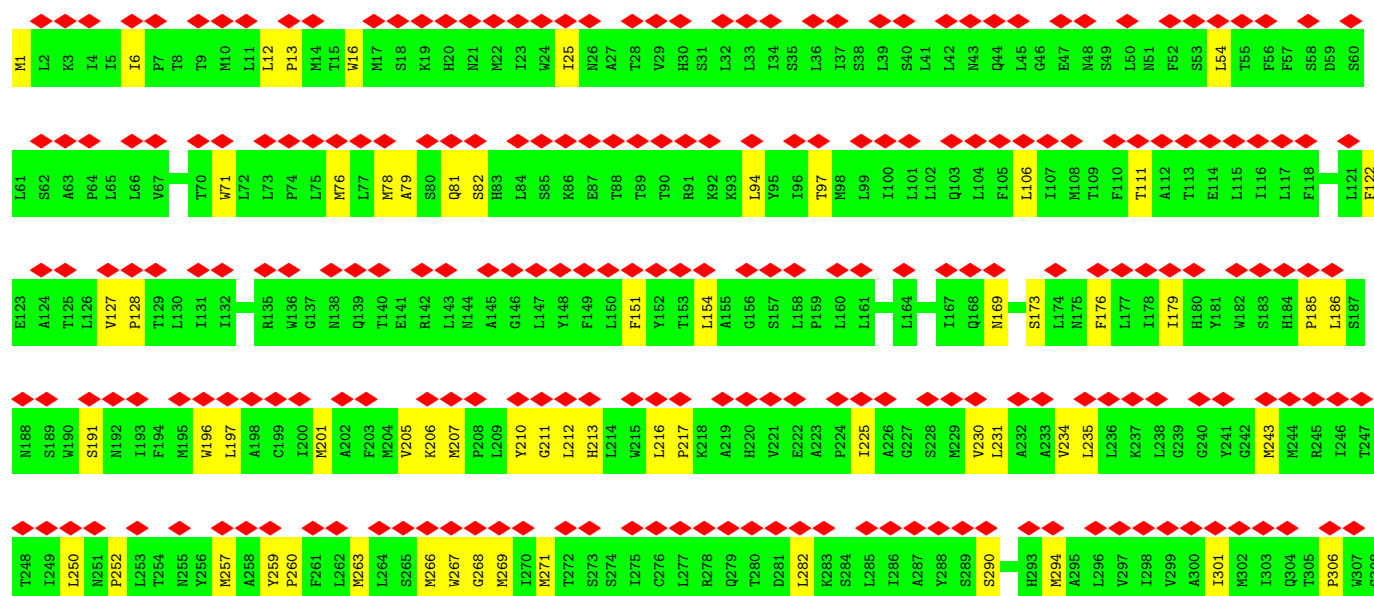
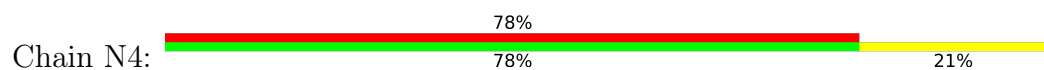
- Molecule 42: NADH-ubiquinone oxidoreductase chain 2

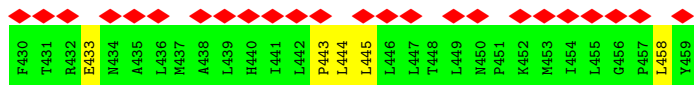


• Molecule 43: NADH-ubiquinone oxidoreductase chain 3

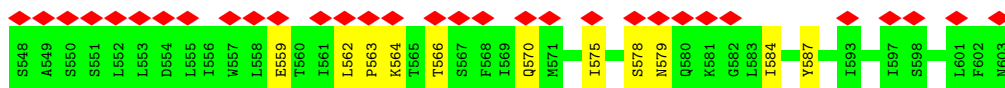


• Molecule 44: NADH-ubiquinone oxidoreductase chain 4

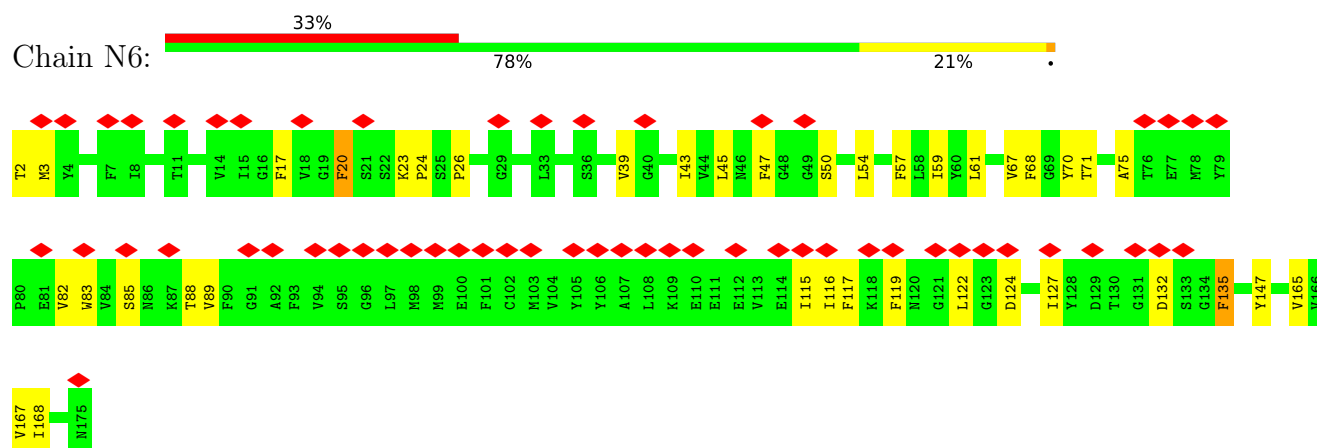




Chain N5:



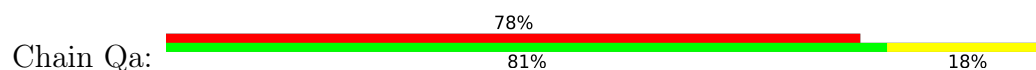
- Molecule 46: NADH-ubiquinone oxidoreductase chain 6

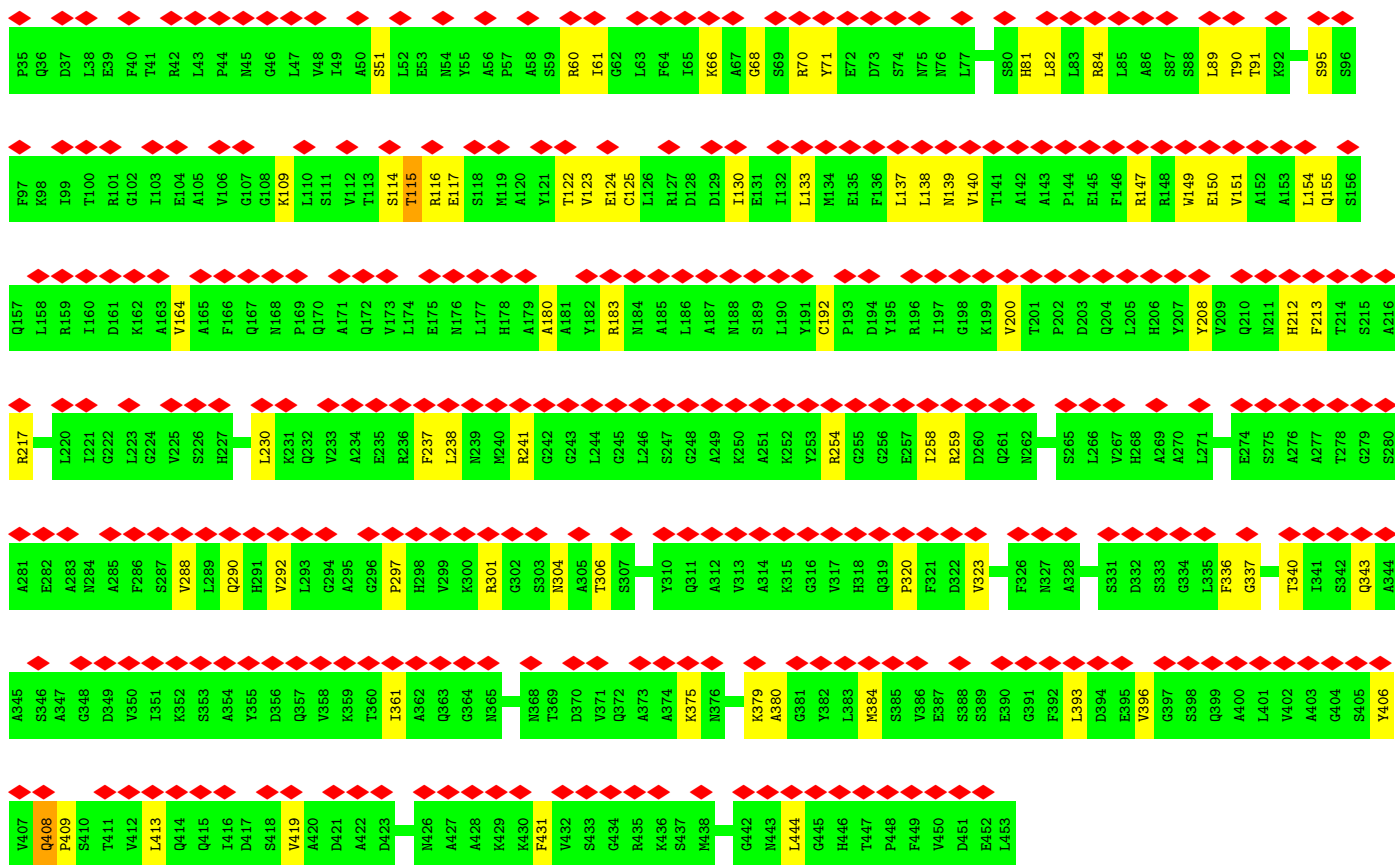


- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

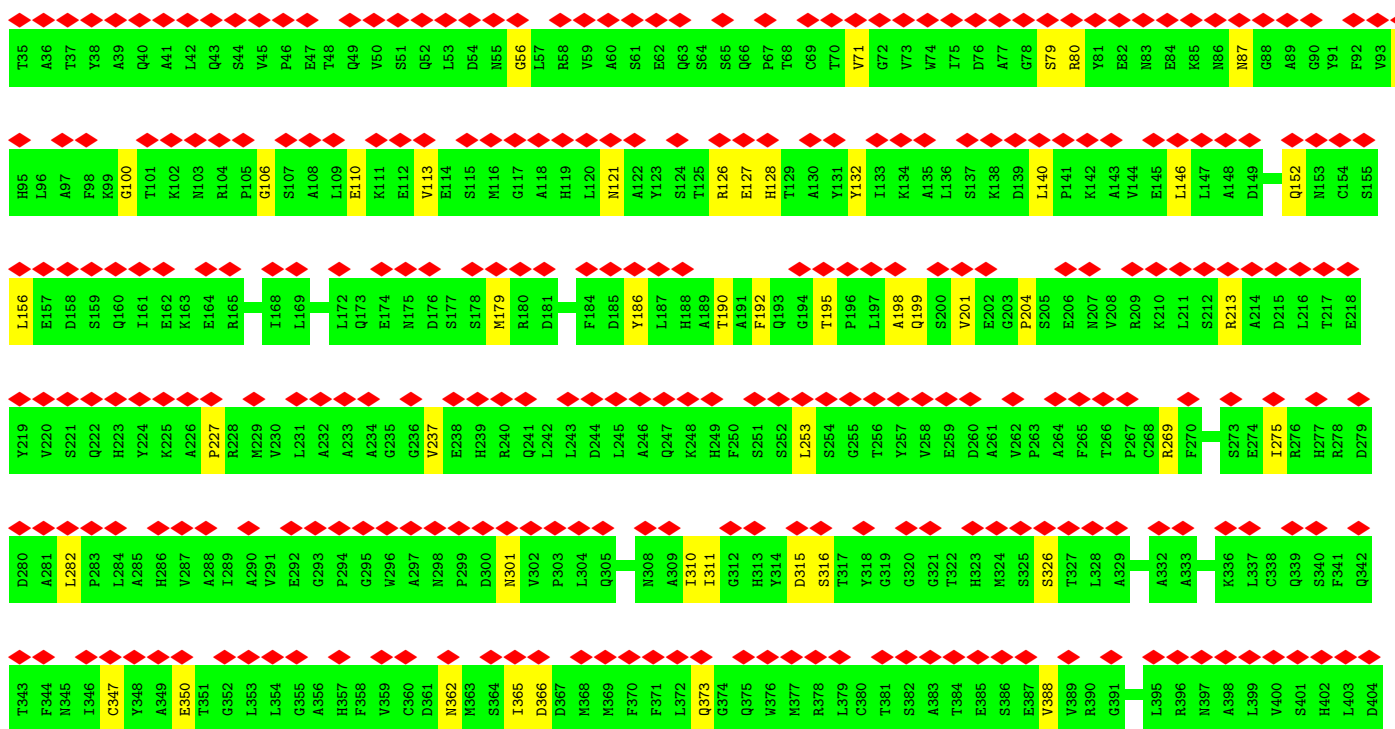
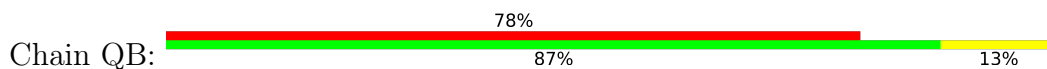


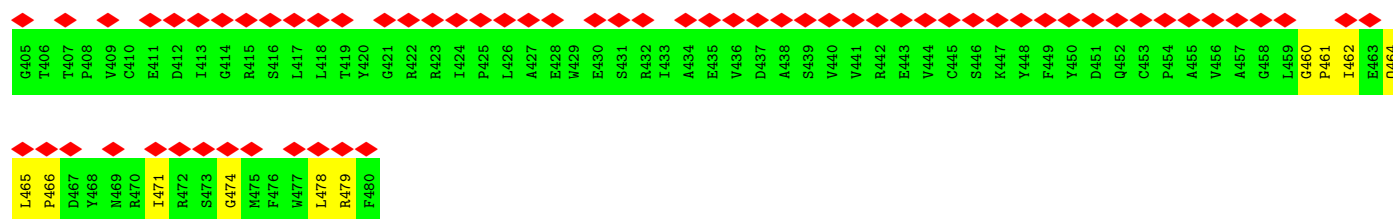
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial





• Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

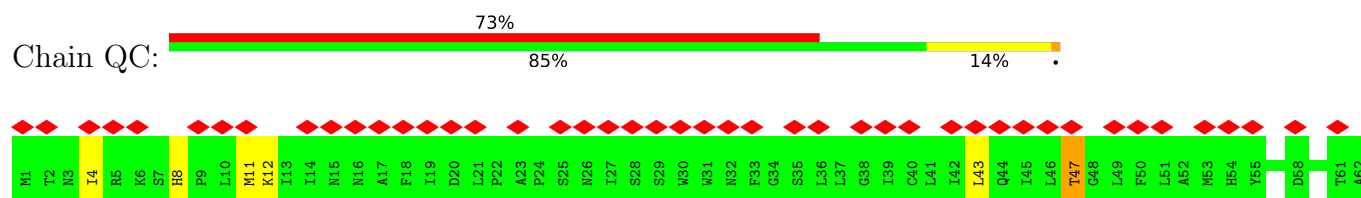


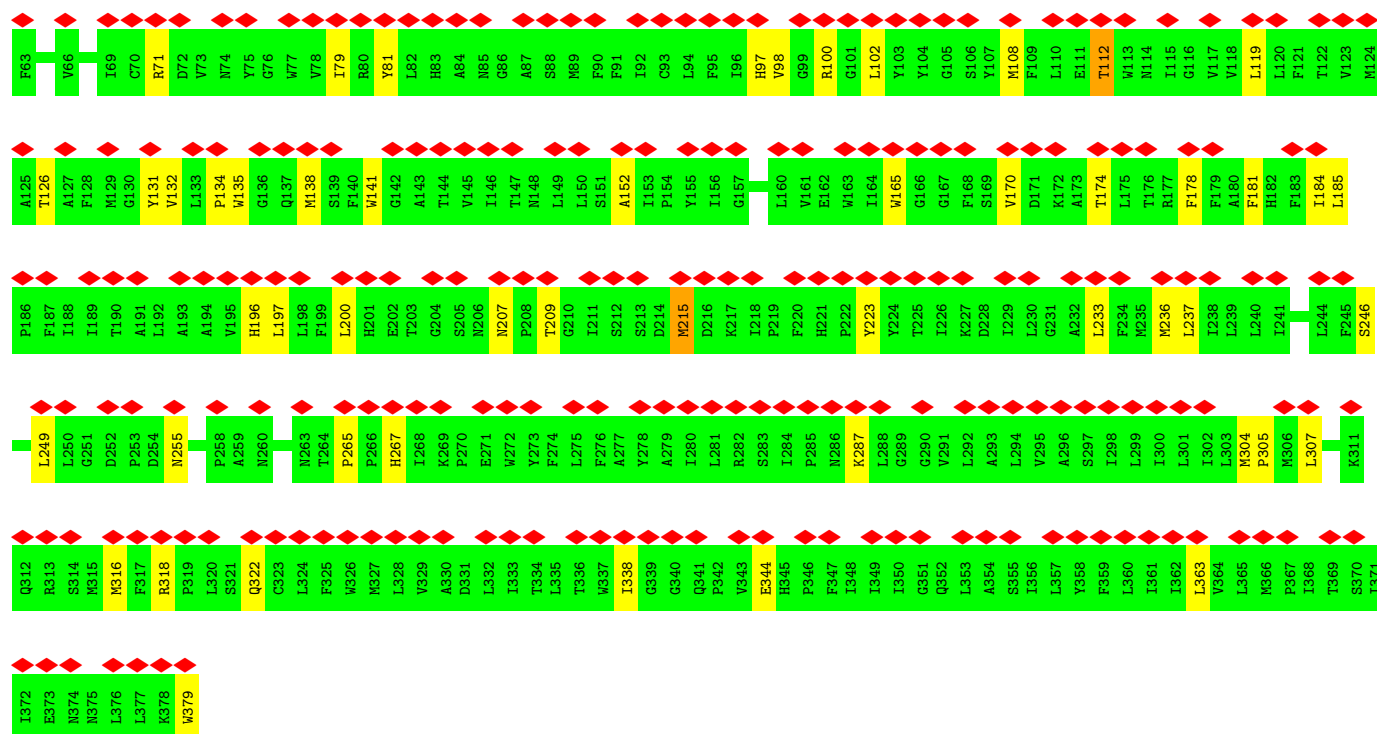


• Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

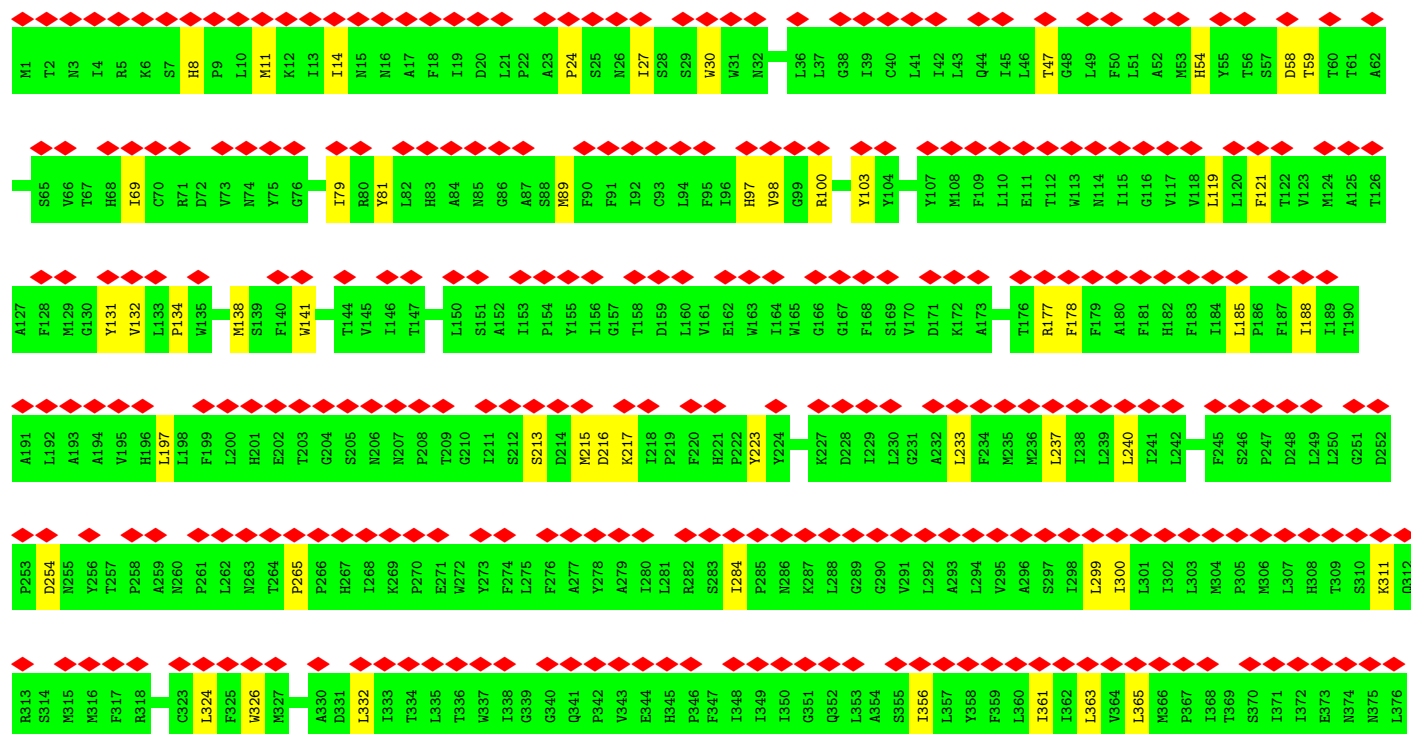
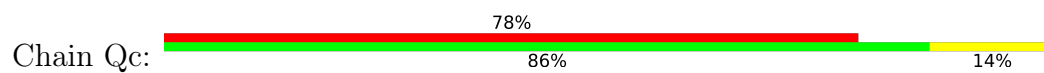


• Molecule 49: Cytochrome b



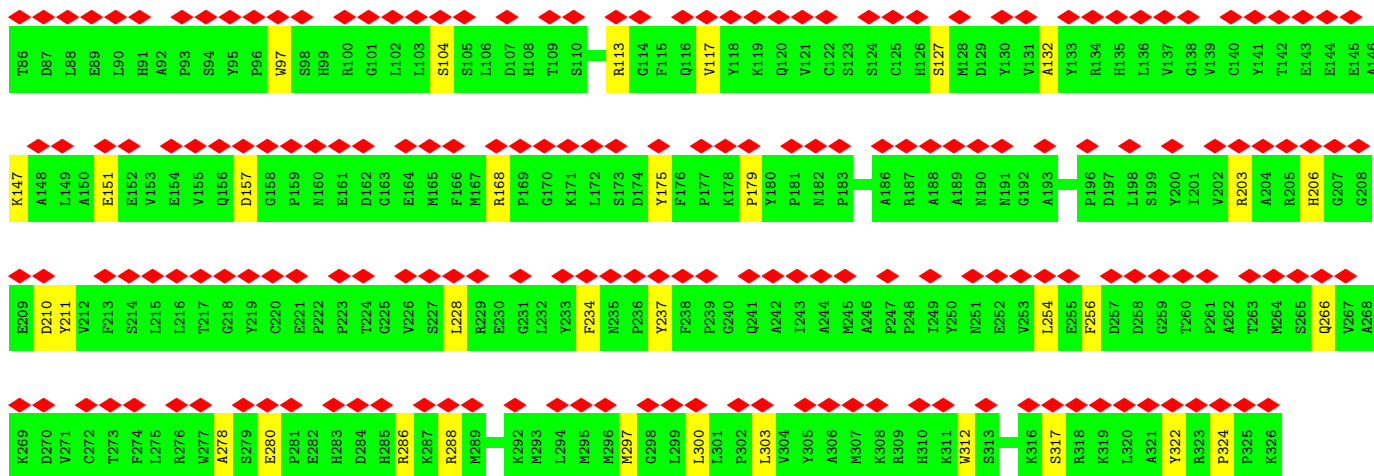
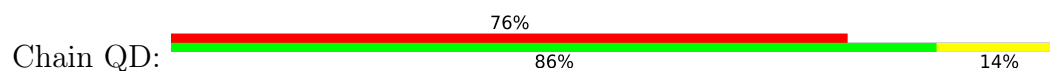


• Molecule 49: Cytochrome b

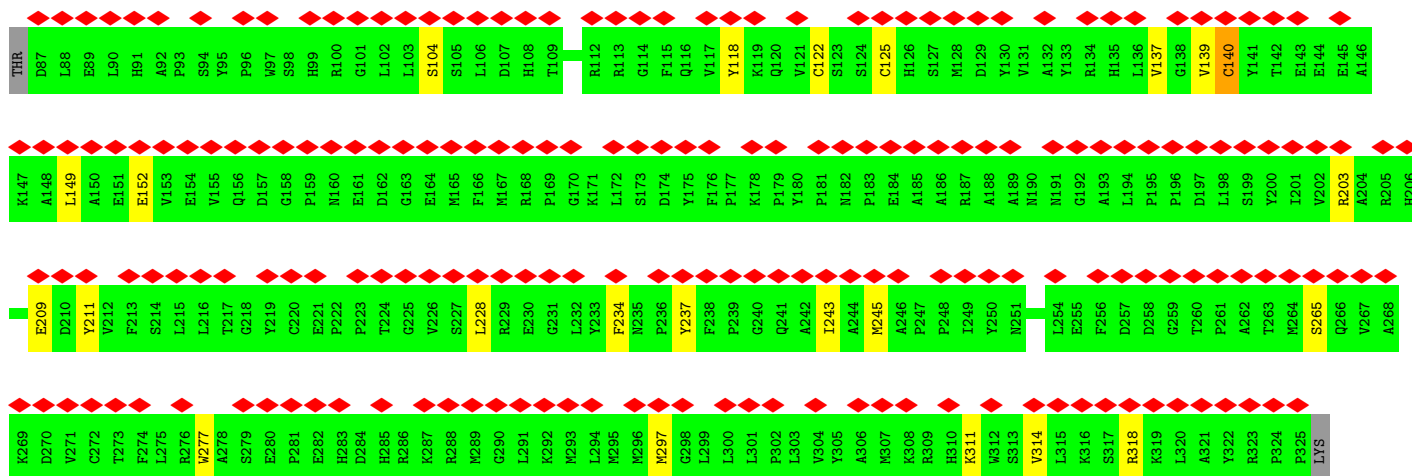
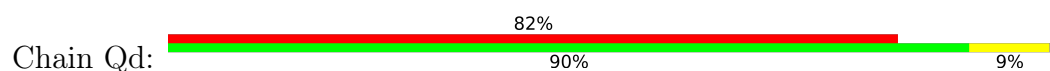




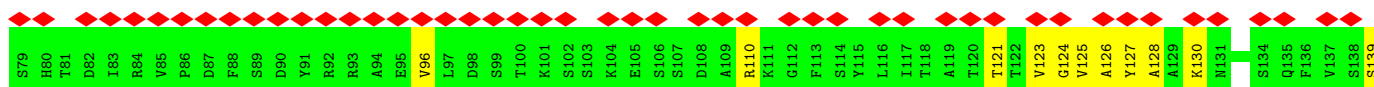
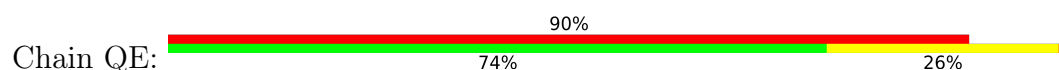
- Molecule 50: Cytochrome c1, heme protein, mitochondrial

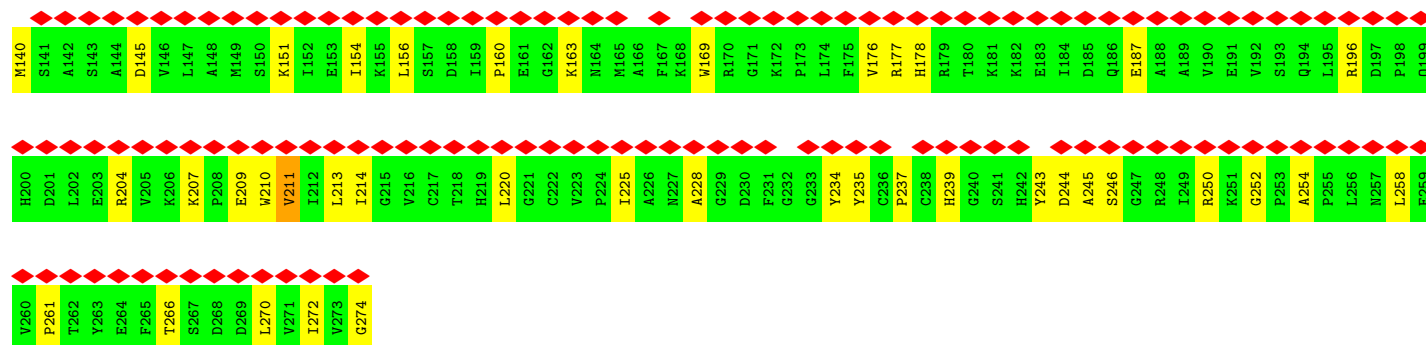


- Molecule 50: Cytochrome c1, heme protein, mitochondrial

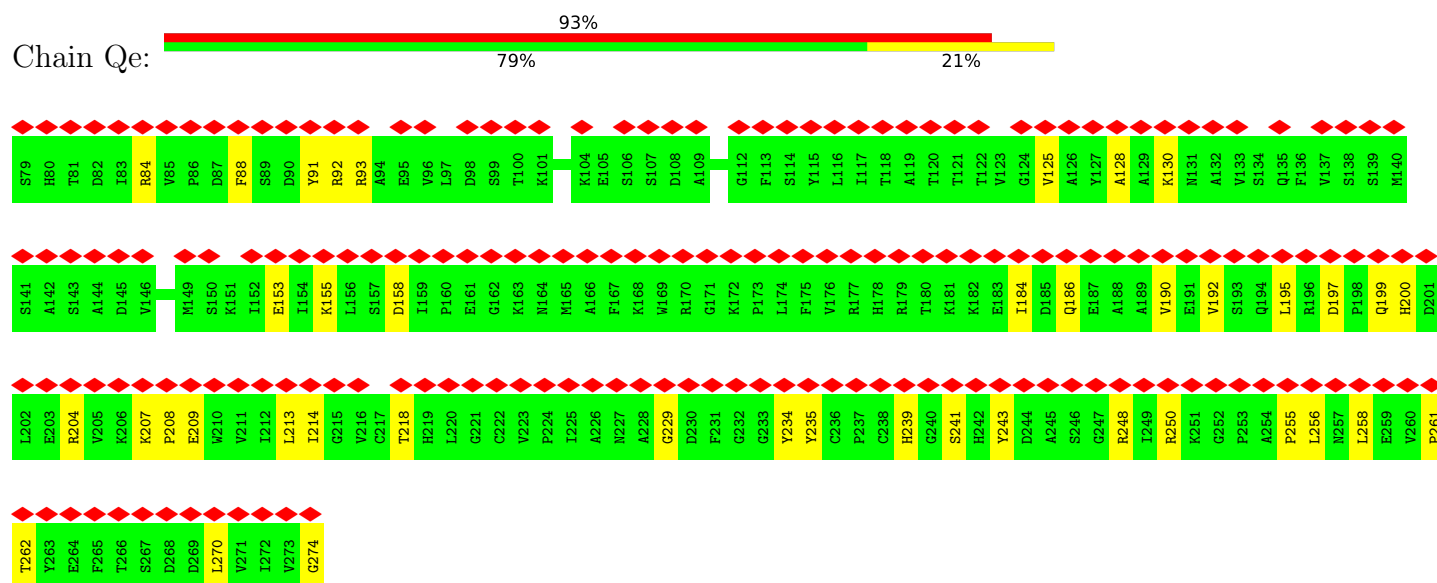


- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial

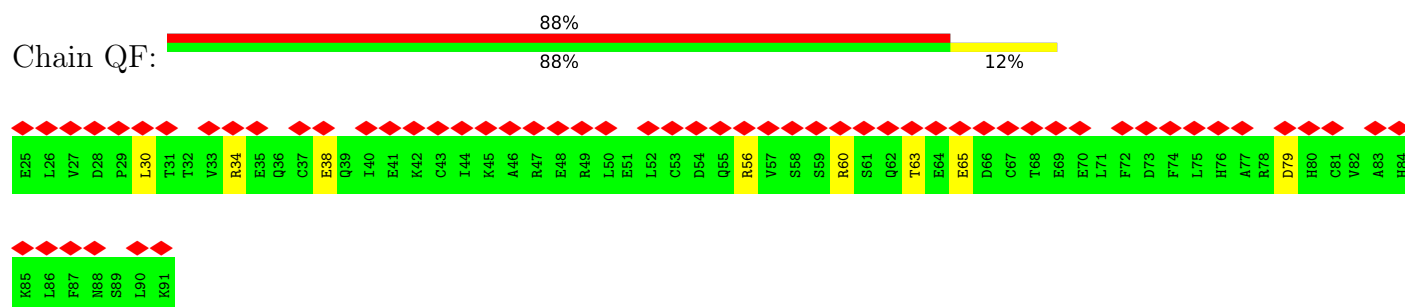




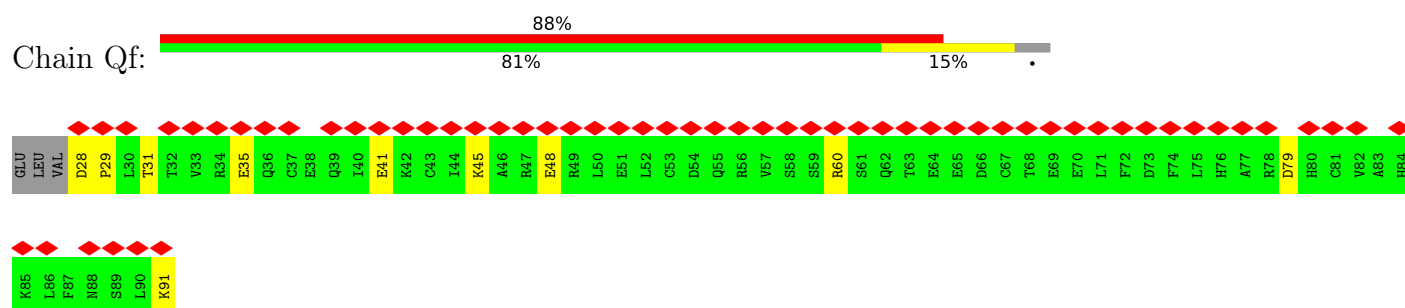
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial



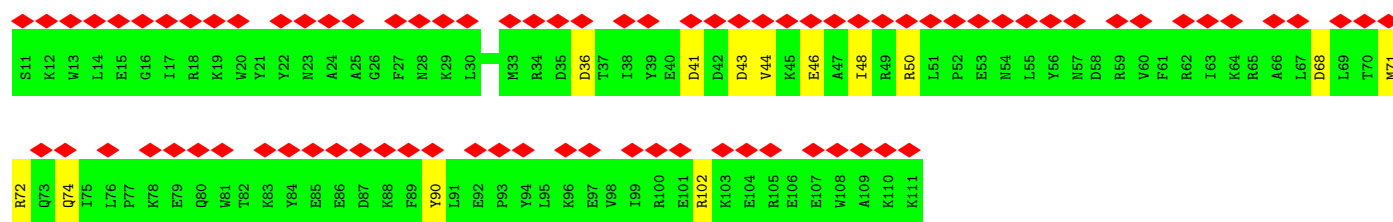
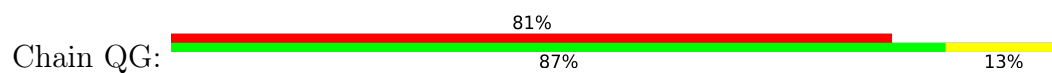
- Molecule 52: Cytochrome b-c1 complex subunit 6



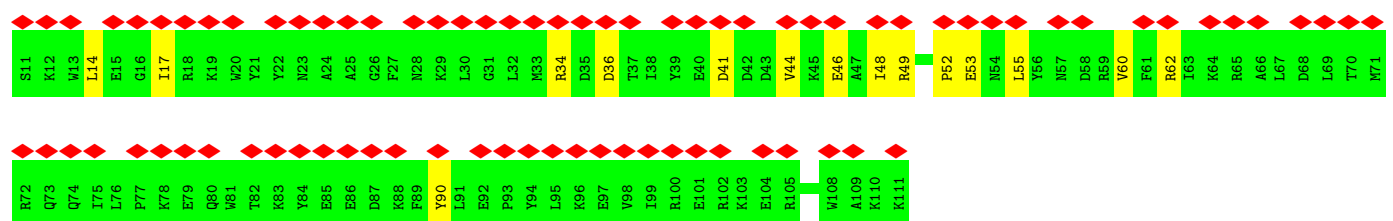
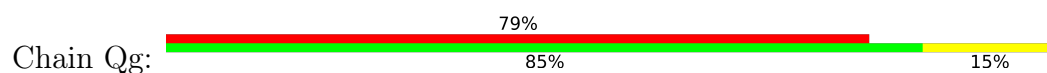
- Molecule 52: Cytochrome b-c1 complex subunit 6



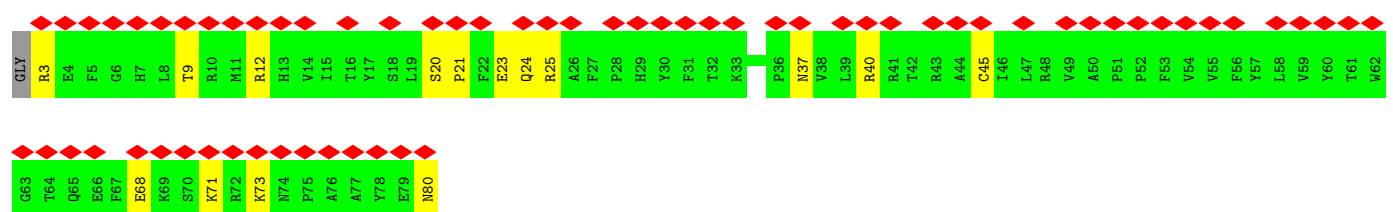
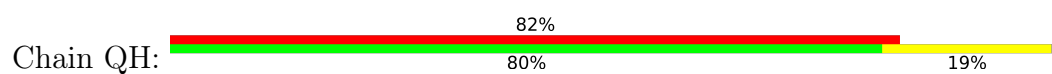
- Molecule 53: Cytochrome b-c1 complex subunit 7



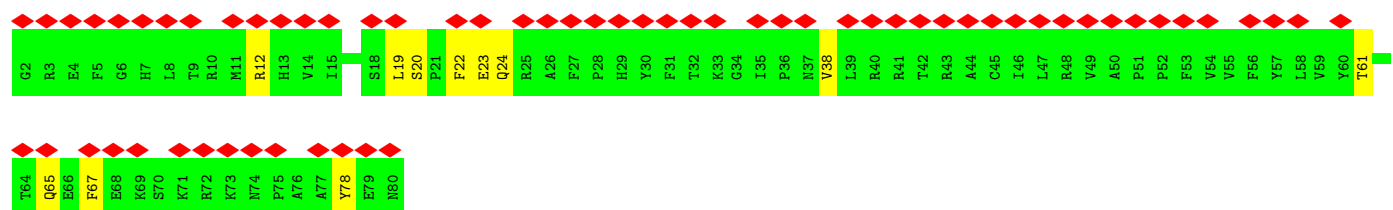
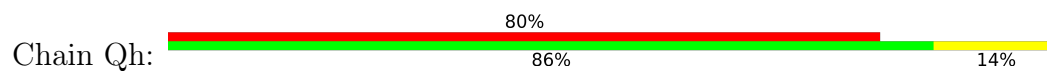
- Molecule 53: Cytochrome b-c1 complex subunit 7



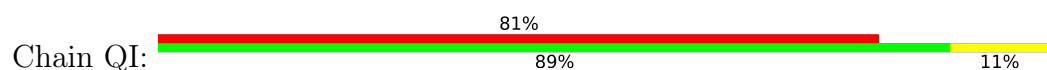
- Molecule 54: Cytochrome b-c1 complex subunit 8

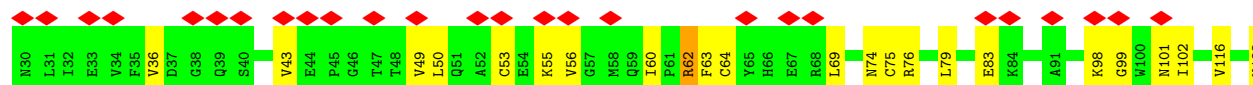


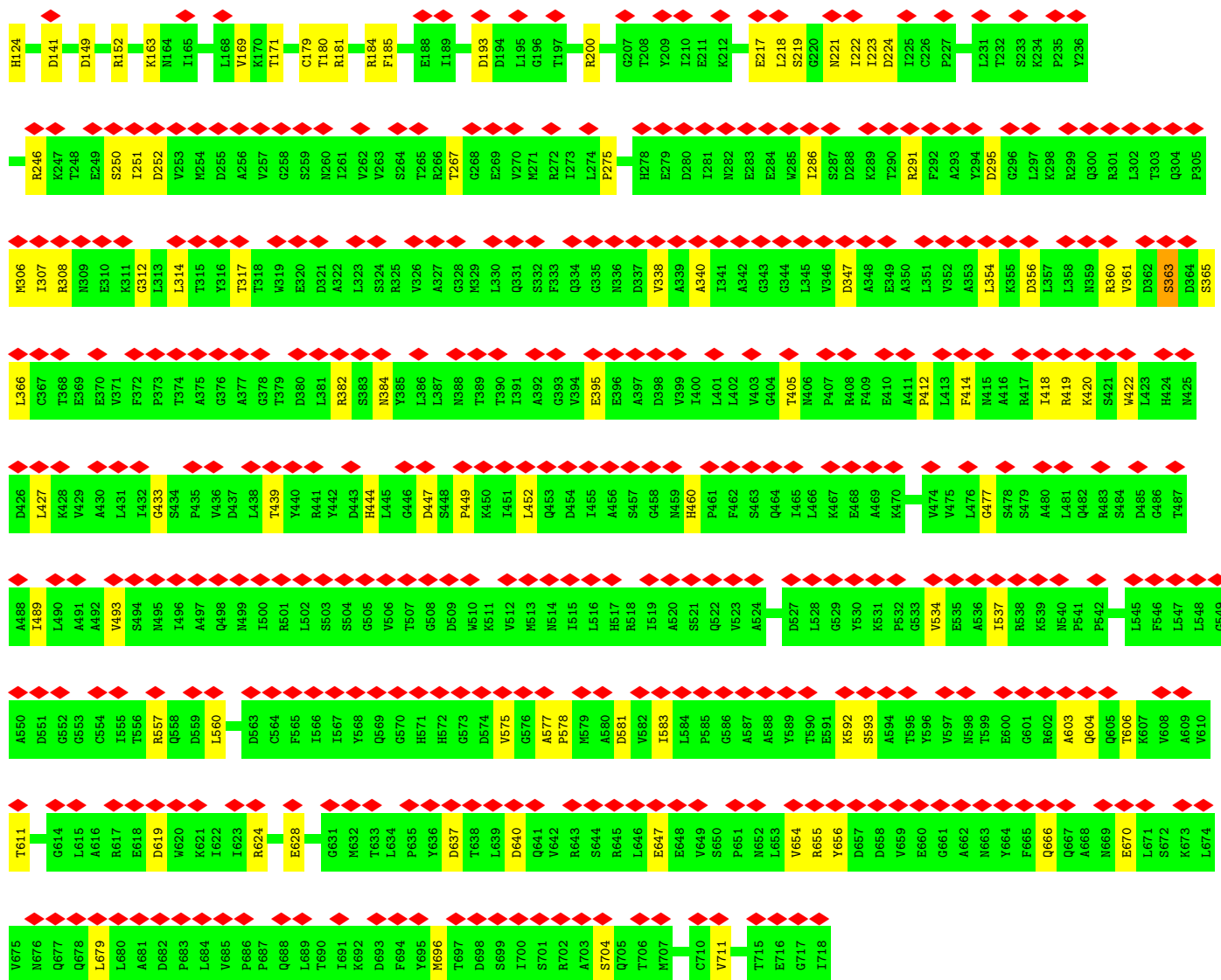
- Molecule 54: Cytochrome b-c1 complex subunit 8



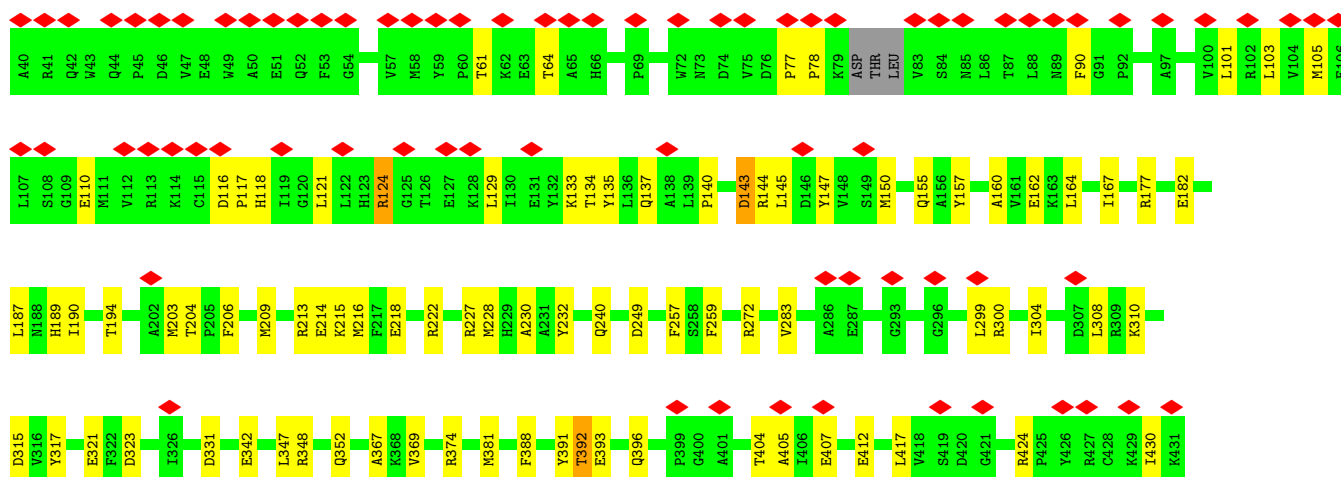
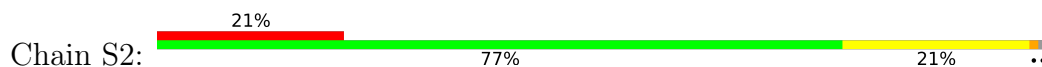
- Molecule 55: Complex III subunit 9

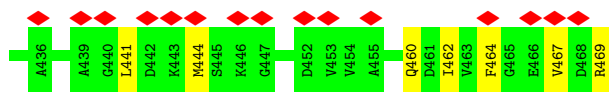




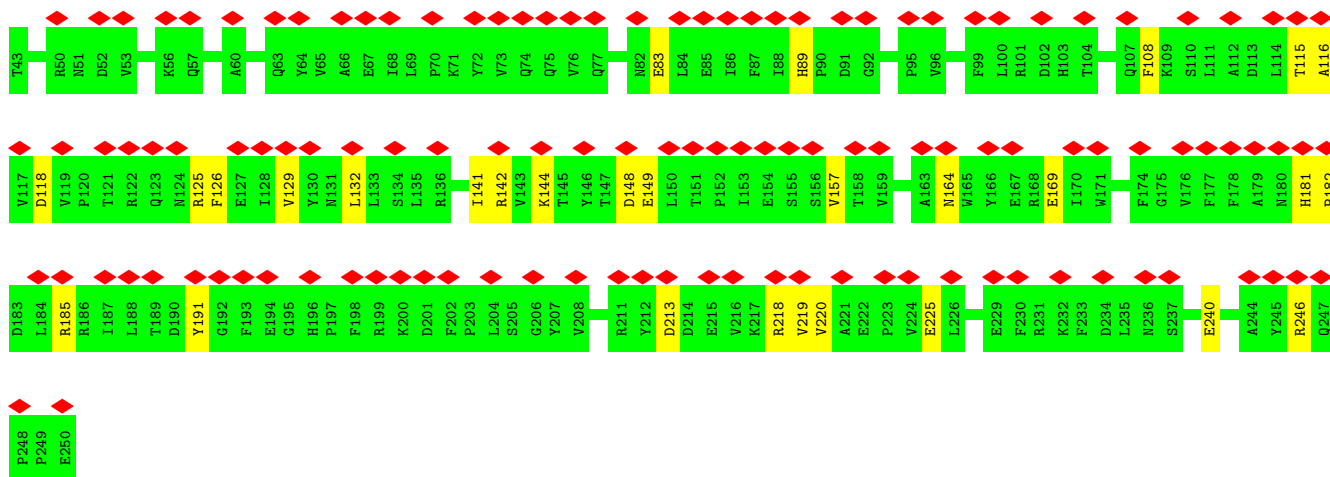
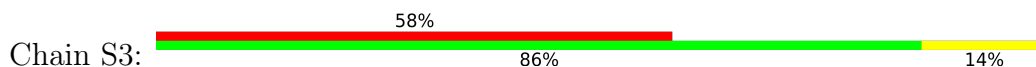


• Molecule 60: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

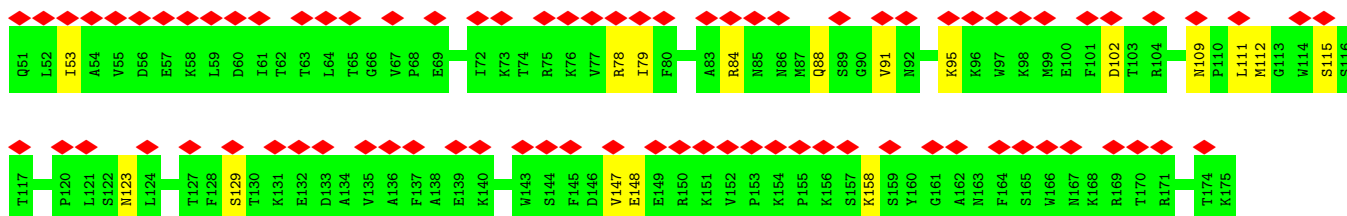
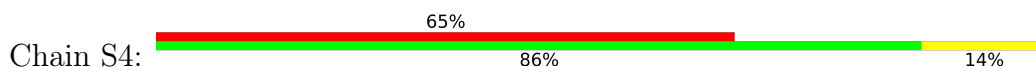




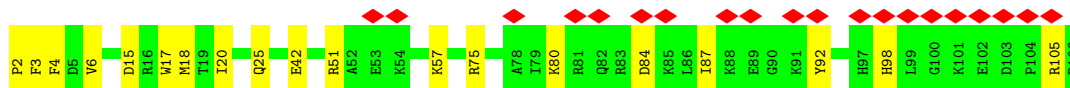
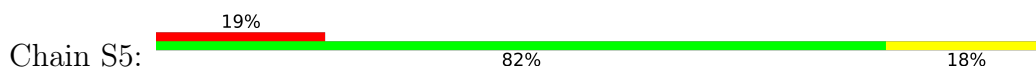
• Molecule 61: Complex I-30kD



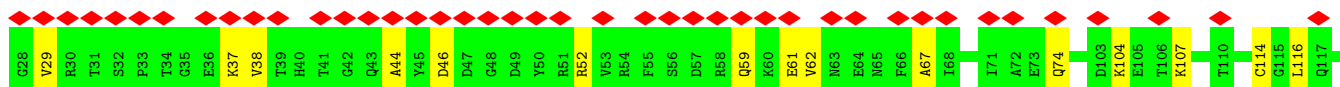
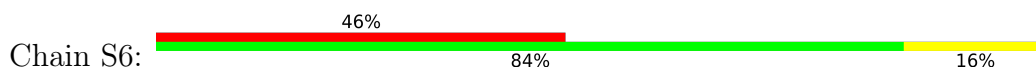
• Molecule 62: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



• Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

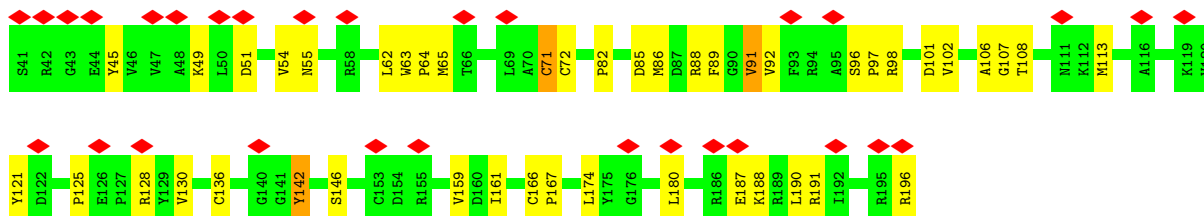
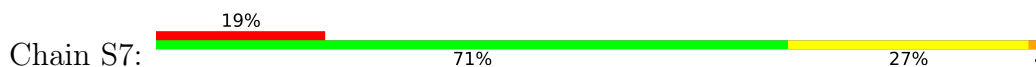


• Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

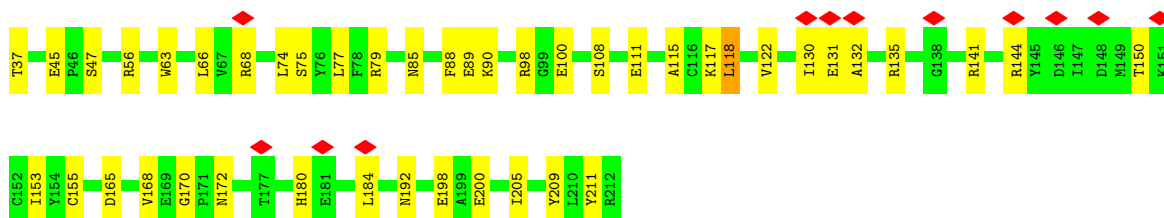
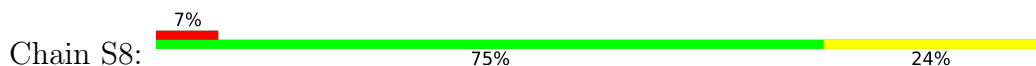




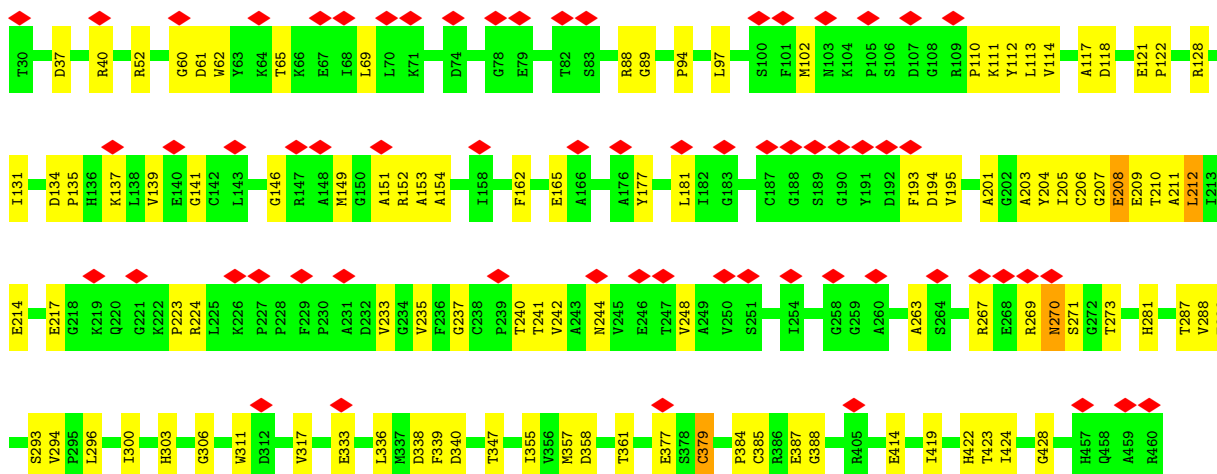
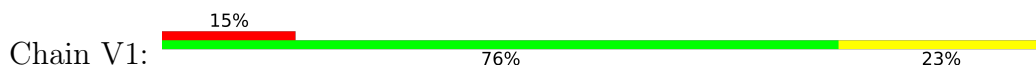
- Molecule 65: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



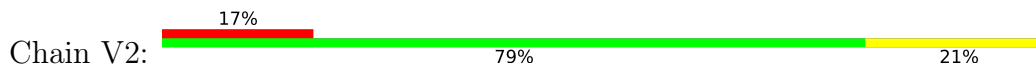
- Molecule 66: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

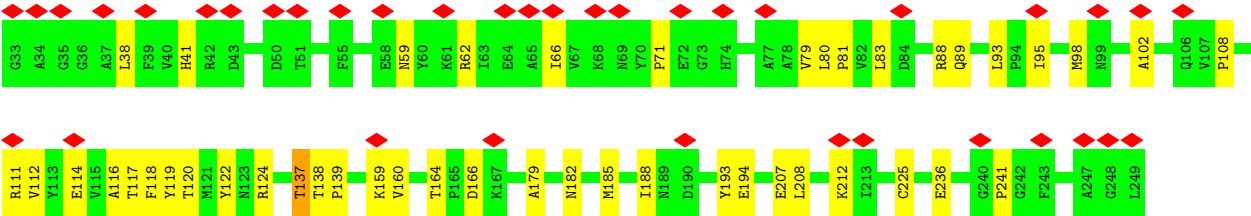


- Molecule 67: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

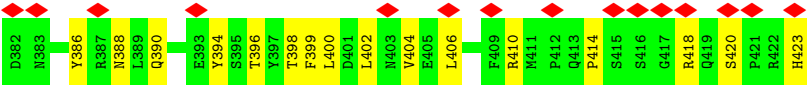


- Molecule 68: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





• Molecule 69: NADH:ubiquinone oxidoreductase subunit V3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89819	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 ($e^-/\text{\AA}^2$)	51.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	131.693	Depositor
Minimum map value	-54.678	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.161	Depositor
Recommended contour level	6	Depositor
Map size (Å)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, HEC, HEA, HEM, 3PE, PEE, FMN, SF4, NDP, 2MR, ADP, FES, CDL, PLX, MG, CU, ZN, PC1

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	4L	0.13	0/759	0.27	0/1029
2	5A	0.13	0/843	0.32	0/1145
3	5B	0.11	0/739	0.28	0/1002
4	6A	0.11	0/637	0.27	0/873
5	6B	0.14	0/704	0.32	0/951
6	6C	0.09	0/587	0.23	0/781
7	7A	0.09	0/457	0.23	0/620
8	7B	0.09	0/405	0.26	0/555
9	7C	0.11	0/400	0.22	0/536
10	8B	0.09	0/349	0.23	0/477
11	A1	0.12	0/577	0.27	0/777
12	A2	0.09	0/697	0.26	0/938
13	A3	0.09	0/664	0.23	0/912
14	A5	0.11	0/929	0.23	0/1258
15	A6	0.11	0/991	0.26	0/1335
16	A7	0.09	0/798	0.23	0/1079
17	A8	0.09	0/1436	0.24	0/1938
18	A9	0.10	0/2820	0.25	0/3823
19	AB	0.08	0/633	0.23	0/851
19	AC	0.11	0/714	0.24	0/965
20	AK	0.10	0/2661	0.26	0/3602
21	AL	0.10	0/1042	0.22	0/1411
22	AM	0.08	0/1245	0.21	0/1694
23	AN	0.12	0/1204	0.26	0/1624
24	B1	0.10	0/491	0.23	0/663
25	B2	0.12	0/610	0.24	0/836
26	B3	0.11	0/660	0.25	0/892
27	B4	0.12	0/1092	0.25	0/1481
28	B5	0.12	0/1184	0.27	0/1603
29	B6	0.13	0/888	0.30	0/1208
30	B7	0.11	0/1092	0.24	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	B8	0.10	0/1371	0.25	0/1875
32	B9	0.11	0/1590	0.26	0/2155
33	BK	0.12	0/1489	0.24	0/2008
34	BL	0.12	0/851	0.27	0/1155
35	C1	0.13	0/4164	0.30	0/5689
36	C2	0.11	0/1880	0.28	0/2564
37	C3	0.11	0/2186	0.26	0/2991
38	C4	0.12	0/1187	0.30	0/1606
39	CA	0.10	0/430	0.20	0/581
40	CB	0.12	0/1031	0.24	0/1394
41	N1	0.14	0/2581	0.32	0/3529
42	N2	0.15	0/2773	0.31	0/3768
43	N3	0.11	0/938	0.26	0/1281
44	N4	0.16	0/3723	0.33	0/5078
45	N5	0.15	0/4914	0.33	0/6683
46	N6	0.13	0/1364	0.30	0/1850
47	QA	0.12	0/3200	0.28	0/4333
47	Qa	0.11	0/3200	0.27	0/4333
48	QB	0.12	0/3531	0.29	0/4793
48	Qb	0.11	0/3436	0.26	0/4659
49	QC	0.14	0/3123	0.30	0/4269
49	Qc	0.15	0/3123	0.30	0/4269
50	QD	0.11	0/1979	0.26	0/2684
50	Qd	0.12	0/1962	0.26	0/2663
51	QE	0.10	0/1550	0.24	0/2098
51	Qe	0.11	0/1550	0.26	0/2098
52	QF	0.09	0/558	0.21	0/747
52	Qf	0.10	0/534	0.22	0/714
53	QG	0.11	0/913	0.25	0/1223
53	Qg	0.11	0/913	0.24	0/1223
54	QH	0.12	0/684	0.28	0/926
54	Qh	0.13	0/688	0.28	0/931
55	QI	0.08	0/520	0.19	0/701
55	Qi	0.12	0/506	0.24	0/683
56	QJ	0.08	0/420	0.21	0/576
57	QK	0.09	0/528	0.26	0/716
58	Qj	0.12	0/437	0.29	0/598
59	S1	0.13	0/5378	0.31	0/7287
60	S2	0.14	0/3514	0.28	0/4761
61	S3	0.12	0/1789	0.28	0/2436
62	S4	0.11	0/1039	0.28	0/1403
63	S5	0.10	0/889	0.22	0/1190
64	S6	0.11	0/755	0.27	0/1018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
65	S7	0.14	0/1279	0.28	0/1730
66	S8	0.13	0/1443	0.26	0/1952
67	V1	0.13	0/3391	0.30	0/4583
68	V2	0.11	0/1711	0.29	0/2328
69	V3	0.08	0/365	0.29	0/493
All	All	0.12	0/115688	0.28	0/156943

