



## Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 02:12 AM EDT

PDB ID : 8ESW  
EMDB ID : EMD-28581  
Title : Structure of mitochondrial complex I from *Drosophila melanogaster*, Flexible-class 1  
Authors : Padavannil, A.; Letts, J.A.  
Deposited on : 2022-10-15  
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

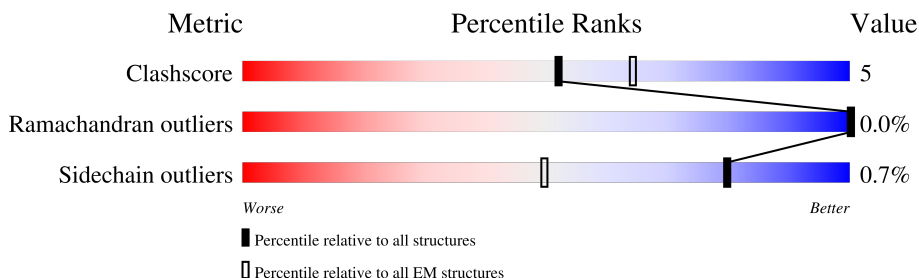
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





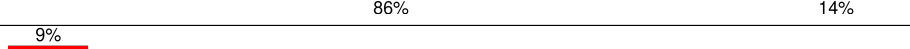




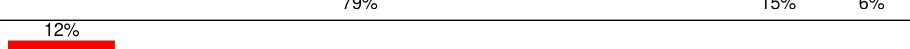
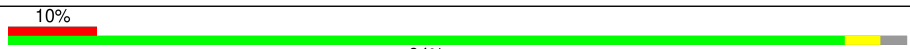


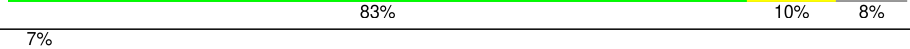

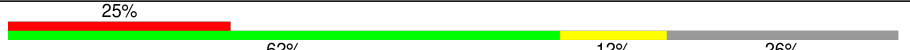

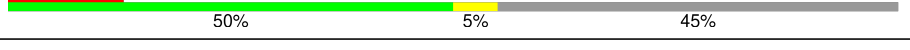
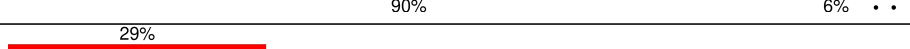







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AN	142	<div> <div>15%</div> <div>83%</div> <div>13%</div> <div>• •</div> </div>
2	S6	126	<div> <div>5%</div> <div>66%</div> <div>6%</div> <div>29%</div> </div>
3	S1	731	<div> <div>8%</div> <div>79%</div> <div>14%</div> <div>7%</div> </div>
4	S3	265	<div> <div>•</div> <div>66%</div> <div>12%</div> <div>22%</div> </div>
5	V2	242	<div> <div>19%</div> <div>75%</div> <div>13%</div> <div>12%</div> </div>
6	S7	221	<div> <div>•</div> <div>64%</div> <div>17%</div> <div>•</div> <div>18%</div> </div>
7	S8	217	<div> <div>•</div> <div>67%</div> <div>19%</div> <div>14%</div> </div>
8	3	117	<div> <div>•</div> <div>68%</div> <div>21%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
9	1	315	
10	4	446	
11	5	577	
12	A8	175	
13	A1	123	
14	AO	154	
15	S5	101	
16	AM	170	
17	BL	159	
18	B6	167	
19	B4	113	
20	B7	117	
21	B5	186	
22	B9	144	
23	BM	150	
24	B8	175	
25	B3	110	
26	AB	152	
26	AC	152	
27	C2	116	
28	B1	56	
29	S4	183	
30	A9	416	
31	B2	94	
32	S2	468	

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Mol	Chain	Length	Quality of chain
33	V3	27	
34	V1	474	
35	2	341	
36	4L	96	
37	6	174	
38	A7	103	
39	A5	124	
40	A3	77	
41	A6	124	
42	AL	407	

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
45	SF4	S7	301	-	-	X	-

## 2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 66555 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 dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AN	137	Total	C	N	O	S	0	0
			1150	750	192	203	5		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S6	90	Total	C	N	O	S	0	0
			722	456	131	130	5		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S1	680	Total	C	N	O	S	0	0
			5168	3239	915	985	29		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S3	208	Total	C	N	O	S	0	0
			1719	1098	302	314	5		

- Molecule 5 is a protein called NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V2	214	Total	C	N	O	S	0	0
			1680	1062	285	321	12		

- Molecule 6 is a protein called LD31474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S7	182	Total	C	N	O	S	0	0
			1435	920	251	250	14		

- Molecule 7 is a protein called NADH dehydrogenase (ubiquinone) 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	186	Total	C	N	O	S	0	0
			1485	935	251	287	12		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3	105	Total	C	N	O	S	0	0
			855	593	119	137	6		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1	315	Total	C	N	O	S	0	0
			2571	1764	367	418	22		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	446	Total	C	N	O	S	0	0
			3604	2448	533	581	42		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	577	Total	C	N	O	S	0	0
			4605	3092	680	773	60		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A8	174	Total	C	N	O	S	0	0
			1384	867	240	267	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	70	Total	C	N	O	S	0	0
			581	375	97	103	6		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	144	Total	C	N	O	S	0	0
			1188	777	201	208	2		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S5	100	Total	C	N	O	S	0	0
			828	523	145	149	11		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AM	164	Total	C	N	O	S	0	0
			1251	813	207	225	6		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BL	150	Total	C	N	O	S	0	0
			1252	786	231	225	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B6	161	Total	C	N	O	S	0	0
			1302	829	242	226	5		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B4	110	Total	C	N	O	S	0	0
			907	578	166	162	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B7	111	Total	C	N	O	S	0	0
			925	589	159	167	10		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B5	143	Total	C	N	O	S	0	0
			1221	787	209	222	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B9	133	Total	C	N	O	S	0	0
			1143	729	216	195	3		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BM	106	Total	C	N	O	S	0	0
			871	560	140	170	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B8	144	Total	C	N	O	S	0	0
			1201	783	191	223	4		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B3	81	Total	C	N	O	S	0	0
			646	421	113	111	1		

- Molecule 26 is a protein called Acyl carrier protein, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
26	AC	84	Total	C	N	O	S	0	0
			677	437	102	136	2		
26	AB	81	Total	C	N	O	S	0	0
			652	421	99	130	2		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C2	115	Total	C	N	O	S	0	0
			904	588	159	156	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B1	55	Total	C	N	O	S	0	0
			430	278	76	74	2		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S4	126	Total	C	N	O	S	0	0
			1023	640	192	187	4		

- Molecule 30 is a protein called NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A9	370	Total	C	N	O	S	0	0
			2972	1895	539	528	10		

- Molecule 31 is a protein called GEO11417p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B2	59	Total	C	N	O	S	0	0
			485	317	85	82	1		

- Molecule 32 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S2	419	Total	C	N	O	S	0	0
			3349	2149	563	614	23		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	V3	27	Total	C	N	O	0	0
			136	81	27	28		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	V1	439	Total	C	N	O	S	0	0
			3368	2126	600	616	26		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2	341	Total	C	N	O	S	0	0
			2797	1893	411	459	34		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	4L	95	Total	C	N	O	S	0	0
			785	535	112	126	12		

- Molecule 37 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	6	165	Total	C	N	O	S	0	0
			1331	902	189	225	15		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A7	90	Total	C	N	O	S	0	0
			725	457	136	131	1		

- Molecule 39 is a protein called NADH dehydrogenase (Ubiquinone) 13 kDa B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A5	117	Total	C	N	O	S	0	0
			914	584	161	165	4		

- Molecule 40 is a protein called RH45008p.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A3	67	Total	C	N	O	S	0	0
			528	331	96	100	1		

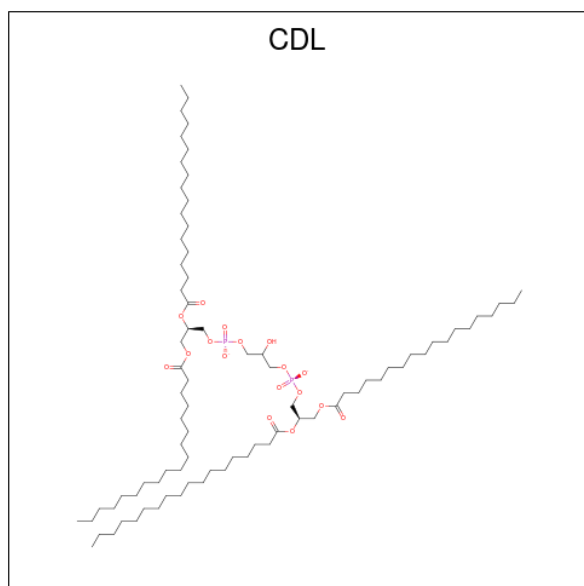
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	A6	114	Total	C	N	O	S	0	0
			968	620	172	170	6		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AL	368	Total	C	N	O	S	0	0
			3008	1927	504	561	16		

- Molecule 43 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
43	AN	1	Total	C	O	P	0
			67	48	17	2	
43	S7	1	Total	C	O	P	0
			71	52	17	2	
43	5	1	Total	C	O	P	0
			68	49	17	2	

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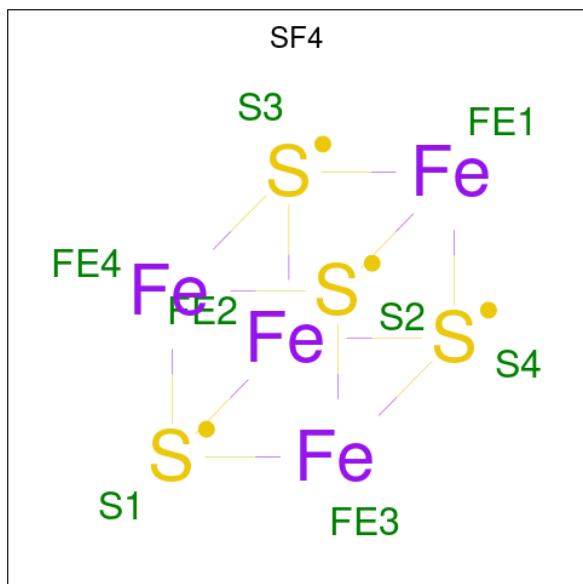
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Mol	Chain	Residues	Atoms				AltConf
43	5	1	Total	C	O	P	0
			75	56	17	2	
43	B6	1	Total	C	O	P	0
			53	34	17	2	
43	B5	1	Total	C	O	P	0
			74	55	17	2	
43	A9	1	Total	C	O	P	0
			54	35	17	2	
43	A9	1	Total	C	O	P	0
			47	28	17	2	

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



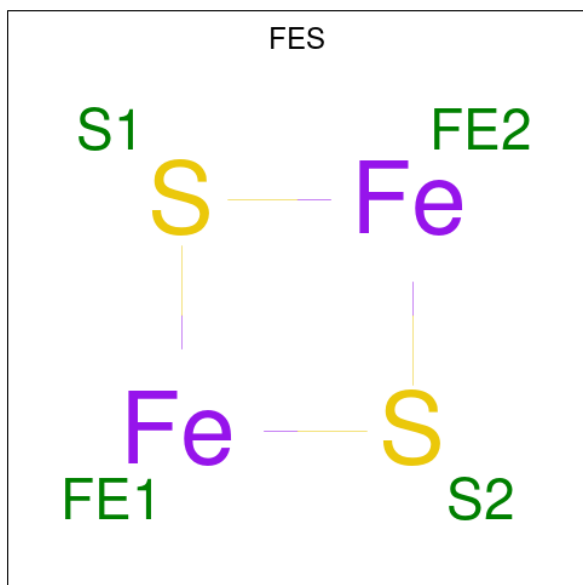
Mol	Chain	Residues	Atoms			AltConf
45	S1	1	Total	Fe	S	0
			8	4	4	
45	S1	1	Total	Fe	S	0
			8	4	4	
45	S7	1	Total	Fe	S	0
			8	4	4	

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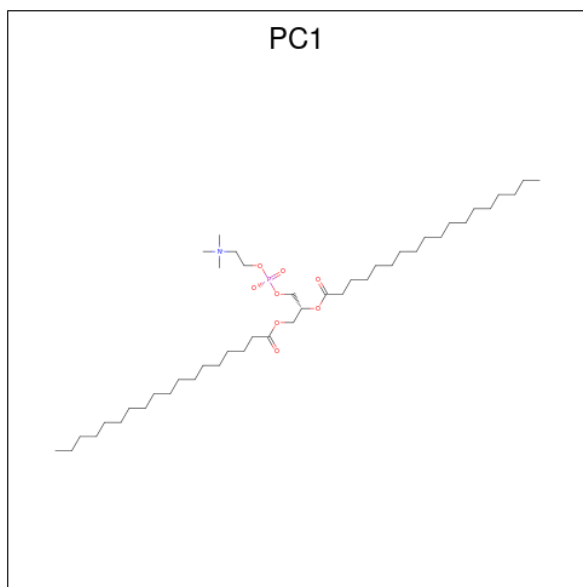
Mol	Chain	Residues	Atoms			AltConf
45	S8	1	Total	Fe	S	0
			8	4	4	
45	S8	1	Total	Fe	S	0
			8	4	4	
45	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



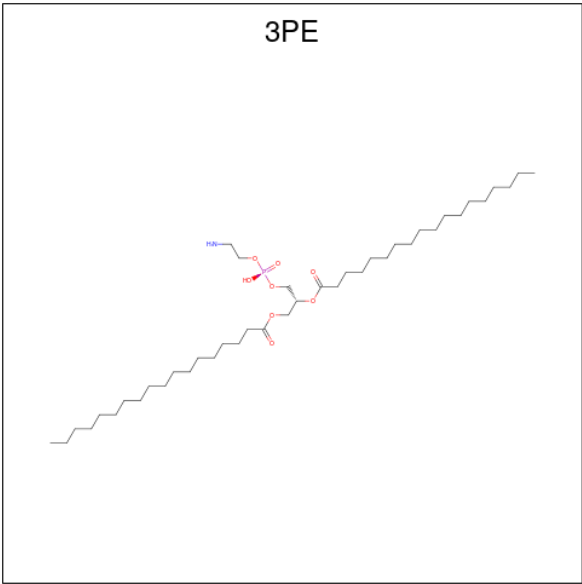
Mol	Chain	Residues	Atoms			AltConf
46	S1	1	Total	Fe	S	0
			4	2	2	
46	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $\text{C}_{44}\text{H}_{88}\text{NO}_8\text{P}$ ).



Mol	Chain	Residues	Atoms					AltConf
47	S7	1	Total	C	N	O	P	0
			36	26	1	8	1	
47	S7	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	1	1	Total	C	N	O	P	0
			54	44	1	8	1	
47	4	1	Total	C	N	O	P	0
			39	29	1	8	1	
47	4	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	AM	1	Total	C	N	O	P	0
			37	27	1	8	1	
47	AM	1	Total	C	N	O	P	0
			33	23	1	8	1	
47	B6	1	Total	C	N	O	P	0
			37	27	1	8	1	
47	B4	1	Total	C	N	O	P	0
			34	24	1	8	1	
47	C2	1	Total	C	N	O	P	0
			39	29	1	8	1	
47	2	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	2	1	Total	C	N	O	P	0
			45	35	1	8	1	
47	6	1	Total	C	N	O	P	0
			36	26	1	8	1	
47	6	1	Total	C	N	O	P	0
			29	19	1	8	1	

- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



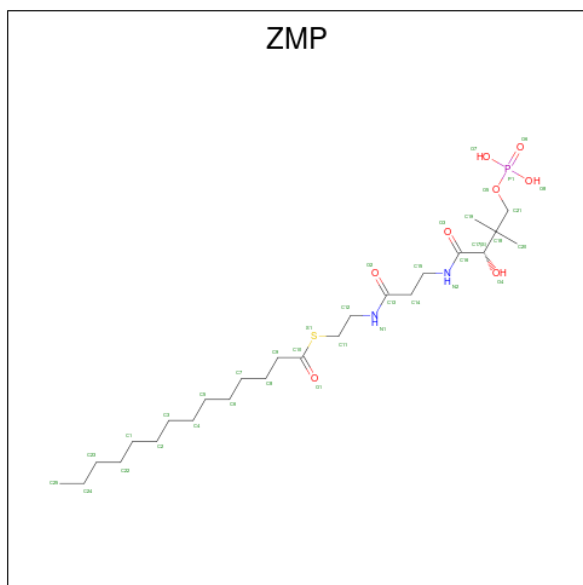
Mol	Chain	Residues	Atoms					AltConf
48	4	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	4	1	Total	C	N	O	P	0
			39	29	1	8	1	
48	5	1	Total	C	N	O	P	0
			32	22	1	8	1	
48	5	1	Total	C	N	O	P	0
			33	23	1	8	1	
48	5	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	5	1	Total	C	N	O	P	0
			36	26	1	8	1	
48	5	1	Total	C	N	O	P	0
			45	35	1	8	1	
48	5	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	AM	1	Total	C	N	O	P	0
			39	29	1	8	1	
48	AM	1	Total	C	N	O	P	0
			36	26	1	8	1	
48	AM	1	Total	C	N	O	P	0
			32	22	1	8	1	
48	B6	1	Total	C	N	O	P	0
			44	34	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
48	2	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 49 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).



Mol	Chain	Residues	Atoms						AltConf
49	B9	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
49	AB	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).





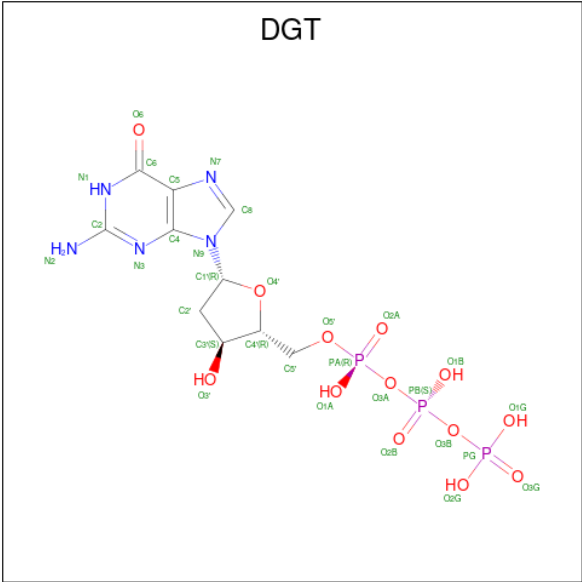
Mol	Chain	Residues	Atoms					AltConf
50	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 51 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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

- Molecule 52 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).

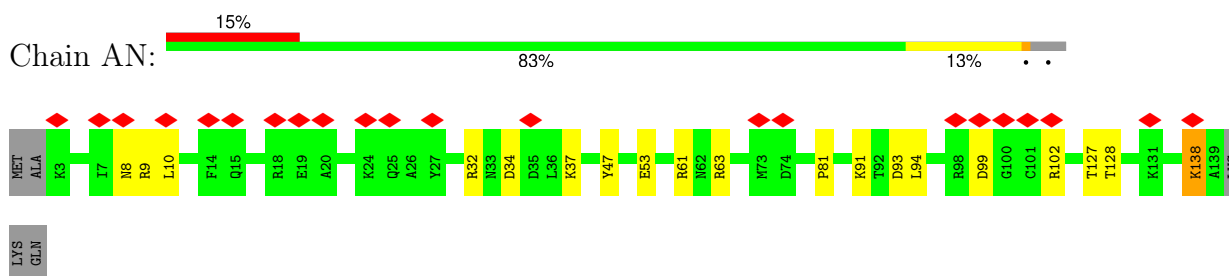


Mol	Chain	Residues	Atoms					AltConf
52	AL	1	Total	C	N	O	P	0
			31	10	5	13	3	

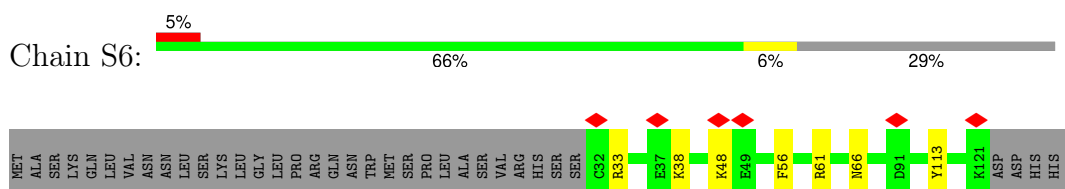
### 3 Residue-property plots [i](#)

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.

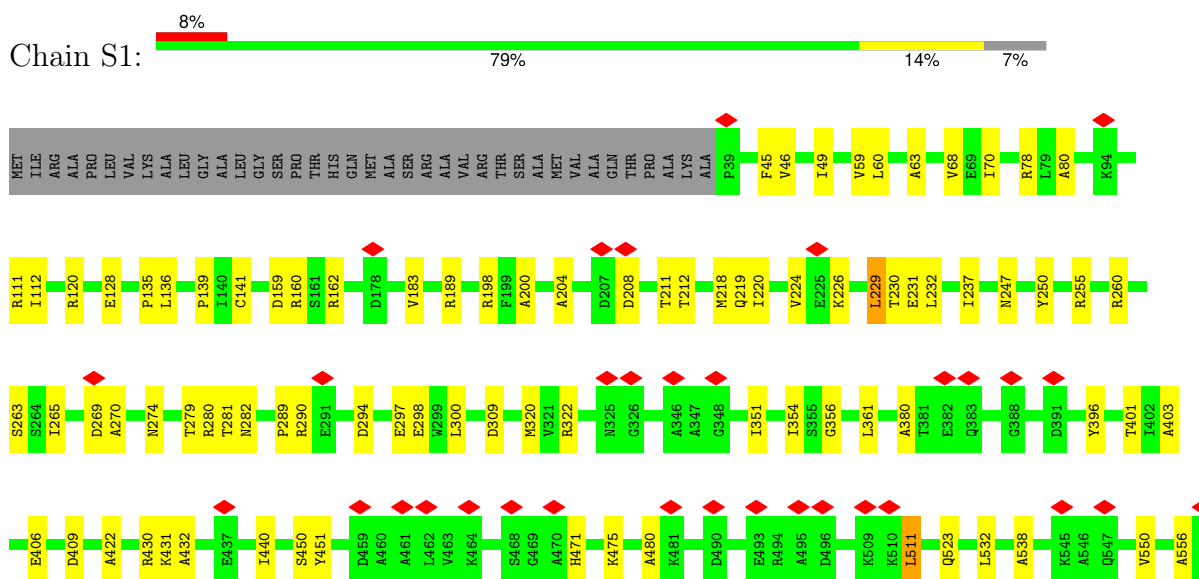
- Molecule 1: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

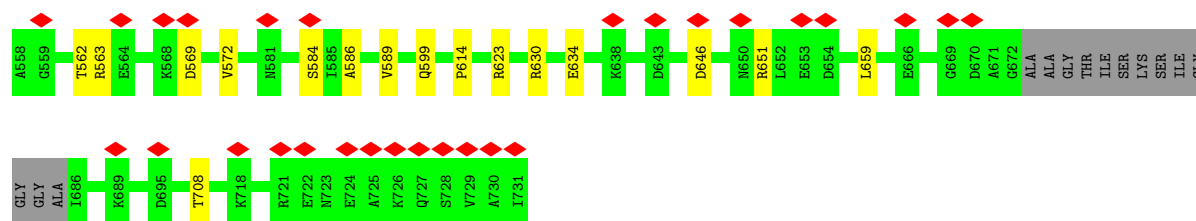


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

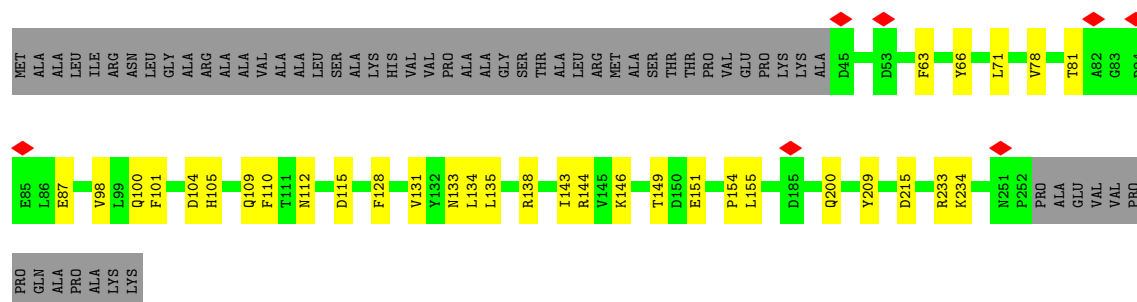


- Molecule 3: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

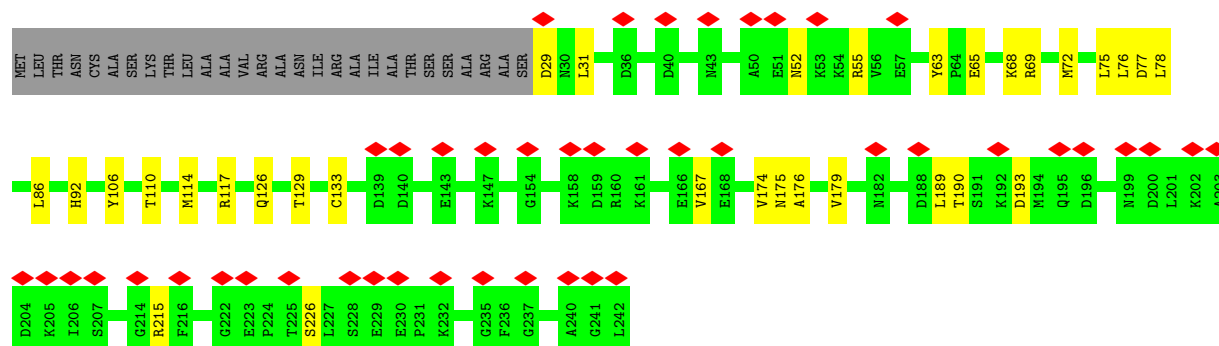
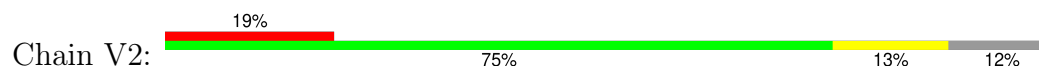




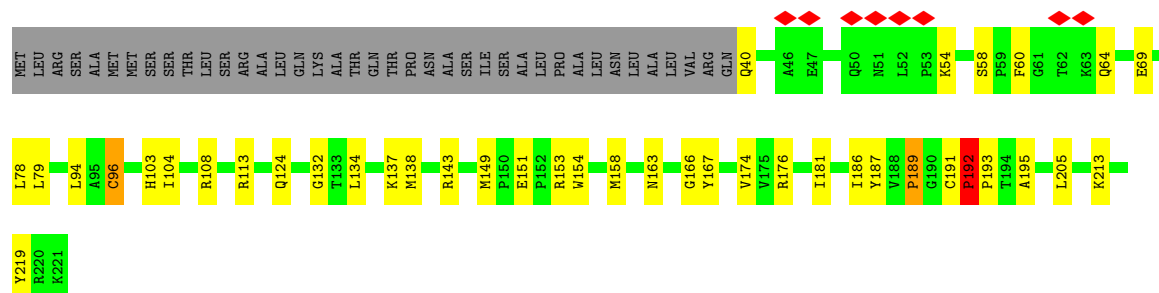
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 5: NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A

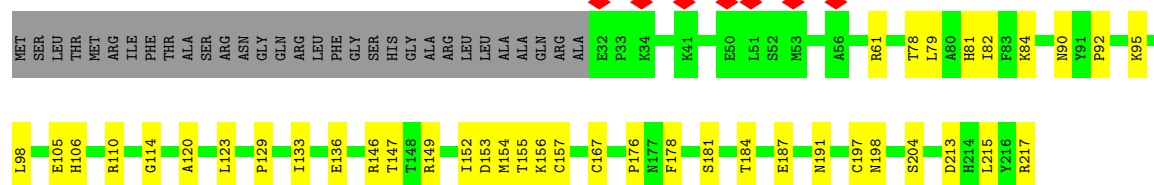


- Molecule 6: LD31474p



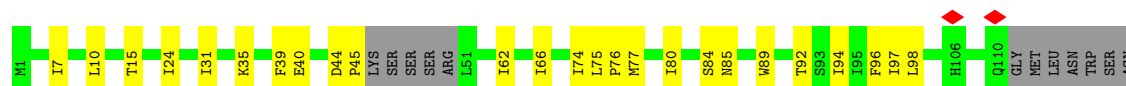
- Molecule 7: NADH dehydrogenase (ubiquinone) 23 kDa subunit

Chain S8: 




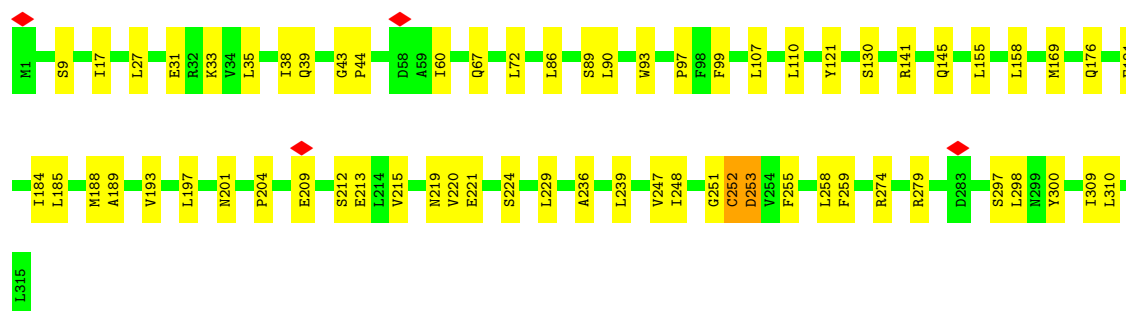
- Molecule 8: NADH-ubiquinone oxidoreductase chain 3

Chain 3: 




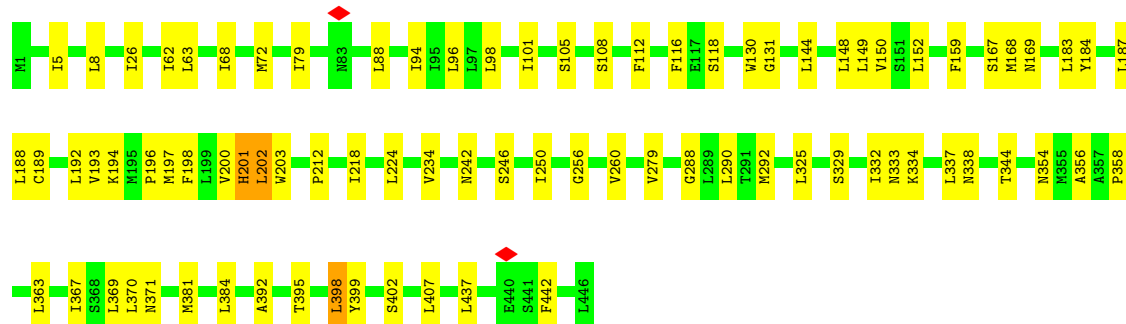
- Molecule 9: NADH-ubiquinone oxidoreductase chain 1

Chain 1: 




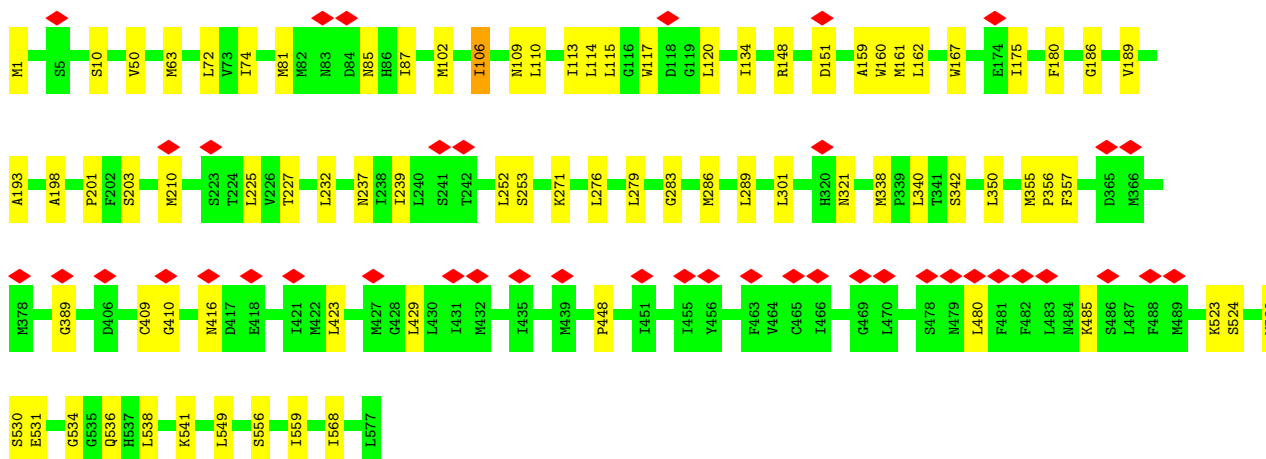
- Molecule 10: NADH-ubiquinone oxidoreductase chain 4

Chain 4: 

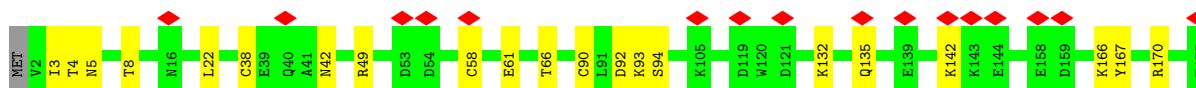


- Molecule 11: NADH-ubiquinone oxidoreductase chain 5

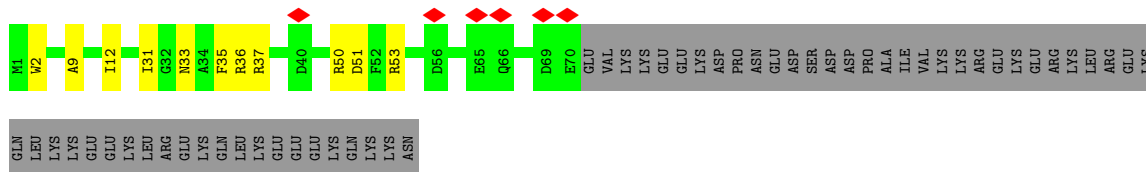
Chain 5: 



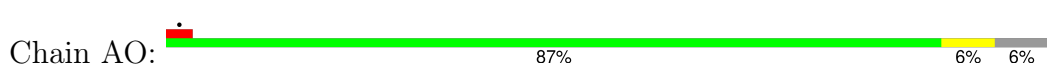
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