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4L	748	0	799	22	0
2	5A	825	0	823	39	0
3	5B	724	0	705	26	0
4	6A	609	0	579	22	0
5	6B	684	0	649	25	0
6	6C	574	0	590	13	0
7	7A	447	0	443	11	0
8	7B	392	0	372	10	0
9	7C	387	0	385	8	0
10	8B	338	0	342	13	0
11	A1	562	0	557	10	0
12	A2	686	0	699	10	0
13	A3	643	0	642	9	0
14	A5	910	0	950	15	0
15	A6	967	0	972	17	0
16	A7	780	0	808	9	0
17	A8	1398	0	1372	27	0
18	A9	2743	0	2762	42	0
19	AB	624	0	625	13	0
19	AC	702	0	694	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	AK	2601	0	2566	42	0
21	AL	1021	0	1025	10	0
22	AM	1204	0	1162	19	0
23	AN	1173	0	1166	21	0
24	B1	479	0	486	7	0
25	B2	584	0	529	6	0
26	B3	641	0	620	9	0
27	B4	1062	0	1072	10	0
28	B5	1151	0	1164	12	0
29	B6	861	0	877	19	0
30	B7	1068	0	1043	17	0
31	B8	1315	0	1208	12	0
32	B9	1534	0	1470	15	0
33	BK	1456	0	1426	14	0
34	BL	828	0	788	10	0
35	C1	4024	0	4005	160	0
36	C2	1833	0	1843	59	0
37	C3	2103	0	2034	82	0
38	C4	1153	0	1130	35	0
39	CA	417	0	422	4	0
40	CB	1000	0	994	10	0
41	N1	2508	0	2607	60	0
42	N2	2710	0	2874	58	0
43	N3	914	0	951	13	0
44	N4	3631	0	3839	69	0
45	N5	4785	0	4933	93	0
46	N6	1329	0	1326	37	0
47	QA	3147	0	3129	37	0
47	Qa	3147	0	3129	48	0
48	QB	3459	0	3350	37	0
48	Qb	3367	0	3262	31	0
49	QC	3025	0	3090	43	0
49	Qc	3025	0	3090	41	0
50	QD	1921	0	1867	26	0
50	Qd	1904	0	1849	18	0
51	QE	1517	0	1500	38	0
51	Qe	1517	0	1500	31	0
52	QF	552	0	536	7	0
52	Qf	528	0	510	8	0
53	QG	893	0	888	8	0
53	Qg	893	0	888	12	0
54	QH	662	0	660	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	Qh	666	0	663	9	0
55	QI	507	0	509	4	0
55	Qi	493	0	491	6	0
56	QJ	405	0	405	3	0
57	QK	520	0	554	9	0
58	Qj	421	0	418	3	0
59	S1	5290	0	5321	76	0
60	S2	3436	0	3373	70	0
61	S3	1738	0	1693	21	0
62	S4	1016	0	1016	15	0
63	S5	867	0	871	19	0
64	S6	741	0	701	11	0
65	S7	1248	0	1254	33	0
66	S8	1412	0	1363	38	0
67	V1	3316	0	3272	67	0
68	V2	1671	0	1673	30	0
69	V3	355	0	329	13	0
70	5B	1	0	0	0	0
70	S6	1	0	0	0	0
71	6A	45	0	64	10	0
71	B4	50	0	77	4	0
71	B5	54	0	88	1	0
71	C3	99	0	152	24	0
71	CB	54	0	88	0	0
71	N1	48	0	73	5	0
71	N4	100	0	154	7	0
71	QB	105	0	167	6	0
71	Qb	48	0	73	2	0
71	Qc	108	0	176	5	0
71	Qh	54	0	88	1	0
71	Qj	43	0	63	0	0
71	S7	54	0	88	2	0
72	6C	31	0	40	3	0
72	AM	52	0	88	4	0
72	B5	52	0	88	1	0
72	N2	52	0	88	4	0
72	N4	52	0	88	3	0
72	QE	46	0	73	6	0
72	QI	52	0	88	4	0
73	A8	83	0	113	6	0
73	AL	180	0	257	5	0
73	B4	80	0	107	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	B5	100	0	156	8	0
73	CB	100	0	156	10	0
73	N1	78	0	103	5	0
73	N2	68	0	80	1	0
73	N5	189	0	284	15	0
73	QB	62	0	68	3	0
73	QD	64	0	72	0	0
73	QH	125	0	138	4	0
73	Qb	64	0	72	3	0
73	Qh	55	0	54	1	0
74	A9	48	0	26	0	0
75	AB	36	0	47	2	0
75	AC	36	0	47	4	0
76	AK	27	0	12	4	0
77	B8	32	0	38	0	0
77	C1	51	0	82	8	0
77	CB	51	0	82	4	0
77	N5	46	0	69	0	0
77	QC	34	0	42	1	0
77	QE	43	0	63	3	0
78	C1	120	0	108	23	0
79	C1	1	0	0	0	0
79	C2	2	0	0	0	0
80	C1	1	0	0	0	0
80	S1	1	0	0	0	0
81	N3	51	0	82	3	0
81	N4	46	0	66	2	0
81	N5	97	0	151	8	0
81	N6	51	0	82	1	0
81	QC	40	0	54	2	0
81	QE	47	0	71	2	0
81	Qc	42	0	61	4	0
81	Qe	44	0	65	4	0
81	S2	48	0	73	3	0
81	S8	51	0	82	2	0
82	QC	86	0	60	8	0
82	Qc	86	0	60	8	0
83	QD	43	0	30	1	0
83	Qd	43	0	32	3	0
84	QE	4	0	0	0	0
84	Qe	4	0	0	2	0
84	S1	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	V2	4	0	0	0	0
85	S1	16	0	0	0	0
85	S7	8	0	0	1	0
85	S8	16	0	0	1	0
85	V1	8	0	0	0	0
86	V1	31	0	19	4	0
All	All	116635	0	117650	1806	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1806) 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)
36:C2:200:CYS:SG	36:C2:207:MET:HE1	1.69	1.33
33:BK:140:GLN:O	33:BK:144:SER:HB2	1.60	1.00
30:B7:92:HIS:HD1	45:N5:481:THR:HG1	1.23	0.87
49:Qc:98:VAL:HG22	82:Qc:403:HEM:HBC2	1.60	0.84
51:Qe:200:HIS:HA	51:Qe:204:ARG:HG3	1.58	0.83
36:C2:161:HIS:CE1	36:C2:200:CYS:SG	2.71	0.83
49:QC:98:VAL:HG22	82:QC:402:HEM:HBC2	1.61	0.81
37:C3:126:PRO:HB3	37:C3:257:TYR:HB3	1.62	0.81
36:C2:161:HIS:HE1	36:C2:200:CYS:SG	2.04	0.80
18:A9:198:ALA:O	18:A9:260:GLY:HA2	1.82	0.79
35:C1:358:LEU:HD13	78:C1:603:HEA:HBA1	1.63	0.79
51:Qe:262:THR:HB	51:Qe:274:GLY:O	1.84	0.78
59:S1:149:ASP:HB2	60:S2:367:ALA:HB3	1.65	0.78
49:QC:237:LEU:HB2	50:QD:297:MET:HE2	1.66	0.77
44:N4:306:PRO:HA	44:N4:458:LEU:HD23	1.67	0.76
67:V1:235:VAL:HG12	67:V1:240:THR:HG21	1.66	0.76
29:B6:88:LEU:HD22	29:B6:92:GLU:HG2	1.68	0.75
21:AL:108:TYR:HB2	73:B4:201:CDL:HB31	1.69	0.75
73:B5:202:CDL:H672	45:N5:12:LEU:HB3	1.66	0.75
59:S1:419:ARG:NH1	59:S1:439:THR:O	2.20	0.74
35:C1:347:LEU:HD13	35:C1:383:MET:HB3	1.68	0.74
77:C1:601:3PE:H2G2	38:C4:113:PHE:HB2	1.70	0.74
5:6B:39:ARG:NH1	5:6B:85:LYS:O	2.20	0.73
59:S1:60:ILE:O	59:S1:62:ARG:NH1	2.22	0.73
3:5B:78:ASN:HB2	3:5B:120:TYR:HD1	1.54	0.73
47:Qa:81:HIS:HD2	47:Qa:192:CYS:H	1.38	0.72
47:Qa:155:GLN:HE22	47:Qa:200:VAL:HB	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:S1:338:VAL:O	59:S1:365:SER:HB2	1.90	0.72
45:N5:530:PRO:O	45:N5:534:HIS:HB2	1.90	0.72
71:C3:302:PC1:H2B1	71:C3:302:PC1:H3G1	1.72	0.71
5:6B:36:ASP:O	5:6B:40:CYS:N	2.16	0.71
12:A2:59:SER:HB2	59:S1:655:ARG:HD3	1.72	0.71
29:B6:132:VAL:O	29:B6:136:LEU:HB3	1.90	0.71
40:CB:2:THR:HB	40:CB:5:SER:HB3	1.72	0.71
51:Qe:204:ARG:NH2	51:Qe:258:LEU:O	2.24	0.71
8:7B:72:VAL:O	38:C4:167:TRP:NE1	2.23	0.71
18:A9:272:LEU:HG	18:A9:375:VAL:HG21	1.72	0.71
55:QI:48:ASN:HD21	50:Qd:104:SER:HA	1.55	0.71
71:6A:101:PC1:H341	37:C3:202:GLY:HA3	1.72	0.71
59:S1:246:ARG:HH22	62:S4:123:ASN:HD21	1.37	0.71
19:AB:116:VAL:HG12	19:AB:120:MET:HE2	1.72	0.70
21:AL:140:LYS:H	42:N2:273:ASN:HD22	1.37	0.70
21:AL:110:ILE:HG13	71:B4:202:PC1:H261	1.71	0.70
35:C1:96:ARG:HH21	71:C3:302:PC1:H112	1.54	0.70
9:7C:53:PHE:HB3	10:8B:57:VAL:HG21	1.73	0.70
73:CB:203:CDL:H231	73:CB:203:CDL:H832	1.72	0.70
42:N2:108:LEU:HD11	42:N2:191:THR:HG21	1.72	0.70
1:4L:71:ALA:O	1:4L:75:LEU:HG	1.91	0.69
22:AM:88:ARG:HD3	66:S8:200:GLU:HG3	1.72	0.69
22:AM:34:ARG:NH2	66:S8:89:GLU:OE2	2.25	0.69
59:S1:124:HIS:HD2	60:S2:381:MET:HE2	1.56	0.69
44:N4:405:LEU:HD21	45:N5:173:LEU:HD12	1.75	0.68
42:N2:342:ALA:HB3	72:N2:401:PLX:H342	1.74	0.68
73:B5:202:CDL:HB21	81:N5:701:PEE:H49	1.75	0.68
1:4L:31:LEU:HD21	46:N6:67:VAL:HG11	1.74	0.68
61:S3:83:GLU:OE1	61:S3:142:ARG:NH2	2.26	0.68
41:N1:137:ALA:HB1	41:N1:286:MET:HE1	1.74	0.68
73:N5:702:CDL:H541	73:N5:702:CDL:HA4	1.76	0.68
2:5A:99:ARG:HH12	38:C4:70:TRP:H	1.42	0.68
2:5A:66:ASP:OD1	2:5A:66:ASP:N	2.24	0.67
68:V2:182:ASN:HB3	68:V2:194:GLU:HB3	1.77	0.67
35:C1:368:HIS:O	36:C2:171:LYS:NZ	2.28	0.67
49:QC:47:THR:HG22	49:QC:79:ILE:HG23	1.75	0.67
35:C1:390:MET:HE1	78:C1:602:HEA:H202	1.75	0.67
35:C1:370:THR:HG23	35:C1:372:TYR:H	1.59	0.67
18:A9:129:LEU:HD23	18:A9:167:ILE:HG13	1.76	0.67
45:N5:387:THR:HG22	45:N5:465:GLY:H	1.59	0.66
33:BK:2:PRO:O	33:BK:7:LYS:NZ	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5A:61:TYR:OH	2:5A:71:GLU:O	2.13	0.66
48:QB:100:GLY:HA2	48:QB:106:GLY:H	1.60	0.66
57:QK:64:LEU:HA	57:QK:78:TYR:HA	1.77	0.66
60:S2:222:ARG:NH1	60:S2:249:ASP:OD2	2.28	0.66
67:V1:205:ILE:HG12	67:V1:379:CYS:HB3	1.77	0.66
46:N6:67:VAL:HA	46:N6:70:TYR:CZ	2.31	0.66
36:C2:194:GLY:N	36:C2:209:ILE:O	2.28	0.66
59:S1:141:ASP:OD2	62:S4:88:GLN:NE2	2.28	0.66
51:Qe:199:GLN:OE1	51:Qe:204:ARG:NH1	2.29	0.66
51:Qe:195:LEU:HD21	51:Qe:248:ARG:HB3	1.78	0.65
35:C1:411:LYS:HA	35:C1:414:PHE:CE2	2.30	0.65
65:S7:85:ASP:HB3	65:S7:88:ARG:HB3	1.76	0.65
54:Qh:61:THR:O	54:Qh:65:GLN:NE2	2.30	0.65
2:5A:136:LEU:HD22	2:5A:141:ILE:HB	1.78	0.65
60:S2:374:ARG:NH2	66:S8:165:ASP:OD1	2.29	0.65
40:CB:13:LEU:HD21	63:S5:4:PHE:HB3	1.79	0.65
47:Qa:155:GLN:NE2	47:Qa:200:VAL:O	2.30	0.65
4:6A:68:ARG:NH1	37:C3:189:SER:OG	2.25	0.65
15:A6:66:TYR:O	15:A6:86:ARG:NH1	2.29	0.65
41:N1:174:MET:HB2	41:N1:242:PHE:HA	1.79	0.65
35:C1:96:ARG:HH22	37:C3:61:ILE:HG12	1.62	0.65
73:QB:501:CDL:HA22	71:QB:503:PC1:H131	1.78	0.65
67:V1:233:VAL:HG13	67:V1:237:GLY:HA2	1.79	0.65
3:5B:105:VAL:HG13	3:5B:111:GLN:HG3	1.79	0.64
30:B7:29:TYR:O	30:B7:104:ARG:NH2	2.30	0.64
35:C1:374:VAL:HA	35:C1:377:PHE:CE2	2.32	0.64
77:C1:601:3PE:H2E1	38:C4:109:PHE:HB3	1.78	0.64
20:AK:120:TYR:HH	76:AK:401:ADP:HO2'	1.43	0.64
49:QC:71:ARG:NH2	50:QD:278:ALA:O	2.28	0.64
73:B5:202:CDL:H191	73:B5:202:CDL:H731	1.80	0.64
47:Qa:237:PHE:HB3	47:Qa:238:LEU:HD12	1.80	0.64
73:CB:203:CDL:H262	73:CB:203:CDL:H751	1.79	0.64
73:AL:201:CDL:H382	71:B4:202:PC1:H2D2	1.79	0.64
45:N5:5:ALA:HB2	45:N5:61:MET:HE1	1.78	0.64
48:QB:195:THR:HG21	48:QB:269:ARG:H	1.63	0.64
20:AK:109:GLN:OE1	20:AK:328:ARG:NH1	2.31	0.64
27:B4:15:PRO:HG2	27:B4:18:LEU:HB2	1.80	0.64
35:C1:420:GLY:O	35:C1:424:THR:OG1	2.14	0.64
41:N1:231:ILE:O	41:N1:235:ASN:ND2	2.31	0.64
45:N5:100:ILE:HG21	45:N5:246:LEU:HB2	1.80	0.64
44:N4:122:PHE:CZ	44:N4:206:LYS:HG3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Qd:243:ILE:HG12	50:Qd:245:MET:H	1.63	0.63
59:S1:308:ARG:NH1	59:S1:312:GLY:O	2.32	0.63
65:S7:51:ASP:HB3	65:S7:190:LEU:HB2	1.80	0.63
13:A3:160:GLY:HA3	17:A8:204:LYS:HD2	1.80	0.63
20:AK:66:GLY:O	20:AK:163:ARG:NH2	2.31	0.63
35:C1:69:MET:HE1	78:C1:602:HEA:HMC1	1.80	0.63
60:S2:137:GLN:O	65:S7:142:TYR:OH	2.17	0.63
66:S8:205:ILE:O	66:S8:209:TYR:HB3	1.98	0.63
4:6A:65:LEU:HA	37:C3:190:ASP:HA	1.80	0.63
13:A3:117:LEU:HD23	41:N1:310:MET:HE1	1.80	0.63
35:C1:447:TYR:O	35:C1:451:ASN:ND2	2.29	0.63
41:N1:34:ARG:HG2	65:S7:82:PRO:HA	1.80	0.63
19:AC:114:ASP:OD1	32:B9:87:ARG:NH2	2.32	0.63
18:A9:61:ALA:HB3	18:A9:82:VAL:HG13	1.81	0.63
12:A2:24:CYS:N	12:A2:58:CYS:SG	2.71	0.63
42:N2:289:ASN:HA	42:N2:292:PHE:CE2	2.34	0.63
73:QB:501:CDL:H521	73:QB:501:CDL:H152	1.81	0.63
23:AN:144:THR:HB	41:N1:96:ILE:HG23	1.81	0.63
51:Qe:155:LYS:HG3	51:Qe:158:ASP:H	1.63	0.63
1:4L:75:LEU:HD13	46:N6:70:TYR:CE2	2.34	0.62
19:AB:111:ASP:OD1	19:AB:111:ASP:N	2.31	0.62
35:C1:51:ASP:O	35:C1:55:ASN:ND2	2.33	0.62
42:N2:170:LEU:HD11	42:N2:288:LEU:HD22	1.81	0.62
59:S1:624:ARG:NH2	59:S1:637:ASP:OD1	2.31	0.62
68:V2:59:ASN:ND2	68:V2:89:GLN:OE1	2.32	0.62
60:S2:388:PHE:O	60:S2:392:THR:OG1	2.16	0.62
6:6C:34:ALA:HB2	36:C2:33:LEU:HB2	1.81	0.62
8:7B:53:TRP:HE1	38:C4:111:ILE:HG22	1.64	0.62
10:8B:62:ASP:OD1	10:8B:62:ASP:N	2.32	0.62
48:Qb:104:ARG:NH2	48:Qb:149:ASP:OD2	2.31	0.62
67:V1:311:TRP:NE1	67:V1:333:GLU:OE1	2.32	0.62
38:C4:59:GLN:HA	38:C4:62:LEU:HB3	1.80	0.62
46:N6:45:LEU:HD23	46:N6:50:SER:HA	1.81	0.62
47:QA:90:THR:HG23	47:QA:95:SER:HA	1.81	0.62
60:S2:393:GLU:OE2	60:S2:396:GLN:NE2	2.33	0.62
37:C3:77:LYS:NZ	37:C3:81:TYR:OH	2.29	0.62
37:C3:136:ILE:HG21	37:C3:173:PHE:HB2	1.82	0.62
48:QB:479:ARG:NH2	71:QB:502:PC1:O12	2.33	0.62
59:S1:250:SER:HB2	59:S1:606:THR:HG23	1.82	0.62
19:AB:82:ARG:HH21	19:AB:125:GLU:HG3	1.65	0.62
35:C1:406:ASN:HB3	35:C1:409:TRP:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:QK:1:MET:O	57:QK:7:ARG:NH1	2.33	0.62
4:6A:81:LEU:HB3	71:6A:101:PC1:H11	1.81	0.62
34:BL:130:GLU:HB3	34:BL:136:LEU:HD21	1.81	0.62
41:N1:58:LYS:HE2	65:S7:125:PRO:HG2	1.82	0.62
73:N5:703:CDL:H402	73:N5:703:CDL:H611	1.82	0.62
15:A6:78:LEU:HD22	15:A6:130:MET:HE3	1.82	0.61
16:A7:27:ARG:HD2	16:A7:31:ILE:HD13	1.81	0.61
30:B7:103:GLU:OE2	30:B7:106:ARG:NH2	2.30	0.61
40:CB:13:LEU:HD11	63:S5:6:VAL:HG22	1.82	0.61
72:N2:401:PLX:H1A2	63:S5:2:PRO:HG2	1.82	0.61
30:B7:15:LYS:HG2	30:B7:113:LYS:HG3	1.82	0.61
22:AM:106:ARG:HB2	22:AM:109:ILE:HG13	1.82	0.61
41:N1:200:LEU:HD22	41:N1:282:TYR:HB3	1.82	0.61
43:N3:68:GLU:HG3	43:N3:98:LEU:HD13	1.82	0.61
20:AK:141:ARG:NH2	76:AK:401:ADP:N7	2.48	0.61
21:AL:41:ILE:HD13	73:AL:202:CDL:H311	1.82	0.61
36:C2:142:VAL:HB	36:C2:211:LEU:HD23	1.83	0.61
20:AK:127:ASP:O	20:AK:132:ARG:NH1	2.33	0.61
49:QC:43:LEU:O	49:QC:47:THR:OG1	2.17	0.61
2:5A:50:THR:O	2:5A:54:PHE:N	2.27	0.61
37:C3:178:ALA:HA	37:C3:181:TYR:HD2	1.64	0.61
41:N1:24:GLU:OE2	41:N1:274:ARG:NH1	2.30	0.61
44:N4:398:MET:HG2	81:N5:704:PEE:H78	1.83	0.61
51:Qe:241:SER:OG	84:Qe:301:FES:S2	2.54	0.61
59:S1:163:LYS:O	59:S1:171:THR:OG1	2.19	0.61
1:4L:73:LEU:HD21	42:N2:41:ILE:HG13	1.82	0.61
6:6C:45:ARG:NH1	36:C2:25:ASP:OD2	2.34	0.61
24:B1:57:TRP:NE1	28:B5:134:GLU:OE1	2.20	0.61
35:C1:404:THR:O	35:C1:480:ARG:NH2	2.33	0.61
60:S2:162:GLU:OE2	60:S2:177:ARG:NH2	2.31	0.61
35:C1:398:PRO:O	35:C1:402:GLY:N	2.31	0.61
37:C3:257:TYR:O	37:C3:261:SER:OG	2.19	0.61
45:N5:362:LEU:HA	45:N5:365:ALA:HB3	1.82	0.61
59:S1:275:PRO:HG3	59:S1:286:ILE:HG12	1.83	0.61
3:5B:84:THR:OG1	3:5B:85:ASN:N	2.34	0.60
5:6B:74:ASP:OD1	5:6B:77:ARG:NH2	2.34	0.60
49:QC:233:LEU:HG	50:QD:297:MET:HE1	1.83	0.60
60:S2:90:PHE:HB3	60:S2:103:LEU:HB3	1.83	0.60
60:S2:140:PRO:HA	60:S2:143:ASP:HB2	1.83	0.60
62:S4:109:ASN:ND2	62:S4:111:LEU:O	2.34	0.60
19:AC:91:ASP:OD1	26:B3:47:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B4:82:PRO:HB2	73:B4:201:CDL:HB61	1.81	0.60
38:C4:55:LEU:HD13	38:C4:63:LYS:HE3	1.81	0.60
38:C4:155:GLY:H	38:C4:158:ALA:HB3	1.64	0.60
37:C3:234:GLY:N	71:C3:301:PC1:O12	2.23	0.60
49:QC:8:HIS:HB3	49:QC:11:MET:HB2	1.83	0.60
35:C1:229:ILE:HD12	35:C1:295:VAL:HB	1.82	0.60
53:Qg:36:ASP:OD2	53:Qg:62:ARG:NH1	2.32	0.60
18:A9:50:SER:OG	61:S3:225:GLU:OE2	2.15	0.60
45:N5:419:THR:HA	45:N5:422:TYR:CE2	2.37	0.60
60:S2:469:ARG:NH2	61:S3:169:GLU:OE2	2.35	0.60
5:6B:9:ILE:HG12	5:6B:56:TRP:HB2	1.84	0.60
49:QC:207:ASN:OD1	49:QC:209:THR:OG1	2.19	0.60
59:S1:224:ASP:OD2	59:S1:291:ARG:NH2	2.27	0.60
67:V1:162:PHE:HB3	67:V1:165:GLU:HB2	1.83	0.60
35:C1:66:ILE:HG23	35:C1:246:LEU:HD11	1.84	0.60
44:N4:408:LEU:HD12	45:N5:172:ILE:HG21	1.84	0.60
52:QF:79:ASP:OD2	50:Qd:237:TYR:OH	2.16	0.60
64:S6:61:GLU:OE2	66:S8:192:ASN:ND2	2.30	0.60
31:B8:83:GLN:HA	31:B8:86:ARG:HG3	1.84	0.60
35:C1:184:PHE:H	35:C1:256:HIS:CE1	2.20	0.60
50:QD:104:SER:HA	55:Qi:48:ASN:HD21	1.65	0.60
2:5A:68:ASP:HB2	2:5A:71:GLU:H	1.66	0.60
35:C1:13:LYS:NZ	35:C1:504:THR:OG1	2.35	0.60
35:C1:211:THR:HA	35:C1:215:LEU:HD13	1.83	0.60
49:QC:233:LEU:HD13	72:QE:301:PLX:H172	1.84	0.60
47:Qa:82:LEU:HD11	47:Qa:154:LEU:HB3	1.84	0.60
2:5A:57:ARG:O	2:5A:61:TYR:N	2.34	0.60
8:7B:74:PRO:HB3	38:C4:143:LYS:HB2	1.84	0.60
37:C3:58:TRP:CG	71:C3:301:PC1:H252	2.36	0.60
50:QD:147:LYS:NZ	50:QD:151:GLU:OE2	2.35	0.60
67:V1:217:GLU:OE2	67:V1:224:ARG:NH2	2.35	0.60
18:A9:87:GLU:HG3	18:A9:89:TYR:H	1.68	0.59
35:C1:438:ARG:NH1	78:C1:603:HEA:O1D	2.34	0.59
5:6B:39:ARG:HA	5:6B:42:LYS:HB3	1.84	0.59
6:6C:10:GLN:NE2	6:6C:12:ARG:O	2.34	0.59
35:C1:28:MET:HE1	78:C1:602:HEA:H212	1.84	0.59
47:Qa:90:THR:HG23	47:Qa:95:SER:HA	1.83	0.59
47:QA:164:VAL:HG22	57:QK:43:LEU:HD21	1.85	0.59
62:S4:91:VAL:O	62:S4:95:LYS:NZ	2.35	0.59
35:C1:82:LEU:HB3	35:C1:86:MET:HE3	1.85	0.59
37:C3:231:HIS:NE2	71:C3:301:PC1:O14	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:N2:88:LYS:HG3	42:N2:148:SER:HB3	1.83	0.59
42:N2:142:LEU:HB3	42:N2:194:LEU:HD21	1.84	0.59
51:QE:196:ARG:NH1	51:QE:254:ALA:O	2.36	0.59
2:5A:98:CYS:O	2:5A:102:ASN:N	2.35	0.59
3:5B:40:ASP:O	3:5B:44:ALA:N	2.21	0.59
18:A9:344:PRO:HG2	18:A9:347:LEU:HD13	1.83	0.59
23:AN:51:MET:HE2	41:N1:311:THR:HB	1.84	0.59
73:B5:202:CDL:H821	73:N5:702:CDL:H473	1.85	0.59
44:N4:383:THR:HG21	45:N5:190:LEU:HD22	1.84	0.59
10:8B:58:LEU:HD23	10:8B:61:LEU:HD11	1.83	0.59
73:B5:202:CDL:H652	45:N5:16:THR:HG21	1.85	0.59
35:C1:383:MET:HE3	35:C1:421:VAL:HG23	1.85	0.59
7:7A:51:ILE:HD11	45:N5:504:LEU:HG	1.84	0.59
11:A1:13:ALA:HB2	41:N1:264:LEU:HD11	1.84	0.59
18:A9:293:LEU:HD12	18:A9:294:PRO:HD2	1.83	0.59
35:C1:2:PHE:HA	35:C1:6:TRP:HD1	1.68	0.59
47:QA:151:VAL:O	47:QA:155:GLN:HG2	2.02	0.59
51:QE:204:ARG:NH2	51:QE:258:LEU:O	2.32	0.59
47:QA:301:ARG:NH2	48:QB:94:GLU:OE2	2.30	0.59
44:N4:211:GLY:H	44:N4:213:HIS:HD2	1.50	0.59
47:QA:60:ARG:NH1	47:QA:124:GLU:OE1	2.35	0.59
47:QA:77:LEU:O	47:QA:196:ARG:NH1	2.30	0.59
60:S2:155:GLN:NE2	60:S2:315:ASP:OD2	2.36	0.59
68:V2:207:GLU:HG3	68:V2:212:LYS:HE2	1.85	0.59
35:C1:358:LEU:HB3	78:C1:603:HEA:HMA	1.85	0.58
5:6B:65:CYS:O	36:C2:98:LYS:NZ	2.32	0.58
17:A8:202:LEU:HD13	23:AN:70:ALA:HB2	1.83	0.58
75:AC:201:ZMP:H22A	32:B9:113:PHE:HA	1.85	0.58
20:AK:145:TYR:OH	20:AK:201:LEU:O	2.20	0.58
59:S1:452:LEU:HD21	59:S1:493:VAL:HG13	1.84	0.58
67:V1:110:PRO:HB3	67:V1:152:ARG:HD3	1.85	0.58
67:V1:112:TYR:HB2	67:V1:240:THR:HG22	1.84	0.58
77:CB:201:3PE:H2D1	42:N2:332:LEU:HD11	1.84	0.58
47:Qa:306:THR:OG1	48:Qb:114:GLU:OE1	2.20	0.58
59:S1:666:GLN:NE2	59:S1:670:GLU:OE2	2.36	0.58
36:C2:96:THR:OG1	36:C2:151:ARG:NH1	2.35	0.58
38:C4:90:PHE:HA	38:C4:93:MET:HG2	1.84	0.58
71:QB:503:PC1:H3B2	77:QE:303:3PE:H2E1	1.84	0.58
54:QH:25:ARG:HG2	51:Qe:93:ARG:HG2	1.85	0.58
51:Qe:195:LEU:HG	51:Qe:197:ASP:H	1.67	0.58
4:6A:69:THR:N	35:C1:216:ASN:OD1	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A5:20:PRO:HB3	14:A5:77:ILE:HG21	1.85	0.58
37:C3:80:ARG:NH2	37:C3:236:GLU:OE1	2.36	0.58
46:N6:2:THR:OG1	46:N6:3:MET:N	2.37	0.58
47:Qa:151:VAL:O	47:Qa:155:GLN:HG2	2.03	0.58
1:4L:56:ALA:HA	63:S5:18:MET:HE3	1.85	0.58
2:5A:59:VAL:HG23	2:5A:90:ILE:HG12	1.85	0.58
41:N1:31:MET:HG2	66:S8:77:LEU:HB2	1.86	0.58
41:N1:117:LEU:HB3	46:N6:68:PHE:CE1	2.39	0.58
68:V2:62:ARG:HD3	69:V3:400:LEU:HB3	1.85	0.58
51:Qe:207:LYS:HD3	51:Qe:208:PRO:HD2	1.86	0.58
12:A2:25:GLN:OE1	12:A2:26:ARG:NH1	2.37	0.58
36:C2:104:TRP:HA	36:C2:207:MET:HE2	1.86	0.58
51:QE:266:THR:OG1	51:QE:270:LEU:O	2.22	0.58
81:QE:302:PEE:H30	81:QE:302:PEE:H67	1.85	0.58
60:S2:308:LEU:HB2	60:S2:407:GLU:HB2	1.86	0.58
5:6B:5:ILE:HG13	5:6B:7:THR:H	1.67	0.58
14:A5:49:GLU:O	14:A5:53:ASN:ND2	2.30	0.58
73:CB:203:CDL:H312	44:N4:94:LEU:HD11	1.85	0.58
48:Qb:152:GLN:HE22	48:Qb:250:PHE:HA	1.69	0.58
67:V1:293:SER:HB3	67:V1:336:LEU:HD23	1.86	0.58
44:N4:122:PHE:HZ	44:N4:206:LYS:HG3	1.67	0.57
4:6A:83:HIS:HA	71:6A:101:PC1:H132	1.86	0.57
35:C1:151:HIS:NE2	35:C1:207:THR:OG1	2.36	0.57
44:N4:392:THR:O	44:N4:396:MET:HG2	2.04	0.57
44:N4:403:THR:HA	44:N4:406:TYR:CE2	2.39	0.57
60:S2:257:PHE:HD2	60:S2:347:LEU:HD11	1.69	0.57
73:A8:301:CDL:H381	42:N2:256:PRO:HB2	1.85	0.57
35:C1:313:ALA:HA	78:C1:603:HEA:H262	1.85	0.57
36:C2:1:MET:HB3	36:C2:193:TYR:HD2	1.69	0.57
44:N4:375:LEU:HD11	45:N5:141:PHE:HE2	1.68	0.57
67:V1:203:ALA:HB3	67:V1:206:CYS:HB2	1.86	0.57
14:A5:48:THR:HA	14:A5:51:ILE:HG12	1.85	0.57
36:C2:128:LEU:HD11	36:C2:134:ARG:HA	1.86	0.57
45:N5:295:GLN:O	45:N5:425:ARG:NH1	2.37	0.57
47:Qa:51:SER:HB3	47:Qa:230:LEU:HD12	1.86	0.57
1:4L:37:MET:HE3	1:4L:67:ALA:HB2	1.87	0.57
3:5B:82:SER:O	3:5B:125:HIS:N	2.37	0.57
3:5B:104:TRP:HE1	35:C1:495:LEU:HB3	1.70	0.57
4:6A:28:TRP:HB3	37:C3:146:TRP:HB2	1.86	0.57
21:AL:140:LYS:HG2	21:AL:141:VAL:HG23	1.86	0.57
35:C1:100:MET:HE3	35:C1:159:LEU:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:240:HIS:HB2	35:C1:291:HIS:HE1	1.69	0.57
37:C3:140:SER:HB3	37:C3:242:TRP:HE1	1.69	0.57
18:A9:135:GLU:HG3	18:A9:140:ASP:HA	1.87	0.57
18:A9:165:ILE:HD13	18:A9:199:THR:HB	1.85	0.57
35:C1:1:MET:N	35:C1:4:ASN:OD1	2.37	0.57
35:C1:38:ARG:NH2	35:C1:451:ASN:O	2.38	0.57
42:N2:42:PRO:HG2	46:N6:167:VAL:HG22	1.86	0.57
59:S1:405:THR:HB	59:S1:477:GLY:HA3	1.86	0.57
67:V1:177:TYR:OH	67:V1:194:ASP:OD1	2.22	0.57
2:5A:56:ALA:O	2:5A:60:THR:OG1	2.20	0.57
37:C3:210:ILE:HD13	71:C3:301:PC1:H3D1	1.87	0.57
48:QB:121:ASN:ND2	48:QB:132:TYR:OH	2.38	0.57
50:QD:97:TRP:NE1	50:QD:210:ASP:OD1	2.31	0.57
73:QH:101:CDL:H131	73:QH:102:CDL:HB4	1.86	0.57
73:QH:102:CDL:H741	73:QH:102:CDL:H532	1.87	0.57
67:V1:52:ARG:HH21	69:V3:390:GLN:HG2	1.69	0.57
30:B7:103:GLU:O	30:B7:107:ARG:HG2	2.05	0.57
35:C1:135:ASN:ND2	35:C1:213:ARG:O	2.38	0.57
38:C4:42:ARG:HE	38:C4:94:ASN:HD21	1.53	0.57
59:S1:83:GLU:HB2	59:S1:101:ASN:HB3	1.86	0.57
60:S2:140:PRO:HB2	65:S7:142:TYR:CE2	2.40	0.57
67:V1:118:ASP:HB3	67:V1:207:GLY:HA2	1.87	0.57
67:V1:94:PRO:HB2	67:V1:97:LEU:HB2	1.86	0.57
10:8B:55:GLY:O	10:8B:59:SER:OG	2.20	0.56
15:A6:89:VAL:HG22	75:AB:201:ZMP:H22	1.86	0.56
51:Qe:255:PRO:HG2	51:Qe:256:LEU:HD23	1.87	0.56
59:S1:449:PRO:HB2	59:S1:679:LEU:HD13	1.86	0.56
1:4L:75:LEU:HD13	46:N6:70:TYR:HE2	1.68	0.56
7:7A:72:GLY:O	7:7A:75:SER:OG	2.22	0.56
35:C1:169:ILE:O	35:C1:172:LYS:NZ	2.36	0.56
42:N2:235:ASN:O	42:N2:315:TRP:NE1	2.37	0.56
36:C2:96:THR:HG1	36:C2:151:ARG:HH11	1.51	0.56
37:C3:221:ARG:HB3	37:C3:226:HIS:HB2	1.88	0.56
50:QD:211:TYR:OH	83:QD:401:HEC:O2A	2.15	0.56
48:Qb:87:ASN:HD22	48:Qb:204:PRO:HD3	1.69	0.56
59:S1:340:ALA:HB3	59:S1:366:LEU:HD23	1.87	0.56
66:S8:100:GLU:O	66:S8:170:GLY:N	2.29	0.56
73:A8:301:CDL:H522	73:A8:301:CDL:H181	1.87	0.56
35:C1:329:GLY:O	36:C2:52:HIS:N	2.37	0.56
42:N2:131:LEU:O	42:N2:135:LYS:HG2	2.06	0.56
60:S2:444:MET:SD	60:S2:460:GLN:NE2	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BL:95:PHE:O	34:BL:99:LEU:HB2	2.05	0.56
49:QC:215:MET:HG2	53:Qg:60:VAL:HG13	1.86	0.56
50:QD:317:SER:OG	54:Qh:24:GLN:OE1	2.18	0.56
59:S1:200:ARG:HH12	68:V2:120:THR:HG23	1.69	0.56
3:5B:78:ASN:HB2	3:5B:120:TYR:CD1	2.39	0.56
17:A8:224:ARG:NH2	63:S5:42:GLU:OE1	2.38	0.56
29:B6:146:LEU:HD11	45:N5:9:LEU:HD12	1.86	0.56
48:Qb:388:VAL:HG21	48:Qb:438:ALA:HA	1.88	0.56
67:V1:60:GLY:HA2	68:V2:241:PRO:HA	1.87	0.56
67:V1:61:ASP:OD1	67:V1:137:LYS:NZ	2.38	0.56
23:AN:89:GLU:OE2	23:AN:128:ARG:NH1	2.35	0.56
36:C2:18:GLU:HA	36:C2:21:LEU:HD12	1.87	0.56
73:CB:203:CDL:HB21	73:CB:203:CDL:HB61	1.88	0.56
54:QH:20:SER:HB3	54:QH:23:GLU:HG2	1.86	0.56
48:Qb:99:LYS:NZ	48:Qb:164:GLU:OE2	2.35	0.56
50:Qd:125:CYS:SG	83:Qd:401:HEC:HAC	2.46	0.56
67:V1:204:TYR:HB3	67:V1:377:GLU:HB3	1.87	0.56
4:6A:68:ARG:HH12	37:C3:189:SER:HG	1.51	0.56
27:B4:98:LEU:HD13	71:N4:503:PC1:H272	1.86	0.56
37:C3:133:ASN:HB3	37:C3:173:PHE:CE2	2.41	0.56
77:CB:201:3PE:H332	42:N2:322:GLN:HE22	1.70	0.56
10:8B:31:ARG:HD3	35:C1:479:LYS:HB3	1.88	0.56
35:C1:508:PRO:HG3	37:C3:6:HIS:HB3	1.88	0.56
36:C2:12:ALA:O	36:C2:188:ARG:NH2	2.31	0.56
45:N5:97:THR:HG21	45:N5:125:LEU:HD22	1.86	0.56
45:N5:400:ASN:HB3	45:N5:486:MET:HE3	1.87	0.56
49:QC:236:MET:HE3	72:QE:301:PLX:H212	1.88	0.56
51:QE:234:TYR:HB2	51:QE:243:TYR:HB2	1.87	0.56
11:A1:12:MET:HE3	41:N1:264:LEU:HD22	1.86	0.56
17:A8:228:ASN:OD1	63:S5:51:ARG:NH1	2.34	0.56
30:B7:92:HIS:ND1	45:N5:481:THR:OG1	2.26	0.56
35:C1:69:MET:SD	78:C1:602:HEA:H18	2.46	0.56
42:N2:252:GLY:HA3	42:N2:290:LEU:HD13	1.88	0.56
51:Qe:214:ILE:HG13	51:Qe:261:PRO:HD3	1.88	0.56
68:V2:108:PRO:HB2	68:V2:111:ARG:HG2	1.88	0.56
7:7A:27:ALA:O	7:7A:31:LYS:HG2	2.06	0.55
35:C1:191:THR:HG23	35:C1:245:ILE:HG23	1.88	0.55
48:Qb:156:LEU:O	48:Qb:213:ARG:NH1	2.38	0.55
61:S3:157:VAL:HG21	61:S3:182:PRO:HD3	1.88	0.55
41:N1:102:VAL:HG11	41:N1:154:LEU:HD11	1.88	0.55
47:QA:70:ARG:NH2	47:QA:332:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B3:27:THR:HG22	26:B3:29:LEU:H	1.71	0.55
35:C1:320:VAL:HG13	35:C1:345:ILE:HD11	1.87	0.55
44:N4:373:ILE:HD11	44:N4:444:LEU:HD23	1.88	0.55
47:QA:399:GLN:HA	47:QA:402:VAL:HG22	1.88	0.55
67:V1:423:THR:HG21	67:V1:428:GLY:HA3	1.87	0.55
23:AN:105:LYS:O	63:S5:75:ARG:NH2	2.40	0.55
71:B4:202:PC1:H3B2	71:N4:504:PC1:H3A2	1.89	0.55
33:BK:114:GLN:HG3	45:N5:203:MET:HG2	1.89	0.55
36:C2:196:CYS:SG	36:C2:204:HIS:HE1	2.28	0.55
42:N2:26:TRP:HB3	42:N2:74:ILE:HD13	1.88	0.55
49:Qc:237:LEU:HD13	50:Qd:297:MET:HG2	1.88	0.55
59:S1:217:GLU:HG3	59:S1:412:PRO:HB3	1.88	0.55
35:C1:383:MET:HG2	35:C1:421:VAL:HB	1.88	0.55
37:C3:231:HIS:CG	71:C3:301:PC1:H122	2.41	0.55
44:N4:369:LEU:HD21	45:N5:149:ILE:HD13	1.89	0.55
62:S4:84:ARG:NH1	62:S4:88:GLN:O	2.38	0.55
18:A9:212:ARG:O	18:A9:216:TYR:N	2.33	0.55
44:N4:1:MET:HE2	44:N4:111:THR:HG21	1.89	0.55
45:N5:332:HIS:O	45:N5:336:LYS:HB2	2.07	0.55
68:V2:179:ALA:HB3	68:V2:185:MET:HE3	1.88	0.55
73:CB:203:CDL:H851	73:CB:203:CDL:H251	1.88	0.55
53:Qg:36:ASP:OD1	53:Qg:90:TYR:OH	2.16	0.55
18:A9:188:GLU:HG3	18:A9:200:ILE:HD13	1.88	0.55
53:QG:36:ASP:OD1	53:QG:90:TYR:OH	2.17	0.55
48:Qb:121:ASN:ND2	48:Qb:132:TYR:OH	2.36	0.55
2:5A:92:ASP:HB2	2:5A:132:LEU:HD21	1.88	0.55
29:B6:89:SER:HB2	29:B6:92:GLU:HB2	1.89	0.55
42:N2:211:MET:HG2	42:N2:333:SER:HB2	1.89	0.55
46:N6:17:PHE:HA	46:N6:20:PHE:CD1	2.42	0.55
51:QE:110:ARG:NH1	54:Qh:22:PHE:O	2.39	0.55
37:C3:86:PHE:CZ	71:C3:301:PC1:H3C1	2.42	0.55
50:QD:280:GLU:OE2	50:QD:286:ARG:NH1	2.40	0.55
71:C3:302:PC1:H362	71:C3:302:PC1:H272	1.89	0.54
7:7A:39:LEU:HB2	7:7A:44:LYS:HB3	1.90	0.54
11:A1:50:ARG:NH2	17:A8:95:VAL:O	2.41	0.54
38:C4:56:SER:N	38:C4:59:GLN:HB2	2.21	0.54
47:QA:70:ARG:HD2	47:QA:117:GLU:HG2	1.89	0.54
47:QA:116:ARG:NH1	47:QA:188:ASN:O	2.40	0.54
49:QC:100:ARG:NH1	82:QC:402:HEM:HBD2	2.22	0.54
67:V1:112:TYR:CD1	67:V1:153:ALA:HB3	2.42	0.54
32:B9:181:GLN:NE2	32:B9:198:PRO:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CA:55:TRP:NE1	40:CB:68:THR:OG1	2.40	0.54
73:N5:702:CDL:H162	73:N5:702:CDL:H581	1.89	0.54
46:N6:17:PHE:HA	46:N6:20:PHE:HD1	1.72	0.54
46:N6:71:THR:HA	46:N6:75:ALA:HB3	1.90	0.54
3:5B:70:ALA:N	3:5B:78:ASN:OD1	2.31	0.54
27:B4:71:ALA:HB2	31:B8:38:PRO:HG2	1.88	0.54
36:C2:9:PHE:HB2	36:C2:21:LEU:HD21	1.88	0.54
67:V1:88:ARG:NH2	67:V1:273:THR:O	2.39	0.54
67:V1:269:ARG:NH1	67:V1:340:ASP:OD2	2.40	0.54
78:C1:602:HEA:HBA2	78:C1:602:HEA:CMA	2.38	0.54
17:A8:84:LEU:O	23:AN:88:ARG:NH1	2.40	0.54
35:C1:74:MET:HE3	35:C1:389:ILE:HG13	1.88	0.54
35:C1:196:LEU:HD11	37:C3:89:SER:HB3	1.90	0.54
45:N5:6:SER:O	45:N5:10:THR:OG1	2.20	0.54
59:S1:251:ILE:HG21	59:S1:604:GLN:HB3	1.88	0.54
73:A8:301:CDL:H511	73:A8:301:CDL:H742	1.88	0.54
38:C4:56:SER:OG	38:C4:59:GLN:N	2.26	0.54
60:S2:230:ALA:O	66:S8:98:ARG:NH2	2.41	0.54
13:A3:127:ALA:HB2	41:N1:312:ALA:HA	1.90	0.54
20:AK:82:LYS:HB2	20:AK:272:VAL:HG21	1.90	0.54
23:AN:98:MET:HE3	23:AN:101:VAL:HG21	1.90	0.54
34:BL:129:ARG:NH1	34:BL:136:LEU:O	2.35	0.54
38:C4:56:SER:N	38:C4:59:GLN:OE1	2.32	0.54
44:N4:196:TRP:CD1	44:N4:250:LEU:HB3	2.43	0.54
47:QA:272:VAL:HA	47:QA:337:GLY:HA3	1.89	0.54
35:C1:369:ASP:HA	35:C1:438:ARG:HD3	1.90	0.54
49:QC:200:LEU:HD13	82:QC:402:HEM:HAD2	1.90	0.54
2:5A:109:ARG:O	2:5A:113:VAL:HG13	2.08	0.54
48:QB:460:GLY:HA2	48:QB:462:ILE:HG12	1.90	0.54
52:QF:56:ARG:NH1	52:QF:65:GLU:OE2	2.41	0.54
65:S7:55:ASN:ND2	65:S7:187:GLU:O	2.35	0.54
18:A9:316:ARG:O	18:A9:320:GLU:HG2	2.08	0.53
35:C1:439:ARG:NH2	78:C1:602:HEA:O1D	2.40	0.53
36:C2:218:TYR:HA	36:C2:221:LYS:HD2	1.90	0.53
48:Qb:467:ASP:OD2	49:Qc:223:TYR:OH	2.22	0.53
71:6A:101:PC1:H381	37:C3:206:LEU:HD22	1.90	0.53
16:A7:71:SER:HB3	16:A7:74:LYS:HE2	1.90	0.53
41:N1:81:LEU:HD21	71:N1:402:PC1:H2B2	1.89	0.53
59:S1:179:CYS:SG	59:S1:181:ARG:HB2	2.48	0.53
59:S1:307:ILE:HG23	59:S1:317:THR:HG21	1.90	0.53
35:C1:181:THR:HG1	35:C1:186:TRP:CD1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Qb:186:TYR:HH	48:Qb:277:HIS:HD1	1.55	0.53
69:V3:418:ARG:NH1	69:V3:423:HIS:O	2.41	0.53
1:4L:1:MET:SD	42:N2:80:TYR:OH	2.66	0.53
71:6A:101:PC1:H3A1	37:C3:206:LEU:HD13	1.89	0.53
57:QK:20:ARG:HH12	57:QK:24:GLY:H	1.57	0.53
48:Qb:302:VAL:HB	48:Qb:303:PRO:HD3	1.91	0.53
29:B6:157:VAL:HG13	45:N5:61:MET:HE3	1.89	0.53
41:N1:160:TYR:OH	43:N3:73:LEU:O	2.27	0.53
49:QC:223:TYR:O	50:QD:312:TRP:NE1	2.35	0.53
4:6A:63:HIS:CD2	5:6B:76:ARG:HE	2.27	0.53
48:QB:301:ASN:ND2	48:QB:347:CYS:SG	2.81	0.53
36:C2:146:MET:N	36:C2:214:VAL:O	2.41	0.53
38:C4:56:SER:O	38:C4:60:LYS:N	2.42	0.53
45:N5:3:PRO:HB2	45:N5:53:MET:HE1	1.90	0.53
48:QB:100:GLY:HA2	48:QB:106:GLY:N	2.24	0.53
59:S1:43:VAL:HG12	59:S1:55:LYS:HD2	1.91	0.53
72:6C:101:PLX:H81	35:C1:433:LEU:HD11	1.91	0.53
44:N4:391:ILE:HG23	44:N4:394:ILE:HD12	1.90	0.53
45:N5:208:CYS:HB2	45:N5:266:LEU:HD22	1.91	0.53
45:N5:15:LEU:HD11	45:N5:94:LEU:HD21	1.91	0.53
12:A2:51:LEU:HD22	12:A2:95:LEU:HD21	1.90	0.53
15:A6:63:ARG:NH2	19:AB:132:ASP:OD2	2.42	0.53
18:A9:167:ILE:HD13	18:A9:201:ILE:HB	1.90	0.53
45:N5:399:VAL:HG12	45:N5:409:LEU:HD13	1.91	0.53
46:N6:82:VAL:HG12	46:N6:85:SER:HB2	1.91	0.53
48:QB:156:LEU:O	48:QB:213:ARG:NH1	2.41	0.52
49:Qc:213:SER:OG	49:Qc:217:LYS:NZ	2.42	0.52
49:Qc:237:LEU:HB2	50:Qd:297:MET:HG2	1.91	0.52
60:S2:190:ILE:HG23	60:S2:209:MET:HB3	1.91	0.52
66:S8:47:SER:O	66:S8:56:ARG:NH2	2.42	0.52
19:AC:94:ASP:HB3	19:AC:97:LYS:HG2	1.90	0.52
36:C2:196:CYS:HB3	36:C2:207:MET:SD	2.49	0.52
41:N1:87:VAL:HG11	43:N3:6:THR:HG21	1.91	0.52
42:N2:42:PRO:HG3	46:N6:167:VAL:HG13	1.91	0.52
55:QI:11:TYR:HA	55:QI:15:PHE:HB2	1.90	0.52
59:S1:347:ASP:OD1	59:S1:347:ASP:N	2.42	0.52
60:S2:321:GLU:O	60:S2:352:GLN:NE2	2.33	0.52
18:A9:199:THR:OG1	18:A9:258:ALA:O	2.24	0.52
18:A9:279:TYR:HB2	18:A9:372:ALA:HB2	1.90	0.52
35:C1:214:ASN:HB2	35:C1:215:LEU:HD12	1.92	0.52
67:V1:113:LEU:HD13	67:V1:149:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:65:MET:HB3	78:C1:602:HEA:CAC	2.40	0.52
37:C3:204:HIS:NE2	37:C3:249:TRP:HB2	2.24	0.52
50:QD:266:GLN:HE22	52:Qf:91:LYS:H	1.58	0.52
67:V1:114:VAL:HG11	67:V1:212:LEU:HD21	1.91	0.52
67:V1:195:VAL:O	69:V3:410:ARG:NH1	2.41	0.52
1:4L:27:MET:HE2	1:4L:78:LEU:HD13	1.91	0.52
35:C1:167:THR:HA	35:C1:171:MET:HG3	1.91	0.52
48:QB:80:ARG:NH2	48:QB:350:GLU:OE1	2.42	0.52
53:QG:46:GLU:OE2	53:QG:50:ARG:NH2	2.42	0.52
72:QI:301:PLX:H331	56:QJ:31:GLY:HA3	1.90	0.52
59:S1:557:ARG:NH2	59:S1:581:ASP:OD1	2.41	0.52
67:V1:211:ALA:HB2	67:V1:223:PRO:HG3	1.91	0.52
35:C1:159:LEU:O	35:C1:162:ILE:HG13	2.09	0.52
36:C2:123:ILE:HD12	36:C2:137:GLU:HB3	1.92	0.52
41:N1:218:GLY:HA3	43:N3:21:ALA:HB1	1.92	0.52
51:QE:207:LYS:HE3	51:QE:210:TRP:HD1	1.75	0.52
49:Qc:300:ILE:HD11	49:Qc:363:LEU:HD21	1.92	0.52
59:S1:361:VAL:HG23	59:S1:363:SER:HB3	1.91	0.52
60:S2:190:ILE:HD11	60:S2:257:PHE:HZ	1.75	0.52
4:6A:62:TYR:HB3	4:6A:64:HIS:HD2	1.75	0.52
14:A5:114:TRP:CD2	14:A5:115:PRO:HA	2.45	0.52
35:C1:3:VAL:HG13	35:C1:7:LEU:HD12	1.90	0.52
42:N2:298:TYR:O	42:N2:303:THR:OG1	2.24	0.52
51:QE:126:ALA:HA	77:QE:303:3PE:H2F1	1.92	0.52
49:Qc:30:TRP:HB3	49:Qc:100:ARG:HG3	1.92	0.52
59:S1:534:VAL:HG22	59:S1:537:ILE:HB	1.92	0.52
68:V2:93:LEU:HD12	68:V2:122:TYR:HB3	1.91	0.52
1:4L:55:LEU:H	63:S5:25:GLN:HE22	1.58	0.52
8:7B:60:ILE:HD13	38:C4:119:ILE:HG12	1.92	0.52
31:B8:96:ASP:OD1	31:B8:96:ASP:N	2.40	0.52
77:C1:601:3PE:H2F1	77:C1:601:3PE:H3G1	1.92	0.52
60:S2:194:THR:HG21	60:S2:209:MET:HB2	1.91	0.52
60:S2:464:PHE:HA	60:S2:467:VAL:HB	1.91	0.52
67:V1:40:ARG:NH1	67:V1:289:GLU:O	2.43	0.52
11:A1:46:ASN:ND2	46:N6:132:ASP:OD2	2.33	0.52
17:A8:174:PHE:HB3	17:A8:178:ARG:HH12	1.75	0.52
34:BL:89:VAL:HG21	44:N4:25:ILE:HG23	1.90	0.52
36:C2:163:TRP:HZ2	36:C2:211:LEU:HD21	1.73	0.52
41:N1:173:TRP:HB3	41:N1:175:ILE:HG22	1.92	0.52
43:N3:70:ALA:HB2	46:N6:59:ILE:HD11	1.91	0.52
43:N3:79:SER:HA	43:N3:87:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QC:141:TRP:CD1	49:QC:265:PRO:HD3	2.44	0.52
67:V1:296:LEU:HD21	67:V1:317:VAL:HG11	1.92	0.52
69:V3:399:PHE:HD2	69:V3:400:LEU:HD12	1.74	0.52
13:A3:144:ASP:HB3	17:A8:209:LYS:HG2	1.91	0.52
45:N5:536:LEU:HB3	45:N5:537:PRO:HD3	1.92	0.52
61:S3:129:VAL:HG22	61:S3:144:LYS:HD2	1.92	0.52
4:6A:74:TRP:NE1	4:6A:79:HIS:O	2.27	0.51
37:C3:180:GLU:HA	37:C3:183:GLU:HB2	1.90	0.51
48:QB:192:PHE:O	48:QB:198:ALA:HB2	2.10	0.51
65:S7:54:VAL:HG21	71:S7:302:PC1:H352	1.90	0.51
37:C3:50:ASN:HD21	71:C3:302:PC1:H392	1.75	0.51
45:N5:293:ILE:HD13	45:N5:418:LEU:HD22	1.92	0.51
48:Qb:396:ARG:NE	48:Qb:430:GLU:OE2	2.42	0.51
23:AN:26:PRO:O	66:S8:68:ARG:NH2	2.41	0.51
48:QB:152:GLN:HG2	48:QB:253:LEU:HD13	1.91	0.51
50:QD:237:TYR:OH	52:Qf:79:ASP:OD2	2.23	0.51
11:A1:44:GLN:HE21	46:N6:135:PHE:HE1	1.57	0.51
18:A9:221:ARG:HH21	18:A9:222:TRP:HE1	1.59	0.51
26:B3:47:ARG:HA	26:B3:50:ALA:HB3	1.92	0.51
28:B5:163:ARG:NH1	40:CB:102:ASP:OD2	2.31	0.51
42:N2:95:MET:HE2	42:N2:149:ILE:HA	1.91	0.51
42:N2:136:LEU:HD12	42:N2:205:LEU:HD21	1.91	0.51
61:S3:132:LEU:HB2	61:S3:141:ILE:HG22	1.92	0.51
67:V1:89:GLY:HA3	86:V1:502:FMN:HM82	1.92	0.51
28:B5:92:PHE:O	33:BK:59:ASN:ND2	2.44	0.51
35:C1:94:PHE:HD1	71:C3:302:PC1:H121	1.74	0.51
59:S1:64:CYS:O	59:S1:184:ARG:NH2	2.27	0.51
62:S4:78:ARG:NE	62:S4:148:GLU:OE2	2.35	0.51
2:5A:68:ASP:O	2:5A:72:LEU:N	2.34	0.51
2:5A:93:ALA:HA	2:5A:96:ARG:HD2	1.91	0.51
6:6C:73:SER:HB2	36:C2:222:TRP:HB2	1.93	0.51
36:C2:217:LYS:HG2	36:C2:221:LYS:HE2	1.93	0.51
41:N1:18:ALA:HB1	41:N1:48:PRO:HB3	1.91	0.51
42:N2:25:HIS:HB2	63:S5:15:ASP:HB3	1.91	0.51
49:Qc:8:HIS:HB3	49:Qc:11:MET:HB2	1.91	0.51
3:5B:83:ILE:N	35:C1:507:GLU:OE2	2.29	0.51
22:AM:69:ASN:HD21	22:AM:112:ASN:HD21	1.57	0.51
35:C1:11:ASN:HD21	35:C1:13:LYS:HD2	1.76	0.51
44:N4:357:THR:HG21	73:N5:702:CDL:H711	1.93	0.51
49:QC:181:PHE:HA	49:QC:184:ILE:HG22	1.93	0.51
51:Qe:239:HIS:HB2	84:Qe:301:FES:S2	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:S2:214:GLU:OE2	60:S2:227:ARG:NH2	2.43	0.51
2:5A:127:TYR:HA	2:5A:130:GLN:HG2	1.93	0.51
23:AN:43:LEU:HG	41:N1:179:TRP:HE1	1.76	0.51
41:N1:72:ILE:HD12	73:N1:401:CDL:H121	1.93	0.51
45:N5:500:LEU:HD12	73:N5:703:CDL:H601	1.93	0.51
59:S1:433:GLY:HA2	59:S1:447:ASP:HA	1.93	0.51
67:V1:112:TYR:O	67:V1:240:THR:HA	2.11	0.51
5:6B:65:CYS:C	36:C2:98:LYS:HZ2	2.16	0.51
22:AM:123:GLN:O	64:S6:59:GLN:NE2	2.43	0.51
36:C2:1:MET:HB3	36:C2:193:TYR:CD2	2.46	0.51
41:N1:273:ILE:HG23	41:N1:277:TYR:HD2	1.76	0.51
45:N5:575:ILE:O	45:N5:579:ASN:HB2	2.11	0.51
49:Qc:284:ILE:HD11	71:Qc:404:PC1:H252	1.93	0.51
59:S1:152:ARG:NH1	67:V1:414:GLU:OE1	2.43	0.51
71:6A:101:PC1:H112	37:C3:187:THR:HA	1.93	0.51
35:C1:308:ALA:O	35:C1:311:ILE:HG12	2.11	0.51
77:C1:601:3PE:H2B1	77:C1:601:3PE:H3C1	1.92	0.51
41:N1:24:GLU:HA	41:N1:271:LEU:HD13	1.93	0.51
47:QA:134:MET:HE2	47:QA:233:VAL:HG21	1.93	0.51
52:QF:34:ARG:O	52:QF:38:GLU:HG2	2.11	0.51
47:Qa:164:VAL:HG21	48:Qb:317:THR:HG21	1.92	0.51
44:N4:216:LEU:HB3	44:N4:217:PRO:HD3	1.93	0.50
60:S2:145:LEU:HD13	60:S2:430:ILE:HG21	1.93	0.50
60:S2:323:ASP:OD1	66:S8:37:THR:OG1	2.28	0.50
65:S7:108:THR:HA	65:S7:136:CYS:HB3	1.93	0.50
67:V1:288:VAL:HG21	67:V1:303:HIS:CD2	2.46	0.50
8:7B:68:PRO:HB3	8:7B:72:VAL:HG21	1.93	0.50
11:A1:66:LEU:O	11:A1:69:ILE:HG13	2.10	0.50
35:C1:140:GLY:O	35:C1:213:ARG:NH2	2.43	0.50
42:N2:112:HIS:O	42:N2:116:PRO:HD2	2.11	0.50
3:5B:105:VAL:HG22	3:5B:111:GLN:HB2	1.93	0.50
35:C1:229:ILE:HD11	36:C2:175:ILE:HG12	1.92	0.50
35:C1:336:PRO:HA	35:C1:414:PHE:HE2	1.76	0.50
39:CA:68:GLU:OE2	39:CA:72:ARG:NE	2.42	0.50
44:N4:266:MET:HB3	44:N4:395:LEU:HD13	1.92	0.50
45:N5:562:LEU:HB3	45:N5:563:PRO:HD3	1.93	0.50
49:QC:112:THR:HG22	49:QC:196:HIS:CE1	2.46	0.50
50:QD:228:LEU:HD11	50:QD:234:PHE:HB2	1.93	0.50
59:S1:200:ARG:NH1	68:V2:118:PHE:O	2.45	0.50
59:S1:306:MET:HE2	59:S1:314:LEU:HB3	1.92	0.50
51:QE:209:GLU:HG3	51:QE:210:TRP:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B4:56:ARG:NH1	27:B4:58:GLY:O	2.45	0.50
34:BL:77:ASP:OD1	34:BL:78:LYS:N	2.44	0.50
35:C1:9:SER:OG	35:C1:99:ASN:ND2	2.44	0.50
35:C1:486:GLU:HB3	38:C4:41:ARG:HD2	1.92	0.50
37:C3:83:MET:HG2	37:C3:237:ALA:HB1	1.94	0.50
68:V2:166:ASP:OD1	68:V2:166:ASP:N	2.42	0.50
14:A5:44:TYR:O	14:A5:48:THR:HG22	2.11	0.50
32:B9:119:PRO:HB3	45:N5:525:MET:HE2	1.94	0.50
38:C4:63:LYS:O	38:C4:66:GLU:HB3	2.11	0.50
44:N4:368:ALA:HB1	44:N4:375:LEU:HD12	1.92	0.50
47:Qa:297:PRO:HB3	47:Qa:304:ASN:HD21	1.77	0.50
65:S7:86:MET:HB2	65:S7:91:VAL:HB	1.93	0.50
32:B9:77:ASP:OD1	32:B9:77:ASP:N	2.45	0.50
32:B9:218:GLU:HG2	32:B9:219:ARG:HG2	1.93	0.50
45:N5:327:LEU:O	45:N5:331:MET:HG2	2.12	0.50
51:QE:140:MET:HE3	49:Qc:177:ARG:HE	1.74	0.50
53:Qg:46:GLU:OE2	53:Qg:49:ARG:NH1	2.43	0.50
59:S1:185:PHE:CZ	59:S1:221:ASN:HB2	2.46	0.50
62:S4:112:MET:HG3	66:S8:184:LEU:HD23	1.93	0.50
7:7A:54:ARG:HB2	45:N5:503:GLU:HG3	1.93	0.50
18:A9:204:SER:HB3	18:A9:266:VAL:HG12	1.94	0.50
36:C2:156:SER:OG	36:C2:174:ALA:O	2.19	0.50
44:N4:366:ASN:ND2	44:N4:407:SER:OG	2.45	0.50
47:QA:313:VAL:HG11	47:QA:350:VAL:HG13	1.94	0.50
49:QC:165:TRP:O	49:QC:174:THR:OG1	2.26	0.50
47:Qa:61:ILE:HG12	47:Qa:130:ILE:HD11	1.94	0.50
48:Qb:74:TRP:CZ2	48:Qb:411:GLU:HA	2.47	0.50
52:Qf:45:LYS:O	52:Qf:48:GLU:HG2	2.12	0.50
66:S8:115:ALA:HB1	66:S8:132:ALA:HB2	1.94	0.50
67:V1:209:GLU:HG3	67:V1:210:THR:H	1.77	0.50
22:AM:127:TYR:OH	64:S6:61:GLU:O	2.24	0.50
29:B6:159:GLU:HG3	45:N5:61:MET:HG2	1.93	0.50
30:B7:17:PRO:HB3	30:B7:105:GLU:HG2	1.92	0.50
35:C1:91:ASP:OD1	35:C1:92:MET:N	2.41	0.50
59:S1:63:PHE:O	59:S1:181:ARG:NH1	2.45	0.50
59:S1:69:LEU:O	62:S4:158:LYS:NZ	2.37	0.50
59:S1:338:VAL:HB	59:S1:363:SER:CB	2.41	0.50
30:B7:12:ASP:OD1	30:B7:14:SER:OG	2.25	0.49
44:N4:443:PRO:HB3	72:N4:502:PLX:H351	1.93	0.49
54:QH:3:ARG:HH22	49:Qc:217:LYS:HE2	1.76	0.49
5:6B:41:GLU:O	5:6B:45:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:316:THR:HG21	78:C1:603:HEA:C14	2.42	0.49
35:C1:425:PHE:HD1	35:C1:428:GLN:HG3	1.76	0.49
35:C1:468:MET:SD	78:C1:602:HEA:H243	2.53	0.49
36:C2:95:LEU:HB3	36:C2:150:ILE:HG13	1.94	0.49
51:QE:214:ILE:HG13	51:QE:261:PRO:HD3	1.94	0.49
49:Qc:216:ASP:OD2	50:Qd:318:ARG:NH2	2.44	0.49
60:S2:145:LEU:HD11	60:S2:430:ILE:HD13	1.94	0.49
15:A6:50:ASP:OD1	15:A6:50:ASP:N	2.42	0.49
22:AM:26:VAL:HG13	22:AM:33:VAL:HG12	1.93	0.49
29:B6:165:PHE:O	29:B6:168:ASP:HB2	2.13	0.49
41:N1:216:ALA:HB2	65:S7:98:ARG:HB3	1.94	0.49
73:N1:401:CDL:H511	73:N1:401:CDL:H732	1.94	0.49
47:QA:61:ILE:HG12	47:QA:130:ILE:HD11	1.93	0.49
49:Qc:47:THR:HG23	49:Qc:79:ILE:HG23	1.93	0.49
42:N2:218:LEU:HD21	42:N2:330:ILE:HD11	1.94	0.49
51:QE:160:PRO:HD2	51:QE:163:LYS:HG2	1.94	0.49
48:Qb:465:LEU:HD12	48:Qb:466:PRO:HD2	1.95	0.49
60:S2:182:GLU:OE2	60:S2:317:TYR:OH	2.18	0.49
6:6C:58:SER:O	6:6C:62:PHE:N	2.34	0.49
22:AM:108:TYR:HE1	66:S8:198:GLU:HG2	1.78	0.49
35:C1:251:PHE:HB3	35:C1:319:LYS:HE2	1.95	0.49
36:C2:104:TRP:CD1	36:C2:203:ASN:HB2	2.48	0.49
44:N4:371:PRO:HD2	73:N5:702:CDL:H402	1.93	0.49
49:QC:81:TYR:OH	50:QD:203:ARG:NH1	2.45	0.49
47:Qa:323:VAL:HG12	47:Qa:340:THR:HG22	1.94	0.49
50:Qd:228:LEU:HD11	50:Qd:234:PHE:HB2	1.93	0.49
67:V1:112:TYR:HD1	67:V1:153:ALA:HB3	1.76	0.49
14:A5:38:ILE:O	14:A5:45:ARG:NH1	2.45	0.49
17:A8:219:TYR:OH	28:B5:189:ASN:ND2	2.39	0.49
22:AM:55:PHE:CZ	22:AM:58:ARG:HG3	2.47	0.49
29:B6:132:VAL:O	29:B6:136:LEU:CB	2.60	0.49
35:C1:151:HIS:CE1	35:C1:206:ILE:HG13	2.47	0.49
60:S2:101:LEU:HB2	60:S2:464:PHE:CZ	2.48	0.49
65:S7:121:TYR:O	65:S7:128:ARG:NH1	2.45	0.49
66:S8:63:TRP:HB3	66:S8:66:LEU:HD12	1.94	0.49
67:V1:146:GLY:HA3	67:V1:193:PHE:CE1	2.46	0.49
20:AK:84:GLY:O	20:AK:157:GLN:NE2	2.36	0.49
20:AK:297:ARG:HA	20:AK:300:VAL:HG22	1.94	0.49
73:AL:202:CDL:H521	46:N6:88:THR:HG23	1.94	0.49
35:C1:173:PRO:HD2	35:C1:176:MET:HE2	1.95	0.49
41:N1:156:MET:HE1	41:N1:177:THR:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:N1:169:GLN:HB3	41:N1:244:GLY:HA3	1.94	0.49
45:N5:249:SER:HA	45:N5:306:THR:HG21	1.94	0.49
53:Qg:53:GLU:OE2	54:Qh:12:ARG:NH1	2.45	0.49
60:S2:190:ILE:HD11	60:S2:257:PHE:CZ	2.47	0.49
18:A9:109:ASN:HB3	18:A9:112:ASP:HB2	1.95	0.49
42:N2:132:THR:HG21	73:N2:402:CDL:H352	1.94	0.49
44:N4:76:MET:SD	44:N4:230:VAL:HB	2.53	0.49
47:Qa:66:LYS:HB2	47:Qa:217:ARG:HB3	1.95	0.49
2:5A:123:GLU:C	2:5A:126:PRO:HD2	2.38	0.49
7:7A:30:GLN:HG2	37:C3:67:PHE:HA	1.95	0.49
25:B2:90:ASP:O	45:N5:385:TYR:OH	2.23	0.49
35:C1:328:HIS:HD2	36:C2:56:MET:HE1	1.78	0.49
49:Qc:54:HIS:HB3	49:Qc:69:ILE:HG12	1.94	0.49
64:S6:67:ALA:HB2	66:S8:111:GLU:HG3	1.93	0.49
35:C1:8:TYR:CZ	37:C3:15:PRO:HB3	2.48	0.49
44:N4:191:SER:HB3	81:N4:501:PEE:H1	1.95	0.49
44:N4:416:ARG:HG2	45:N5:159:HIS:HB3	1.94	0.49
51:QE:220:LEU:HD12	51:QE:239:HIS:HE1	1.77	0.49
68:V2:111:ARG:NH1	68:V2:114:GLU:OE2	2.46	0.49
4:6A:88:ASN:ND2	71:6A:101:PC1:H151	2.28	0.48
9:7C:59:GLN:NE2	35:C1:116:SER:O	2.34	0.48
18:A9:359:TYR:HB2	41:N1:65:THR:HA	1.95	0.48
23:AN:85:GLN:OE1	63:S5:105:ARG:NH1	2.44	0.48
37:C3:15:PRO:O	37:C3:19:THR:OG1	2.24	0.48
49:Qc:356:ILE:HG13	71:Qc:404:PC1:H261	1.95	0.48
1:4L:28:SER:HB3	46:N6:23:LYS:HD2	1.94	0.48
17:A8:141:ASN:HD21	23:AN:81:ARG:HH21	1.60	0.48
36:C2:196:CYS:CB	36:C2:207:MET:SD	3.01	0.48
37:C3:9:HIS:NE2	37:C3:64:GLU:OE1	2.45	0.48
81:N5:701:PEE:H36	73:N5:702:CDL:H231	1.96	0.48
52:QF:60:ARG:NH2	54:QH:80:ASN:O	2.45	0.48
59:S1:217:GLU:HG2	59:S1:218:LEU:HG	1.94	0.48
67:V1:355:ILE:HD13	68:V2:139:PRO:HG3	1.95	0.48
12:A2:65:LEU:HD12	12:A2:79:LEU:HD11	1.94	0.48
18:A9:64:PHE:O	18:A9:67:ARG:HG2	2.13	0.48
35:C1:352:GLY:HA3	78:C1:603:HEA:H162	1.95	0.48
41:N1:149:ILE:HG21	41:N1:185:TRP:HB2	1.95	0.48
82:Qc:403:HEM:HBA1	82:Qc:403:HEM:HHA	1.95	0.48
51:Qe:153:GLU:HB3	51:Qe:270:LEU:HD11	1.95	0.48
60:S2:189:HIS:NE2	60:S2:342:GLU:OE1	2.45	0.48
66:S8:153:ILE:HG12	85:S8:302:SF4:S1	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:V1:300:ILE:HG22	67:V1:306:GLY:HA2	1.96	0.48
68:V2:41:HIS:CD2	68:V2:95:ILE:HG13	2.48	0.48
2:5A:102:ASN:ND2	38:C4:67:LYS:HA	2.28	0.48
3:5B:69:ALA:HB2	35:C1:512:ASN:HB3	1.96	0.48
35:C1:96:ARG:HH21	71:C3:302:PC1:H142	1.78	0.48
35:C1:491:ASN:HB3	35:C1:494:TRP:HD1	1.78	0.48
73:N1:401:CDL:HB31	46:N6:82:VAL:HG21	1.94	0.48
71:QB:502:PC1:H231	49:QC:4:ILE:HD11	1.95	0.48
48:Qb:274:GLU:OE2	48:Qb:276:ARG:NE	2.41	0.48
60:S2:299:LEU:HD22	60:S2:304:ILE:HD12	1.95	0.48
65:S7:188:LYS:HB3	65:S7:191:ARG:HB2	1.94	0.48
22:AM:124:TYR:OH	66:S8:184:LEU:O	2.28	0.48
24:B1:29:ARG:NH2	72:B5:201:PLX:O2	2.47	0.48
35:C1:372:TYR:N	35:C1:432:GLY:HA3	2.28	0.48
36:C2:118:PHE:HB3	36:C2:226:MET:HE1	1.96	0.48
77:CB:201:3PE:H391	42:N2:324:LYS:HA	1.95	0.48
71:N4:504:PC1:H371	71:N4:504:PC1:H292	1.95	0.48
51:Qe:213:LEU:HD23	51:Qe:258:LEU:HD12	1.95	0.48
52:Qf:28:ASP:HB3	52:Qf:29:PRO:HD3	1.95	0.48
66:S8:74:LEU:HD12	66:S8:77:LEU:HD23	1.94	0.48
67:V1:102:MET:SD	67:V1:241:THR:OG1	2.67	0.48
2:5A:65:PRO:HA	2:5A:100:ARG:HH11	1.79	0.48
20:AK:87:HIS:HE1	20:AK:162:GLU:HG3	1.77	0.48
32:B9:161:PHE:O	32:B9:165:GLU:HG2	2.14	0.48
41:N1:103:LEU:HB2	46:N6:54:LEU:HD13	1.94	0.48
41:N1:141:SER:HB2	41:N1:289:LEU:HG	1.96	0.48
43:N3:66:ASP:O	43:N3:69:ILE:HG13	2.12	0.48
44:N4:318:ALA:HB2	44:N4:373:ILE:HG13	1.95	0.48
51:QE:156:LEU:HB3	51:QE:210:TRP:CZ2	2.49	0.48
57:QK:32:ALA:HB1	47:Qa:164:VAL:HB	1.96	0.48
51:Qe:128:ALA:HB1	81:Qe:302:PEE:H56	1.96	0.48
59:S1:593:SER:HA	59:S1:606:THR:O	2.13	0.48
6:6C:15:LEU:O	6:6C:19:LEU:N	2.40	0.48
21:AL:118:MET:HA	21:AL:121:THR:HG22	1.96	0.48
35:C1:94:PHE:CD1	71:C3:302:PC1:H121	2.49	0.48
35:C1:407:GLN:H	77:C1:601:3PE:H112	1.79	0.48
36:C2:104:TRP:CG	36:C2:203:ASN:HB2	2.48	0.48
42:N2:190:MET:HG2	42:N2:204:ASN:HB3	1.94	0.48
42:N2:197:ASN:HB2	42:N2:269:GLU:HG2	1.95	0.48
48:QB:190:THR:HG22	48:QB:275:ILE:HG23	1.96	0.48
60:S2:228:MET:SD	65:S7:167:PRO:HG3	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A8:246:PHE:HE1	73:A8:301:CDL:H341	1.77	0.48
19:AB:117:GLU:HA	19:AB:120:MET:HE3	1.96	0.48
35:C1:96:ARG:CZ	37:C3:57:TRP:HE1	2.26	0.48
41:N1:301:CYS:O	41:N1:305:ILE:HG13	2.14	0.48
72:N2:401:PLX:H221	63:S5:2:PRO:HD3	1.96	0.48
50:QD:132:ALA:HA	50:QD:175:TYR:HA	1.96	0.48
51:QE:207:LYS:HE3	51:QE:210:TRP:CD1	2.49	0.48
71:Qc:404:PC1:H2F1	71:Qc:404:PC1:H2B1	1.96	0.48
59:S1:36:VAL:HG22	59:S1:102:ILE:HD12	1.96	0.48
65:S7:62:LEU:O	65:S7:91:VAL:HA	2.13	0.48
19:AC:111:ASP:N	19:AC:111:ASP:OD1	2.46	0.48
24:B1:47:ARG:NH2	24:B1:53:GLU:OE2	2.46	0.48
26:B3:24:ILE:O	26:B3:30:GLU:HB3	2.14	0.48
36:C2:161:HIS:HB2	36:C2:174:ALA:HB3	1.94	0.48
37:C3:126:PRO:HA	37:C3:130:PRO:HG2	1.95	0.48
71:N4:503:PC1:H3A2	71:N4:504:PC1:H3D1	1.96	0.48
48:QB:126:ARG:NH1	48:QB:199:GLN:O	2.47	0.48
67:V1:154:ALA:HB2	67:V1:193:PHE:CZ	2.49	0.48
2:5A:97:ALA:O	2:5A:101:LEU:N	2.47	0.48
5:6B:72:ALA:O	5:6B:76:ARG:HD3	2.14	0.48
28:B5:147:ALA:HB2	44:N4:173:SER:HB2	1.96	0.48
29:B6:141:ILE:HG23	81:N5:701:PEE:H60	1.95	0.48
42:N2:190:MET:HE1	42:N2:205:LEU:HD13	1.94	0.48
44:N4:382:ILE:HG12	44:N4:396:MET:HG3	1.96	0.48
9:7C:59:GLN:O	9:7C:63:LYS:N	2.38	0.47
35:C1:88:GLY:HA2	35:C1:505:PHE:CZ	2.49	0.47
37:C3:207:HIS:CE1	71:C3:301:PC1:H3G2	2.49	0.47
45:N5:248:HIS:O	45:N5:253:VAL:HG22	2.14	0.47
47:QA:222:GLY:HA3	47:QA:230:LEU:HD11	1.95	0.47
59:S1:624:ARG:NH1	59:S1:628:GLU:OE1	2.46	0.47
60:S2:61:THR:H	60:S2:64:THR:HG1	1.59	0.47
1:4L:62:ILE:HG21	42:N2:31:ILE:HD11	1.95	0.47
6:6C:53:TYR:OH	36:C2:188:ARG:NH2	2.26	0.47
28:B5:133:TYR:OH	33:BK:87:GLU:OE1	2.18	0.47
35:C1:406:ASN:CG	35:C1:409:TRP:HD1	2.22	0.47
37:C3:188:ILE:HD13	37:C3:198:PHE:CG	2.49	0.47
73:CB:203:CDL:H232	44:N4:97:THR:HG21	1.96	0.47
42:N2:291:TYR:HA	44:N4:151:PHE:HZ	1.79	0.47
44:N4:185:PRO:HB3	44:N4:252:PRO:HD3	1.96	0.47
48:QB:113:VAL:HG12	48:QB:146:LEU:HD23	1.96	0.47
48:QB:311:ILE:O	48:QB:326:SER:OG	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Qa:183:ARG:HG3	47:Qa:254:ARG:HB2	1.96	0.47
50:Qd:211:TYR:OH	83:Qd:401:HEC:O1A	2.18	0.47
68:V2:38:LEU:O	68:V2:124:ARG:NH2	2.42	0.47
37:C3:60:ASP:HA	37:C3:63:ARG:HD2	1.95	0.47
42:N2:172:GLN:OE1	45:N5:578:SER:OG	2.25	0.47
42:N2:265:MET:HE3	42:N2:340:THR:HG21	1.95	0.47
48:QB:269:ARG:NH1	51:QE:96:VAL:O	2.43	0.47
51:QE:244:ASP:OD2	51:QE:250:ARG:NH2	2.47	0.47
69:V3:386:TYR:CZ	69:V3:388:ASN:HB3	2.49	0.47
37:C3:140:SER:HB3	37:C3:242:TRP:NE1	2.29	0.47
44:N4:400:MET:HE1	45:N5:183:VAL:HG21	1.96	0.47
81:N5:701:PEE:H53	81:N5:701:PEE:H58	1.62	0.47
46:N6:124:ASP:HA	46:N6:127:ILE:HG12	1.96	0.47
51:QE:177:ARG:HB3	51:QE:211:VAL:HG13	1.95	0.47
51:QE:213:LEU:HD13	51:QE:258:LEU:HD12	1.95	0.47
51:QE:228:ALA:HB3	51:QE:235:TYR:HB3	1.96	0.47
48:Qb:315:ASP:OD1	48:Qb:316:SER:N	2.48	0.47
49:Qc:326:TRP:HZ2	81:Qc:401:PEE:H7	1.80	0.47
59:S1:603:ALA:HB3	59:S1:656:TYR:HA	1.97	0.47
64:S6:38:VAL:HG22	64:S6:44:ALA:HB2	1.95	0.47
25:B2:65:THR:HB	25:B2:68:GLN:HG2	1.96	0.47
25:B2:101:PRO:HD2	30:B7:99:MET:HE1	1.97	0.47
29:B6:146:LEU:HA	29:B6:150:VAL:HB	1.95	0.47
32:B9:178:GLU:OE2	32:B9:209:TRP:NE1	2.43	0.47
33:BK:74:ILE:HG23	33:BK:156:LEU:HD22	1.96	0.47
42:N2:112:HIS:CE1	42:N2:164:ILE:HG21	2.50	0.47
44:N4:243:MET:HB3	44:N4:301:ILE:HG21	1.96	0.47
48:QB:192:PHE:HB3	48:QB:195:THR:OG1	2.13	0.47
49:Qc:132:VAL:HG11	49:Qc:178:PHE:HD2	1.80	0.47
60:S2:117:PRO:HG3	60:S2:441:LEU:HD23	1.96	0.47
60:S2:124:2MR:O	65:S7:146:SER:OG	2.20	0.47
2:5A:58:TRP:CE2	2:5A:79:LEU:HD13	2.49	0.47
71:6A:101:PC1:H152	37:C3:187:THR:HA	1.96	0.47
10:8B:27:ALA:HB2	35:C1:404:THR:HG21	1.95	0.47
25:B2:79:MET:SD	45:N5:375:ILE:HG12	2.54	0.47
41:N1:273:ILE:HG23	41:N1:277:TYR:CD2	2.49	0.47
45:N5:295:GLN:HB2	45:N5:301:ILE:HG12	1.97	0.47
67:V1:388:GLY:HA3	67:V1:419:ILE:HD11	1.96	0.47
2:5A:104:PHE:CE2	2:5A:141:ILE:HA	2.49	0.47
5:6B:58:ARG:HA	5:6B:61:TYR:CE1	2.50	0.47
13:A3:137:ASN:OD1	13:A3:137:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AK:87:HIS:CE1	20:AK:162:GLU:HG3	2.50	0.47
22:AM:96:ASP:HB3	22:AM:101:LYS:HD3	1.97	0.47
26:B3:23:LYS:HB3	26:B3:25:GLU:HG2	1.96	0.47
29:B6:134:HIS:NE2	45:N5:35:TYR:OH	2.37	0.47
41:N1:61:LEU:HD11	65:S7:98:ARG:HD2	1.97	0.47
45:N5:288:THR:HG21	45:N5:307:SER:HB3	1.97	0.47
47:QA:85:LEU:HD12	47:QA:158:LEU:HD23	1.97	0.47
48:QB:56:GLY:HA3	48:QB:227:PRO:HB3	1.96	0.47
51:QE:178:HIS:HB2	51:QE:210:TRP:CZ3	2.49	0.47
47:Qa:301:ARG:NH2	48:Qb:94:GLU:OE2	2.48	0.47
63:S5:84:ASP:HA	63:S5:87:ILE:HG12	1.96	0.47
65:S7:64:PRO:HA	65:S7:102:VAL:O	2.15	0.47
5:6B:42:LYS:O	5:6B:45:THR:OG1	2.32	0.47
17:A8:115:LYS:HB3	17:A8:116:PRO:HD3	1.97	0.47
18:A9:106:MET:HE2	18:A9:118:LYS:HE3	1.97	0.47
45:N5:559:GLU:O	45:N5:564:LYS:HB2	2.15	0.47
48:QB:479:ARG:HH21	73:QB:501:CDL:HB21	1.78	0.47
47:Qa:375:LYS:NZ	47:Qa:419:VAL:O	2.34	0.47
50:Qd:118:TYR:HA	50:Qd:122:CYS:SG	2.54	0.47
5:6B:30:CYS:HB2	5:6B:65:CYS:SG	2.55	0.47
18:A9:85:ARG:HH22	65:S7:196:ARG:HG3	1.79	0.47
20:AK:253:GLU:O	20:AK:282:LYS:NZ	2.47	0.47
37:C3:137:LEU:HD12	37:C3:249:TRP:CD1	2.49	0.47
41:N1:273:ILE:HD11	81:S8:303:PEE:H65	1.97	0.47
42:N2:96:THR:HG22	42:N2:100:MET:HE2	1.97	0.47
44:N4:282:LEU:HD21	44:N4:359:TRP:HH2	1.80	0.47
45:N5:208:CYS:HA	45:N5:209:PRO:HD3	1.73	0.47
27:B4:88:LEU:HD11	73:B4:201:CDL:H322	1.95	0.47
35:C1:70:VAL:HB	35:C1:246:LEU:HD22	1.97	0.47
8:7B:34:HIS:NE2	77:C1:601:3PE:O22	2.46	0.46
11:A1:54:ILE:HD11	17:A8:98:SER:HA	1.96	0.46
18:A9:79:GLN:NE2	18:A9:102:GLN:O	2.48	0.46
35:C1:397:PHE:HB3	35:C1:405:LEU:HD11	1.97	0.46
37:C3:54:MET:HB3	37:C3:58:TRP:CZ3	2.50	0.46
45:N5:174:TYR:CD2	45:N5:232:TRP:HB3	2.50	0.46
45:N5:241:THR:HG21	45:N5:344:GLY:HA3	1.96	0.46
48:QB:179:MET:HE1	48:QB:282:LEU:HD13	1.96	0.46
15:A6:89:VAL:CG2	75:AB:201:ZMP:H22	2.45	0.46
17:A8:117:ASN:HB3	23:AN:73:PRO:HG2	1.97	0.46
20:AK:141:ARG:NE	20:AK:168:ASP:OD1	2.46	0.46
37:C3:57:TRP:O	37:C3:61:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C3:79:LEU:HB3	37:C3:233:PHE:CE2	2.50	0.46
37:C3:187:THR:OG1	37:C3:188:ILE:N	2.48	0.46
56:QJ:14:ALA:O	56:QJ:18:ILE:HG12	2.15	0.46
57:QK:24:GLY:HA3	47:Qa:109:LYS:HE3	1.96	0.46
47:Qa:70:ARG:NH1	47:Qa:117:GLU:OE2	2.48	0.46
49:Qc:119:LEU:HD22	82:Qc:403:HEM:HBB2	1.97	0.46
61:S3:126:PHE:HE2	61:S3:149:GLU:HG3	1.80	0.46
67:V1:117:ALA:HB1	67:V1:131:ILE:HD11	1.96	0.46
35:C1:442:ASP:OD2	36:C2:134:ARG:NH1	2.35	0.46
78:C1:602:HEA:H212	78:C1:602:HEA:H271	1.69	0.46
46:N6:117:PHE:HB2	46:N6:119:PHE:CZ	2.51	0.46
47:QA:72:GLU:OE2	47:QA:80:SER:N	2.30	0.46
48:QB:315:ASP:OD1	48:QB:316:SER:N	2.48	0.46
81:Qe:302:PEE:H16	81:Qe:302:PEE:H22	1.46	0.46
17:A8:160:THR:HA	17:A8:163:TRP:NE1	2.30	0.46
20:AK:138:TYR:HE1	20:AK:165:ILE:HG23	1.80	0.46
24:B1:42:SER:O	24:B1:46:LYS:HB2	2.15	0.46
31:B8:62:TYR:OH	31:B8:74:ASP:O	2.24	0.46
42:N2:288:LEU:HD23	81:S2:501:PEE:H58	1.98	0.46
81:N4:501:PEE:H72	81:N4:501:PEE:H67	1.80	0.46
45:N5:80:PHE:HB3	45:N5:82:MET:HE2	1.97	0.46
45:N5:292:ALA:HB2	45:N5:304:PHE:HB3	1.98	0.46
46:N6:57:PHE:O	46:N6:61:LEU:HG	2.14	0.46
50:QD:288:ARG:NH1	55:Qi:41:ASP:OD1	2.49	0.46
51:QE:123:VAL:HG13	55:Qi:29:ALA:HA	1.96	0.46
59:S1:340:ALA:HB1	59:S1:354:LEU:HD21	1.97	0.46
60:S2:164:LEU:HD12	60:S2:417:LEU:HD23	1.97	0.46
69:V3:420:SER:HB3	69:V3:423:HIS:ND1	2.29	0.46
1:4L:6:MET:HB2	46:N6:119:PHE:CD1	2.51	0.46
2:5A:110:ILE:O	2:5A:113:VAL:HG22	2.16	0.46
72:6C:101:PLX:H1A2	72:6C:101:PLX:H21	1.63	0.46
7:7A:40:PRO:HG2	7:7A:43:LEU:HB2	1.98	0.46
7:7A:71:LEU:HD21	35:C1:114:ALA:HB2	1.98	0.46
9:7C:49:PHE:CD2	10:8B:50:PHE:HB3	2.49	0.46
17:A8:120:PHE:HE2	23:AN:76:GLN:HB3	1.80	0.46
20:AK:83:LEU:HG	20:AK:272:VAL:HG13	1.97	0.46
22:AM:78:ASP:OD2	22:AM:80:SER:OG	2.32	0.46
37:C3:157:LYS:HE3	37:C3:158:HIS:CE1	2.51	0.46
42:N2:217:MET:HE2	42:N2:326:LEU:HB2	1.97	0.46
47:QA:271:LEU:HD22	47:QA:453:LEU:HD13	1.97	0.46
49:QC:197:LEU:HD11	82:QC:402:HEM:HMA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Qa:70:ARG:HD2	47:Qa:117:GLU:HG2	1.96	0.46
49:Qc:197:LEU:HD11	82:Qc:403:HEM:HMA3	1.96	0.46
51:Qe:88:PHE:O	51:Qe:92:ARG:HG3	2.15	0.46
62:S4:102:ASP:OD1	62:S4:102:ASP:N	2.45	0.46
67:V1:194:ASP:OD1	69:V3:410:ARG:NH1	2.49	0.46
4:6A:88:ASN:OD1	71:6A:101:PC1:H141	2.15	0.46
18:A9:237:LYS:HA	18:A9:326:ASP:HB2	1.97	0.46
23:AN:68:ARG:O	23:AN:72:MET:HG3	2.15	0.46
29:B6:148:TYR:CE1	33:BK:49:ARG:HG2	2.50	0.46
35:C1:96:ARG:NH2	37:C3:61:ILE:HG12	2.30	0.46
54:QH:12:ARG:NH1	48:Qb:279:ASP:OD1	2.49	0.46
47:Qa:71:TYR:HB3	47:Qa:212:HIS:CE1	2.50	0.46
9:7C:33:ASN:HD21	9:7C:35:TRP:HB2	1.81	0.46
10:8B:51:LEU:HD13	38:C4:117:LEU:HD21	1.98	0.46
30:B7:107:ARG:HA	30:B7:110:GLN:HG2	1.98	0.46
35:C1:74:MET:HA	35:C1:78:PHE:HD2	1.81	0.46
35:C1:202:LEU:HD22	35:C1:238:PHE:CZ	2.51	0.46
78:C1:602:HEA:HBA2	78:C1:602:HEA:HMA	1.98	0.46
36:C2:215:PRO:HB2	36:C2:218:TYR:HD1	1.81	0.46
37:C3:83:MET:HE3	37:C3:87:ILE:HD11	1.97	0.46
41:N1:99:ASN:HB2	71:N1:402:PC1:H152	1.97	0.46
41:N1:272:TRP:CZ2	66:S8:74:LEU:HB2	2.51	0.46
45:N5:103:PHE:HB2	45:N5:341:MET:HE3	1.97	0.46
45:N5:504:LEU:HD12	73:N5:703:CDL:H511	1.98	0.46
49:QC:132:VAL:HG11	49:QC:178:PHE:HD2	1.80	0.46
51:QE:151:LYS:HB3	51:QE:272:ILE:HD11	1.98	0.46
47:Qa:60:ARG:NH2	47:Qa:124:GLU:OE1	2.48	0.46
3:5B:47:LEU:HD11	3:5B:62:TYR:CE2	2.51	0.46
5:6B:31:TRP:CD2	37:C3:110:PRO:HB3	2.51	0.46
20:AK:131:TYR:CD1	20:AK:185:CYS:HB3	2.50	0.46
20:AK:355:TRP:H	20:AK:355:TRP:CD1	2.34	0.46
22:AM:84:PRO:HD3	22:AM:113:HIS:HD2	1.81	0.46
47:QA:233:VAL:HG22	47:QA:236:ARG:HH12	1.79	0.46
49:QC:379:TRP:HB3	53:Qg:34:ARG:HH12	1.81	0.46
50:QD:300:LEU:HD21	51:QE:124:GLY:HA3	1.97	0.46
51:QE:225:ILE:HG12	51:QE:237:PRO:HD3	1.97	0.46
47:Qa:123:VAL:HG22	47:Qa:137:LEU:HD22	1.98	0.46
35:C1:416:ILE:HG22	35:C1:464:ALA:HB2	1.98	0.46
38:C4:145:MET:HA	38:C4:148:MET:HG2	1.97	0.46
44:N4:225:ILE:HD13	44:N4:331:ASN:HB2	1.97	0.46
49:QC:126:THR:HG21	82:QC:401:HEM:HBB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Qf:60:ARG:NH1	54:Qh:78:TYR:O	2.47	0.46
59:S1:219:SER:O	59:S1:222:ILE:HG12	2.15	0.46
60:S2:160:ALA:HA	60:S2:404:THR:HG21	1.97	0.46
65:S7:130:VAL:HB	65:S7:159:VAL:HA	1.98	0.46
2:5A:140:GLY:O	38:C4:78:LYS:NZ	2.48	0.46
5:6B:6:GLN:O	5:6B:10:LYS:N	2.47	0.46
71:B4:202:PC1:H382	71:B4:202:PC1:H3C1	1.97	0.46
36:C2:116:LEU:HD12	36:C2:227:LEU:HG	1.97	0.46
44:N4:336:ARG:NH1	44:N4:433:GLU:OE2	2.47	0.46
45:N5:421:ALA:O	45:N5:424:THR:OG1	2.29	0.46
54:QH:20:SER:O	54:QH:24:GLN:HG2	2.16	0.46
67:V1:208:GLU:O	67:V1:212:LEU:N	2.42	0.46
86:V1:502:FMN:H9	86:V1:502:FMN:H4'	1.97	0.46
68:V2:83:LEU:HD21	68:V2:116:ALA:HB2	1.98	0.46
35:C1:307:SER:O	35:C1:311:ILE:HG23	2.17	0.45
73:N1:401:CDL:H592	71:N1:402:PC1:H2H1	1.96	0.45
44:N4:260:PRO:HB3	71:N4:503:PC1:H241	1.97	0.45
45:N5:298:ILE:O	45:N5:302:VAL:HG23	2.16	0.45
47:QA:82:LEU:HD11	47:QA:154:LEU:HB3	1.98	0.45
66:S8:100:GLU:OE1	66:S8:172:ASN:ND2	2.47	0.45
54:QH:37:ASN:OD1	54:QH:40:ARG:NH2	2.49	0.45
49:Qc:81:TYR:OH	50:Qd:203:ARG:NH1	2.49	0.45
49:Qc:240:LEU:HD21	81:Qe:302:PEE:H19	1.97	0.45
64:S6:46:ASP:OD1	64:S6:46:ASP:N	2.43	0.45
64:S6:104:LYS:HE3	64:S6:107:LYS:HD3	1.98	0.45
2:5A:65:PRO:HA	2:5A:100:ARG:NH1	2.32	0.45
2:5A:144:PRO:O	2:5A:148:GLY:N	2.49	0.45
8:7B:63:GLU:H	8:7B:63:GLU:CD	2.25	0.45
14:A5:30:LYS:NZ	20:AK:273:GLU:OE1	2.48	0.45
20:AK:120:TYR:OH	76:AK:401:ADP:O2'	2.16	0.45
35:C1:75:ILE:HD11	35:C1:191:THR:HG21	1.98	0.45
35:C1:396:TRP:CD1	35:C1:399:LEU:HD23	2.52	0.45
49:QC:307:LEU:HD11	49:QC:363:LEU:HD23	1.99	0.45
49:Qc:138:MET:HG2	49:Qc:254:ASP:HB2	1.98	0.45
59:S1:433:GLY:O	59:S1:444:HIS:NE2	2.42	0.45
60:S2:194:THR:HB	60:S2:206:PHE:HA	1.98	0.45
13:A3:135:PRO:HB2	23:AN:69:ILE:HD11	1.99	0.45
73:B4:201:CDL:H352	73:B4:201:CDL:H381	1.79	0.45
30:B7:99:MET:HG3	31:B8:156:VAL:HG12	1.98	0.45
36:C2:134:ARG:NH1	36:C2:135:LEU:HD21	2.31	0.45
41:N1:114:TYR:HA	41:N1:117:LEU:HG	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QC:138:MET:HB2	49:QC:255:ASN:HD22	1.80	0.45
50:QD:157:ASP:HB2	50:QD:168:ARG:HG2	1.99	0.45
47:Qa:380:ALA:HB1	47:Qa:384:MET:HE3	1.98	0.45
49:Qc:121:PHE:HE2	49:Qc:299:LEU:HD13	1.81	0.45
51:Qe:190:VAL:HG21	51:Qe:250:ARG:HH22	1.81	0.45
59:S1:53:CYS:HA	59:S1:56:VAL:HG22	1.99	0.45
60:S2:430:ILE:HB	60:S2:469:ARG:HD2	1.97	0.45
2:5A:81:GLY:O	36:C2:53:THR:N	2.49	0.45
18:A9:198:ALA:O	18:A9:260:GLY:CA	2.60	0.45
36:C2:28:LEU:HA	36:C2:31:VAL:HG22	1.99	0.45
41:N1:9:LEU:O	41:N1:13:ILE:HG12	2.15	0.45
41:N1:286:MET:HE3	41:N1:286:MET:HB2	1.76	0.45
42:N2:197:ASN:HD22	42:N2:200:MET:HG2	1.81	0.45
44:N4:197:LEU:O	44:N4:201:MET:HB2	2.17	0.45
48:Qb:102:LYS:HG2	48:Qb:153:ASN:HB3	1.98	0.45
67:V1:281:HIS:ND1	67:V1:358:ASP:OD1	2.50	0.45
3:5B:87:ARG:NE	35:C1:507:GLU:HG2	2.31	0.45
8:7B:35:ASP:OD1	38:C4:98:ASN:ND2	2.50	0.45
20:AK:328:ARG:HH21	34:BL:58:ASP:CG	2.25	0.45
22:AM:78:ASP:OD1	22:AM:78:ASP:N	2.50	0.45
35:C1:202:LEU:O	35:C1:206:ILE:HG12	2.17	0.45
35:C1:336:PRO:HG3	35:C1:411:LYS:HG3	1.99	0.45
73:CB:203:CDL:H561	44:N4:13:PRO:HB3	1.98	0.45
44:N4:207:MET:HE1	44:N4:294:MET:HE3	1.99	0.45
48:QB:465:LEU:HD12	48:QB:466:PRO:HD2	1.98	0.45
73:Qb:501:CDL:H762	49:Qc:14:ILE:HG21	1.97	0.45
2:5A:123:GLU:OE1	2:5A:123:GLU:N	2.50	0.45
4:6A:62:TYR:HB3	4:6A:64:HIS:CD2	2.51	0.45
23:AN:93:GLU:OE1	63:S5:92:TYR:OH	2.31	0.45
36:C2:105:TYR:HB2	36:C2:120:SER:O	2.16	0.45
43:N3:60:ILE:HG22	46:N6:168:ILE:HD13	1.99	0.45
44:N4:267:TRP:O	44:N4:271:MET:HG2	2.16	0.45
44:N4:357:THR:OG1	73:N5:702:CDL:HA21	2.17	0.45
49:QC:344:GLU:HG3	54:Qh:67:PHE:HE1	1.82	0.45
47:Qa:68:GLY:O	47:Qa:208:TYR:OH	2.35	0.45
53:Qg:41:ASP:OD1	53:Qg:41:ASP:N	2.45	0.45
59:S1:50:LEU:HA	59:S1:60:ILE:HD12	1.99	0.45
67:V1:384:PRO:HG2	67:V1:422:HIS:O	2.16	0.45
3:5B:83:ILE:HD11	37:C3:2:THR:N	2.32	0.45
15:A6:136:THR:HG21	61:S3:220:VAL:HB	1.98	0.45
18:A9:56:ALA:HA	18:A9:125:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AB:90:TYR:HD2	19:AB:93:ILE:HG13	1.81	0.45
29:B6:181:LYS:HG3	30:B7:40:VAL:HG13	1.99	0.45
35:C1:28:MET:HE3	35:C1:469:ILE:HD11	1.98	0.45
35:C1:41:LEU:HD22	35:C1:443:TYR:HE2	1.81	0.45
35:C1:360:ASN:HB2	35:C1:363:LEU:HB3	1.98	0.45
37:C3:125:ASN:HD22	37:C3:128:GLU:H	1.64	0.45
48:QB:127:GLU:O	48:QB:128:HIS:ND1	2.50	0.45
49:QC:8:HIS:O	49:QC:12:LYS:N	2.41	0.45
50:QD:127:SER:HB3	50:QD:179:PRO:HD2	1.99	0.45
47:Qa:379:LYS:HG2	47:Qa:413:LEU:HD22	1.99	0.45
59:S1:74:ASN:OD1	59:S1:75:CYS:N	2.50	0.45
69:V3:402:LEU:O	69:V3:406:LEU:HG	2.17	0.45
2:5A:76:MET:HE2	2:5A:110:ILE:HG12	1.99	0.45
3:5B:82:SER:N	3:5B:123:VAL:O	2.50	0.45
5:6B:66:PRO:HB3	36:C2:100:MET:HE3	1.97	0.45
22:AM:88:ARG:HG3	22:AM:93:MET:HB2	1.99	0.45
23:AN:93:GLU:HG3	63:S5:98:HIS:CD2	2.52	0.45
35:C1:412:ILE:HG12	38:C4:103:ILE:HA	1.98	0.45
37:C3:24:ALA:HB2	71:C3:302:PC1:H3A2	1.99	0.45
38:C4:38:TYR:CE2	38:C4:47:PRO:HG2	2.52	0.45
42:N2:83:GLN:HE22	63:S5:20:ILE:HG22	1.82	0.45
43:N3:38:GLU:HB3	43:N3:41:PHE:O	2.16	0.45
59:S1:647:GLU:HB2	59:S1:654:VAL:HG11	1.98	0.45
8:7B:46:ALA:HA	38:C4:108:LEU:HD13	1.99	0.45
16:A7:39:PRO:HG3	66:S8:211:TYR:CZ	2.52	0.45
35:C1:51:ASP:OD1	35:C1:51:ASP:N	2.49	0.45
37:C3:16:TRP:NE1	37:C3:60:ASP:OD2	2.50	0.45
44:N4:106:LEU:HD13	44:N4:234:VAL:HG11	1.99	0.45
45:N5:389:PHE:O	45:N5:393:ASP:HB3	2.17	0.45
73:N5:703:CDL:H541	73:N5:703:CDL:H731	1.99	0.45
47:Qa:396:VAL:HG22	47:Qa:406:TYR:HE1	1.82	0.45
51:Qe:218:THR:HG21	51:Qe:256:LEU:HG	1.98	0.45
61:S3:240:GLU:OE1	61:S3:246:ARG:NH2	2.48	0.45
2:5A:77:ASN:HD22	38:C4:45:PRO:HD2	1.82	0.44
3:5B:92:ILE:HG12	3:5B:100:VAL:HG22	1.98	0.44
4:6A:82:PHE:O	71:6A:101:PC1:H143	2.16	0.44
14:A5:113:LYS:NZ	14:A5:116:ILE:HD13	2.32	0.44
35:C1:443:TYR:O	36:C2:134:ARG:NH2	2.49	0.44
45:N5:14:ILE:HD11	45:N5:43:ALA:HA	1.98	0.44
47:QA:89:LEU:HD22	47:QA:150:GLU:HB3	1.98	0.44
49:QC:97:HIS:HD2	82:QC:402:HEM:C1C	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:QH:68:GLU:HA	54:QH:71:LYS:HE2	1.98	0.44
47:Qa:81:HIS:CD2	47:Qa:192:CYS:H	2.25	0.44
60:S2:272:ARG:NH1	81:S8:303:PEE:H1	2.32	0.44
2:5A:102:ASN:HA	38:C4:70:TRP:CZ2	2.52	0.44
75:AC:201:ZMP:H22	75:AC:201:ZMP:H25B	1.68	0.44
20:AK:83:LEU:HB3	20:AK:85:LEU:HG	1.99	0.44
31:B8:161:TYR:HB3	31:B8:166:LEU:HG	2.00	0.44
35:C1:19:TYR:CE2	35:C1:102:PHE:HB2	2.52	0.44
37:C3:148:HIS:HE1	37:C3:152:MET:HE3	1.82	0.44
37:C3:217:VAL:HG11	71:C3:301:PC1:H251	1.99	0.44
46:N6:82:VAL:HG22	46:N6:83:TRP:H	1.82	0.44
51:QE:130:LYS:HD2	58:Qj:34:TRP:CE2	2.52	0.44
51:QE:140:MET:O	49:Qc:177:ARG:NH2	2.49	0.44
53:QG:41:ASP:OD1	53:QG:41:ASP:N	2.50	0.44
59:S1:557:ARG:HA	59:S1:560:LEU:HB2	2.00	0.44
66:S8:168:VAL:HG11	66:S8:205:ILE:HD11	1.99	0.44
1:4L:38:LEU:O	1:4L:42:ILE:HG12	2.18	0.44
13:A3:152:PRO:HG3	17:A8:204:LYS:HE3	1.99	0.44
73:B5:202:CDL:H111	81:N5:701:PEE:H63	1.98	0.44
35:C1:144:ASP:HA	35:C1:147:ILE:HD12	1.99	0.44
35:C1:378:HIS:HE1	78:C1:602:HEA:NA	2.13	0.44
41:N1:134:ARG:NH2	60:S2:110:GLU:OE2	2.35	0.44
45:N5:23:ASN:HD22	73:N5:702:CDL:HB4	1.81	0.44
45:N5:233:LEU:HB3	45:N5:234:PRO:HD3	1.99	0.44
45:N5:297:ASP:O	45:N5:301:ILE:HG13	2.18	0.44
45:N5:566:THR:O	45:N5:570:GLN:HG2	2.17	0.44
57:QK:71:ASN:OD1	57:QK:71:ASN:N	2.50	0.44
47:Qa:320:PRO:HG2	47:Qa:343:GLN:HE21	1.82	0.44
73:Qb:501:CDL:HB4	73:Qb:501:CDL:H122	2.00	0.44
59:S1:123:ASN:ND2	67:V1:387:GLU:OE1	2.49	0.44
60:S2:190:ILE:HD12	60:S2:216:MET:HE1	1.99	0.44
1:4L:35:GLY:HA3	46:N6:20:PHE:CZ	2.52	0.44
4:6A:40:VAL:O	4:6A:44:THR:OG1	2.31	0.44
20:AK:134:GLN:HE22	76:AK:401:ADP:HN62	1.64	0.44
23:AN:88:ARG:O	23:AN:92:GLU:HG2	2.16	0.44
35:C1:254:ILE:HG13	35:C1:344:PHE:CD2	2.52	0.44
43:N3:71:LEU:O	46:N6:147:TYR:OH	2.34	0.44
44:N4:79:ALA:O	44:N4:82:SER:HB3	2.18	0.44
53:QG:43:ASP:OD2	53:QG:102:ARG:NH1	2.51	0.44
48:Qb:80:ARG:NH2	48:Qb:268:CYS:SG	2.91	0.44
49:Qc:311:LYS:NZ	49:Qc:379:TRP:OXT	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Qc:361:ILE:HG12	49:Qc:365:LEU:HD12	1.98	0.44
60:S2:187:LEU:HD23	60:S2:213:ARG:HG2	2.00	0.44
66:S8:153:ILE:HG13	66:S8:155:CYS:HB3	2.00	0.44
2:5A:113:VAL:HG11	38:C4:45:PRO:HB3	1.99	0.44
18:A9:173:ASP:HB3	18:A9:176:SER:HB2	2.00	0.44
24:B1:27:LEU:HD12	44:N4:6:ILE:HD11	1.98	0.44
37:C3:58:TRP:HA	37:C3:61:ILE:HD12	2.00	0.44
49:QC:102:LEU:HD22	49:QC:304:MET:HE2	1.99	0.44
47:Qa:147:ARG:HD3	47:Qa:149:TRP:CZ2	2.53	0.44
48:Qb:152:GLN:NE2	48:Qb:250:PHE:HA	2.31	0.44
53:Qg:14:LEU:HD12	53:Qg:17:ILE:HD11	1.98	0.44
54:Qh:20:SER:HB3	54:Qh:23:GLU:HG2	1.98	0.44
68:V2:71:PRO:HB3	69:V3:414:PRO:HG2	1.99	0.44
1:4L:37:MET:SD	1:4L:63:LEU:HG	2.58	0.44
2:5A:143:THR:O	2:5A:147:LEU:N	2.43	0.44
14:A5:9:THR:HG21	14:A5:14:LEU:HD23	2.00	0.44
17:A8:246:PHE:CE1	73:A8:301:CDL:H341	2.52	0.44
20:AK:62:ILE:HG12	20:AK:205:VAL:HB	1.99	0.44
23:AN:49:SER:HB2	41:N1:172:ILE:HD13	1.98	0.44
30:B7:43:GLN:NE2	31:B8:169:GLU:OE2	2.45	0.44
30:B7:92:HIS:O	30:B7:96:VAL:HG13	2.18	0.44
35:C1:94:PHE:HB3	35:C1:97:MET:HG3	1.99	0.44
41:N1:179:TRP:CG	41:N1:180:PRO:HD3	2.53	0.44
42:N2:254:LEU:HD21	44:N4:154:LEU:HD11	1.99	0.44
43:N3:101:SER:HB3	46:N6:165:VAL:HG21	2.00	0.44
49:QC:152:ALA:HB2	49:QC:287:LYS:HG2	1.98	0.44
51:QE:125:VAL:HG11	72:QE:301:PLX:H132	1.98	0.44
52:QF:30:LEU:HB2	50:Qd:265:SER:HB3	1.99	0.44
47:Qa:91:THR:OG1	47:Qa:139:ASN:ND2	2.51	0.44
59:S1:267:THR:HB	62:S4:115:SER:HB2	2.00	0.44
4:6A:65:LEU:HD22	37:C3:190:ASP:HB3	2.00	0.44
10:8B:28:LYS:HD2	35:C1:481:GLU:HB2	2.00	0.44
18:A9:246:SER:O	18:A9:250:ILE:HG12	2.18	0.44
23:AN:140:PHE:O	71:N1:402:PC1:H143	2.18	0.44
35:C1:13:LYS:HB3	35:C1:81:TRP:CZ3	2.53	0.44
37:C3:58:TRP:CD1	37:C3:61:ILE:HD12	2.53	0.44
73:CB:203:CDL:H362	42:N2:243:LEU:HD23	1.99	0.44
45:N5:151:SER:HB2	45:N5:252:MET:SD	2.58	0.44
48:QB:140:LEU:HD22	48:QB:237:VAL:HG12	1.99	0.44
48:Qb:76:ASP:HB2	48:Qb:418:LEU:HD22	2.00	0.44
59:S1:76:ARG:O	59:S1:116:VAL:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:S2:203:MET:O	60:S2:206:PHE:HB3	2.17	0.44
65:S7:72:CYS:HB3	65:S7:106:ALA:HB1	2.00	0.44
67:V1:37:ASP:HB2	68:V2:236:GLU:HG2	2.00	0.44
67:V1:209:GLU:HG3	67:V1:210:THR:N	2.33	0.44
9:7C:44:TYR:O	9:7C:47:SER:OG	2.31	0.44
20:AK:357:LYS:HD3	39:CA:36:HIS:O	2.17	0.44
29:B6:143:HIS:CD2	33:BK:45:VAL:HG21	2.53	0.44
33:BK:107:GLN:HE22	45:N5:194:ASN:ND2	2.16	0.44
35:C1:168:ILE:HD11	35:C1:188:VAL:HG23	2.00	0.44
35:C1:175:ALA:HB3	35:C1:511:ILE:HB	1.99	0.44
35:C1:342:LEU:HD13	36:C2:46:LEU:HD11	2.00	0.44
60:S2:232:TYR:OH	60:S2:240:GLN:O	2.21	0.44
64:S6:37:LYS:HB2	64:S6:62:VAL:HG21	1.99	0.44
1:4L:4:VAL:O	1:4L:8:ILE:HG12	2.18	0.44
15:A6:124:LYS:O	15:A6:125:GLN:NE2	2.51	0.44
15:A6:135:GLU:OE1	61:S3:218:ARG:NH2	2.45	0.44
38:C4:56:SER:H	38:C4:59:GLN:HB2	1.83	0.44
42:N2:243:LEU:HD22	42:N2:330:ILE:HG21	1.99	0.44
44:N4:127:VAL:HB	44:N4:128:PRO:HD3	1.99	0.44
45:N5:265:PRO:O	45:N5:269:THR:HG23	2.17	0.44
47:QA:138:LEU:O	47:QA:142:ALA:HB3	2.18	0.44
81:Qc:401:PEE:H20	81:Qc:401:PEE:H14	1.64	0.44
51:Qe:213:LEU:HD23	51:Qe:258:LEU:HB2	1.99	0.44
60:S2:144:ARG:NH2	65:S7:166:CYS:SG	2.82	0.44
64:S6:74:GLN:HG3	66:S8:108:SER:HB2	1.99	0.44
65:S7:65:MET:HE2	65:S7:97:PRO:HB3	1.98	0.44
2:5A:124:ILE:HG12	6:6C:9:PRO:HG2	1.99	0.43
6:6C:51:ASP:OD1	6:6C:54:ARG:NH2	2.43	0.43
12:A2:31:GLN:NE2	12:A2:35:ASP:OD1	2.51	0.43
17:A8:160:THR:HA	17:A8:163:TRP:CD1	2.53	0.43
20:AK:83:LEU:HA	20:AK:83:LEU:HD23	1.86	0.43
27:B4:70:TYR:HD2	31:B8:38:PRO:HD2	1.83	0.43
35:C1:181:THR:OG1	35:C1:186:TRP:NE1	2.51	0.43
48:QB:79:SER:OG	48:QB:201:VAL:HA	2.18	0.43
50:QD:303:LEU:HB3	51:QE:121:THR:OG1	2.18	0.43
50:Qd:139:VAL:HG21	50:Qd:277:TRP:CZ2	2.53	0.43
20:AK:208:TYR:O	20:AK:259:GLN:HA	2.18	0.43
21:AL:34:LEU:HD21	73:AL:202:CDL:H421	2.00	0.43
29:B6:86:GLN:NE2	32:B9:160:TYR:OH	2.42	0.43
35:C1:202:LEU:HB2	35:C1:238:PHE:CG	2.53	0.43
35:C1:468:MET:HE2	35:C1:468:MET:HB3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N5:373:LEU:HD22	45:N5:431:PHE:HE2	1.82	0.43
45:N5:375:ILE:HD12	45:N5:458:LEU:HD11	2.00	0.43
47:QA:313:VAL:HG21	47:QA:323:VAL:HG21	2.00	0.43
49:QC:131:TYR:O	49:QC:134:PRO:HD2	2.18	0.43
54:QH:45:CYS:SG	73:QH:101:CDL:H311	2.58	0.43
72:QI:301:PLX:H131	51:Qe:125:VAL:HG21	2.00	0.43
82:Qc:402:HEM:HBC2	82:Qc:402:HEM:HMC1	1.99	0.43
65:S7:62:LEU:C	65:S7:63:TRP:HD1	2.26	0.43
65:S7:89:PHE:CE2	65:S7:174:LEU:HD21	2.53	0.43
67:V1:201:ALA:HB3	68:V2:119:TYR:CD1	2.53	0.43
5:6B:63:SER:HA	36:C2:111:THR:HG23	1.99	0.43
14:A5:76:GLN:HG3	16:A7:103:ARG:HH22	1.83	0.43
73:A8:301:CDL:H601	73:A8:301:CDL:H572	1.87	0.43
72:AM:201:PLX:H331	72:AM:201:PLX:H362	1.80	0.43
73:B5:202:CDL:H312	81:N5:701:PEE:H61	1.99	0.43
30:B7:95:TYR:CZ	31:B8:156:VAL:HG11	2.53	0.43
35:C1:302:ARG:HH21	36:C2:84:LEU:HD11	1.83	0.43
77:C1:601:3PE:H361	77:C1:601:3PE:H271	2.00	0.43
73:CB:203:CDL:H272	44:N4:16:TRP:CE2	2.52	0.43
44:N4:205:VAL:HG22	44:N4:212:LEU:HD13	2.00	0.43
44:N4:210:TYR:CG	44:N4:268:GLY:HA3	2.53	0.43
44:N4:445:LEU:HB3	73:N5:702:CDL:H442	1.99	0.43
45:N5:49:VAL:HB	45:N5:50:PRO:HD3	1.99	0.43
48:QB:373:GLN:HE22	48:QB:471:ILE:HG23	1.83	0.43
81:Qe:302:PEE:H69	81:Qe:302:PEE:H62	1.67	0.43
59:S1:74:ASN:HA	67:V1:424:ILE:HD11	1.99	0.43
60:S2:405:ALA:HB1	60:S2:412:GLU:HG3	2.01	0.43
14:A5:105:GLU:HB3	61:S3:89:HIS:HE2	1.83	0.43
17:A8:111:ALA:HB2	17:A8:197:PRO:HG3	2.01	0.43
35:C1:12:HIS:HB3	35:C1:92:MET:HG2	2.01	0.43
35:C1:74:MET:SD	35:C1:249:PRO:HG2	2.59	0.43
47:Qa:89:LEU:HD22	47:Qa:150:GLU:HB3	2.00	0.43
47:Qa:138:LEU:HB3	47:Qa:238:LEU:HD13	2.01	0.43
48:Qb:38:TYR:CZ	48:Qb:42:LEU:HD11	2.53	0.43
49:Qc:233:LEU:HD23	49:Qc:233:LEU:HA	1.86	0.43
50:Qd:122:CYS:SG	83:Qd:401:HEC:HAB	2.59	0.43
53:Qg:46:GLU:HA	53:Qg:49:ARG:HG2	2.00	0.43
58:Qj:39:ARG:HH12	58:Qj:52:PHE:HB3	1.84	0.43
59:S1:246:ARG:HH22	62:S4:123:ASN:ND2	2.11	0.43
59:S1:395:GLU:OE2	59:S1:420:LYS:NZ	2.46	0.43
60:S2:116:ASP:OD1	61:S3:185:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:V1:338:ASP:OD1	67:V1:339:PHE:N	2.51	0.43
3:5B:79:LEU:HD23	3:5B:121:LYS:HB3	2.00	0.43
75:AC:201:ZMP:H14	32:B9:102:ALA:HB1	2.00	0.43
42:N2:190:MET:HE3	42:N2:205:LEU:HB2	2.00	0.43
44:N4:176:PHE:HA	44:N4:179:ILE:HG12	2.01	0.43
51:QE:128:ALA:HB1	81:QE:302:PEE:H60	2.00	0.43
47:Qa:213:PHE:O	47:Qa:241:ARG:NE	2.51	0.43
64:S6:114:CYS:SG	64:S6:116:LEU:HB2	2.59	0.43
65:S7:107:GLY:HA2	85:S7:301:SF4:S4	2.58	0.43
67:V1:267:ARG:HB2	67:V1:270:ASN:OD1	2.19	0.43
2:5A:125:TYR:O	2:5A:129:ILE:HG12	2.18	0.43
14:A5:116:ILE:HG13	62:S4:129:SER:HB2	1.99	0.43
15:A6:54:ALA:HB1	15:A6:105:VAL:HG11	2.00	0.43
35:C1:181:THR:HG1	35:C1:186:TRP:NE1	2.17	0.43
35:C1:463:THR:HA	35:C1:466:MET:HE2	1.99	0.43
72:QI:301:PLX:H111	51:Qe:125:VAL:HG21	2.01	0.43
57:QK:20:ARG:NH1	57:QK:24:GLY:H	2.15	0.43
47:Qa:290:GLN:HB2	47:Qa:336:PHE:HE2	1.84	0.43
61:S3:115:THR:OG1	61:S3:116:ALA:N	2.52	0.43
14:A5:106:GLU:OE1	14:A5:106:GLU:N	2.50	0.43
17:A8:124:ARG:HA	17:A8:124:ARG:HD2	1.81	0.43
18:A9:66:GLY:HA2	18:A9:129:LEU:HD13	2.00	0.43
73:B5:202:CDL:H182	73:B5:202:CDL:H211	1.82	0.43
30:B7:22:MET:HE1	30:B7:102:PHE:HD2	1.83	0.43
37:C3:45:LEU:HD12	37:C3:45:LEU:HA	1.90	0.43
45:N5:66:TRP:CD1	81:N5:701:PEE:H14	2.54	0.43
45:N5:290:LEU:O	45:N5:523:SER:OG	2.36	0.43
51:Qe:184:ILE:HD11	51:Qe:209:GLU:HA	2.01	0.43
60:S2:392:THR:HG23	66:S8:118:LEU:HD22	1.99	0.43
67:V1:65:THR:O	67:V1:69:LEU:HG	2.19	0.43
67:V1:128:ARG:NE	67:V1:165:GLU:OE2	2.51	0.43
12:A2:18:GLU:HG2	12:A2:68:ARG:HB3	1.99	0.43
19:AB:115:GLN:O	19:AB:119:ILE:HG12	2.18	0.43
22:AM:44:TYR:OH	22:AM:113:HIS:N	2.42	0.43
28:B5:139:ILE:HG23	44:N4:54:LEU:HD23	2.01	0.43
33:BK:67:GLU:OE2	34:BL:124:ARG:NH2	2.49	0.43
35:C1:38:ARG:NH2	35:C1:454:SER:HB2	2.34	0.43
38:C4:166:GLU:HG2	38:C4:167:TRP:O	2.18	0.43
41:N1:277:TYR:OH	66:S8:66:LEU:HB3	2.19	0.43
42:N2:43:VAL:HG11	42:N2:129:LEU:HD23	2.00	0.43
81:N3:201:PEE:H24	81:N3:201:PEE:H29	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:QA:183:ARG:HG3	47:QA:254:ARG:HB2	2.00	0.43
77:QC:404:3PE:H121	77:QC:404:3PE:H2	2.00	0.43
47:Qa:84:ARG:HD3	47:Qa:114:SER:OG	2.19	0.43
49:Qc:134:PRO:HG3	82:Qc:402:HEM:O2D	2.19	0.43
52:Qf:41:GLU:O	52:Qf:45:LYS:HG2	2.17	0.43
59:S1:98:LYS:HD3	59:S1:99:GLY:N	2.34	0.43
60:S2:134:THR:HA	60:S2:424:ARG:HG2	2.00	0.43
1:4L:41:PHE:O	1:4L:45:THR:HG22	2.18	0.43
8:7B:71:ARG:HG3	8:7B:72:VAL:HG23	2.00	0.43
24:B1:30:ARG:O	24:B1:33:GLU:HG2	2.19	0.43
27:B4:47:TYR:HB2	31:B8:101:TRP:CE3	2.53	0.43
28:B5:74:TYR:O	34:BL:96:SER:OG	2.29	0.43
35:C1:38:ARG:O	35:C1:42:GLY:N	2.52	0.43
35:C1:438:ARG:NH2	78:C1:603:HEA:O2D	2.51	0.43
37:C3:33:MET:HB3	37:C3:39:SER:HB2	2.00	0.43
47:QA:64:PHE:HB3	47:QA:401:LEU:HD11	2.01	0.43
51:QE:130:LYS:HA	77:QE:303:3PE:H282	2.01	0.43
73:Qb:501:CDL:HA32	71:Qb:502:PC1:H151	2.01	0.43
49:Qc:332:LEU:HD12	81:Qc:401:PEE:H36	1.99	0.43
68:V2:137:THR:HG22	68:V2:138:THR:H	1.84	0.43
1:4L:55:LEU:HD13	63:S5:17:TRP:HE3	1.84	0.43
3:5B:40:ASP:HA	3:5B:43:GLN:HB2	2.01	0.43
72:AM:201:PLX:H281	72:AM:201:PLX:H252	1.84	0.43
33:BK:33:LEU:HD13	45:N5:49:VAL:HG13	2.01	0.43
35:C1:212:ASP:OD1	35:C1:217:THR:OG1	2.33	0.43
45:N5:327:LEU:HG	45:N5:331:MET:HE2	2.00	0.43
46:N6:122:LEU:HD11	63:S5:80:LYS:HE2	2.00	0.43
81:N6:201:PEE:H53	81:N6:201:PEE:H14	1.99	0.43
49:QC:379:TRP:HB3	53:Qg:34:ARG:NH1	2.34	0.43
52:QF:60:ARG:HD3	52:QF:63:THR:HG21	2.01	0.43
47:Qa:91:THR:HG21	47:Qa:140:VAL:HA	2.01	0.43
61:S3:118:ASP:OD2	61:S3:125:ARG:NH2	2.44	0.43
20:AK:62:ILE:HG23	20:AK:205:VAL:HB	2.01	0.42
21:AL:76:ILE:HG21	71:Qh:102:PC1:H221	2.01	0.42
73:AL:202:CDL:H212	73:AL:202:CDL:H342	2.00	0.42
35:C1:469:ILE:HD13	35:C1:469:ILE:HA	1.87	0.42
42:N2:271:THR:HG22	44:N4:169:ASN:HD22	1.84	0.42
44:N4:231:LEU:HD23	44:N4:235:LEU:HD12	2.01	0.42
45:N5:11:THR:HG22	45:N5:46:LEU:HB3	2.01	0.42
46:N6:26:PRO:HB2	46:N6:71:THR:HG21	2.01	0.42
47:QA:177:LEU:HD21	47:QA:272:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:QA:337:GLY:HA2	47:QA:431:PHE:CE1	2.54	0.42
48:QB:310:ILE:HD11	48:QB:388:VAL:HA	2.01	0.42
49:Qc:185:LEU:HD23	49:Qc:188:ILE:HD12	2.01	0.42
66:S8:131:GLU:HG3	66:S8:144:ARG:HD2	2.00	0.42
25:B2:59:ARG:HH12	26:B3:48:ASN:HA	1.84	0.42
35:C1:274:VAL:HG12	35:C1:278:MET:HE2	2.01	0.42
47:QA:300:LYS:HE2	47:QA:301:ARG:NH1	2.34	0.42
49:QC:135:TRP:HH2	49:QC:170:VAL:HG12	1.84	0.42
51:QE:145:ASP:OD1	51:QE:145:ASP:N	2.52	0.42
54:QH:9:THR:HG21	49:Qc:215:MET:HA	2.02	0.42
47:Qa:408:GLN:HE21	47:Qa:409:PRO:HD2	1.84	0.42
71:Qc:405:PC1:H362	71:Qc:405:PC1:H391	1.74	0.42
65:S7:45:TYR:O	65:S7:49:LYS:HG2	2.19	0.42
67:V1:134:ASP:N	67:V1:135:PRO:HD3	2.35	0.42
67:V1:263:ALA:HA	67:V1:271:SER:HB3	2.01	0.42
68:V2:188:ILE:HB	68:V2:193:TYR:HE2	1.84	0.42
69:V3:400:LEU:O	69:V3:404:VAL:HG23	2.19	0.42
3:5B:100:VAL:HB	3:5B:102:TRP:CZ2	2.53	0.42
24:B1:50:ARG:HB2	24:B1:53:GLU:HG2	2.01	0.42
35:C1:393:PHE:O	35:C1:397:PHE:N	2.52	0.42
35:C1:456:MET:O	35:C1:460:ILE:HG13	2.20	0.42
40:CB:74:GLY:O	40:CB:78:LEU:HG	2.19	0.42
41:N1:233:MET:HE3	41:N1:233:MET:HB3	1.77	0.42
42:N2:137:ALA:HB3	42:N2:138:PRO:HD3	2.02	0.42
42:N2:175:LEU:O	42:N2:179:MET:HG2	2.20	0.42
42:N2:287:LEU:HD12	81:S2:501:PEE:H64	2.01	0.42
54:QH:21:PRO:HG3	50:Qd:314:VAL:HG23	2.01	0.42
55:QI:45:GLU:OE2	55:QI:54:LYS:NZ	2.43	0.42
48:Qb:126:ARG:NH1	48:Qb:199:GLN:O	2.52	0.42
59:S1:49:VAL:HG13	59:S1:102:ILE:HD13	2.01	0.42
60:S2:150:MET:SD	60:S2:228:MET:HB2	2.59	0.42
68:V2:59:ASN:OD1	68:V2:62:ARG:NH1	2.52	0.42
5:6B:45:THR:HG23	5:6B:51:VAL:HG11	2.00	0.42
5:6B:76:ARG:O	5:6B:81:THR:N	2.51	0.42
15:A6:67:ARG:NH2	19:AB:120:MET:HG2	2.33	0.42
18:A9:122:HIS:HE1	64:S6:52:ARG:NH2	2.17	0.42
20:AK:251:MET:SD	20:AK:254:LYS:HD2	2.59	0.42
28:B5:152:LYS:HD3	40:CB:96:VAL:HG21	2.01	0.42
41:N1:295:PRO:HA	81:N3:201:PEE:H32	2.01	0.42
45:N5:8:THR:O	45:N5:11:THR:OG1	2.30	0.42
47:QA:148:ARG:NH2	53:QG:50:ARG:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:QA:180:ALA:HA	47:QA:254:ARG:NH2	2.34	0.42
49:QC:338:ILE:HD13	49:QC:338:ILE:HA	1.93	0.42
81:QC:403:PEE:H23	81:QC:403:PEE:H30	1.53	0.42
48:Qb:294:PRO:HB2	48:Qb:298:ASN:HB3	2.01	0.42
59:S1:489:ILE:O	59:S1:493:VAL:HG22	2.19	0.42
67:V1:141:GLY:HA3	67:V1:248:VAL:O	2.19	0.42
67:V1:214:GLU:OE2	67:V1:224:ARG:NE	2.37	0.42
6:6C:72:GLN:CD	36:C2:141:ARG:H	2.27	0.42
19:AB:137:LYS:HE3	19:AB:137:LYS:HB2	1.93	0.42
20:AK:102:ASP:OD1	20:AK:102:ASP:N	2.51	0.42
22:AM:91:HIS:CE1	66:S8:90:LYS:HB3	2.54	0.42
45:N5:149:ILE:HD11	73:N5:702:CDL:H172	2.02	0.42
51:QE:169:TRP:HZ2	51:QE:274:GLY:HA2	1.85	0.42
53:QG:44:VAL:O	53:QG:48:ILE:HG12	2.20	0.42
54:QH:25:ARG:N	51:Qe:91:TYR:O	2.51	0.42
50:Qd:311:LYS:HD3	50:Qd:311:LYS:HA	1.90	0.42
51:Qe:234:TYR:N	51:Qe:243:TYR:O	2.30	0.42
54:Qh:38:VAL:HG13	73:Qh:101:CDL:H311	2.01	0.42
60:S2:300:ARG:NH2	60:S2:407:GLU:OE2	2.50	0.42
61:S3:108:PHE:HB3	61:S3:132:LEU:HB3	2.01	0.42
4:6A:70:LYS:O	35:C1:216:ASN:ND2	2.44	0.42
16:A7:25:GLN:O	60:S2:215:LYS:NZ	2.42	0.42
21:AL:14:GLU:HA	21:AL:21:LYS:HE3	2.01	0.42
37:C3:86:PHE:O	37:C3:89:SER:OG	2.27	0.42
41:N1:123:SER:HB3	41:N1:214:GLU:HG3	2.00	0.42
73:N1:401:CDL:HB4	73:N1:401:CDL:H322	2.00	0.42
71:N1:402:PC1:H351	71:N1:402:PC1:H322	1.88	0.42
44:N4:269:MET:SD	44:N4:399:ASN:ND2	2.93	0.42
46:N6:39:VAL:O	46:N6:43:ILE:HG13	2.20	0.42
53:QG:68:ASP:HA	53:QG:71:MET:HG2	2.00	0.42
48:Qb:407:THR:HB	48:Qb:408:PRO:HD3	2.01	0.42
49:Qc:24:PRO:HB2	49:Qc:27:ILE:HG23	2.00	0.42
53:Qg:44:VAL:O	53:Qg:48:ILE:HG12	2.20	0.42
67:V1:114:VAL:O	67:V1:242:VAL:HA	2.19	0.42
68:V2:79:VAL:HG23	68:V2:80:LEU:HD12	2.01	0.42
3:5B:104:TRP:NE1	35:C1:495:LEU:HB3	2.34	0.42
14:A5:116:ILE:HD12	14:A5:116:ILE:HA	1.80	0.42
17:A8:235:LEU:HD23	17:A8:235:LEU:HA	1.90	0.42
19:AB:85:TYR:O	19:AB:89:LEU:HG	2.20	0.42
19:AC:112:SER:HB2	32:B9:59:LEU:HD21	2.02	0.42
21:AL:45:PRO:HA	21:AL:46:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:147:ILE:HG21	35:C1:210:LEU:HB2	2.02	0.42
44:N4:12:LEU:HB2	44:N4:13:PRO:HD3	2.01	0.42
44:N4:290:SER:HA	44:N4:319:HIS:HE2	1.83	0.42
45:N5:260:LEU:HD23	45:N5:260:LEU:HA	1.90	0.42
49:QC:316:MET:HE3	81:QC:403:PEE:H10	2.02	0.42
49:Qc:97:HIS:HD2	82:Qc:403:HEM:C1C	2.38	0.42
49:Qc:103:TYR:CG	81:Qc:401:PEE:H16	2.54	0.42
58:Qj:39:ARG:O	58:Qj:43:ASP:HB2	2.20	0.42
60:S2:101:LEU:HD22	60:S2:464:PHE:HZ	1.84	0.42
60:S2:283:VAL:HG22	60:S2:331:ASP:HB3	2.01	0.42
68:V2:159:LYS:HD3	68:V2:159:LYS:HA	1.89	0.42
11:A1:17:PHE:HE1	41:N1:257:ILE:HA	1.83	0.42
20:AK:138:TYR:OH	20:AK:193:LYS:HA	2.20	0.42
20:AK:283:GLY:O	20:AK:286:PRO:HD2	2.19	0.42
22:AM:58:ARG:HD2	66:S8:89:GLU:OE1	2.20	0.42
31:B8:78:LEU:HD12	31:B8:106:HIS:HA	2.02	0.42
35:C1:67:PHE:HA	35:C1:71:MET:HE2	2.01	0.42
35:C1:413:HIS:CE1	35:C1:468:MET:HB2	2.55	0.42
37:C3:86:PHE:HZ	71:C3:301:PC1:H3C1	1.82	0.42
44:N4:322:THR:HG21	44:N4:366:ASN:HA	2.02	0.42
47:QA:51:SER:OG	47:QA:230:LEU:HD12	2.19	0.42
47:QA:147:ARG:HD3	47:QA:149:TRP:CZ2	2.55	0.42
50:QD:266:GLN:NE2	52:Qf:91:LYS:H	2.18	0.42
53:QG:72:ARG:NH1	53:QG:74:GLN:OE1	2.47	0.42
73:QH:102:CDL:H312	73:QH:102:CDL:H712	2.02	0.42
50:Qd:149:LEU:O	50:Qd:152:GLU:HG2	2.19	0.42
59:S1:696:MET:HG2	59:S1:711:VAL:HG21	2.02	0.42
66:S8:45:GLU:CD	66:S8:45:GLU:H	2.28	0.42
67:V1:62:TRP:CZ3	67:V1:181:LEU:HB3	2.54	0.42
69:V3:394:TYR:CD1	69:V3:398:THR:HG21	2.54	0.42
1:4L:35:GLY:HA3	46:N6:20:PHE:HZ	1.85	0.42
5:6B:66:PRO:O	5:6B:70:VAL:HG23	2.20	0.42
13:A3:94:LEU:HD11	81:N3:201:PEE:H67	2.02	0.42
31:B8:136:PHE:O	31:B8:140:MET:HG2	2.20	0.42
32:B9:143:GLU:HB2	32:B9:164:ARG:HH21	1.85	0.42
35:C1:28:MET:CE	78:C1:602:HEA:H271	2.50	0.42
35:C1:31:THR:OG1	78:C1:602:HEA:H14	2.20	0.42
35:C1:399:LEU:HB2	35:C1:494:TRP:CH2	2.55	0.42
36:C2:145:PRO:HG3	36:C2:219:PHE:CG	2.55	0.42
37:C3:25:LEU:O	37:C3:28:THR:OG1	2.34	0.42
37:C3:144:ILE:HD13	37:C3:166:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C3:165:ILE:O	37:C3:169:LEU:HG	2.20	0.42
41:N1:40:VAL:HG12	41:N1:46:LEU:HB2	2.02	0.42
45:N5:289:ALA:O	45:N5:293:ILE:HG23	2.19	0.42
49:Qc:131:TYR:O	49:Qc:134:PRO:HD2	2.19	0.42
59:S1:422:TRP:HA	59:S1:427:LEU:HB3	2.02	0.42
60:S2:129:LEU:O	60:S2:133:LYS:HG2	2.20	0.42
72:6C:101:PLX:H72	36:C2:28:LEU:HD11	2.02	0.42
12:A2:37:ILE:HD12	12:A2:55:ILE:HD13	2.02	0.42
17:A8:141:ASN:HD21	23:AN:81:ARG:NH2	2.18	0.42
18:A9:126:VAL:HG23	18:A9:161:VAL:HG11	2.02	0.42
18:A9:306:GLU:HB3	18:A9:315:THR:HG22	2.01	0.42
20:AK:260:TYR:CE2	20:AK:271:VAL:HG22	2.55	0.42
20:AK:284:PRO:O	20:AK:288:GLN:HG2	2.20	0.42
34:BL:98:VAL:HG11	44:N4:71:TRP:CZ3	2.54	0.42
35:C1:52:GLN:HB2	36:C2:202:SER:HB3	2.01	0.42
35:C1:297:MET:O	35:C1:302:ARG:NH1	2.44	0.42
37:C3:130:PRO:HA	37:C3:133:ASN:ND2	2.34	0.42
37:C3:231:HIS:ND1	71:C3:301:PC1:H133	2.34	0.42
71:C3:302:PC1:H351	71:C3:302:PC1:H322	1.88	0.42
41:N1:142:TYR:CE1	41:N1:289:LEU:HD23	2.55	0.42
45:N5:264:TYR:CD2	45:N5:265:PRO:HD3	2.55	0.42
45:N5:526:LEU:HD12	45:N5:530:PRO:HG3	2.02	0.42
47:QA:185:ALA:HB3	47:QA:251:ALA:HB2	2.02	0.42
55:QI:50:GLY:H	55:QI:55:HIS:CD2	2.38	0.42
72:QI:301:PLX:H71	71:Qb:502:PC1:H372	2.02	0.42
47:Qa:115:THR:HG22	47:Qa:116:ARG:H	1.84	0.42
47:Qa:125:CYS:HB3	47:Qa:133:LEU:HD22	2.01	0.42
47:Qa:154:LEU:HD23	47:Qa:154:LEU:HA	1.88	0.42
52:Qf:31:THR:O	52:Qf:35:GLU:HG2	2.20	0.42
59:S1:414:PHE:O	59:S1:418:ILE:HG13	2.20	0.42
7:7A:36:ASP:CG	26:B3:35:LYS:HD2	2.44	0.41
7:7A:39:LEU:HD11	45:N5:510:TYR:HB3	2.01	0.41
9:7C:60:LEU:HD23	10:8B:64:TYR:HB2	2.02	0.41
15:A6:45:PRO:HB3	62:S4:53:ILE:HD13	2.00	0.41
16:A7:27:ARG:NH1	60:S2:218:GLU:OE1	2.37	0.41
17:A8:117:ASN:O	17:A8:121:MET:HG2	2.20	0.41
20:AK:316:LEU:HB2	20:AK:319:ILE:HG12	2.02	0.41
35:C1:19:TYR:CZ	35:C1:102:PHE:HB2	2.55	0.41
48:Qb:73:VAL:HG23	48:Qb:147:LEU:HD13	2.02	0.41
49:Qc:141:TRP:CD1	49:Qc:265:PRO:HD3	2.55	0.41
60:S2:121:LEU:HD23	65:S7:113:MET:SD	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:S2:147:TYR:HB2	65:S7:71:CYS:HB3	2.02	0.41
61:S3:148:ASP:OD1	61:S3:148:ASP:N	2.53	0.41
65:S7:188:LYS:HD2	65:S7:191:ARG:HE	1.85	0.41
3:5B:72:GLY:N	3:5B:76:ASP:O	2.53	0.41
10:8B:52:ILE:HB	10:8B:53:PRO:HD3	2.02	0.41
16:A7:43:VAL:HG22	16:A7:47:HIS:CG	2.54	0.41
18:A9:127:ILE:HD11	18:A9:253:ILE:HD11	2.01	0.41
45:N5:228:GLY:H	45:N5:230:HIS:HD2	1.68	0.41
45:N5:496:MET:HE1	73:N5:703:CDL:H431	2.03	0.41
49:QC:304:MET:HB2	49:QC:305:PRO:HD3	2.03	0.41
52:QF:65:GLU:HG3	54:QH:73:LYS:NZ	2.35	0.41
47:Qa:288:VAL:O	47:Qa:292:VAL:HG23	2.20	0.41
50:Qd:139:VAL:HG23	50:Qd:140:CYS:SG	2.60	0.41
60:S2:348:ARG:HG2	60:S2:352:GLN:HE21	1.84	0.41
66:S8:117:LYS:NZ	66:S8:130:ILE:O	2.53	0.41
2:5A:60:THR:O	2:5A:63:ASN:HB2	2.21	0.41
4:6A:63:HIS:CE1	5:6B:76:ARG:HE	2.38	0.41
13:A3:152:PRO:HB3	13:A3:159:GLN:HB2	2.01	0.41
18:A9:54:ILE:HD12	18:A9:76:MET:HE1	2.02	0.41
19:AB:99:SER:N	19:AB:102:SER:OG	2.53	0.41
29:B6:135:VAL:HG21	45:N5:42:TYR:HD2	1.86	0.41
29:B6:137:ILE:HB	29:B6:138:PRO:HD3	2.02	0.41
29:B6:161:LYS:HG3	30:B7:50:GLN:NE2	2.35	0.41
41:N1:63:PRO:O	41:N1:66:SER:OG	2.36	0.41
41:N1:209:SER:HB2	65:S7:96:SER:HB2	2.02	0.41
42:N2:95:MET:HE1	42:N2:145:ILE:HD12	2.02	0.41
45:N5:407:TRP:O	45:N5:411:MET:HG2	2.21	0.41
48:QB:110:GLU:HA	48:QB:113:VAL:HG22	2.02	0.41
48:QB:362:ASN:HB3	48:QB:461:PRO:HG2	2.01	0.41
59:S1:76:ARG:HD3	59:S1:79:LEU:HD21	2.01	0.41
59:S1:169:VAL:HG22	59:S1:223:ILE:HD11	2.01	0.41
59:S1:338:VAL:HB	59:S1:363:SER:HB2	2.02	0.41
67:V1:111:LYS:HB2	67:V1:151:ALA:HA	2.03	0.41
17:A8:121:MET:HE3	17:A8:125:TRP:HZ3	1.85	0.41
18:A9:75:ARG:NH2	61:S3:213:ASP:OD2	2.54	0.41
33:BK:140:GLN:O	33:BK:144:SER:CB	2.50	0.41
35:C1:393:PHE:CE2	78:C1:602:HEA:H251	2.55	0.41
37:C3:9:HIS:NE2	37:C3:11:VAL:HG22	2.35	0.41
39:CA:31:ILE:HG13	39:CA:32:ARG:N	2.36	0.41
40:CB:30:ASP:OD1	40:CB:31:PRO:HD2	2.21	0.41
40:CB:62:ARG:HE	77:CB:201:3PE:H341	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:N1:142:TYR:HA	41:N1:145:THR:OG1	2.20	0.41
41:N1:305:ILE:HD13	43:N3:91:ALA:HB1	2.03	0.41
42:N2:36:ASN:OD1	42:N2:134:GLN:NE2	2.36	0.41
44:N4:398:MET:O	44:N4:402:ILE:HG13	2.20	0.41
45:N5:264:TYR:CG	45:N5:265:PRO:HD3	2.55	0.41
48:QB:373:GLN:NE2	48:QB:471:ILE:HG23	2.35	0.41
51:QE:125:VAL:HG21	72:QE:301:PLX:H111	2.03	0.41
47:Qa:60:ARG:NH1	47:Qa:122:THR:HG21	2.35	0.41
47:Qa:180:ALA:HB2	47:Qa:258:ILE:HG13	2.02	0.41
51:Qe:229:GLY:HA2	51:Qe:235:TYR:HB2	2.02	0.41
53:Qg:52:PRO:HD2	53:Qg:55:LEU:HD12	2.01	0.41
60:S2:135:TYR:O	60:S2:157:TYR:OH	2.37	0.41
60:S2:167:ILE:HD13	60:S2:369:VAL:HG11	2.02	0.41
65:S7:161:ILE:HG13	65:S7:180:LEU:HB2	2.02	0.41
66:S8:75:SER:O	66:S8:79:ARG:HG3	2.20	0.41
67:V1:244:ASN:O	67:V1:248:VAL:HG22	2.21	0.41
3:5B:72:GLY:HA2	3:5B:77:PRO:HA	2.03	0.41
3:5B:82:SER:OG	3:5B:84:THR:O	2.24	0.41
28:B5:116:PRO:HB2	71:B5:203:PC1:H321	2.02	0.41
35:C1:405:LEU:H	35:C1:405:LEU:HD12	1.84	0.41
36:C2:108:TYR:O	36:C2:117:THR:HA	2.21	0.41
38:C4:55:LEU:HD22	38:C4:84:LEU:HD13	2.03	0.41
42:N2:20:VAL:HG23	42:N2:32:GLY:HA3	2.01	0.41
42:N2:136:LEU:HD11	72:N2:401:PLX:H211	2.02	0.41
72:N4:502:PLX:H22	72:N4:502:PLX:H1A3	1.75	0.41
45:N5:188:TRP:CZ2	45:N5:209:PRO:HG2	2.54	0.41
46:N6:24:PRO:HA	46:N6:89:VAL:HG21	2.01	0.41
57:QK:67:SER:OG	57:QK:77:ARG:NH2	2.53	0.41
48:Qb:84:GLU:HG2	51:Qe:84:ARG:HH12	1.85	0.41
3:5B:42:GLU:H	3:5B:42:GLU:HG3	1.71	0.41
3:5B:44:ALA:O	3:5B:49:ARG:HD2	2.21	0.41
18:A9:228:LEU:O	18:A9:292:PRO:HA	2.20	0.41
27:B4:14:LEU:HD12	27:B4:15:PRO:HD2	2.02	0.41
32:B9:120:GLN:HB2	45:N5:524:ASN:HD21	1.86	0.41
35:C1:52:GLN:O	35:C1:56:VAL:HG23	2.20	0.41
35:C1:61:HIS:HE1	78:C1:602:HEA:NC	2.18	0.41
37:C3:50:ASN:ND2	71:C3:302:PC1:H392	2.36	0.41
73:CB:203:CDL:H473	44:N4:127:VAL:HB	2.02	0.41
59:S1:575:VAL:C	59:S1:578:PRO:HD2	2.45	0.41
60:S2:391:TYR:HD1	66:S8:122:VAL:HG21	1.86	0.41
60:S2:462:ILE:HG23	60:S2:467:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5B:68:LYS:O	35:C1:512:ASN:ND2	2.53	0.41
9:7C:60:LEU:HB3	10:8B:64:TYR:HB3	2.02	0.41
15:A6:127:THR:O	15:A6:131:ARG:HG3	2.21	0.41
15:A6:127:THR:HG23	61:S3:219:VAL:O	2.21	0.41
17:A8:105:ALA:HB2	17:A8:159:PHE:CE1	2.55	0.41
35:C1:416:ILE:HD11	38:C4:107:ALA:HA	2.03	0.41
40:CB:15:PHE:O	40:CB:80:ARG:NH1	2.47	0.41
44:N4:257:MET:HE1	71:N4:503:PC1:H321	2.02	0.41
47:QA:60:ARG:HG2	47:QA:393:LEU:HD22	2.02	0.41
71:QB:503:PC1:H3E2	71:Qc:405:PC1:H2H2	2.02	0.41
49:QC:185:LEU:HD23	49:QC:185:LEU:HA	1.88	0.41
49:QC:318:ARG:O	49:QC:322:GLN:HG3	2.21	0.41
51:QE:187:GLU:CD	51:QE:245:ALA:HB3	2.46	0.41
47:Qa:60:ARG:HD3	47:Qa:393:LEU:HD22	2.02	0.41
63:S5:57:LYS:HE3	63:S5:57:LYS:HB3	1.94	0.41
68:V2:88:ARG:HD3	69:V3:396:THR:HG22	2.03	0.41
1:4L:72:ALA:HB1	43:N3:60:ILE:HG23	2.03	0.41
6:6C:72:GLN:NE2	36:C2:141:ARG:HG3	2.36	0.41
33:BK:8:ASP:OD2	34:BL:127:LYS:NZ	2.53	0.41
33:BK:73:ASP:OD1	33:BK:73:ASP:N	2.42	0.41
36:C2:106:TRP:HB2	36:C2:120:SER:OG	2.21	0.41
48:QB:478:LEU:C	55:Qi:18:THR:HG21	2.45	0.41
50:QD:254:LEU:HD23	50:QD:256:PHE:CE1	2.56	0.41
50:QD:322:TYR:CE2	50:QD:324:PRO:HG3	2.56	0.41
72:QE:301:PLX:H182	72:QE:301:PLX:H151	1.68	0.41
63:S5:2:PRO:HB2	63:S5:3:PHE:H	1.62	0.41
66:S8:85:ASN:HD22	66:S8:88:PHE:HB2	1.86	0.41
2:5A:109:ARG:NH1	38:C4:45:PRO:O	2.54	0.41
4:6A:64:HIS:O	37:C3:191:GLY:N	2.54	0.41
4:6A:76:ASP:OD1	4:6A:79:HIS:ND1	2.54	0.41
5:6B:7:THR:HA	5:6B:10:LYS:HB3	2.01	0.41
5:6B:10:LYS:HE3	5:6B:10:LYS:HB2	1.84	0.41
6:6C:43:GLU:HB2	6:6C:44:PRO:HD3	2.02	0.41
11:A1:17:PHE:CE1	41:N1:257:ILE:HA	2.56	0.41
11:A1:29:PHE:HE2	41:N1:1:MET:HE3	1.86	0.41
15:A6:49:ARG:HH21	62:S4:53:ILE:HG22	1.86	0.41
17:A8:174:PHE:O	17:A8:178:ARG:NH1	2.54	0.41
18:A9:49:SER:HB2	61:S3:225:GLU:HG2	2.02	0.41
18:A9:135:GLU:OE1	18:A9:179:ARG:NH2	2.54	0.41
19:AB:78:ALA:HA	19:AB:81:ASP:OD2	2.20	0.41
75:AC:201:ZMP:H20B	32:B9:55:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B3:24:ILE:HG22	26:B3:50:ALA:HB2	2.02	0.41
35:C1:37:ILE:HG23	35:C1:54:TYR:CE1	2.56	0.41
35:C1:151:HIS:NE2	35:C1:206:ILE:HG13	2.35	0.41
35:C1:409:TRP:CD1	77:C1:601:3PE:H222	2.56	0.41
36:C2:98:LYS:HB2	36:C2:98:LYS:HE3	1.87	0.41
36:C2:165:VAL:HG12	36:C2:168:LEU:H	1.86	0.41
37:C3:86:PHE:CE1	71:C3:302:PC1:H232	2.55	0.41
37:C3:98:PHE:O	37:C3:102:TYR:HD1	2.04	0.41
37:C3:147:ALA:HB1	37:C3:159:MET:SD	2.61	0.41
38:C4:112:GLY:O	38:C4:116:LEU:HG	2.21	0.41
41:N1:267:THR:O	41:N1:271:LEU:HG	2.19	0.41
42:N2:250:SER:O	42:N2:259:GLY:HA3	2.21	0.41
44:N4:78:MET:O	44:N4:81:GLN:HG2	2.20	0.41
44:N4:259:TYR:O	44:N4:263:MET:HG2	2.21	0.41
44:N4:357:THR:O	44:N4:361:VAL:HG23	2.21	0.41
45:N5:96:VAL:O	45:N5:100:ILE:HG12	2.21	0.41
45:N5:324:LEU:HD23	45:N5:324:LEU:HA	1.93	0.41
47:QA:173:VAL:HG21	47:QA:268:HIS:HB2	2.01	0.41
51:QE:154:ILE:HD13	51:QE:176:VAL:HG21	2.02	0.41
72:QE:301:PLX:H91	72:QE:301:PLX:H122	1.60	0.41
49:Qc:58:ASP:OD1	49:Qc:59:THR:N	2.54	0.41
49:Qc:97:HIS:CD2	82:Qc:403:HEM:NC	2.88	0.41
51:Qe:192:VAL:HG11	51:Qe:200:HIS:HB3	2.03	0.41
59:S1:180:THR:O	59:S1:184:ARG:NE	2.33	0.41
59:S1:382:ARG:C	59:S1:384:ASN:H	2.29	0.41
60:S2:77:PRO:HA	60:S2:78:PRO:HD3	1.98	0.41
60:S2:310:LYS:HE2	66:S8:37:THR:N	2.36	0.41
81:S2:501:PEE:H49	81:S2:501:PEE:H54	1.90	0.41
61:S3:164:ASN:HA	61:S3:181:HIS:HE2	1.85	0.41
67:V1:37:ASP:HA	67:V1:40:ARG:HG3	2.03	0.41
67:V1:121:GLU:HA	67:V1:122:PRO:HD3	1.95	0.41
68:V2:102:ALA:HB2	68:V2:112:VAL:HG21	2.02	0.41
4:6A:62:TYR:HE2	37:C3:120:GLY:HA3	1.86	0.41
12:A2:91:LEU:HD23	12:A2:91:LEU:HA	1.88	0.41
16:A7:28:TYR:N	16:A7:30:GLU:OE1	2.54	0.41
19:AC:120:MET:HE1	32:B9:66:LEU:HB3	2.03	0.41
20:AK:97:ASP:OD1	20:AK:97:ASP:N	2.54	0.41
20:AK:327:ASP:O	20:AK:331:GLN:HG2	2.21	0.41
22:AM:49:TYR:HB2	22:AM:61:TRP:CE2	2.56	0.41
35:C1:238:PHE:C	35:C1:241:PRO:HD2	2.46	0.41
72:N4:502:PLX:H371	72:N4:502:PLX:H342	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N6:115:ILE:HG22	46:N6:116:ILE:H	1.85	0.41
56:QJ:34:TRP:CE2	51:Qe:130:LYS:HD2	2.56	0.41
49:Qc:324:LEU:HD23	49:Qc:324:LEU:HA	1.94	0.41
60:S2:90:PHE:HB2	60:S2:105:MET:HE2	2.02	0.41
1:4L:27:MET:HE3	46:N6:70:TYR:CE1	2.55	0.40
2:5A:84:LEU:HD13	6:6C:12:ARG:HH12	1.86	0.40
4:6A:57:PRO:HB3	37:C3:122:HIS:NE2	2.36	0.40
5:6B:58:ARG:O	5:6B:62:LYS:HB2	2.21	0.40
14:A5:31:ILE:O	14:A5:35:LEU:HG	2.20	0.40
16:A7:23:LYS:HG3	60:S2:259:PHE:CD1	2.56	0.40
18:A9:207:PHE:HB2	18:A9:214:LEU:HG	2.01	0.40
72:AM:201:PLX:H222	71:S7:302:PC1:H391	2.03	0.40
26:B3:16:LEU:HD12	26:B3:16:LEU:H	1.86	0.40
27:B4:106:LYS:HE2	71:N4:503:PC1:H112	2.03	0.40
28:B5:53:ARG:NH2	29:B6:89:SER:O	2.53	0.40
28:B5:108:GLU:OE1	28:B5:108:GLU:N	2.54	0.40
35:C1:283:LEU:HD13	35:C1:311:ILE:HG13	2.02	0.40
37:C3:58:TRP:CD2	71:C3:301:PC1:H252	2.56	0.40
48:QB:87:ASN:HD22	48:QB:204:PRO:HD3	1.85	0.40
48:QB:186:TYR:O	48:QB:190:THR:HG23	2.21	0.40
48:QB:365:ILE:HD13	48:QB:462:ILE:HG22	2.02	0.40
49:QC:119:LEU:HD22	82:QC:402:HEM:HBB2	2.03	0.40
49:QC:215:MET:HE3	49:QC:215:MET:HB2	1.83	0.40
49:QC:267:HIS:HE1	50:QD:206:HIS:CE1	2.39	0.40
47:Qa:259:ARG:NH2	47:Qa:444:LEU:HB3	2.35	0.40
59:S1:306:MET:HB2	59:S1:583:ILE:HB	2.03	0.40
60:S2:118:HIS:ND1	61:S3:191:TYR:OH	2.53	0.40
60:S2:164:LEU:HD23	60:S2:164:LEU:HA	1.88	0.40
66:S8:150:THR:HG21	66:S8:180:HIS:CD2	2.56	0.40
68:V2:98:MET:HE1	68:V2:124:ARG:HG2	2.03	0.40
15:A6:81:SER:OG	18:A9:367:GLU:OE2	2.29	0.40
18:A9:338:LEU:HD23	18:A9:338:LEU:HA	1.97	0.40
20:AK:68:ILE:O	20:AK:216:ILE:HD12	2.21	0.40
20:AK:182:ARG:NH1	20:AK:184:GLN:OE1	2.55	0.40
20:AK:208:TYR:HE1	20:AK:210:ASP:HB2	1.86	0.40
25:B2:69:LEU:HD22	45:N5:367:PRO:HG2	2.03	0.40
35:C1:155:VAL:O	35:C1:159:LEU:HG	2.20	0.40
35:C1:409:TRP:HA	35:C1:412:ILE:HD12	2.03	0.40
37:C3:34:TRP:HA	37:C3:39:SER:H	1.86	0.40
37:C3:109:THR:H	37:C3:112:LEU:HD12	1.86	0.40
42:N2:40:MET:HE3	42:N2:44:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:N2:112:HIS:HB2	42:N2:184:ILE:HD13	2.04	0.40
47:QA:70:ARG:HA	47:QA:185:ALA:O	2.20	0.40
50:QD:104:SER:HA	55:Qi:48:ASN:ND2	2.35	0.40
50:QD:113:ARG:O	50:QD:117:VAL:HG23	2.21	0.40
48:Qb:57:LEU:HD12	48:Qb:229:MET:O	2.22	0.40
59:S1:592:LYS:NZ	59:S1:619:ASP:OD2	2.37	0.40
66:S8:135:ARG:HD3	66:S8:141:ARG:HG3	2.03	0.40
67:V1:135:PRO:O	67:V1:139:VAL:HG23	2.21	0.40
20:AK:64:VAL:HG21	20:AK:76:ALA:HB2	2.04	0.40
20:AK:287:ASP:OD1	20:AK:287:ASP:N	2.54	0.40
72:AM:201:PLX:H6	72:AM:201:PLX:H91	1.75	0.40
37:C3:214:PHE:HA	71:C3:301:PC1:H282	2.03	0.40
71:C3:301:PC1:H371	71:C3:302:PC1:H222	2.02	0.40
51:QE:211:VAL:HG21	51:QE:246:SER:HA	2.04	0.40
48:Qb:286:HIS:HD2	48:Qb:357:HIS:HE1	1.69	0.40
65:S7:188:LYS:HD2	65:S7:191:ARG:NE	2.36	0.40
67:V1:287:THR:HB	68:V2:225:CYS:SG	2.61	0.40
67:V1:357:MET:HB3	67:V1:361:THR:HG21	2.02	0.40
68:V2:188:ILE:HG21	68:V2:208:LEU:HD11	2.03	0.40
2:5A:107:ALA:HB1	2:5A:141:ILE:HD13	2.04	0.40
7:7A:43:LEU:HD22	7:7A:50:ASN:ND2	2.37	0.40
15:A6:59:ARG:NH1	19:AB:136:GLU:OE1	2.55	0.40
35:C1:200:PRO:HB3	37:C3:93:PHE:HB2	2.02	0.40
35:C1:397:PHE:HB3	35:C1:398:PRO:HD3	2.02	0.40
37:C3:163:LEU:HD23	37:C3:163:LEU:HA	1.96	0.40
42:N2:162:ILE:HD12	42:N2:282:MET:HG2	2.04	0.40
42:N2:168:GLY:O	42:N2:172:GLN:HG2	2.22	0.40
45:N5:584:ILE:HG22	45:N5:587:TYR:OH	2.21	0.40
47:QA:207:TYR:O	47:QA:211:ASN:ND2	2.37	0.40
48:QB:474:GLY:HA2	71:QB:503:PC1:H142	2.03	0.40
49:QC:246:SER:HB2	49:QC:249:LEU:HB2	2.03	0.40
82:QC:401:HEM:HBC2	82:QC:401:HEM:HMC1	2.04	0.40
47:Qa:337:GLY:HA2	47:Qa:431:PHE:CE1	2.57	0.40
49:Qc:89:MET:HE2	49:Qc:89:MET:HB2	1.96	0.40
54:Qh:19:LEU:HD23	54:Qh:24:GLN:HB3	2.03	0.40
59:S1:295:ASP:OD1	59:S1:704:SER:OG	2.37	0.40
59:S1:577:ALA:HB3	59:S1:578:PRO:HD3	2.02	0.40
62:S4:79:ILE:HB	62:S4:147:VAL:HG22	2.03	0.40
68:V2:66:ILE:HG21	68:V2:81:PRO:HB2	2.04	0.40
2:5A:110:ILE:O	2:5A:114:VAL:HG23	2.22	0.40
10:8B:43:LEU:HG	35:C1:470:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A2:44:LEU:O	12:A2:48:ASN:ND2	2.54	0.40
20:AK:61:VAL:O	20:AK:204:HIS:N	2.54	0.40
35:C1:240:HIS:HB3	35:C1:241:PRO:HD3	2.03	0.40
35:C1:390:MET:SD	78:C1:602:HEA:H242	2.62	0.40
41:N1:288:LEU:O	41:N1:292:SER:HB2	2.22	0.40
45:N5:504:LEU:HD23	45:N5:504:LEU:HA	1.86	0.40
46:N6:24:PRO:HG3	46:N6:83:TRP:CE2	2.56	0.40
48:QB:366:ASP:HB2	48:QB:464:GLN:HG2	2.02	0.40
51:QE:127:TYR:HE1	55:Qi:33:GLU:HG3	1.86	0.40
51:QE:196:ARG:NH2	51:QE:252:GLY:O	2.45	0.40
51:Qe:186:GLN:O	51:Qe:190:VAL:HG23	2.22	0.40
51:Qe:234:TYR:HB2	51:Qe:243:TYR:HB2	2.02	0.40
59:S1:193:ASP:N	59:S1:193:ASP:OD1	2.54	0.40
59:S1:356:ASP:O	59:S1:360:ARG:HG2	2.21	0.40
67:V1:118:ASP:C	86:V1:502:FMN:HM73	2.46	0.40
86:V1:502:FMN:H9	86:V1:502:FMN:H1'2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4L	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
2	5A	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
3	5B	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
4	6A	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
5	6B	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
6	6C	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
7	7A	55/57 (96%)	54 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7B	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
9	7C	45/47 (96%)	45 (100%)	0	0	100	100
10	8B	41/43 (95%)	41 (100%)	0	0	100	100
11	A1	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
12	A2	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
13	A3	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
14	A5	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
15	A6	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
16	A7	93/112 (83%)	92 (99%)	1 (1%)	0	100	100
17	A8	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
18	A9	339/341 (99%)	329 (97%)	10 (3%)	0	100	100
19	AB	75/87 (86%)	74 (99%)	1 (1%)	0	100	100
19	AC	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
20	AK	319/321 (99%)	313 (98%)	6 (2%)	0	100	100
21	AL	138/140 (99%)	138 (100%)	0	0	100	100
22	AM	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
23	AN	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
24	B1	54/56 (96%)	54 (100%)	0	0	100	100
25	B2	65/67 (97%)	65 (100%)	0	0	100	100
26	B3	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
27	B4	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
28	B5	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
29	B6	97/126 (77%)	94 (97%)	3 (3%)	0	100	100
30	B7	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
31	B8	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
32	B9	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
33	BK	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
34	BL	97/102 (95%)	88 (91%)	9 (9%)	0	100	100
35	C1	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
36	C2	226/228 (99%)	221 (98%)	5 (2%)	0	100	100
37	C3	258/260 (99%)	246 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	C4	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
39	CA	47/49 (96%)	47 (100%)	0	0	100	100
40	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
41	N1	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
42	N2	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
43	N3	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
44	N4	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
45	N5	601/603 (100%)	573 (95%)	28 (5%)	0	100	100
46	N6	172/174 (99%)	162 (94%)	10 (6%)	0	100	100
47	QA	417/419 (100%)	410 (98%)	7 (2%)	0	100	100
47	Qa	417/419 (100%)	408 (98%)	9 (2%)	0	100	100
48	QB	444/446 (100%)	430 (97%)	14 (3%)	0	100	100
48	Qb	429/446 (96%)	419 (98%)	10 (2%)	0	100	100
49	QC	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
49	Qc	377/379 (100%)	368 (98%)	9 (2%)	0	100	100
50	QD	239/241 (99%)	230 (96%)	9 (4%)	0	100	100
50	Qd	237/241 (98%)	230 (97%)	7 (3%)	0	100	100
51	QE	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
51	Qe	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
52	QF	65/67 (97%)	65 (100%)	0	0	100	100
52	Qf	62/67 (92%)	62 (100%)	0	0	100	100
53	QG	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
53	Qg	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
54	QH	76/79 (96%)	72 (95%)	4 (5%)	0	100	100
54	Qh	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
55	QI	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
55	Qi	58/62 (94%)	58 (100%)	0	0	100	100
56	QJ	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
57	QK	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
58	Qj	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
59	S1	687/689 (100%)	656 (96%)	31 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	S2	422/430 (98%)	405 (96%)	17 (4%)	0	100	100
61	S3	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
62	S4	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
63	S5	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
64	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
65	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
66	S8	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
67	V1	429/431 (100%)	409 (95%)	20 (5%)	0	100	100
68	V2	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
69	V3	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
All	All	13964/14217 (98%)	13550 (97%)	414 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	4L	85/85 (100%)	85 (100%)	0	100	100
2	5A	89/89 (100%)	85 (96%)	4 (4%)	23	51
3	5B	80/80 (100%)	78 (98%)	2 (2%)	42	67
4	6A	65/65 (100%)	62 (95%)	3 (5%)	23	51
5	6B	73/73 (100%)	72 (99%)	1 (1%)	62	79
6	6C	57/57 (100%)	57 (100%)	0	100	100
7	7A	48/48 (100%)	45 (94%)	3 (6%)	15	41
8	7B	39/39 (100%)	39 (100%)	0	100	100
9	7C	40/40 (100%)	40 (100%)	0	100	100
10	8B	37/37 (100%)	36 (97%)	1 (3%)	40	65
11	A1	58/58 (100%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	A2	76/76 (100%)	75 (99%)	1 (1%)	65	80
13	A3	69/69 (100%)	69 (100%)	0	100	100
14	A5	99/99 (100%)	98 (99%)	1 (1%)	73	85
15	A6	107/107 (100%)	107 (100%)	0	100	100
16	A7	87/97 (90%)	86 (99%)	1 (1%)	70	83
17	A8	153/153 (100%)	153 (100%)	0	100	100
18	A9	295/295 (100%)	294 (100%)	1 (0%)	91	95
19	AB	71/80 (89%)	70 (99%)	1 (1%)	62	79
19	AC	80/80 (100%)	79 (99%)	1 (1%)	65	80
20	AK	284/284 (100%)	282 (99%)	2 (1%)	81	90
21	AL	101/101 (100%)	100 (99%)	1 (1%)	73	85
22	AM	130/130 (100%)	130 (100%)	0	100	100
23	AN	123/123 (100%)	123 (100%)	0	100	100
24	B1	53/53 (100%)	52 (98%)	1 (2%)	52	73
25	B2	62/62 (100%)	62 (100%)	0	100	100
26	B3	62/62 (100%)	61 (98%)	1 (2%)	58	77
27	B4	113/113 (100%)	113 (100%)	0	100	100
28	B5	121/121 (100%)	121 (100%)	0	100	100
29	B6	96/119 (81%)	95 (99%)	1 (1%)	73	85
30	B7	112/112 (100%)	112 (100%)	0	100	100
31	B8	141/141 (100%)	141 (100%)	0	100	100
32	B9	159/159 (100%)	158 (99%)	1 (1%)	84	91
33	BK	155/156 (99%)	155 (100%)	0	100	100
34	BL	91/94 (97%)	91 (100%)	0	100	100
35	C1	425/425 (100%)	410 (96%)	15 (4%)	31	59
36	C2	212/212 (100%)	209 (99%)	3 (1%)	62	79
37	C3	224/224 (100%)	219 (98%)	5 (2%)	47	69
38	C4	123/123 (100%)	119 (97%)	4 (3%)	33	60
39	CA	45/45 (100%)	45 (100%)	0	100	100
40	CB	108/108 (100%)	108 (100%)	0	100	100
41	N1	275/275 (100%)	269 (98%)	6 (2%)	47	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	N2	311/311 (100%)	310 (100%)	1 (0%)	91	95
43	N3	100/100 (100%)	99 (99%)	1 (1%)	73	85
44	N4	410/410 (100%)	408 (100%)	2 (0%)	86	92
45	N5	537/537 (100%)	535 (100%)	2 (0%)	89	94
46	N6	140/140 (100%)	137 (98%)	3 (2%)	48	71
47	QA	330/330 (100%)	328 (99%)	2 (1%)	84	91
47	Qa	330/330 (100%)	327 (99%)	3 (1%)	75	87
48	QB	372/372 (100%)	371 (100%)	1 (0%)	91	95
48	Qb	362/372 (97%)	360 (99%)	2 (1%)	84	91
49	QC	332/332 (100%)	328 (99%)	4 (1%)	67	82
49	Qc	332/332 (100%)	332 (100%)	0	100	100
50	QD	206/206 (100%)	206 (100%)	0	100	100
50	Qd	204/206 (99%)	201 (98%)	3 (2%)	60	78
51	QE	166/166 (100%)	164 (99%)	2 (1%)	67	82
51	Qe	166/166 (100%)	166 (100%)	0	100	100
52	QF	64/64 (100%)	64 (100%)	0	100	100
52	Qf	61/64 (95%)	61 (100%)	0	100	100
53	QG	93/93 (100%)	93 (100%)	0	100	100
53	Qg	93/93 (100%)	93 (100%)	0	100	100
54	QH	70/70 (100%)	70 (100%)	0	100	100
54	Qh	70/70 (100%)	70 (100%)	0	100	100
55	QI	50/50 (100%)	50 (100%)	0	100	100
55	Qi	49/50 (98%)	49 (100%)	0	100	100
56	QJ	40/40 (100%)	40 (100%)	0	100	100
57	QK	55/59 (93%)	54 (98%)	1 (2%)	54	75
58	Qj	41/41 (100%)	41 (100%)	0	100	100
59	S1	579/579 (100%)	573 (99%)	6 (1%)	73	85
60	S2	367/370 (99%)	364 (99%)	3 (1%)	79	89
61	S3	190/190 (100%)	190 (100%)	0	100	100
62	S4	113/113 (100%)	113 (100%)	0	100	100
63	S5	93/93 (100%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	S6	79/79 (100%)	78 (99%)	1 (1%)	65	80
65	S7	132/132 (100%)	127 (96%)	5 (4%)	28	57
66	S8	151/151 (100%)	150 (99%)	1 (1%)	81	90
67	V1	344/344 (100%)	337 (98%)	7 (2%)	50	72
68	V2	183/183 (100%)	179 (98%)	4 (2%)	47	69
69	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	12179/12248 (99%)	12065 (99%)	114 (1%)	74	87