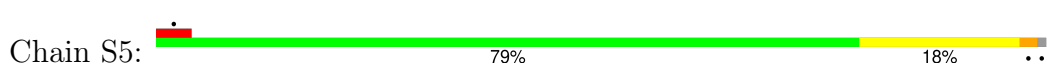
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



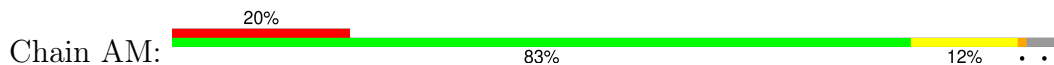
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

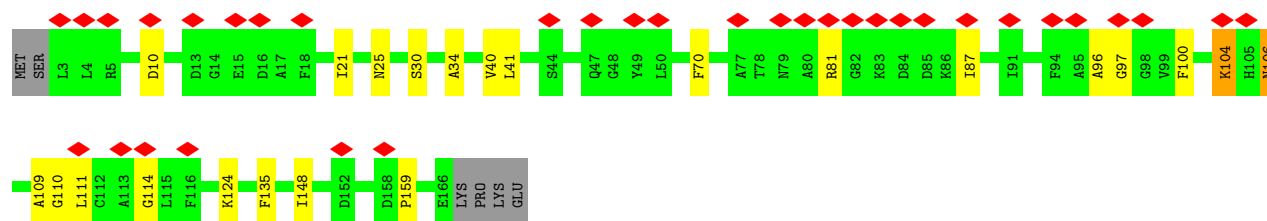


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



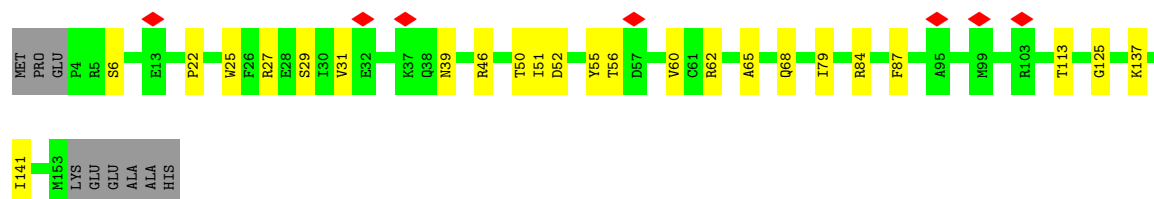
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11





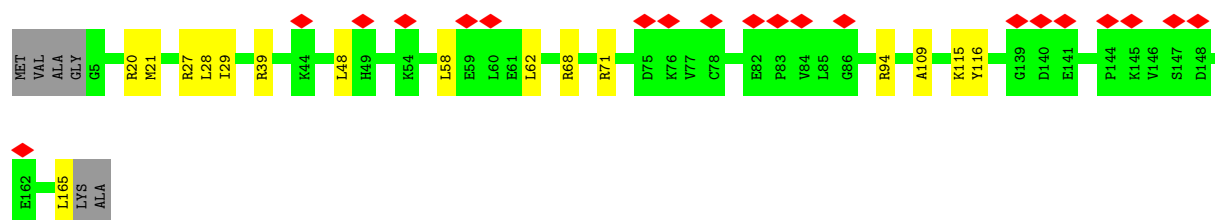
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BL: 79% 15% 6%



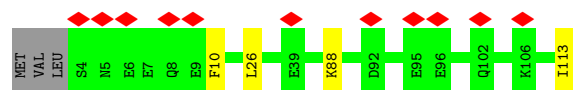
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6: 12% 87% 10%



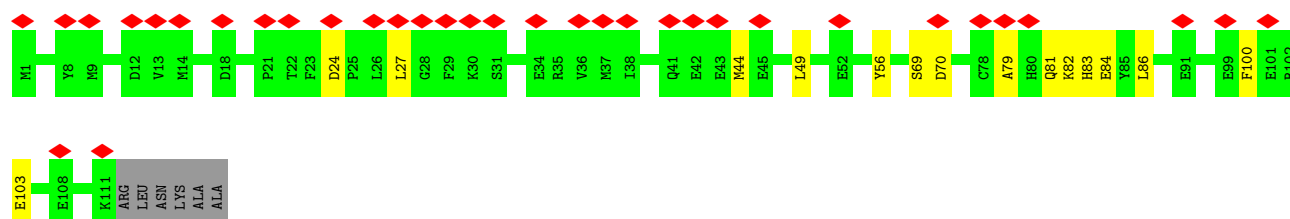
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain B4: 10% 94% 5%

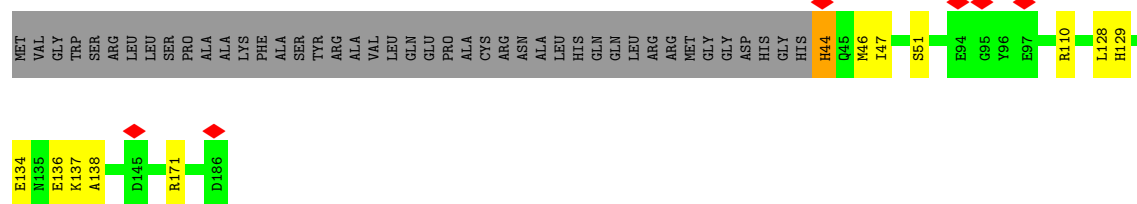


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

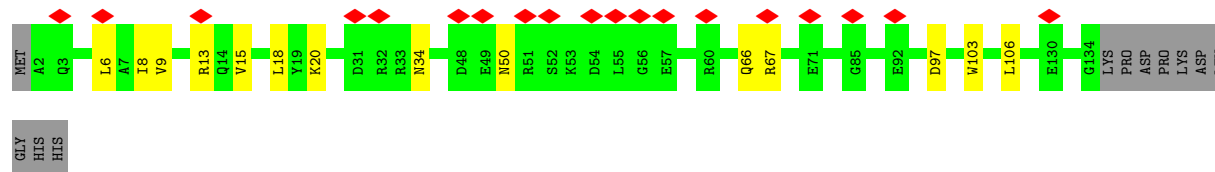
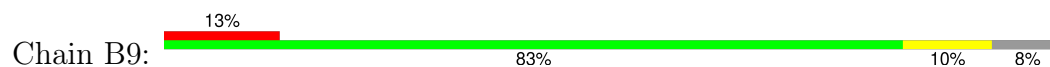
Chain B7: 29% 82% 13% 5%



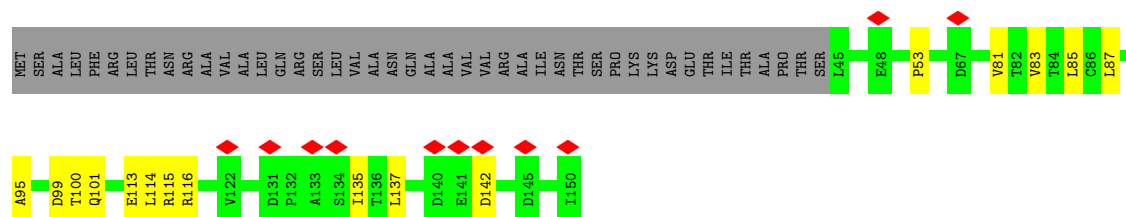
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



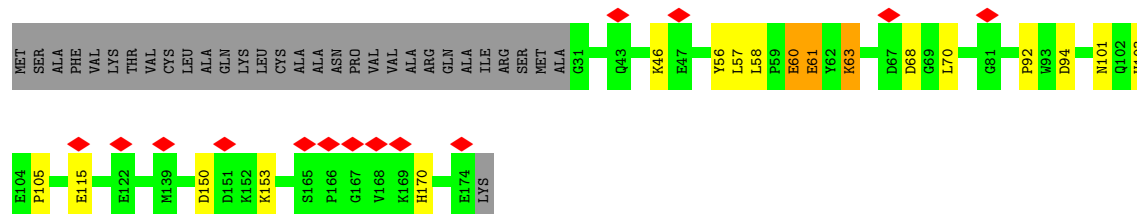
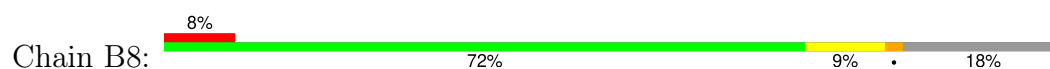
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



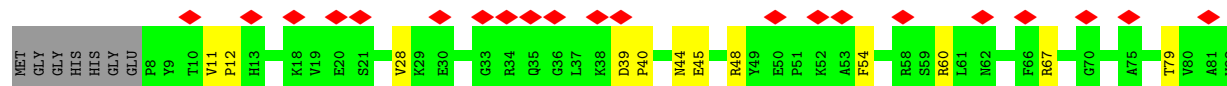
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



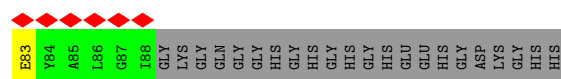
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



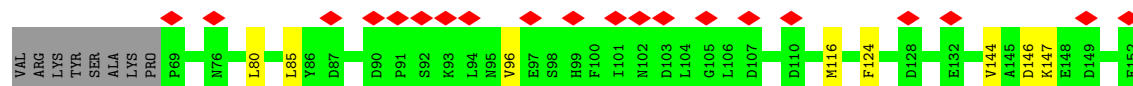
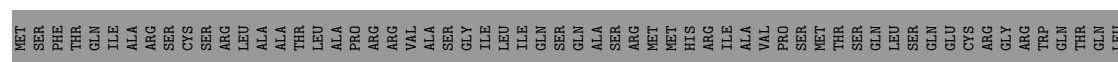
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



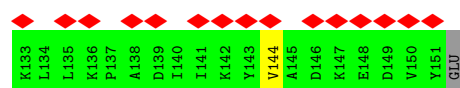
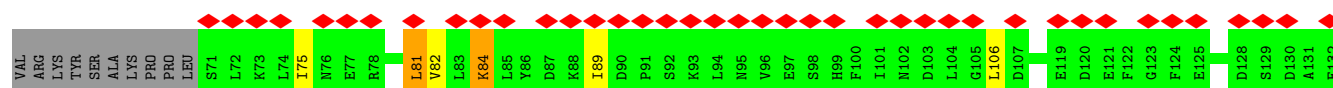
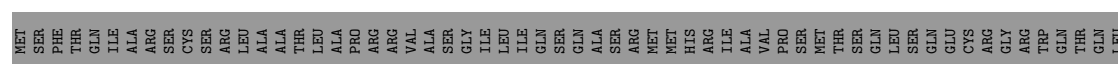




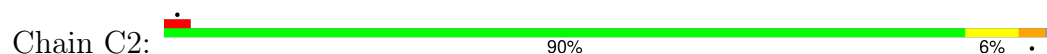
- Molecule 26: Acyl carrier protein, mitochondrial



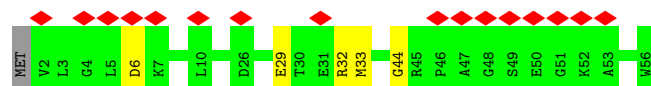
- Molecule 26: Acyl carrier protein, mitochondrial



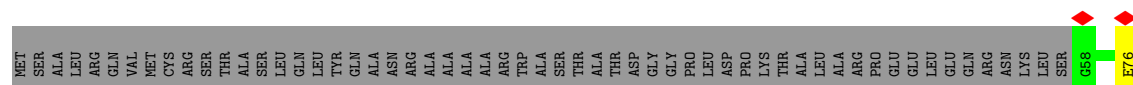
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2

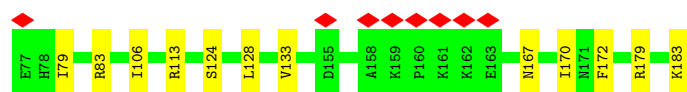


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

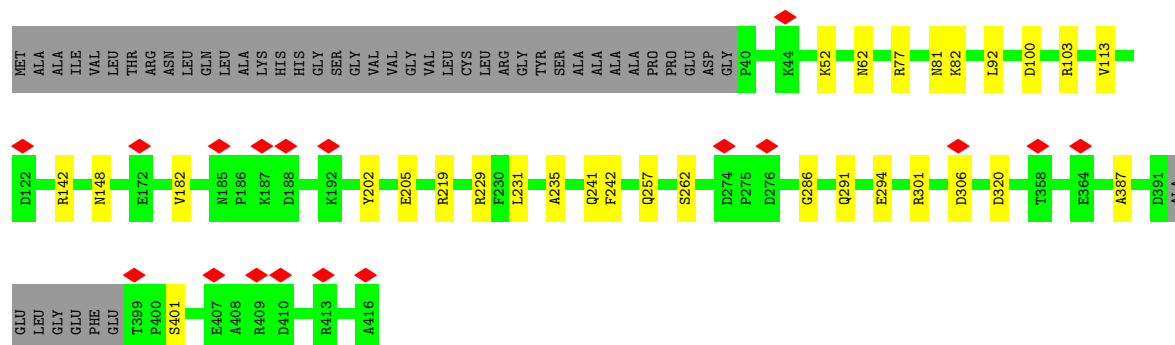
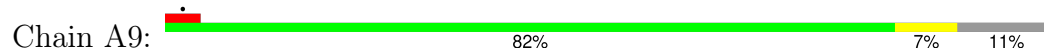


- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

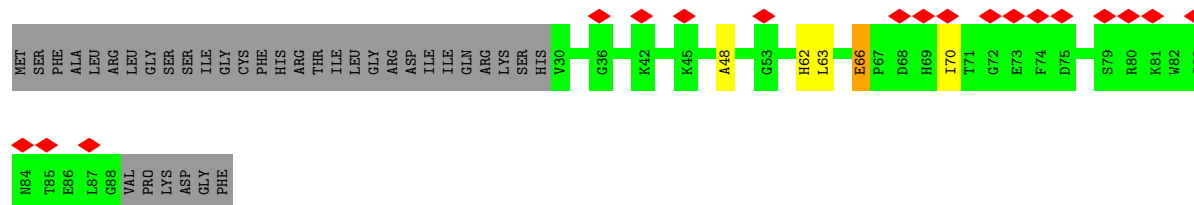




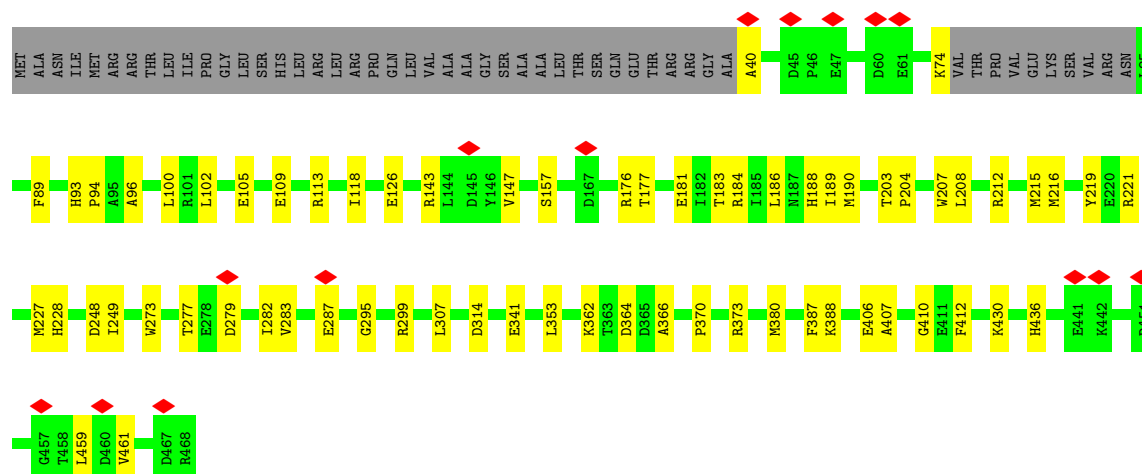
- Molecule 30: NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A



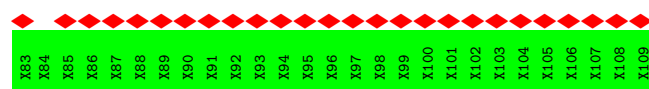
- Molecule 31: GEO11417p1



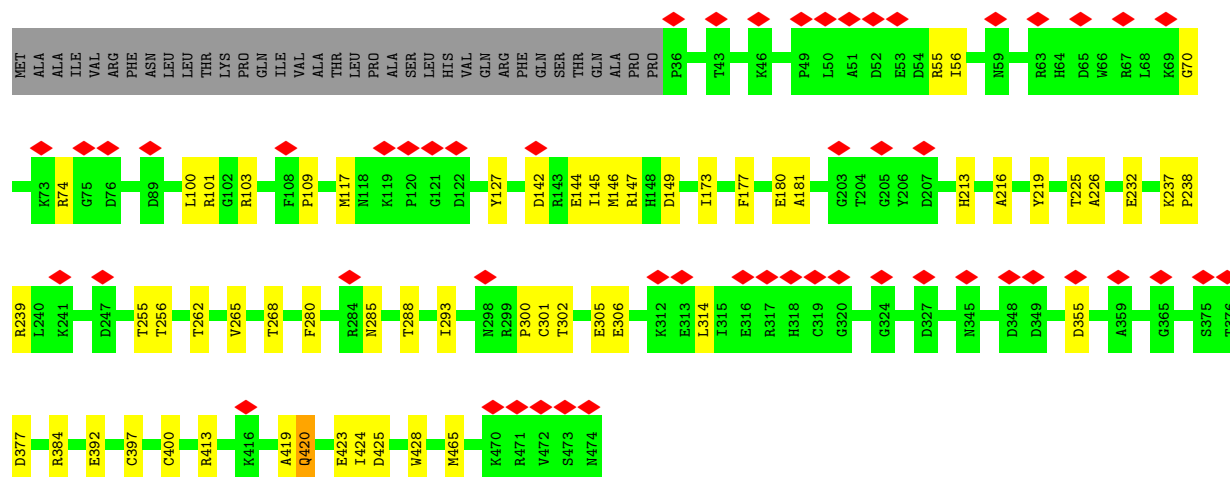
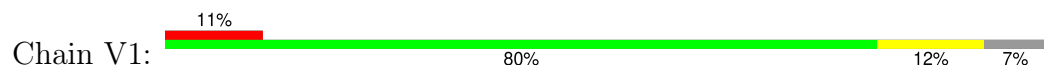
- Molecule 32: Complex I-49kD



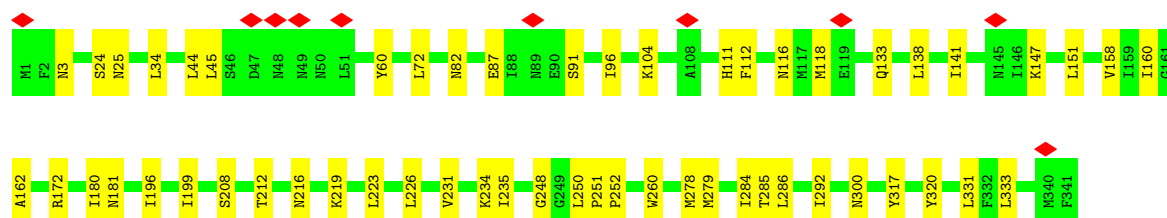
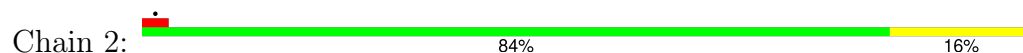
- Molecule 33: NADH dehydrogenase [ubiquinone] flavoprotein 3



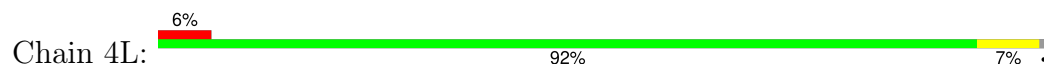
- Molecule 34: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



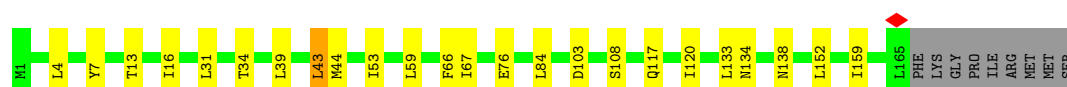
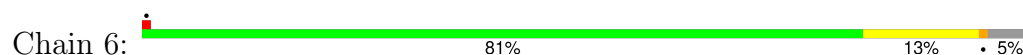
- Molecule 35: NADH-ubiquinone oxidoreductase chain 2



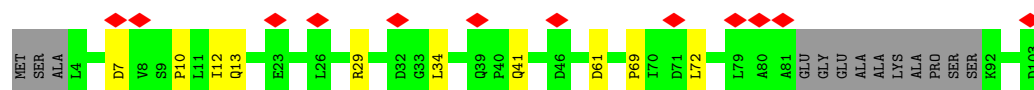
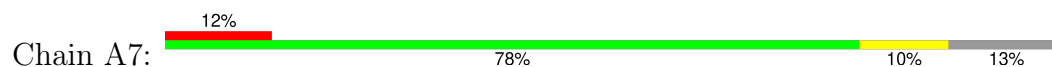
- Molecule 36: NADH-ubiquinone oxidoreductase chain 4L



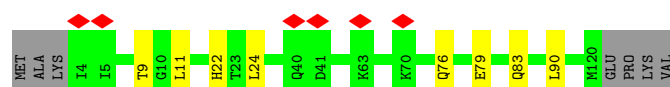
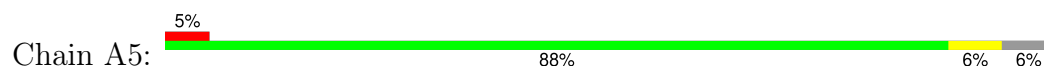
- Molecule 37: NADH-ubiquinone oxidoreductase chain 6



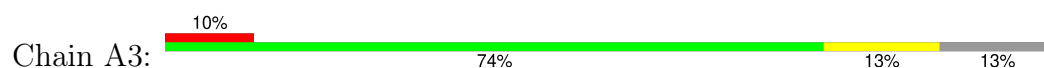
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



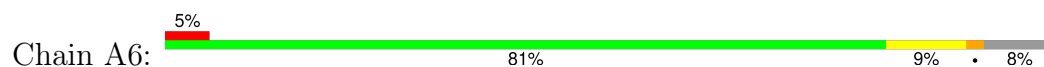
- Molecule 39: NADH dehydrogenase (Ubiquinone) 13 kDa B subunit



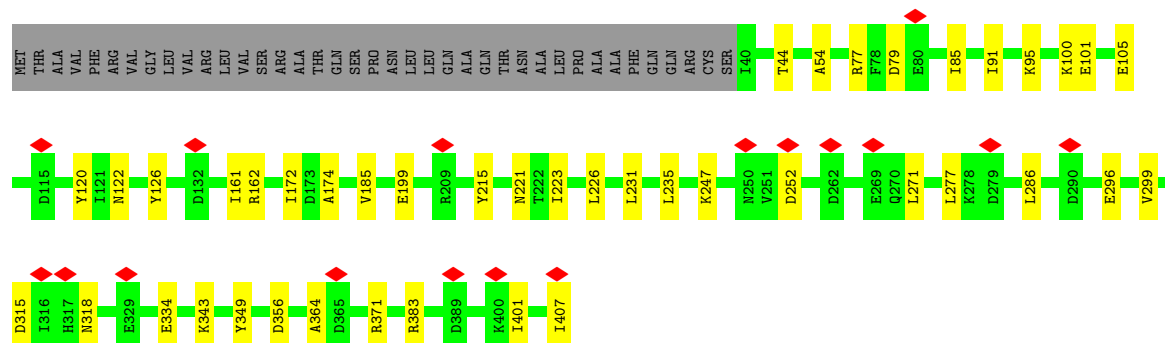
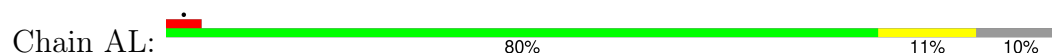
- Molecule 40: RH45008p



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	293389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.017	Depositor
Minimum map value	-2.064	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	450.56, 450.56, 450.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	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, NDP, FES, 3PE, CDL, DGT, FMN, ZN, PC1, SF4

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	AN	0.31	0/1190	0.58	0/1612
2	S6	0.29	0/739	0.55	0/995
3	S1	0.29	0/5251	0.57	0/7117
4	S3	0.28	0/1766	0.56	0/2400
5	V2	0.29	0/1719	0.58	0/2328
6	S7	0.34	0/1473	0.66	2/1997 (0.1%)
7	S8	0.33	0/1518	0.60	0/2050
8	3	0.32	0/875	0.61	0/1187
9	1	0.33	0/2651	0.60	0/3593
10	4	0.32	0/3708	0.61	1/5024 (0.0%)
11	5	0.33	0/4725	0.65	0/6396
12	A8	0.29	0/1417	0.53	0/1911
13	A1	0.29	0/594	0.60	0/801
14	AO	0.30	0/1224	0.56	0/1659
15	S5	0.35	0/846	0.61	0/1128
16	AM	0.31	0/1287	0.53	0/1749
17	BL	0.30	0/1285	0.57	0/1734
18	B6	0.27	0/1338	0.57	0/1808
19	B4	0.28	0/928	0.52	0/1241
20	B7	0.30	0/948	0.56	0/1275
21	B5	0.28	0/1255	0.53	0/1694
22	B9	0.27	0/1176	0.57	0/1586
23	BM	0.27	0/896	0.52	0/1222
24	B8	0.29	0/1250	0.57	0/1701
25	B3	0.28	0/665	0.56	0/903
26	AB	0.30	0/662	0.64	0/894
26	AC	0.26	0/688	0.54	0/928
27	C2	0.36	0/932	0.65	1/1266 (0.1%)
28	B1	0.27	0/441	0.56	0/590
29	S4	0.27	0/1051	0.57	0/1424
30	A9	0.30	0/3045	0.60	0/4118
31	B2	0.30	0/508	0.55	0/698

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	S2	0.32	0/3432	0.60	0/4650
34	V1	0.32	0/3446	0.61	0/4654
35	2	0.32	0/2876	0.58	0/3890
36	4L	0.30	0/806	0.53	0/1085
37	6	0.30	0/1356	0.57	0/1836
38	A7	0.27	0/741	0.60	0/1006
39	A5	0.27	0/933	0.56	0/1265
40	A3	0.25	0/537	0.55	0/725
41	A6	0.29	0/988	0.54	0/1329
42	AL	0.28	0/3083	0.56	0/4168
All	All	0.30	0/66249	0.59	4/89637 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
27	C2	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	S7	192	PRO	N-CA-C	-7.61	92.32	112.10
6	S7	189	PRO	N-CA-C	5.92	127.50	112.10
10	4	212	PRO	N-CA-CB	5.83	110.29	103.30
27	C2	111	SER	N-CA-C	5.49	125.82	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	C2	116	ARG	Sidechain

## 5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	1150	0	1107	18	0
2	S6	722	0	705	5	0
3	S1	5168	0	5214	65	0
4	S3	1719	0	1666	27	0
5	V2	1680	0	1657	20	0
6	S7	1435	0	1448	35	0
7	S8	1485	0	1422	34	0
8	3	855	0	927	21	0
9	1	2571	0	2628	54	0
10	4	3604	0	3734	63	0
11	5	4605	0	4742	59	0
12	A8	1384	0	1324	17	0
13	A1	581	0	582	8	0
14	AO	1188	0	1196	9	0
15	S5	828	0	805	13	0
16	AM	1251	0	1230	17	0
17	BL	1252	0	1195	24	0
18	B6	1302	0	1295	11	0
19	B4	907	0	896	8	0
20	B7	925	0	906	10	0
21	B5	1221	0	1188	12	0
22	B9	1143	0	1111	10	0
23	BM	871	0	822	12	0
24	B8	1201	0	1107	18	0
25	B3	646	0	641	9	0
26	AB	652	0	655	4	0
26	AC	677	0	681	6	0
27	C2	904	0	892	10	0
28	B1	430	0	436	4	0
29	S4	1023	0	994	9	0
30	A9	2972	0	2983	18	0
31	B2	485	0	450	5	0
32	S2	3349	0	3314	44	0
33	V3	136	0	30	0	0
34	V1	3368	0	3345	42	0
35	2	2797	0	2879	39	0
36	4L	785	0	809	8	0
37	6	1331	0	1439	19	0
38	A7	725	0	721	11	0
39	A5	914	0	944	8	0
40	A3	528	0	521	9	0
41	A6	968	0	991	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	AL	3008	0	2945	28	0
43	5	143	0	177	1	0
43	A9	101	0	90	2	0
43	AN	67	0	78	3	0
43	B5	74	0	95	4	0
43	B6	53	0	50	1	0
43	S7	71	0	86	2	0
44	S6	1	0	0	0	0
45	S1	16	0	0	0	0
45	S7	8	0	0	5	0
45	S8	16	0	0	1	0
45	V1	8	0	0	1	0
46	S1	4	0	0	0	0
46	V2	4	0	0	0	0
47	1	54	0	88	1	0
47	2	89	0	132	3	0
47	4	83	0	114	7	0
47	6	65	0	78	2	0
47	AM	70	0	88	3	0
47	B4	34	0	42	1	0
47	B6	37	0	48	1	0
47	C2	39	0	52	2	0
47	S7	82	0	115	3	0
48	2	39	0	52	3	0
48	4	74	0	96	4	0
48	5	248	0	358	8	0
48	AM	107	0	136	4	0
48	B6	44	0	65	2	0
49	AB	34	0	40	0	0
49	B9	34	0	40	2	0
50	A9	48	0	26	0	0
51	V1	31	0	19	0	0
52	AL	31	0	12	3	0
All	All	66555	0	66754	690	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 5.