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	5A	60	THR
2	5A	66	ASP
2	5A	115	LYS
2	5A	130	GLN
3	5B	42	GLU
3	5B	84	THR
4	6A	44	THR
4	6A	46	ASN
4	6A	47	SER
5	6B	51	VAL
7	7A	28	GLU
7	7A	49	ASP
7	7A	53	TYR
10	8B	62	ASP
12	A2	98	LYS
14	A5	77	ILE
16	A7	58	ASP
18	A9	129	LEU
19	AB	111	ASP
19	AC	112	SER
20	AK	97	ASP
20	AK	243	TYR
21	AL	115	CYS
24	B1	5	LEU
26	B3	47	ARG
29	B6	77	GLU
32	B9	147	ASP
35	C1	34	SER
35	C1	43	GLN

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Mol	Chain	Res	Type
35	C1	51	ASP
35	C1	104	LEU
35	C1	127	THR
35	C1	128	VAL
35	C1	132	LEU
35	C1	202	LEU
35	C1	209	LEU
35	C1	214	ASN
35	C1	366	VAL
35	C1	426	PHE
35	C1	440	TYR
35	C1	496	HIS
35	C1	504	THR
36	C2	98	LYS
36	C2	127	ASP
36	C2	199	ILE
37	C3	68	GLN
37	C3	133	ASN
37	C3	140	SER
37	C3	144	ILE
37	C3	213	THR
38	C4	56	SER
38	C4	58	SER
38	C4	62	LEU
38	C4	66	GLU
41	N1	61	LEU
41	N1	117	LEU
41	N1	129	LEU
41	N1	145	THR
41	N1	282	TYR
41	N1	289	LEU
42	N2	139	LEU
43	N3	63	LEU
44	N4	186	LEU
44	N4	375	LEU
45	N5	286	LEU
45	N5	336	LYS
46	N6	20	PHE
46	N6	47	PHE
46	N6	135	PHE
47	QA	138	LEU
47	QA	451	ASP

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Mol	Chain	Res	Type
48	QB	71	VAL
49	QC	47	THR
49	QC	108	MET
49	QC	112	THR
49	QC	215	MET
51	QE	139	SER
51	QE	211	VAL
57	QK	43	LEU
47	Qa	115	THR
47	Qa	361	ILE
47	Qa	408	GLN
48	Qb	92	PHE
48	Qb	154	CYS
50	Qd	137	VAL
50	Qd	140	CYS
50	Qd	209	GLU
59	S1	62	ARG
59	S1	252	ASP
59	S1	363	SER
59	S1	460	HIS
59	S1	611	THR
59	S1	640	ASP
60	S2	143	ASP
60	S2	204	THR
60	S2	392	THR
64	S6	29	VAL
65	S7	71	CYS
65	S7	91	VAL
65	S7	92	VAL
65	S7	101	ASP
65	S7	142	TYR
66	S8	118	LEU
67	V1	208	GLU
67	V1	212	LEU
67	V1	270	ASN
67	V1	294	VAL
67	V1	347	THR
67	V1	379	CYS
67	V1	385	CYS
68	V2	117	THR
68	V2	137	THR
68	V2	160	VAL

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Mol	Chain	Res	Type
68	V2	164	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (254) such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	7	ASN
2	5A	77	ASN
3	5B	43	GLN
3	5B	97	ASN
3	5B	125	HIS
4	6A	46	ASN
4	6A	53	HIS
4	6A	54	HIS
4	6A	63	HIS
4	6A	64	HIS
5	6B	24	GLN
5	6B	26	GLN
5	6B	33	ASN
5	6B	38	HIS
7	7A	50	ASN
11	A1	61	HIS
12	A2	86	GLN
12	A2	93	ASN
14	A5	71	GLN
14	A5	86	ASN
15	A6	74	HIS
15	A6	84	GLN
17	A8	107	HIS
17	A8	141	ASN
17	A8	142	GLN
18	A9	38	HIS
18	A9	122	HIS
18	A9	323	HIS
18	A9	356	HIS
18	A9	376	ASN
19	AB	101	ASN
19	AC	142	GLN
20	AK	134	GLN
20	AK	221	GLN
20	AK	346	ASN
21	AL	79	GLN
22	AM	31	ASN

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Mol	Chain	Res	Type
22	AM	52	ASN
22	AM	69	ASN
22	AM	91	HIS
22	AM	113	HIS
23	AN	24	ASN
23	AN	61	GLN
23	AN	90	ASN
25	B2	63	GLN
25	B2	68	GLN
25	B2	71	GLN
26	B3	21	GLN
26	B3	33	GLN
26	B3	91	GLN
27	B4	50	GLN
28	B5	170	GLN
28	B5	189	ASN
29	B6	86	GLN
29	B6	149	HIS
30	B7	47	ASN
30	B7	76	ASN
30	B7	85	HIS
30	B7	110	GLN
31	B8	94	HIS
31	B8	115	ASN
31	B8	154	GLN
32	B9	56	GLN
32	B9	117	GLN
33	BK	59	ASN
33	BK	91	GLN
33	BK	107	GLN
33	BK	124	ASN
33	BK	149	HIS
35	C1	55	ASN
35	C1	80	ASN
35	C1	99	ASN
35	C1	170	ASN
35	C1	256	HIS
35	C1	291	HIS
35	C1	328	HIS
35	C1	360	ASN
35	C1	368	HIS
35	C1	422	ASN

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Mol	Chain	Res	Type
35	C1	496	HIS
35	C1	512	ASN
36	C2	22	HIS
36	C2	59	GLN
36	C2	180	ASN
36	C2	195	GLN
36	C2	203	ASN
37	C3	50	ASN
37	C3	70	HIS
37	C3	71	HIS
37	C3	125	ASN
37	C3	148	HIS
37	C3	161	GLN
37	C3	222	GLN
38	C4	54	ASN
38	C4	98	ASN
38	C4	154	GLN
40	CB	63	GLN
41	N1	138	GLN
41	N1	194	ASN
41	N1	287	HIS
41	N1	304	HIS
42	N2	77	ASN
42	N2	83	GLN
42	N2	112	HIS
42	N2	171	ASN
42	N2	186	HIS
42	N2	273	ASN
42	N2	310	ASN
42	N2	322	GLN
42	N2	347	ASN
43	N3	26	GLN
44	N4	30	HIS
44	N4	175	ASN
44	N4	213	HIS
44	N4	304	GLN
44	N4	366	ASN
44	N4	399	ASN
44	N4	422	HIS
45	N5	2	ASN
45	N5	23	ASN
45	N5	34	ASN

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Mol	Chain	Res	Type
45	N5	136	ASN
45	N5	139	GLN
45	N5	175	ASN
45	N5	226	GLN
45	N5	230	HIS
45	N5	309	GLN
45	N5	447	ASN
45	N5	518	GLN
45	N5	524	ASN
45	N5	546	GLN
45	N5	580	GLN
47	QA	167	GLN
47	QA	176	ASN
47	QA	291	HIS
47	QA	298	HIS
47	QA	365	ASN
47	QA	415	GLN
47	QA	426	ASN
47	QA	446	HIS
48	QB	49	GLN
48	QB	87	ASN
48	QB	152	GLN
48	QB	160	GLN
48	QB	173	GLN
48	QB	188	HIS
48	QB	239	HIS
48	QB	301	ASN
48	QB	308	ASN
48	QB	357	HIS
49	QC	32	ASN
49	QC	54	HIS
49	QC	114	ASN
49	QC	137	GLN
49	QC	255	ASN
49	QC	308	HIS
49	QC	322	GLN
50	QD	206	HIS
50	QD	266	GLN
51	QE	135	GLN
51	QE	186	GLN
51	QE	199	GLN
51	QE	227	ASN

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Mol	Chain	Res	Type
51	QE	257	ASN
52	QF	88	ASN
53	QG	54	ASN
55	QI	38	GLN
55	QI	46	HIS
55	QI	48	ASN
55	QI	55	HIS
56	QJ	16	ASN
47	Qa	81	HIS
47	Qa	139	ASN
47	Qa	167	GLN
47	Qa	172	GLN
47	Qa	178	HIS
47	Qa	211	ASN
47	Qa	212	HIS
47	Qa	284	ASN
47	Qa	290	GLN
47	Qa	304	ASN
47	Qa	311	GLN
47	Qa	343	GLN
47	Qa	376	ASN
47	Qa	408	GLN
48	Qb	43	GLN
48	Qb	87	ASN
48	Qb	95	HIS
48	Qb	119	HIS
48	Qb	170	GLN
48	Qb	188	HIS
48	Qb	207	ASN
48	Qb	239	HIS
48	Qb	247	GLN
48	Qb	286	HIS
48	Qb	313	HIS
48	Qb	357	HIS
49	Qc	32	ASN
49	Qc	54	HIS
49	Qc	137	GLN
49	Qc	375	ASN
50	Qd	190	ASN
50	Qd	251	ASN
50	Qd	283	HIS
50	Qd	310	HIS

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Mol	Chain	Res	Type
51	Qe	135	GLN
51	Qe	186	GLN
51	Qe	219	HIS
52	Qf	36	GLN
52	Qf	55	GLN
53	Qg	23	ASN
54	Qh	7	HIS
55	Qi	38	GLN
55	Qi	48	ASN
58	Qj	16	ASN
59	S1	39	GLN
59	S1	101	ASN
59	S1	282	ASN
59	S1	304	GLN
59	S1	336	ASN
59	S1	415	ASN
59	S1	425	ASN
59	S1	569	GLN
59	S1	604	GLN
59	S1	652	ASN
59	S1	663	ASN
59	S1	688	GLN
60	S2	98	HIS
60	S2	166	ASN
60	S2	271	ASN
61	S3	77	GLN
61	S3	123	GLN
61	S3	196	HIS
62	S4	123	ASN
62	S4	163	ASN
63	S5	21	GLN
63	S5	25	GLN
63	S5	45	HIS
63	S5	98	HIS
64	S6	74	GLN
64	S6	117	GLN
64	S6	123	HIS
66	S8	85	ASN
67	V1	277	ASN
67	V1	284	HIS
67	V1	303	HIS
67	V1	393	ASN

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Mol	Chain	Res	Type
68	V2	74	HIS
68	V2	90	ASN
68	V2	131	HIS
68	V2	133	GLN
68	V2	191	ASN
68	V2	246	GLN
69	V3	419	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
60	2MR	S2	124	60	10,12,13	2.42	2 (20%)	5,13,15	1.07	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
60	2MR	S2	124	60	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	S2	124	2MR	CZ-NE	5.09	1.45	1.34
60	S2	124	2MR	CZ-NH2	5.07	1.44	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	S2	124	2MR	NE-CD-CG-CB
60	S2	124	2MR	CA-CB-CG-CD
60	S2	124	2MR	CG-CD-NE-CZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	S2	124	2MR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 7 are monoatomic - leaving 80 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	$\# Z > 2$
71	PC1	6A	101	-	44,44,53	0.32	0	50,52,61	0.32	0
71	PC1	N4	504	-	51,51,53	0.30	0	57,59,61	0.28	0
82	HEM	QC	401	49	41,50,50	1.21	4 (9%)	45,82,82	1.70	9 (20%)
84	FES	V2	301	68	0,4,4	-	-	-	-	-
71	PC1	Qb	502	-	47,47,53	0.31	0	53,55,61	0.37	0
73	CDL	QH	101	-	60,60,99	0.37	0	66,72,111	0.32	0
77	3PE	CB	201	-	50,50,50	0.31	0	53,55,55	0.29	0
85	SF4	S1	801	59	0,12,12	-	-	-	-	-
81	PEE	N5	701	-	45,45,50	1.39	5 (11%)	48,50,55	1.21	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	HEM	Qc	403	49	41,50,50	1.23	3 (7%)	45,82,82	1.69	8 (17%)
81	PEE	N5	704	-	50,50,50	1.33	5 (10%)	53,55,55	1.15	2 (3%)
73	CDL	A8	301	-	82,82,99	0.32	0	88,94,111	0.36	0
73	CDL	QB	501	-	61,61,99	0.38	0	67,73,111	0.42	0
81	PEE	N6	201	-	50,50,50	1.33	5 (10%)	53,55,55	1.17	2 (3%)
73	CDL	B5	202	-	99,99,99	0.31	0	105,111,111	0.27	0
72	PLX	N4	502	-	51,51,51	1.11	4 (7%)	55,59,59	0.88	1 (1%)
71	PC1	N1	402	-	47,47,53	0.31	0	53,55,61	0.30	0
73	CDL	AL	201	-	90,90,99	0.32	0	96,102,111	0.38	0
84	FES	Qe	301	51	0,4,4	-	-	-	-	-
71	PC1	C3	301	-	48,48,53	0.31	0	54,56,61	0.49	0
73	CDL	QH	102	-	63,63,99	0.36	0	69,75,111	0.31	0
84	FES	S1	803	59	0,4,4	-	-	-	-	-
72	PLX	AM	201	-	51,51,51	1.10	4 (7%)	55,59,59	0.88	1 (1%)
81	PEE	S8	303	-	50,50,50	1.32	5 (10%)	53,55,55	1.16	3 (5%)
73	CDL	N5	702	-	88,88,99	0.31	0	94,100,111	0.29	0
83	HEC	QD	401	50	32,50,50	2.03	4 (12%)	24,82,82	2.35	15 (62%)
81	PEE	QE	302	-	46,46,50	1.37	5 (10%)	49,51,55	1.20	3 (6%)
86	FMN	V1	502	-	33,33,33	0.21	0	48,50,50	0.46	0
85	SF4	S8	301	66	0,12,12	-	-	-	-	-
71	PC1	QB	502	-	50,50,53	0.30	0	56,58,61	0.30	0
73	CDL	QD	402	-	63,63,99	0.37	0	69,75,111	0.36	0
72	PLX	B5	201	-	51,51,51	1.10	4 (7%)	55,59,59	0.89	1 (1%)
73	CDL	CB	203	-	99,99,99	0.30	0	105,111,111	0.26	0
71	PC1	C3	302	-	49,49,53	0.31	0	55,57,61	0.30	0
81	PEE	QC	403	-	39,39,50	1.32	4 (10%)	42,44,55	1.13	3 (7%)
71	PC1	Qj	101	-	42,42,53	0.33	0	48,50,61	0.31	0
73	CDL	N1	401	-	77,77,99	0.34	0	83,89,111	0.30	0
77	3PE	B8	201	-	31,31,50	0.37	0	34,36,55	0.34	0
85	SF4	S1	802	59	0,12,12	-	-	-	-	-
76	ADP	AK	401	-	24,29,29	0.96	1 (4%)	29,45,45	1.44	4 (13%)
71	PC1	N4	503	-	47,47,53	0.31	0	53,55,61	0.31	0
73	CDL	N5	703	-	99,99,99	0.30	0	105,111,111	0.29	0
83	HEC	Qd	401	50	32,50,50	2.02	4 (12%)	24,82,82	2.27	13 (54%)
74	NDP	A9	401	-	45,52,52	0.51	0	53,80,80	0.55	1 (1%)
82	HEM	Qc	402	49	41,50,50	1.20	4 (9%)	45,82,82	1.70	8 (17%)
71	PC1	B4	202	-	49,49,53	0.30	0	55,57,61	0.31	0
71	PC1	QB	503	-	53,53,53	0.30	0	59,61,61	0.29	0
84	FES	QE	304	51	0,4,4	-	-	-	-	-
85	SF4	S7	301	65	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	PLX	QI	301	-	51,51,51	1.12	5 (9%)	55,59,59	0.89	1 (1%)
73	CDL	AL	202	-	88,88,99	0.32	0	94,100,111	0.33	0
73	CDL	B4	201	-	79,79,99	0.33	0	85,91,111	0.31	0
81	PEE	S2	501	-	47,47,50	1.36	5 (10%)	50,52,55	1.17	3 (6%)
81	PEE	N4	501	-	45,45,50	1.38	5 (11%)	48,50,55	1.22	3 (6%)
71	PC1	B5	203	-	53,53,53	0.29	0	59,61,61	0.28	0
77	3PE	QE	303	-	42,42,50	0.32	0	45,47,55	0.35	0
71	PC1	S7	302	-	53,53,53	0.29	0	59,61,61	0.27	0
72	PLX	6C	101	-	30,30,51	1.32	3 (10%)	34,38,59	0.79	1 (2%)
85	SF4	V1	501	67	0,12,12	-	-	-	-	-
77	3PE	N5	705	-	45,45,50	0.32	0	48,50,55	0.29	0
77	3PE	QC	404	-	33,33,50	0.36	0	36,38,55	0.33	0
71	PC1	CB	202	-	53,53,53	0.29	0	59,61,61	0.28	0
82	HEM	QC	402	49	41,50,50	1.24	3 (7%)	45,82,82	1.67	7 (15%)
72	PLX	QE	301	-	45,45,51	1.16	4 (8%)	49,53,59	0.88	1 (2%)
71	PC1	Qc	404	-	53,53,53	0.30	0	59,61,61	0.28	0
75	ZMP	AB	201	19	29,35,36	0.65	1 (3%)	34,42,45	0.73	0
78	HEA	C1	602	35	57,67,67	2.00	17 (29%)	61,103,103	2.69	26 (42%)
72	PLX	N2	401	-	51,51,51	1.11	4 (7%)	55,59,59	0.86	1 (1%)
81	PEE	N3	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.17	2 (3%)
85	SF4	S8	302	66	0,12,12	-	-	-	-	-
73	CDL	N2	402	-	67,67,99	0.36	0	73,79,111	0.35	0
81	PEE	Qe	302	-	43,43,50	1.38	5 (11%)	46,48,55	1.25	4 (8%)
81	PEE	Qc	401	-	41,41,50	1.28	4 (9%)	44,46,55	1.19	3 (6%)
73	CDL	Qb	501	-	63,63,99	0.37	0	69,75,111	0.38	0
71	PC1	Qc	405	-	53,53,53	0.29	0	59,61,61	0.32	0
75	ZMP	AC	201	19	29,35,36	0.65	1 (3%)	34,42,45	0.74	0
71	PC1	Qh	102	-	53,53,53	0.29	0	59,61,61	0.28	0
78	HEA	C1	603	35	57,67,67	2.00	15 (26%)	61,103,103	2.71	28 (45%)
73	CDL	Qh	101	-	54,54,99	0.39	0	60,66,111	0.34	0
77	3PE	C1	601	-	50,50,50	0.32	0	53,55,55	0.27	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
71	PC1	6A	101	-	-	9/48/48/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PC1	N4	504	-	-	6/55/55/57	-
82	HEM	QC	401	49	-	7/12/54/54	-
84	FES	V2	301	68	-	-	0/1/1/1
71	PC1	Qb	502	-	-	12/51/51/57	-
73	CDL	QH	101	-	-	16/71/71/110	-
77	3PE	CB	201	-	-	16/54/54/54	-
85	SF4	S1	801	59	-	-	0/6/5/5
81	PEE	N5	701	-	-	22/49/49/54	-
82	HEM	Qc	403	49	-	9/12/54/54	-
81	PEE	N5	704	-	-	26/54/54/54	-
73	CDL	A8	301	-	-	21/93/93/110	-
73	CDL	QB	501	-	-	20/72/72/110	-
81	PEE	N6	201	-	-	23/54/54/54	-
73	CDL	B5	202	-	-	18/110/110/110	-
72	PLX	N4	502	-	-	18/55/55/55	-
71	PC1	N1	402	-	-	14/51/51/57	-
73	CDL	AL	201	-	-	17/101/101/110	-
84	FES	Qe	301	51	-	-	0/1/1/1
71	PC1	C3	301	-	-	12/52/52/57	-
73	CDL	QH	102	-	-	19/74/74/110	-
84	FES	S1	803	59	-	-	0/1/1/1
72	PLX	AM	201	-	-	23/55/55/55	-
81	PEE	S8	303	-	-	25/54/54/54	-
73	CDL	N5	702	-	-	25/99/99/110	-
83	HEC	QD	401	50	-	2/10/54/54	-
81	PEE	QE	302	-	-	18/50/50/54	-
86	FMN	V1	502	-	-	6/18/18/18	0/3/3/3
85	SF4	S8	301	66	-	-	0/6/5/5
71	PC1	QB	502	-	-	16/54/54/57	-
73	CDL	QD	402	-	-	13/74/74/110	-
72	PLX	B5	201	-	-	19/55/55/55	-
73	CDL	CB	203	-	-	21/110/110/110	-
71	PC1	C3	302	-	-	13/53/53/57	-
81	PEE	QC	403	-	-	19/43/43/54	-
71	PC1	Qj	101	-	-	14/46/46/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
73	CDL	N1	401	-	-	16/88/88/110	-
77	3PE	B8	201	-	-	5/35/35/54	-
85	SF4	S1	802	59	-	-	0/6/5/5
76	ADP	AK	401	-	-	1/12/32/32	0/3/3/3
71	PC1	N4	503	-	-	24/51/51/57	-
73	CDL	N5	703	-	-	25/110/110/110	-
83	HEC	Qd	401	50	-	1/10/54/54	-
74	NDP	A9	401	-	-	7/30/77/77	0/5/5/5
82	HEM	Qc	402	49	-	7/12/54/54	-
71	PC1	B4	202	-	-	10/53/53/57	-
71	PC1	QB	503	-	-	9/57/57/57	-
84	FES	QE	304	51	-	-	0/1/1/1
85	SF4	S7	301	65	-	-	0/6/5/5
72	PLX	QI	301	-	-	20/55/55/55	-
73	CDL	AL	202	-	-	16/99/99/110	-
73	CDL	B4	201	-	-	16/90/90/110	-
81	PEE	S2	501	-	-	30/51/51/54	-
81	PEE	N4	501	-	-	26/49/49/54	-
71	PC1	B5	203	-	-	14/57/57/57	-
77	3PE	QE	303	-	-	10/46/46/54	-
71	PC1	S7	302	-	-	9/57/57/57	-
72	PLX	6C	101	-	-	14/34/34/55	-
85	SF4	V1	501	67	-	-	0/6/5/5
77	3PE	N5	705	-	-	12/49/49/54	-
77	3PE	QC	404	-	-	3/37/37/54	-
71	PC1	CB	202	-	-	6/57/57/57	-
82	HEM	QC	402	49	-	6/12/54/54	-
72	PLX	QE	301	-	-	23/49/49/55	-
71	PC1	Qc	404	-	-	14/57/57/57	-
75	ZMP	AB	201	19	-	22/40/42/43	-
78	HEA	C1	602	35	-	11/32/76/76	-
72	PLX	N2	401	-	-	26/55/55/55	-
81	PEE	N3	201	-	-	29/54/54/54	-
85	SF4	S8	302	66	-	-	0/6/5/5
73	CDL	N2	402	-	-	20/78/78/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	PEE	Qe	302	-	-	22/47/47/54	-
81	PEE	Qc	401	-	-	25/45/45/54	-
73	CDL	Qb	501	-	-	21/74/74/110	-
71	PC1	Qc	405	-	-	11/57/57/57	-
75	ZMP	AC	201	19	-	16/40/42/43	-
71	PC1	Qh	102	-	-	10/57/57/57	-
78	HEA	C1	603	35	-	11/32/76/76	-
73	CDL	Qh	101	-	-	5/65/65/110	-
77	3PE	C1	601	-	-	14/54/54/54	-

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	QD	401	HEC	C3C-C2C	-6.54	1.33	1.40
83	Qd	401	HEC	C3C-C2C	-6.44	1.34	1.40
83	Qd	401	HEC	C2B-C3B	-6.13	1.34	1.40
83	QD	401	HEC	C2B-C3B	-6.06	1.34	1.40
78	C1	602	HEA	C3B-C2B	5.45	1.47	1.34
78	C1	603	HEA	C3B-C2B	5.00	1.46	1.34
78	C1	602	HEA	CHC-C4B	4.47	1.46	1.35
78	C1	603	HEA	C4B-NB	-4.46	1.32	1.40
78	C1	602	HEA	C3A-C2A	4.41	1.46	1.40
78	C1	603	HEA	CHC-C4B	4.30	1.46	1.35
78	C1	603	HEA	C3A-C2A	4.29	1.46	1.40
78	C1	603	HEA	C3D-C2D	4.22	1.45	1.36
78	C1	603	HEA	C3C-C2C	4.12	1.46	1.40
78	C1	602	HEA	CHD-C1D	4.09	1.45	1.35
81	N5	704	PEE	C18-C19	4.06	1.55	1.31
81	N6	201	PEE	C18-C19	4.06	1.55	1.31
81	QC	403	PEE	C18-C19	4.05	1.55	1.31
81	QE	302	PEE	C18-C19	4.04	1.55	1.31
81	N4	501	PEE	C18-C19	4.04	1.55	1.31
81	S2	501	PEE	C18-C19	4.03	1.55	1.31
78	C1	602	HEA	C1D-ND	-4.03	1.33	1.40
81	N3	201	PEE	C18-C19	4.03	1.55	1.31
81	S8	303	PEE	C18-C19	4.03	1.55	1.31
81	N5	701	PEE	C18-C19	4.03	1.55	1.31
81	Qc	401	PEE	C18-C19	4.01	1.55	1.31
78	C1	602	HEA	C4B-NB	-4.00	1.33	1.40
78	C1	602	HEA	C3C-C2C	3.97	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	C1	603	HEA	C1D-ND	-3.96	1.33	1.40
81	S2	501	PEE	C39-C38	3.95	1.54	1.31
81	Qe	302	PEE	C39-C38	3.95	1.54	1.31
81	S8	303	PEE	C39-C38	3.94	1.54	1.31
81	N6	201	PEE	C39-C38	3.94	1.54	1.31
81	N5	701	PEE	C39-C38	3.94	1.54	1.31
81	N3	201	PEE	C39-C38	3.94	1.54	1.31
81	QE	302	PEE	C39-C38	3.94	1.54	1.31
81	N5	704	PEE	C39-C38	3.93	1.54	1.31
81	N4	501	PEE	C39-C38	3.92	1.54	1.31
82	Qc	403	HEM	C4D-ND	-3.85	1.33	1.40
78	C1	603	HEA	CHD-C1D	3.84	1.44	1.35
78	C1	602	HEA	C3D-C2D	3.68	1.44	1.36
82	Qc	402	HEM	C4D-ND	-3.61	1.34	1.40
82	QC	402	HEM	C4D-ND	-3.58	1.34	1.40
82	QC	401	HEM	C4D-ND	-3.56	1.34	1.40
81	Qe	302	PEE	C18-C19	3.40	1.55	1.29
83	Qd	401	HEC	CBC-CAC	-3.38	1.36	1.49
83	QD	401	HEC	CBC-CAC	-3.37	1.36	1.49
81	N5	704	PEE	O3-C30	3.32	1.43	1.33
81	N6	201	PEE	O3-C30	3.29	1.42	1.33
81	N5	701	PEE	O3-C30	3.29	1.42	1.33
81	S8	303	PEE	O3-C30	3.26	1.42	1.33
81	QE	302	PEE	O3-C30	3.25	1.42	1.33
81	QC	403	PEE	O3-C30	3.25	1.42	1.33
81	Qc	401	PEE	O3-C30	3.23	1.42	1.33
81	Qe	302	PEE	O3-C30	3.22	1.42	1.33
81	N3	201	PEE	O3-C30	3.22	1.42	1.33
81	S2	501	PEE	O3-C30	3.21	1.42	1.33
81	N4	501	PEE	O3-C30	3.15	1.42	1.33
82	Qc	403	HEM	C1B-NB	-3.07	1.35	1.40
82	QC	402	HEM	C1B-NB	-3.05	1.35	1.40
82	QC	401	HEM	C1B-NB	-2.98	1.35	1.40
72	N2	401	PLX	O6-C4	-2.97	1.40	1.44
72	QI	301	PLX	O6-C4	-2.95	1.40	1.44
72	N4	502	PLX	O6-C4	-2.94	1.40	1.44
72	QE	301	PLX	O6-C4	-2.94	1.40	1.44
82	Qc	402	HEM	C1B-NB	-2.94	1.35	1.40
72	AM	201	PLX	O6-C4	-2.93	1.40	1.44
72	B5	201	PLX	O6-C4	-2.88	1.40	1.44
72	6C	101	PLX	O6-C4	-2.87	1.40	1.44
78	C1	603	HEA	C4B-C3B	2.86	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	S8	303	PEE	O2-C10	2.74	1.42	1.34
78	C1	602	HEA	C1B-NB	-2.72	1.33	1.38
81	N3	201	PEE	O2-C10	2.67	1.41	1.34
81	N6	201	PEE	O2-C10	2.66	1.41	1.34
81	N5	701	PEE	O2-C10	2.66	1.41	1.34
81	QE	302	PEE	O2-C10	2.65	1.41	1.34
81	S2	501	PEE	O2-C10	2.65	1.41	1.34
78	C1	603	HEA	FE-ND	2.64	2.09	1.96
81	Qe	302	PEE	O2-C10	2.62	1.41	1.34
81	N5	704	PEE	O2-C10	2.62	1.41	1.34
81	Qc	401	PEE	O2-C2	-2.60	1.40	1.46
78	C1	603	HEA	FE-NB	2.59	2.09	1.96
82	QC	402	HEM	C1D-ND	-2.59	1.33	1.38
82	Qc	403	HEM	C1D-ND	-2.58	1.33	1.38
81	QC	403	PEE	O2-C10	2.58	1.41	1.34
78	C1	602	HEA	FE-ND	2.57	2.09	1.96
81	N4	501	PEE	O2-C2	-2.57	1.40	1.46
81	N4	501	PEE	O2-C10	2.57	1.41	1.34
81	QC	403	PEE	O2-C2	-2.53	1.40	1.46
81	Qe	302	PEE	O2-C2	-2.52	1.40	1.46
81	Qc	401	PEE	O2-C10	2.52	1.41	1.34
78	C1	602	HEA	FE-NB	2.51	2.09	1.96
82	QC	401	HEM	C1D-ND	-2.51	1.33	1.38
78	C1	603	HEA	C1B-NB	-2.50	1.33	1.38
75	AB	201	ZMP	C9-C10	-2.50	1.48	1.50
82	Qc	402	HEM	C1D-ND	-2.50	1.33	1.38
81	N5	704	PEE	O2-C2	-2.49	1.40	1.46
81	S2	501	PEE	O2-C2	-2.47	1.40	1.46
81	N3	201	PEE	O2-C2	-2.47	1.40	1.46
76	AK	401	ADP	C5-C4	2.45	1.47	1.40
81	QE	302	PEE	O2-C2	-2.45	1.40	1.46
78	C1	602	HEA	C4D-ND	-2.44	1.33	1.38
81	N6	201	PEE	O2-C2	-2.42	1.40	1.46
75	AC	201	ZMP	C9-C10	-2.41	1.48	1.50
81	N5	701	PEE	O2-C2	-2.40	1.40	1.46
78	C1	602	HEA	O2D-CGD	-2.39	1.22	1.30
78	C1	602	HEA	CAA-C2A	-2.37	1.48	1.52
78	C1	602	HEA	O2A-CGA	-2.36	1.22	1.30
78	C1	603	HEA	CAA-C2A	-2.36	1.48	1.52
78	C1	603	HEA	O2D-CGD	-2.36	1.22	1.30
83	Qd	401	HEC	CBB-CAB	-2.34	1.40	1.49
78	C1	603	HEA	O2A-CGA	-2.32	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	QD	401	HEC	CBB-CAB	-2.31	1.40	1.49
81	S8	303	PEE	O2-C2	-2.24	1.41	1.46
72	QE	301	PLX	C1B-N1	-2.18	1.43	1.50
72	N4	502	PLX	C1B-N1	-2.16	1.43	1.50
72	QI	301	PLX	C1B-N1	-2.15	1.43	1.50
72	B5	201	PLX	C1B-N1	-2.14	1.43	1.50
72	N2	401	PLX	C1B-N1	-2.11	1.43	1.50
72	6C	101	PLX	C1B-N1	-2.11	1.43	1.50
72	QE	301	PLX	C1A-N1	-2.10	1.43	1.50
78	C1	602	HEA	C1C-CHC	2.10	1.46	1.41
72	AM	201	PLX	C1B-N1	-2.09	1.43	1.50
72	QI	301	PLX	C1A-N1	-2.09	1.43	1.50
78	C1	602	HEA	C4B-C3B	2.08	1.48	1.44
82	Qc	402	HEM	CHB-C1B	2.05	1.40	1.35
72	N2	401	PLX	C1A-N1	-2.05	1.44	1.50
72	6C	101	PLX	P1-O4	2.05	1.67	1.59
72	N4	502	PLX	P1-O4	2.05	1.67	1.59
82	QC	401	HEM	CHB-C1B	2.03	1.40	1.35
72	AM	201	PLX	P1-O4	2.03	1.67	1.59
72	N4	502	PLX	C1A-N1	-2.02	1.44	1.50
72	B5	201	PLX	P1-O4	2.02	1.67	1.59
72	QE	301	PLX	P1-O4	2.01	1.67	1.59
72	QI	301	PLX	P1-O4	2.01	1.67	1.59
72	AM	201	PLX	C1A-N1	-2.01	1.44	1.50
72	N2	401	PLX	P1-O4	2.01	1.67	1.59
72	B5	201	PLX	C1A-N1	-2.01	1.44	1.50
72	QI	301	PLX	C7-C6	2.00	1.55	1.50

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	C1	602	HEA	CAD-CBD-CGD	-9.17	93.88	113.60
78	C1	603	HEA	CAD-CBD-CGD	-8.53	95.25	113.60
78	C1	603	HEA	C3D-C4D-ND	5.79	115.96	110.36
78	C1	603	HEA	C2D-C1D-ND	5.26	116.08	109.84
78	C1	603	HEA	CHB-C1B-C2B	-5.04	117.10	124.98
78	C1	602	HEA	C2B-C1B-NB	4.97	115.84	109.88
78	C1	602	HEA	C2D-C1D-ND	4.95	115.71	109.84
78	C1	603	HEA	C13-C12-C11	-4.93	106.94	114.35
78	C1	602	HEA	CHB-C1B-C2B	-4.84	117.41	124.98
78	C1	602	HEA	C1D-C2D-C3D	-4.83	101.88	106.96
78	C1	603	HEA	C2B-C1B-NB	4.77	115.59	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	C1	603	HEA	C1D-C2D-C3D	-4.71	102.00	106.96
82	QC	401	HEM	CHC-C4B-NB	4.59	129.42	124.43
78	C1	602	HEA	C3C-C4C-NC	4.59	115.14	109.21
78	C1	602	HEA	C3D-C4D-ND	4.58	114.79	110.36
82	Qc	402	HEM	CHC-C4B-NB	4.54	129.36	124.43
82	Qc	403	HEM	CHC-C4B-NB	4.40	129.22	124.43
82	QC	402	HEM	CHC-C4B-NB	4.40	129.21	124.43
78	C1	603	HEA	CAA-CBA-CGA	-4.39	101.45	113.76
78	C1	602	HEA	C3B-C4B-NB	4.37	115.02	109.84
78	C1	602	HEA	C13-C12-C11	-4.34	107.83	114.35
78	C1	602	HEA	CAA-CBA-CGA	-4.33	101.63	113.76
81	N5	701	PEE	O2-C10-C11	4.13	120.40	111.50
81	QE	302	PEE	O2-C10-C11	4.12	120.38	111.50
83	QD	401	HEC	CMD-C2D-C1D	-4.09	122.18	128.46
81	N4	501	PEE	O2-C10-C11	4.04	120.21	111.50
81	N6	201	PEE	O2-C10-C11	3.99	120.10	111.50
83	Qd	401	HEC	CMD-C2D-C1D	-3.99	122.33	128.46
82	QC	402	HEM	C4D-ND-C1D	3.97	109.17	105.07
81	S8	303	PEE	O2-C10-C11	3.92	119.95	111.50
78	C1	603	HEA	C3C-C4C-NC	3.92	114.28	109.21
78	C1	603	HEA	C3B-C4B-NB	3.91	114.47	109.84
81	S2	501	PEE	O2-C10-C11	3.90	119.90	111.50
81	Qc	401	PEE	O2-C10-C11	3.90	119.90	111.50
82	QC	401	HEM	CHB-C1B-NB	3.89	129.18	124.38
81	N3	201	PEE	O2-C10-C11	3.88	119.85	111.50
81	Qe	302	PEE	O2-C10-C11	3.87	119.85	111.50
82	Qc	403	HEM	C4D-ND-C1D	3.84	109.04	105.07
81	N5	704	PEE	O2-C10-C11	3.82	119.73	111.50
82	Qc	402	HEM	CHB-C1B-NB	3.80	129.08	124.38
81	QC	403	PEE	O2-C10-C11	3.80	119.69	111.50
82	QC	402	HEM	CHB-C1B-NB	3.78	129.06	124.38
78	C1	602	HEA	C4B-C3B-C2B	-3.68	101.12	107.41
82	Qc	403	HEM	CHB-C1B-NB	3.66	128.90	124.38
78	C1	603	HEA	CHA-C4D-C3D	-3.64	119.49	124.84
78	C1	602	HEA	CMC-C2C-C3C	3.56	131.34	124.68
76	AK	401	ADP	PA-O3A-PB	-3.56	120.60	132.83
83	QD	401	HEC	CBD-CAD-C3D	3.47	118.54	112.62
83	Qd	401	HEC	CMB-C2B-C1B	-3.36	123.31	128.46
78	C1	603	HEA	C4B-C3B-C2B	-3.33	101.73	107.41
83	Qd	401	HEC	CMB-C2B-C3B	3.32	129.72	125.82
83	QD	401	HEC	CMB-C2B-C1B	-3.31	123.37	128.46
82	Qc	402	HEM	C4D-ND-C1D	3.30	108.48	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	C1	603	HEA	CMC-C2C-C3C	3.28	130.82	124.68
83	QD	401	HEC	CMC-C2C-C3C	3.28	129.67	125.82
82	Qc	402	HEM	C1B-NB-C4B	3.25	108.43	105.07
82	QC	401	HEM	C4D-ND-C1D	3.25	108.42	105.07
83	QD	401	HEC	CMB-C2B-C3B	3.24	129.63	125.82
76	AK	401	ADP	N3-C2-N1	-3.19	123.70	128.68
82	Qc	402	HEM	CHA-C4D-ND	3.16	128.29	124.38
83	Qd	401	HEC	CMC-C2C-C3C	3.15	129.52	125.82
78	C1	602	HEA	C27-C19-C20	3.14	120.56	115.27
82	Qc	403	HEM	C1B-NB-C4B	3.10	108.28	105.07
83	Qd	401	HEC	CBD-CAD-C3D	3.06	117.84	112.62
82	QC	401	HEM	C1B-NB-C4B	3.04	108.22	105.07
83	QD	401	HEC	C4C-C3C-C2C	3.01	109.60	106.35
83	Qd	401	HEC	C4C-C3C-C2C	3.00	109.59	106.35
78	C1	602	HEA	CHA-C4D-C3D	-3.00	120.43	124.84
82	QC	401	HEM	CHA-C4D-ND	2.99	128.07	124.38
82	QC	402	HEM	C1B-NB-C4B	2.99	108.16	105.07
78	C1	602	HEA	C13-C14-C15	-2.98	120.50	127.66
82	Qc	403	HEM	CHA-C4D-ND	2.96	128.04	124.38
78	C1	603	HEA	C27-C19-C20	2.91	120.17	115.27
76	AK	401	ADP	C3'-C2'-C1'	2.84	105.26	100.98
82	QC	402	HEM	CHD-C1D-ND	2.83	127.50	124.43
76	AK	401	ADP	C4-C5-N7	-2.81	106.47	109.40
83	Qd	401	HEC	O1D-CGD-CBD	-2.78	114.14	123.08
83	QD	401	HEC	O1D-CGD-CBD	-2.77	114.18	123.08
81	Qe	302	PEE	C17-C18-C19	-2.77	109.07	131.07
82	QC	401	HEM	CHD-C1D-ND	2.75	127.42	124.43
81	Qe	302	PEE	O3-C30-C31	2.73	120.48	111.91
81	Qc	401	PEE	O3-C30-C31	2.73	120.47	111.91
81	N5	704	PEE	O3-C30-C31	2.71	120.42	111.91
83	QD	401	HEC	CBA-CAA-C2A	2.71	117.17	112.60
82	Qc	402	HEM	CHD-C1D-ND	2.71	127.37	124.43
81	N5	701	PEE	O3-C30-C31	2.69	120.35	111.91
78	C1	603	HEA	C13-C14-C15	-2.68	121.21	127.66
81	S8	303	PEE	O3-C30-C31	2.67	120.30	111.91
78	C1	603	HEA	CHB-C1B-NB	2.65	127.31	124.43
81	QC	403	PEE	O3-C30-C31	2.64	120.18	111.91
78	C1	602	HEA	C17-C18-C19	-2.63	121.32	127.66
81	QE	302	PEE	O3-C30-C31	2.63	120.15	111.91
78	C1	603	HEA	C1B-C2B-C3B	-2.61	103.68	106.80
78	C1	603	HEA	C17-C18-C19	-2.60	121.41	127.66
81	N4	501	PEE	O3-C30-C31	2.60	120.05	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	Qc	403	HEM	CHD-C1D-ND	2.59	127.25	124.43
81	S2	501	PEE	O3-C30-C31	2.59	120.03	111.91
78	C1	602	HEA	CBA-CAA-C2A	-2.58	108.25	112.60
81	N6	201	PEE	O3-C30-C31	2.58	119.99	111.91
83	QD	401	HEC	CMC-C2C-C1C	-2.55	124.55	128.46
82	QC	402	HEM	CHA-C4D-ND	2.53	127.50	124.38
81	N3	201	PEE	O3-C30-C31	2.51	119.78	111.91
83	Qd	401	HEC	CMC-C2C-C1C	-2.50	124.62	128.46
78	C1	603	HEA	C1D-ND-C4D	-2.48	102.52	105.07
78	C1	603	HEA	CHC-C4B-NB	-2.47	121.33	124.38
78	C1	602	HEA	CMB-C2B-C1B	-2.45	121.30	125.04
83	Qd	401	HEC	CMA-C3A-C2A	2.45	129.57	124.94
78	C1	603	HEA	CMB-C2B-C3B	2.45	135.01	130.34
78	C1	603	HEA	CMB-C2B-C1B	-2.45	121.31	125.04
78	C1	602	HEA	C1B-C2B-C3B	-2.38	103.95	106.80
83	QD	401	HEC	O1A-CGA-CBA	-2.37	115.45	123.08
78	C1	603	HEA	C4D-C3D-C2D	-2.37	103.44	106.90
78	C1	603	HEA	O1D-CGD-CBD	-2.36	115.49	123.08
83	QD	401	HEC	CMD-C2D-C3D	2.34	129.35	124.94
82	QC	402	HEM	CHB-C1B-C2B	-2.33	120.28	126.72
78	C1	602	HEA	CMB-C2B-C3B	2.31	134.74	130.34
82	QC	401	HEM	CHB-C1B-C2B	-2.31	120.34	126.72
78	C1	602	HEA	O1D-CGD-CBD	-2.30	115.68	123.08
74	A9	401	NDP	C5A-C6A-N6A	2.30	123.85	120.35
83	Qd	401	HEC	CMD-C2D-C3D	2.30	129.28	124.94
82	Qc	403	HEM	CAD-CBD-CGD	-2.29	108.68	113.60
72	N4	502	PLX	O3-P1-O2	-2.28	100.99	112.24
83	QD	401	HEC	CMA-C3A-C2A	2.27	129.21	124.94
72	N2	401	PLX	O3-P1-O2	-2.25	101.09	112.24
78	C1	602	HEA	CHC-C4B-NB	-2.25	121.61	124.38
72	6C	101	PLX	O3-P1-O2	-2.24	101.19	112.24
78	C1	603	HEA	C26-C15-C14	-2.23	117.97	123.68
82	Qc	403	HEM	CHB-C1B-C2B	-2.22	120.58	126.72
78	C1	602	HEA	C26-C15-C16	2.22	119.00	115.27
82	Qc	402	HEM	CHB-C1B-C2B	-2.22	120.59	126.72
72	AM	201	PLX	O3-P1-O2	-2.21	101.33	112.24
72	QE	301	PLX	O3-P1-O2	-2.21	101.33	112.24
72	B5	201	PLX	O3-P1-O2	-2.20	101.35	112.24
83	Qd	401	HEC	O2A-CGA-O1A	2.20	128.78	123.30
72	QI	301	PLX	O3-P1-O2	-2.19	101.41	112.24
78	C1	602	HEA	C27-C19-C18	-2.18	118.08	123.68
78	C1	602	HEA	CHD-C1D-C2D	-2.18	120.69	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	Qd	401	HEC	O1A-CGA-CBA	-2.15	116.18	123.08
82	QC	401	HEM	CAD-CBD-CGD	-2.15	108.98	113.60
83	QD	401	HEC	O2A-CGA-O1A	2.15	128.65	123.30
78	C1	602	HEA	CHB-C1B-NB	2.13	126.75	124.43
83	QD	401	HEC	C1D-C2D-C3D	2.12	108.47	107.00
81	Qc	401	PEE	C17-C18-C19	-2.10	108.63	124.73
83	QD	401	HEC	C2B-C3B-C4B	2.08	108.59	106.35
82	QC	401	HEM	CBA-CAA-C2A	-2.06	109.10	112.62
81	S8	303	PEE	C17-C18-C19	-2.05	109.02	124.73
78	C1	603	HEA	C27-C19-C18	-2.04	118.44	123.68
83	Qd	401	HEC	C2B-C3B-C4B	2.04	108.55	106.35
81	S2	501	PEE	C37-C38-C39	-2.04	109.10	124.73
82	Qc	402	HEM	CBA-CAA-C2A	-2.04	109.15	112.62
81	N4	501	PEE	C37-C38-C39	-2.03	109.13	124.73
81	QC	403	PEE	C20-C19-C18	-2.03	109.18	124.73
81	QE	302	PEE	C37-C38-C39	-2.03	109.18	124.73
78	C1	603	HEA	OMA-CMA-C3A	-2.02	120.52	124.91
78	C1	603	HEA	O1A-CGA-CBA	-2.01	116.61	123.08
81	N5	701	PEE	C20-C19-C18	-2.01	109.27	124.73
81	Qe	302	PEE	C20-C19-C18	-2.01	109.80	126.37
81	N5	701	PEE	C40-C39-C38	-2.00	109.35	124.73
81	N5	701	PEE	C17-C18-C19	-2.00	109.35	124.73

There are no chirality outliers.

All (1066) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
71	6A	101	PC1	C11-O13-P-O12
71	6A	101	PC1	C1-O11-P-O13
71	6A	101	PC1	C12-C11-O13-P
71	B4	202	PC1	C1-O11-P-O14
71	B5	203	PC1	C11-O13-P-O12
71	B5	203	PC1	C11-O13-P-O14
71	B5	203	PC1	C11-O13-P-O11
71	C3	301	PC1	C1-O11-P-O12
71	C3	301	PC1	C2-C1-O11-P
71	C3	301	PC1	O21-C2-C3-O31
71	C3	302	PC1	C11-O13-P-O12
71	C3	302	PC1	C11-O13-P-O14
71	CB	202	PC1	C1-O11-P-O14
71	N1	402	PC1	C11-O13-P-O12
71	N1	402	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
71	N4	503	PC1	C11-O13-P-O12
71	N4	503	PC1	C11-O13-P-O14
71	N4	503	PC1	C11-O13-P-O11
71	N4	503	PC1	C1-O11-P-O12
71	N4	503	PC1	C1-O11-P-O14
71	N4	503	PC1	C1-O11-P-O13
71	QB	502	PC1	C11-O13-P-O12
71	QB	502	PC1	C1-O11-P-O12
71	QB	502	PC1	C1-O11-P-O14
71	QB	503	PC1	C11-O13-P-O12
71	QB	503	PC1	C11-O13-P-O14
71	Qb	502	PC1	O13-C11-C12-N
71	Qc	405	PC1	C11-O13-P-O12
71	Qc	405	PC1	C1-O11-P-O14
71	Qh	102	PC1	C11-O13-P-O12
71	Qh	102	PC1	C11-O13-P-O14
71	Qh	102	PC1	C11-O13-P-O11
71	Qh	102	PC1	C1-O11-P-O12
71	Qh	102	PC1	C1-O11-P-O14
71	Qj	101	PC1	C11-O13-P-O12
71	Qj	101	PC1	C11-O13-P-O14
71	Qj	101	PC1	C1-O11-P-O12
71	Qj	101	PC1	C1-O11-P-O14
71	Qj	101	PC1	C1-O11-P-O13
72	6C	101	PLX	C2-O1-P1-O2
72	6C	101	PLX	O9-C24-O8-C5
72	6C	101	PLX	O9-C24-C25-C26
72	AM	201	PLX	O7-C6-O6-C4
72	AM	201	PLX	C3-O4-P1-O3
72	AM	201	PLX	C2-O1-P1-O3
72	B5	201	PLX	O7-C6-O6-C4
72	N2	401	PLX	O7-C6-C7-C8
72	N2	401	PLX	O7-C6-O6-C4
72	N2	401	PLX	C3-O4-P1-O2
72	N2	401	PLX	C3-O4-P1-O3
72	N2	401	PLX	O9-C24-C25-C26
72	N4	502	PLX	O7-C6-O6-C4
72	N4	502	PLX	C3-O4-P1-O2
72	N4	502	PLX	C25-C24-O8-C5
72	N4	502	PLX	O9-C24-C25-C26
72	QE	301	PLX	O7-C6-C7-C8
72	QE	301	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
72	QE	301	PLX	O9-C24-C25-C26
72	QI	301	PLX	O7-C6-C7-C8
72	QI	301	PLX	C3-O4-P1-O2
72	QI	301	PLX	C2-O1-P1-O2
72	QI	301	PLX	C2-O1-P1-O3
72	QI	301	PLX	N1-C1-C2-O1
72	QI	301	PLX	C25-C24-O8-C5
72	QI	301	PLX	O9-C24-C25-C26
73	A8	301	CDL	CA2-OA2-PA1-OA3
73	A8	301	CDL	CA3-OA5-PA1-OA3
73	A8	301	CDL	CA3-OA5-PA1-OA4
73	A8	301	CDL	CB2-OB2-PB2-OB3
73	A8	301	CDL	CB2-OB2-PB2-OB4
73	A8	301	CDL	CB3-OB5-PB2-OB3
73	AL	201	CDL	CB2-OB2-PB2-OB3
73	AL	201	CDL	CB2-OB2-PB2-OB4
73	AL	201	CDL	CB2-OB2-PB2-OB5
73	AL	201	CDL	CB3-OB5-PB2-OB3
73	AL	201	CDL	CB3-OB5-PB2-OB4
73	AL	202	CDL	CA2-OA2-PA1-OA3
73	AL	202	CDL	CB2-OB2-PB2-OB3
73	AL	202	CDL	CB2-OB2-PB2-OB4
73	B4	201	CDL	CA2-OA2-PA1-OA3
73	B4	201	CDL	CA2-OA2-PA1-OA4
73	B4	201	CDL	CA2-OA2-PA1-OA5
73	B4	201	CDL	CB2-OB2-PB2-OB4
73	B5	202	CDL	CA2-OA2-PA1-OA3
73	B5	202	CDL	CA3-OA5-PA1-OA3
73	B5	202	CDL	CA3-OA5-PA1-OA4
73	B5	202	CDL	CB3-OB5-PB2-OB3
73	B5	202	CDL	CB3-OB5-PB2-OB4
73	CB	203	CDL	CA3-OA5-PA1-OA3
73	CB	203	CDL	CB2-OB2-PB2-OB3
73	CB	203	CDL	CB2-OB2-PB2-OB4
73	CB	203	CDL	CB3-OB5-PB2-OB2
73	CB	203	CDL	CB3-OB5-PB2-OB3
73	N1	401	CDL	CB2-OB2-PB2-OB3
73	N2	402	CDL	CA2-OA2-PA1-OA3
73	N2	402	CDL	CA2-OA2-PA1-OA4
73	N2	402	CDL	CA2-OA2-PA1-OA5
73	N2	402	CDL	CB2-OB2-PB2-OB4
73	N5	702	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
73	N5	702	CDL	CA3-OA5-PA1-OA3
73	N5	702	CDL	CB3-OB5-PB2-OB2
73	N5	702	CDL	CB3-OB5-PB2-OB3
73	N5	702	CDL	CB3-OB5-PB2-OB4
73	QB	501	CDL	CA3-OA5-PA1-OA2
73	QB	501	CDL	CA3-OA5-PA1-OA3
73	QB	501	CDL	CA3-OA5-PA1-OA4
73	QH	101	CDL	CB3-OB5-PB2-OB4
73	QH	102	CDL	O1-C1-CA2-OA2
73	QH	102	CDL	CB2-OB2-PB2-OB3
73	QH	102	CDL	OB5-CB3-CB4-OB6
73	Qb	501	CDL	CA2-OA2-PA1-OA3
73	Qb	501	CDL	CA3-OA5-PA1-OA3
73	Qb	501	CDL	CB2-OB2-PB2-OB4
73	Qb	501	CDL	OB5-CB3-CB4-OB6
73	Qh	101	CDL	CB2-OB2-PB2-OB3
74	A9	401	NDP	C2B-O2B-P2B-O3X
75	AB	201	ZMP	C17-C18-C21-O5
75	AB	201	ZMP	C16-C17-C18-C21
75	AB	201	ZMP	C16-C17-C18-C19
75	AB	201	ZMP	C16-C17-C18-C20
75	AB	201	ZMP	C12-C11-S1-C10
75	AB	201	ZMP	O1-C10-S1-C11
75	AB	201	ZMP	C9-C10-S1-C11
75	AC	201	ZMP	C9-C10-S1-C11
75	AC	201	ZMP	S1-C10-C9-C8
75	AC	201	ZMP	O1-C10-C9-C8
75	AC	201	ZMP	C7-C8-C9-C10
77	B8	201	3PE	C1-O11-P-O13
77	B8	201	3PE	C1-O11-P-O14
77	B8	201	3PE	O13-C11-C12-N
77	C1	601	3PE	C11-O13-P-O11
77	C1	601	3PE	C11-O13-P-O12
77	C1	601	3PE	C11-O13-P-O14
77	C1	601	3PE	O13-C11-C12-N
77	CB	201	3PE	C1-O11-P-O14
77	CB	201	3PE	O13-C11-C12-N
77	N5	705	3PE	C1-O11-P-O14
77	N5	705	3PE	C11-O13-P-O12
77	N5	705	3PE	C11-O13-P-O14
77	QE	303	3PE	C1-O11-P-O12
77	QE	303	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
78	C1	602	HEA	C1A-C2A-CAA-CBA
78	C1	602	HEA	C3A-C2A-CAA-CBA
78	C1	603	HEA	C1A-C2A-CAA-CBA
78	C1	603	HEA	C3A-C2A-CAA-CBA
78	C1	603	HEA	C17-C18-C19-C20
78	C1	603	HEA	C18-C19-C20-C21
78	C1	603	HEA	C19-C20-C21-C22
81	N3	201	PEE	C1-O3P-P-O1P
81	N3	201	PEE	C5-C4-O4P-P
81	N3	201	PEE	O4P-C4-C5-N
81	N4	501	PEE	C4-O4P-P-O3P
81	N5	701	PEE	C4-O4P-P-O1P
81	N5	701	PEE	C37-C38-C39-C40
81	N5	704	PEE	C4-O4P-P-O2P
81	N5	704	PEE	C37-C38-C39-C40
81	QC	403	PEE	O2-C2-C3-O3
81	QC	403	PEE	C1-O3P-P-O2P
81	Qe	302	PEE	C17-C18-C19-C20
81	S2	501	PEE	C2-C1-O3P-P
81	S2	501	PEE	C1-O3P-P-O2P
81	S8	303	PEE	C4-O4P-P-O2P
81	S8	303	PEE	C4-O4P-P-O1P
82	QC	401	HEM	C2B-C3B-CAB-CBB
82	QC	401	HEM	C4B-C3B-CAB-CBB
82	QC	402	HEM	C2B-C3B-CAB-CBB
82	QC	402	HEM	C4B-C3B-CAB-CBB
82	Qc	402	HEM	C2B-C3B-CAB-CBB
82	Qc	402	HEM	C4B-C3B-CAB-CBB
82	Qc	403	HEM	C1A-C2A-CAA-CBA
82	Qc	403	HEM	C3A-C2A-CAA-CBA
82	Qc	403	HEM	C2B-C3B-CAB-CBB
82	Qc	403	HEM	C4B-C3B-CAB-CBB
86	V1	502	FMN	N10-C1'-C2'-O2'
86	V1	502	FMN	N10-C1'-C2'-C3'
86	V1	502	FMN	C5'-O5'-P-O1P
86	V1	502	FMN	C5'-O5'-P-O2P
86	V1	502	FMN	C5'-O5'-P-O3P
81	Qe	302	PEE	O5-C30-O3-C3
81	Qe	302	PEE	C31-C30-O3-C3
81	N3	201	PEE	O5-C30-O3-C3
81	N4	501	PEE	O5-C30-O3-C3
81	Qc	401	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
81	S8	303	PEE	O4-C10-O2-C2
81	N3	201	PEE	C31-C30-O3-C3
81	N4	501	PEE	C31-C30-O3-C3
81	Qc	401	PEE	C31-C30-O3-C3
81	S8	303	PEE	C11-C10-O2-C2
78	C1	602	HEA	C27-C19-C20-C21
78	C1	603	HEA	C27-C19-C20-C21
81	N3	201	PEE	C17-C18-C19-C20
81	N4	501	PEE	C37-C38-C39-C40
78	C1	602	HEA	C17-C18-C19-C27
78	C1	603	HEA	C17-C18-C19-C27
78	C1	602	HEA	C17-C18-C19-C20
75	AC	201	ZMP	C3-C4-C5-C6
81	Qe	302	PEE	C12-C13-C14-C15
73	B5	202	CDL	CB2-C1-CA2-OA2
81	N5	704	PEE	O5-C30-O3-C3
71	B4	202	PC1	C11-C12-N-C14
81	N5	704	PEE	C31-C30-O3-C3
72	B5	201	PLX	C14-C15-C16-C17
73	B5	202	CDL	O1-C1-CA2-OA2
73	QB	501	CDL	O1-C1-CA2-OA2
81	QC	403	PEE	C11-C12-C13-C14
81	N4	501	PEE	C10-C11-C12-C13
81	N3	201	PEE	C37-C38-C39-C40
81	N5	704	PEE	C17-C18-C19-C20
81	Qc	401	PEE	C11-C12-C13-C14
73	B4	201	CDL	CB5-C51-C52-C53
81	N3	201	PEE	C30-C31-C32-C33
81	Qc	401	PEE	C10-C11-C12-C13
81	Qc	401	PEE	C30-C31-C32-C33
71	B4	202	PC1	C11-C12-N-C15
71	N4	503	PC1	C11-C12-N-C15
71	Qb	502	PC1	C11-C12-N-C15
81	N6	201	PEE	C30-C31-C32-C33
81	S2	501	PEE	C17-C18-C19-C20
81	S8	303	PEE	C37-C38-C39-C40
71	6A	101	PC1	C11-O13-P-O11
71	B4	202	PC1	C1-O11-P-O13
71	C3	301	PC1	C1-O11-P-O13
71	C3	302	PC1	C11-O13-P-O11
71	CB	202	PC1	C1-O11-P-O13
71	N1	402	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
71	QB	502	PC1	C11-O13-P-O11
71	QB	502	PC1	C1-O11-P-O13
71	QB	503	PC1	C11-O13-P-O11
71	QB	503	PC1	C1-O11-P-O13
71	Qc	404	PC1	C11-O13-P-O11
71	Qc	405	PC1	C11-O13-P-O11
71	Qh	102	PC1	C1-O11-P-O13
71	Qj	101	PC1	C11-O13-P-O11
71	S7	302	PC1	C1-O11-P-O13
72	6C	101	PLX	C2-O1-P1-O4
72	AM	201	PLX	C3-O4-P1-O1
72	AM	201	PLX	C2-O1-P1-O4
72	B5	201	PLX	C2-O1-P1-O4
72	N2	401	PLX	C3-O4-P1-O1
72	N2	401	PLX	C2-O1-P1-O4
72	QI	301	PLX	C3-O4-P1-O1
73	A8	301	CDL	CA3-OA5-PA1-OA2
73	A8	301	CDL	CB2-OB2-PB2-OB5
73	A8	301	CDL	CB3-OB5-PB2-OB2
73	AL	201	CDL	CA2-OA2-PA1-OA5
73	AL	201	CDL	CB3-OB5-PB2-OB2
73	AL	202	CDL	CA2-OA2-PA1-OA5
73	AL	202	CDL	CA3-OA5-PA1-OA2
73	AL	202	CDL	CB2-OB2-PB2-OB5
73	B5	202	CDL	CA2-OA2-PA1-OA5
73	B5	202	CDL	CA3-OA5-PA1-OA2
73	B5	202	CDL	CB3-OB5-PB2-OB2
73	CB	203	CDL	CB2-OB2-PB2-OB5
73	N1	401	CDL	CA3-OA5-PA1-OA2
73	N1	401	CDL	CB2-OB2-PB2-OB5
73	N2	402	CDL	CA3-OA5-PA1-OA2
73	N5	702	CDL	CA2-OA2-PA1-OA5
73	N5	702	CDL	CA3-OA5-PA1-OA2
73	N5	703	CDL	CB2-OB2-PB2-OB5
73	N5	703	CDL	CB3-OB5-PB2-OB2
73	QD	402	CDL	CA2-OA2-PA1-OA5
73	QD	402	CDL	CB3-OB5-PB2-OB2
73	QH	102	CDL	CA3-OA5-PA1-OA2
73	Qb	501	CDL	CA2-OA2-PA1-OA5
73	Qb	501	CDL	CB2-OB2-PB2-OB5
73	Qb	501	CDL	CB3-OB5-PB2-OB2
77	C1	601	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
77	CB	201	3PE	C11-O13-P-O11
77	N5	705	3PE	C1-O11-P-O13
77	N5	705	3PE	C11-O13-P-O11
77	QE	303	3PE	C1-O11-P-O13
81	N5	704	PEE	C4-O4P-P-O3P
81	N6	201	PEE	C4-O4P-P-O3P
81	QC	403	PEE	C1-O3P-P-O4P
81	S2	501	PEE	C1-O3P-P-O4P
81	S2	501	PEE	C4-O4P-P-O3P
81	S8	303	PEE	C4-O4P-P-O3P
73	A8	301	CDL	CB7-C71-C72-C73
73	QH	102	CDL	CB2-C1-CA2-OA2
77	CB	201	3PE	C23-C24-C25-C26
71	Qj	101	PC1	C11-C12-N-C15
72	QI	301	PLX	O6-C6-C7-C8
81	QE	302	PEE	C11-C12-C13-C14
81	Qc	401	PEE	C11-C10-O2-C2
71	S7	302	PC1	C27-C28-C29-C2A
72	QI	301	PLX	C30-C31-C32-C33
75	AC	201	ZMP	C1-C22-C23-C24
75	AB	201	ZMP	C20-C18-C21-O5
72	QE	301	PLX	C26-C27-C28-C29
73	N1	401	CDL	C12-C13-C14-C15
81	N3	201	PEE	C34-C35-C36-C37
81	N6	201	PEE	C22-C23-C24-C25
81	N6	201	PEE	C33-C34-C35-C36
81	Qc	401	PEE	O4-C10-O2-C2
71	N4	504	PC1	C29-C2A-C2B-C2C
72	B5	201	PLX	C30-C31-C32-C33
81	S8	303	PEE	C22-C23-C24-C25
81	S8	303	PEE	C12-C13-C14-C15
71	C3	302	PC1	C2-C1-O11-P
81	QE	302	PEE	C17-C18-C19-C20
81	N3	201	PEE	C14-C15-C16-C17
81	N6	201	PEE	C34-C35-C36-C37
81	QE	302	PEE	C33-C34-C35-C36
73	N5	702	CDL	O1-C1-CA2-OA2
72	AM	201	PLX	C31-C32-C33-C34
81	N6	201	PEE	C21-C22-C23-C24
71	N1	402	PC1	C31-C32-C33-C34
72	N2	401	PLX	C32-C33-C34-C35
72	B5	201	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
81	Qe	302	PEE	C14-C15-C16-C17
71	Qc	405	PC1	C36-C37-C38-C39
71	Qh	102	PC1	C3A-C3B-C3C-C3D
81	N3	201	PEE	C12-C13-C14-C15
81	Qe	302	PEE	C11-C12-C13-C14
81	Qe	302	PEE	C32-C33-C34-C35
81	S8	303	PEE	C13-C14-C15-C16
73	AL	202	CDL	C16-C17-C18-C19
81	N3	201	PEE	C11-C12-C13-C14
73	N5	703	CDL	C39-C40-C41-C42
81	N3	201	PEE	C33-C34-C35-C36
81	N4	501	PEE	C35-C36-C37-C38
71	N4	504	PC1	C3C-C3D-C3E-C3F
73	AL	202	CDL	C12-C13-C14-C15
81	N4	501	PEE	C14-C15-C16-C17
72	N2	401	PLX	C16-C17-C18-C19
72	N4	502	PLX	C30-C31-C32-C33
81	N5	704	PEE	C12-C13-C14-C15
81	S2	501	PEE	O4P-C4-C5-N
71	C3	302	PC1	C3C-C3D-C3E-C3F
75	AB	201	ZMP	C22-C1-C2-C3
75	AC	201	ZMP	C6-C7-C8-C9
77	C1	601	3PE	C25-C26-C27-C28
72	N2	401	PLX	C31-C32-C33-C34
72	N4	502	PLX	C31-C32-C33-C34
81	N6	201	PEE	C40-C41-C42-C43
77	CB	201	3PE	C36-C37-C38-C39
77	N5	705	3PE	C26-C27-C28-C29
81	S8	303	PEE	C33-C34-C35-C36
81	N5	704	PEE	C30-C31-C32-C33
72	AM	201	PLX	O7-C6-C7-C8
72	AM	201	PLX	O9-C24-C25-C26
72	B5	201	PLX	O9-C24-C25-C26
81	S2	501	PEE	C14-C15-C16-C17
81	N6	201	PEE	C35-C36-C37-C38
81	N5	701	PEE	C11-C12-C13-C14
81	Qe	302	PEE	C13-C14-C15-C16
81	S8	303	PEE	C42-C43-C44-C45
81	N5	701	PEE	C14-C15-C16-C17
71	N4	503	PC1	C2-C1-O11-P
71	B4	202	PC1	C11-C12-N-C13
71	N1	402	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
71	QB	502	PC1	C11-C12-N-C14
71	Qc	404	PC1	C2E-C2F-C2G-C2H
81	QC	403	PEE	C14-C15-C16-C17
81	S2	501	PEE	C31-C30-O3-C3
82	QC	401	HEM	C3D-CAD-CBD-CGD
73	N5	703	CDL	C18-C19-C20-C21
73	Qb	501	CDL	CA5-C11-C12-C13
81	QC	403	PEE	C10-C11-C12-C13
81	N5	701	PEE	C17-C18-C19-C20
81	S2	501	PEE	C38-C39-C40-C41
81	N3	201	PEE	C35-C36-C37-C38
81	N5	704	PEE	C35-C36-C37-C38
75	AB	201	ZMP	C3-C4-C5-C6
81	N6	201	PEE	C12-C13-C14-C15
71	C3	302	PC1	C38-C39-C3A-C3B
71	N4	503	PC1	C35-C36-C37-C38
72	QE	301	PLX	C29-C30-C31-C32
71	C3	302	PC1	C31-C32-C33-C34
81	S2	501	PEE	C10-C11-C12-C13
71	QB	503	PC1	C34-C35-C36-C37
81	Qc	401	PEE	C22-C23-C24-C25
81	S2	501	PEE	C11-C12-C13-C14
81	N4	501	PEE	C11-C10-O2-C2
81	N5	704	PEE	C11-C10-O2-C2
72	QI	301	PLX	O4-C3-C4-O6
81	N4	501	PEE	O3P-C1-C2-O2
72	AM	201	PLX	C27-C28-C29-C30
75	AC	201	ZMP	C4-C5-C6-C7
81	S8	303	PEE	C21-C22-C23-C24
81	N4	501	PEE	O4-C10-O2-C2
81	N5	704	PEE	O4-C10-O2-C2
81	N5	704	PEE	C10-C11-C12-C13
71	Qc	404	PC1	C3B-C3C-C3D-C3E
75	AB	201	ZMP	C1-C22-C23-C24
72	AM	201	PLX	O6-C4-C5-O8
71	Qb	502	PC1	C11-C12-N-C14
71	Qj	101	PC1	C11-C12-N-C13
71	Qj	101	PC1	C11-C12-N-C14
81	QC	403	PEE	C22-C23-C24-C25
81	QE	302	PEE	C14-C15-C16-C17
81	N5	701	PEE	C35-C36-C37-C38
81	Qe	302	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
81	Qc	401	PEE	C31-C32-C33-C34
75	AB	201	ZMP	C5-C6-C7-C8
72	QE	301	PLX	C25-C26-C27-C28
71	N4	503	PC1	C21-C22-C23-C24
72	AM	201	PLX	C11-C10-C9-C8
81	S2	501	PEE	O5-C30-O3-C3
81	QC	403	PEE	C16-C17-C18-C19
72	QI	301	PLX	C2-O1-P1-O4
73	N5	703	CDL	CA3-OA5-PA1-OA2
73	QB	501	CDL	CA2-OA2-PA1-OA5
73	QH	101	CDL	CA2-OA2-PA1-OA5
73	QH	101	CDL	CB3-OB5-PB2-OB2
73	QH	102	CDL	CB3-OB5-PB2-OB2
73	Qb	501	CDL	CA3-OA5-PA1-OA2
73	Qh	101	CDL	CB2-OB2-PB2-OB5
81	N3	201	PEE	C1-O3P-P-O4P
73	N5	703	CDL	C60-C61-C62-C63
71	Qj	101	PC1	C22-C23-C24-C25
71	N4	503	PC1	O11-C1-C2-C3
73	N5	703	CDL	OB5-CB3-CB4-CB6
73	QH	102	CDL	OB5-CB3-CB4-CB6
71	Qc	405	PC1	C37-C38-C39-C3A
75	AB	201	ZMP	C6-C7-C8-C9
75	AB	201	ZMP	C2-C3-C4-C5
72	N2	401	PLX	C34-C35-C36-C37
72	QI	301	PLX	C9-C10-C11-C12
77	N5	705	3PE	C21-C22-C23-C24
77	CB	201	3PE	C38-C39-C3A-C3B
81	N4	501	PEE	C12-C13-C14-C15
72	N2	401	PLX	C14-C15-C16-C17
81	Qe	302	PEE	C38-C39-C40-C41
71	N4	503	PC1	C11-C12-N-C13
71	N4	503	PC1	C11-C12-N-C14
71	Qb	502	PC1	C11-C12-N-C13
71	C3	301	PC1	C1-C2-C3-O31
71	Qj	101	PC1	C1-C2-C3-O31
72	6C	101	PLX	C3-C4-C5-O8
72	QE	301	PLX	C3-C4-C5-O8
73	N2	402	CDL	C36-C37-C38-C39
73	QH	102	CDL	CA3-CA4-CA6-OA8
77	CB	201	3PE	C1-C2-C3-O31
81	N3	201	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
81	N4	501	PEE	C1-C2-C3-O3
81	N5	701	PEE	C1-C2-C3-O3
72	QI	301	PLX	C33-C34-C35-C36
81	N5	704	PEE	C11-C12-C13-C14
75	AC	201	ZMP	O3-C16-C17-O4
78	C1	602	HEA	C19-C20-C21-C22
73	B5	202	CDL	C63-C64-C65-C66
81	QE	302	PEE	C21-C22-C23-C24
81	QE	302	PEE	C35-C36-C37-C38
81	Qe	302	PEE	C39-C40-C41-C42
81	S2	501	PEE	C35-C36-C37-C38
81	S8	303	PEE	C15-C16-C17-C18
81	S8	303	PEE	C35-C36-C37-C38
72	QI	301	PLX	C7-C8-C9-C10
73	B5	202	CDL	C21-C22-C23-C24
81	N4	501	PEE	C21-C22-C23-C24
75	AB	201	ZMP	C19-C18-C21-O5
81	N3	201	PEE	C10-C11-C12-C13
72	QE	301	PLX	C12-C13-C14-C15
72	B5	201	PLX	C18-C19-C20-C21
81	QE	302	PEE	C22-C23-C24-C25
81	Qc	401	PEE	C33-C34-C35-C36
73	CB	203	CDL	OB5-CB3-CB4-OB6
71	N1	402	PC1	C11-C12-N-C14
71	QB	502	PC1	C11-C12-N-C15
71	Qc	405	PC1	C21-C22-C23-C24
81	Qc	401	PEE	C13-C14-C15-C16
73	QH	101	CDL	OA6-CA4-CA6-OA8
73	A8	301	CDL	C11-C12-C13-C14
73	A8	301	CDL	C31-C32-C33-C34
75	AC	201	ZMP	C1-C2-C3-C4
81	QE	302	PEE	C32-C33-C34-C35
72	N2	401	PLX	C18-C19-C20-C21
81	N3	201	PEE	C11-C10-O2-C2
81	Qe	302	PEE	C11-C10-O2-C2
77	C1	601	3PE	C2C-C2D-C2E-C2F
81	N5	704	PEE	C18-C19-C20-C21
71	QB	502	PC1	O11-C1-C2-C3
72	QI	301	PLX	O4-C3-C4-C5
73	B5	202	CDL	OB5-CB3-CB4-CB6
73	Qb	501	CDL	OB5-CB3-CB4-CB6
81	N4	501	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
81	QC	403	PEE	O3P-C1-C2-C3
81	QE	302	PEE	O3P-C1-C2-C3
73	AL	202	CDL	C41-C42-C43-C44
81	N4	501	PEE	O4P-C4-C5-N
81	Qc	401	PEE	O4P-C4-C5-N
73	N1	401	CDL	C76-C77-C78-C79
73	CB	203	CDL	C81-C82-C83-C84
81	S2	501	PEE	C12-C13-C14-C15
71	Qb	502	PC1	O21-C21-C22-C23
81	N6	201	PEE	C10-C11-C12-C13
81	N4	501	PEE	C2-C1-O3P-P
75	AC	201	ZMP	S1-C11-C12-N1
82	Qc	402	HEM	C3D-CAD-CBD-CGD
75	AB	201	ZMP	C4-C5-C6-C7
71	N4	503	PC1	C1-C2-C3-O31
72	B5	201	PLX	C3-C4-C5-O8
72	N2	401	PLX	C3-C4-C5-O8
72	N4	502	PLX	C3-C4-C5-O8
72	N2	401	PLX	C17-C18-C19-C20
81	N6	201	PEE	C17-C18-C19-C20
75	AC	201	ZMP	C22-C23-C24-C25
81	N5	701	PEE	C23-C24-C25-C26
81	N5	701	PEE	C33-C34-C35-C36
75	AB	201	ZMP	N2-C16-C17-C18
73	Qb	501	CDL	C51-C52-C53-C54
71	N1	402	PC1	C1-O11-P-O13
72	B5	201	PLX	C3-C4-O6-C6
72	B5	201	PLX	C5-C4-O6-C6
72	N4	502	PLX	C5-C4-O6-C6
72	N4	502	PLX	C3-O4-P1-O1
73	N1	401	CDL	CA2-OA2-PA1-OA5
77	CB	201	3PE	C1-O11-P-O13
81	N5	701	PEE	C10-C11-C12-C13
71	6A	101	PC1	C33-C34-C35-C36
71	N1	402	PC1	C2A-C2B-C2C-C2D
81	N5	704	PEE	C33-C34-C35-C36
71	N4	503	PC1	O11-C1-C2-O21
71	Qc	404	PC1	O11-C1-C2-O21
72	N2	401	PLX	O4-C3-C4-O6
73	B5	202	CDL	OB5-CB3-CB4-OB6
73	N5	702	CDL	OB5-CB3-CB4-OB6
81	Qe	302	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
81	N5	701	PEE	C12-C13-C14-C15
81	Qe	302	PEE	C40-C41-C42-C43
77	QE	303	3PE	O21-C21-C22-C23
73	AL	201	CDL	C55-C56-C57-C58
81	S2	501	PEE	C44-C45-C46-C47
71	Qj	101	PC1	O21-C2-C3-O31
72	6C	101	PLX	O6-C4-C5-O8
72	N2	401	PLX	O6-C4-C5-O8
72	N4	502	PLX	O6-C4-C5-O8
73	B4	201	CDL	OB6-CB4-CB6-OB8
73	N5	703	CDL	OB6-CB4-CB6-OB8
73	QH	102	CDL	OA6-CA4-CA6-OA8
81	N4	501	PEE	O2-C2-C3-O3
81	N5	701	PEE	O2-C2-C3-O3
81	Qe	302	PEE	O2-C2-C3-O3
81	N5	701	PEE	C21-C22-C23-C24
81	S8	303	PEE	C11-C12-C13-C14
73	CB	203	CDL	C58-C59-C60-C61
81	N3	201	PEE	O4-C10-O2-C2
81	Qe	302	PEE	O4-C10-O2-C2
81	N3	201	PEE	C42-C43-C44-C45
77	QC	404	3PE	O31-C31-C32-C33
71	C3	302	PC1	C25-C26-C27-C28
71	N1	402	PC1	C27-C28-C29-C2A
72	QE	301	PLX	C7-C8-C9-C10
72	B5	201	PLX	C16-C17-C18-C19
73	N2	402	CDL	C1-CB2-OB2-PB2
73	Qh	101	CDL	CA4-CA3-OA5-PA1
72	N2	401	PLX	C2-C1-N1-C1C
81	N3	201	PEE	C22-C23-C24-C25
81	N3	201	PEE	C16-C17-C18-C19
71	Qc	404	PC1	C27-C28-C29-C2A
72	B5	201	PLX	C25-C26-C27-C28
75	AC	201	ZMP	O1-C10-S1-C11
81	N6	201	PEE	C32-C33-C34-C35
71	C3	302	PC1	O31-C31-C32-C33
73	AL	201	CDL	C75-C76-C77-C78
72	6C	101	PLX	O8-C24-C25-C26
72	AM	201	PLX	O6-C6-C7-C8
72	N2	401	PLX	O8-C24-C25-C26
72	QE	301	PLX	O6-C6-C7-C8
72	N2	401	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
81	Qc	401	PEE	C16-C17-C18-C19
81	QC	403	PEE	C19-C20-C21-C22
73	N5	703	CDL	C54-C55-C56-C57
75	AC	201	ZMP	C14-C15-N2-C16
75	AC	201	ZMP	N2-C16-C17-O4
72	N4	502	PLX	C18-C19-C20-C21
72	N2	401	PLX	C2-C1-N1-C1A
81	S8	303	PEE	C3-C2-O2-C10
72	N4	502	PLX	C12-C13-C14-C15
81	N4	501	PEE	C30-C31-C32-C33
73	QB	501	CDL	CB3-CB4-CB6-OB8
73	QH	101	CDL	CB3-CB4-CB6-OB8
81	N5	701	PEE	C2-C1-O3P-P
81	QE	302	PEE	C1-C2-C3-O3
81	S2	501	PEE	C1-C2-C3-O3
81	S8	303	PEE	C1-C2-C3-O3
72	6C	101	PLX	O4-C3-C4-O6
72	AM	201	PLX	O4-C3-C4-O6
73	QD	402	CDL	OB5-CB3-CB4-OB6
81	QC	403	PEE	O3P-C1-C2-O2
81	QE	302	PEE	O3P-C1-C2-O2
71	QB	502	PC1	C24-C25-C26-C27
72	N4	502	PLX	C24-C25-C26-C27
71	B4	202	PC1	C39-C3A-C3B-C3C
71	N4	503	PC1	O21-C2-C3-O31
72	B5	201	PLX	O6-C4-C5-O8
77	CB	201	3PE	O21-C2-C3-O31
81	N3	201	PEE	O2-C2-C3-O3
81	S2	501	PEE	O2-C2-C3-O3
78	C1	603	HEA	C20-C21-C22-C23
81	N5	704	PEE	C39-C40-C41-C42
73	CB	203	CDL	C75-C76-C77-C78
71	C3	302	PC1	C39-C3A-C3B-C3C
81	Qc	401	PEE	C32-C33-C34-C35
81	N5	701	PEE	C32-C33-C34-C35
74	A9	401	NDP	PN-O3-PA-O2A
72	N4	502	PLX	C27-C28-C29-C30
73	QD	402	CDL	C52-C51-CB5-OB6
77	C1	601	3PE	O31-C31-C32-C33
71	N4	503	PC1	C34-C35-C36-C37
71	Qc	405	PC1	C1-O11-P-O13
73	B4	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
73	QH	102	CDL	CB2-OB2-PB2-OB5
81	N5	701	PEE	C4-O4P-P-O3P
81	Qc	401	PEE	C1-O3P-P-O4P
73	CB	203	CDL	C60-C61-C62-C63
72	N4	502	PLX	C4-C3-O4-P1
73	AL	201	CDL	CA4-CA3-OA5-PA1
73	AL	201	CDL	CB4-CB3-OB5-PB2
73	N5	703	CDL	CA4-CA3-OA5-PA1
72	QE	301	PLX	C16-C17-C18-C19
71	6A	101	PC1	C1-O11-P-O12
71	B4	202	PC1	C1-O11-P-O12
71	CB	202	PC1	C1-O11-P-O12
71	QB	502	PC1	C11-O13-P-O14
71	QB	503	PC1	C1-O11-P-O12
71	QB	503	PC1	C1-O11-P-O14
71	Qc	404	PC1	C11-O13-P-O14
71	S7	302	PC1	C1-O11-P-O14
72	6C	101	PLX	C3-O4-P1-O2
72	AM	201	PLX	C3-O4-P1-O2
72	AM	201	PLX	C2-O1-P1-O2
72	B5	201	PLX	C2-O1-P1-O3
72	N2	401	PLX	C2-O1-P1-O3
72	QE	301	PLX	C3-O4-P1-O3
72	QI	301	PLX	C3-O4-P1-O3
73	A8	301	CDL	CB3-OB5-PB2-OB4
73	AL	201	CDL	CA2-OA2-PA1-OA3
73	AL	202	CDL	CA2-OA2-PA1-OA4
73	AL	202	CDL	CA3-OA5-PA1-OA3
73	AL	202	CDL	CA3-OA5-PA1-OA4
73	B4	201	CDL	CB2-OB2-PB2-OB3
73	B5	202	CDL	CA2-OA2-PA1-OA4
73	N1	401	CDL	CA3-OA5-PA1-OA3
73	N1	401	CDL	CB2-OB2-PB2-OB4
73	N2	402	CDL	CA3-OA5-PA1-OA3
73	N2	402	CDL	CA3-OA5-PA1-OA4
73	N5	702	CDL	CA2-OA2-PA1-OA3
73	N5	702	CDL	CA3-OA5-PA1-OA4
73	N5	703	CDL	CA3-OA5-PA1-OA4
73	N5	703	CDL	CB2-OB2-PB2-OB3
73	N5	703	CDL	CB3-OB5-PB2-OB3
73	N5	703	CDL	CB3-OB5-PB2-OB4
73	QD	402	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
73	QD	402	CDL	CB3-OB5-PB2-OB3
73	QH	101	CDL	CA2-OA2-PA1-OA4
73	QH	101	CDL	CB3-OB5-PB2-OB3
73	QH	102	CDL	CA3-OA5-PA1-OA3
73	QH	102	CDL	CB3-OB5-PB2-OB3
73	QH	102	CDL	CB3-OB5-PB2-OB4
73	Qb	501	CDL	CA2-OA2-PA1-OA4
73	Qb	501	CDL	CB3-OB5-PB2-OB3
73	Qb	501	CDL	CB3-OB5-PB2-OB4
77	C1	601	3PE	C1-O11-P-O14
77	CB	201	3PE	C11-O13-P-O14
77	N5	705	3PE	C1-O11-P-O12
81	N5	704	PEE	C1-O3P-P-O1P
81	N5	704	PEE	C4-O4P-P-O1P
81	N6	201	PEE	C4-O4P-P-O2P
81	N6	201	PEE	C4-O4P-P-O1P
81	S2	501	PEE	C4-O4P-P-O2P
81	S2	501	PEE	C4-O4P-P-O1P
71	Qc	404	PC1	O11-C1-C2-C3
72	6C	101	PLX	O4-C3-C4-C5
73	AL	202	CDL	OB5-CB3-CB4-CB6
73	CB	203	CDL	OB5-CB3-CB4-CB6
73	N2	402	CDL	OB5-CB3-CB4-CB6
73	N5	702	CDL	OB5-CB3-CB4-CB6
73	QD	402	CDL	OB5-CB3-CB4-CB6
73	QH	101	CDL	OB5-CB3-CB4-CB6
77	CB	201	3PE	O11-C1-C2-C3
73	Qb	501	CDL	C72-C71-CB7-OB8
71	B4	202	PC1	C25-C26-C27-C28
77	CB	201	3PE	C24-C25-C26-C27
71	CB	202	PC1	C12-C11-O13-P
71	QB	502	PC1	C12-C11-O13-P
71	S7	302	PC1	C12-C11-O13-P
72	6C	101	PLX	C1-C2-O1-P1
72	B5	201	PLX	C25-C24-O8-C5
81	N6	201	PEE	C5-C4-O4P-P
71	N4	503	PC1	C25-C26-C27-C28
71	B4	202	PC1	C34-C35-C36-C37
81	N4	501	PEE	C19-C20-C21-C22
81	N5	701	PEE	C19-C20-C21-C22
81	N5	701	PEE	C15-C16-C17-C18
81	N6	201	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
73	N5	702	CDL	CB2-C1-CA2-OA2
71	QB	502	PC1	O11-C1-C2-O21
73	AL	202	CDL	OB5-CB3-CB4-OB6
73	N2	402	CDL	OB5-CB3-CB4-OB6
73	N5	703	CDL	OB5-CB3-CB4-OB6
73	QH	101	CDL	OB5-CB3-CB4-OB6
71	Qh	102	PC1	C39-C3A-C3B-C3C
73	A8	301	CDL	C22-C23-C24-C25
77	C1	601	3PE	C23-C24-C25-C26
71	B5	203	PC1	C25-C26-C27-C28
71	N1	402	PC1	C11-C12-N-C15
71	QB	502	PC1	C11-C12-N-C13
81	N3	201	PEE	C20-C21-C22-C23
73	QB	501	CDL	CB5-C51-C52-C53
73	QD	402	CDL	CA7-C31-C32-C33
71	6A	101	PC1	O13-C11-C12-N
71	C3	301	PC1	O13-C11-C12-N
71	N4	503	PC1	O13-C11-C12-N
71	N4	504	PC1	O13-C11-C12-N
71	QB	503	PC1	O13-C11-C12-N
71	Qc	404	PC1	O13-C11-C12-N
71	Qc	405	PC1	O13-C11-C12-N
71	Qh	102	PC1	O13-C11-C12-N
71	S7	302	PC1	O13-C11-C12-N
72	AM	201	PLX	C3-C4-C5-O8
72	QE	301	PLX	N1-C1-C2-O1
73	N5	703	CDL	CB3-CB4-CB6-OB8
81	QC	403	PEE	C1-C2-C3-O3
81	Qc	401	PEE	O2-C2-C3-O3
73	QH	102	CDL	C32-C33-C34-C35
81	QE	302	PEE	C10-C11-C12-C13
72	QE	301	PLX	O8-C24-C25-C26
75	AB	201	ZMP	O3-C16-C17-O4
71	N4	503	PC1	O31-C31-C32-C33
77	B8	201	3PE	O21-C21-C22-C23
74	A9	401	NDP	O4D-C1D-N1N-C6N
72	N2	401	PLX	C2-C1-N1-C1B
81	S2	501	PEE	C11-C10-O2-C2
71	C3	301	PC1	C37-C38-C39-C3A
81	S2	501	PEE	C21-C22-C23-C24
73	AL	201	CDL	CA3-CA4-OA6-CA5
72	B5	201	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
81	S2	501	PEE	O4-C10-O2-C2
78	C1	602	HEA	C11-C12-C13-C14
73	N5	703	CDL	C53-C54-C55-C56
73	AL	202	CDL	C12-C11-CA5-OA6
72	QE	301	PLX	C17-C18-C19-C20
73	N1	401	CDL	C1-CB2-OB2-PB2
77	B8	201	3PE	C2-C1-O11-P
73	CB	203	CDL	C18-C19-C20-C21
73	N2	402	CDL	C34-C35-C36-C37
81	S8	303	PEE	C41-C42-C43-C44
77	CB	201	3PE	O11-C1-C2-O21
81	QE	302	PEE	C23-C24-C25-C26
73	N5	702	CDL	C20-C21-C22-C23
81	S8	303	PEE	C34-C35-C36-C37
73	N5	702	CDL	C60-C61-C62-C63
72	QE	301	PLX	O6-C4-C5-O8
73	QB	501	CDL	OB6-CB4-CB6-OB8
73	QH	101	CDL	OB6-CB4-CB6-OB8
71	N4	504	PC1	C11-O13-P-O11
71	Qc	404	PC1	C1-O11-P-O13
72	N4	502	PLX	C2-O1-P1-O4
73	CB	203	CDL	CA3-OA5-PA1-OA2
73	N1	401	CDL	CB3-OB5-PB2-OB2
73	QB	501	CDL	CB2-OB2-PB2-OB5
73	QH	102	CDL	CA2-OA2-PA1-OA5
77	QE	303	3PE	C11-O13-P-O11
81	N5	704	PEE	C1-O3P-P-O4P
81	N6	201	PEE	C1-O3P-P-O4P
81	QE	302	PEE	C1-O3P-P-O4P
81	Qe	302	PEE	C4-O4P-P-O3P
74	A9	401	NDP	C2D-C1D-N1N-C6N
75	AB	201	ZMP	O4-C17-C18-C19
73	Qb	501	CDL	CA7-C31-C32-C33
72	B5	201	PLX	C13-C14-C15-C16
81	S2	501	PEE	C42-C43-C44-C45
73	QH	101	CDL	CA3-CA4-CA6-OA8
81	Qc	401	PEE	C1-C2-C3-O3
71	S7	302	PC1	C2B-C2C-C2D-C2E
72	QI	301	PLX	C26-C27-C28-C29
81	Qe	302	PEE	C42-C43-C44-C45
71	B5	203	PC1	C21-C22-C23-C24
71	N4	504	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
71	S7	302	PC1	C2-C1-O11-P
73	N2	402	CDL	C1-CA2-OA2-PA1
73	N5	702	CDL	C1-CB2-OB2-PB2
86	V1	502	FMN	C4'-C5'-O5'-P
81	S2	501	PEE	C33-C34-C35-C36
81	N6	201	PEE	C18-C19-C20-C21
81	S8	303	PEE	C36-C37-C38-C39
72	AM	201	PLX	C6-C7-C8-C9
81	N5	704	PEE	C31-C32-C33-C34
77	C1	601	3PE	C3F-C3G-C3H-C3I
73	B5	202	CDL	C18-C19-C20-C21
81	Qc	401	PEE	C34-C35-C36-C37
81	S8	303	PEE	O4P-C4-C5-N
82	QC	401	HEM	CAD-CBD-CGD-O1D
71	B5	203	PC1	C31-C32-C33-C34
71	B5	203	PC1	C26-C27-C28-C29
81	N4	501	PEE	C39-C40-C41-C42
81	S2	501	PEE	C34-C35-C36-C37
73	QH	102	CDL	C12-C11-CA5-OA6
73	N5	703	CDL	C57-C58-C59-C60
82	Qc	402	HEM	CAA-CBA-CGA-O2A
82	Qc	403	HEM	CAA-CBA-CGA-O2A
72	AM	201	PLX	O8-C24-C25-C26
71	Qh	102	PC1	C3D-C3E-C3F-C3G
73	N5	702	CDL	C24-C25-C26-C27
73	QD	402	CDL	CA4-CA3-OA5-PA1
82	QC	402	HEM	CAA-CBA-CGA-O1A
82	Qc	402	HEM	CAD-CBD-CGD-O1D
73	B4	201	CDL	C52-C51-CB5-OB6
82	Qc	403	HEM	CAD-CBD-CGD-O2D
81	QC	403	PEE	C15-C16-C17-C18
77	N5	705	3PE	C37-C38-C39-C3A
71	Qc	405	PC1	C27-C28-C29-C2A
73	CB	203	CDL	C21-C22-C23-C24
82	Qc	403	HEM	CAA-CBA-CGA-O1A
73	Qb	501	CDL	C54-C55-C56-C57
81	Qc	401	PEE	C35-C36-C37-C38
71	B5	203	PC1	C1-C2-C3-O31
73	B4	201	CDL	CA3-CA4-CA6-OA8
82	Qc	402	HEM	CAA-CBA-CGA-O1A
81	QC	403	PEE	C31-C30-O3-C3
81	Qc	401	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
78	C1	602	HEA	CAD-CBD-CGD-O1D
72	QI	301	PLX	C16-C17-C18-C19
82	QC	401	HEM	CAD-CBD-CGD-O2D
82	Qc	403	HEM	CAD-CBD-CGD-O1D
71	C3	301	PC1	C1-C2-O21-C21
71	Qb	502	PC1	C3-C2-O21-C21
73	AL	202	CDL	CA6-CA4-OA6-CA5
73	N2	402	CDL	CA6-CA4-OA6-CA5
73	Qb	501	CDL	CA3-CA4-OA6-CA5
81	N5	704	PEE	C43-C44-C45-C46
82	QC	401	HEM	CAA-CBA-CGA-O1A
71	Qc	405	PC1	O21-C21-C22-C23
82	Qc	402	HEM	CAD-CBD-CGD-O2D
81	QC	403	PEE	C31-C32-C33-C34
71	Qj	101	PC1	C33-C34-C35-C36
72	N2	401	PLX	C7-C8-C9-C10
73	Qh	101	CDL	CA7-C31-C32-C33
82	QC	401	HEM	CAA-CBA-CGA-O2A
73	CB	203	CDL	C39-C40-C41-C42
72	AM	201	PLX	O4-C3-C4-C5
81	QC	403	PEE	O5-C30-O3-C3
73	N5	702	CDL	C19-C20-C21-C22
73	B4	201	CDL	OA6-CA4-CA6-OA8
73	N5	702	CDL	OB6-CB4-CB6-OB8
73	B4	201	CDL	C74-C75-C76-C77
73	A8	301	CDL	C72-C73-C74-C75
81	N6	201	PEE	C31-C32-C33-C34
78	C1	603	HEA	CAD-CBD-CGD-O2D
82	QC	402	HEM	CAA-CBA-CGA-O2A
81	N3	201	PEE	C40-C41-C42-C43
73	N5	703	CDL	C12-C11-CA5-OA6
71	B4	202	PC1	C23-C24-C25-C26
72	6C	101	PLX	C25-C26-C27-C28
73	CB	203	CDL	CB4-CB3-OB5-PB2
73	Qh	101	CDL	C1-CA2-OA2-PA1
73	N2	402	CDL	C52-C51-CB5-OB6
77	N5	705	3PE	C36-C37-C38-C39
73	N5	703	CDL	C40-C41-C42-C43
73	B5	202	CDL	C37-C38-C39-C40
81	N4	501	PEE	C17-C18-C19-C20
75	AB	201	ZMP	C22-C23-C24-C25
73	A8	301	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
72	AM	201	PLX	C4-C5-O8-C24
71	Qb	502	PC1	O11-C1-C2-O21
73	N2	402	CDL	C12-C11-CA5-OA6
81	N3	201	PEE	O3P-C1-C2-C3
78	C1	602	HEA	C18-C19-C20-C21
82	QC	402	HEM	CAD-CBD-CGD-O1D
72	QE	301	PLX	C11-C12-C13-C14
73	CB	203	CDL	C37-C38-C39-C40
81	N4	501	PEE	C18-C19-C20-C21
82	QC	402	HEM	CAD-CBD-CGD-O2D
73	QB	501	CDL	CB2-C1-CA2-OA2
73	A8	301	CDL	OB6-CB4-CB6-OB8
73	AL	201	CDL	OB6-CB4-CB6-OB8
77	QE	303	3PE	O21-C2-C3-O31
72	QE	301	PLX	C6-C7-C8-C9
71	Qb	502	PC1	O22-C21-C22-C23
72	AM	201	PLX	C15-C16-C17-C18
73	N1	401	CDL	C81-C82-C83-C84
71	Qc	404	PC1	O21-C21-C22-C23
81	S8	303	PEE	C31-C30-O3-C3
81	QC	403	PEE	C18-C19-C20-C21
81	S8	303	PEE	O5-C30-O3-C3
72	AM	201	PLX	C30-C31-C32-C33
75	AB	201	ZMP	N2-C16-C17-O4
71	Qb	502	PC1	C31-C32-C33-C34
71	N4	503	PC1	C36-C37-C38-C39
72	QE	301	PLX	C9-C10-C11-C12
74	A9	401	NDP	C2D-C1D-N1N-C2N
81	Qc	401	PEE	O2-C10-C11-C12
71	S7	302	PC1	C34-C35-C36-C37
73	B4	201	CDL	C32-C33-C34-C35
81	S8	303	PEE	C17-C18-C19-C20
73	N1	401	CDL	C74-C75-C76-C77
73	AL	201	CDL	C32-C31-CA7-OA8
71	6A	101	PC1	C25-C26-C27-C28
73	QB	501	CDL	CA6-CA4-OA6-CA5
73	QB	501	CDL	CB6-CB4-OB6-CB5
73	QD	402	CDL	CB6-CB4-OB6-CB5
81	N5	704	PEE	C3-C2-O2-C10
73	N1	401	CDL	CA5-C11-C12-C13
71	N4	503	PC1	O21-C21-C22-C23
71	QB	503	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
72	6C	101	PLX	C6-C7-C8-C9
73	A8	301	CDL	C38-C39-C40-C41
81	N6	201	PEE	C24-C25-C26-C27
75	AC	201	ZMP	C11-C12-N1-C13
71	6A	101	PC1	O31-C31-C32-C33
73	N5	703	CDL	C32-C31-CA7-OA8
73	QH	102	CDL	C72-C71-CB7-OB8
71	B5	203	PC1	C2A-C2B-C2C-C2D
72	N4	502	PLX	C25-C26-C27-C28
81	N5	701	PEE	C38-C39-C40-C41
81	Qe	302	PEE	C36-C37-C38-C39
73	Qb	501	CDL	C1-CB2-OB2-PB2
81	Qe	302	PEE	C1-C2-C3-O3
73	QH	101	CDL	C73-C74-C75-C76
73	QB	501	CDL	OA5-CA3-CA4-OA6
81	N3	201	PEE	O3P-C1-C2-O2
71	C3	301	PC1	O31-C31-C32-C33
71	N1	402	PC1	O21-C21-C22-C23
77	C1	601	3PE	O21-C21-C22-C23
77	CB	201	3PE	O31-C31-C32-C33
81	N5	701	PEE	O2-C10-C11-C12
81	S2	501	PEE	O2-C10-C11-C12
81	S2	501	PEE	C31-C32-C33-C34
77	QE	303	3PE	O22-C21-C22-C23
78	C1	602	HEA	CAD-CBD-CGD-O2D
78	C1	603	HEA	CAD-CBD-CGD-O1D
81	N4	501	PEE	C40-C41-C42-C43
81	Qc	401	PEE	C24-C25-C26-C27
71	CB	202	PC1	C2D-C2E-C2F-C2G
81	Qe	302	PEE	O2-C10-C11-C12
73	B4	201	CDL	C82-C83-C84-C85
81	N6	201	PEE	C16-C17-C18-C19
73	B5	202	CDL	C74-C75-C76-C77
71	QB	502	PC1	C34-C35-C36-C37
81	S2	501	PEE	C32-C33-C34-C35
83	QD	401	HEC	CAD-CBD-CGD-O2D
81	S8	303	PEE	C39-C40-C41-C42
74	A9	401	NDP	O4D-C1D-N1N-C2N
71	N4	503	PC1	C37-C38-C39-C3A
81	N4	501	PEE	O2-C10-C11-C12
73	CB	203	CDL	C53-C54-C55-C56
71	B5	203	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
73	N5	702	CDL	OA6-CA4-CA6-OA8
77	QC	404	3PE	O21-C2-C3-O31
81	N5	704	PEE	O2-C2-C3-O3
71	B5	203	PC1	O31-C31-C32-C33
72	QE	301	PLX	C11-C10-C9-C8
73	N5	703	CDL	C52-C51-CB5-OB6
81	QE	302	PEE	C19-C20-C21-C22
71	Qj	101	PC1	C2-C1-O11-P
73	QH	101	CDL	C1-CA2-OA2-PA1
72	B5	201	PLX	C24-C25-C26-C27
71	C3	301	PC1	C36-C37-C38-C39
77	QE	303	3PE	C2C-C2D-C2E-C2F
74	A9	401	NDP	O4B-C4B-C5B-O5B
76	AK	401	ADP	O4'-C4'-C5'-O5'
71	C3	302	PC1	O32-C31-C32-C33
71	B5	203	PC1	C28-C29-C2A-C2B
73	N5	702	CDL	C41-C42-C43-C44
73	CB	203	CDL	C52-C51-CB5-OB6
73	N1	401	CDL	C72-C71-CB7-OB8
72	B5	201	PLX	C34-C35-C36-C37
72	QE	301	PLX	C13-C14-C15-C16
73	QH	101	CDL	C74-C75-C76-C77
71	N4	504	PC1	C2C-C2D-C2E-C2F
72	QI	301	PLX	O8-C24-C25-C26
73	QH	102	CDL	C72-C71-CB7-OB9
81	S2	501	PEE	O4-C10-C11-C12
71	Qb	502	PC1	C22-C23-C24-C25
71	N4	503	PC1	O22-C21-C22-C23
71	QB	502	PC1	C36-C37-C38-C39
77	C1	601	3PE	C3E-C3F-C3G-C3H
71	Qc	404	PC1	O22-C21-C22-C23
81	N5	701	PEE	O4-C10-C11-C12
73	B4	201	CDL	CB3-CB4-CB6-OB8
73	Qb	501	CDL	CB3-CB4-CB6-OB8
81	N5	704	PEE	C1-C2-C3-O3
71	C3	302	PC1	C37-C38-C39-C3A
73	A8	301	CDL	CA2-OA2-PA1-OA5
73	N2	402	CDL	CB2-OB2-PB2-OB5
73	A8	301	CDL	C57-C58-C59-C60
71	C3	301	PC1	O32-C31-C32-C33
81	N4	501	PEE	O4-C10-C11-C12
72	N4	502	PLX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
81	S2	501	PEE	C40-C41-C42-C43
73	AL	201	CDL	C1-CA2-OA2-PA1
77	CB	201	3PE	O32-C31-C32-C33
77	QC	404	3PE	O32-C31-C32-C33
81	Qc	401	PEE	O4-C10-C11-C12
78	C1	602	HEA	C14-C15-C16-C17
73	N5	702	CDL	C33-C34-C35-C36
83	QD	401	HEC	CAD-CBD-CGD-O1D
71	C3	301	PC1	C11-O13-P-O14
71	CB	202	PC1	C11-O13-P-O14
71	N1	402	PC1	C1-O11-P-O12
71	Qc	404	PC1	C11-O13-P-O12
73	N2	402	CDL	CB2-OB2-PB2-OB3
73	N2	402	CDL	CB3-OB5-PB2-OB3
73	QB	501	CDL	CA2-OA2-PA1-OA3
73	QB	501	CDL	CB2-OB2-PB2-OB3
73	QD	402	CDL	CA3-OA5-PA1-OA3
73	QH	102	CDL	CA2-OA2-PA1-OA3
73	Qb	501	CDL	CA3-OA5-PA1-OA4
77	QE	303	3PE	C11-O13-P-O14
81	N3	201	PEE	C4-O4P-P-O1P
81	N4	501	PEE	C4-O4P-P-O2P
81	N5	701	PEE	C1-O3P-P-O1P
81	N6	201	PEE	C1-O3P-P-O1P
81	QE	302	PEE	C4-O4P-P-O1P
77	C1	601	3PE	O22-C21-C22-C23
77	QE	303	3PE	O11-C1-C2-C3
81	N5	704	PEE	O4P-C4-C5-N
71	B5	203	PC1	O32-C31-C32-C33
73	AL	201	CDL	C32-C31-CA7-OA9
73	N5	703	CDL	C32-C31-CA7-OA9
81	Qe	302	PEE	O4-C10-C11-C12
72	6C	101	PLX	C7-C8-C9-C10
73	N5	702	CDL	C52-C51-CB5-OB6
73	QB	501	CDL	C32-C31-CA7-OA8
73	N1	401	CDL	C72-C71-CB7-OB9
71	C3	302	PC1	C23-C24-C25-C26
72	N2	401	PLX	C25-C24-O8-C5
73	N2	402	CDL	CA3-CA4-OA6-CA5
73	QB	501	CDL	CA3-CA4-OA6-CA5
73	QB	501	CDL	CB3-CB4-OB6-CB5
73	QD	402	CDL	CB3-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
75	AB	201	ZMP	O3-C16-C17-C18
77	N5	705	3PE	C12-C11-O13-P
81	N5	704	PEE	C1-C2-O2-C10
81	QC	403	PEE	C5-C4-O4P-P
81	Qc	401	PEE	C5-C4-O4P-P
71	N1	402	PC1	O22-C21-C22-C23
72	N2	401	PLX	C11-C10-C9-C8
73	QD	402	CDL	C32-C31-CA7-OA8
72	QE	301	PLX	C10-C11-C12-C13
81	Qc	401	PEE	C14-C15-C16-C17
71	Qc	405	PC1	C3A-C3B-C3C-C3D
71	B5	203	PC1	C11-C12-N-C15
71	QB	502	PC1	O31-C31-C32-C33
71	Qb	502	PC1	O31-C31-C32-C33
73	N1	401	CDL	C78-C79-C80-C81
71	Qc	404	PC1	C2C-C2D-C2E-C2F
73	N5	702	CDL	C12-C11-CA5-OA6
73	QH	101	CDL	C32-C31-CA7-OA8
81	QE	302	PEE	O2-C10-C11-C12
83	Qd	401	HEC	CAA-CBA-CGA-O2A
73	N5	703	CDL	C52-C51-CB5-OB7
73	A8	301	CDL	C71-C72-C73-C74
77	CB	201	3PE	C29-C2A-C2B-C2C
82	Qc	403	HEM	C2A-CAA-CBA-CGA
72	AM	201	PLX	C29-C30-C31-C32
73	QB	501	CDL	C52-C51-CB5-OB6
72	QE	301	PLX	C15-C16-C17-C18
73	CB	203	CDL	C52-C51-CB5-OB7
73	N5	702	CDL	C12-C11-CA5-OA7
73	B4	201	CDL	C35-C36-C37-C38
81	QC	403	PEE	C12-C13-C14-C15
81	N3	201	PEE	O2-C10-C11-C12
71	N1	402	PC1	C32-C33-C34-C35
81	N6	201	PEE	C39-C40-C41-C42
71	Qb	502	PC1	O32-C31-C32-C33
73	QB	501	CDL	C52-C51-CB5-OB7
73	QH	101	CDL	C32-C31-CA7-OA9
81	QE	302	PEE	O4-C10-C11-C12
73	N5	703	CDL	C51-C52-C53-C54
77	N5	705	3PE	C3A-C3B-C3C-C3D
71	Qc	404	PC1	O31-C31-C32-C33
71	S7	302	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
78	C1	603	HEA	CAA-CBA-CGA-O2A

There are no ring outliers.