All (690) 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)
34:V1:397:CYS:SG	34:V1:400:CYS:HB3	1.99	1.02
34:V1:413:ARG:NH2	34:V1:423:GLU:OE2	1.93	1.00
10:4:197:MET:HB2	10:4:200:VAL:HG22	1.50	0.91
22:B9:15:VAL:HG11	49:B9:201:ZMP:H19B	1.51	0.90
34:V1:419:ALA:HB1	34:V1:423:GLU:OE1	1.73	0.87
6:S7:191:CYS:HB3	6:S7:192:PRO:HD3	1.62	0.82
10:4:242:ASN:O	10:4:246:SER:HB3	1.82	0.79
34:V1:413:ARG:HH22	34:V1:423:GLU:CD	1.84	0.79
42:AL:91:ILE:HB	52:AL:501:DGT:H5'	1.66	0.78
17:BL:56:THR:HG23	27:C2:103:LYS:O	1.84	0.78
7:S8:106:HIS:HE1	45:S8:301:SF4:S4	2.07	0.76
34:V1:70:GLY:O	34:V1:74:ARG:HB2	1.90	0.72
4:S3:154:PRO:HG3	41:A6:17:ILE:HB	1.72	0.70
9:1:193:VAL:HG11	47:1:401:PC1:H391	1.74	0.70
6:S7:96:CYS:SG	45:S7:301:SF4:FE4	1.84	0.70
6:S7:191:CYS:SG	45:S7:301:SF4:FE3	1.83	0.69
11:5:134:ILE:HG12	24:B8:115:GLU:HG2	1.76	0.68
3:S1:211:THR:HB	3:S1:220:ILE:HD13	1.76	0.68
3:S1:230:THR:HG22	3:S1:232:LEU:H	1.59	0.67
3:S1:218:MET:CE	34:V1:237:LYS:HE2	2.26	0.66
10:4:198:PHE:HB2	10:4:256:GLY:HA3	1.77	0.65
41:A6:19:SER:HB3	41:A6:77:ASP:OD2	1.97	0.64
15:S5:18:LEU:HD21	36:4L:59:PHE:CE1	2.33	0.64
30:A9:242:PHE:H	43:A9:502:CDL:HB61	1.64	0.63
3:S1:218:MET:HE1	34:V1:237:LYS:HE2	1.81	0.63
17:BL:25:TRP:O	17:BL:29:SER:HB2	1.98	0.62
8:3:39:PHE:HE2	9:1:215:VAL:HG21	1.63	0.62
3:S1:289:PRO:HG3	3:S1:300:LEU:HB2	1.80	0.62
3:S1:260:ARG:HB2	3:S1:279:THR:O	2.00	0.61
34:V1:142:ASP:HA	34:V1:145:ILE:HD12	1.82	0.61
11:5:568:ILE:HD12	35:2:96:ILE:HG23	1.83	0.61
16:AM:124:LYS:HG2	48:AM:201:3PE:H332	1.84	0.60
30:A9:387:ALA:HB1	37:6:76:GLU:HB2	1.83	0.60
18:B6:109:ALA:HB1	43:B5:201:CDL:H311	1.84	0.60
12:A8:166:LYS:HE3	27:C2:13:ASN:HA	1.82	0.60
11:5:113:ILE:O	11:5:117:TRP:HB2	2.02	0.60
10:4:196:PRO:HD3	10:4:224:LEU:HD22	1.84	0.59
6:S7:108:ARG:HH22	38:A7:29:ARG:HH21	1.51	0.59
34:V1:101:ARG:HA	34:V1:109:PRO:HA	1.85	0.59
9:1:247:VAL:HG13	9:1:252:CYS:SG	2.43	0.59
29:S4:113:ARG:HG3	29:S4:124:SER:HB3	1.85	0.59
32:S2:204:PRO:HA	32:S2:207:TRP:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V2:92:HIS:HE2	5:V2:106:TYR:HH	1.46	0.58
35:2:181:ASN:ND2	35:2:285:THR:OG1	2.36	0.58
42:AL:122:ASN:HD21	42:AL:126:TYR:HB3	1.67	0.58
10:4:381:MET:SD	11:5:160:TRP:NE1	2.72	0.58
29:S4:172:PHE:HZ	29:S4:183:LYS:HZ3	1.51	0.58
12:A8:90:CYS:O	12:A8:94:SER:HB3	2.02	0.58
6:S7:191:CYS:HG	45:S7:301:SF4:FE3	1.17	0.58
11:5:193:ALA:HB2	11:5:232:LEU:HD23	1.84	0.58
15:S5:18:LEU:HD21	36:4L:59:PHE:CD1	2.39	0.58
9:1:213:GLU:OE1	9:1:279:ARG:NH2	2.37	0.58
9:1:176:GLN:OE1	9:1:251:GLY:HA2	2.04	0.57
47:4:502:PC1:H281	48:4:504:3PE:H2A2	1.85	0.57
15:S5:77:ARG:NH1	15:S5:91:PHE:O	2.37	0.57
41:A6:40:ILE:HD12	41:A6:56:CYS:HB3	1.84	0.57
38:A7:10:PRO:HA	38:A7:13:GLN:HB2	1.87	0.57
6:S7:163:ASN:HD22	6:S7:187:TYR:HB3	1.68	0.57
11:5:180:PHE:HB2	48:5:607:3PE:H111	1.85	0.57
19:B4:10:PHE:CD1	24:B8:60:GLU:HG3	2.39	0.57
42:AL:174:ALA:HB1	42:AL:185:VAL:HG21	1.87	0.57
9:1:31:GLU:O	9:1:35:LEU:HB2	2.04	0.57
9:1:253:ASP:HB3	9:1:259:PHE:HB2	1.86	0.57
13:A1:31:ILE:HG22	13:A1:33:ASN:H	1.69	0.56
17:BL:137:LYS:HB3	27:C2:109:LEU:HD12	1.87	0.56
9:1:197:LEU:HD13	9:1:204:PRO:HG2	1.86	0.56
10:4:202:LEU:H	10:4:202:LEU:HD22	1.70	0.56
42:AL:85:ILE:HG12	42:AL:231:LEU:HB3	1.87	0.56
31:B2:62:HIS:O	31:B2:66:GLU:HG3	2.04	0.56
47:4:501:PC1:H11	23:BM:95:ALA:HA	1.86	0.56
9:1:185:LEU:HB3	9:1:188:MET:HB2	1.88	0.56
10:4:371:ASN:HD22	11:5:159:ALA:HA	1.71	0.56
32:S2:190:MET:SD	32:S2:212:ARG:NH1	2.79	0.56
26:AB:81:LEU:HG	26:AB:82:VAL:N	2.20	0.56
1:AN:128:THR:OG1	7:S8:149:ARG:NH2	2.39	0.56
10:4:356:ALA:HB3	11:5:148:ARG:HH12	1.70	0.56
35:2:44:LEU:O	35:2:45:LEU:HB3	2.06	0.56
10:4:196:PRO:HB2	10:4:279:VAL:HG13	1.88	0.55
40:A3:51:ASN:ND2	40:A3:70:LYS:O	2.40	0.55
4:S3:104:ASP:HB2	39:A5:90:LEU:HD12	1.88	0.55
9:1:39:GLN:HG3	32:S2:203:THR:HG23	1.88	0.55
11:5:102:MET:O	11:5:106:ILE:HG13	2.06	0.55
3:S1:211:THR:OG1	3:S1:218:MET:CG	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1:176:GLN:NE2	9:1:248:ILE:O	2.39	0.55
11:5:161:MET:HG2	11:5:167:TRP:HA	1.89	0.55
16:AM:81:ARG:HH12	16:AM:87:ILE:HD11	1.71	0.55
9:1:310:LEU:HD22	40:A3:36:MET:HB2	1.89	0.55
3:S1:599:GLN:HB2	3:S1:614:PRO:HD3	1.89	0.55
10:4:108:SER:HB3	10:4:168:MET:HB3	1.88	0.55
11:5:50:VAL:O	11:5:109:ASN:ND2	2.39	0.55
11:5:340:LEU:HD23	11:5:423:LEU:HD23	1.87	0.55
34:V1:413:ARG:NH1	34:V1:423:GLU:OE1	2.39	0.54
35:2:300:ASN:HB3	42:AL:364:ALA:HB1	1.89	0.54
6:S7:163:ASN:ND2	6:S7:187:TYR:HB3	2.22	0.54
8:3:75:LEU:HD23	9:1:158:LEU:HD13	1.88	0.54
9:1:27:LEU:HD22	9:1:239:LEU:HG	1.89	0.54
4:S3:78:VAL:HG23	38:A7:72:LEU:HB2	1.88	0.54
9:1:184:ILE:HG23	9:1:185:LEU:HG	1.89	0.54
42:AL:91:ILE:HD12	52:AL:501:DGT:H3'	1.89	0.54
3:S1:623:ARG:NH1	41:A6:119:PHE:O	2.40	0.54
11:5:523:LYS:NZ	24:B8:70:LEU:O	2.39	0.54
15:S5:16:GLY:HA2	35:2:25:ASN:OD1	2.07	0.54
3:S1:59:VAL:HG13	3:S1:112:ILE:HD13	1.89	0.54
4:S3:215:ASP:OD1	30:A9:81:ASN:ND2	2.41	0.54
18:B6:58:LEU:O	18:B6:62:LEU:HB2	2.07	0.54
32:S2:183:THR:OG1	32:S2:219:TYR:OH	2.26	0.54
10:4:150:VAL:HG11	10:4:193:VAL:HG21	1.89	0.54
34:V1:177:PHE:HB3	34:V1:180:GLU:HB2	1.89	0.54
10:4:131:GLY:O	32:S2:40:ALA:N	2.41	0.54
15:S5:39:GLU:OE1	21:B5:171:ARG:NH2	2.41	0.54
6:S7:167:TYR:HE1	7:S8:129:PRO:HB2	1.71	0.54
12:A8:66:THR:OG1	14:AO:85:ARG:NH2	2.41	0.54
34:V1:226:ALA:HB2	34:V1:238:PRO:HG3	1.90	0.54
47:C2:201:PC1:H372	35:2:331:LEU:HD23	1.89	0.54
1:AN:34:ASP:OD2	6:S7:113:ARG:NH2	2.41	0.53
4:S3:66:TYR:HH	4:S3:105:HIS:HE2	1.55	0.53
12:A8:38:CYS:O	12:A8:42:ASN:ND2	2.41	0.53
30:A9:241:GLN:NE2	30:A9:320:ASP:OD1	2.42	0.53
3:S1:263:SER:HB3	3:S1:290:ARG:HH11	1.73	0.53
3:S1:297:GLU:OE2	3:S1:431:LYS:NZ	2.39	0.53
9:1:220:VAL:HG13	9:1:221:GLU:HG2	1.91	0.53
11:5:63:MET:HG2	11:5:102:MET:HG3	1.88	0.53
12:A8:92:ASP:OD1	12:A8:93:LYS:HG2	2.09	0.53
23:BM:81:VAL:HA	23:BM:85:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:S2:147:VAL:HG11	32:S2:190:MET:HG2	1.89	0.53
2:S6:66:ASN:O	7:S8:110:ARG:NH2	2.41	0.53
6:S7:174:VAL:O	6:S7:176:ARG:NH1	2.41	0.53
34:V1:419:ALA:CB	34:V1:423:GLU:OE1	2.54	0.53
10:4:96:LEU:HD21	10:4:218:ILE:HG12	1.90	0.53
12:A8:22:LEU:O	13:A1:50:ARG:NH1	2.42	0.53
7:S8:167:CYS:O	32:S2:373:ARG:NH2	2.40	0.53
2:S6:113:TYR:O	7:S8:146:ARG:NH2	2.42	0.53
10:4:62:ILE:HG23	10:4:101:ILE:HG12	1.90	0.53
11:5:253:SER:OG	11:5:283:GLY:O	2.26	0.53
10:4:201:HIS:O	10:4:203:TRP:N	2.42	0.53
6:S7:191:CYS:O	45:S7:301:SF4:S2	2.67	0.53
18:B6:71:ARG:HD2	18:B6:94:ARG:HH22	1.74	0.53
10:4:26:ILE:HG23	23:BM:81:VAL:HG11	1.91	0.53
7:S8:110:ARG:NH1	7:S8:114:GLY:O	2.42	0.52
34:V1:117:MET:SD	34:V1:256:THR:OG1	2.62	0.52
9:1:181:PHE:HB3	9:1:185:LEU:HD12	1.91	0.52
10:4:8:LEU:HD12	10:4:94:ILE:HG23	1.91	0.52
11:5:1:MET:N	43:B6:203:CDL:OA3	2.42	0.52
42:AL:120:TYR:OH	42:AL:162:ARG:NH1	2.42	0.52
1:AN:53:GLU:HG3	1:AN:63:ARG:HG2	1.90	0.52
4:S3:115:ASP:HB3	32:S2:430:LYS:HG3	1.92	0.52
9:1:31:GLU:OE2	9:1:274:ARG:NH1	2.38	0.52
13:A1:53:ARG:NH2	14:AO:82:GLU:OE2	2.42	0.52
32:S2:295:GLY:HA3	32:S2:410:GLY:HA2	1.92	0.52
22:B9:20:LYS:HE2	26:AC:116:MET:HG2	1.92	0.52
17:BL:79:ILE:HG23	23:BM:114:LEU:HD13	1.92	0.52
34:V1:74:ARG:NH2	34:V1:149:ASP:OD1	2.43	0.52
35:2:231:VAL:O	42:AL:371:ARG:NH1	2.41	0.52
37:6:134:ASN:OD1	37:6:138:ASN:ND2	2.42	0.52
10:4:358:PRO:HG2	43:5:604:CDL:H822	1.90	0.52
11:5:10:SER:HB2	11:5:74:ILE:HG21	1.92	0.52
38:A7:7:ASP:OD2	38:A7:13:GLN:NE2	2.43	0.52
34:V1:425:ASP:O	34:V1:428:TRP:HB3	2.09	0.51
16:AM:159:PRO:O	21:B5:171:ARG:NH1	2.43	0.51
2:S6:33:ARG:NH1	2:S6:56:PHE:O	2.44	0.51
3:S1:630:ARG:NH1	3:S1:634:GLU:OE1	2.44	0.51
18:B6:21:MET:HB3	18:B6:39:ARG:HD3	1.92	0.51
35:2:111:HIS:HD2	35:2:180:ILE:HD13	1.76	0.51
48:2:401:3PE:H331	48:2:401:3PE:H241	1.93	0.51
3:S1:430:ARG:NH1	3:S1:450:SER:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S8:213:ASP:OD2	7:S8:217:ARG:NH2	2.43	0.51
37:6:34:THR:HB	37:6:59:LEU:HD12	1.92	0.51
3:S1:282:ASN:ND2	29:S4:113:ARG:O	2.43	0.51
4:S3:200:GLN:HE22	32:S2:126:GLU:HB2	1.76	0.51
7:S8:136:GLU:OE2	7:S8:149:ARG:NH1	2.44	0.51
32:S2:221:ARG:NH1	32:S2:248:ASP:OD2	2.44	0.51
16:AM:70:PHE:HB2	16:AM:96:ALA:HB2	1.92	0.51
22:B9:97:ASP:N	22:B9:97:ASP:OD1	2.42	0.51
26:AB:81:LEU:O	26:AB:84:LYS:HG3	2.11	0.51
5:V2:175:ASN:OD1	5:V2:215:ARG:NH1	2.44	0.51
10:4:371:ASN:ND2	11:5:159:ALA:HA	2.26	0.51
6:S7:60:PHE:HE1	6:S7:213:LYS:HG2	1.76	0.51
9:1:97:PRO:HG3	9:1:169:MET:HB3	1.93	0.51
11:5:110:LEU:HB2	11:5:167:TRP:HB3	1.93	0.51
24:B8:57:LEU:HG	24:B8:105:PRO:HG3	1.93	0.51
32:S2:74:LYS:NZ	42:AL:349:TYR:OH	2.44	0.51
35:2:158:VAL:HG11	35:2:278:MET:HG2	1.93	0.51
17:BL:84:ARG:NH2	19:B4:113:ILE:OXT	2.44	0.50
32:S2:177:THR:OG1	32:S2:314:ASP:O	2.28	0.50
5:V2:52:ASN:OD1	5:V2:55:ARG:NH1	2.44	0.50
11:5:175:ILE:HG13	17:BL:87:PHE:HZ	1.77	0.50
12:A8:135:GLN:HG2	40:A3:63:HIS:CE1	2.46	0.50
18:B6:29:ILE:HG21	24:B8:92:PRO:HG3	1.93	0.50
34:V1:100:LEU:HD21	34:V1:262:THR:HG23	1.93	0.50
8:3:39:PHE:CE2	9:1:215:VAL:HG21	2.46	0.50
8:3:62:ILE:HG21	37:6:159:ILE:HG21	1.92	0.50
17:BL:22:PRO:HB3	43:B5:201:CDL:H802	1.94	0.50
17:BL:39:ASN:O	21:B5:110:ARG:NH2	2.44	0.50
20:B7:79:ALA:O	20:B7:82:LYS:HB3	2.11	0.50
32:S2:105:GLU:OE1	32:S2:113:ARG:NH2	2.44	0.50
9:1:67:GLN:NE2	9:1:224:SER:O	2.44	0.50
10:4:329:SER:O	10:4:333:ASN:ND2	2.44	0.50
11:5:350:LEU:HB3	11:5:355:MET:HB2	1.94	0.50
32:S2:89:PHE:HB2	32:S2:102:LEU:HB3	1.93	0.50
32:S2:189:ILE:HG23	32:S2:208:LEU:HB3	1.93	0.50
3:S1:135:PRO:HG2	3:S1:189:ARG:HG3	1.93	0.50
5:V2:29:ASP:N	5:V2:29:ASP:OD1	2.44	0.50
10:4:338:ASN:HB2	10:4:407:LEU:HD11	1.93	0.50
4:S3:87:GLU:OE2	4:S3:144:ARG:NH1	2.45	0.50
5:V2:129:THR:HB	34:V1:384:ARG:HH21	1.77	0.50
7:S8:153:ASP:OD1	7:S8:155:THR:OG1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A1:33:ASN:ND2	13:A1:35:PHE:O	2.45	0.50
30:A9:205:GLU:OE2	30:A9:219:ARG:NH2	2.41	0.50
7:S8:92:PRO:O	7:S8:95:LYS:NZ	2.43	0.50
10:4:288:GLY:HA3	10:4:369:LEU:HD22	1.94	0.50
24:B8:58:LEU:HB2	24:B8:61:GLU:HG3	1.93	0.50
35:2:44:LEU:O	35:2:45:LEU:CB	2.59	0.50
35:2:138:LEU:HD23	35:2:141:ILE:HD12	1.94	0.50
3:S1:322:ARG:NH2	3:S1:584:SER:O	2.45	0.49
18:B6:165:LEU:O	23:BM:115:ARG:NH1	2.45	0.49
3:S1:160:ARG:NH2	32:S2:364:ASP:O	2.45	0.49
43:AN:201:CDL:OB4	13:A1:2:TRP:NE1	2.46	0.49
32:S2:299:ARG:NH2	32:S2:341:GLU:OE2	2.45	0.49
35:2:216:ASN:O	35:2:219:LYS:NZ	2.43	0.49
9:1:31:GLU:O	9:1:35:LEU:CB	2.60	0.49
18:B6:48:LEU:HB2	21:B5:44:HIS:O	2.12	0.49
42:AL:315:ASP:HB3	42:AL:318:ASN:HB2	1.94	0.49
43:AN:201:CDL:H712	38:A7:12:ILE:HD11	1.92	0.49
7:S8:98:LEU:HD11	7:S8:178:PHE:HE2	1.77	0.49
3:S1:135:PRO:CG	3:S1:189:ARG:HG3	2.43	0.49
11:5:530:SER:O	11:5:534:GLY:HA3	2.13	0.49
20:B7:100:PHE:O	20:B7:103:GLU:HB3	2.12	0.49
8:3:24:ILE:HG22	43:A9:503:CDL:H711	1.94	0.49
17:BL:6:SER:OG	20:B7:69:SER:O	2.29	0.49
39:A5:9:THR:HG23	39:A5:11:LEU:H	1.77	0.49
26:AB:89:ILE:HD11	26:AB:106:LEU:HD11	1.92	0.49
1:AN:91:LYS:HZ2	7:S8:176:PRO:HB3	1.75	0.49
15:S5:74:ARG:NH2	37:6:103:ASP:OD2	2.42	0.49
42:AL:79:ASP:OD1	42:AL:79:ASP:N	2.46	0.49
3:S1:136:LEU:HG	32:S2:380:MET:SD	2.52	0.49
6:S7:78:LEU:HB2	43:S7:302:CDL:H732	1.95	0.49
10:4:152:LEU:HD13	35:2:279:MET:HB3	1.95	0.49
14:AO:142:LYS:O	14:AO:146:LYS:HB2	2.13	0.49
42:AL:221:ASN:ND2	42:AL:349:TYR:O	2.45	0.49
9:1:130:SER:HB3	9:1:221:GLU:HG3	1.95	0.49
17:BL:137:LYS:HG2	23:BM:135:ILE:HD11	1.94	0.49
3:S1:646:ASP:OD1	29:S4:83:ARG:NH1	2.46	0.48
32:S2:96:ALA:HB1	32:S2:100:LEU:HB3	1.94	0.48
40:A3:22:ASP:OD1	40:A3:22:ASP:N	2.45	0.48
9:1:141:ARG:NH1	32:S2:109:GLU:OE1	2.46	0.48
32:S2:181:GLU:OE2	32:S2:184:ARG:NH1	2.46	0.48
4:S3:233:ARG:NH2	7:S8:133:ILE:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:S2:362:LYS:HE2	32:S2:370:PRO:HD2	1.94	0.48
1:AN:63:ARG:NH2	1:AN:93:ASP:OD1	2.38	0.48
3:S1:183:VAL:HG22	3:S1:237:ILE:HD11	1.95	0.48
7:S8:120:ALA:HB2	7:S8:147:THR:HG22	1.94	0.48
9:1:155:LEU:HD23	9:1:158:LEU:HD23	1.94	0.48
47:4:502:PC1:H232	27:C2:40:ILE:HG21	1.96	0.48
35:2:3:ASN:HB3	42:AL:334:GLU:HG3	1.95	0.48
3:S1:354:ILE:HG12	3:S1:380:ALA:HB3	1.95	0.48
10:4:88:LEU:HD22	35:2:235:ILE:HG23	1.95	0.48
48:5:602:3PE:H352	48:B6:202:3PE:H291	1.95	0.48
20:B7:56:TYR:OH	24:B8:170:HIS:ND1	2.46	0.48
30:A9:100:ASP:O	30:A9:103:ARG:NH1	2.46	0.48
34:V1:413:ARG:HH12	34:V1:423:GLU:CD	2.16	0.48
35:2:333:LEU:HD21	47:2:403:PC1:H2B2	1.94	0.48
3:S1:280:ARG:HG2	3:S1:281:THR:HG23	1.96	0.48
32:S2:407:ALA:HB2	32:S2:412:PHE:HB2	1.95	0.48
35:2:162:ALA:HB1	35:2:284:ILE:HB	1.95	0.48
5:V2:174:VAL:HG21	34:V1:302:THR:HB	1.96	0.48
35:2:248:GLY:HA3	35:2:286:LEU:HD13	1.95	0.48
3:S1:231:GLU:HG2	3:S1:232:LEU:HG	1.96	0.48
25:B3:39:ASP:HA	25:B3:40:PRO:HD3	1.74	0.48
4:S3:100:GLN:NE2	4:S3:104:ASP:OD1	2.45	0.48
13:A1:37:ARG:NH1	13:A1:51:ASP:OD1	2.47	0.47
17:BL:50:THR:OG1	17:BL:52:ASP:OD1	2.32	0.47
2:S6:38:LYS:O	2:S6:61:ARG:NH1	2.48	0.47
6:S7:94:LEU:HB2	6:S7:132:GLY:HA3	1.96	0.47
7:S8:105:GLU:OE2	7:S8:198:ASN:ND2	2.47	0.47
3:S1:532:LEU:HD21	3:S1:538:ALA:HB2	1.97	0.47
42:AL:277:LEU:HB3	42:AL:286:LEU:HD11	1.96	0.47
5:V2:65:GLU:HA	5:V2:68:LYS:HE2	1.97	0.47
6:S7:151:GLU:HA	6:S7:153:ARG:HG3	1.97	0.47
9:1:209:GLU:OE2	9:1:219:ASN:ND2	2.47	0.47
10:4:325:LEU:HD23	10:4:332:ILE:HG22	1.96	0.47
11:5:409:CYS:SG	11:5:410:GLY:N	2.85	0.47
11:5:538:LEU:HD23	48:5:601:3PE:H321	1.95	0.47
7:S8:61:ARG:NH2	40:A3:18:ASN:OD1	2.47	0.47
7:S8:133:ILE:HG12	7:S8:152:ILE:HG12	1.95	0.47
11:5:389:GLY:HA3	48:5:603:3PE:H2C2	1.96	0.47
1:AN:9:ARG:NH2	38:A7:7:ASP:O	2.45	0.47
4:S3:128:PHE:HB2	4:S3:149:THR:O	2.14	0.47
4:S3:138:ARG:HH21	39:A5:79:GLU:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S7:124:GLN:NE2	9:1:219:ASN:O	2.42	0.47
8:3:40:GLU:HG3	8:3:45:PRO:HB3	1.96	0.47
9:1:212:SER:OG	9:1:279:ARG:NH1	2.47	0.47
10:4:144:LEU:O	10:4:148:LEU:HB2	2.14	0.47
15:S5:21:HIS:NE2	15:S5:61:VAL:HG21	2.30	0.47
7:S8:78:THR:HG23	9:1:38:ILE:HG23	1.96	0.47
9:1:86:LEU:HD22	9:1:229:LEU:HD22	1.96	0.47
10:4:187:LEU:HB3	10:4:234:VAL:HG11	1.95	0.47
22:B9:9:VAL:HG22	22:B9:13:ARG:HH21	1.80	0.47
10:4:63:LEU:HD23	10:4:442:PHE:HZ	1.80	0.47
47:4:502:PC1:H292	48:4:504:3PE:H282	1.97	0.47
48:5:605:3PE:O14	31:B2:62:HIS:NE2	2.48	0.47
34:V1:280:PHE:HB3	34:V1:306:GLU:HG3	1.97	0.47
40:A3:48:ASP:O	40:A3:72:ARG:NH2	2.47	0.47
10:4:358:PRO:HB3	11:5:115:LEU:HG	1.97	0.47
27:C2:47:ARG:NH1	42:AL:407:ILE:OXT	2.48	0.47
30:A9:257:GLN:NE2	30:A9:286:GLY:O	2.47	0.47
34:V1:225:THR:HB	34:V1:239:ARG:HG3	1.96	0.47
3:S1:361:LEU:HD21	3:S1:659:LEU:HD13	1.97	0.46
6:S7:158:MET:HG2	6:S7:193:PRO:HG2	1.96	0.46
29:S4:76:GLU:HA	29:S4:79:ILE:HG22	1.96	0.46
42:AL:101:GLU:O	42:AL:105:GLU:HB2	2.14	0.46
10:4:149:LEU:HD13	48:5:601:3PE:H331	1.97	0.46
22:B9:34:ASN:HB2	25:B3:28:VAL:HG21	1.97	0.46
32:S2:388:LYS:HA	32:S2:388:LYS:HD2	1.77	0.46
34:V1:144:GLU:OE1	34:V1:147:ARG:NH2	2.48	0.46
42:AL:356:ASP:N	42:AL:356:ASP:OD1	2.45	0.46
5:V2:190:THR:H	5:V2:193:ASP:HB2	1.80	0.46
10:4:118:SER:HA	35:2:252:PRO:HD3	1.98	0.46
10:4:193:VAL:HA	10:4:200:VAL:HG21	1.97	0.46
3:S1:78:ARG:NH1	3:S1:298:GLU:OE1	2.48	0.46
10:4:159:PHE:HZ	35:2:260:TRP:HE1	1.63	0.46
11:5:227:THR:HB	11:5:301:LEU:HD11	1.96	0.46
13:A1:9:ALA:O	13:A1:12:ILE:HB	2.15	0.46
34:V1:397:CYS:N	45:V1:502:SF4:S3	2.80	0.46
3:S1:45:PHE:O	3:S1:111:ARG:HA	2.16	0.46
7:S8:81:HIS:HA	7:S8:84:LYS:HD2	1.97	0.46
8:3:77:MET:HB2	8:3:89:TRP:HE1	1.80	0.46
11:5:549:LEU:HD11	35:2:160:ILE:HG23	1.97	0.46
15:S5:15:THR:HG21	35:2:24:SER:HA	1.98	0.46
42:AL:199:GLU:HB2	42:AL:271:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S3:131:VAL:HG22	4:S3:146:LYS:HG2	1.98	0.46
17:BL:51:ILE:HD11	17:BL:62:ARG:HG2	1.96	0.46
20:B7:24:ASP:HB3	20:B7:27:LEU:HB2	1.98	0.46
24:B8:58:LEU:HB2	24:B8:61:GLU:CG	2.46	0.46
34:V1:127:TYR:O	34:V1:255:THR:HA	2.14	0.46
6:S7:137:LYS:NZ	32:S2:118:ILE:O	2.43	0.46
42:AL:161:ILE:HG12	42:AL:215:TYR:HD1	1.81	0.46
4:S3:128:PHE:HE2	4:S3:151:GLU:HB3	1.80	0.46
6:S7:189:PRO:HD3	7:S8:181:SER:HA	1.98	0.46
7:S8:215:LEU:HD12	38:A7:41:GLN:HB3	1.98	0.46
9:1:184:ILE:HD11	14:AO:51:LEU:HD23	1.97	0.46
25:B3:67:ARG:HD3	31:B2:48:ALA:HB1	1.98	0.46
34:V1:56:ILE:HG21	34:V1:265:VAL:HG12	1.98	0.46
34:V1:219:TYR:HB3	34:V1:392:GLU:HB3	1.98	0.46
3:S1:351:ILE:HG22	3:S1:550:VAL:HB	1.99	0.45
5:V2:75:LEU:O	5:V2:78:LEU:HB3	2.16	0.45
11:5:531:GLU:HB3	11:5:536:GLN:HB2	1.97	0.45
32:S2:459:LEU:HB3	32:S2:461:VAL:HG13	1.97	0.45
3:S1:141:CYS:O	3:S1:255:ARG:NH1	2.50	0.45
10:4:260:VAL:HG11	10:4:279:VAL:HB	1.99	0.45
11:5:120:LEU:HD13	11:5:225:LEU:HA	1.98	0.45
4:S3:71:LEU:HD13	4:S3:98:VAL:HG22	1.98	0.45
10:4:392:ALA:HB3	11:5:148:ARG:HG2	1.99	0.45
16:AM:111:LEU:O	16:AM:114:GLY:N	2.49	0.45
17:BL:141:ILE:HG13	23:BM:137:LEU:HD22	1.97	0.45
6:S7:166:GLY:HA2	7:S8:156:LYS:HA	1.99	0.45
10:4:112:PHE:O	10:4:116:PHE:CB	2.64	0.45
10:4:167:SER:HB2	21:B5:138:ALA:HB2	1.98	0.45
10:4:292:MET:O	17:BL:125:GLY:N	2.45	0.45
10:4:367:ILE:HD11	11:5:114:LEU:HD23	1.98	0.45
11:5:276:LEU:HD23	11:5:279:LEU:HD12	1.98	0.45
12:A8:167:TYR:OH	21:B5:136:GLU:OE1	2.35	0.45
30:A9:52:LYS:HG3	30:A9:62:ASN:HA	1.98	0.45
34:V1:377:ASP:N	34:V1:377:ASP:OD1	2.45	0.45
11:5:72:LEU:HD13	11:5:429:LEU:HB2	1.99	0.45
20:B7:81:GLN:O	20:B7:84:GLU:HB3	2.17	0.45
3:S1:46:VAL:HG23	3:S1:112:ILE:HB	1.99	0.45
3:S1:294:ASP:HA	3:S1:403:ALA:HB2	1.99	0.45
5:V2:126:GLN:HB3	5:V2:167:VAL:HG11	1.97	0.45
48:5:602:3PE:H342	48:B6:202:3PE:H371	1.97	0.45
19:B4:10:PHE:HE1	24:B8:61:GLU:HG2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:B4:201:PC1:H331	47:B4:201:PC1:H232	1.99	0.45
30:A9:142:ARG:HD3	30:A9:142:ARG:HA	1.80	0.45
35:2:196:ILE:HD13	35:2:199:ILE:HD12	1.98	0.45
1:AN:127:THR:OG1	7:S8:191:ASN:ND2	2.47	0.45
11:5:357:PHE:HE2	31:B2:63:LEU:HD23	1.80	0.45
12:A8:49:ARG:HH21	37:6:120:ILE:HD13	1.81	0.45
1:AN:94:LEU:HB3	1:AN:99:ASP:HB2	1.99	0.45
6:S7:103:HIS:NE2	32:S2:216:MET:SD	2.90	0.45
8:3:92:THR:O	8:3:96:PHE:HB2	2.16	0.45
11:5:356:PRO:HB3	31:B2:70:ILE:HD11	1.99	0.45
14:AO:83:ARG:HD2	37:6:120:ILE:HG23	1.99	0.45
3:S1:200:ALA:HA	3:S1:204:ALA:HB3	1.98	0.45
4:S3:154:PRO:HD2	41:A6:15:ARG:HD3	1.99	0.45
9:1:212:SER:O	32:S2:93:HIS:NE2	2.49	0.45
16:AM:148:ILE:HD11	47:AM:205:PC1:H152	1.97	0.45
19:B4:10:PHE:CE1	24:B8:60:GLU:HG3	2.52	0.45
5:V2:76:LEU:HD22	5:V2:86:LEU:HD21	1.99	0.45
5:V2:174:VAL:HG13	34:V1:300:PRO:HB2	1.98	0.45
7:S8:123:LEU:HD21	32:S2:387:PHE:HA	1.98	0.45
10:4:183:LEU:HB2	47:2:402:PC1:H221	1.99	0.45
22:B9:6:LEU:HG	22:B9:8:ILE:HG12	1.99	0.45
30:A9:301:ARG:NH1	30:A9:401:SER:O	2.50	0.45
32:S2:436:HIS:HB3	32:S2:459:LEU:HD22	1.99	0.45
35:2:87:GLU:OE2	35:2:91:SER:OG	2.34	0.45
24:B8:68:ASP:OD1	24:B8:68:ASP:N	2.45	0.44
34:V1:293:ILE:HB	34:V1:301:CYS:HB3	1.99	0.44
36:4L:61:MET:HE2	37:6:53:ILE:HG21	1.98	0.44
41:A6:16:PRO:HB2	41:A6:19:SER:O	2.17	0.44
3:S1:208:ASP:N	3:S1:208:ASP:OD1	2.48	0.44
12:A8:58:CYS:HB3	12:A8:61:GLU:HB2	1.98	0.44
25:B3:54:PHE:O	25:B3:60:ARG:NH1	2.50	0.44
32:S2:227:MET:HG3	32:S2:228:HIS:ND1	2.33	0.44
4:S3:112:ASN:HD22	4:S3:135:LEU:HD23	1.83	0.44
8:3:94:ILE:O	8:3:98:LEU:HB2	2.16	0.44
9:1:33:LYS:NZ	9:1:44:PRO:O	2.50	0.44
11:5:448:PRO:HG3	20:B7:82:LYS:HG3	2.00	0.44
32:S2:186:LEU:HD21	32:S2:215:MET:HB2	1.99	0.44
35:2:223:LEU:HA	35:2:226:LEU:HD12	2.00	0.44
3:S1:80:ALA:O	3:S1:198:ARG:NH1	2.50	0.44
3:S1:320:MET:HB2	3:S1:589:VAL:HB	2.00	0.44
4:S3:115:ASP:OD1	4:S3:133:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:242:ASN:HB3	10:4:292:MET:HE1	2.00	0.44
22:B9:18:LEU:HD12	22:B9:66:GLN:HG3	1.98	0.44
23:BM:83:VAL:HA	23:BM:87:LEU:HD12	2.00	0.44
25:B3:45:GLU:HG2	25:B3:48:ARG:HE	1.81	0.44
1:AN:102:ARG:HD3	7:S8:204:SER:HB3	2.00	0.44
3:S1:270:ALA:HB3	3:S1:422:ALA:HB2	1.99	0.44
5:V2:69:ARG:O	5:V2:72:MET:HB2	2.18	0.44
5:V2:114:MET:HB2	34:V1:216:ALA:HB1	1.98	0.44
7:S8:106:HIS:CD2	7:S8:157:CYS:SG	2.90	0.44
16:AM:21:ILE:O	16:AM:25:ASN:HB2	2.18	0.44
30:A9:77:ARG:HE	30:A9:103:ARG:HE	1.66	0.44
10:4:116:PHE:HZ	10:4:194:LYS:HG3	1.82	0.44
10:4:152:LEU:HB3	35:2:279:MET:HE3	2.00	0.44
3:S1:218:MET:HE2	34:V1:237:LYS:HE2	1.98	0.44
11:5:186:GLY:HA3	11:5:239:ILE:HG21	2.00	0.44
18:B6:27:ARG:NH1	26:AC:146:ASP:O	2.48	0.44
28:B1:29:GLU:OE1	28:B1:32:ARG:NH2	2.45	0.44
32:S2:143:ARG:HG3	32:S2:228:HIS:CD2	2.53	0.44
42:AL:95:LYS:HG2	42:AL:235:LEU:HD12	2.00	0.44
1:AN:37:LYS:HB2	1:AN:37:LYS:HE2	1.80	0.44
17:BL:137:LYS:HB3	27:C2:109:LEU:CD1	2.48	0.44
35:2:60:TYR:OH	35:2:133:GLN:OE1	2.31	0.44
25:B3:79:THR:O	25:B3:83:GLU:HB2	2.18	0.44
3:S1:247:ASN:HB3	3:S1:250:TYR:HB3	2.00	0.43
9:1:107:LEU:HB3	9:1:110:LEU:HD12	2.00	0.43
9:1:215:VAL:HG12	32:S2:94:PRO:HD3	2.00	0.43
10:4:354:ASN:HB3	10:4:395:THR:HG21	2.00	0.43
32:S2:307:LEU:HB2	32:S2:406:GLU:HB2	2.00	0.43
34:V1:420:GLN:O	34:V1:465:MET:HE3	2.18	0.43
36:4L:32:LEU:HB3	37:6:66:PHE:HE1	1.82	0.43
6:S7:79:LEU:HD13	47:S7:304:PC1:H392	2.00	0.43
11:5:198:ALA:HB1	11:5:203:SER:HA	2.00	0.43
12:A8:142:LYS:HD3	12:A8:142:LYS:HA	1.83	0.43
16:AM:34:ALA:HA	48:2:401:3PE:H2A2	2.00	0.43
23:BM:99:ASP:OD1	23:BM:99:ASP:N	2.51	0.43
30:A9:306:ASP:OD1	30:A9:306:ASP:N	2.52	0.43
10:4:184:TYR:O	10:4:188:LEU:HB2	2.19	0.43
5:V2:226:SER:HB2	34:V1:55:ARG:HH21	1.83	0.43
7:S8:136:GLU:HB2	7:S8:149:ARG:HB3	2.00	0.43
10:4:68:ILE:O	10:4:72:MET:HB2	2.17	0.43
11:5:286:MET:HA	11:5:289:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S5:41:TYR:HB3	15:S5:45:ARG:HB3	2.00	0.43
49:B9:201:ZMP:H1A	49:B9:201:ZMP:H4A	1.62	0.43
3:S1:224:VAL:HG23	3:S1:226:LYS:HG3	2.00	0.43
3:S1:396:TYR:HB2	3:S1:523:GLN:HE22	1.83	0.43
4:S3:134:LEU:HB2	4:S3:143:ILE:HG22	2.00	0.43
10:4:79:ILE:HD12	10:4:130:TRP:HD1	1.84	0.43
10:4:334:LYS:HE3	10:4:334:LYS:HB3	1.84	0.43
11:5:189:VAL:HG22	11:5:232:LEU:HD21	2.01	0.43
12:A8:49:ARG:NH1	14:AO:84:ASP:OD2	2.52	0.43
16:AM:100:PHE:CE1	16:AM:104:LYS:HE3	2.54	0.43
32:S2:184:ARG:NH2	32:S2:406:GLU:O	2.52	0.43
42:AL:54:ALA:HB3	42:AL:77:ARG:HB3	2.00	0.43
1:AN:138:LYS:HE3	1:AN:138:LYS:HB3	1.51	0.43
8:3:76:PRO:HB3	37:6:133:LEU:HD13	2.01	0.43
30:A9:92:LEU:HD12	30:A9:113:VAL:HG13	2.00	0.43
35:2:112:PHE:O	35:2:116:ASN:ND2	2.51	0.43
35:2:208:SER:O	35:2:212:THR:OG1	2.31	0.43
6:S7:54:LYS:HB2	6:S7:54:LYS:HE2	1.83	0.43
10:4:5:ILE:HG23	10:4:98:LEU:HD11	2.00	0.43
11:5:81:MET:HB2	11:5:87:ILE:HD13	2.00	0.43
17:BL:113:THR:HG22	19:B4:113:ILE:HG12	2.00	0.43
24:B8:94:ASP:HB2	24:B8:101:ASN:HA	2.01	0.43
25:B3:44:ASN:HA	26:AC:85:LEU:HD13	2.01	0.43
32:S2:279:ASP:HA	32:S2:282:ILE:HD11	2.00	0.43
42:AL:383:ARG:NH1	42:AL:401:ILE:O	2.52	0.43
3:S1:572:VAL:HB	3:S1:586:ALA:HA	2.00	0.43
10:4:398:LEU:HG	10:4:399:TYR:N	2.32	0.43
15:S5:14:LEU:H	15:S5:14:LEU:HG	1.63	0.43
17:BL:137:LYS:HE3	27:C2:109:LEU:HD12	2.01	0.43
21:B5:129:HIS:ND1	28:B1:33:MET:HG2	2.33	0.43
24:B8:63:LYS:HB2	24:B8:63:LYS:HE3	1.51	0.43
35:2:34:LEU:HD22	35:2:104:LYS:HE2	2.00	0.43
39:A5:9:THR:OG1	39:A5:76:GLN:OE1	2.37	0.43
3:S1:229:LEU:H	3:S1:229:LEU:HG	1.65	0.43
6:S7:143:ARG:NH1	6:S7:181:ILE:O	2.52	0.43
11:5:559:ILE:HG23	16:AM:41:LEU:HB3	2.01	0.43
15:S5:6:PHE:HA	47:AM:205:PC1:H143	2.01	0.43
32:S2:283:VAL:HG13	32:S2:287:GLU:HG2	2.01	0.43
34:V1:103:ARG:NH1	34:V1:288:THR:O	2.48	0.43
3:S1:120:ARG:NH2	38:A7:61:ASP:OD2	2.51	0.43
4:S3:209:TYR:HE1	29:S4:128:LEU:HD11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S8:79:LEU:HD12	7:S8:82:ILE:HD12	2.01	0.43
9:1:121:TYR:HE1	37:6:67:ILE:HG13	1.83	0.43
26:AB:75:ILE:HD12	26:AB:144:VAL:HG13	2.00	0.43
3:S1:569:ASP:OD1	3:S1:569:ASP:N	2.47	0.42
8:3:66:ILE:HG23	37:6:152:LEU:HB3	2.01	0.42
10:4:356:ALA:HB1	10:4:363:LEU:HD13	2.01	0.42
21:B5:51:SER:HB2	22:B9:103:TRP:HA	2.01	0.42
34:V1:173:ILE:HG21	34:V1:181:ALA:HB2	2.01	0.42
3:S1:128:GLU:OE2	3:S1:162:ARG:NH2	2.45	0.42
4:S3:63:PHE:HE2	4:S3:143:ILE:HD12	1.84	0.42
4:S3:81:THR:HA	38:A7:69:PRO:HB3	2.00	0.42
9:1:89:SER:HB3	9:1:236:ALA:HB3	2.00	0.42
11:5:480:LEU:HD11	25:B3:28:VAL:HG22	2.01	0.42
16:AM:97:GLY:O	16:AM:110:GLY:HA2	2.19	0.42
17:BL:60:VAL:HG13	21:B5:128:LEU:HD22	2.01	0.42
24:B8:46:LYS:HA	24:B8:46:LYS:HD3	1.84	0.42
35:2:72:LEU:HD23	36:4L:42:LEU:HD13	2.00	0.42
1:AN:61:ARG:HE	1:AN:61:ARG:HB3	1.71	0.42
6:S7:219:TYR:O	30:A9:148:ASN:ND2	2.52	0.42
8:3:15:THR:HG22	9:1:86:LEU:HD23	2.01	0.42
10:4:189:CYS:HA	10:4:192:LEU:HB2	2.01	0.42
26:AC:124:PHE:HZ	26:AC:144:VAL:HG22	1.84	0.42
37:6:13:THR:HA	37:6:16:ILE:HG12	2.01	0.42
40:A3:70:LYS:HB3	40:A3:70:LYS:HE3	1.82	0.42
4:S3:110:PHE:HB3	4:S3:134:LEU:HB3	2.01	0.42
6:S7:40:GLN:HE22	7:S8:197:CYS:HB3	1.84	0.42
10:4:337:LEU:HD13	10:4:344:THR:HG21	2.00	0.42
11:5:106:ILE:HG13	11:5:106:ILE:H	1.62	0.42
11:5:523:LYS:HE3	24:B8:70:LEU:HB3	2.01	0.42
15:S5:21:HIS:CE1	36:4L:53:LEU:HD21	2.53	0.42
26:AC:80:LEU:HD21	26:AC:96:VAL:HG12	2.01	0.42
32:S2:249:ILE:HG22	32:S2:353:LEU:HD11	2.02	0.42
3:S1:309:ASP:OD2	3:S1:708:THR:OG1	2.36	0.42
3:S1:440:ILE:HD13	3:S1:451:TYR:HE2	1.84	0.42
6:S7:104:ILE:HG22	6:S7:195:ALA:HB1	2.02	0.42
24:B8:150:ASP:O	24:B8:153:LYS:NZ	2.53	0.42
1:AN:32:ARG:HA	47:S7:303:PC1:H152	2.01	0.42
3:S1:78:ARG:HE	3:S1:297:GLU:HG2	1.85	0.42
5:V2:133:CYS:HA	5:V2:176:ALA:HB1	2.01	0.42
6:S7:149:MET:O	8:3:35:LYS:NZ	2.53	0.42
7:S8:184:THR:HB	7:S8:187:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3:31:ILE:HD12	9:1:72:LEU:HD11	2.01	0.42
9:1:189:ALA:O	9:1:193:VAL:HG23	2.20	0.42
8:3:77:MET:HA	8:3:80:ILE:HD12	2.01	0.42
48:4:503:3PE:H232	48:AM:203:3PE:H32	2.02	0.42
11:5:321:ASN:ND2	11:5:416:ASN:O	2.53	0.42
35:2:234:LYS:HD3	35:2:234:LYS:HA	1.84	0.42
42:AL:252:ASP:N	42:AL:252:ASP:OD1	2.53	0.42
3:S1:401:THR:HG22	3:S1:403:ALA:H	1.84	0.42
6:S7:58:SER:HB2	43:S7:302:CDL:HB32	2.00	0.42
10:4:371:ASN:HB3	11:5:162:LEU:HD22	2.01	0.42
17:BL:46:ARG:HH21	28:B1:44:GLY:HA3	1.85	0.42
25:B3:11:VAL:HA	25:B3:12:PRO:HD3	1.90	0.42
32:S2:157:SER:OG	32:S2:176:ARG:NH1	2.52	0.42
3:S1:409:ASP:HB3	3:S1:480:ALA:HB1	2.02	0.42
8:3:74:ILE:HB	9:1:158:LEU:HD21	2.01	0.42
9:1:155:LEU:HB3	9:1:297:SER:HB3	2.02	0.42
10:4:169:ASN:HB2	21:B5:134:GLU:HG2	2.02	0.42
15:S5:27:CYS:HB2	15:S5:30:PHE:HD2	1.85	0.42
22:B9:106:LEU:HD23	23:BM:53:PRO:HG2	2.00	0.42
37:6:84:LEU:HD23	47:6:202:PC1:H31	2.02	0.42
4:S3:155:LEU:HD12	4:S3:155:LEU:HA	1.95	0.42
6:S7:154:TRP:HB3	6:S7:205:LEU:HD11	2.02	0.42
8:3:7:ILE:HD12	8:3:7:ILE:HA	1.93	0.42
9:1:300:TYR:HD1	40:A3:29:LEU:HD13	1.84	0.42
16:AM:104:LYS:HA	16:AM:104:LYS:HD3	1.72	0.42
16:AM:135:PHE:CG	35:2:151:LEU:HD21	2.55	0.42
17:BL:27:ARG:HA	17:BL:31:VAL:HB	2.02	0.42
17:BL:65:ALA:HA	17:BL:68:GLN:HG2	2.02	0.42
30:A9:182:VAL:HB	30:A9:202:TYR:HB2	2.01	0.42
37:6:39:LEU:O	37:6:43:LEU:HD22	2.20	0.42
6:S7:134:LEU:HD12	6:S7:138:MET:HB3	2.02	0.41
9:1:309:ILE:HD13	9:1:309:ILE:HA	1.91	0.41
10:4:437:LEU:HB3	47:4:501:PC1:H2	2.01	0.41
11:5:338:MET:O	11:5:342:SER:OG	2.37	0.41
20:B7:83:HIS:HA	20:B7:86:LEU:HB2	2.01	0.41
34:V1:142:ASP:O	34:V1:146:MET:HG2	2.20	0.41
6:S7:113:ARG:HA	9:1:44:PRO:HA	2.01	0.41
47:4:502:PC1:H132	47:4:502:PC1:H111	1.91	0.41
48:4:503:3PE:H12	19:B4:88:LYS:HE2	2.01	0.41
11:5:524:SER:O	11:5:529:TRP:N	2.49	0.41
17:BL:55:TYR:HA	27:C2:104:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BM:100:THR:OG1	23:BM:101:GLN:N	2.53	0.41
30:A9:291:GLN:HE21	30:A9:294:GLU:HG2	1.84	0.41
35:2:226:LEU:HD13	35:2:292:ILE:HG23	2.01	0.41
3:S1:60:LEU:HA	3:S1:70:ILE:HD13	2.02	0.41
4:S3:234:LYS:HB3	4:S3:234:LYS:HE3	1.84	0.41
20:B7:44:MET:HG3	20:B7:49:LEU:HD12	2.01	0.41
28:B1:6:ASP:OD1	28:B1:6:ASP:N	2.45	0.41
29:S4:179:ARG:HH22	34:V1:232:GLU:HB3	1.85	0.41
34:V1:56:ILE:HG12	34:V1:268:THR:HG21	2.03	0.41
1:AN:8:ASN:OD1	1:AN:8:ASN:N	2.52	0.41
3:S1:212:THR:HB	5:V2:110:THR:HG21	2.03	0.41
4:S3:101:PHE:HD1	39:A5:90:LEU:HD21	1.85	0.41
11:5:148:ARG:HD2	11:5:151:ASP:HB2	2.02	0.41
32:S2:188:HIS:NE2	32:S2:341:GLU:OE1	2.45	0.41
39:A5:22:HIS:NE2	42:AL:44:THR:O	2.50	0.41
3:S1:63:ALA:HB1	3:S1:68:VAL:HG13	2.02	0.41
6:S7:96:CYS:SG	45:S7:301:SF4:S3	3.13	0.41
10:4:62:ILE:HD11	10:4:105:SER:HB3	2.02	0.41
12:A8:3:ILE:HG22	14:AO:95:ARG:HD3	2.02	0.41
17:BL:55:TYR:CD2	27:C2:102:ARG:HB3	2.55	0.41
23:BM:113:GLU:HA	23:BM:116:ARG:HG2	2.01	0.41
34:V1:285:ASN:HD21	34:V1:355:ASP:H	1.69	0.41
38:A7:29:ARG:HD2	38:A7:34:LEU:HD11	2.01	0.41
3:S1:159:ASP:HB2	32:S2:366:ALA:HB3	2.02	0.41
3:S1:471:HIS:O	3:S1:475:LYS:NZ	2.53	0.41
11:5:338:MET:O	11:5:342:SER:CB	2.68	0.41
32:S2:273:TRP:O	32:S2:277:THR:OG1	2.30	0.41
37:6:44:MET:H	37:6:44:MET:HG2	1.70	0.41
41:A6:94:TRP:O	41:A6:96:GLN:NE2	2.53	0.41
6:S7:113:ARG:NH2	7:S8:90:ASN:OD1	2.53	0.41
8:3:80:ILE:H	8:3:80:ILE:HG13	1.71	0.41
8:3:84:SER:OG	8:3:85:ASN:N	2.54	0.41
8:3:97:ILE:HG23	9:1:298:LEU:HD22	2.03	0.41
9:1:33:LYS:HA	9:1:43:GLY:HA3	2.01	0.41
9:1:99:PHE:HB2	9:1:255:PHE:CE1	2.55	0.41
10:4:202:LEU:HD21	11:5:530:SER:HB2	2.02	0.41
12:A8:132:LYS:HB2	40:A3:60:VAL:HG12	2.02	0.41
12:A8:4:THR:OG1	12:A8:5:ASN:N	2.53	0.41
16:AM:106:ASN:HD22	16:AM:109:ALA:HB2	1.85	0.41
39:A5:24:LEU:HD23	39:A5:24:LEU:HA	1.95	0.41
3:S1:46:VAL:O	3:S1:49:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:269:ASP:OD1	3:S1:269:ASP:N	2.52	0.41
3:S1:356:GLY:HA2	3:S1:556:ALA:HB2	2.03	0.41
4:S3:109:GLN:HE21	39:A5:83:GLN:HG2	1.85	0.41
9:1:93:TRP:HZ2	9:1:239:LEU:HB3	1.86	0.41
10:4:250:ILE:HD11	10:4:290:LEU:HB2	2.03	0.41
10:4:398:LEU:O	10:4:402:SER:OG	2.31	0.41
10:4:437:LEU:HD13	47:4:501:PC1:H242	2.02	0.41
11:5:541:LYS:HA	11:5:541:LYS:HD2	1.82	0.41
12:A8:170:ARG:HG2	21:B5:137:LYS:HG2	2.03	0.41
47:AM:205:PC1:H261	47:2:403:PC1:H322	2.02	0.41
18:B6:115:LYS:HG3	18:B6:116:TYR:HD2	1.85	0.41
20:B7:86:LEU:HD23	20:B7:86:LEU:HA	1.96	0.41
22:B9:67:ARG:HA	22:B9:67:ARG:HD2	1.97	0.41
27:C2:27:ASN:HD21	47:C2:201:PC1:H141	1.85	0.41
29:S4:167:ASN:HB3	29:S4:170:ILE:HG23	2.03	0.41
30:A9:82:LYS:NZ	30:A9:262:SER:OG	2.45	0.41
35:2:317:TYR:HA	35:2:320:TYR:HB3	2.03	0.41
37:6:4:LEU:HD23	37:6:7:TYR:HD2	1.85	0.41
47:6:201:PC1:H142	47:6:201:PC1:H111	1.92	0.41
41:A6:39:GLN:HG2	41:A6:91:VAL:HG22	2.03	0.41
42:AL:100:LYS:HB3	42:AL:100:LYS:HE3	1.92	0.41
47:S7:304:PC1:H3C1	9:1:60:ILE:HG23	2.03	0.41
11:5:201:PRO:HD3	11:5:252:LEU:HD22	2.03	0.41
16:AM:40:VAL:HG23	16:AM:41:LEU:HD12	2.02	0.41
24:B8:56:TYR:CD2	24:B8:103:HIS:HB3	2.56	0.41
38:A7:34:LEU:HD23	38:A7:34:LEU:HA	1.96	0.41
1:AN:10:LEU:HD11	43:AN:201:CDL:H522	2.01	0.40
1:AN:37:LYS:HD3	1:AN:61:ARG:HH21	1.86	0.40
1:AN:47:TYR:HE2	1:AN:81:PRO:HB3	1.84	0.40
5:V2:63:TYR:OH	34:V1:213:HIS:ND1	2.39	0.40
8:3:10:LEU:HD23	8:3:10:LEU:HA	1.90	0.40
9:1:9:SER:HB2	13:A1:36:ARG:HH22	1.86	0.40
10:4:370:LEU:HD22	10:4:384:LEU:HD13	2.03	0.40
11:5:85:ASN:OD1	21:B5:47:ILE:HG21	2.21	0.40
14:AO:133:LYS:NZ	37:6:108:SER:O	2.40	0.40
16:AM:10:ASP:OD1	16:AM:10:ASP:N	2.53	0.40
29:S4:106:ILE:HG12	29:S4:133:VAL:HB	2.03	0.40
35:2:250:LEU:HA	35:2:251:PRO:HD3	1.91	0.40
3:S1:265:ILE:HG22	3:S1:274:ASN:HD22	1.86	0.40
3:S1:562:THR:OG1	3:S1:563:ARG:N	2.54	0.40
7:S8:154:MET:HA	7:S8:157:CYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:5:210:MET:SD	11:5:271:LYS:HB3	2.61	0.40
12:A8:8:THR:O	12:A8:8:THR:OG1	2.38	0.40
14:AO:147:ARG:NH2	37:6:117:GLN:O	2.54	0.40
34:V1:305:GLU:HG2	34:V1:314:LEU:HD13	2.02	0.40
52:AL:501:DGT:H8	52:AL:501:DGT:H5'A	2.02	0.40
3:S1:406:GLU:HA	3:S1:432:ALA:HB2	2.04	0.40
5:V2:179:VAL:HG22	5:V2:189:LEU:HD11	2.02	0.40
10:4:201:HIS:O	10:4:202:LEU:C	2.58	0.40
11:5:556:SER:HB2	36:4L:95:ILE:H	1.85	0.40
48:AM:204:3PE:H262	48:2:401:3PE:H381	2.04	0.40
30:A9:231:LEU:O	30:A9:235:ALA:HB2	2.22	0.40
35:2:118:MET:HG3	35:2:172:ARG:HB3	2.04	0.40
36:4L:61:MET:HA	36:4L:64:LEU:HB2	2.04	0.40
42:AL:172:ILE:HG21	42:AL:343:LYS:HG3	2.02	0.40
42:AL:223:ILE:HD12	42:AL:226:LEU:HD21	2.03	0.40
1:AN:128:THR:HG23	7:S8:149:ARG:HB2	2.04	0.40
2:S6:113:TYR:OH	3:S1:139:PRO:HD2	2.22	0.40
5:V2:31:LEU:O	5:V2:117:ARG:NH1	2.41	0.40
9:1:17:ILE:HG23	9:1:90:LEU:HD13	2.02	0.40
9:1:145:GLN:NE2	9:1:201:ASN:OD1	2.54	0.40
9:1:258:LEU:HD23	9:1:258:LEU:HA	1.96	0.40
11:5:485:LYS:HB2	48:5:603:3PE:H31	2.03	0.40
16:AM:30:SER:HB2	48:AM:204:3PE:H221	2.03	0.40
18:B6:20:ARG:HD2	19:B4:26:LEU:HD13	2.02	0.40
47:B6:201:PC1:H112	43:B5:201:CDL:H131	2.03	0.40
35:2:104:LYS:HB3	35:2:104:LYS:HE3	1.88	0.40
42:AL:296:GLU:HB2	42:AL:299:VAL:HG12	2.03	0.40
3:S1:511:LEU:HD12	3:S1:511:LEU:O	2.22	0.40
6:S7:64:GLN:HG2	6:S7:69:GLU:HG3	2.04	0.40
17:BL:27:ARG:NH1	43:B5:201:CDL:OB3	2.54	0.40
18:B6:28:LEU:HD21	26:AC:147:LYS:HB2	2.03	0.40
19:B4:10:PHE:CE1	24:B8:61:GLU:HG2	2.56	0.40
35:2:147:LYS:HE3	35:2:147:LYS:HB3	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AN	135/142 (95%)	134 (99%)	1 (1%)	0	100	100
2	S6	88/126 (70%)	87 (99%)	1 (1%)	0	100	100
3	S1	676/731 (92%)	653 (97%)	23 (3%)	0	100	100
4	S3	206/265 (78%)	202 (98%)	4 (2%)	0	100	100
5	V2	212/242 (88%)	206 (97%)	6 (3%)	0	100	100
6	S7	180/221 (81%)	173 (96%)	6 (3%)	1 (1%)	22	53
7	S8	184/217 (85%)	178 (97%)	6 (3%)	0	100	100
8	3	101/117 (86%)	101 (100%)	0	0	100	100
9	1	313/315 (99%)	300 (96%)	13 (4%)	0	100	100
10	4	444/446 (100%)	430 (97%)	13 (3%)	1 (0%)	44	71
11	5	575/577 (100%)	547 (95%)	28 (5%)	0	100	100
12	A8	172/175 (98%)	167 (97%)	5 (3%)	0	100	100
13	A1	68/123 (55%)	66 (97%)	2 (3%)	0	100	100
14	AO	142/154 (92%)	141 (99%)	1 (1%)	0	100	100
15	S5	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
16	AM	162/170 (95%)	159 (98%)	3 (2%)	0	100	100
17	BL	148/159 (93%)	144 (97%)	4 (3%)	0	100	100
18	B6	159/167 (95%)	154 (97%)	5 (3%)	0	100	100
19	B4	108/113 (96%)	106 (98%)	2 (2%)	0	100	100
20	B7	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
21	B5	141/186 (76%)	139 (99%)	2 (1%)	0	100	100
22	B9	131/144 (91%)	130 (99%)	1 (1%)	0	100	100
23	BM	104/150 (69%)	102 (98%)	2 (2%)	0	100	100
24	B8	142/175 (81%)	134 (94%)	8 (6%)	0	100	100
25	B3	79/110 (72%)	75 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	AB	79/152 (52%)	78 (99%)	1 (1%)	0	100	100
26	AC	82/152 (54%)	81 (99%)	1 (1%)	0	100	100
27	C2	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
28	B1	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
29	S4	124/183 (68%)	120 (97%)	4 (3%)	0	100	100
30	A9	366/416 (88%)	352 (96%)	14 (4%)	0	100	100
31	B2	57/94 (61%)	57 (100%)	0	0	100	100
32	S2	415/468 (89%)	404 (97%)	11 (3%)	0	100	100
34	V1	437/474 (92%)	417 (95%)	19 (4%)	1 (0%)	44	71
35	2	339/341 (99%)	330 (97%)	9 (3%)	0	100	100
36	4L	93/96 (97%)	93 (100%)	0	0	100	100
37	6	163/174 (94%)	157 (96%)	6 (4%)	0	100	100
38	A7	86/103 (84%)	85 (99%)	1 (1%)	0	100	100
39	A5	115/124 (93%)	111 (96%)	4 (4%)	0	100	100
40	A3	65/77 (84%)	65 (100%)	0	0	100	100
41	A6	112/124 (90%)	108 (96%)	4 (4%)	0	100	100
42	AL	366/407 (90%)	353 (96%)	13 (4%)	0	100	100
All	All	7942/9000 (88%)	7702 (97%)	237 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	4	202	LEU
6	S7	192	PRO
34	V1	424	ILE

### 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	AN	118/122 (97%)	117 (99%)	1 (1%)	79	87
2	S6	78/111 (70%)	77 (99%)	1 (1%)	65	79
3	S1	549/582 (94%)	545 (99%)	4 (1%)	81	88
4	S3	186/225 (83%)	186 (100%)	0	100	100
5	V2	185/205 (90%)	184 (100%)	1 (0%)	86	91
6	S7	152/184 (83%)	150 (99%)	2 (1%)	65	79
7	S8	159/182 (87%)	159 (100%)	0	100	100
8	3	98/110 (89%)	97 (99%)	1 (1%)	73	84
9	1	282/282 (100%)	280 (99%)	2 (1%)	81	88
10	4	402/404 (100%)	400 (100%)	2 (0%)	86	91
11	5	518/518 (100%)	516 (100%)	2 (0%)	89	93
12	A8	150/151 (99%)	150 (100%)	0	100	100
13	A1	63/115 (55%)	63 (100%)	0	100	100
14	AO	126/134 (94%)	126 (100%)	0	100	100
15	S5	88/89 (99%)	81 (92%)	7 (8%)	10	32
16	AM	125/131 (95%)	123 (98%)	2 (2%)	58	76
17	BL	133/141 (94%)	133 (100%)	0	100	100
18	B6	133/136 (98%)	132 (99%)	1 (1%)	79	87
19	B4	91/94 (97%)	91 (100%)	0	100	100
20	B7	100/104 (96%)	99 (99%)	1 (1%)	73	84
21	B5	129/162 (80%)	127 (98%)	2 (2%)	58	76
22	B9	116/126 (92%)	115 (99%)	1 (1%)	75	85
23	BM	95/131 (72%)	94 (99%)	1 (1%)	70	82
24	B8	121/145 (83%)	118 (98%)	3 (2%)	42	67
25	B3	66/84 (79%)	66 (100%)	0	100	100
26	AB	75/136 (55%)	73 (97%)	2 (3%)	40	65
26	AC	78/136 (57%)	78 (100%)	0	100	100
27	C2	92/94 (98%)	87 (95%)	5 (5%)	18	46
28	B1	42/43 (98%)	42 (100%)	0	100	100
29	S4	110/154 (71%)	110 (100%)	0	100	100
30	A9	313/346 (90%)	312 (100%)	1 (0%)	91	94
31	B2	50/80 (62%)	49 (98%)	1 (2%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	S2	358/398 (90%)	358 (100%)	0	100	100
34	V1	351/381 (92%)	350 (100%)	1 (0%)	91	94
35	2	317/317 (100%)	316 (100%)	1 (0%)	91	94
36	4L	90/91 (99%)	90 (100%)	0	100	100
37	6	159/167 (95%)	157 (99%)	2 (1%)	65	79
38	A7	77/86 (90%)	77 (100%)	0	100	100
39	A5	96/102 (94%)	96 (100%)	0	100	100
40	A3	53/59 (90%)	53 (100%)	0	100	100
41	A6	107/114 (94%)	104 (97%)	3 (3%)	38	64
42	AL	324/356 (91%)	323 (100%)	1 (0%)	91	94
All	All	6955/7728 (90%)	6904 (99%)	51 (1%)	80	88

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AN	138	LYS
2	S6	48	LYS
3	S1	219	GLN
3	S1	229	LEU
3	S1	511	LEU
3	S1	651	ARG
5	V2	77	ASP
6	S7	96	CYS
6	S7	186	ILE
8	3	44	ASP
9	1	252	CYS
9	1	253	ASP
10	4	201	HIS
10	4	398	LEU
11	5	106	ILE
11	5	237	ASN
15	S5	8	ARG
15	S5	14	LEU
15	S5	15	THR
15	S5	23	THR
15	S5	24	TYR
15	S5	26	LYS
15	S5	29	LYS

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Mol	Chain	Res	Type
16	AM	104	LYS
16	AM	106	ASN
18	B6	68	ARG
20	B7	70	ASP
21	B5	44	HIS
21	B5	46	MET
22	B9	50	ASN
23	BM	142	ASP
24	B8	60	GLU
24	B8	61	GLU
24	B8	63	LYS
27	C2	103	LYS
27	C2	104	THR
27	C2	108	VAL
27	C2	109	LEU
27	C2	116	ARG
30	A9	229	ARG
31	B2	66	GLU
34	V1	420	GLN
35	2	82	ASN
37	6	31	LEU
37	6	43	LEU
41	A6	17	ILE
41	A6	18	LEU
41	A6	19	SER
42	AL	247	LYS
26	AB	81	LEU
26	AB	84	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	S1	134	HIS
35	2	181	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 1 is monoatomic - leaving 48 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	$\# Z  > 2$
47	PC1	1	401	-	53,53,53	0.32	0	59,61,61	0.54	1 (1%)
48	3PE	5	607	-	50,50,50	0.30	0	53,55,55	0.30	0
47	PC1	6	202	-	28,28,53	0.41	0	34,36,61	0.40	0
45	SF4	S1	802	3	0,12,12	-	-	-		
48	3PE	B6	202	-	43,43,50	0.35	0	46,48,55	0.73	3 (6%)
43	CDL	5	604	-	67,67,99	0.35	0	73,79,111	0.32	0
46	FES	S1	803	3	0,4,4	-	-	-		
47	PC1	C2	201	-	38,38,53	0.33	0	44,46,61	0.35	0
49	ZMP	AB	201	-	28,33,36	0.81	2 (7%)	32,40,45	3.16	9 (28%)
45	SF4	S8	302	7	0,12,12	-	-	-		
51	FMN	V1	501	-	33,33,33	0.25	0	48,50,50	0.37	0
48	3PE	5	603	-	50,50,50	0.30	0	53,55,55	0.29	0
43	CDL	S7	302	-	70,70,99	0.34	0	76,82,111	0.28	0
45	SF4	S7	301	6	0,12,12	-	-	-		
47	PC1	S7	303	-	35,35,53	0.35	0	41,43,61	0.43	0
48	3PE	5	601	-	31,31,50	0.37	0	34,36,55	0.33	0
48	3PE	AM	204	-	31,31,50	0.37	0	34,36,55	0.32	0
52	DGT	AL	501	-	29,33,33	0.97	3 (10%)	37,52,52	0.75	1 (2%)
43	CDL	B6	203	-	52,52,99	0.41	0	58,64,111	0.56	1 (1%)
47	PC1	AM	205	-	32,32,53	0.36	0	38,40,61	0.37	0
45	SF4	S8	301	7	0,12,12	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
43	CDL	A9	503	-	46,46,99	0.44	0	52,58,111	0.59	1 (1%)
47	PC1	2	402	-	43,43,53	0.31	0	49,51,61	0.33	0
43	CDL	A9	502	-	53,53,99	0.40	0	59,65,111	0.36	0
43	CDL	5	608	-	74,74,99	0.34	0	80,86,111	0.30	0
48	3PE	4	503	-	34,34,50	0.36	0	37,39,55	0.36	0
48	3PE	AM	201	-	38,38,50	0.34	0	41,43,55	0.29	0
43	CDL	B5	201	-	73,73,99	0.34	0	79,85,111	0.31	0
48	3PE	2	401	-	38,38,50	0.37	0	41,43,55	0.63	1 (2%)
47	PC1	4	502	-	43,43,53	0.33	0	49,51,61	0.32	0
48	3PE	AM	203	-	35,35,50	0.36	0	38,40,55	0.32	0
47	PC1	B4	201	-	33,33,53	0.35	0	39,41,61	0.36	0
48	3PE	5	605	-	35,35,50	0.38	0	38,40,55	0.65	1 (2%)
48	3PE	5	602	-	32,32,50	0.37	0	35,37,55	0.36	0
45	SF4	S1	801	3	0,12,12	-	-	-	-	-
47	PC1	B6	201	-	36,36,53	0.36	0	42,44,61	0.64	1 (2%)
47	PC1	2	403	-	44,44,53	0.34	0	50,52,61	0.33	0
47	PC1	4	501	-	38,38,53	0.33	0	44,46,61	0.36	0
48	3PE	5	606	-	44,44,50	0.32	0	47,49,55	0.43	0
45	SF4	V1	502	34	0,12,12	-	-	-	-	-
47	PC1	AM	202	-	36,36,53	0.34	0	42,44,61	0.34	0
46	FES	V2	301	5	0,4,4	-	-	-	-	-
50	NDP	A9	501	-	47,52,52	0.55	0	61,80,80	0.53	1 (1%)
48	3PE	4	504	-	38,38,50	0.36	0	41,43,55	0.64	1 (2%)
47	PC1	6	201	-	35,35,53	0.34	0	41,43,61	0.35	0
49	ZMP	B9	201	-	28,33,36	0.23	0	32,40,45	0.34	0
43	CDL	AN	201	-	66,66,99	0.35	0	72,78,111	0.31	0
47	PC1	S7	304	-	45,45,53	0.33	0	51,53,61	0.31	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
47	PC1	1	401	-	-	18/57/57/57	-
48	3PE	5	607	-	-	12/54/54/54	-
47	PC1	6	202	-	-	9/32/32/57	-
48	3PE	B6	202	-	-	12/47/47/54	-
45	SF4	S1	802	3	-	-	0/6/5/5
43	CDL	5	604	-	-	15/78/78/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FES	S1	803	3	-	-	0/1/1/1
47	PC1	C2	201	-	-	11/42/42/57	-
49	ZMP	AB	201	-	-	20/38/40/43	-
45	SF4	S8	302	7	-	-	0/6/5/5
51	FMN	V1	501	-	-	8/18/18/18	0/3/3/3
48	3PE	5	603	-	-	11/54/54/54	-
43	CDL	S7	302	-	-	10/81/81/110	-
47	PC1	S7	303	-	-	9/39/39/57	-
48	3PE	5	601	-	-	4/35/35/54	-
48	3PE	AM	204	-	-	4/35/35/54	-
52	DGT	AL	501	-	-	4/18/34/34	0/3/3/3
45	SF4	S7	301	6	-	-	0/6/5/5
43	CDL	B6	203	-	-	17/63/63/110	-
47	PC1	AM	205	-	-	12/36/36/57	-
45	SF4	S8	301	7	-	-	0/6/5/5
43	CDL	A9	503	-	-	18/57/57/110	-
47	PC1	2	402	-	-	8/47/47/57	-
43	CDL	A9	502	-	-	15/64/64/110	-
43	CDL	5	608	-	-	11/85/85/110	-
48	3PE	4	503	-	-	7/38/38/54	-
48	3PE	AM	201	-	-	7/42/42/54	-
43	CDL	B5	201	-	-	17/84/84/110	-
48	3PE	2	401	-	-	10/42/42/54	-
47	PC1	4	502	-	-	9/47/47/57	-
48	3PE	AM	203	-	-	12/39/39/54	-
47	PC1	B4	201	-	-	9/37/37/57	-
48	3PE	5	605	-	-	3/39/39/54	-
48	3PE	5	602	-	-	6/36/36/54	-
45	SF4	S1	801	3	-	-	0/6/5/5
47	PC1	B6	201	-	-	11/40/40/57	-
47	PC1	2	403	-	-	12/48/48/57	-
47	PC1	4	501	-	-	4/42/42/57	-
48	3PE	5	606	-	-	15/48/48/54	-
47	PC1	AM	202	-	-	5/40/40/57	-
45	SF4	V1	502	34	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FES	V2	301	5	-	-	0/1/1/1
50	NDP	A9	501	-	-	5/30/77/77	0/5/5/5
48	3PE	4	504	-	-	6/42/42/54	-
47	PC1	6	201	-	-	11/39/39/57	-
49	ZMP	B9	201	-	-	26/38/40/43	-
43	CDL	AN	201	-	-	13/77/77/110	-
47	PC1	S7	304	-	-	10/49/49/57	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	AL	501	DGT	C5-C6	-2.77	1.42	1.47
49	AB	201	ZMP	C9-C10	2.33	1.53	1.50
49	AB	201	ZMP	O4-C17	2.23	1.46	1.42
52	AL	501	DGT	C8-N7	-2.19	1.31	1.34
52	AL	501	DGT	C5-C4	-2.04	1.38	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	AB	201	ZMP	C19-C18-C17	-7.99	95.14	108.77
49	AB	201	ZMP	C19-C18-C21	7.69	120.91	108.22
49	AB	201	ZMP	C20-C18-C21	7.68	120.90	108.22
49	AB	201	ZMP	C20-C18-C17	-7.50	95.98	108.77
49	AB	201	ZMP	C20-C18-C19	4.49	118.16	109.20
49	AB	201	ZMP	C15-N2-C16	4.00	129.73	122.55
49	AB	201	ZMP	C17-C16-N2	3.35	122.84	116.48
48	2	401	3PE	C2-O21-C21	2.69	124.22	117.80
47	B6	201	PC1	C2-O21-C21	2.63	124.10	117.80
43	B6	203	CDL	CB4-OB6-CB5	2.55	123.89	117.80
48	5	605	3PE	C2-O21-C21	2.51	123.81	117.80
49	AB	201	ZMP	O1-C10-C9	-2.51	121.08	123.98
43	A9	503	CDL	CB4-OB6-CB5	2.51	123.80	117.80
48	4	504	3PE	C2-O21-C21	2.49	123.76	117.80
47	1	401	PC1	C2-O21-C21	2.45	123.67	117.80
48	B6	202	3PE	O31-C3-C2	2.37	115.22	108.40
48	B6	202	3PE	C2-O21-C21	2.33	123.37	117.80
50	A9	501	NDP	C5A-C6A-N6A	2.31	123.83	120.31
48	B6	202	3PE	O21-C2-C3	2.30	116.59	108.34
49	AB	201	ZMP	O4-C17-C18	2.02	114.86	110.18
52	AL	501	DGT	O6-C6-C5	2.02	128.32	124.32

There are no chirality outliers.