67 monomers are involved in 251 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	6A	101	PC1	10	0
71	N4	504	PC1	3	0
82	QC	401	HEM	2	0
71	Qb	502	PC1	2	0
73	QH	101	CDL	2	0
77	CB	201	3PE	4	0
81	N5	701	PEE	7	0
82	Qc	403	HEM	6	0
81	N5	704	PEE	1	0
73	A8	301	CDL	6	0
73	QB	501	CDL	3	0
81	N6	201	PEE	1	0
73	B5	202	CDL	8	0
72	N4	502	PLX	3	0
71	N1	402	PC1	5	0
73	AL	201	CDL	1	0
84	Qe	301	FES	2	0
71	C3	301	PC1	13	0
73	QH	102	CDL	3	0
72	AM	201	PLX	4	0
81	S8	303	PEE	2	0
73	N5	702	CDL	10	0
83	QD	401	HEC	1	0
81	QE	302	PEE	2	0
86	V1	502	FMN	4	0
71	QB	502	PC1	2	0
72	B5	201	PLX	1	0
73	CB	203	CDL	10	0
71	C3	302	PC1	12	0
81	QC	403	PEE	2	0
73	N1	401	CDL	5	0
76	AK	401	ADP	4	0
71	N4	503	PC1	5	0
73	N5	703	CDL	5	0
83	Qd	401	HEC	3	0
82	Qc	402	HEM	2	0

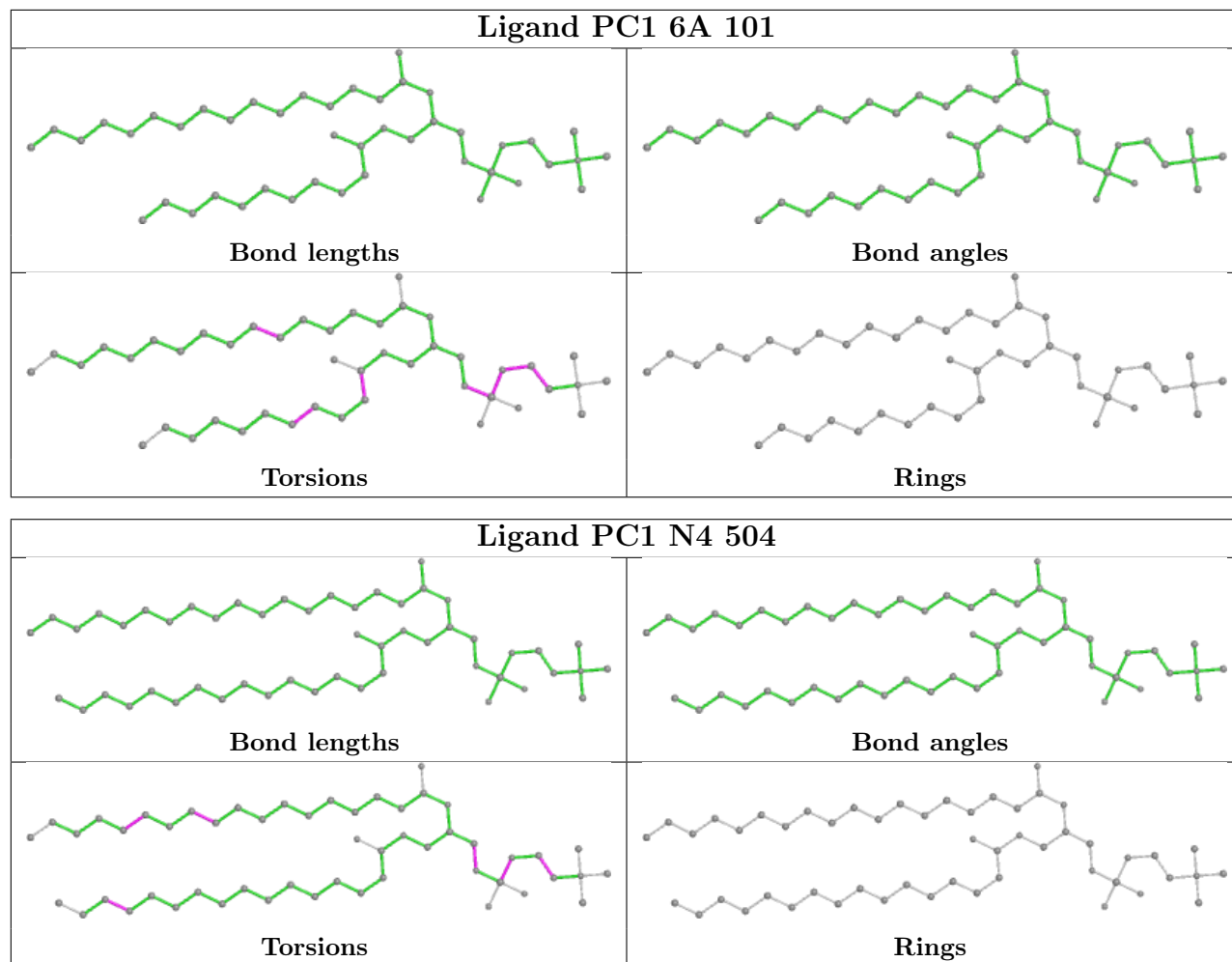
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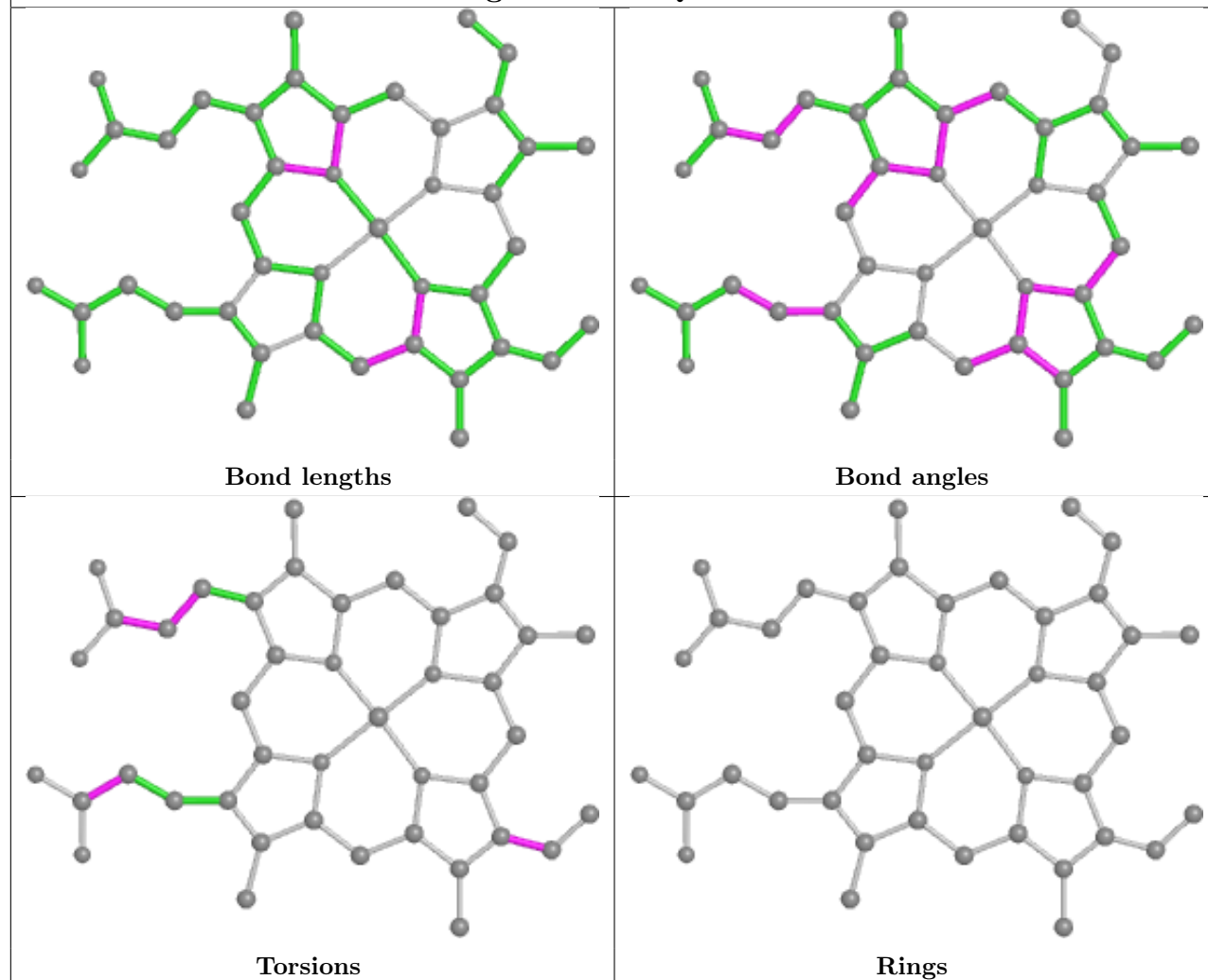
Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	B4	202	PC1	4	0
71	QB	503	PC1	4	0
85	S7	301	SF4	1	0
72	QI	301	PLX	4	0
73	AL	202	CDL	4	0
73	B4	201	CDL	4	0
81	S2	501	PEE	3	0
81	N4	501	PEE	2	0
71	B5	203	PC1	1	0
77	QE	303	3PE	3	0
71	S7	302	PC1	2	0
72	6C	101	PLX	3	0
77	QC	404	3PE	1	0
82	QC	402	HEM	6	0
72	QE	301	PLX	6	0
71	Qc	404	PC1	3	0
75	AB	201	ZMP	2	0
78	C1	602	HEA	16	0
72	N2	401	PLX	4	0
81	N3	201	PEE	3	0
85	S8	302	SF4	1	0
73	N2	402	CDL	1	0
81	Qe	302	PEE	4	0
81	Qc	401	PEE	4	0
73	Qb	501	CDL	3	0
71	Qc	405	PC1	2	0
75	AC	201	ZMP	4	0
71	Qh	102	PC1	1	0
78	C1	603	HEA	7	0
73	Qh	101	CDL	1	0
77	C1	601	3PE	8	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

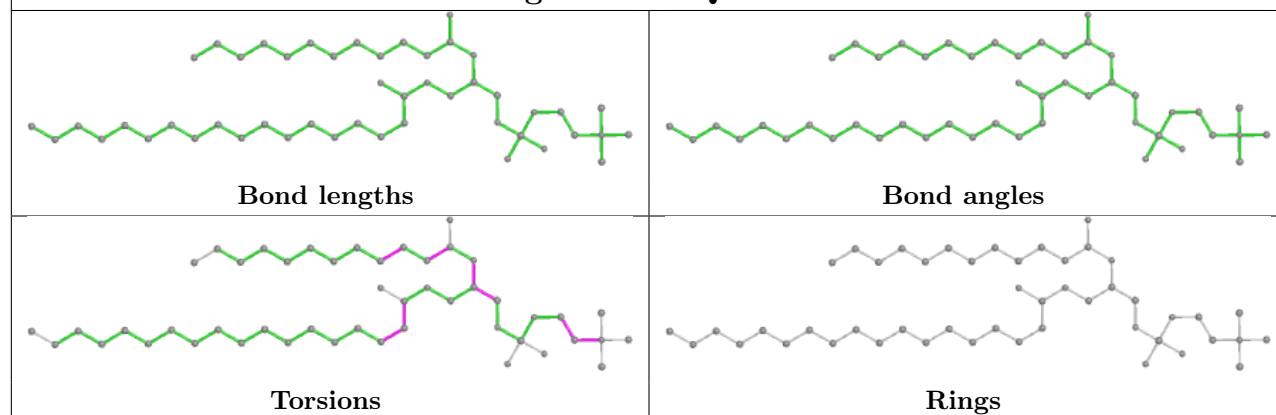
equivalents in the CSD to analyse the geometry.

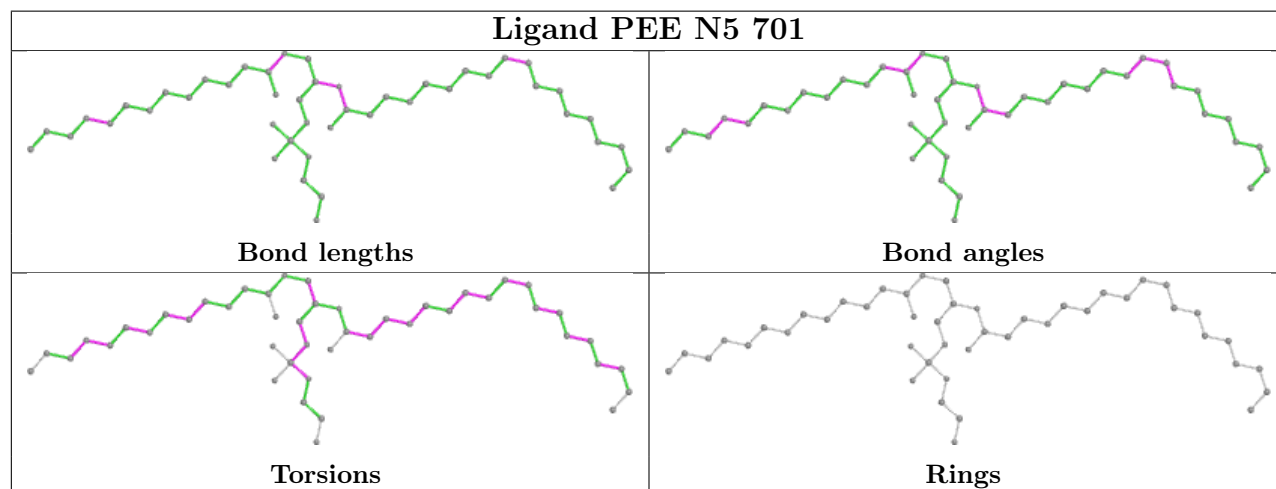
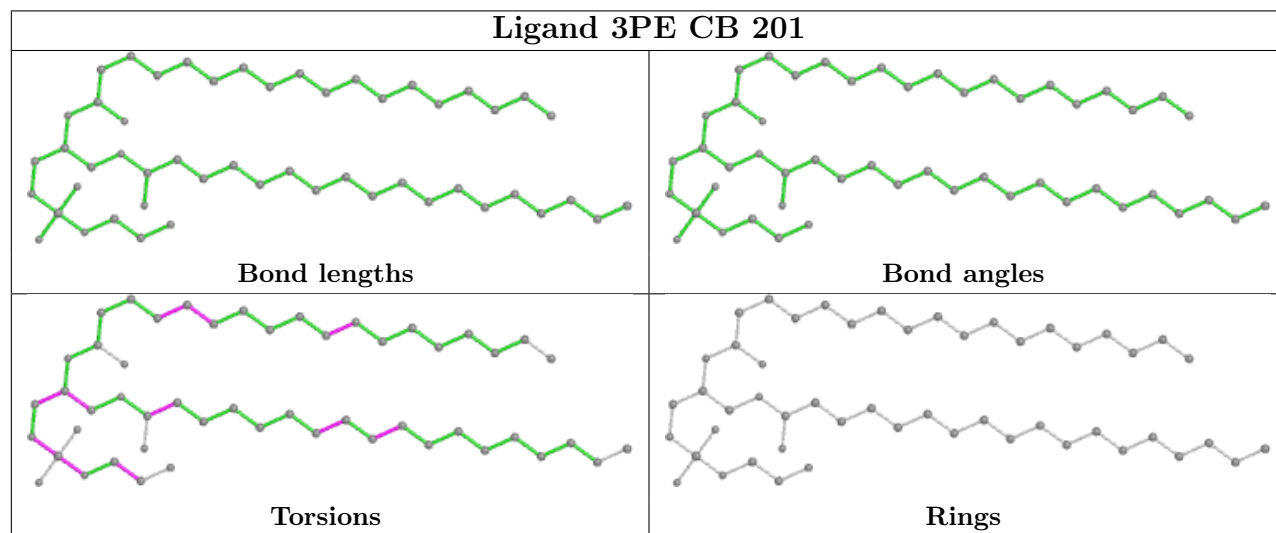
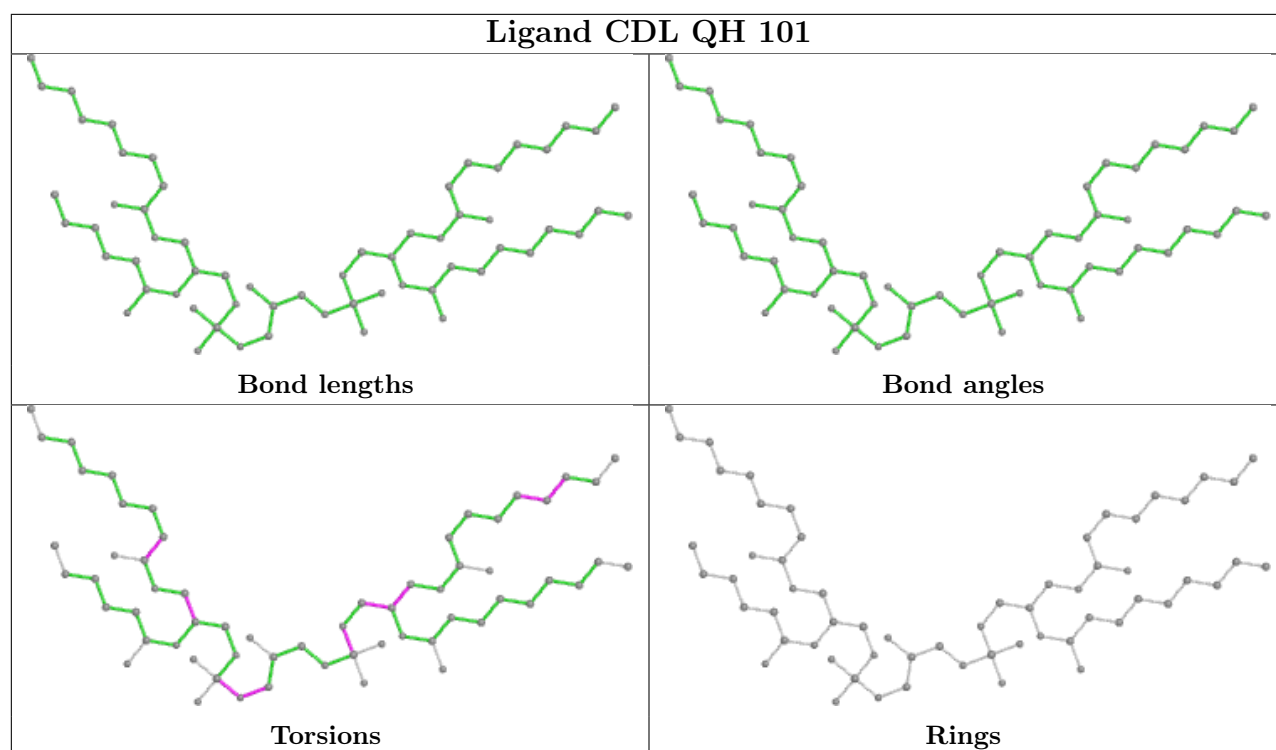


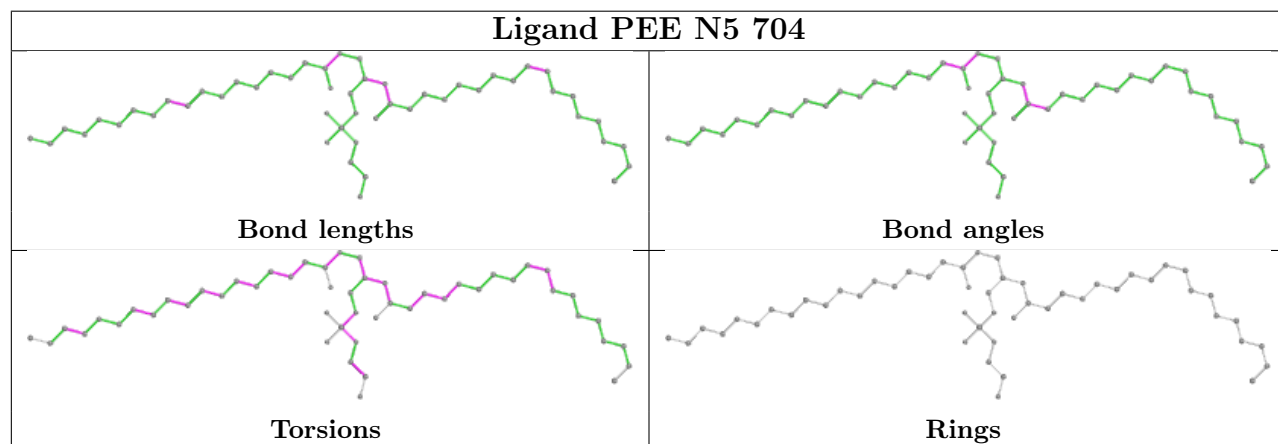
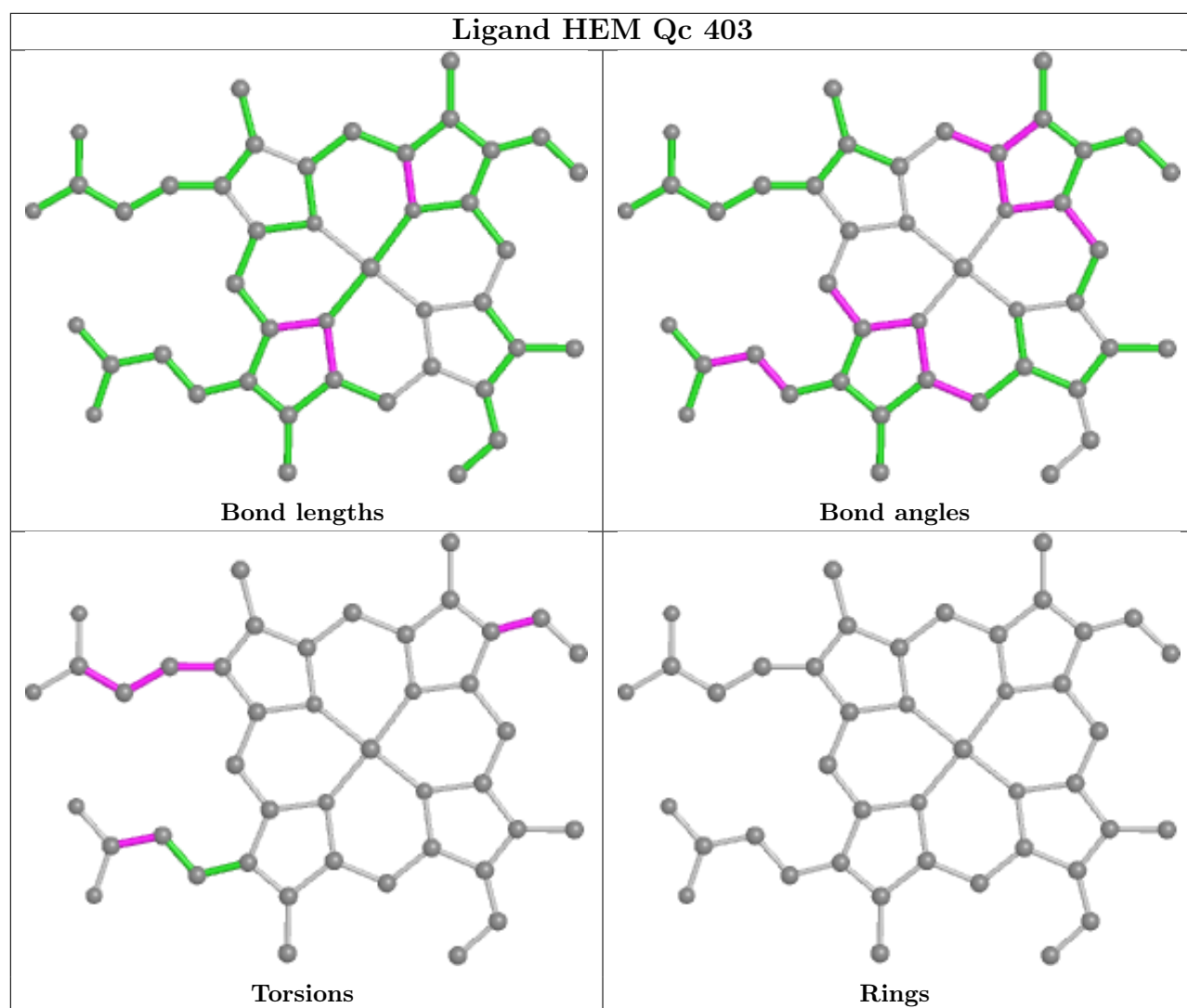
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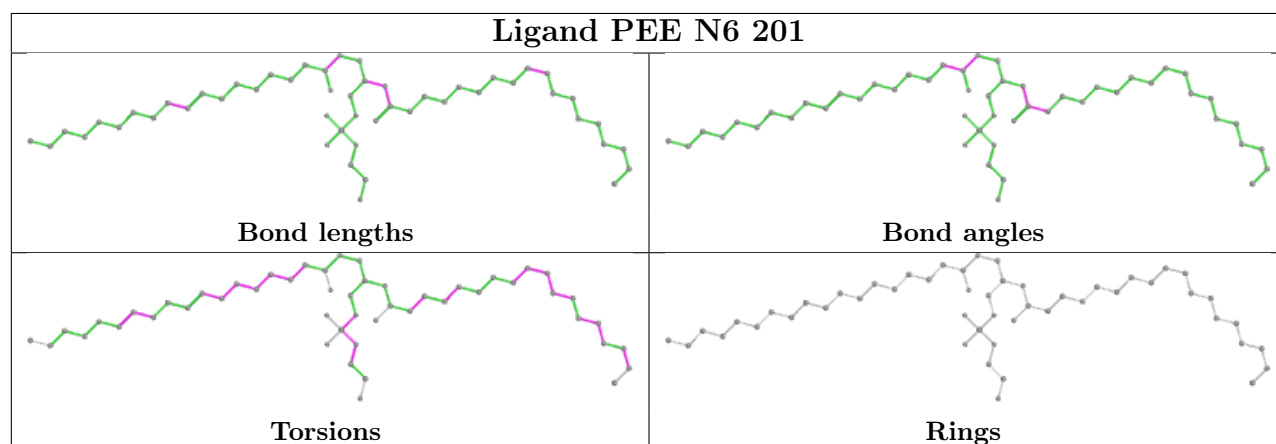
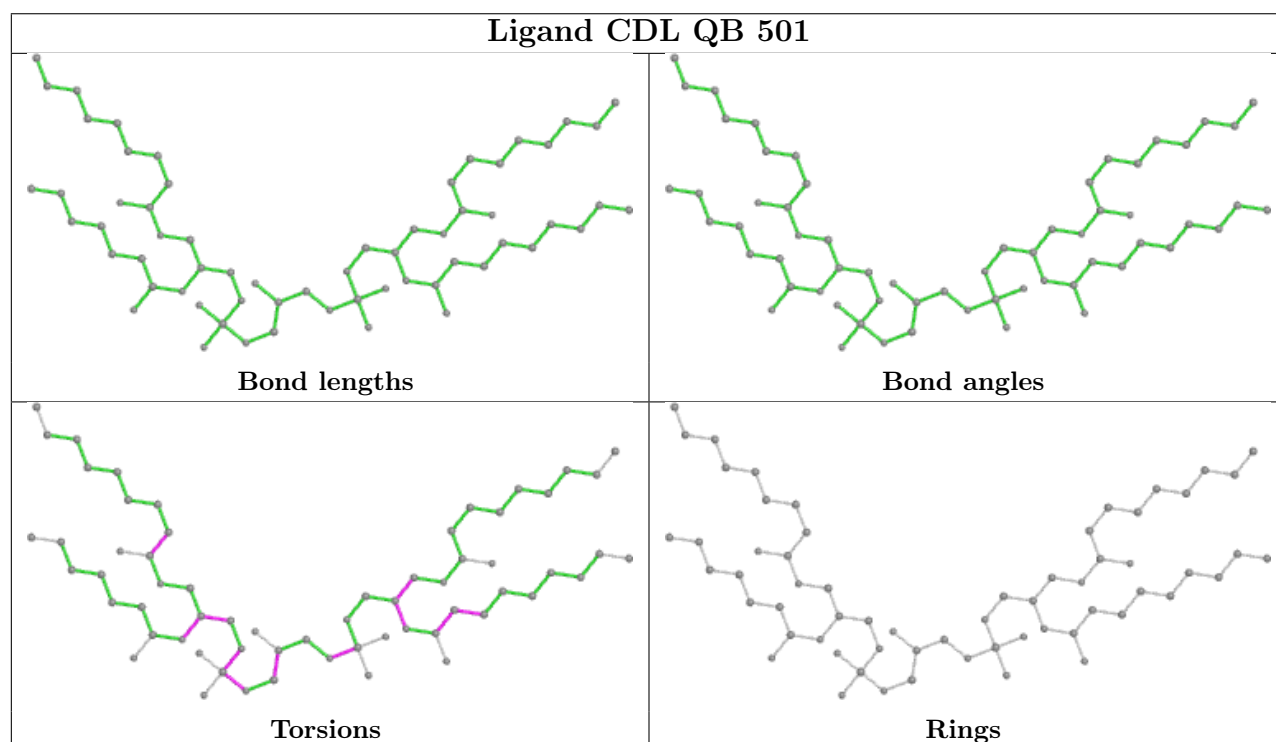
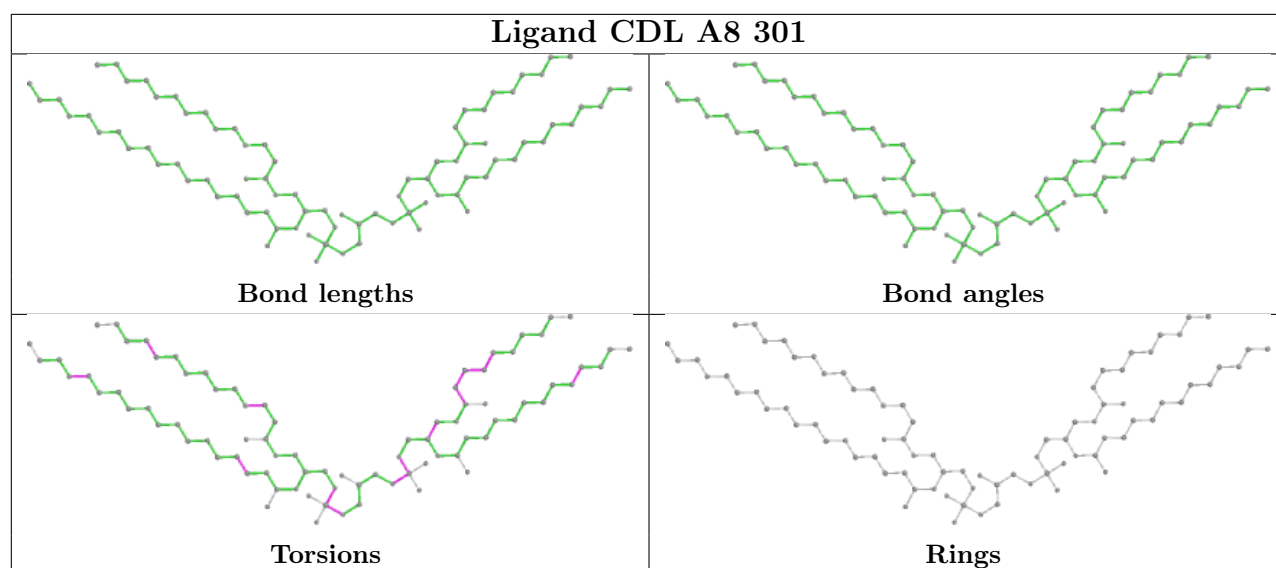


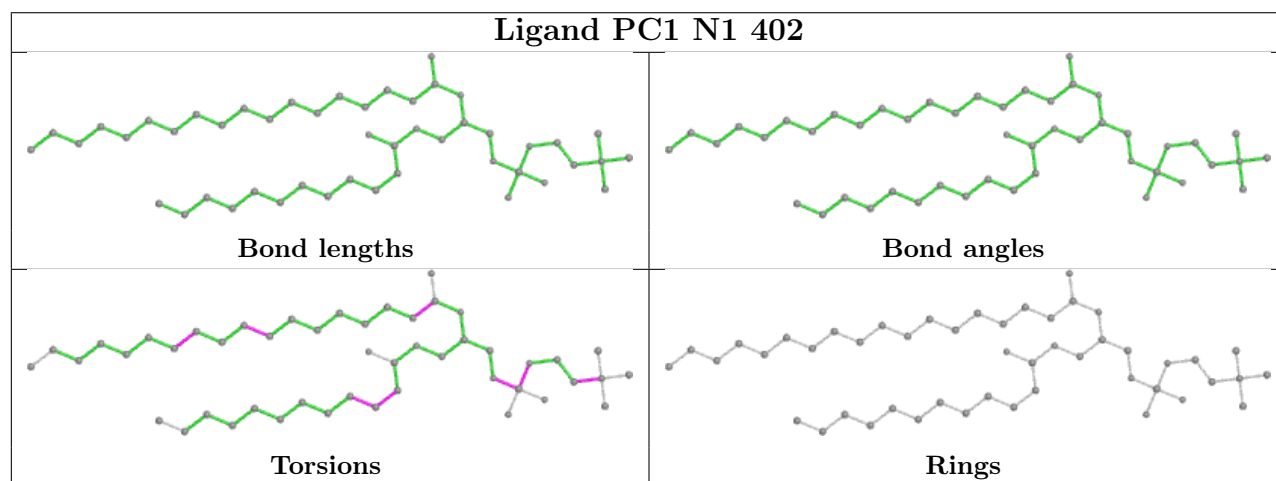
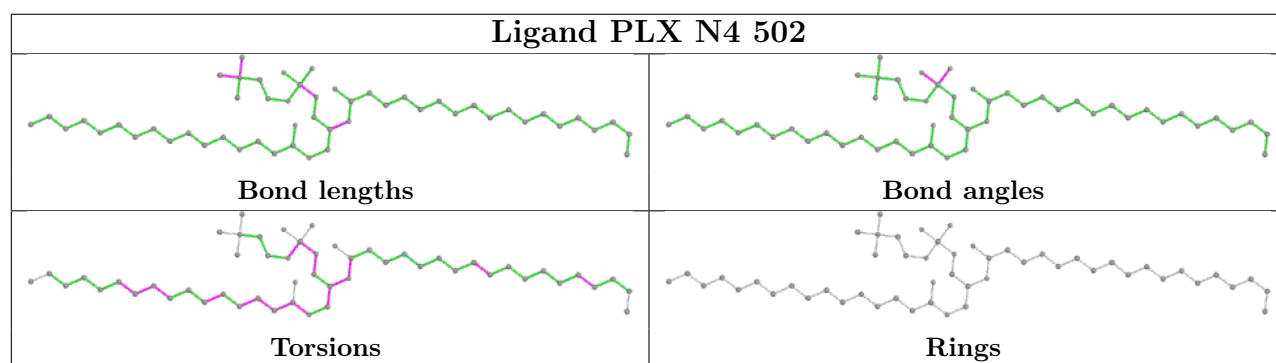
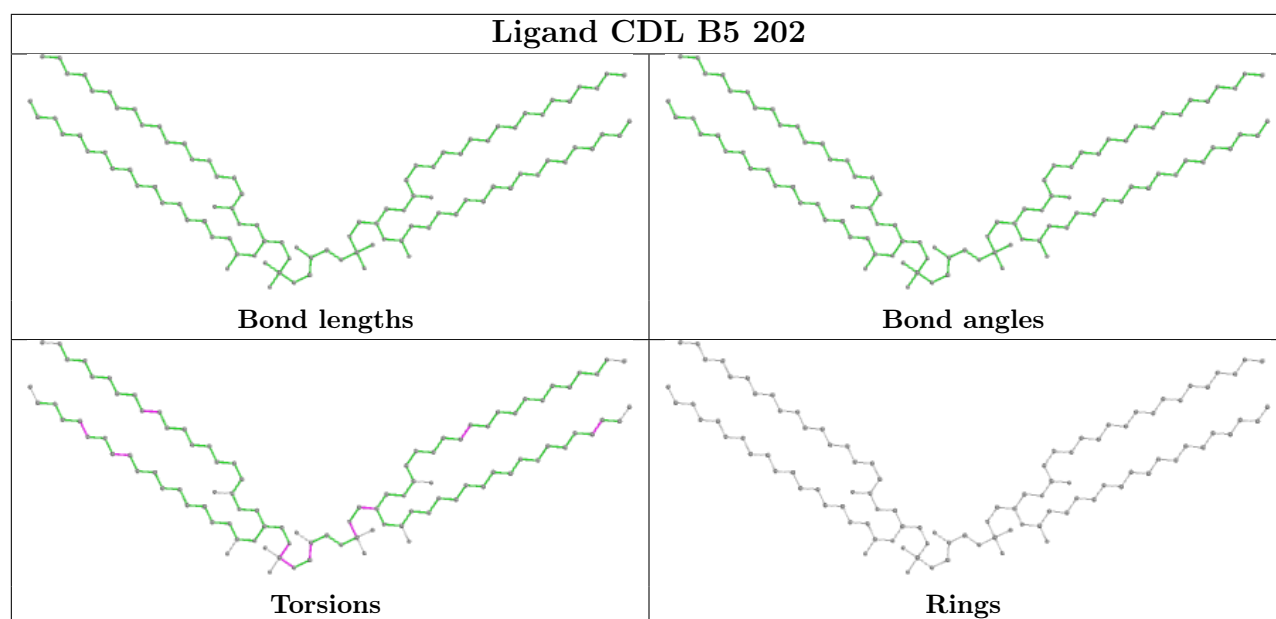
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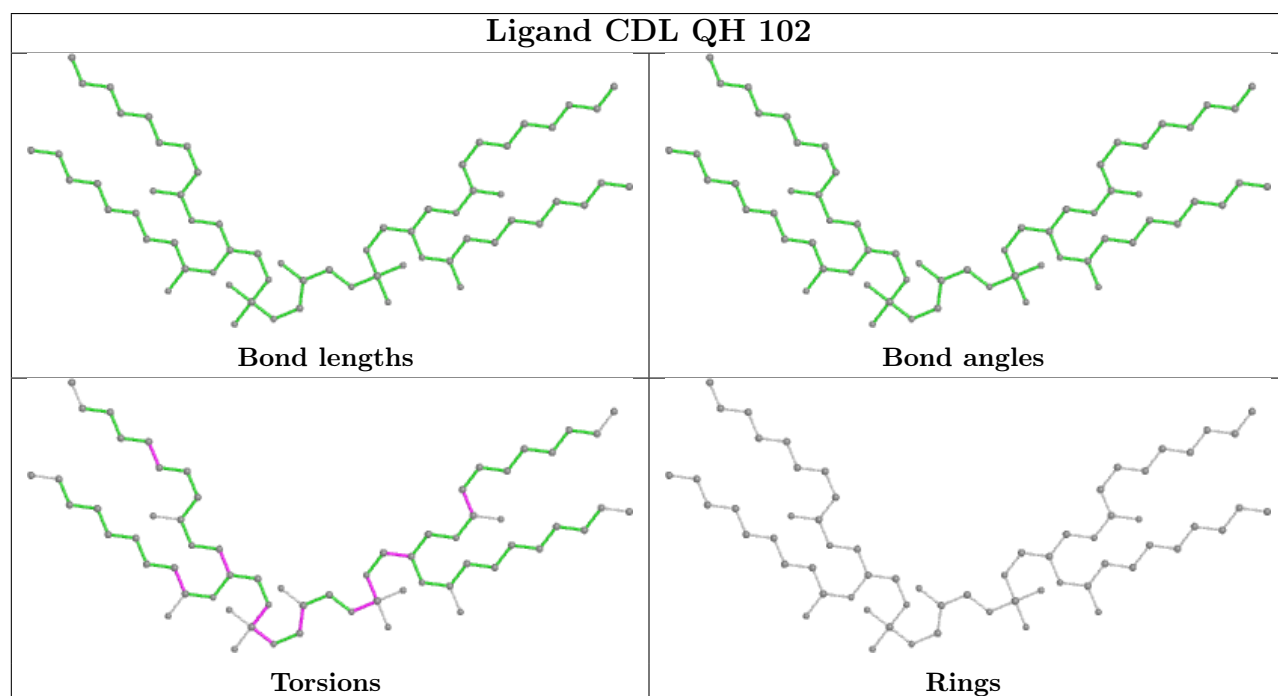
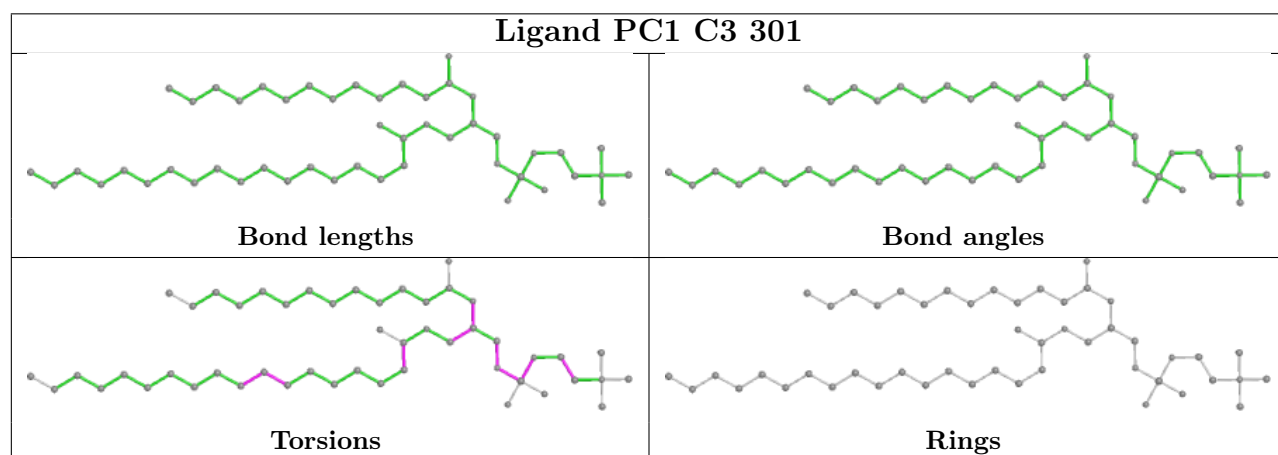
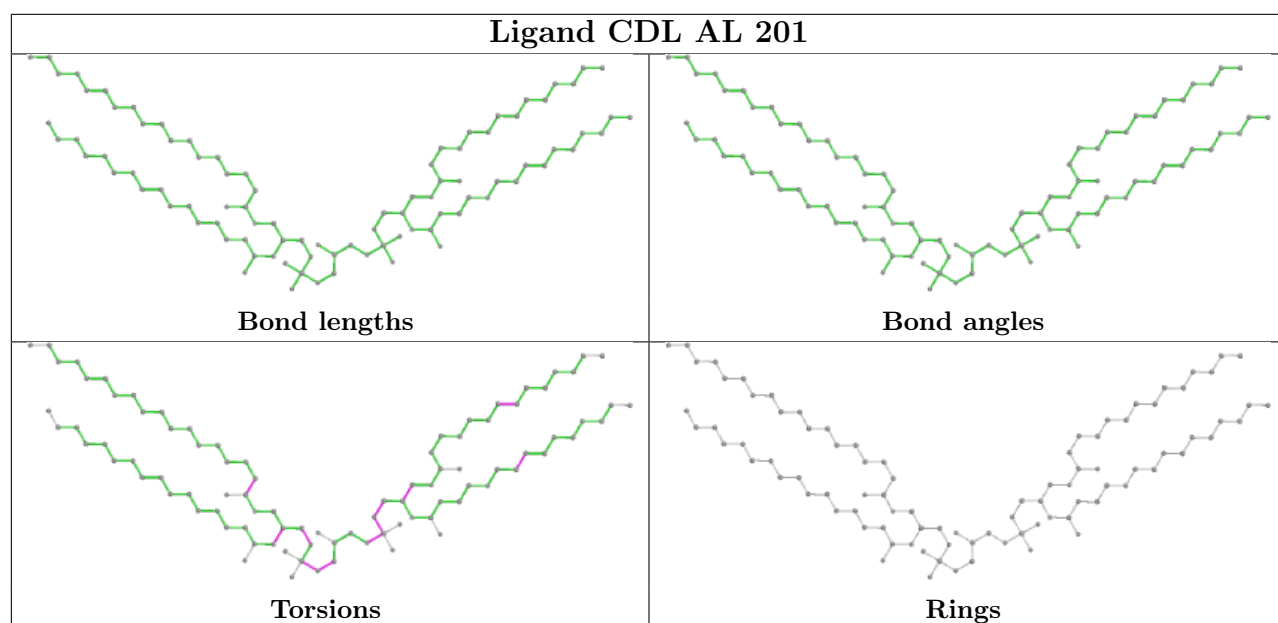


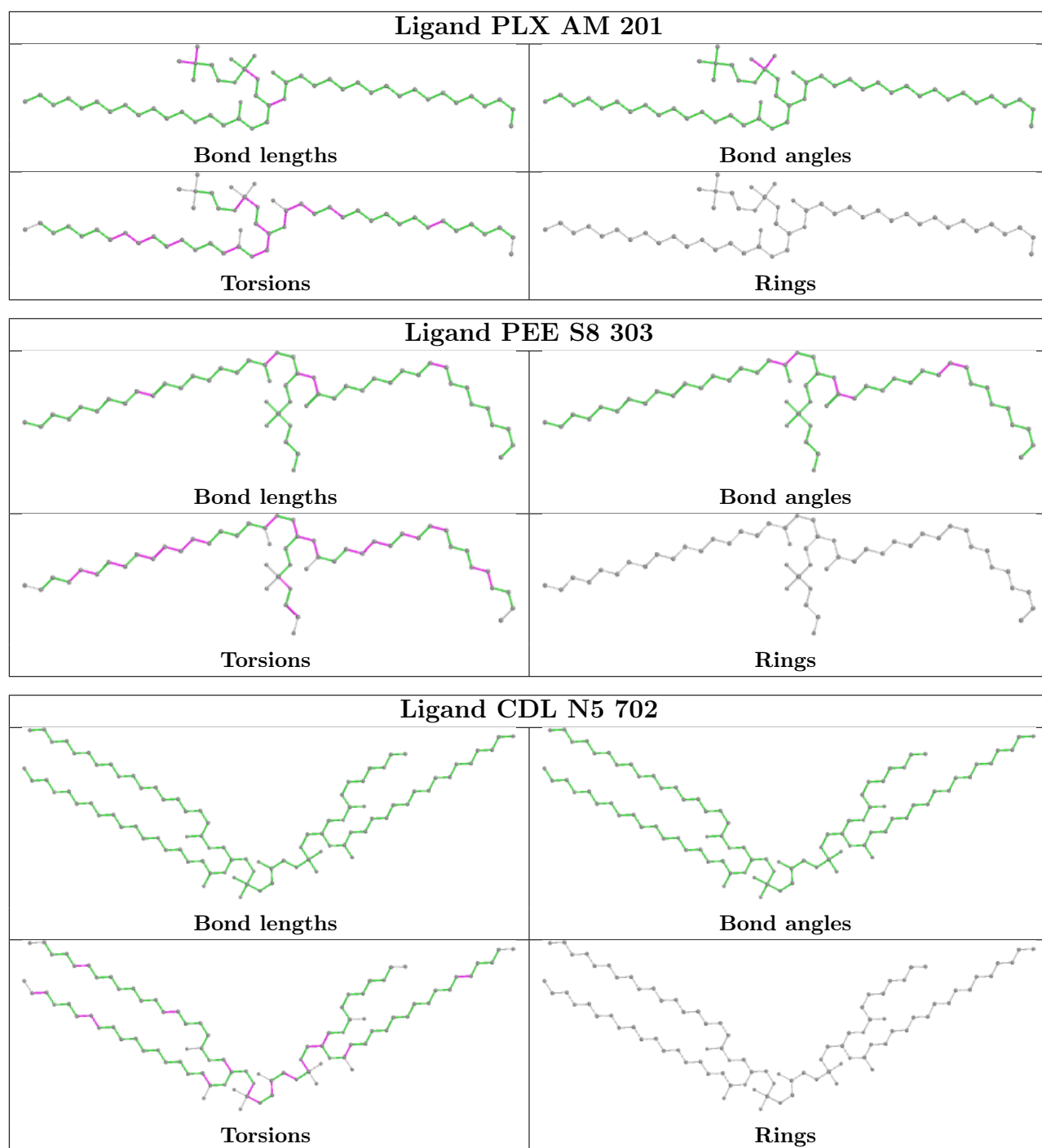




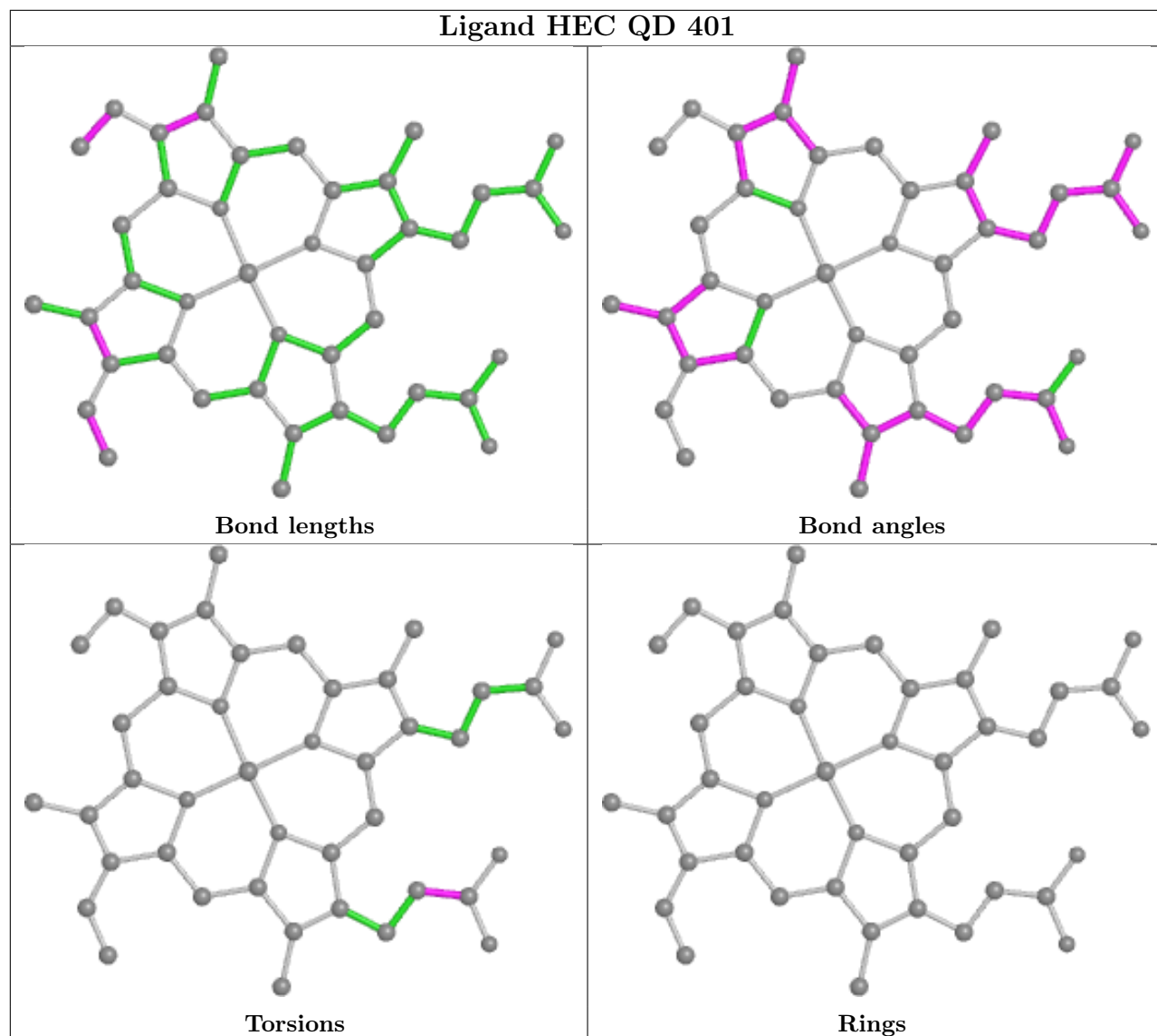




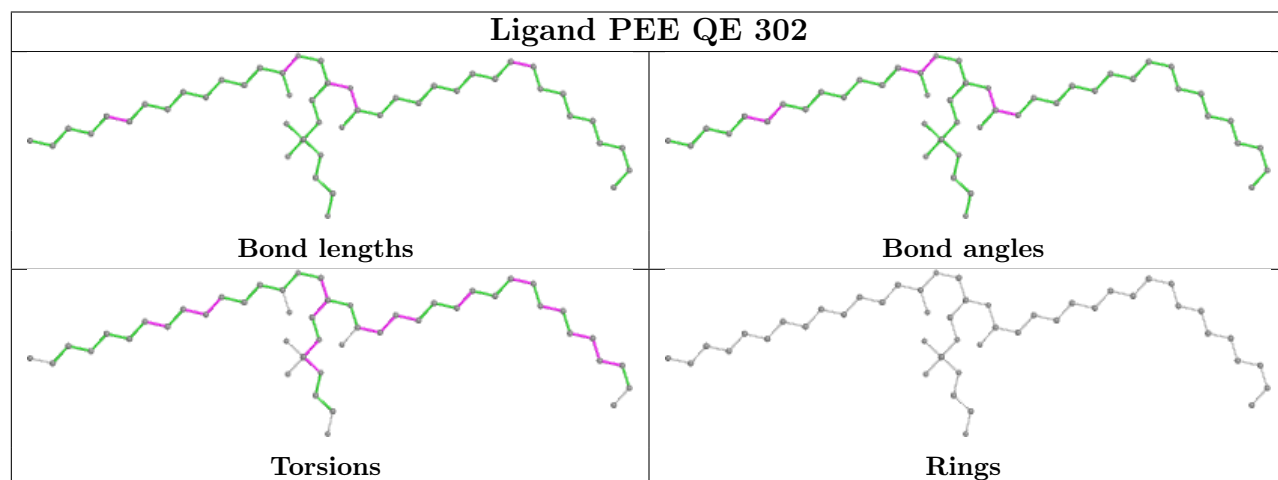


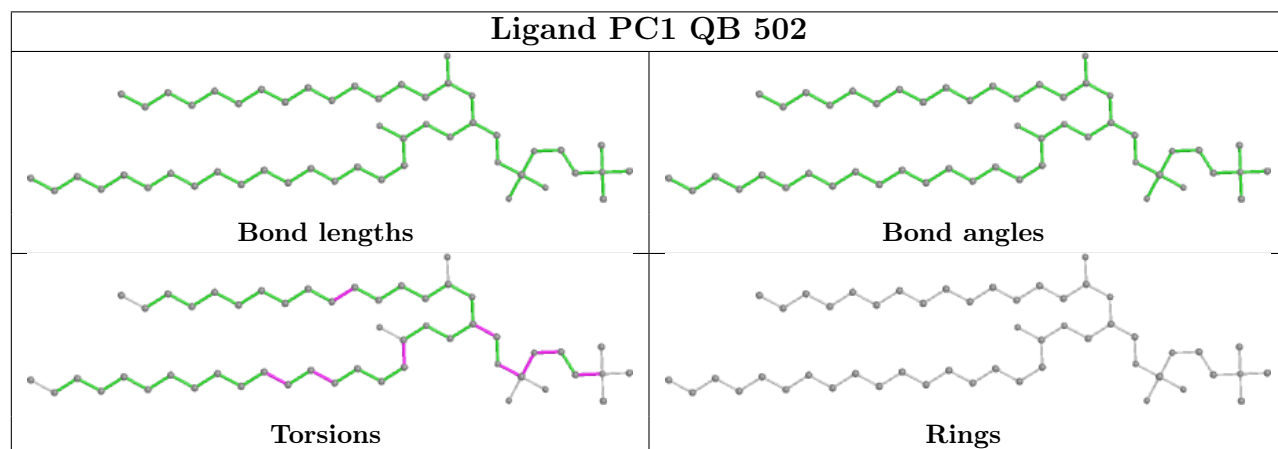
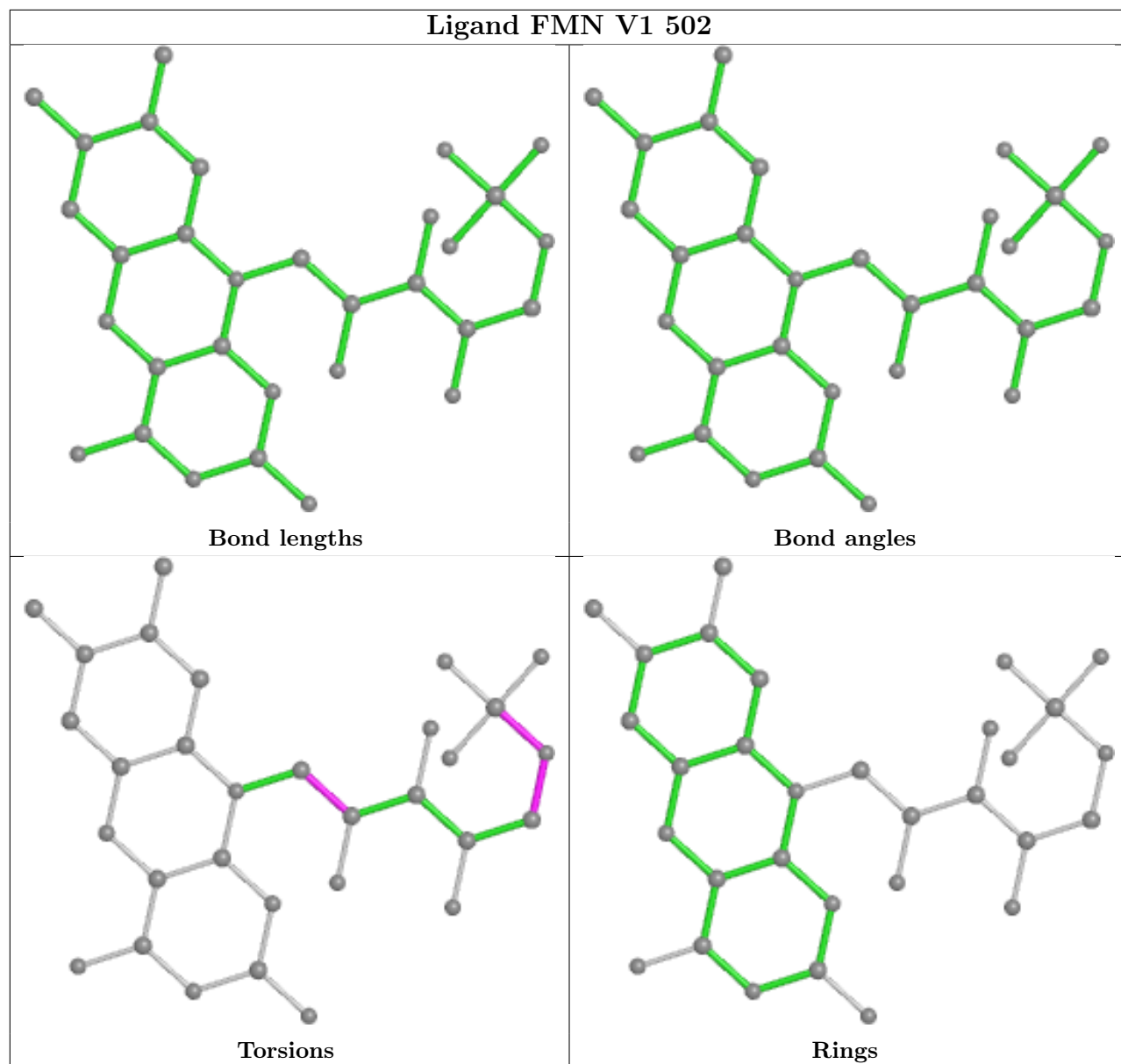


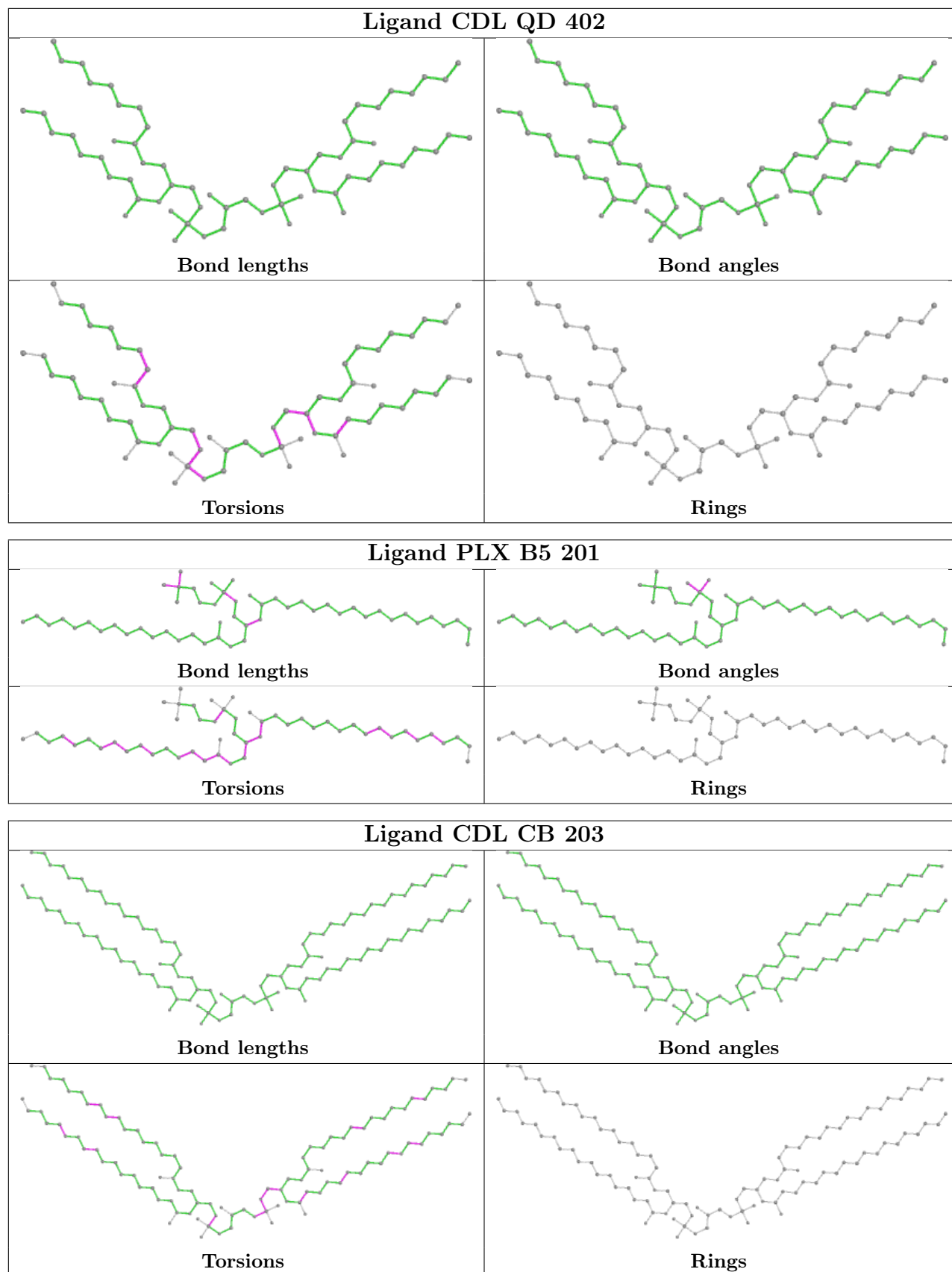
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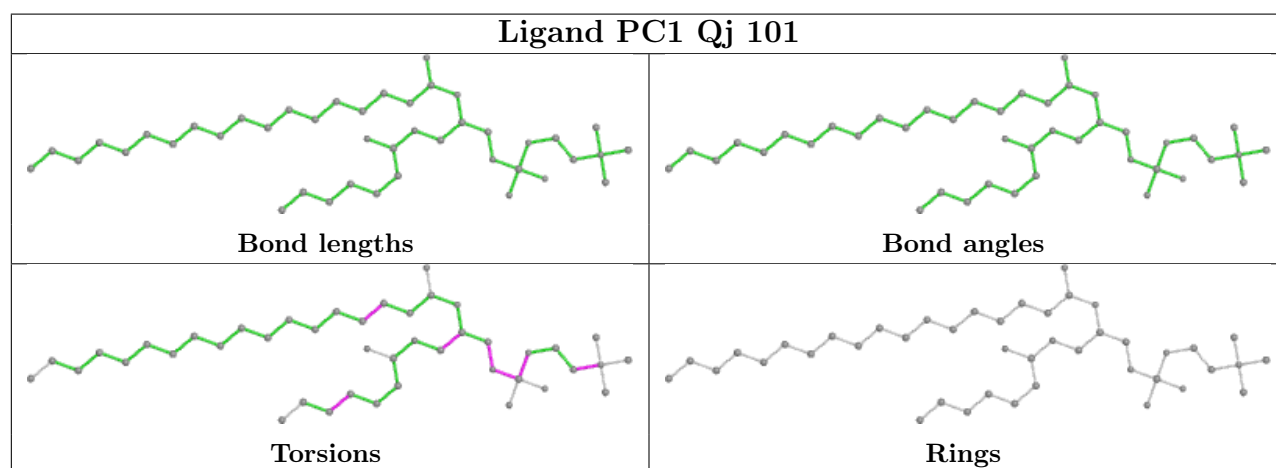
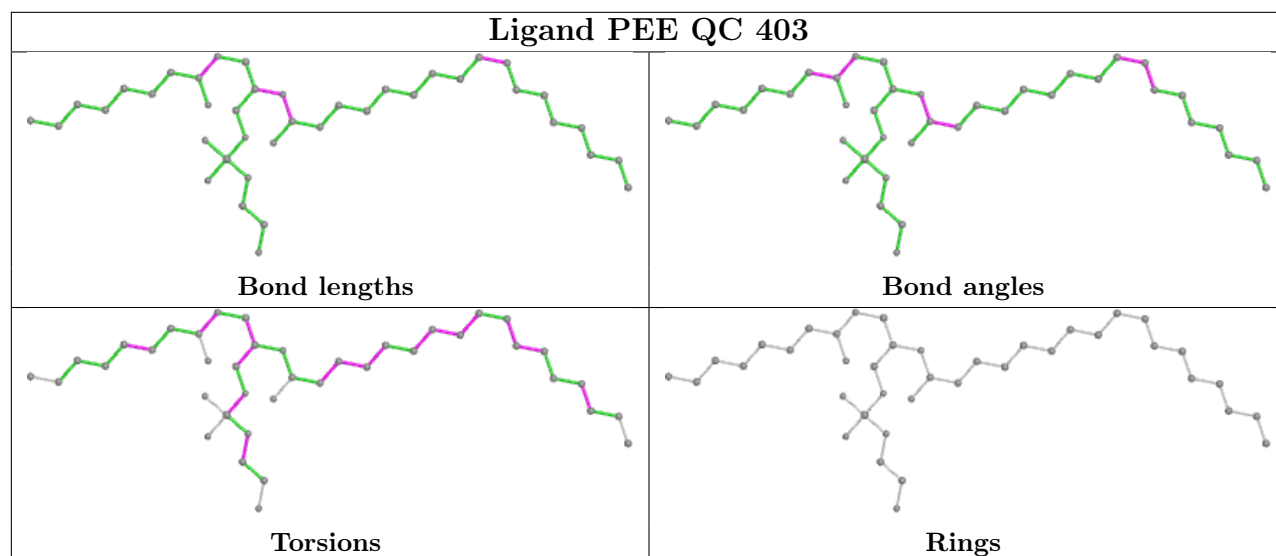
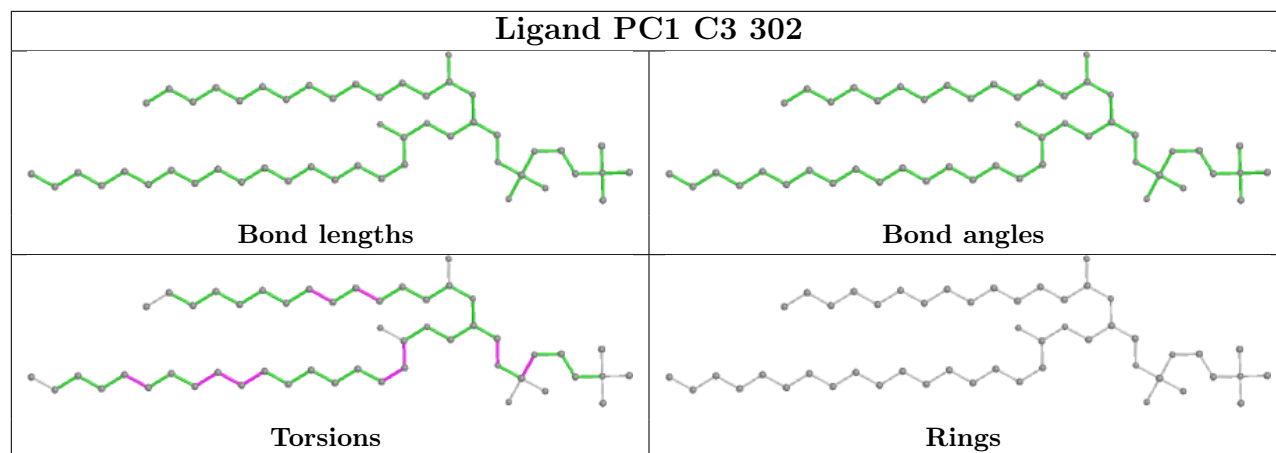


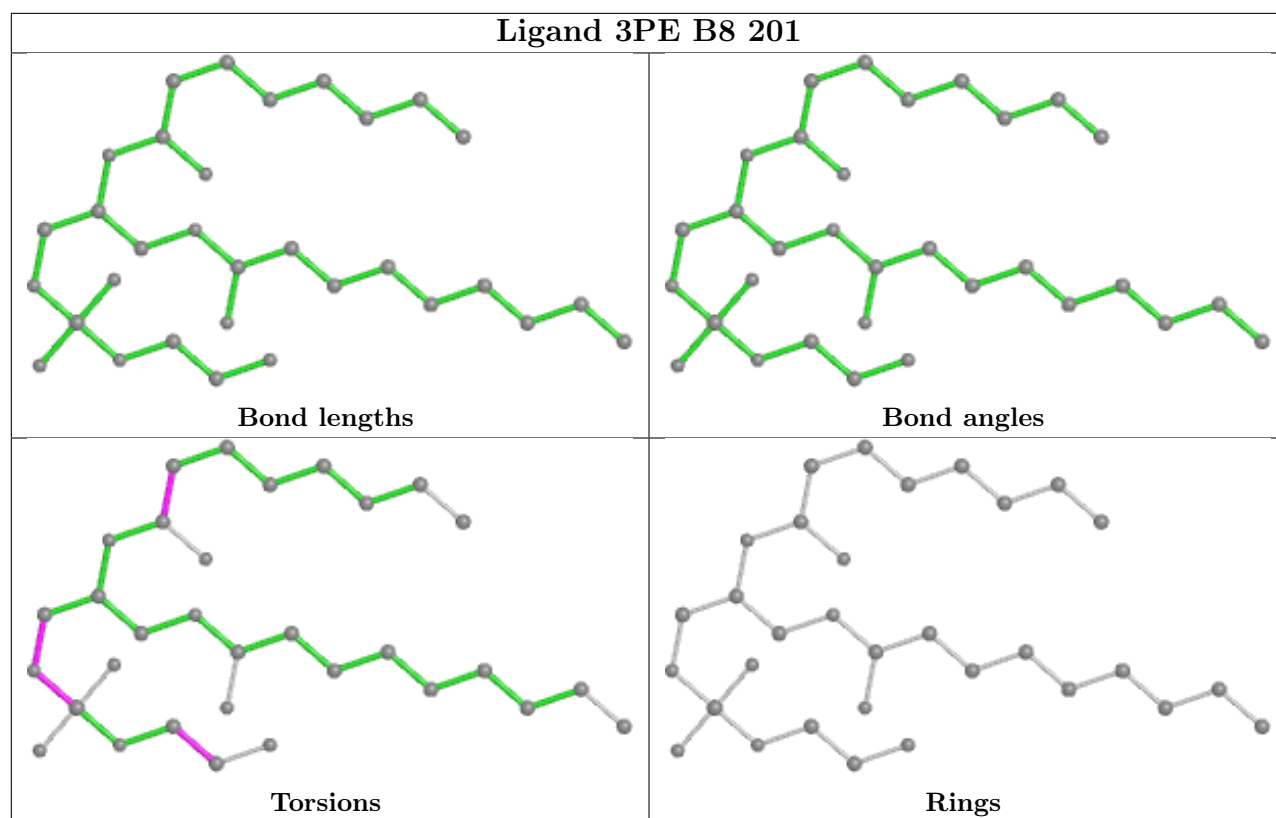
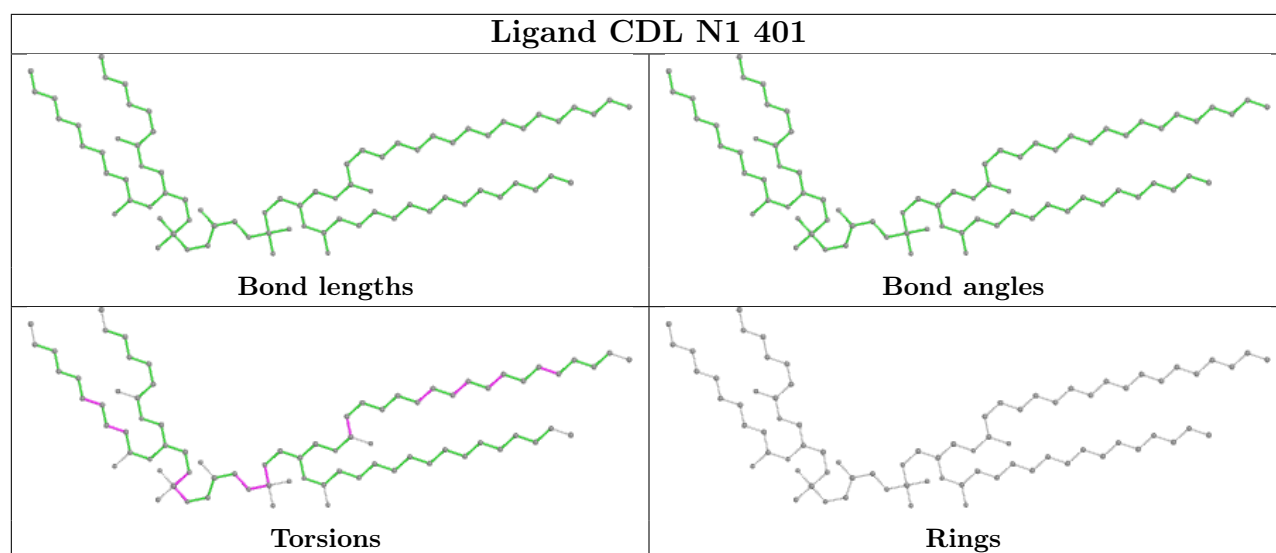
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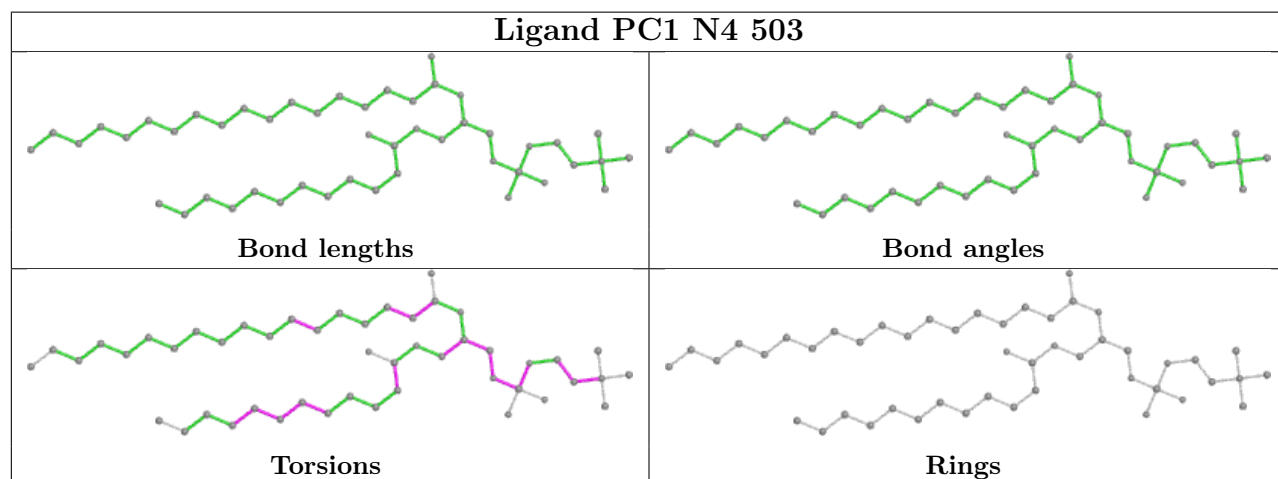
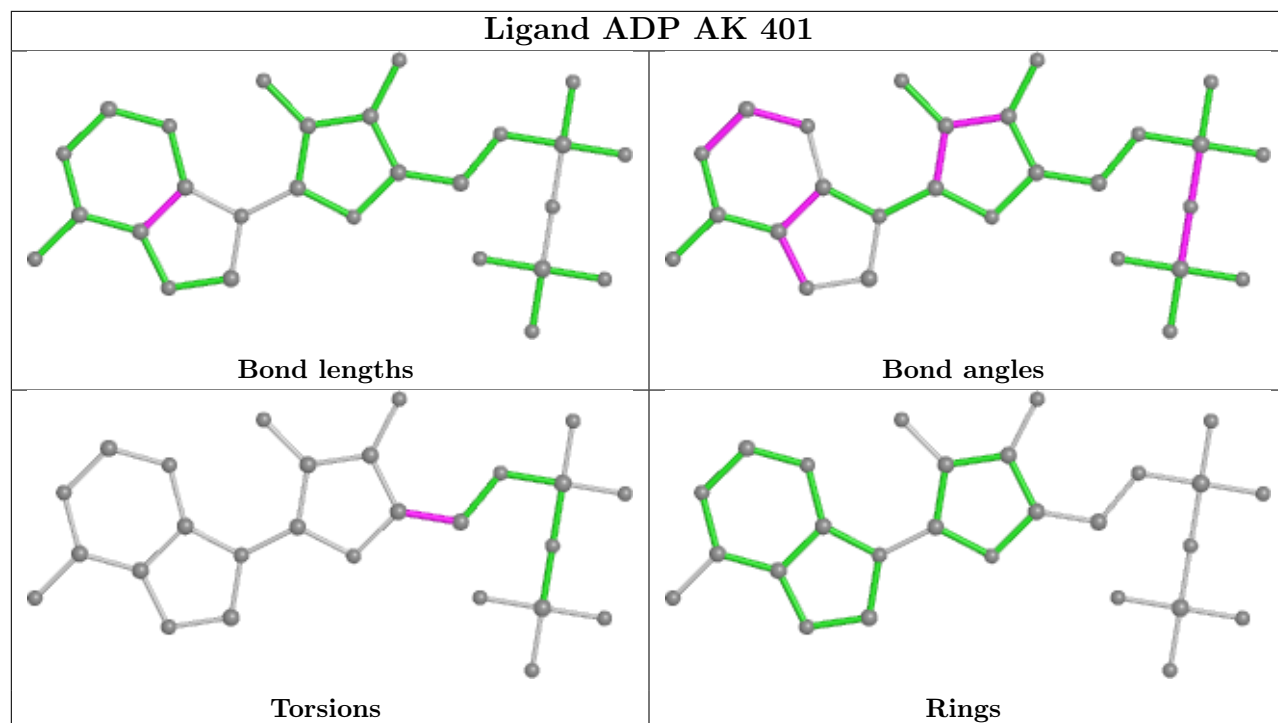




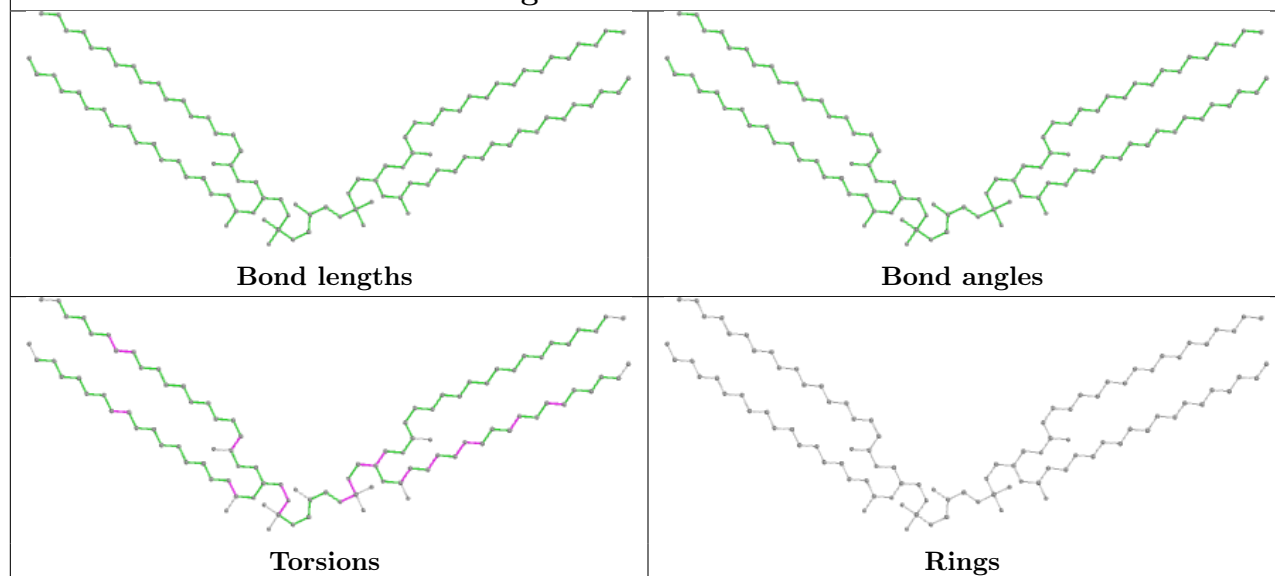




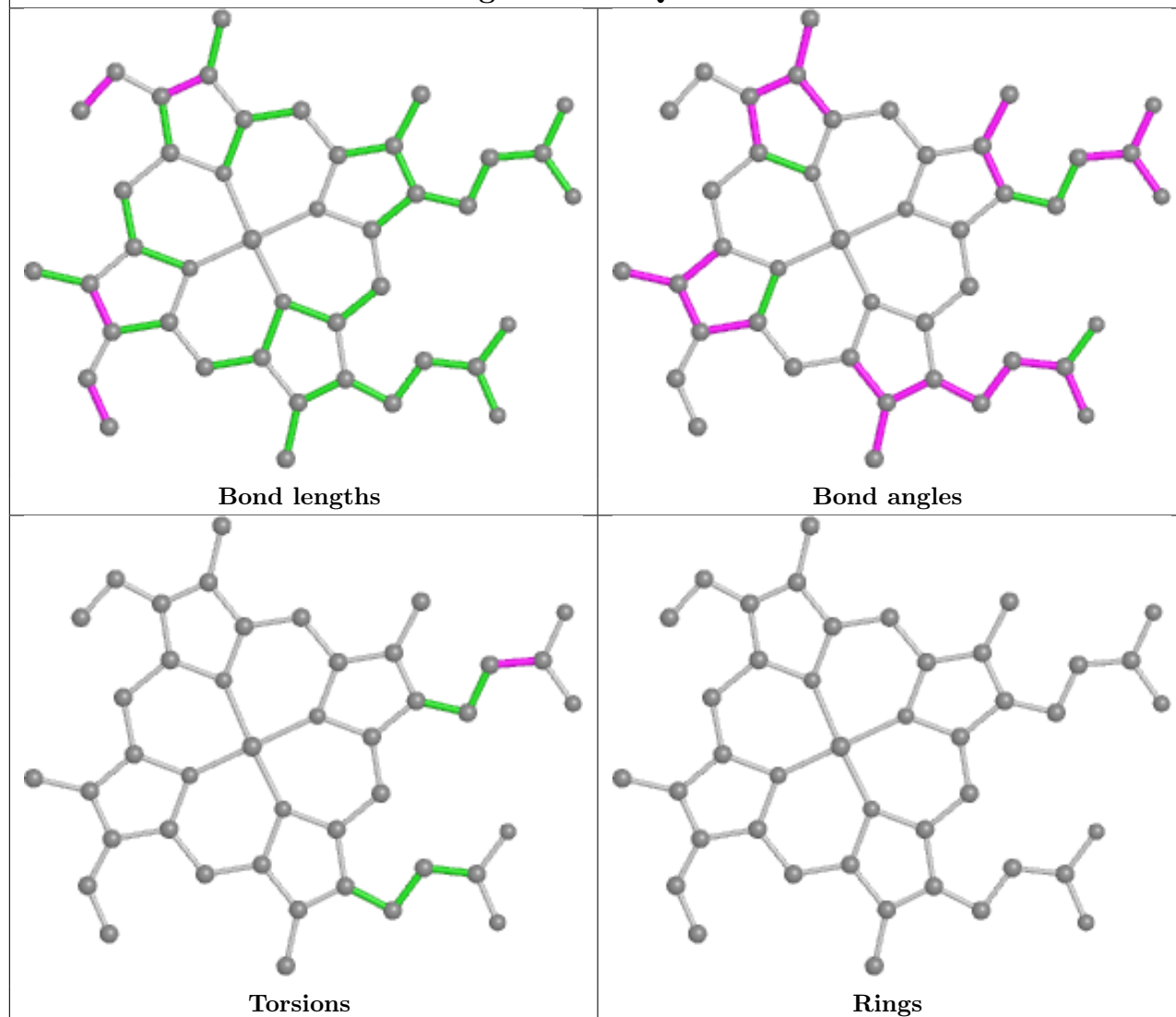


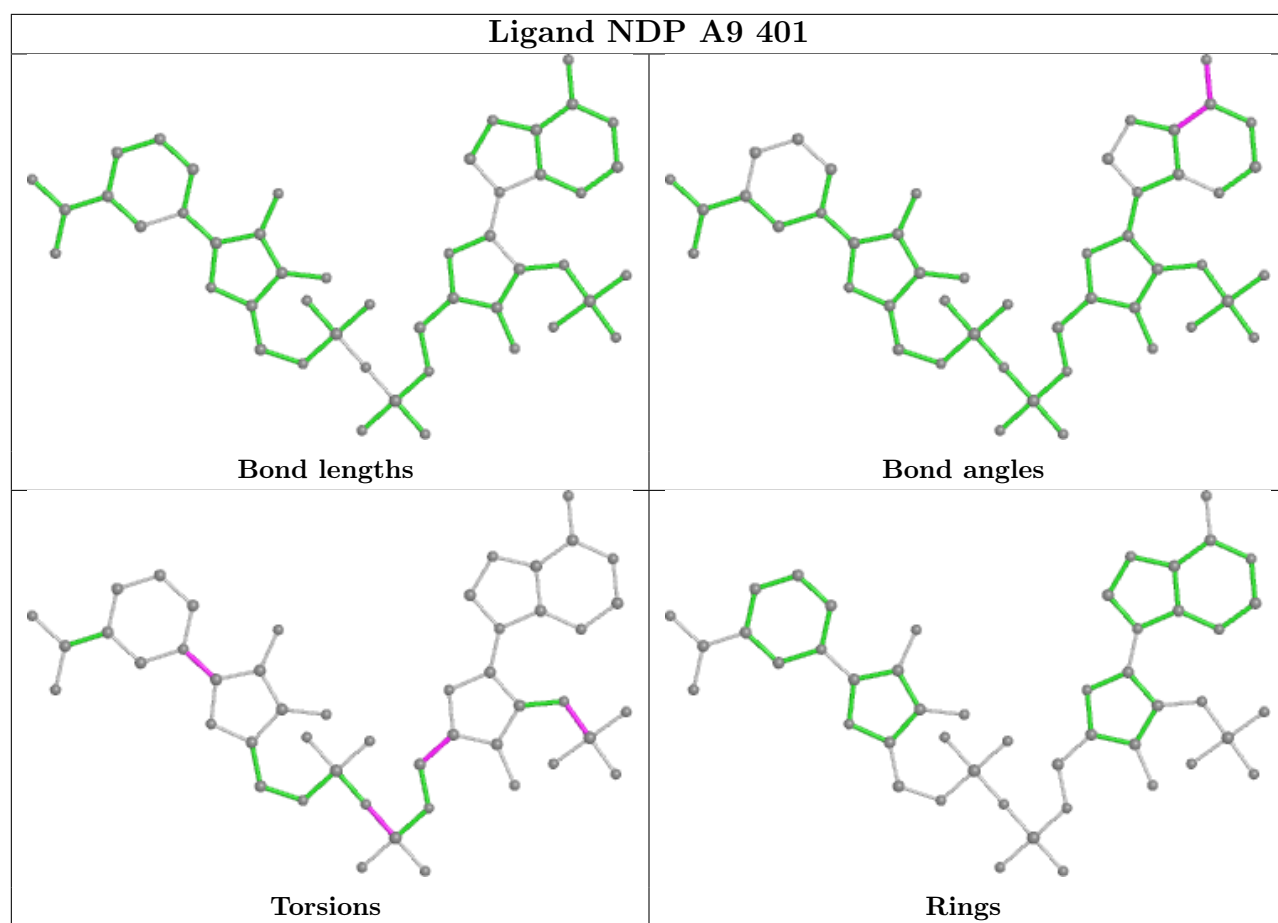


Ligand CDL N5 703

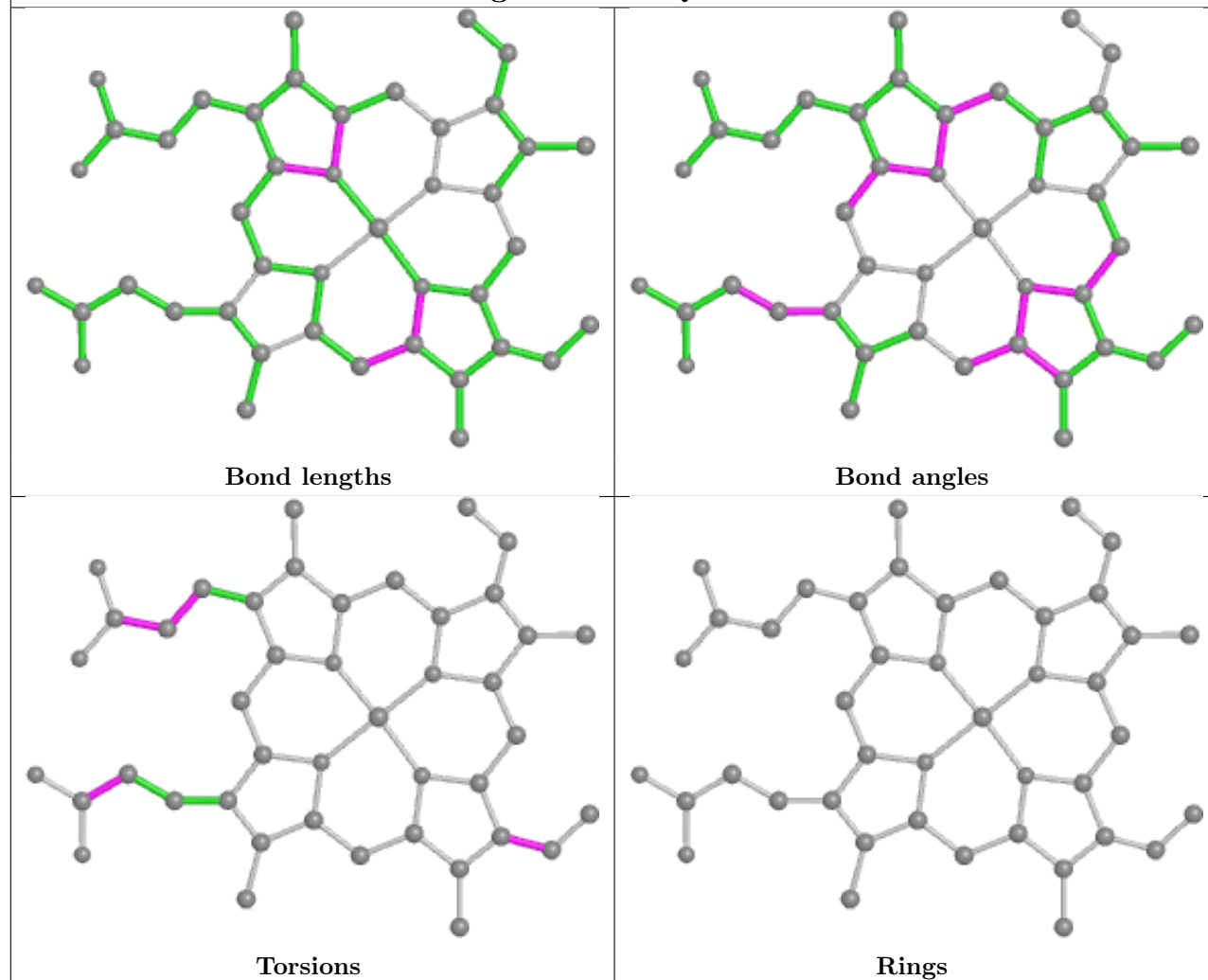


Ligand HEC Qd 401

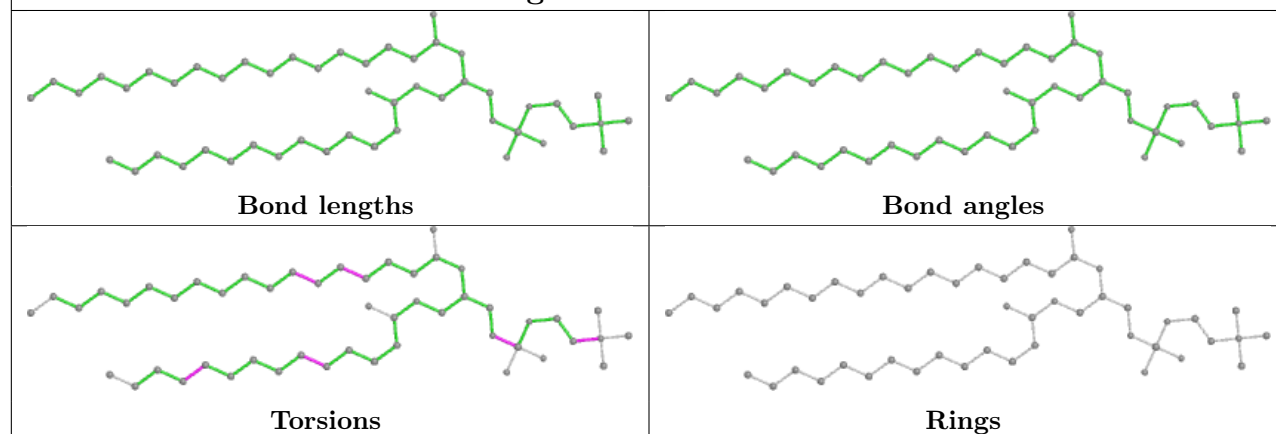


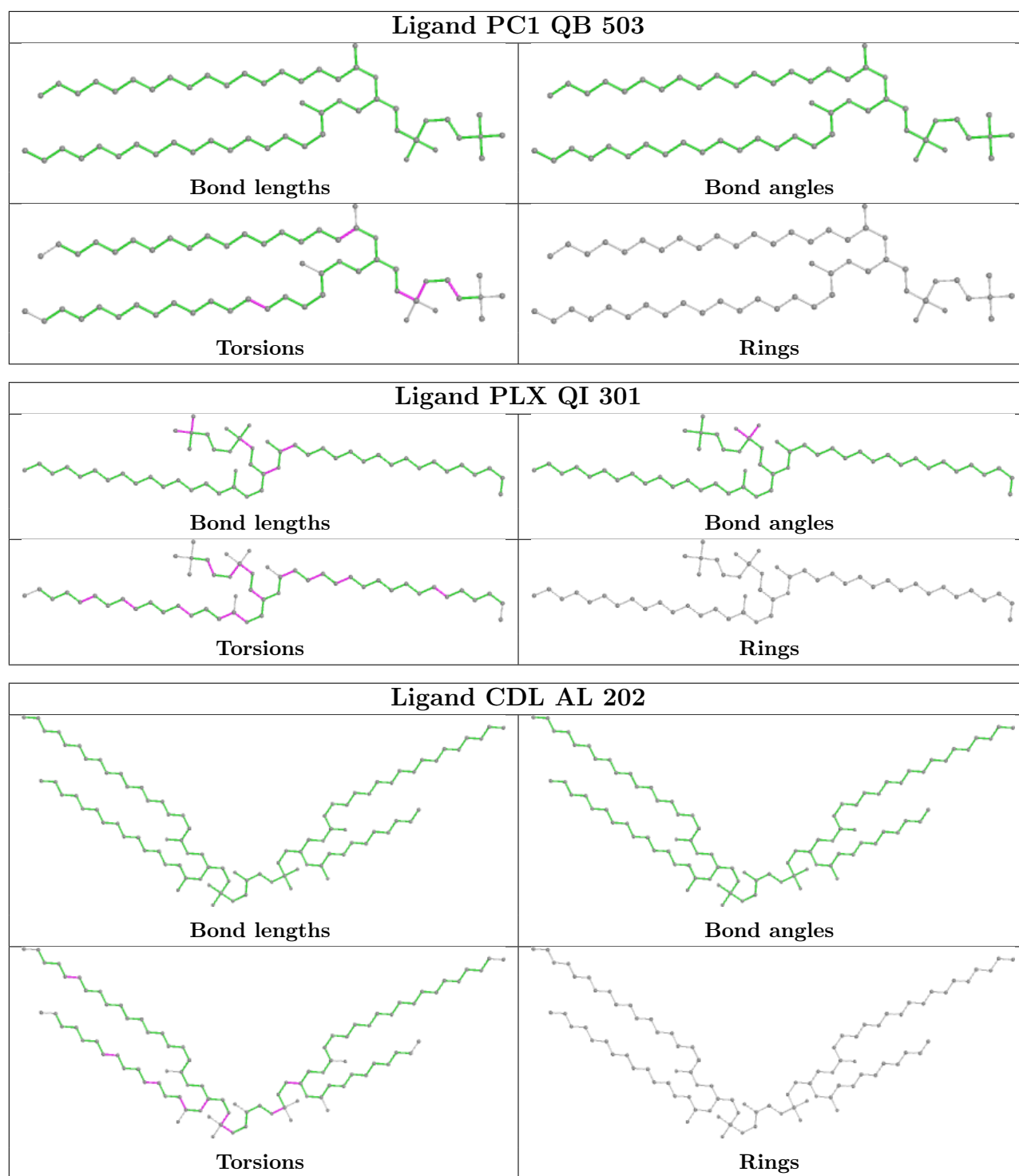


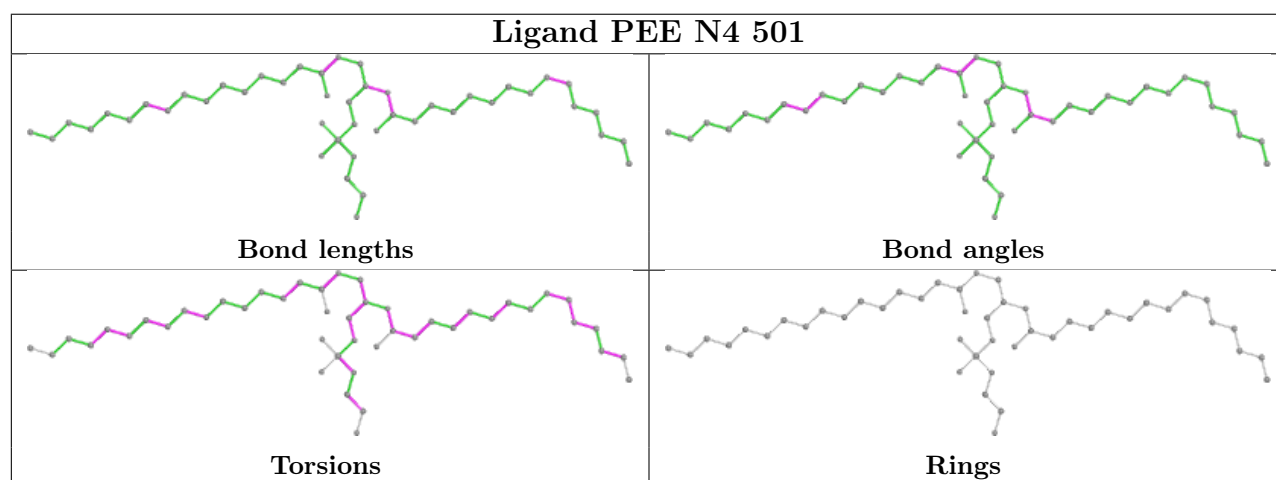
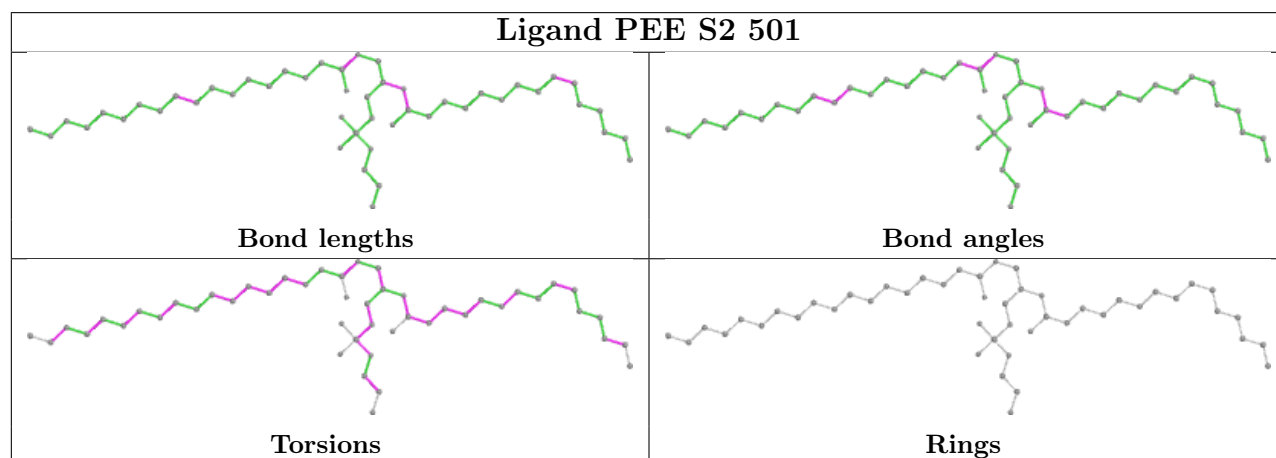
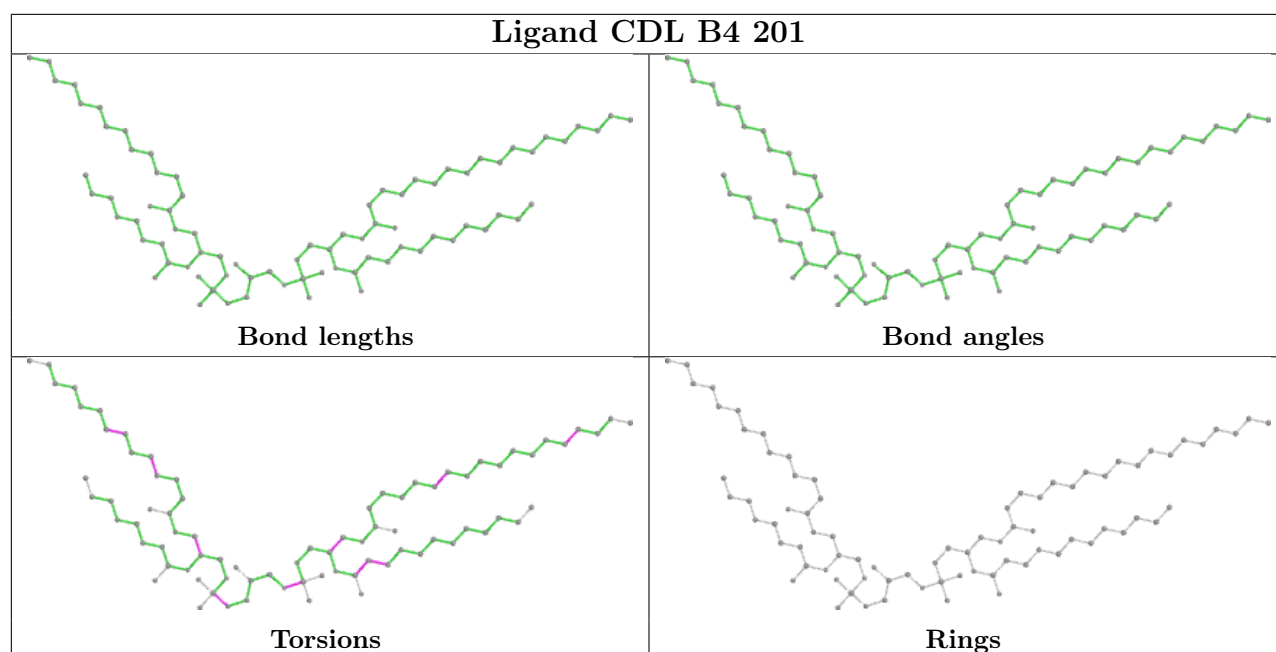
Ligand HEM Qc 402

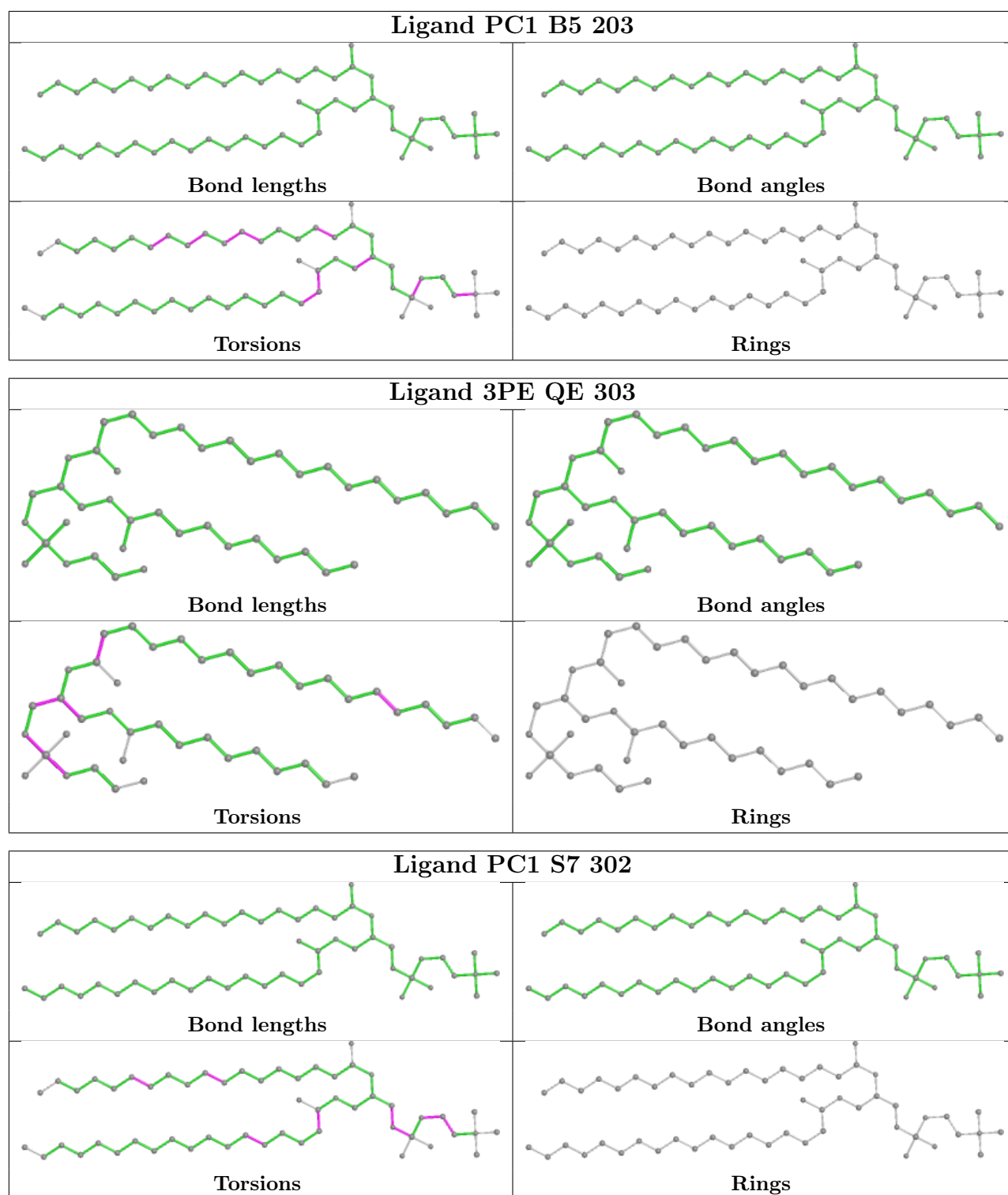


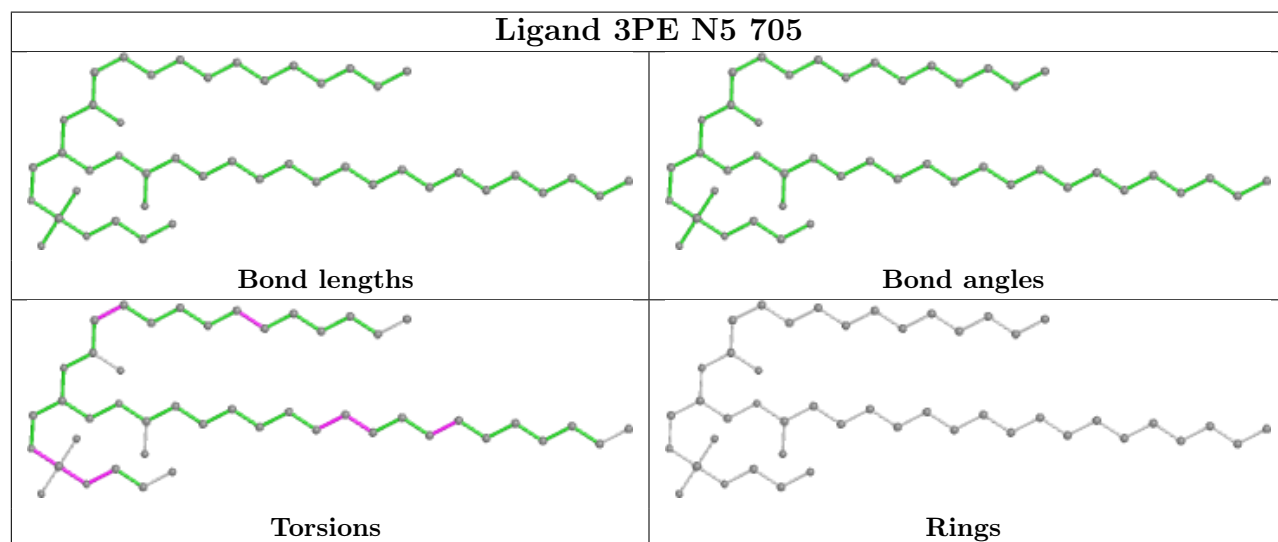
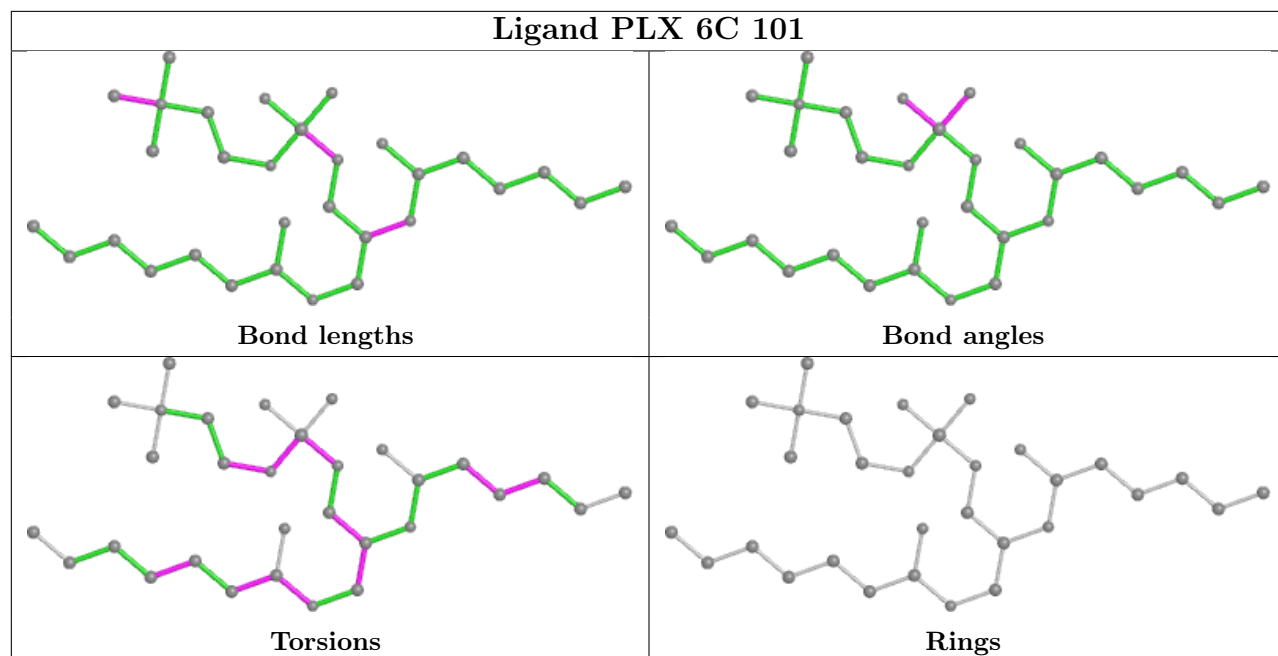
Ligand PC1 B4 202

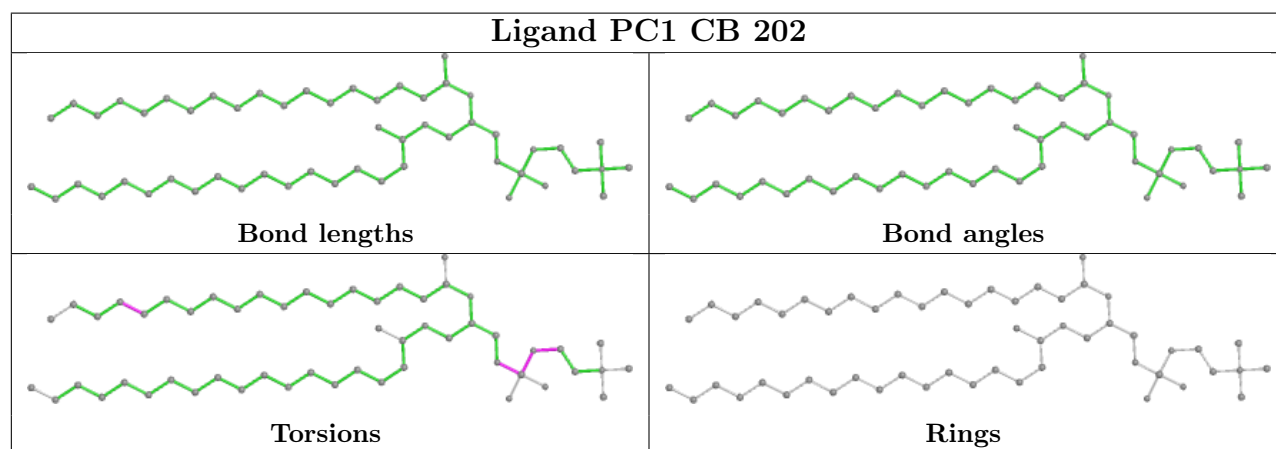
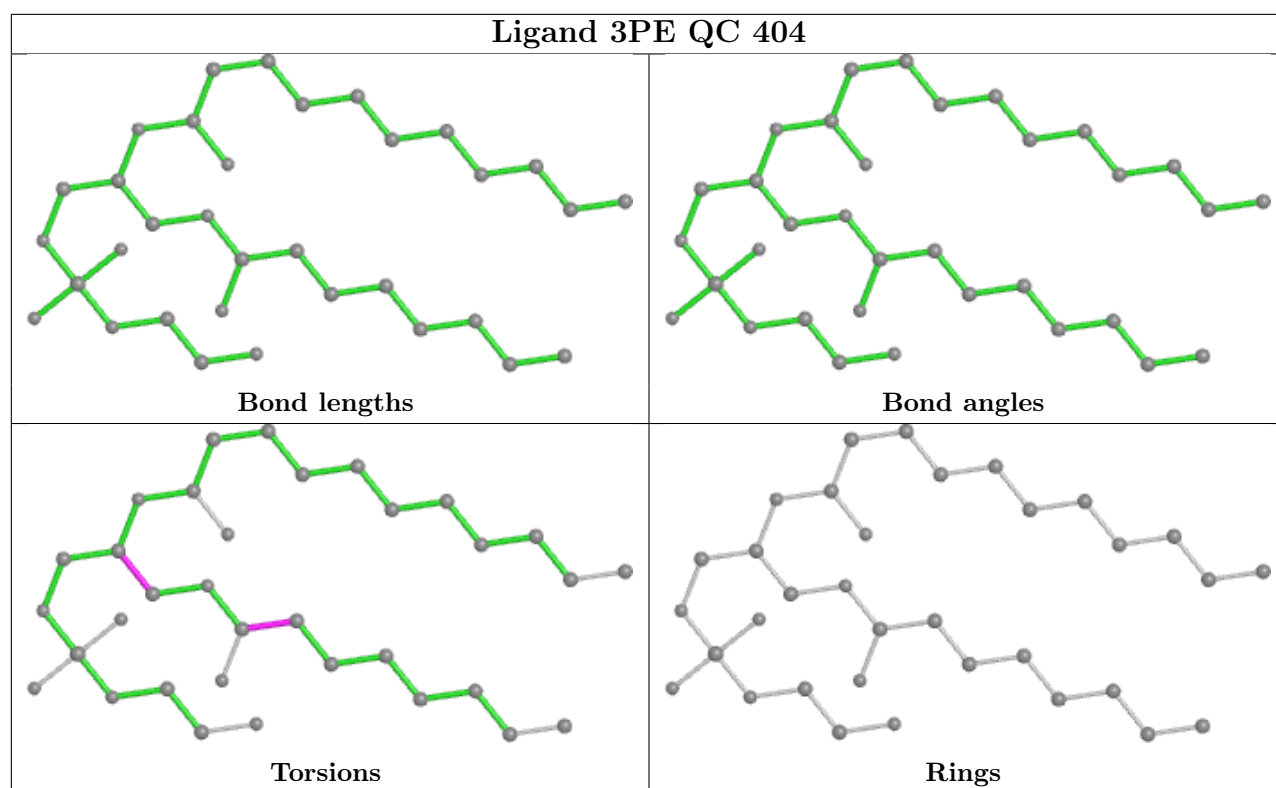


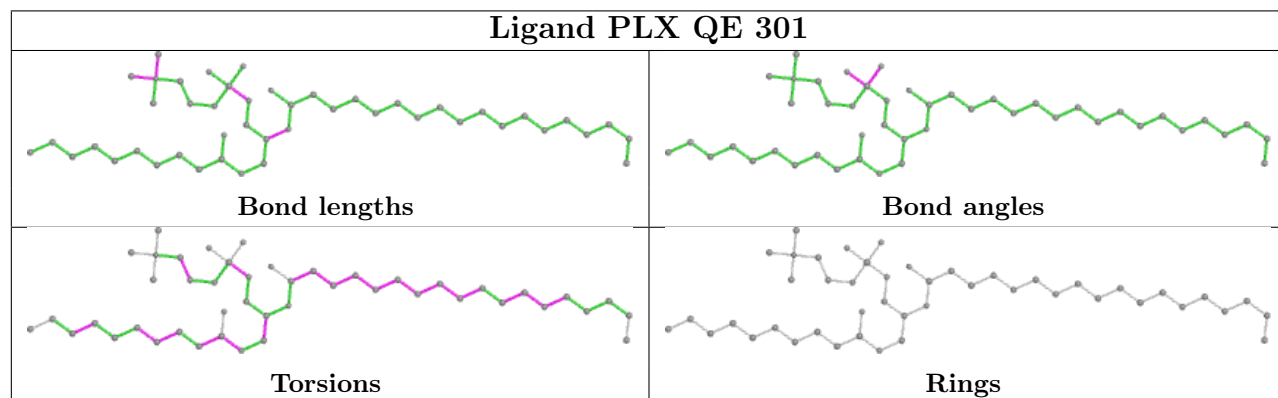
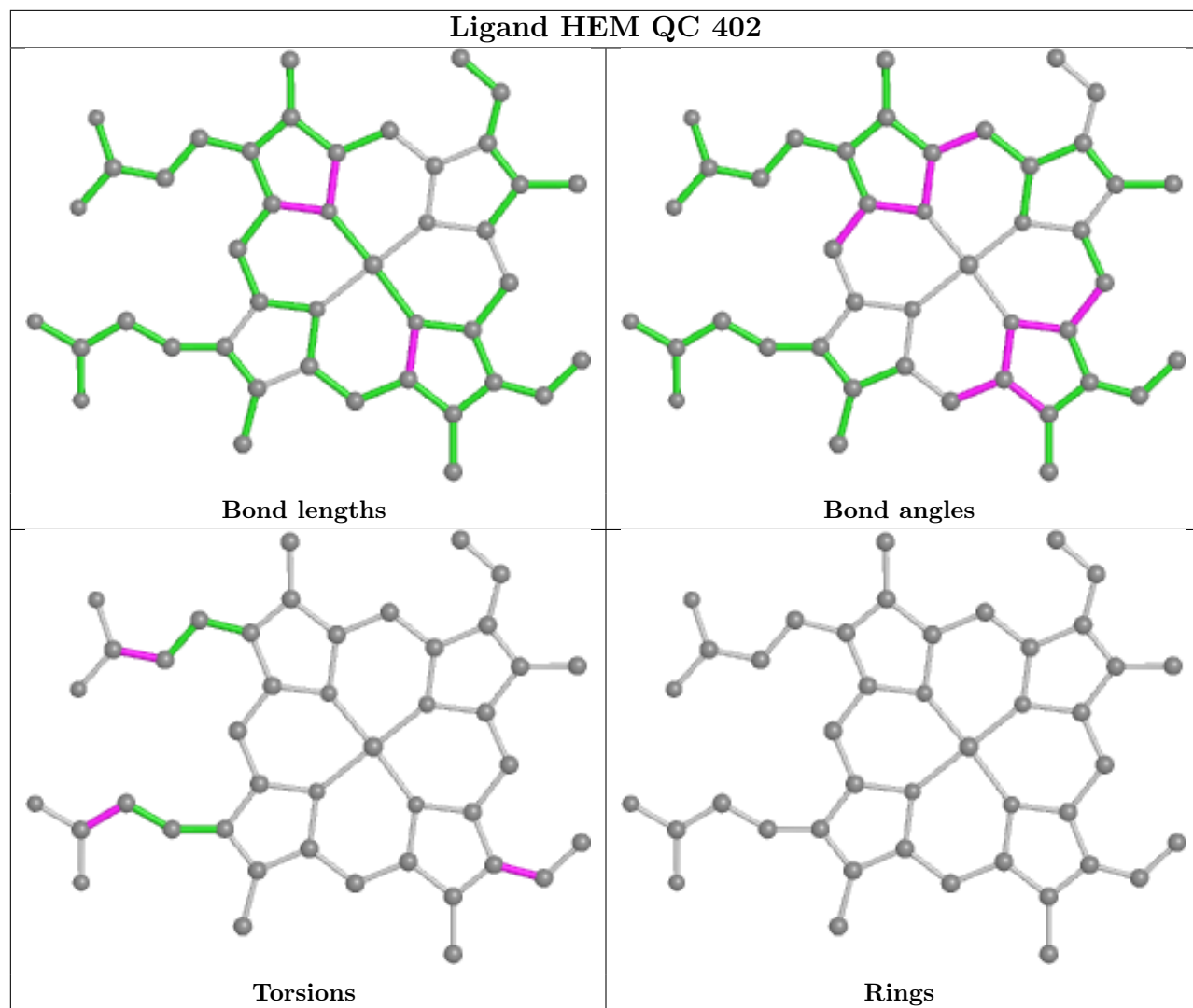