All (426) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	AN	201	CDL	CA2-OA2-PA1-OA3
43	AN	201	CDL	CA2-OA2-PA1-OA4
43	AN	201	CDL	CA2-OA2-PA1-OA5
43	AN	201	CDL	CA3-OA5-PA1-OA2
43	AN	201	CDL	CB3-OB5-PB2-OB2
43	AN	201	CDL	CB3-OB5-PB2-OB4
43	S7	302	CDL	CB2-OB2-PB2-OB4
43	S7	302	CDL	CB3-OB5-PB2-OB2
43	S7	302	CDL	CB3-OB5-PB2-OB4
43	5	604	CDL	CA2-OA2-PA1-OA3
43	5	604	CDL	CA2-OA2-PA1-OA4
43	5	604	CDL	CA2-OA2-PA1-OA5
43	5	604	CDL	CA3-OA5-PA1-OA4
43	5	604	CDL	CB2-OB2-PB2-OB4
43	5	608	CDL	CA2-OA2-PA1-OA4
43	5	608	CDL	CA2-OA2-PA1-OA5
43	5	608	CDL	CA3-OA5-PA1-OA2
43	5	608	CDL	CA3-OA5-PA1-OA4
43	5	608	CDL	CA4-CA3-OA5-PA1
43	5	608	CDL	CB3-OB5-PB2-OB2
43	5	608	CDL	CB3-OB5-PB2-OB4
43	B6	203	CDL	CA2-OA2-PA1-OA5
43	B6	203	CDL	CA3-OA5-PA1-OA2
43	B6	203	CDL	C1-CB2-OB2-PB2
43	B6	203	CDL	CB2-OB2-PB2-OB4
43	B6	203	CDL	CB2-OB2-PB2-OB5
43	B6	203	CDL	CB3-OB5-PB2-OB2
43	B6	203	CDL	CB3-OB5-PB2-OB3
43	B6	203	CDL	CB3-OB5-PB2-OB4
43	B5	201	CDL	CA3-OA5-PA1-OA2
43	B5	201	CDL	CA3-OA5-PA1-OA3
43	B5	201	CDL	CB2-OB2-PB2-OB3
43	B5	201	CDL	CB2-OB2-PB2-OB4
43	B5	201	CDL	CB2-OB2-PB2-OB5
43	B5	201	CDL	CB3-OB5-PB2-OB2
43	B5	201	CDL	CB3-OB5-PB2-OB3
43	B5	201	CDL	CB3-OB5-PB2-OB4
43	A9	502	CDL	CA2-OA2-PA1-OA4
43	A9	502	CDL	CA3-OA5-PA1-OA2
43	A9	502	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
43	A9	502	CDL	CB2-OB2-PB2-OB5
43	A9	502	CDL	CB3-OB5-PB2-OB3
43	A9	502	CDL	OB5-CB3-CB4-OB6
43	A9	503	CDL	CA3-OA5-PA1-OA2
43	A9	503	CDL	CA3-OA5-PA1-OA3
43	A9	503	CDL	CA3-OA5-PA1-OA4
43	A9	503	CDL	CB2-OB2-PB2-OB3
43	A9	503	CDL	CB2-OB2-PB2-OB4
43	A9	503	CDL	CB2-OB2-PB2-OB5
43	A9	503	CDL	CB3-OB5-PB2-OB2
43	A9	503	CDL	CB3-OB5-PB2-OB3
43	A9	503	CDL	CB3-OB5-PB2-OB4
47	S7	303	PC1	C1-O11-P-O12
47	S7	303	PC1	C1-O11-P-O13
47	S7	304	PC1	C11-O13-P-O12
47	S7	304	PC1	C11-O13-P-O11
47	S7	304	PC1	C1-O11-P-O14
47	1	401	PC1	C11-O13-P-O12
47	1	401	PC1	C11-O13-P-O14
47	1	401	PC1	C11-O13-P-O11
47	4	501	PC1	C11-O13-P-O12
47	4	501	PC1	C1-O11-P-O14
47	4	502	PC1	C11-O13-P-O12
47	4	502	PC1	C11-O13-P-O11
47	AM	202	PC1	C11-O13-P-O14
47	AM	202	PC1	C11-O13-P-O11
47	AM	202	PC1	C1-O11-P-O12
47	AM	205	PC1	C11-O13-P-O14
47	AM	205	PC1	C11-O13-P-O11
47	AM	205	PC1	C1-O11-P-O14
47	AM	205	PC1	C1-O11-P-O13
47	B6	201	PC1	C11-O13-P-O12
47	B6	201	PC1	C11-O13-P-O14
47	B6	201	PC1	C11-O13-P-O11
47	B6	201	PC1	C1-O11-P-O12
47	B6	201	PC1	C1-O11-P-O14
47	B6	201	PC1	C1-O11-P-O13
47	C2	201	PC1	C11-O13-P-O12
47	C2	201	PC1	C11-O13-P-O14
47	C2	201	PC1	C11-O13-P-O11
47	C2	201	PC1	C1-O11-P-O13
47	C2	201	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
47	2	402	PC1	C11-O13-P-O12
47	2	402	PC1	C11-O13-P-O11
47	2	403	PC1	C11-O13-P-O12
47	2	403	PC1	C11-O13-P-O11
47	2	403	PC1	C1-O11-P-O12
47	2	403	PC1	C1-O11-P-O14
47	2	403	PC1	C1-O11-P-O13
47	6	201	PC1	C11-O13-P-O12
47	6	201	PC1	C11-O13-P-O14
47	6	201	PC1	C11-O13-P-O11
47	6	201	PC1	C1-O11-P-O14
47	6	202	PC1	C11-O13-P-O12
47	6	202	PC1	C11-O13-P-O14
47	6	202	PC1	C11-O13-P-O11
47	6	202	PC1	C1-O11-P-O12
48	4	503	3PE	C1-O11-P-O12
48	4	503	3PE	C1-O11-P-O13
48	4	503	3PE	C1-O11-P-O14
48	4	503	3PE	C11-O13-P-O11
48	4	503	3PE	C11-O13-P-O12
48	4	504	3PE	C1-O11-P-O13
48	4	504	3PE	C1-O11-P-O14
48	4	504	3PE	C11-O13-P-O14
48	5	601	3PE	C1-O11-P-O12
48	5	601	3PE	C1-O11-P-O13
48	5	602	3PE	C11-O13-P-O11
48	5	602	3PE	C11-O13-P-O12
48	5	602	3PE	C11-O13-P-O14
48	5	602	3PE	O13-C11-C12-N
48	5	603	3PE	C11-O13-P-O11
48	5	603	3PE	C11-O13-P-O12
48	5	603	3PE	C11-O13-P-O14
48	5	603	3PE	O13-C11-C12-N
48	5	605	3PE	O13-C11-C12-N
48	5	606	3PE	C1-O11-P-O13
48	5	606	3PE	C11-O13-P-O11
48	5	606	3PE	C11-O13-P-O12
48	5	606	3PE	C2-C1-O11-P
48	5	607	3PE	C1-O11-P-O13
48	5	607	3PE	C11-O13-P-O12
48	5	607	3PE	O13-C11-C12-N
48	AM	201	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
48	AM	201	3PE	C11-O13-P-O12
48	AM	201	3PE	C11-O13-P-O14
48	AM	203	3PE	C11-O13-P-O11
48	AM	203	3PE	C11-O13-P-O14
48	AM	204	3PE	C1-O11-P-O12
48	AM	204	3PE	C1-O11-P-O14
48	B6	202	3PE	C1-O11-P-O12
48	B6	202	3PE	C11-O13-P-O11
48	B6	202	3PE	C11-O13-P-O14
48	B6	202	3PE	O13-C11-C12-N
48	2	401	3PE	C1-O11-P-O13
48	2	401	3PE	C1-O11-P-O14
49	B9	201	ZMP	C19-C18-C21-O5
49	B9	201	ZMP	C20-C18-C21-O5
49	B9	201	ZMP	C17-C18-C21-O5
49	B9	201	ZMP	O4-C17-C18-C21
49	B9	201	ZMP	C16-C17-C18-C21
49	B9	201	ZMP	C16-C17-C18-C19
49	B9	201	ZMP	O4-C17-C18-C20
49	B9	201	ZMP	C16-C17-C18-C20
49	B9	201	ZMP	C17-C16-N2-C15
49	B9	201	ZMP	O3-C16-N2-C15
49	B9	201	ZMP	C13-C14-C15-N2
49	B9	201	ZMP	C14-C13-N1-C12
49	B9	201	ZMP	S1-C11-C12-N1
49	B9	201	ZMP	S1-C10-C9-C8
49	B9	201	ZMP	O1-C10-C9-C8
49	B9	201	ZMP	C7-C8-C9-C10
49	AB	201	ZMP	C20-C18-C21-O5
49	AB	201	ZMP	C17-C18-C21-O5
49	AB	201	ZMP	C16-C17-C18-C21
49	AB	201	ZMP	C16-C17-C18-C19
49	AB	201	ZMP	C16-C17-C18-C20
49	AB	201	ZMP	O3-C16-C17-O4
49	AB	201	ZMP	N2-C16-C17-O4
49	AB	201	ZMP	C17-C16-N2-C15
49	AB	201	ZMP	S1-C11-C12-N1
49	AB	201	ZMP	O1-C10-S1-C11
49	AB	201	ZMP	C9-C10-S1-C11
50	A9	501	NDP	PN-O3-PA-O5B
50	A9	501	NDP	C5D-O5D-PN-O3
50	A9	501	NDP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
51	V1	501	FMN	C3'-C4'-C5'-O5'
52	AL	501	DGT	C5'-O5'-PA-O3A
52	AL	501	DGT	C3'-C4'-C5'-O5'
49	B9	201	ZMP	O2-C13-N1-C12
43	B6	203	CDL	O1-C1-CB2-OB2
43	A9	503	CDL	O1-C1-CA2-OA2
49	AB	201	ZMP	O3-C16-N2-C15
52	AL	501	DGT	O4'-C4'-C5'-O5'
49	B9	201	ZMP	C1-C2-C3-C4
43	B6	203	CDL	CA2-C1-CB2-OB2
47	2	403	PC1	C11-C12-N-C14
49	B9	201	ZMP	C3-C4-C5-C6
43	A9	503	CDL	CB7-C71-C72-C73
48	5	607	3PE	C31-C32-C33-C34
43	A9	502	CDL	CA7-C31-C32-C33
49	B9	201	ZMP	C6-C7-C8-C9
47	1	401	PC1	C11-C12-N-C14
47	2	403	PC1	C11-C12-N-C13
47	6	202	PC1	C11-C12-N-C13
47	1	401	PC1	C3A-C3B-C3C-C3D
47	AM	205	PC1	C32-C33-C34-C35
43	S7	302	CDL	C52-C53-C54-C55
43	5	608	CDL	CB5-C51-C52-C53
48	AM	203	3PE	C31-C32-C33-C34
47	2	402	PC1	C31-C32-C33-C34
47	4	501	PC1	C23-C24-C25-C26
43	A9	503	CDL	CA7-C31-C32-C33
47	1	401	PC1	C11-C12-N-C13
47	2	403	PC1	C11-C12-N-C15
47	2	402	PC1	C21-C22-C23-C24
43	5	608	CDL	C39-C40-C41-C42
47	6	201	PC1	C31-C32-C33-C34
47	1	401	PC1	C11-C12-N-C15
47	6	202	PC1	C11-C12-N-C14
47	6	202	PC1	C11-C12-N-C15
48	5	606	3PE	C29-C2A-C2B-C2C
47	1	401	PC1	C21-C22-C23-C24
47	4	502	PC1	C26-C27-C28-C29
43	B6	203	CDL	OA6-CA4-CA6-OA8
49	AB	201	ZMP	C6-C7-C8-C9
50	A9	501	NDP	O4D-C1D-N1N-C6N
48	4	504	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
43	A9	503	CDL	CB2-C1-CA2-OA2
49	B9	201	ZMP	C4-C5-C6-C7
48	5	603	3PE	C25-C26-C27-C28
43	A9	502	CDL	OB5-CB3-CB4-CB6
47	AM	205	PC1	O11-C1-C2-C3
51	V1	501	FMN	C2'-C3'-C4'-O4'
47	S7	303	PC1	C1-C2-C3-O31
47	1	401	PC1	C1-C2-C3-O31
48	B6	202	3PE	C1-C2-C3-O31
51	V1	501	FMN	C5'-O5'-P-O1P
43	S7	302	CDL	OB5-CB3-CB4-OB6
48	5	603	3PE	O21-C2-C3-O31
48	AM	203	3PE	O21-C2-C3-O31
48	B6	202	3PE	O21-C2-C3-O31
49	B9	201	ZMP	C2-C3-C4-C5
49	B9	201	ZMP	O4-C17-C18-C19
49	AB	201	ZMP	O4-C17-C18-C19
49	AB	201	ZMP	O4-C17-C18-C20
51	V1	501	FMN	O4'-C4'-C5'-O5'
43	B5	201	CDL	OB5-CB3-CB4-CB6
47	B4	201	PC1	O11-C1-C2-C3
43	B5	201	CDL	C80-C81-C82-C83
49	B9	201	ZMP	C5-C6-C7-C8
47	4	502	PC1	C31-C32-C33-C34
47	1	401	PC1	O11-C1-C2-O21
47	AM	205	PC1	O11-C1-C2-O21
47	S7	303	PC1	O21-C2-C3-O31
49	AB	201	ZMP	S1-C10-C9-C8
49	AB	201	ZMP	O1-C10-C9-C8
43	5	608	CDL	C37-C38-C39-C40
47	S7	304	PC1	C11-C12-N-C15
51	V1	501	FMN	C5'-O5'-P-O2P
47	6	201	PC1	O31-C31-C32-C33
47	S7	303	PC1	O11-C1-C2-O21
48	5	607	3PE	O11-C1-C2-O21
43	AN	201	CDL	CA3-CA4-CA6-OA8
43	B6	203	CDL	CA3-CA4-CA6-OA8
48	5	601	3PE	C31-C32-C33-C34
47	4	501	PC1	C12-C11-O13-P
48	5	602	3PE	C12-C11-O13-P
47	2	402	PC1	C27-C28-C29-C2A
48	AM	203	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
43	AN	201	CDL	OA6-CA4-CA6-OA8
47	1	401	PC1	O21-C2-C3-O31
47	S7	304	PC1	C11-C12-N-C13
47	AM	202	PC1	O13-C11-C12-N
47	AM	205	PC1	O13-C11-C12-N
47	B6	201	PC1	O13-C11-C12-N
47	B4	201	PC1	O13-C11-C12-N
47	2	402	PC1	O13-C11-C12-N
47	2	402	PC1	C26-C27-C28-C29
43	S7	302	CDL	OB5-CB3-CB4-CB6
43	B6	203	CDL	OB5-CB3-CB4-CB6
47	S7	303	PC1	O11-C1-C2-C3
43	B5	201	CDL	C1-CA2-OA2-PA1
43	A9	502	CDL	C1-CB2-OB2-PB2
47	B4	201	PC1	C2-C1-O11-P
48	AM	204	3PE	C2-C1-O11-P
43	B6	203	CDL	OB5-CB3-CB4-OB6
43	B5	201	CDL	OB5-CB3-CB4-OB6
47	B4	201	PC1	O11-C1-C2-O21
48	5	606	3PE	O11-C1-C2-O21
47	C2	201	PC1	C26-C27-C28-C29
48	5	603	3PE	C1-C2-C3-O31
48	5	606	3PE	C1-C2-C3-O31
43	AN	201	CDL	CA3-OA5-PA1-OA3
43	S7	302	CDL	CB2-OB2-PB2-OB5
43	5	604	CDL	CA3-OA5-PA1-OA2
43	5	604	CDL	CA3-OA5-PA1-OA3
43	5	604	CDL	CB2-OB2-PB2-OB3
43	5	604	CDL	CB2-OB2-PB2-OB5
43	B6	203	CDL	CA3-OA5-PA1-OA3
43	B5	201	CDL	CA3-OA5-PA1-OA4
43	A9	502	CDL	CA2-OA2-PA1-OA3
43	A9	502	CDL	CA2-OA2-PA1-OA5
43	A9	502	CDL	CB2-OB2-PB2-OB3
43	A9	502	CDL	CB2-OB2-PB2-OB4
47	S7	303	PC1	C1-O11-P-O14
47	S7	304	PC1	C1-O11-P-O12
47	S7	304	PC1	C1-O11-P-O13
47	S7	304	PC1	C11-C12-N-C14
47	4	502	PC1	C11-O13-P-O14
47	B4	201	PC1	C1-O11-P-O14
47	C2	201	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
47	2	402	PC1	C11-O13-P-O14
47	6	201	PC1	C1-O11-P-O12
47	6	201	PC1	C1-O11-P-O13
47	6	202	PC1	C1-O11-P-O14
47	6	202	PC1	C1-O11-P-O13
48	4	503	3PE	C11-O13-P-O14
48	5	601	3PE	C1-O11-P-O14
48	5	606	3PE	C1-O11-P-O14
48	5	607	3PE	C1-O11-P-O14
48	5	607	3PE	C11-O13-P-O11
48	5	607	3PE	C11-O13-P-O14
48	AM	203	3PE	C1-O11-P-O12
48	AM	203	3PE	C1-O11-P-O13
48	AM	203	3PE	C1-O11-P-O14
48	AM	203	3PE	O13-C11-C12-N
48	AM	204	3PE	C1-O11-P-O13
48	B6	202	3PE	C1-O11-P-O13
48	B6	202	3PE	C1-O11-P-O14
48	B6	202	3PE	C11-O13-P-O12
48	2	401	3PE	C1-O11-P-O12
49	AB	201	ZMP	O4-C17-C18-C21
50	A9	501	NDP	C5D-O5D-PN-O2N
52	AL	501	DGT	C5'-O5'-PA-O2A
43	S7	302	CDL	C1-CA2-OA2-PA1
43	5	604	CDL	CA4-CA3-OA5-PA1
43	B5	201	CDL	CA4-CA3-OA5-PA1
47	S7	303	PC1	C2-C1-O11-P
47	B6	201	PC1	C2-C1-O11-P
48	2	401	3PE	C2-C1-O11-P
47	2	403	PC1	C2A-C2B-C2C-C2D
47	4	502	PC1	C22-C23-C24-C25
48	B6	202	3PE	C31-C32-C33-C34
48	5	606	3PE	O11-C1-C2-C3
48	AM	203	3PE	C21-C22-C23-C24
48	5	606	3PE	O21-C2-C3-O31
48	5	603	3PE	O21-C21-C22-C23
49	AB	201	ZMP	C13-C14-C15-N2
48	AM	203	3PE	C1-C2-C3-O31
47	B4	201	PC1	C24-C25-C26-C27
43	AN	201	CDL	C1-CA2-OA2-PA1
48	5	606	3PE	C28-C29-C2A-C2B
51	V1	501	FMN	O3'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
47	1	401	PC1	C2-C1-O11-P
48	5	605	3PE	C28-C29-C2A-C2B
48	5	605	3PE	C1-C2-C3-O31
47	2	403	PC1	C28-C29-C2A-C2B
43	5	608	CDL	C41-C42-C43-C44
47	2	403	PC1	C21-C22-C23-C24
48	2	401	3PE	C23-C24-C25-C26
47	1	401	PC1	C34-C35-C36-C37
43	B5	201	CDL	C12-C13-C14-C15
48	5	603	3PE	C33-C34-C35-C36
47	B4	201	PC1	C22-C23-C24-C25
47	AM	205	PC1	C2-C1-O11-P
51	V1	501	FMN	O3'-C3'-C4'-C5'
47	AM	202	PC1	C34-C35-C36-C37
47	6	201	PC1	C1-C2-C3-O31
48	4	503	3PE	C33-C34-C35-C36
47	C2	201	PC1	C25-C26-C27-C28
47	2	403	PC1	O31-C31-C32-C33
48	5	603	3PE	C32-C33-C34-C35
48	5	606	3PE	C21-C22-C23-C24
43	B5	201	CDL	C71-C72-C73-C74
47	C2	201	PC1	C2-C1-O11-P
48	B6	202	3PE	C1-C2-O21-C21
48	2	401	3PE	C28-C29-C2A-C2B
49	AB	201	ZMP	C2-C1-C22-C23
47	1	401	PC1	C2A-C2B-C2C-C2D
48	5	607	3PE	C1-C2-C3-O31
48	2	401	3PE	O31-C31-C32-C33
49	B9	201	ZMP	C22-C1-C2-C3
48	4	504	3PE	O31-C31-C32-C33
48	AM	201	3PE	O31-C31-C32-C33
48	2	401	3PE	C27-C28-C29-C2A
43	A9	503	CDL	C1-CA2-OA2-PA1
47	S7	303	PC1	O13-C11-C12-N
47	6	201	PC1	O13-C11-C12-N
43	5	604	CDL	C72-C71-CB7-OB8
47	S7	304	PC1	C39-C3A-C3B-C3C
47	C2	201	PC1	C11-C12-N-C13
47	B6	201	PC1	C24-C25-C26-C27
43	A9	503	CDL	C72-C71-CB7-OB8
47	B6	201	PC1	O31-C31-C32-C33
48	5	606	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
47	6	201	PC1	O32-C31-C32-C33
48	5	602	3PE	C21-C22-C23-C24
48	2	401	3PE	O21-C21-C22-C23
48	B6	202	3PE	C32-C33-C34-C35
43	AN	201	CDL	CB4-CB3-OB5-PB2
48	AM	203	3PE	C2-C1-O11-P
43	A9	502	CDL	C72-C71-CB7-OB8
47	AM	205	PC1	O21-C21-C22-C23
43	S7	302	CDL	C12-C11-CA5-OA6
43	A9	503	CDL	C32-C31-CA7-OA8
47	C2	201	PC1	O11-C1-C2-C3
51	V1	501	FMN	N10-C1'-C2'-O2'
43	5	604	CDL	C32-C31-CA7-OA8
47	1	401	PC1	C1-C2-O21-C21
48	5	607	3PE	C32-C33-C34-C35
47	S7	304	PC1	C3B-C3C-C3D-C3E
43	B6	203	CDL	C52-C51-CB5-OB6
47	4	502	PC1	O31-C31-C32-C33
47	B6	201	PC1	O32-C31-C32-C33
47	1	401	PC1	C29-C2A-C2B-C2C
48	AM	201	3PE	O21-C21-C22-C23
48	5	606	3PE	O32-C31-C32-C33
47	1	401	PC1	C28-C29-C2A-C2B
47	AM	205	PC1	O22-C21-C22-C23
48	2	401	3PE	O22-C21-C22-C23
48	AM	201	3PE	C35-C36-C37-C38
43	A9	503	CDL	C32-C31-CA7-OA9
43	AN	201	CDL	C52-C53-C54-C55
48	AM	201	3PE	O32-C31-C32-C33
48	5	606	3PE	C2A-C2B-C2C-C2D
43	5	604	CDL	C72-C71-CB7-OB9
48	4	504	3PE	O32-C31-C32-C33
48	5	607	3PE	O21-C2-C3-O31
47	4	502	PC1	C33-C34-C35-C36
43	A9	502	CDL	C72-C71-CB7-OB9
43	5	604	CDL	C56-C57-C58-C59
47	1	401	PC1	C39-C3A-C3B-C3C
49	B9	201	ZMP	N2-C16-C17-O4
43	5	604	CDL	C32-C31-CA7-OA9
48	5	607	3PE	C2-C1-O11-P
43	A9	503	CDL	C72-C71-CB7-OB9
43	AN	201	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
43	S7	302	CDL	C12-C11-CA5-OA7
47	B4	201	PC1	O21-C21-C22-C23
47	B4	201	PC1	O31-C31-C32-C33
47	4	502	PC1	C21-C22-C23-C24
43	B5	201	CDL	C77-C78-C79-C80
43	B6	203	CDL	C72-C71-CB7-OB8
47	AM	205	PC1	O31-C31-C32-C33
48	5	603	3PE	C3B-C3C-C3D-C3E

There are no ring outliers.

37 monomers are involved in 61 short contacts:

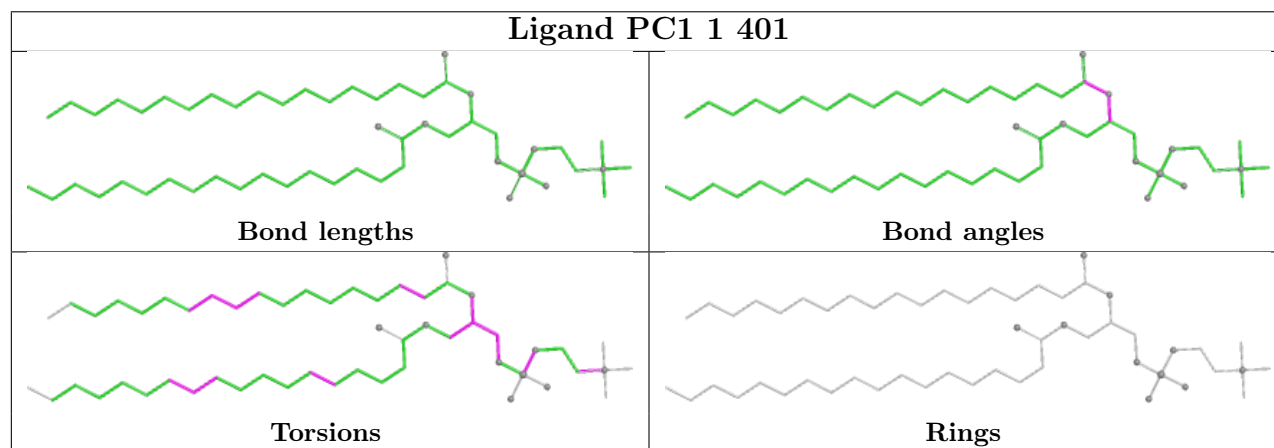
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	1	401	PC1	1	0
48	5	607	3PE	1	0
47	6	202	PC1	1	0
48	B6	202	3PE	2	0
43	5	604	CDL	1	0
47	C2	201	PC1	2	0
48	5	603	3PE	2	0
43	S7	302	CDL	2	0
45	S7	301	SF4	5	0
47	S7	303	PC1	1	0
48	5	601	3PE	2	0
48	AM	204	3PE	2	0
52	AL	501	DGT	3	0
43	B6	203	CDL	1	0
47	AM	205	PC1	3	0
45	S8	301	SF4	1	0
43	A9	503	CDL	1	0
47	2	402	PC1	1	0
43	A9	502	CDL	1	0
48	4	503	3PE	2	0
48	AM	201	3PE	1	0
43	B5	201	CDL	4	0
48	2	401	3PE	3	0
47	4	502	PC1	4	0
48	AM	203	3PE	1	0
47	B4	201	PC1	1	0
48	5	605	3PE	1	0
48	5	602	3PE	2	0
47	B6	201	PC1	1	0

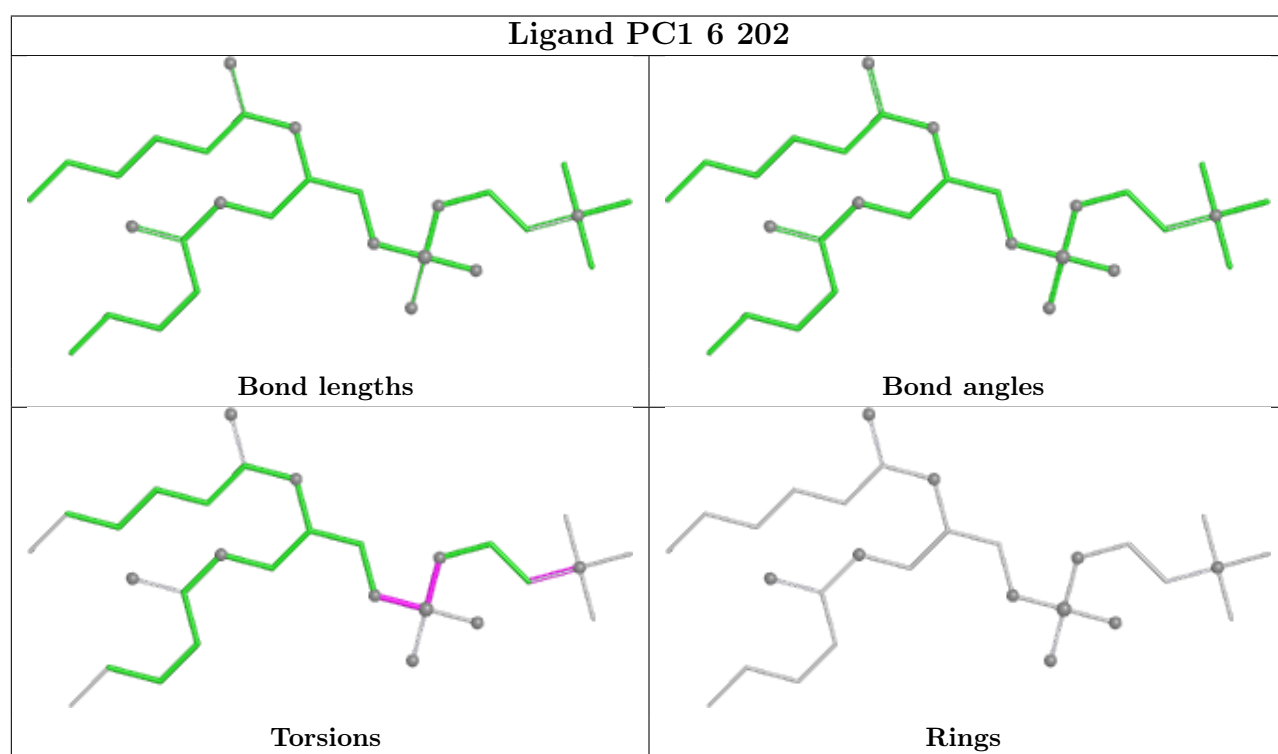
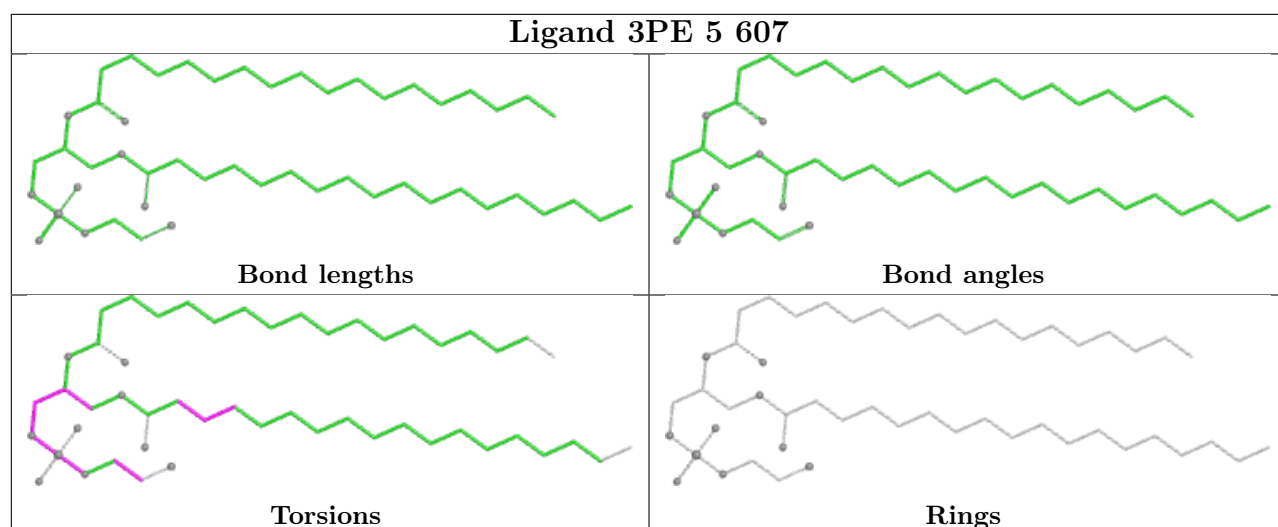
*Continued on next page...*

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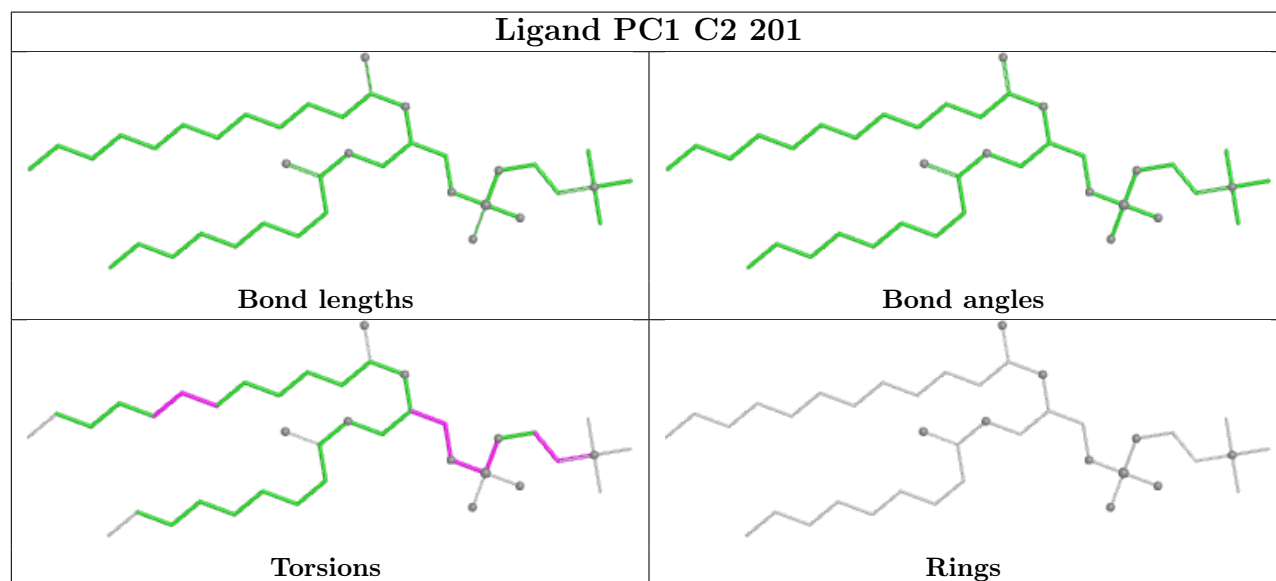
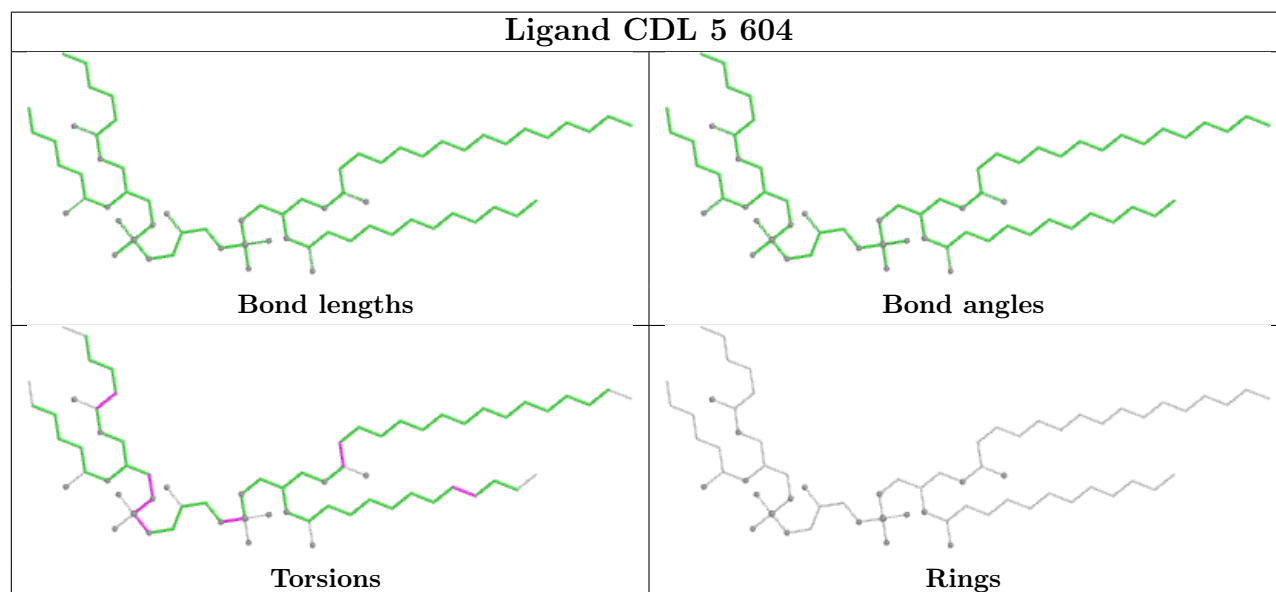
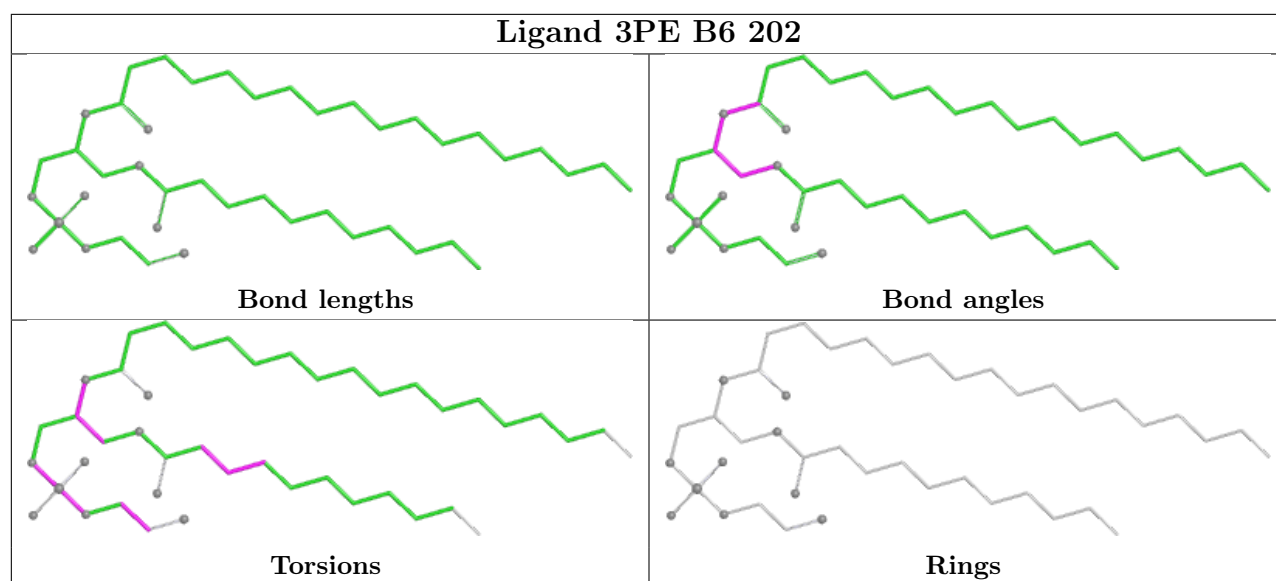
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	2	403	PC1	2	0
47	4	501	PC1	3	0
45	V1	502	SF4	1	0
48	4	504	3PE	2	0
47	6	201	PC1	1	0
49	B9	201	ZMP	2	0
43	AN	201	CDL	3	0
47	S7	304	PC1	2	0

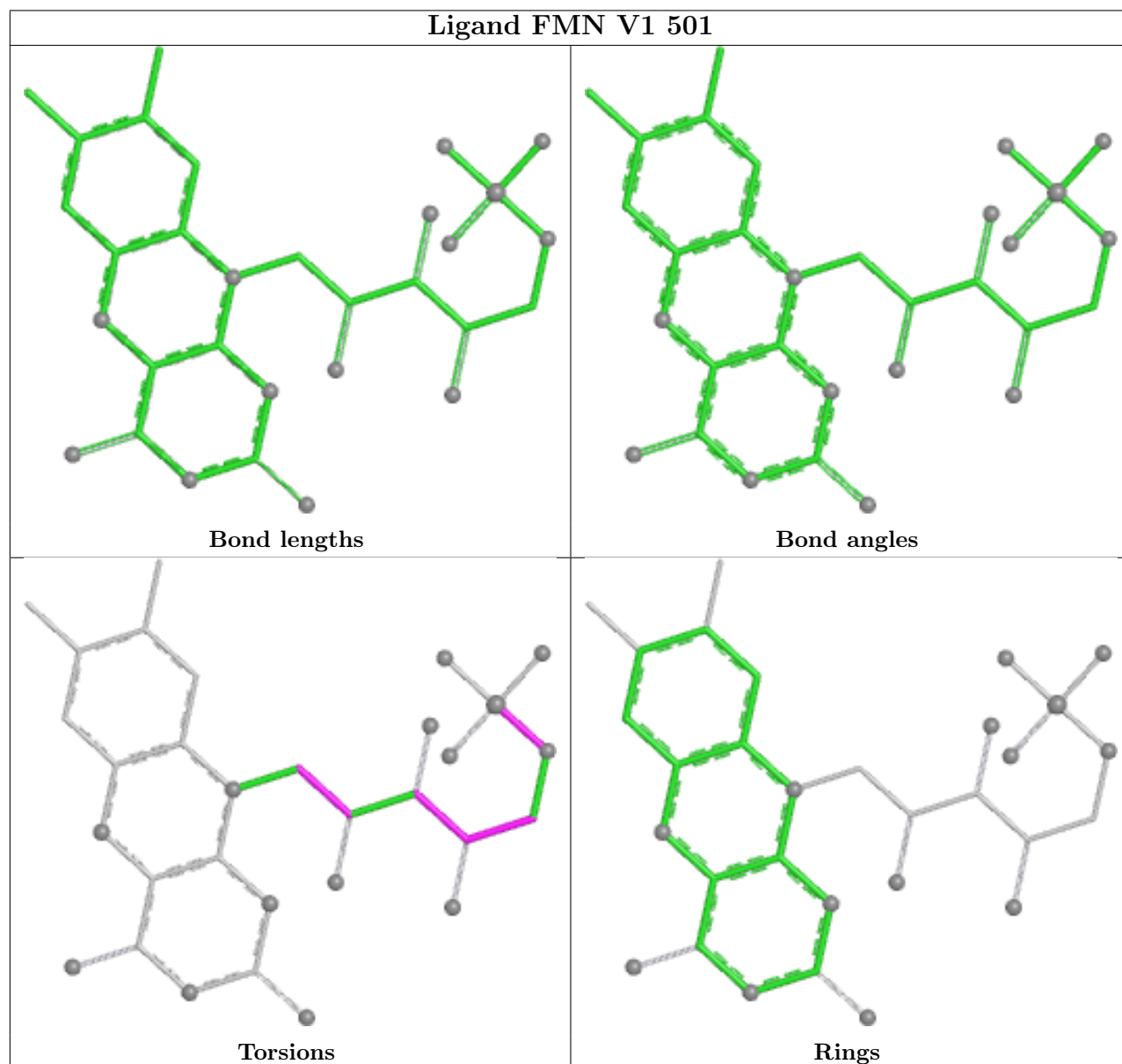
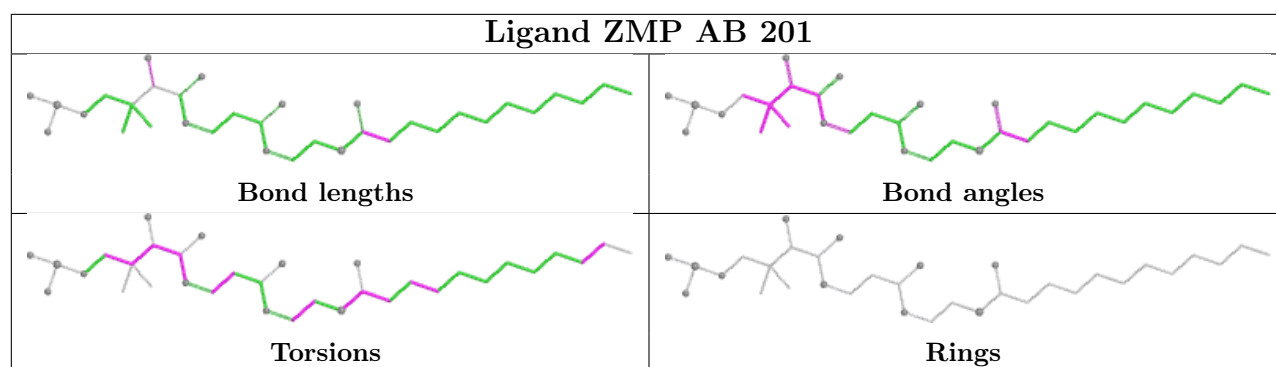
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

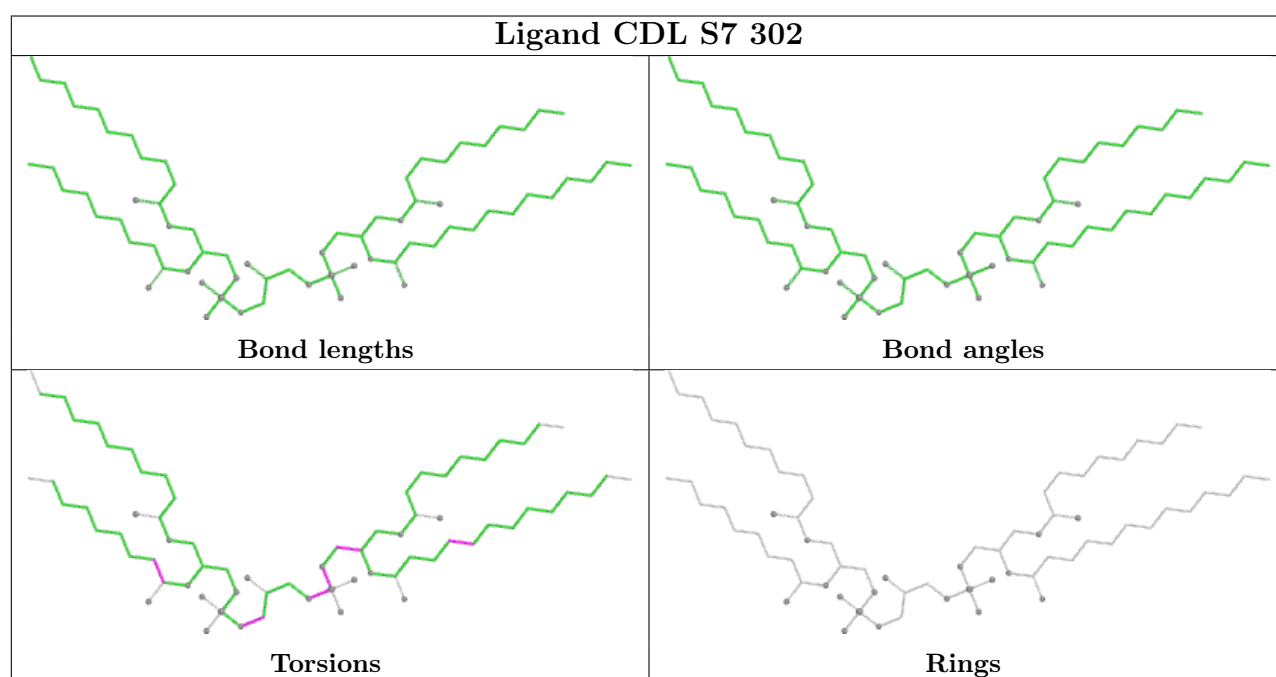
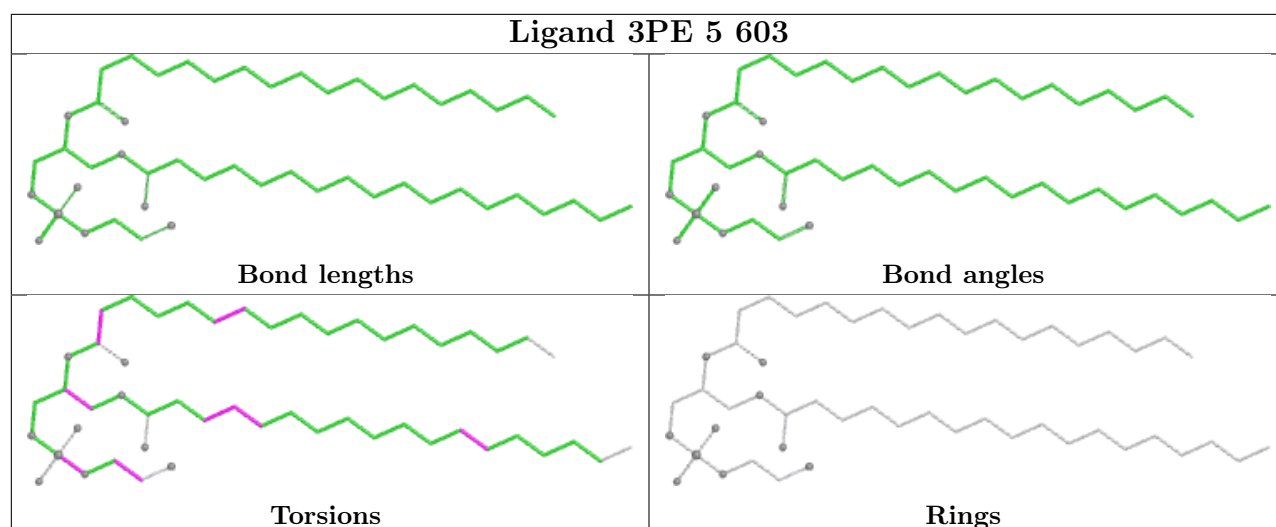


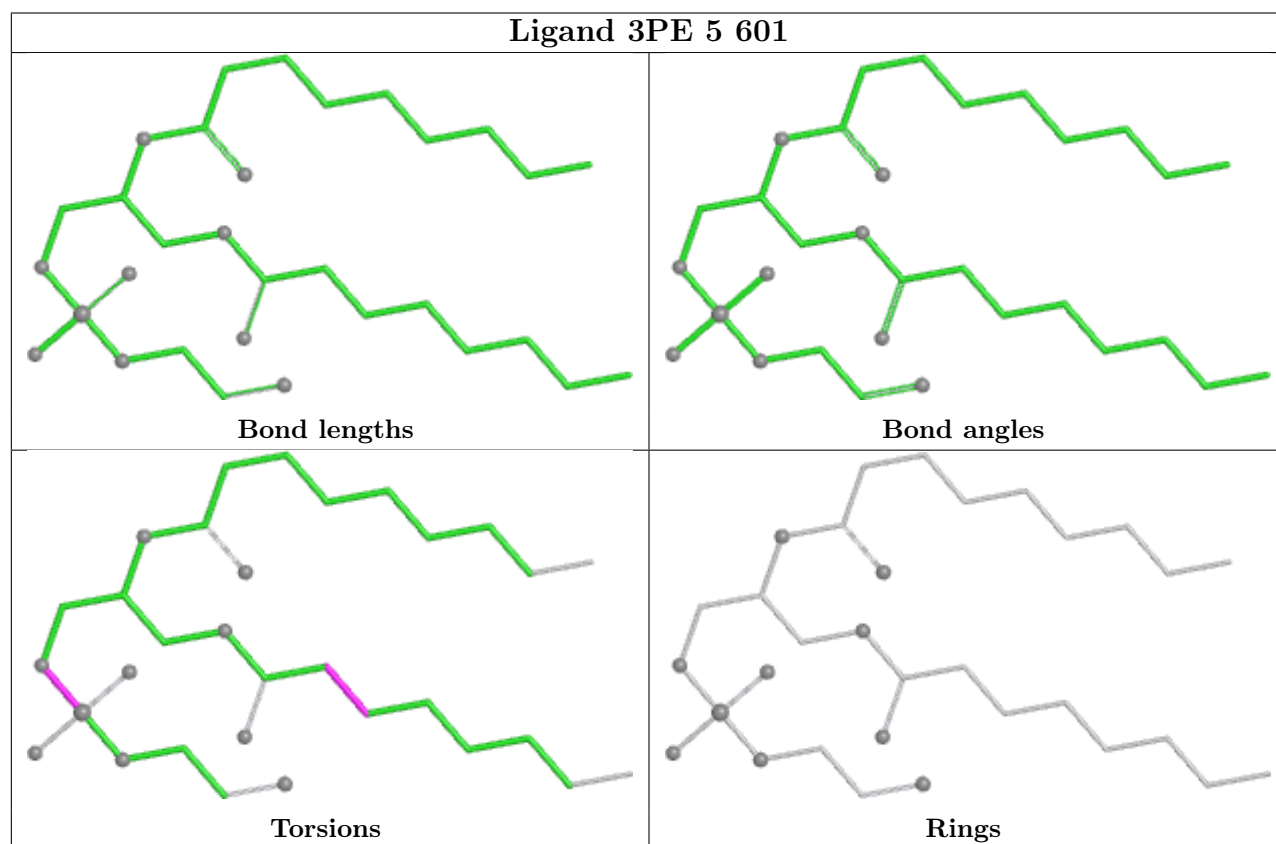
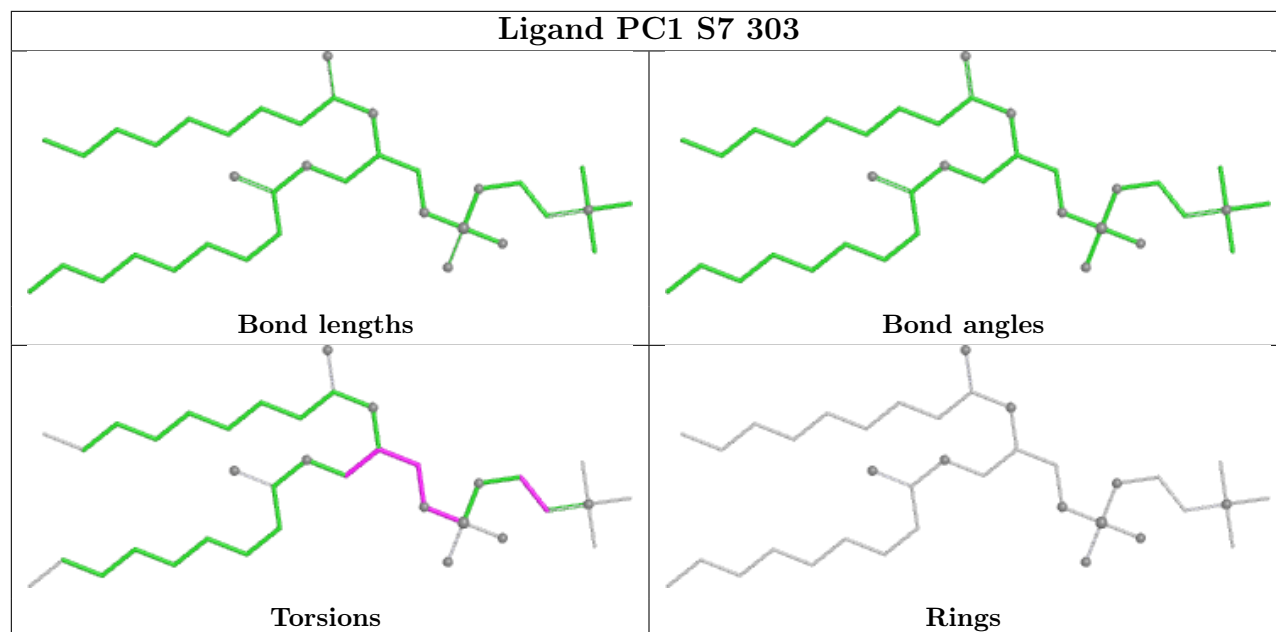


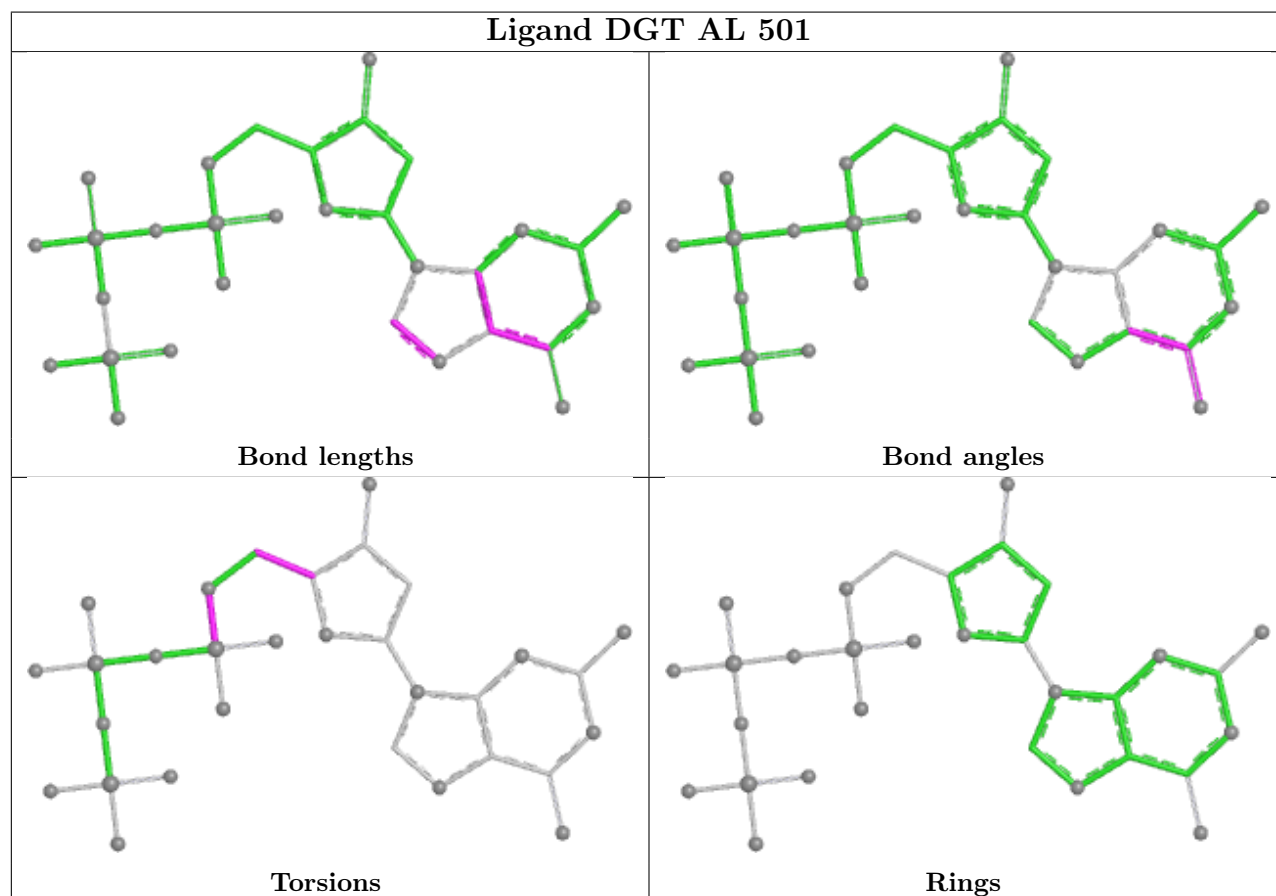
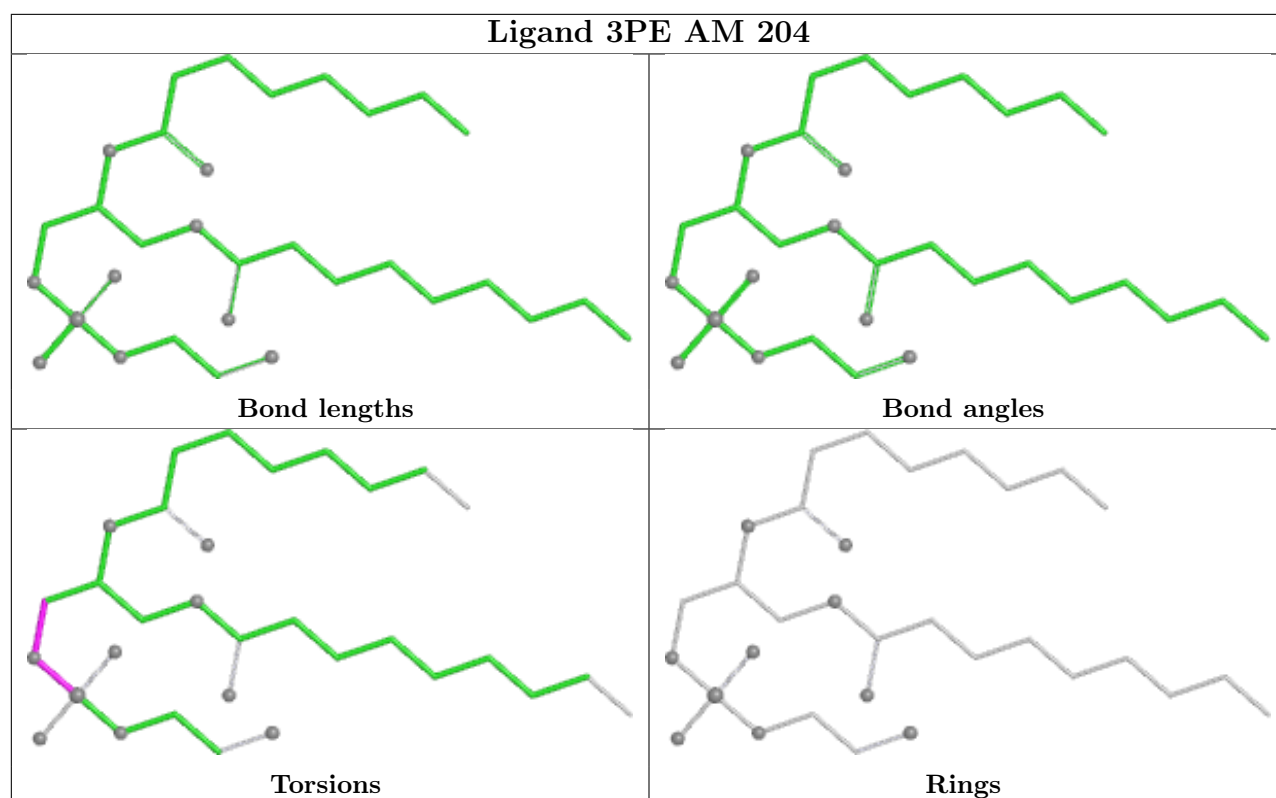


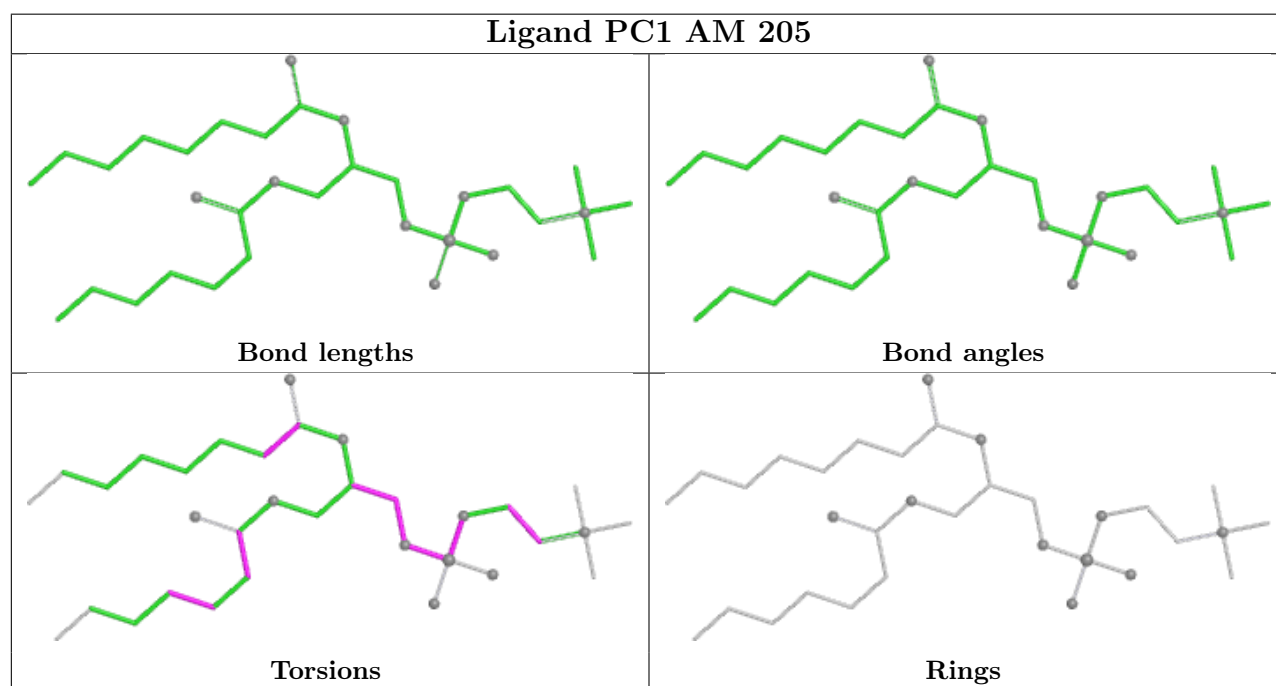
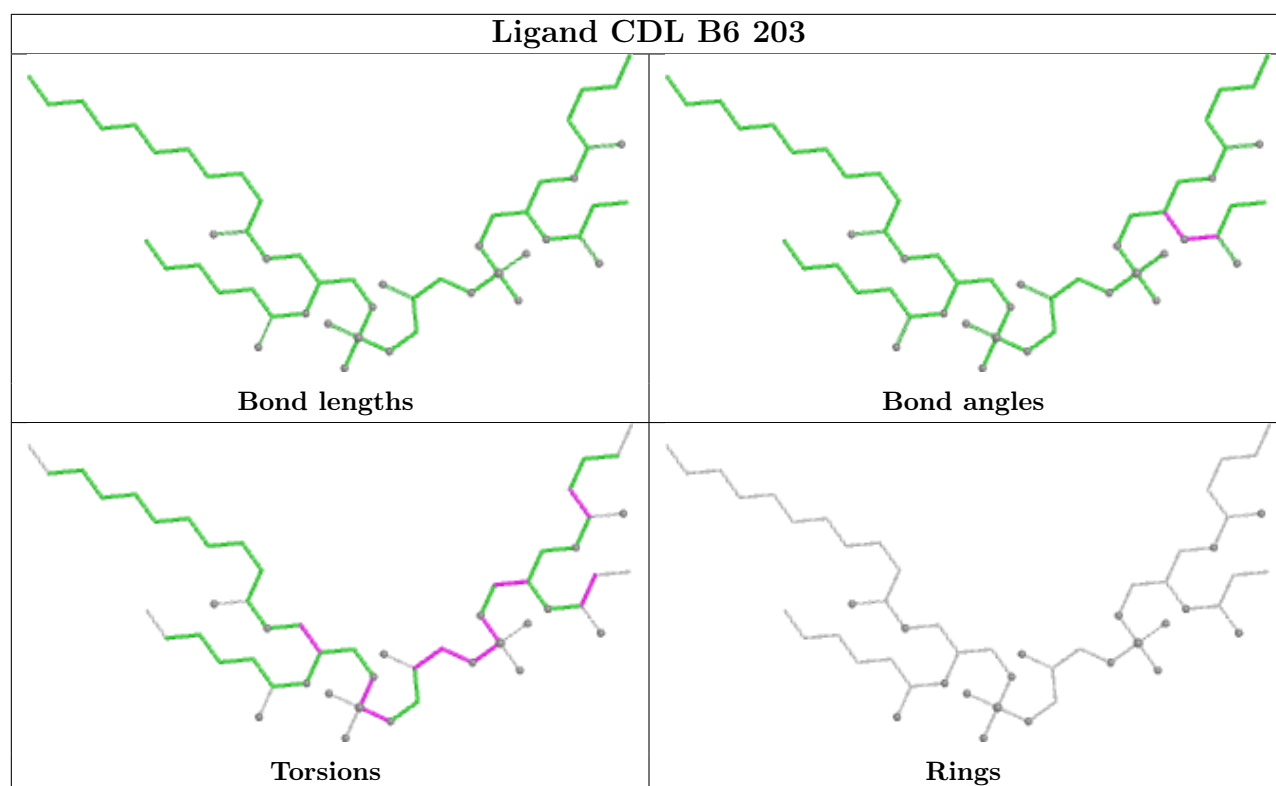