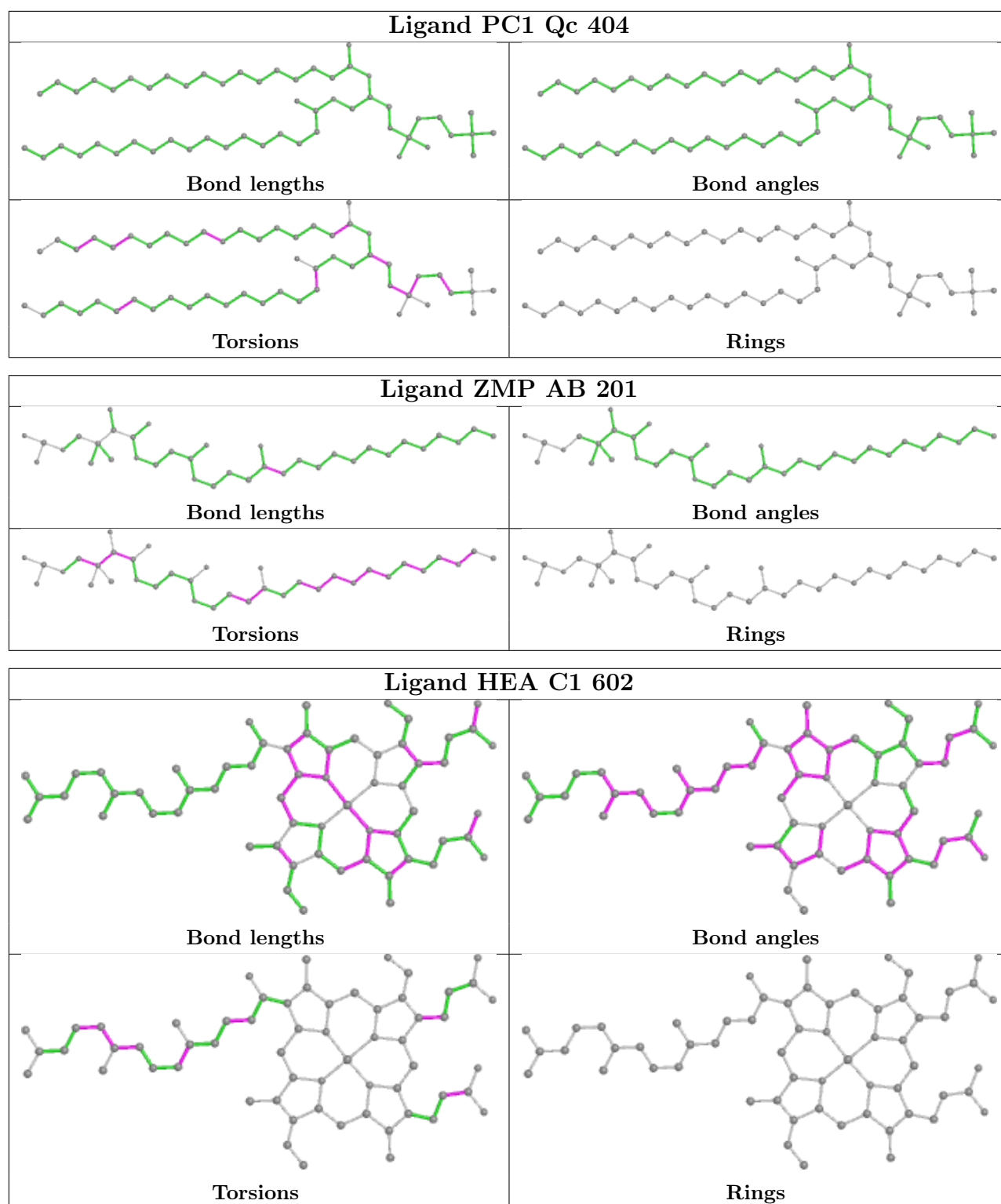


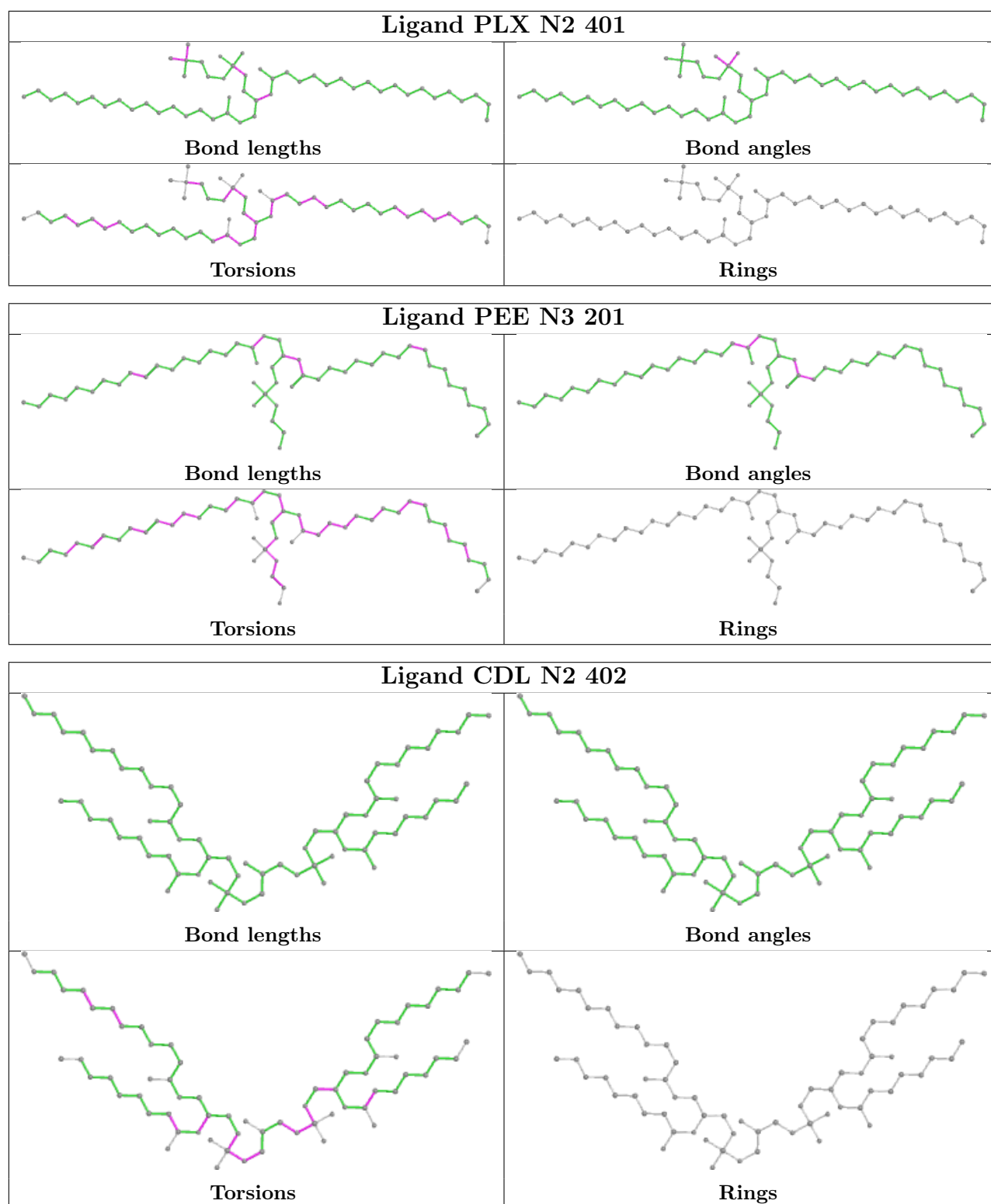


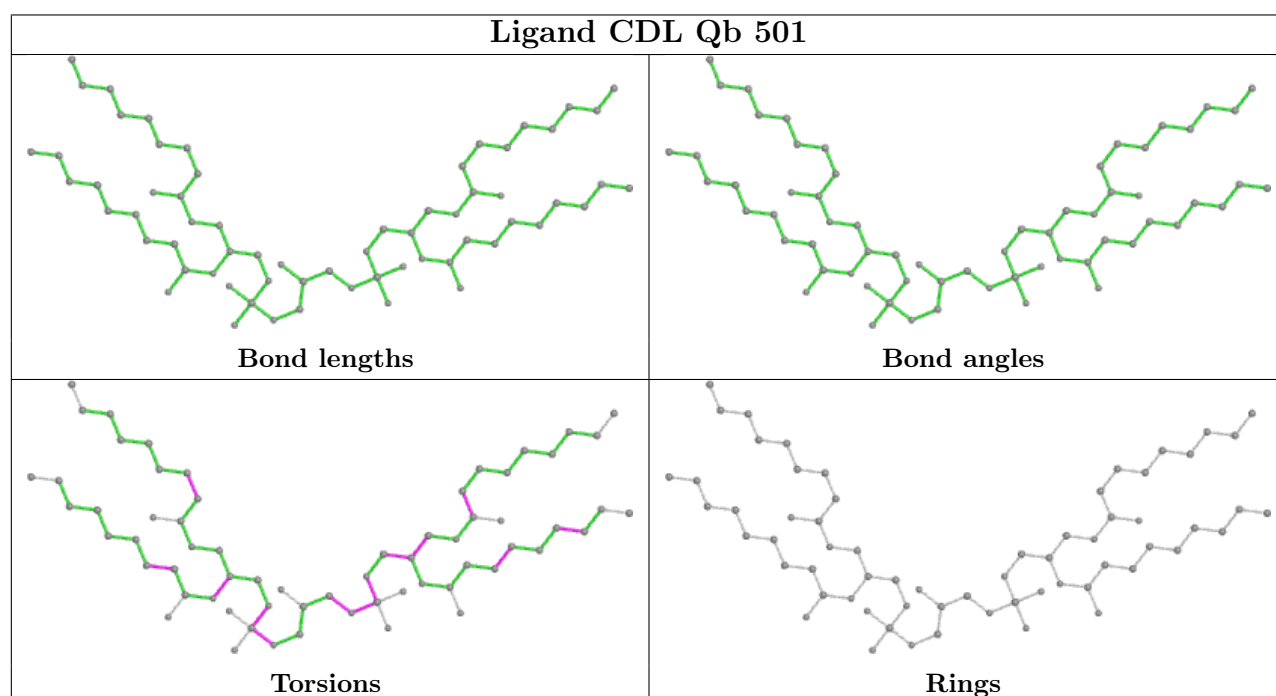
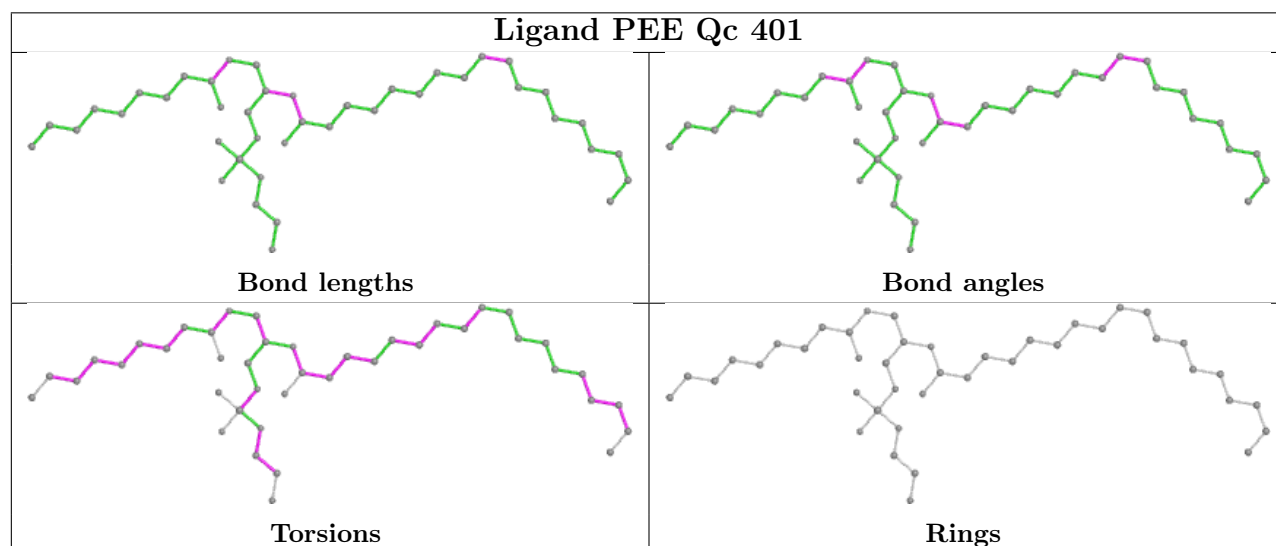
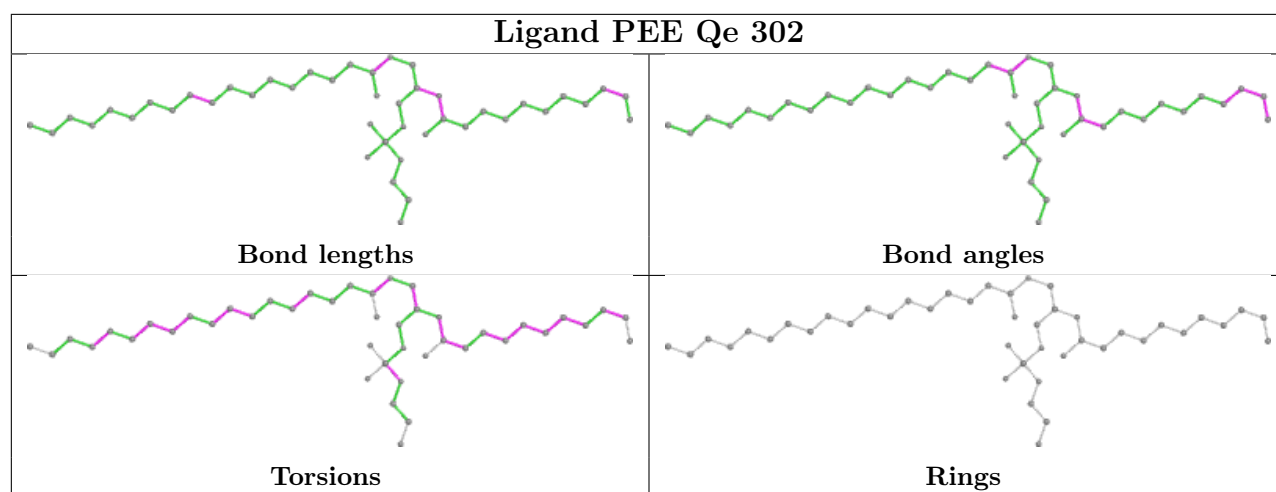


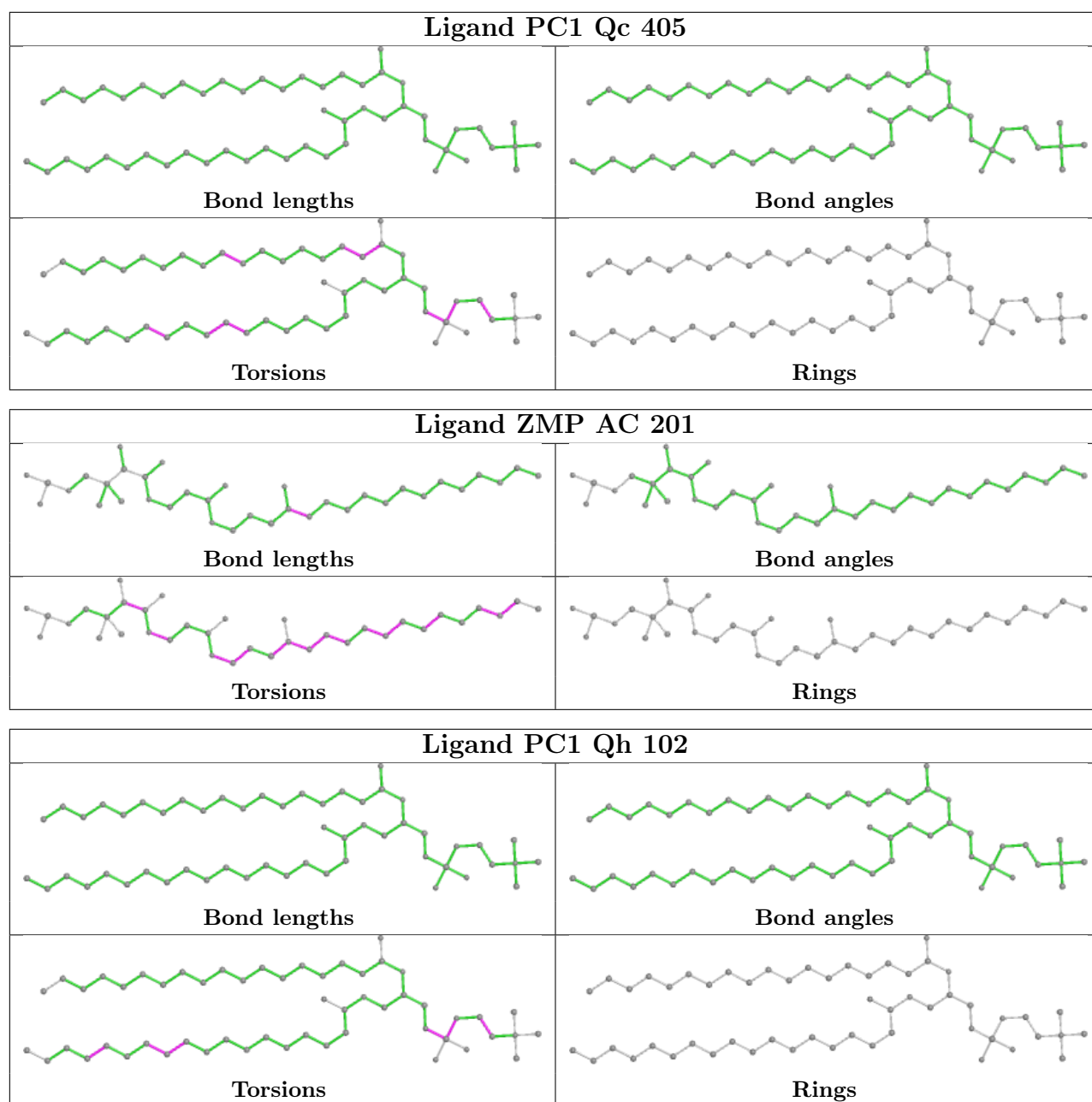


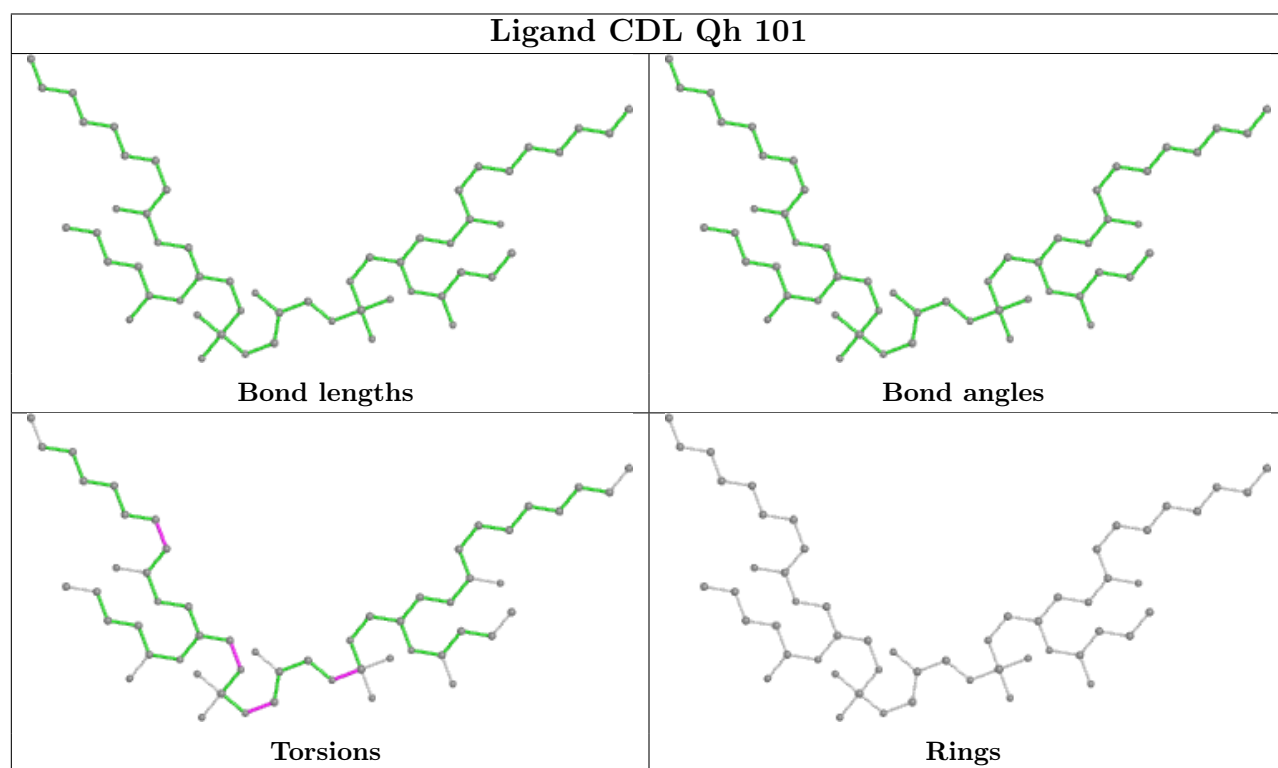
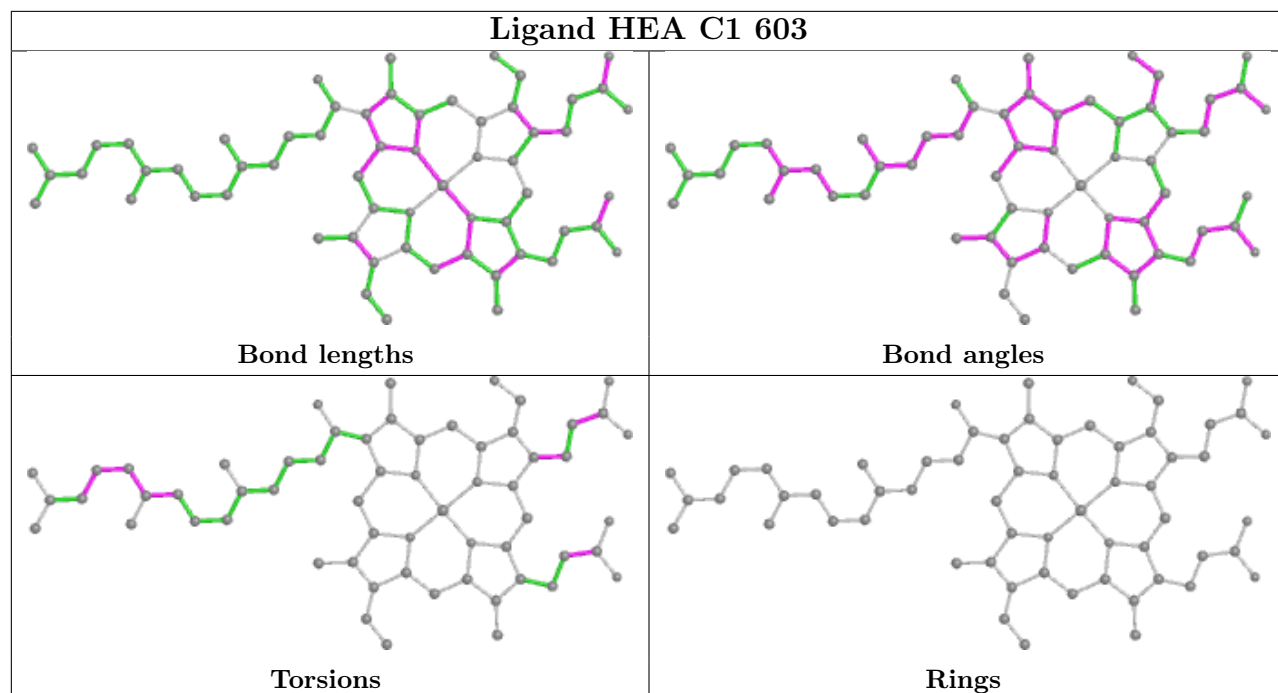


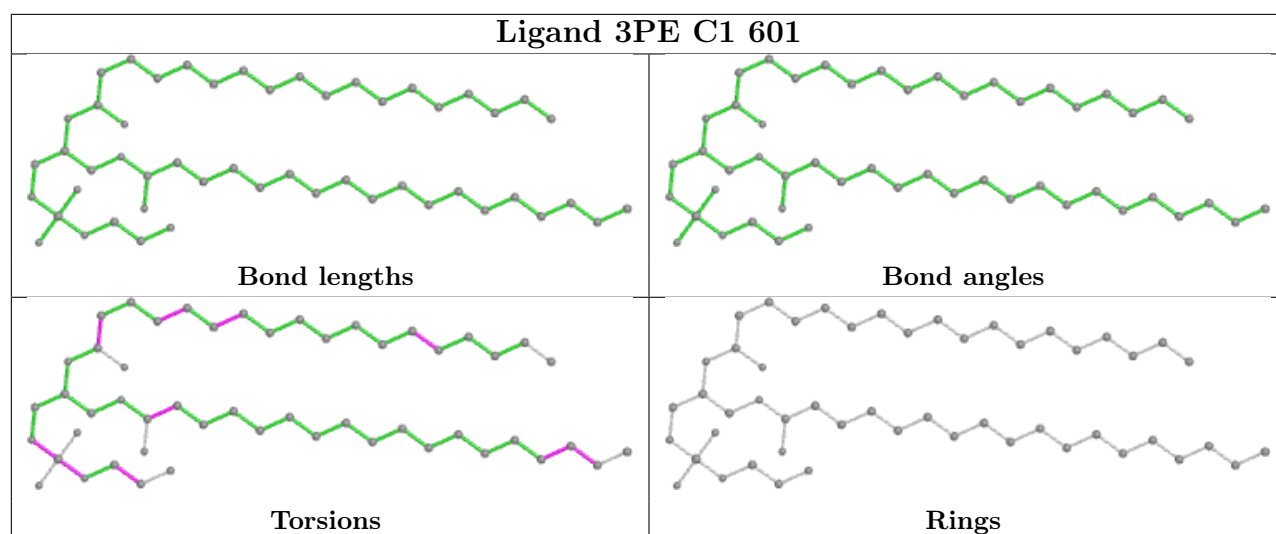












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

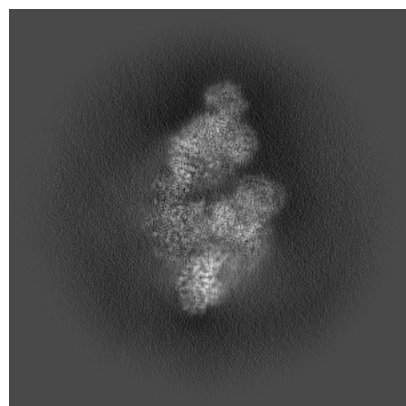
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60422. These allow visual inspection of the internal detail of the map and identification of artifacts.

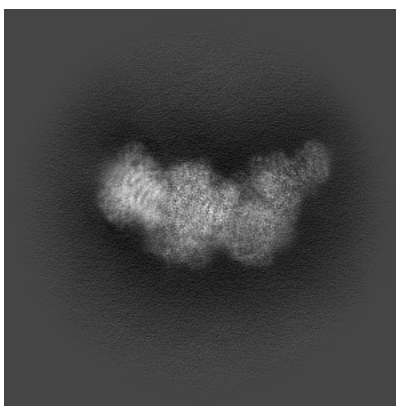
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

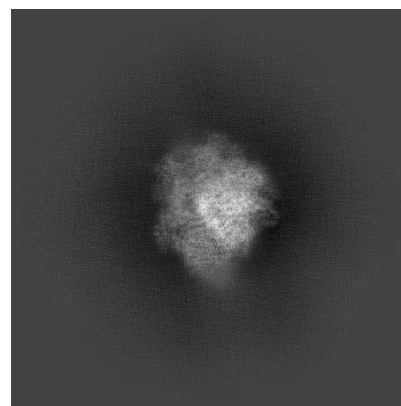
6.1.1 Primary map



X

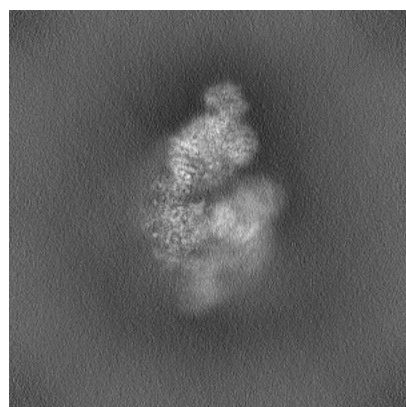


Y

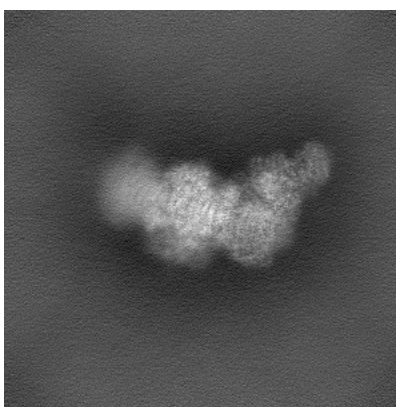


Z

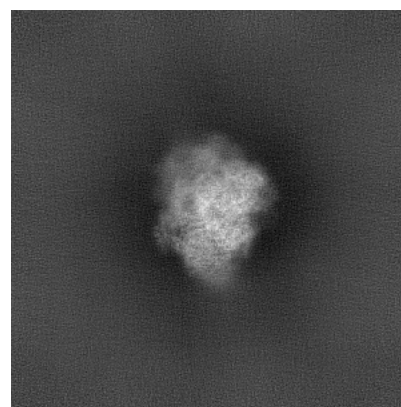
6.1.2 Raw map



X



Y

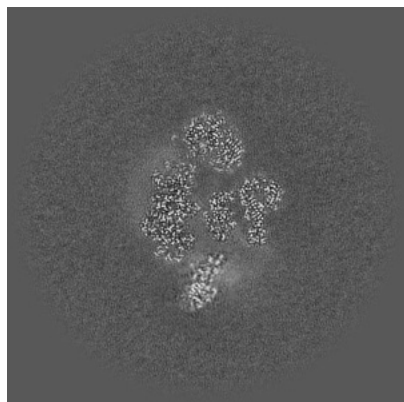


Z

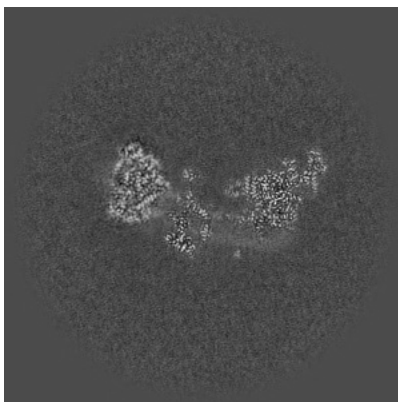
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

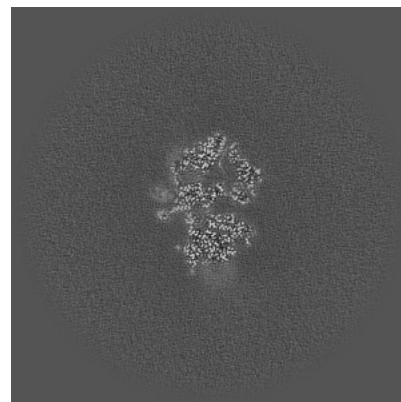
6.2.1 Primary map



X Index: 240

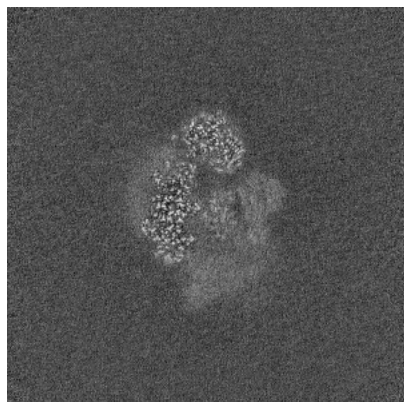


Y Index: 240

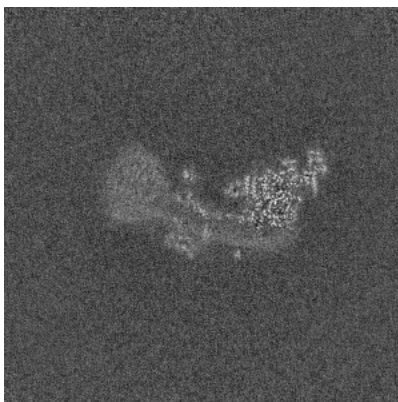


Z Index: 240

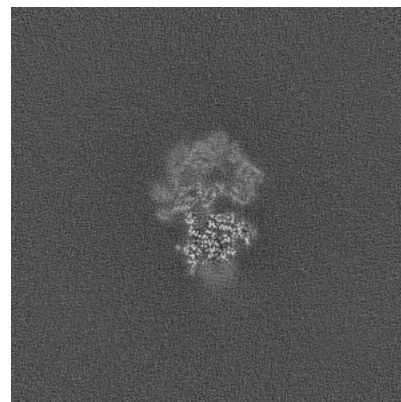
6.2.2 Raw map



X Index: 240



Y Index: 240

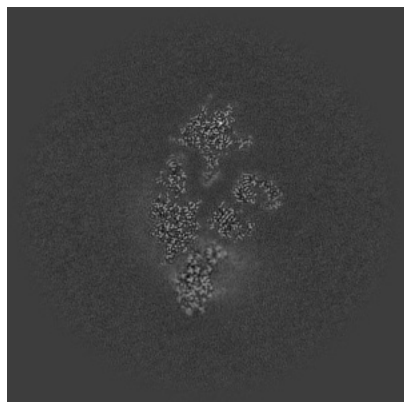


Z Index: 240

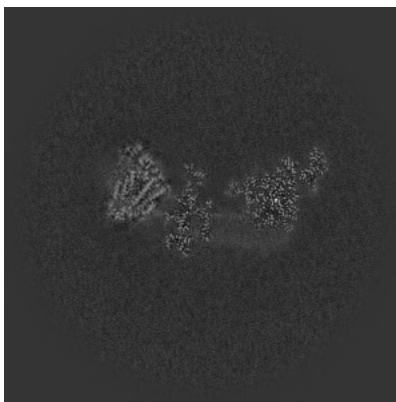
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

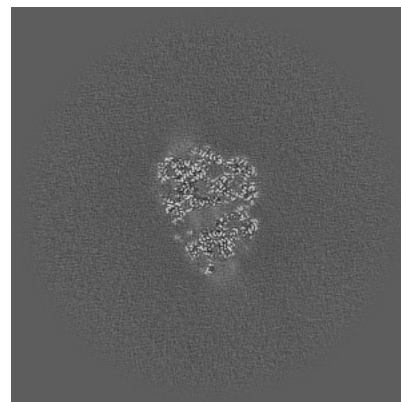
6.3.1 Primary map



X Index: 256

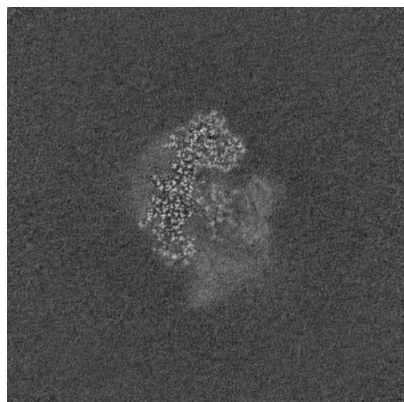


Y Index: 243

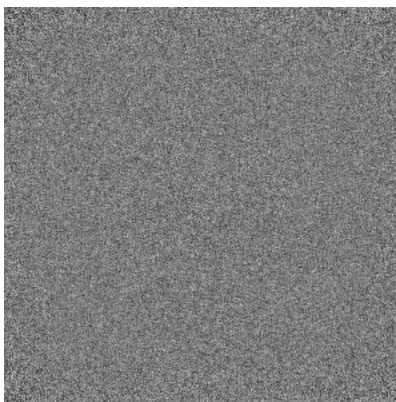


Z Index: 217

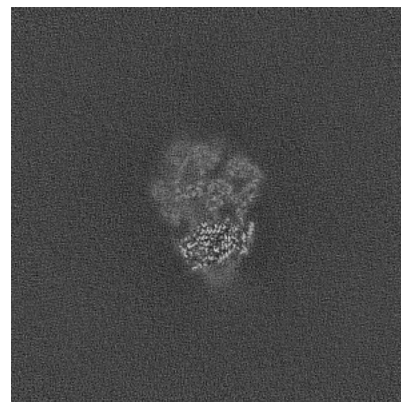
6.3.2 Raw map



X Index: 234



Y Index: 0

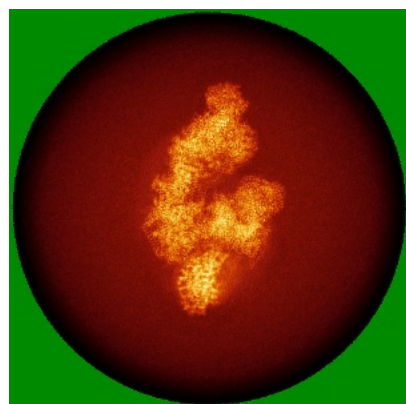


Z Index: 230

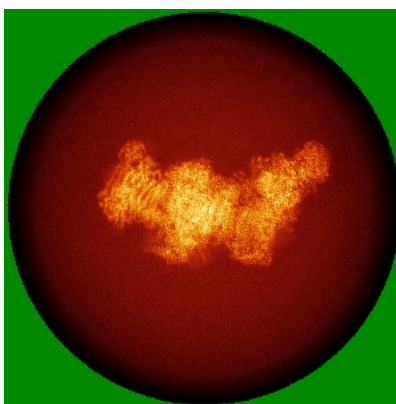
The images above show the largest variance slices of the map in three orthogonal directions.

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

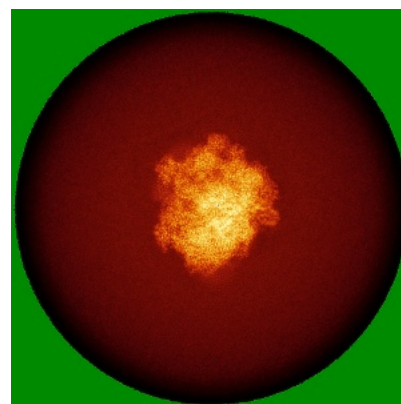
6.4.1 Primary map



X

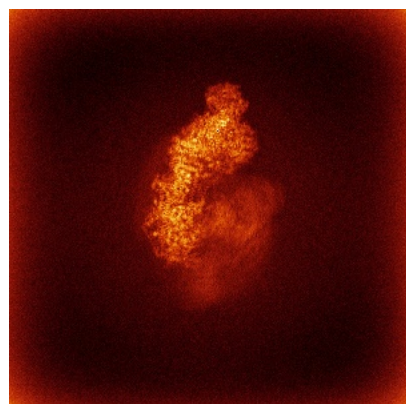


Y

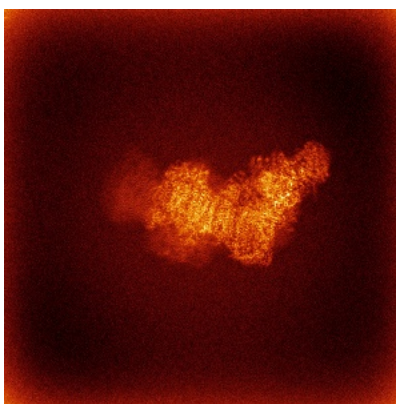


Z

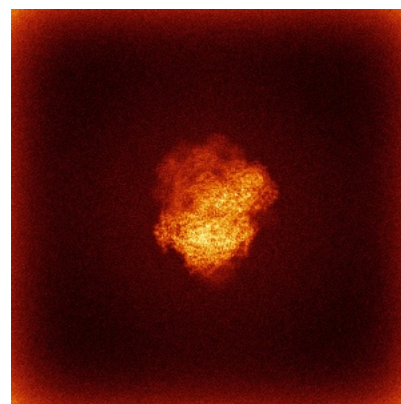
6.4.2 Raw map



X



Y

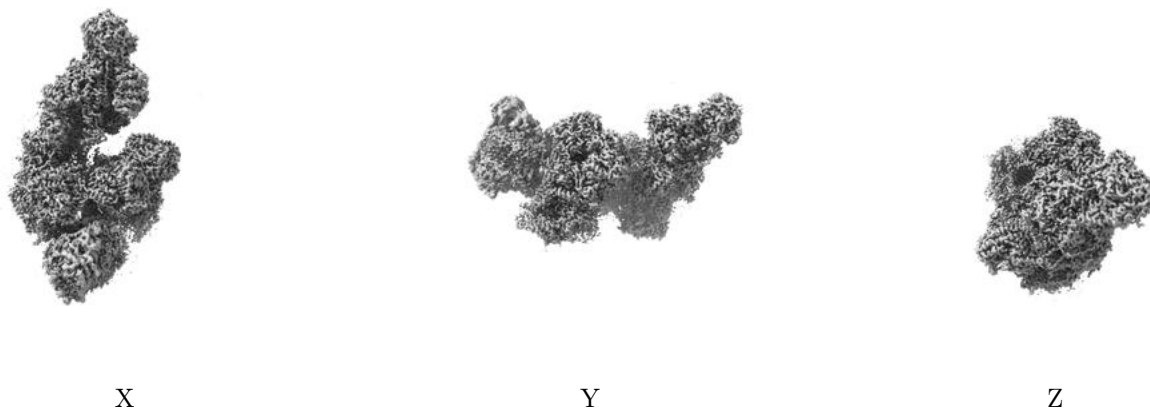


Z

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.

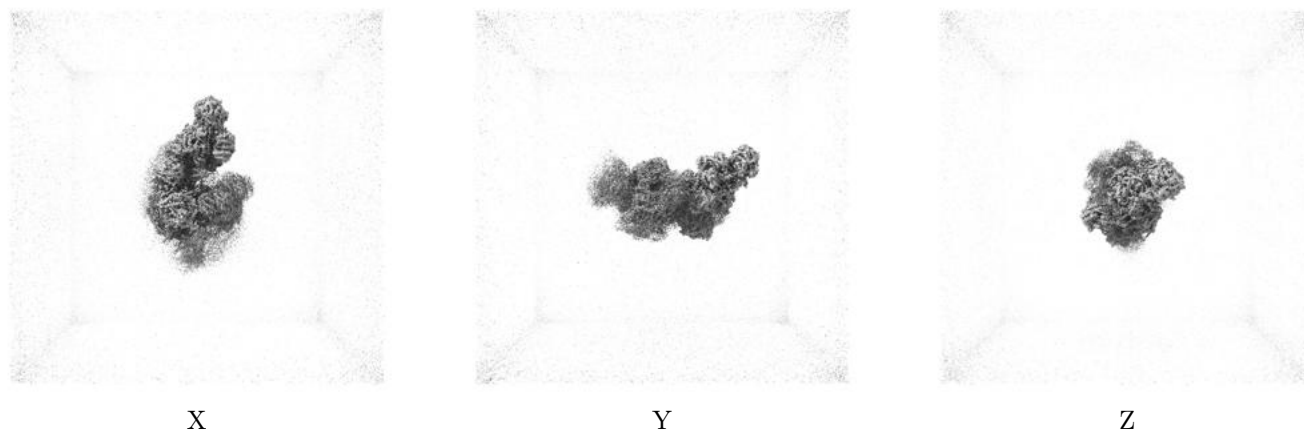
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. 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.

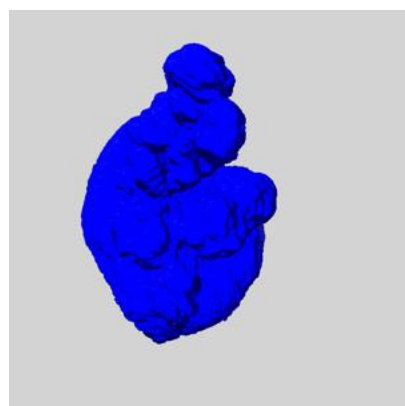
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

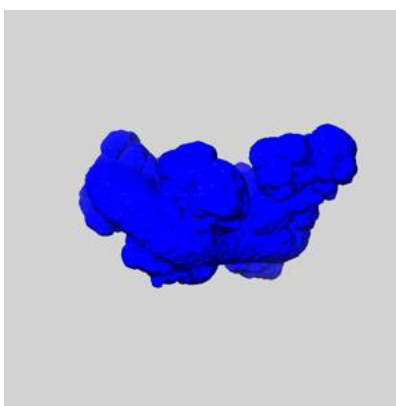
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

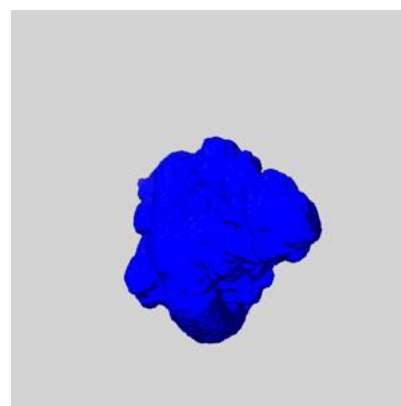
6.6.1 emd_60422_msk_1.map [i](#)



X



Y

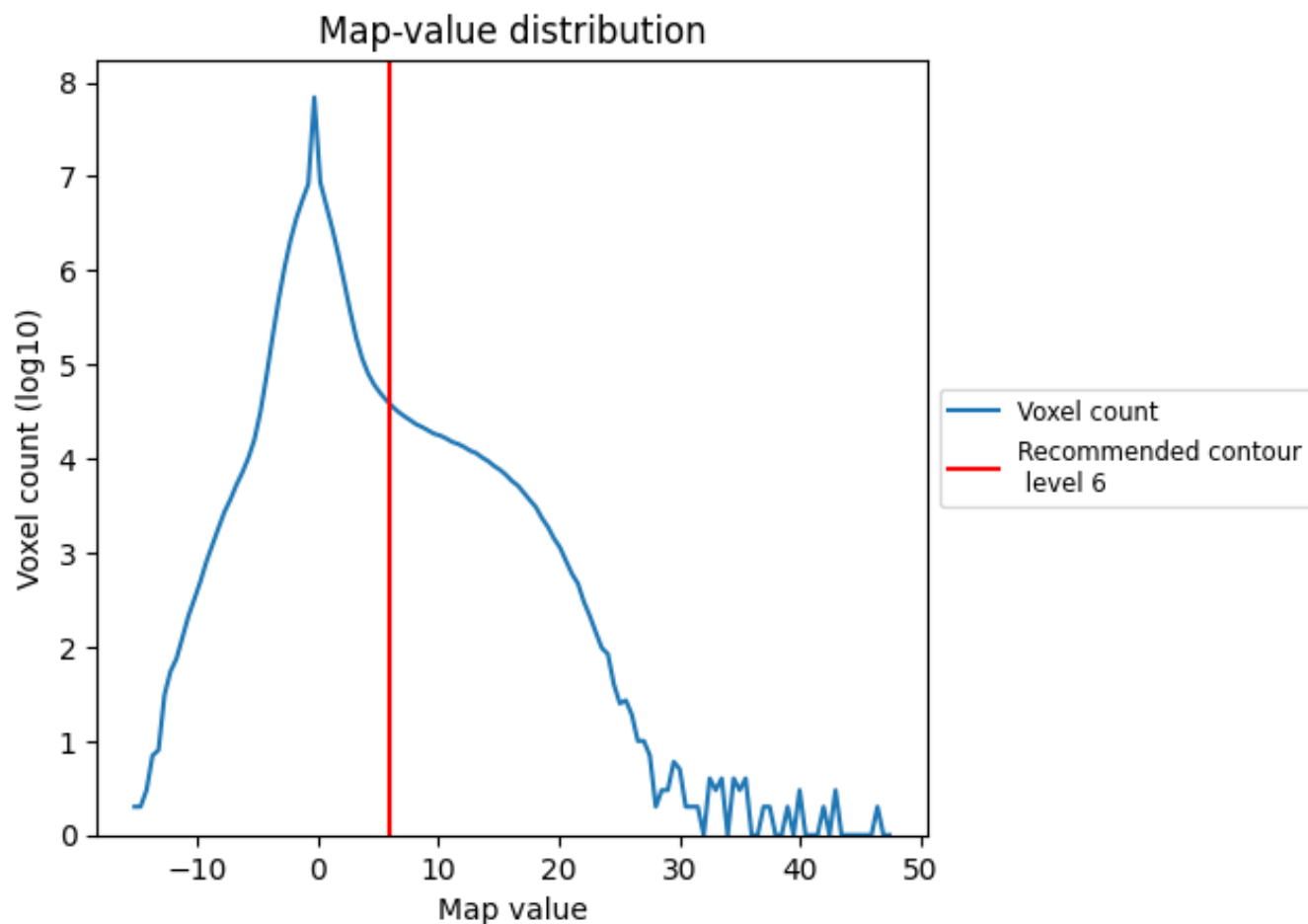


Z

7 Map analysis [i](#)

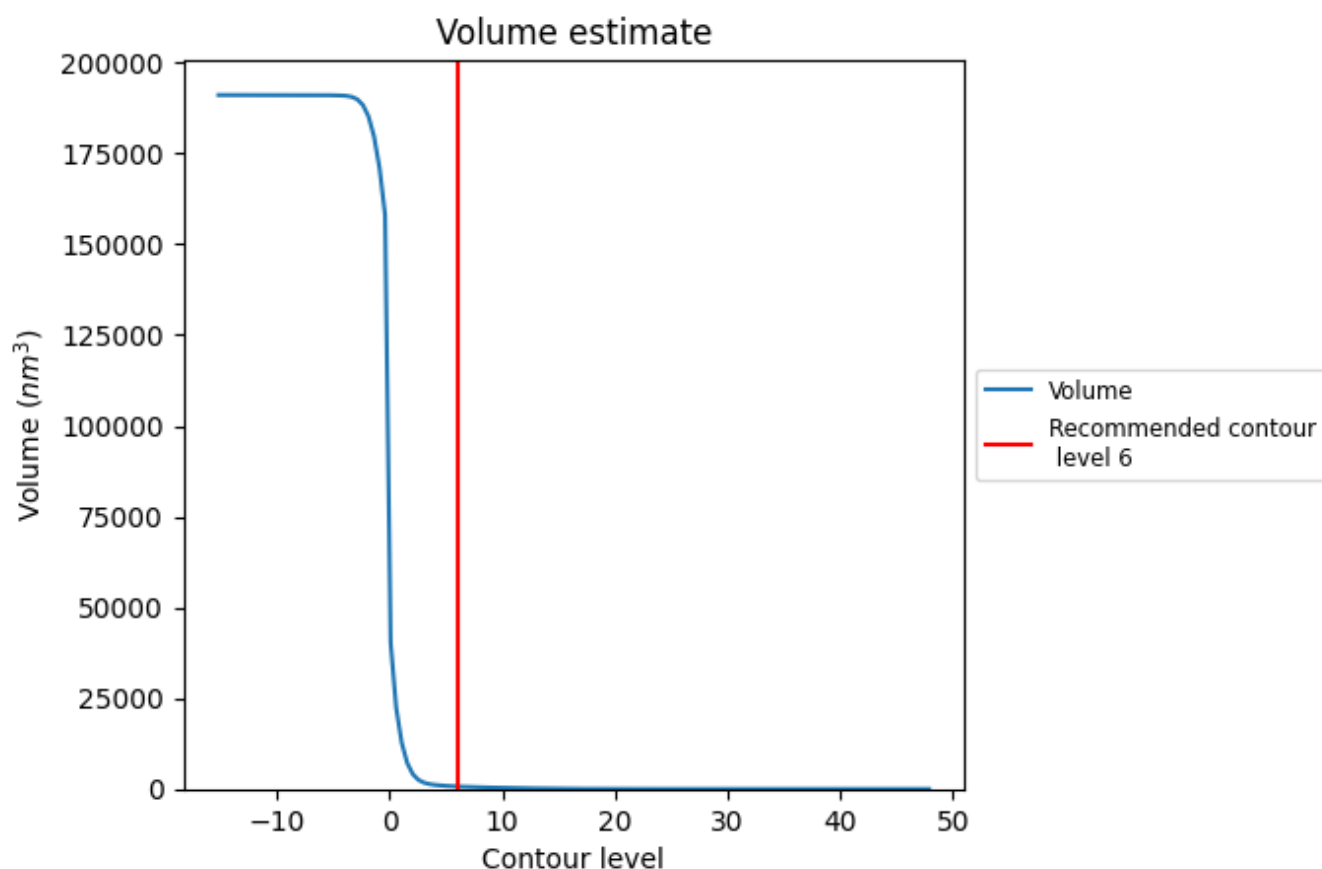
This section contains the results of statistical analysis of the map.

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.

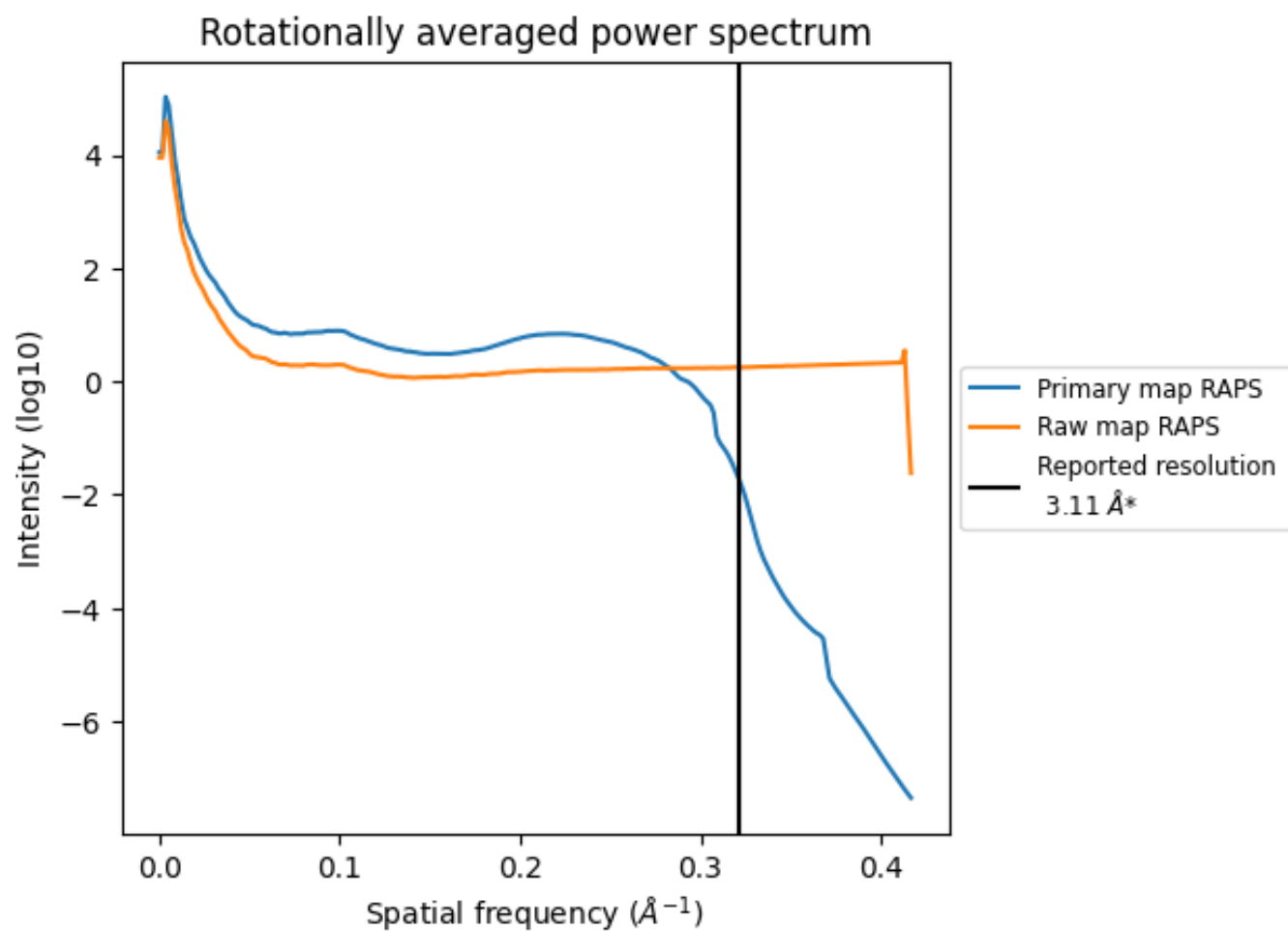
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 677 nm³; this corresponds to an approximate mass of 611 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 ⓘ

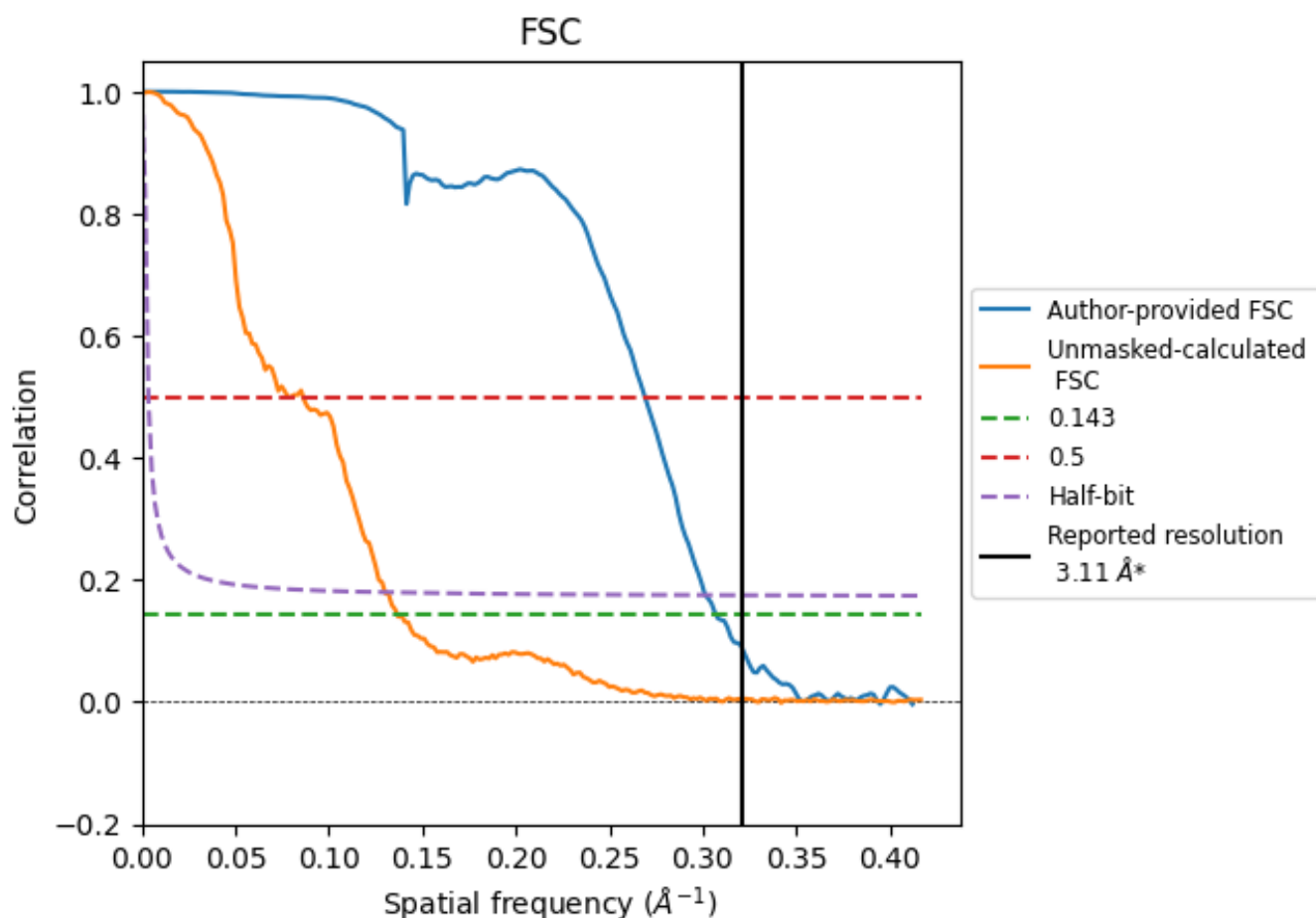


*Reported resolution corresponds to spatial frequency of 0.322 \AA^{-1}

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 0.322 \AA^{-1}

8.2 Resolution estimates [i](#)

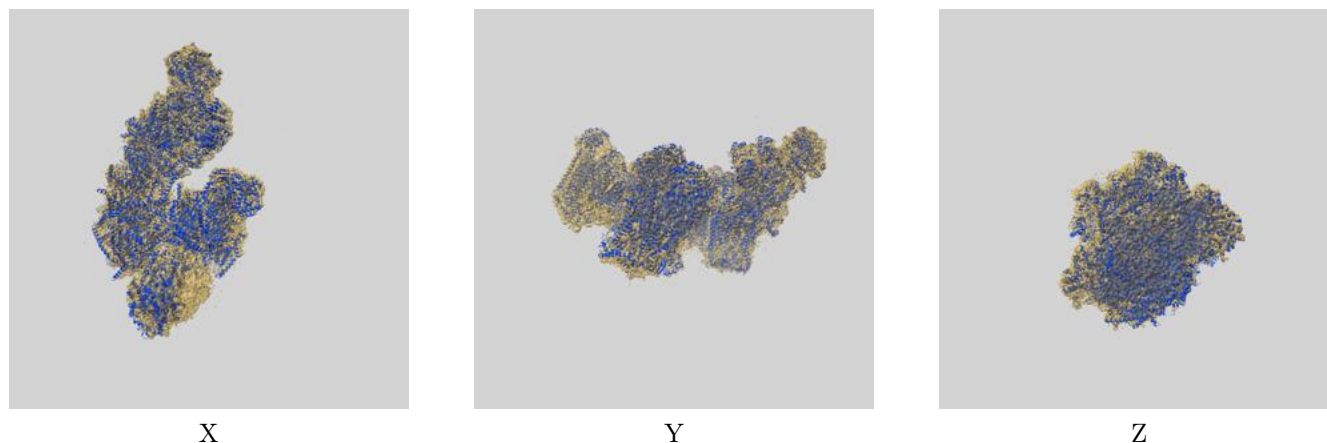
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.26	3.72	3.32
Unmasked-calculated*	7.32	12.82	7.69

*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 7.32 differs from the reported value 3.11 by more than 10 %

9 Map-model fit [i](#)

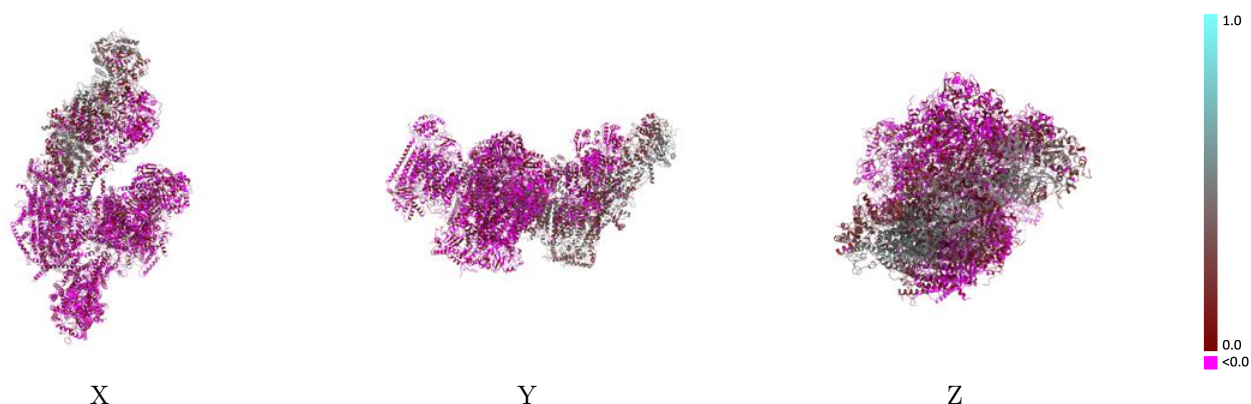
This section contains information regarding the fit between EMDB map EMD-60422 and PDB model 8ZSO. Per-residue inclusion information can be found in section [3](#) on page [30](#).

9.1 Map-model overlay [i](#)



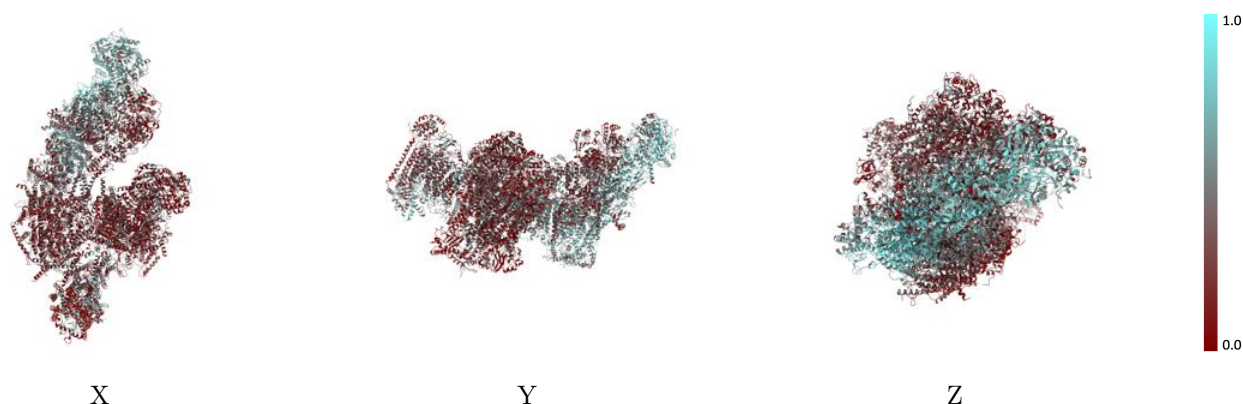
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



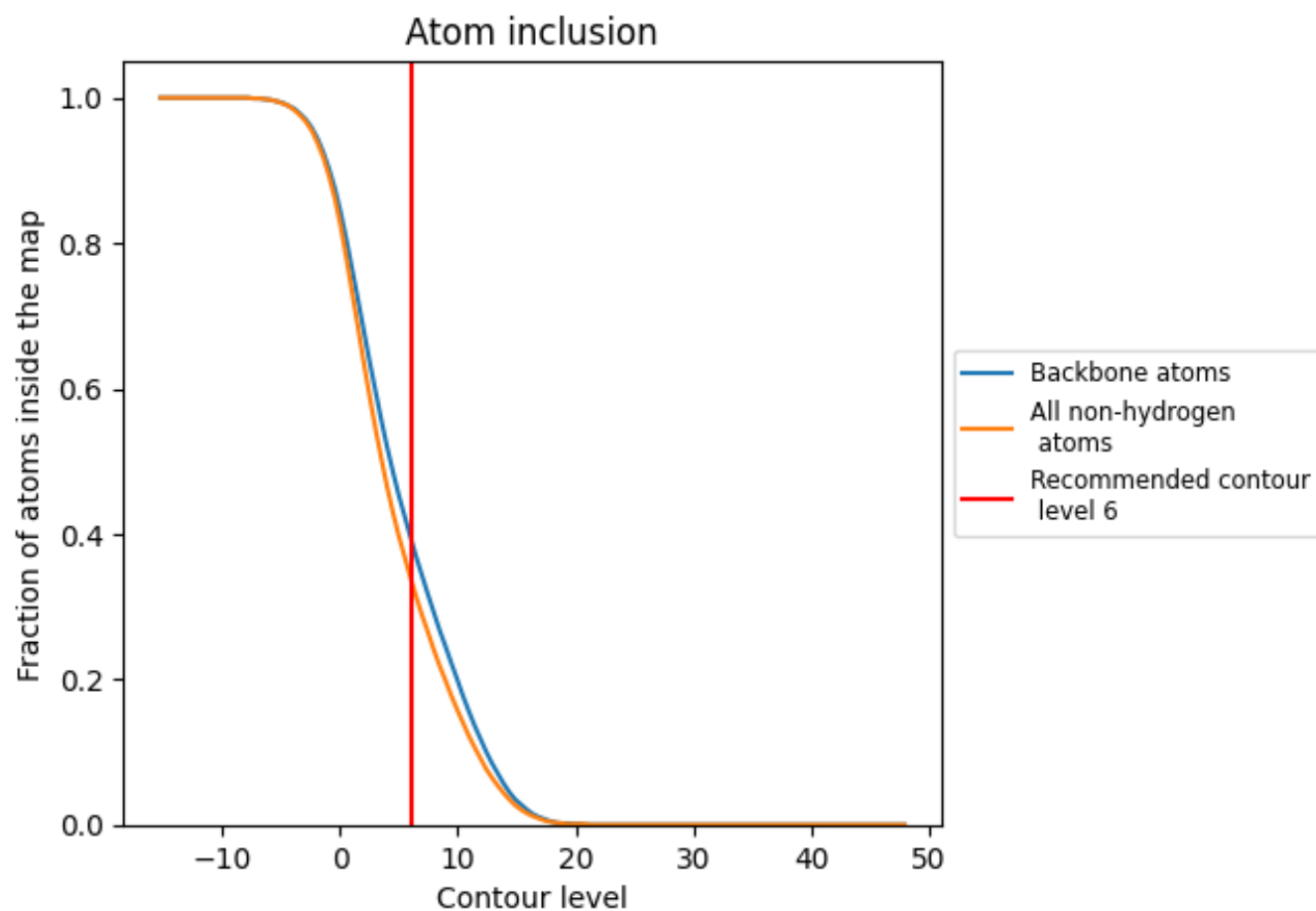
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 34% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3390	 0.0830
4L	 0.6310	 0.3660
5A	 0.2190	 -0.0300
5B	 0.3280	 -0.0290
6A	 0.3900	 -0.0110
6B	 0.5320	 0.0310
6C	 0.1700	 -0.0220
7A	 0.2190	 -0.0060
7B	 0.0550	 -0.0010
7C	 0.3450	 0.0400
8B	 0.1480	 -0.0470
A1	 0.6060	 0.3150
A2	 0.2410	 0.0140
A3	 0.7220	 0.4490
A5	 0.3120	 0.0990
A6	 0.2700	 0.0320
A7	 0.5030	 0.3660
A8	 0.5770	 0.3130
A9	 0.2600	 -0.0080
AB	 0.1740	 0.0290
AC	 0.2310	 0.0260
AK	 0.3940	 0.1700
AL	 0.2720	 0.0240
AM	 0.4170	 0.2530
AN	 0.6460	 0.3810
B1	 0.2310	 -0.0230
B2	 0.1930	 0.0190
B3	 0.1790	 0.0240
B4	 0.1930	 -0.0690
B5	 0.3180	 0.0340
B6	 0.1900	 -0.0050
B7	 0.2870	 0.0240
B8	 0.2060	 -0.0550
B9	 0.2000	 -0.0040
BK	 0.2100	 -0.0470









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Chain	Atom inclusion	Q-score
BL	 0.2040	 -0.0380
C1	 0.3640	 -0.0380
C2	 0.3820	 0.0080
C3	 0.3810	 -0.0010
C4	 0.1980	 -0.0110
CA	 0.3420	 0.0850
CB	 0.3950	 0.1270
N1	 0.6410	 0.3750
N2	 0.5170	 0.2280
N3	 0.5890	 0.3610
N4	 0.2410	 -0.0760
N5	 0.2270	 -0.0300
N6	 0.5070	 0.3170
QA	 0.2370	 0.0180
QB	 0.2310	 0.0190
QC	 0.2550	 -0.0330
QD	 0.2360	 -0.0190
QE	 0.1260	 0.0380
QF	 0.1480	 -0.0090
QG	 0.2140	 -0.0070
QH	 0.1870	 -0.0020
QI	 0.2230	 -0.0280
QJ	 0.1780	 0.0020
QK	 0.1230	 -0.0020
Qa	 0.2190	 0.0060
Qb	 0.2360	 -0.0040
Qc	 0.2200	 0.0080
Qd	 0.2190	 0.0020
Qe	 0.0950	 -0.0240
Qf	 0.1940	 -0.0450
Qg	 0.2370	 -0.0080
Qh	 0.1940	 -0.0330
Qi	 0.2020	 0.0360
Qj	 0.2110	 0.0490
S1	 0.3490	 0.0710
S2	 0.6190	 0.3260
S3	 0.3940	 0.1080
S4	 0.3290	 0.0790
S5	 0.6050	 0.3740
S6	 0.4560	 0.1940
S7	 0.5750	 0.2630
S8	 0.6830	 0.3730

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Chain	Atom inclusion	Q-score
V1	 0.6430	 0.3620
V2	 0.6090	 0.3610
V3	 0.5260	 0.3240