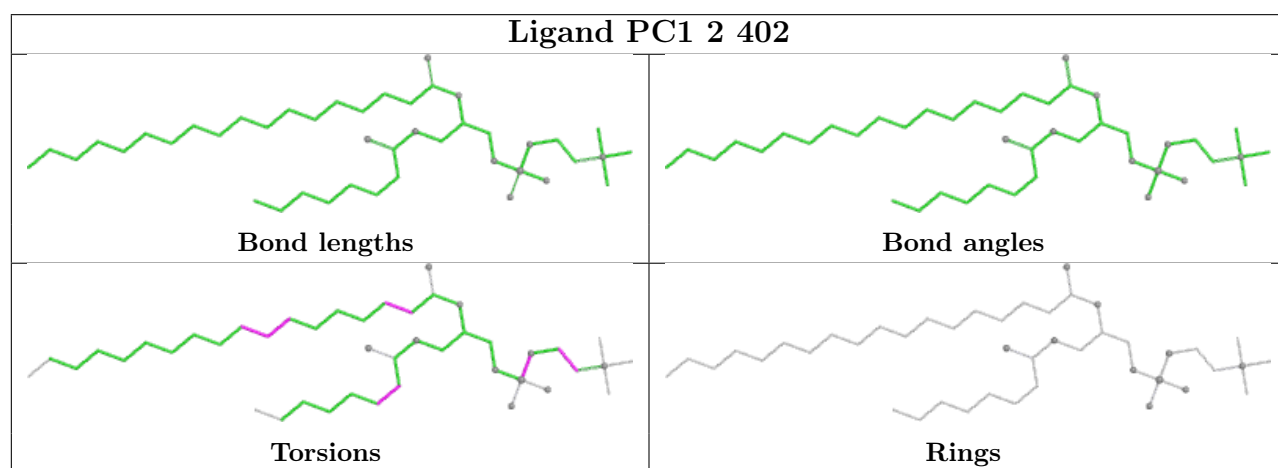
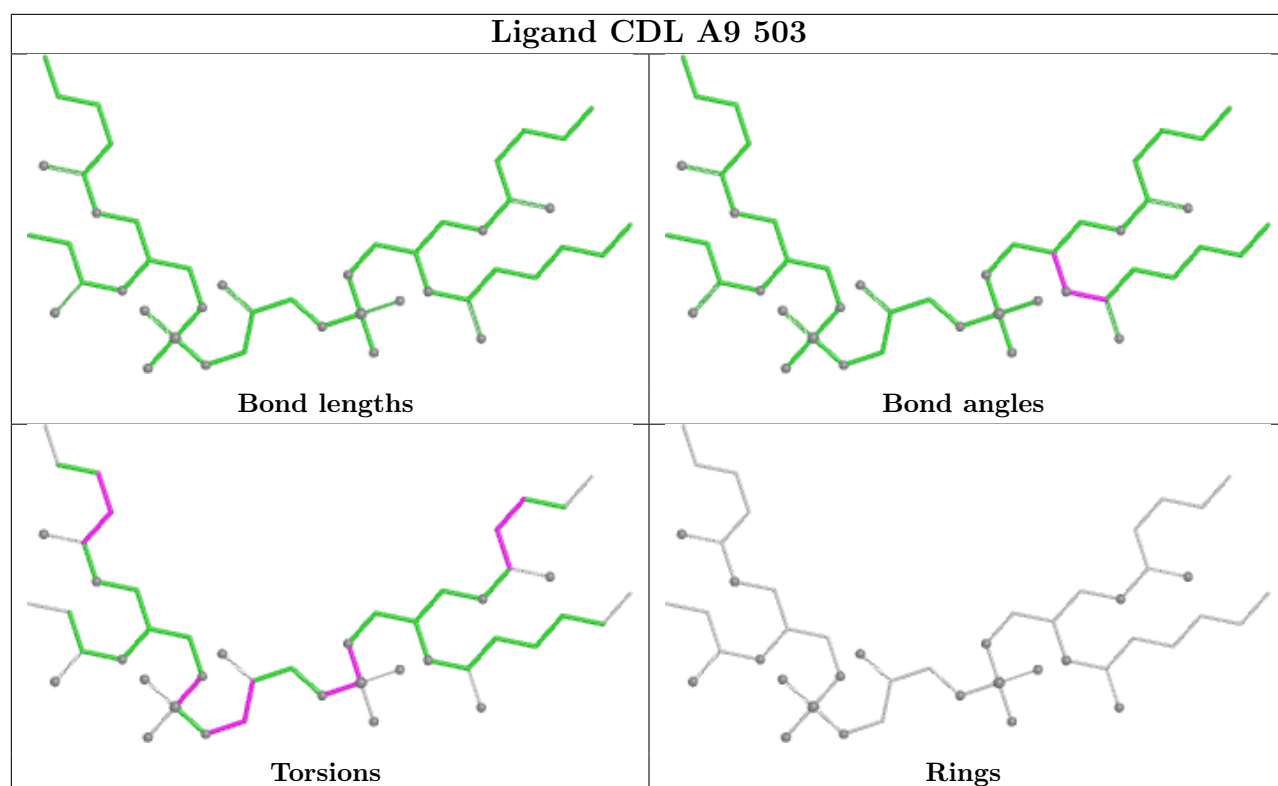


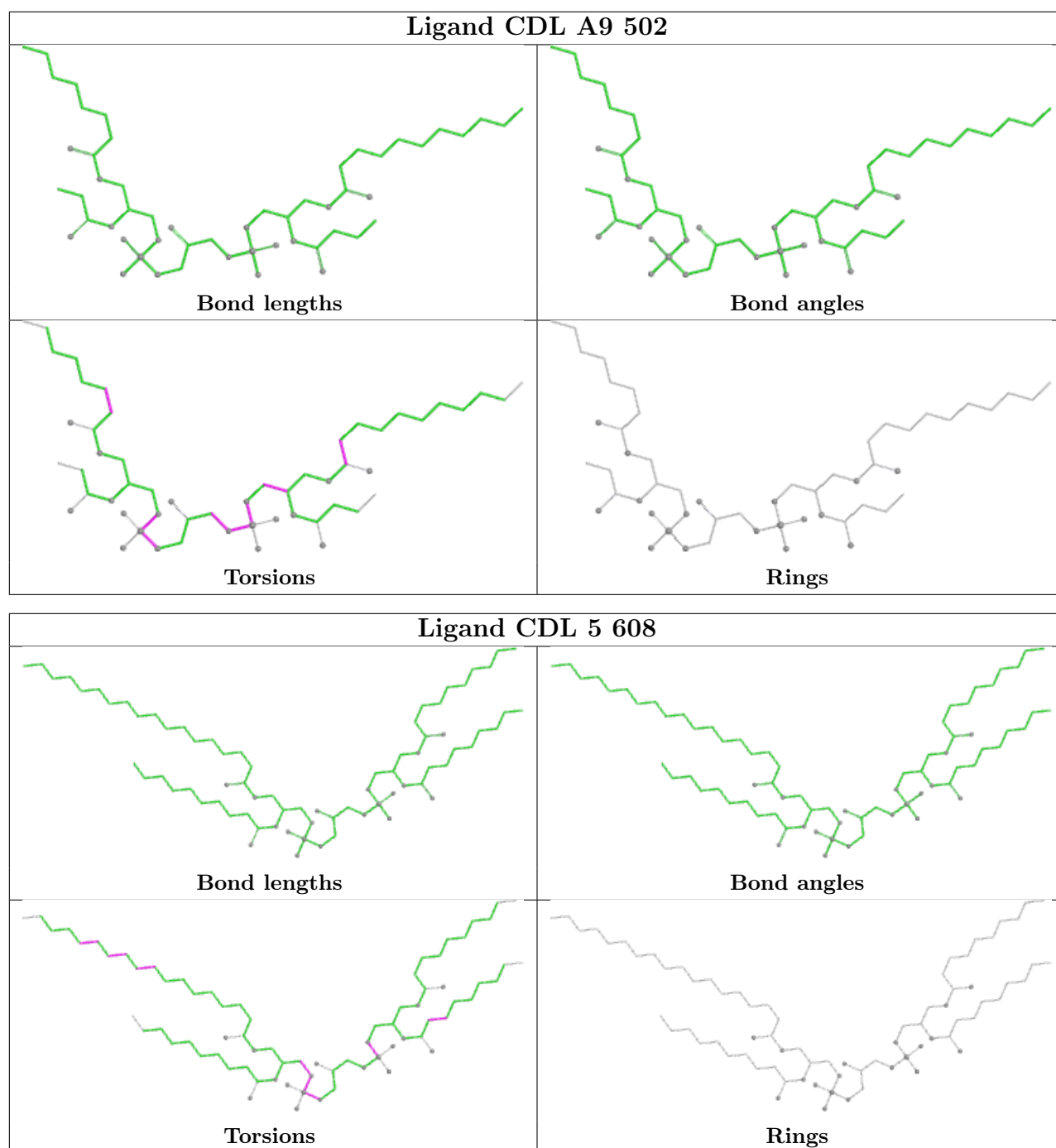




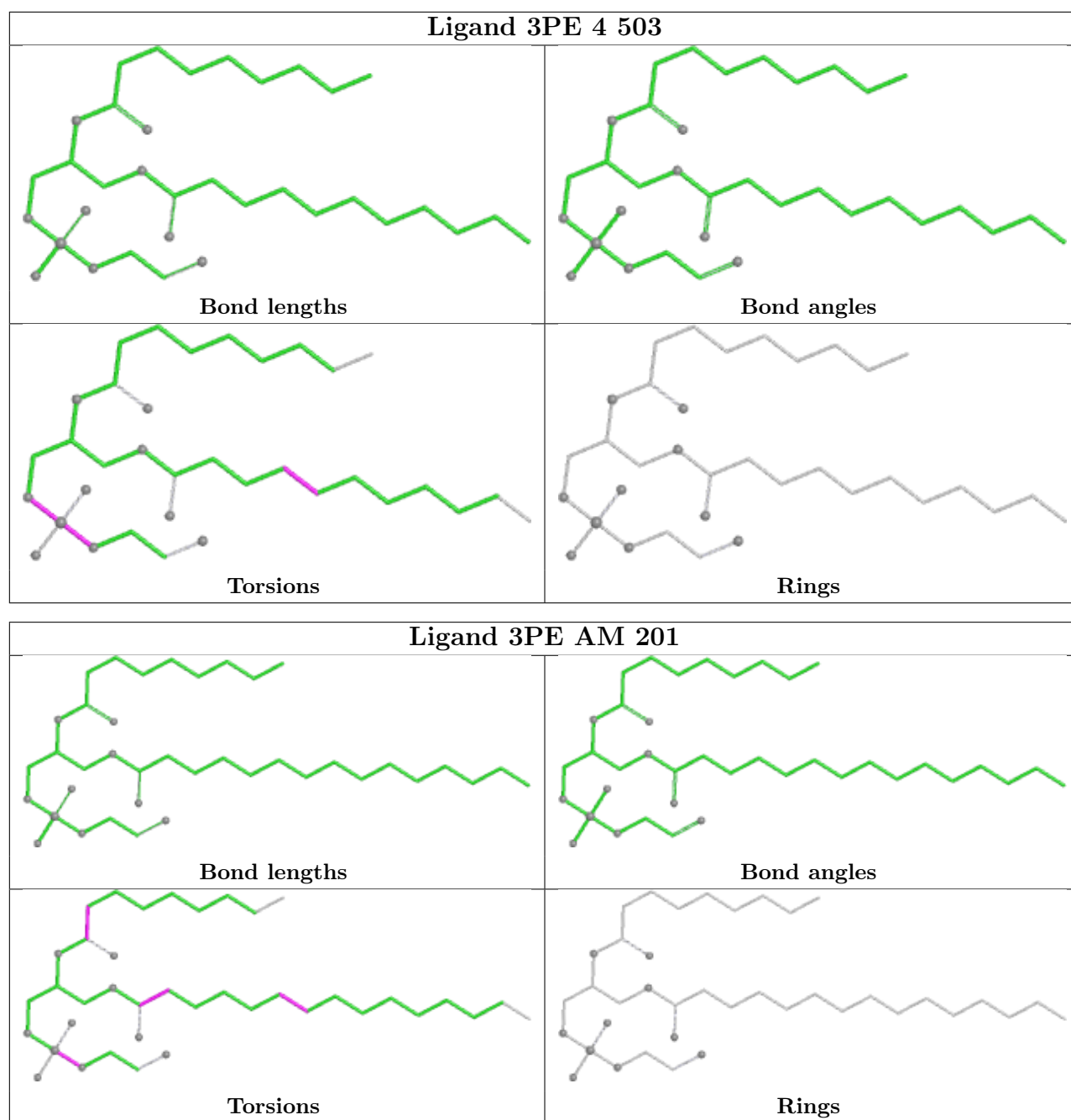


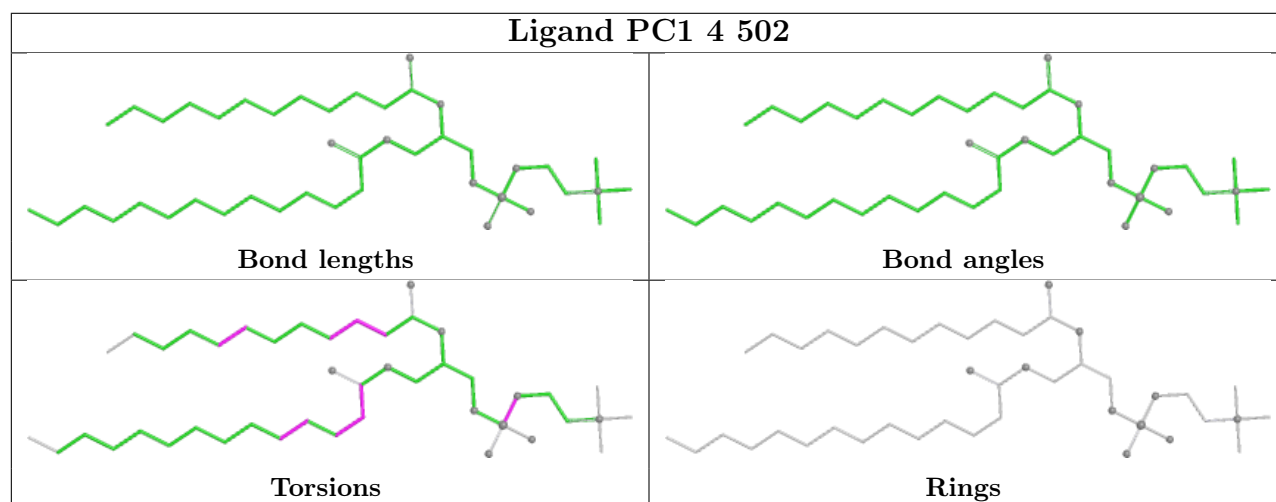
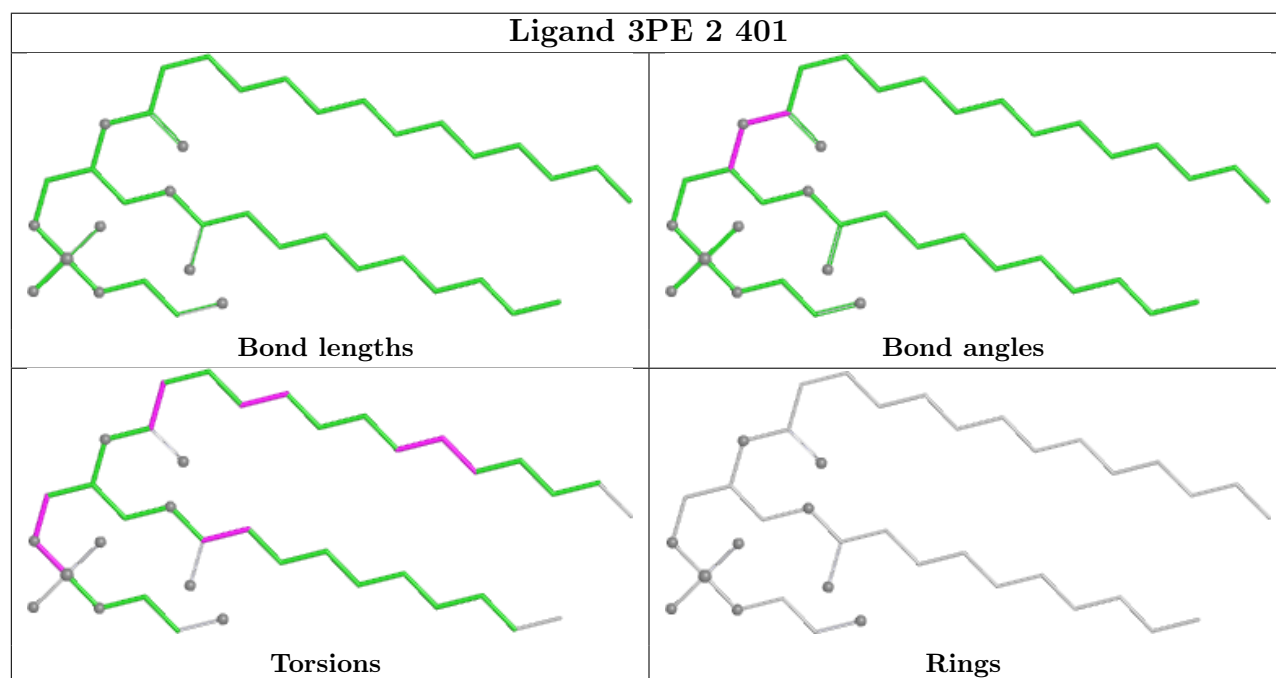
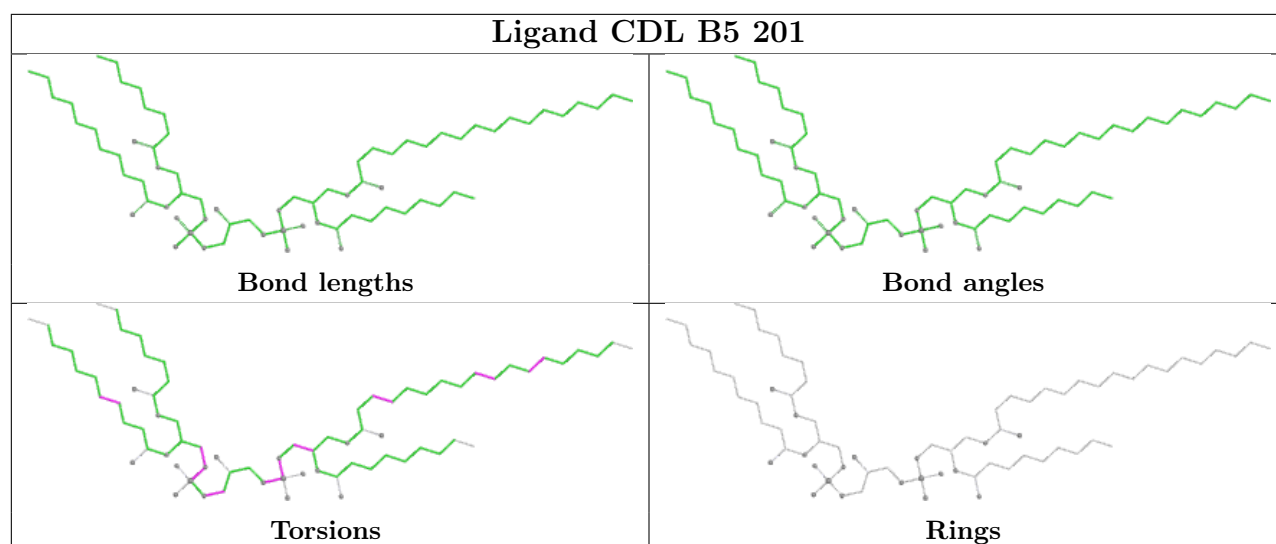


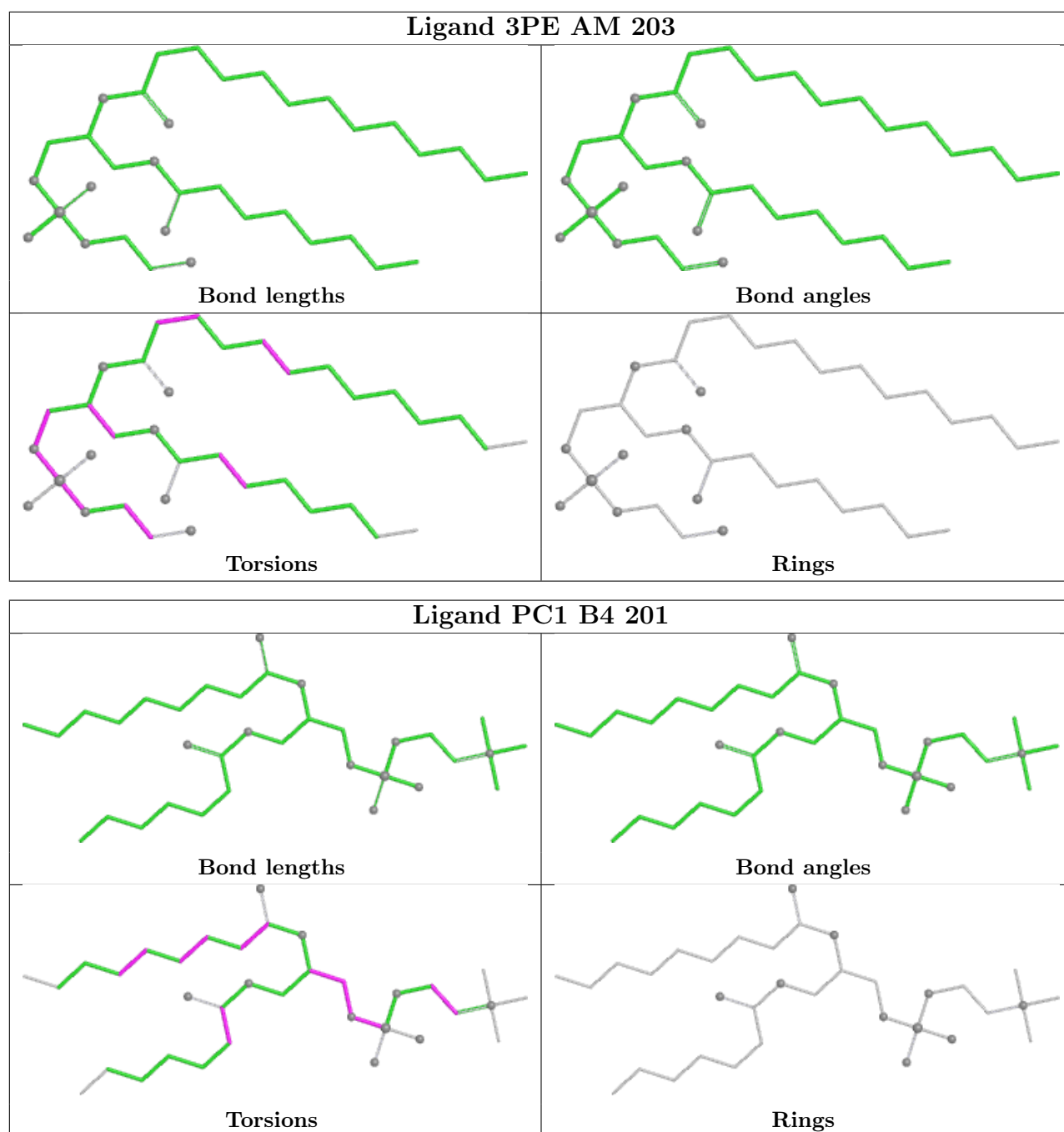


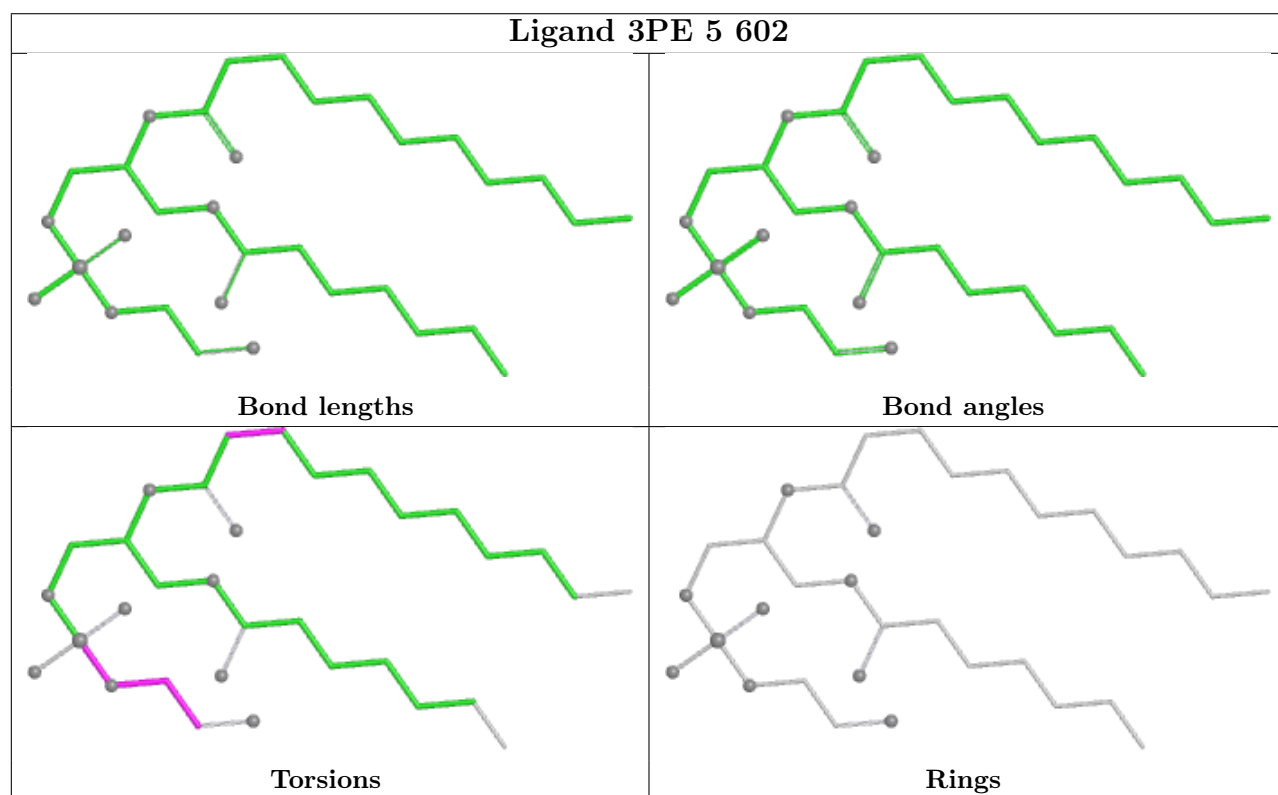
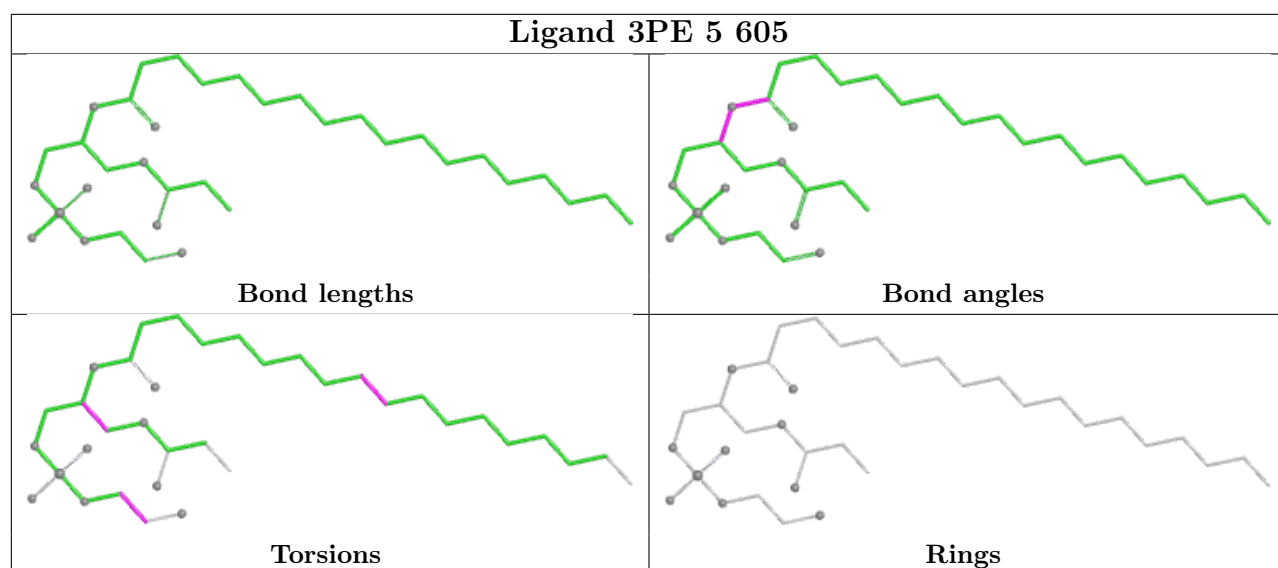


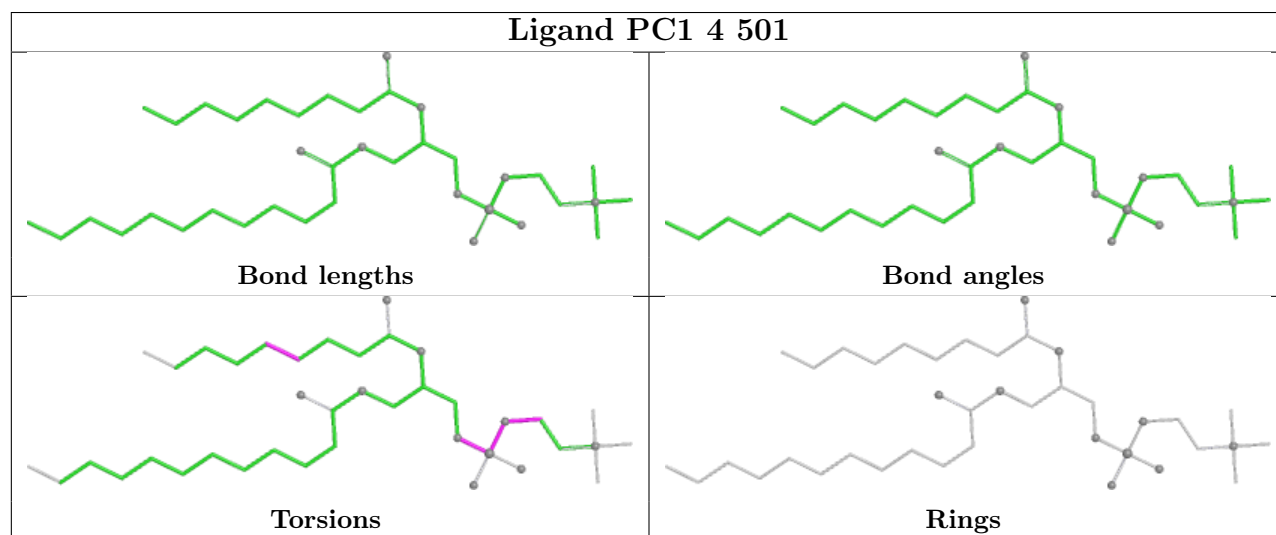
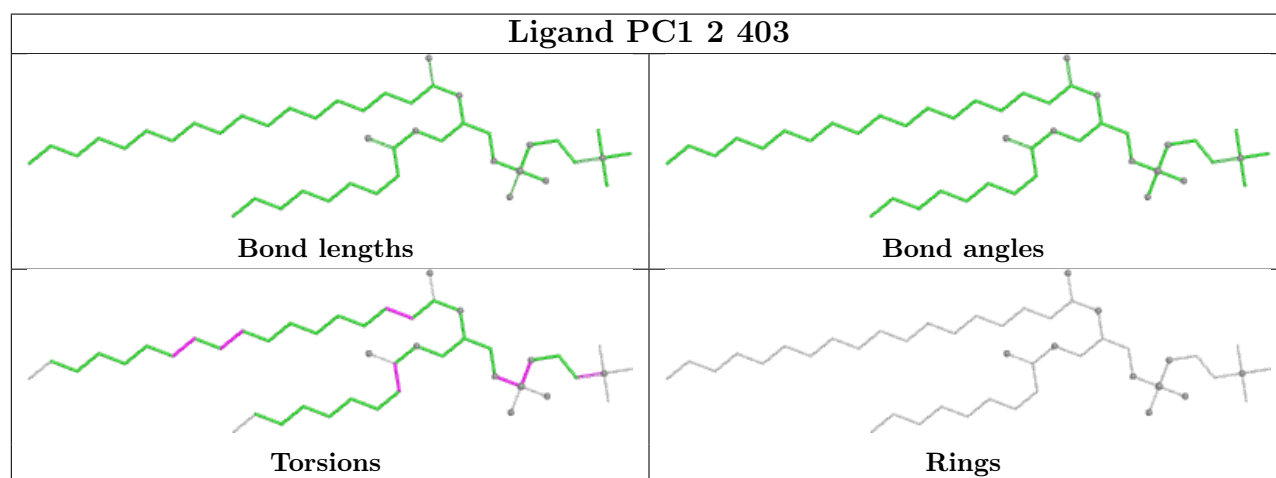
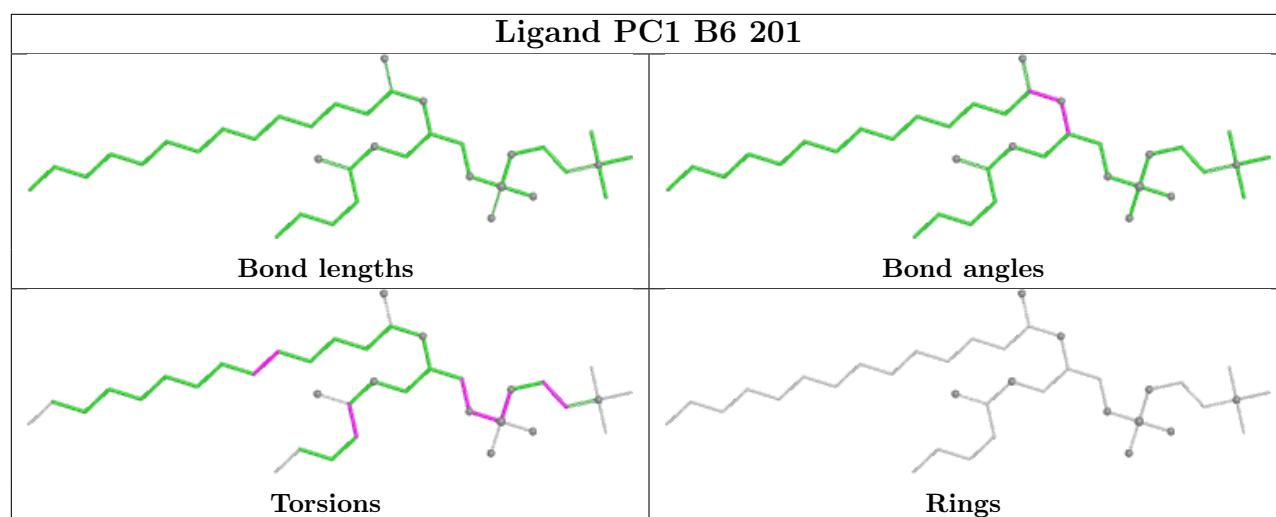


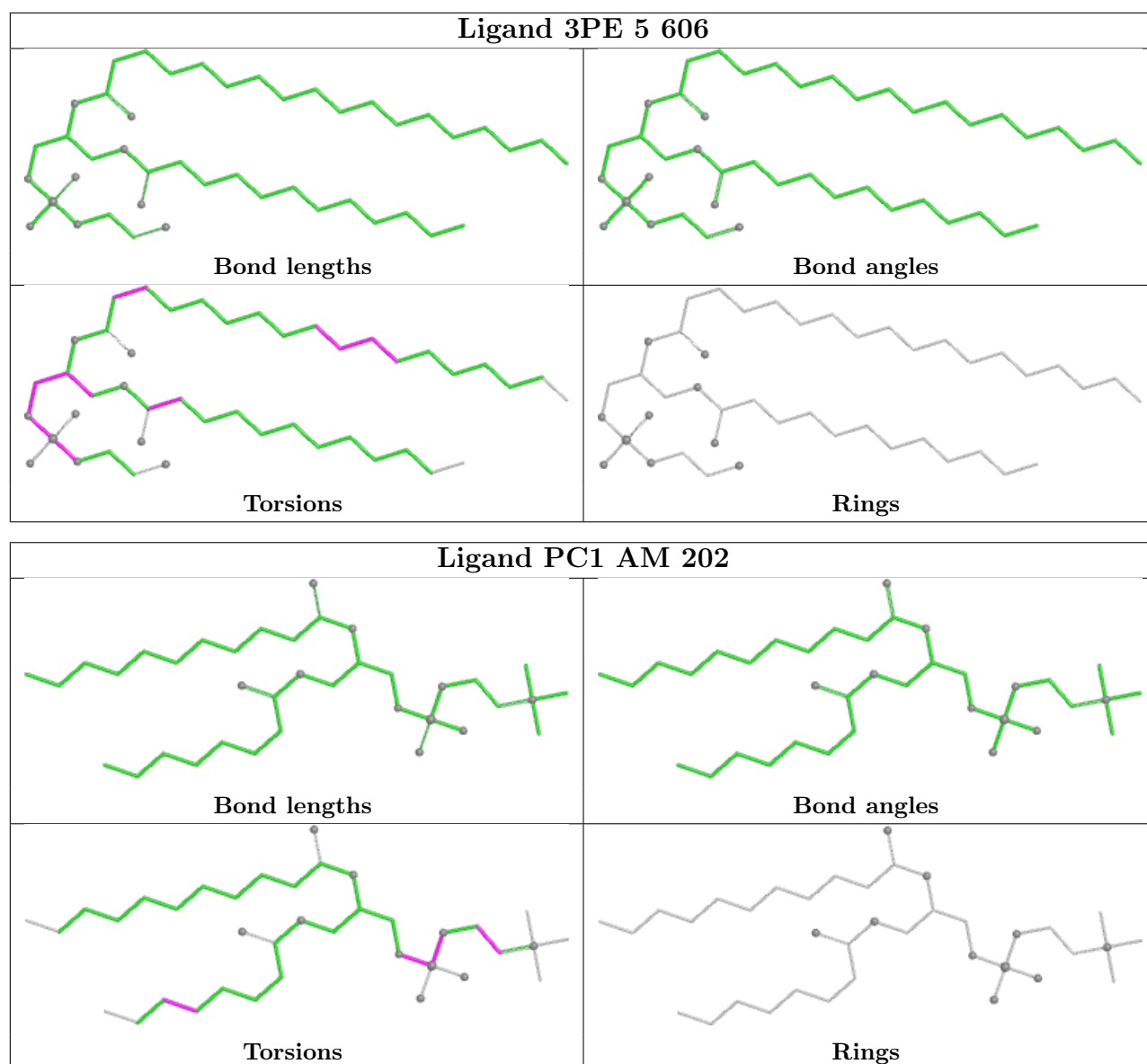


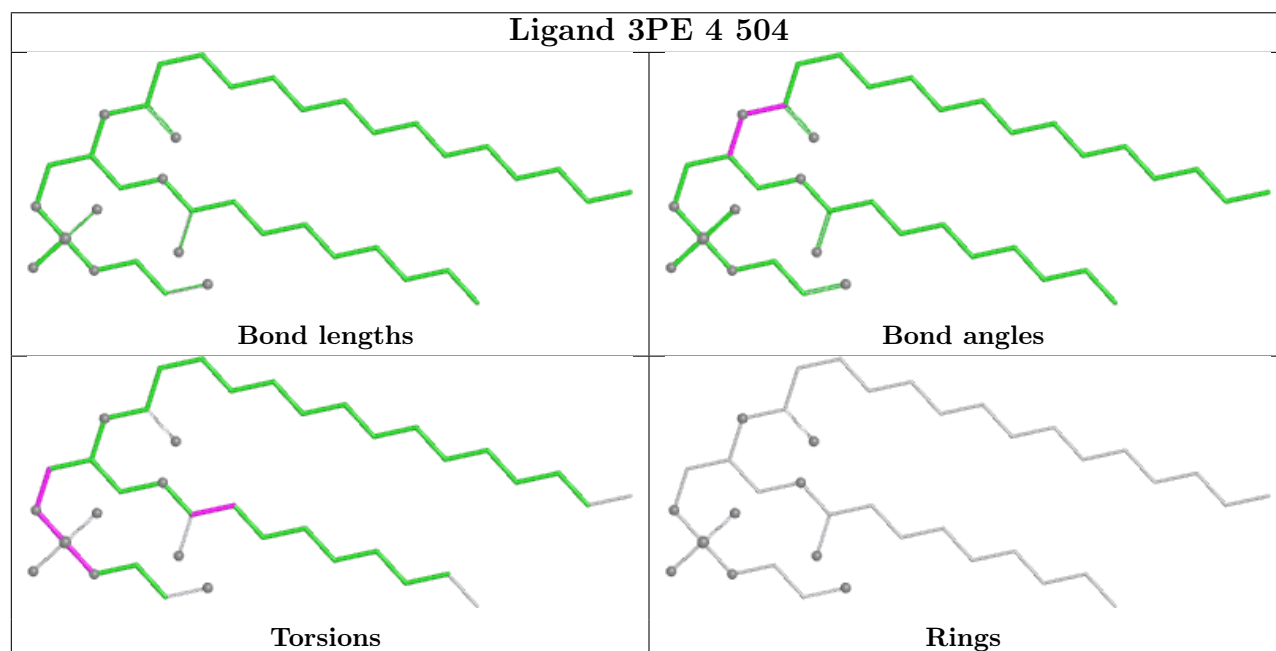
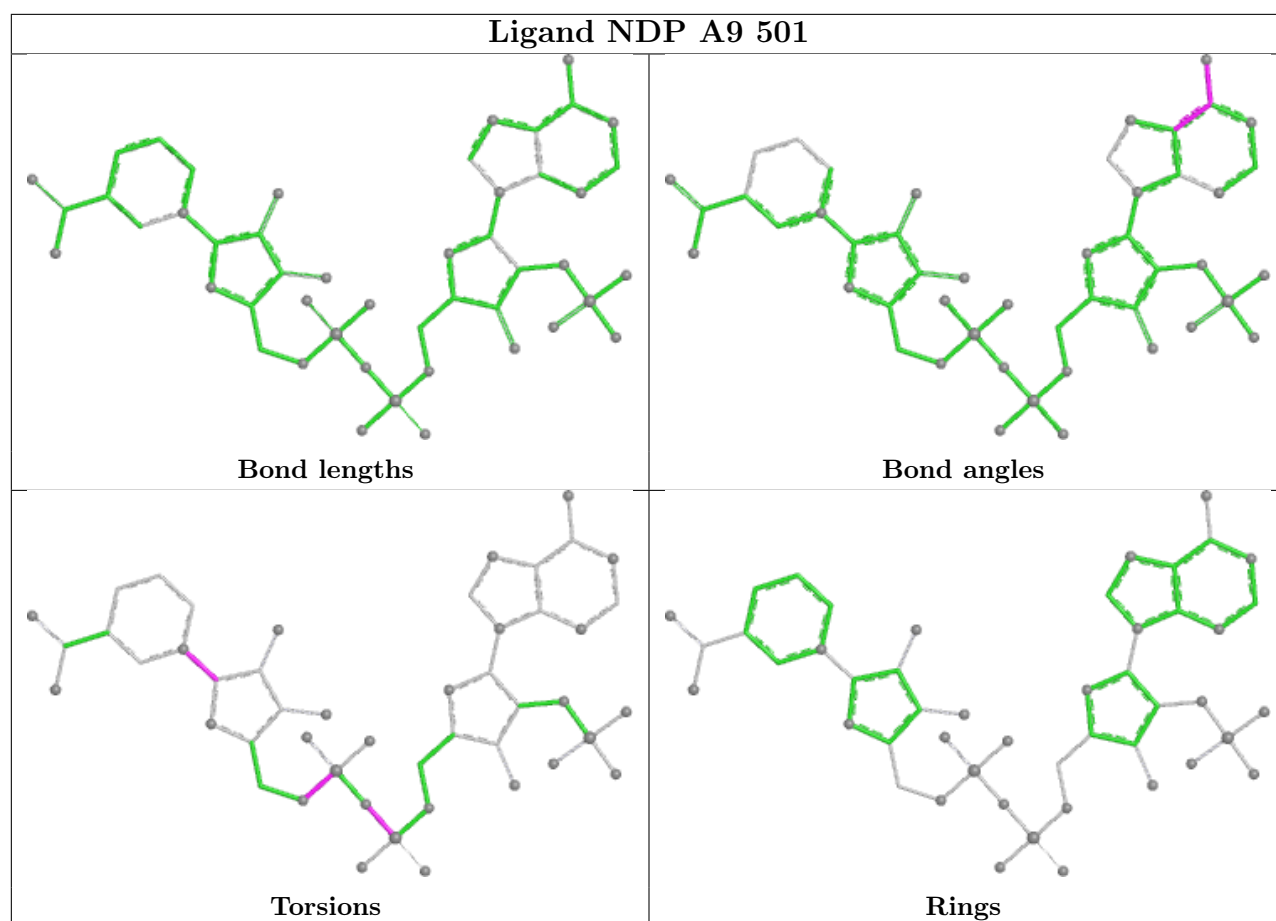


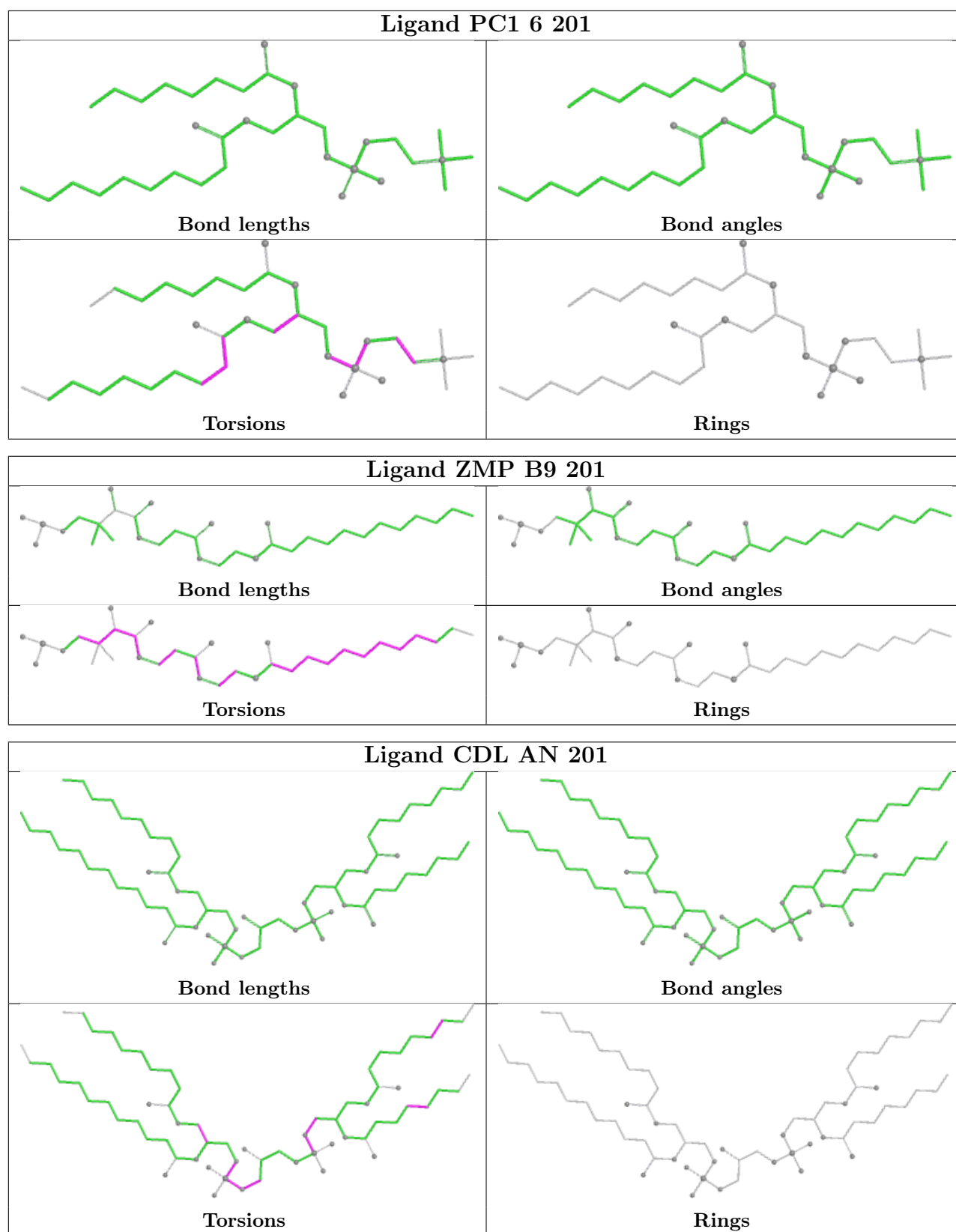




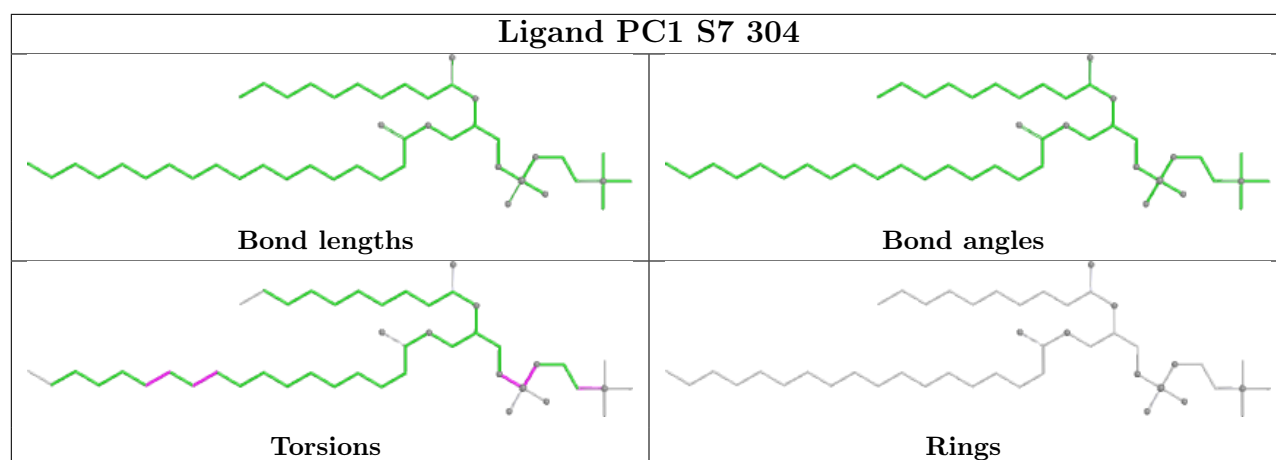












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

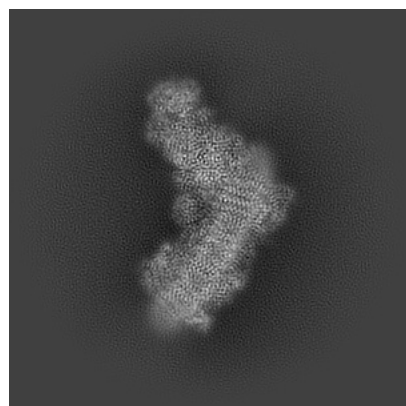
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28581. These allow visual inspection of the internal detail of the map and identification of artifacts.

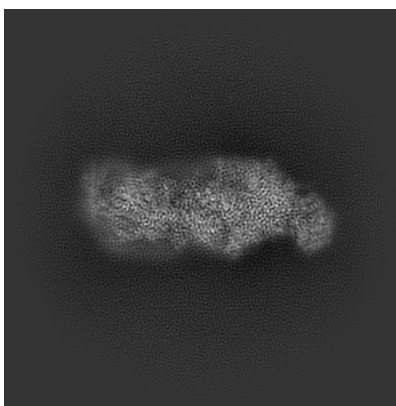
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

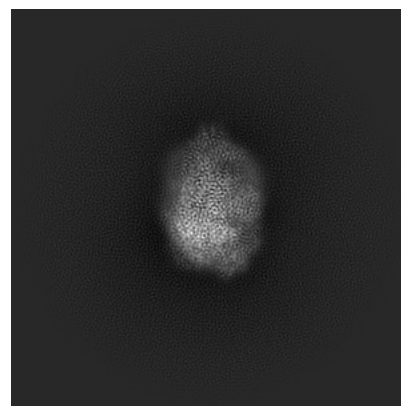
#### 6.1.1 Primary map



X

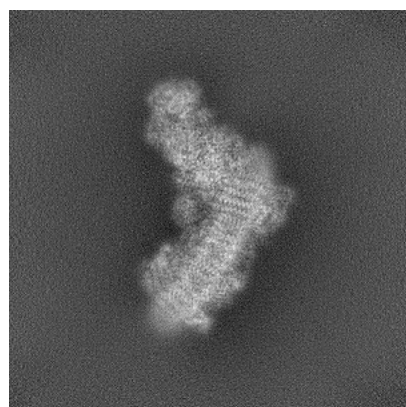


Y

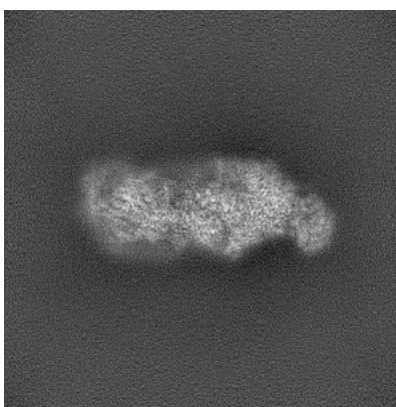


Z

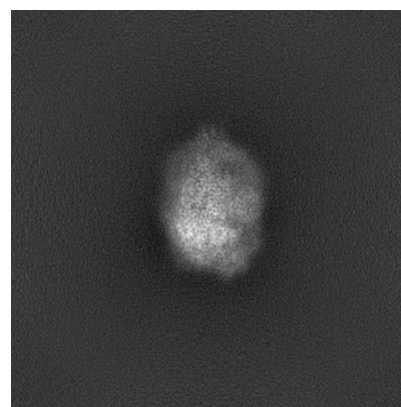
#### 6.1.2 Raw map



X



Y

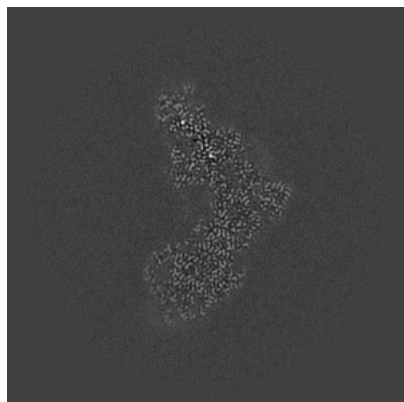


Z

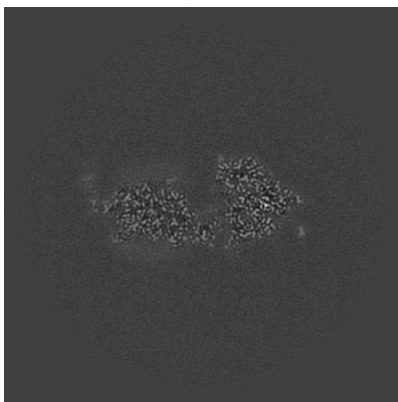
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

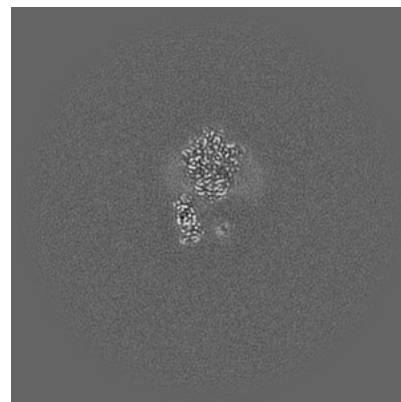
### 6.2.1 Primary map



X Index: 256

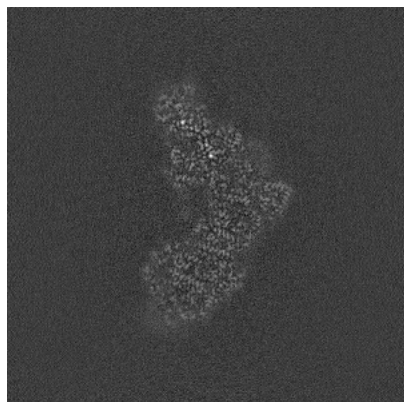


Y Index: 256

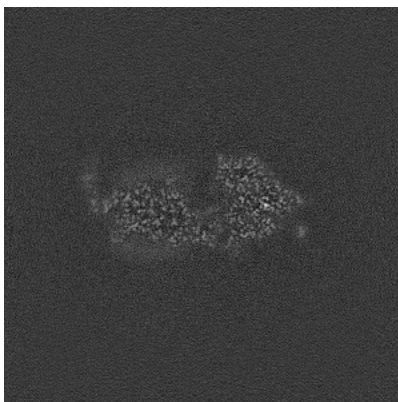


Z Index: 256

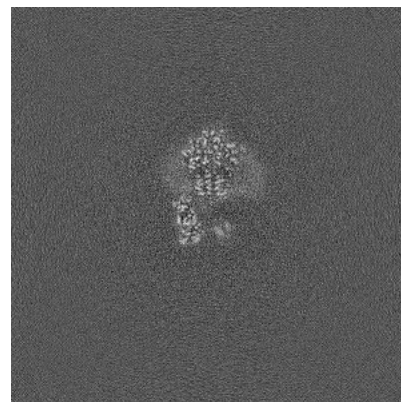
### 6.2.2 Raw map



X Index: 256



Y Index: 256

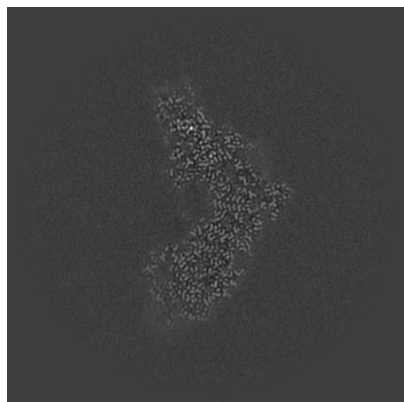


Z Index: 256

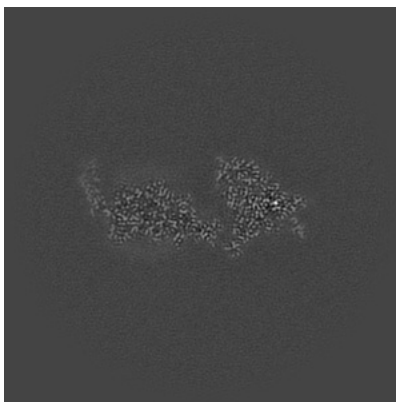
The images above show central slices of the map in three orthogonal directions.

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

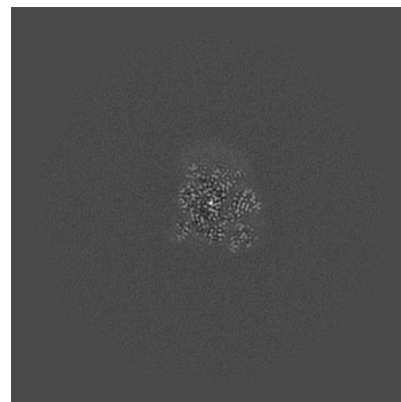
### 6.3.1 Primary map



X Index: 254

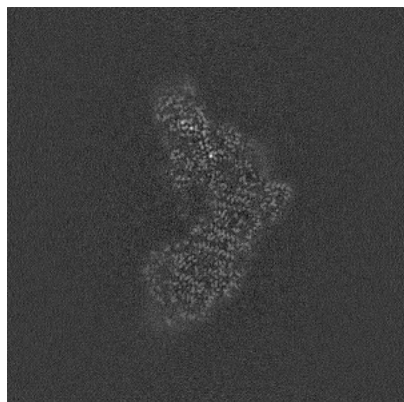


Y Index: 251

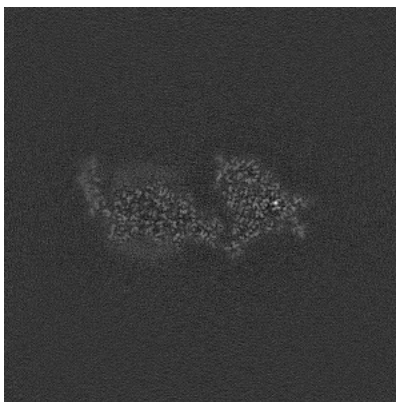


Z Index: 320

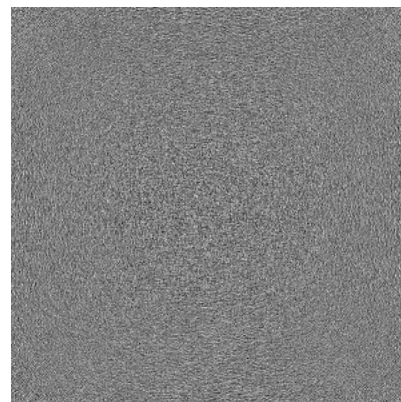
### 6.3.2 Raw map



X Index: 255



Y Index: 251



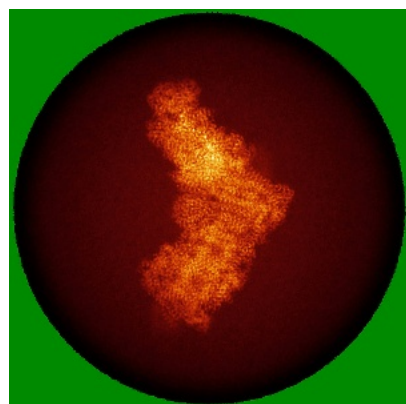
Z Index: 0

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

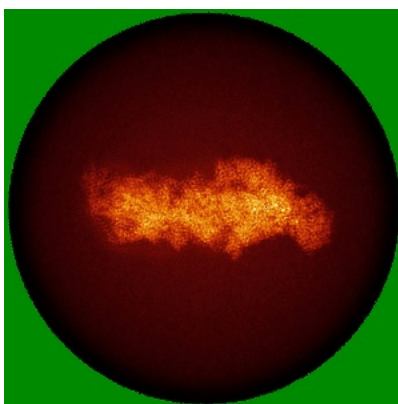


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

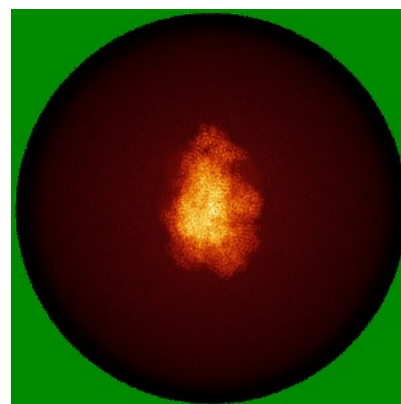
### 6.4.1 Primary map



X

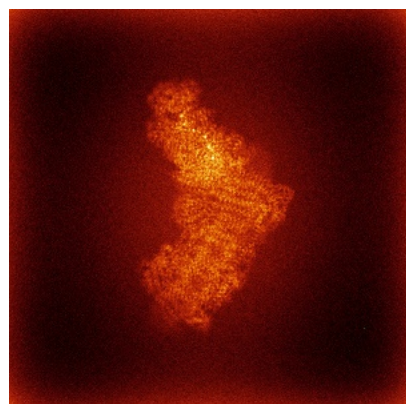


Y

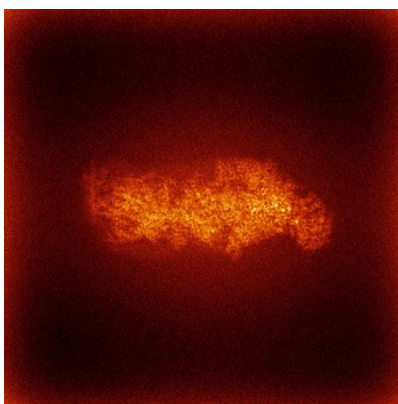


Z

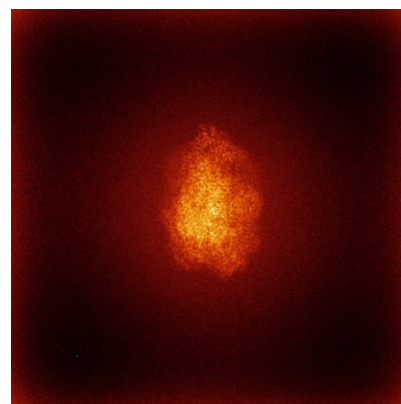
### 6.4.2 Raw map



X



Y

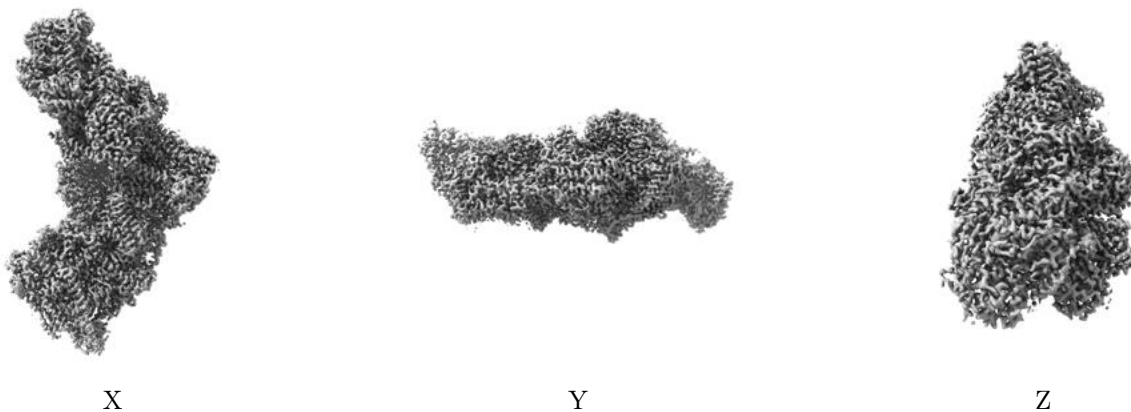


Z

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

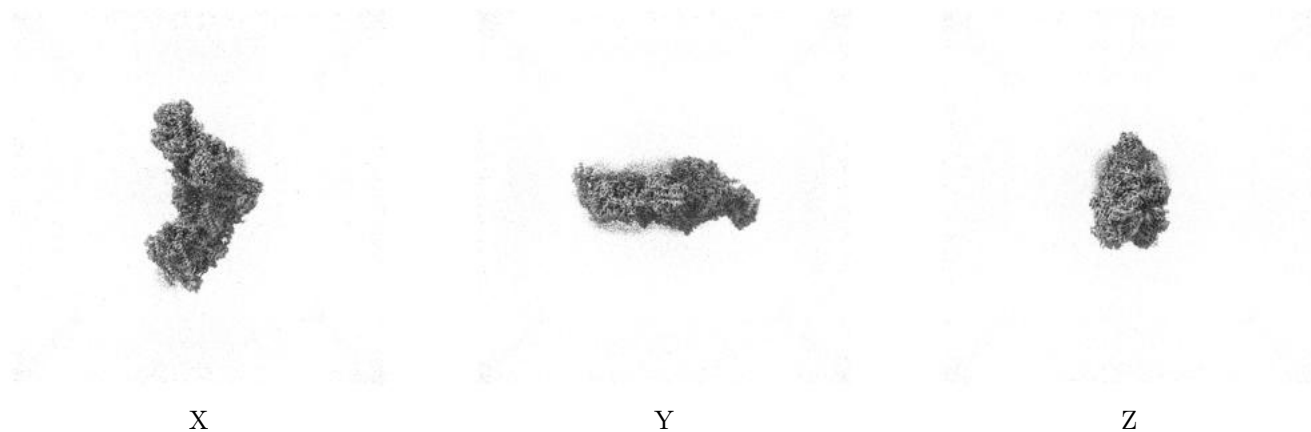
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

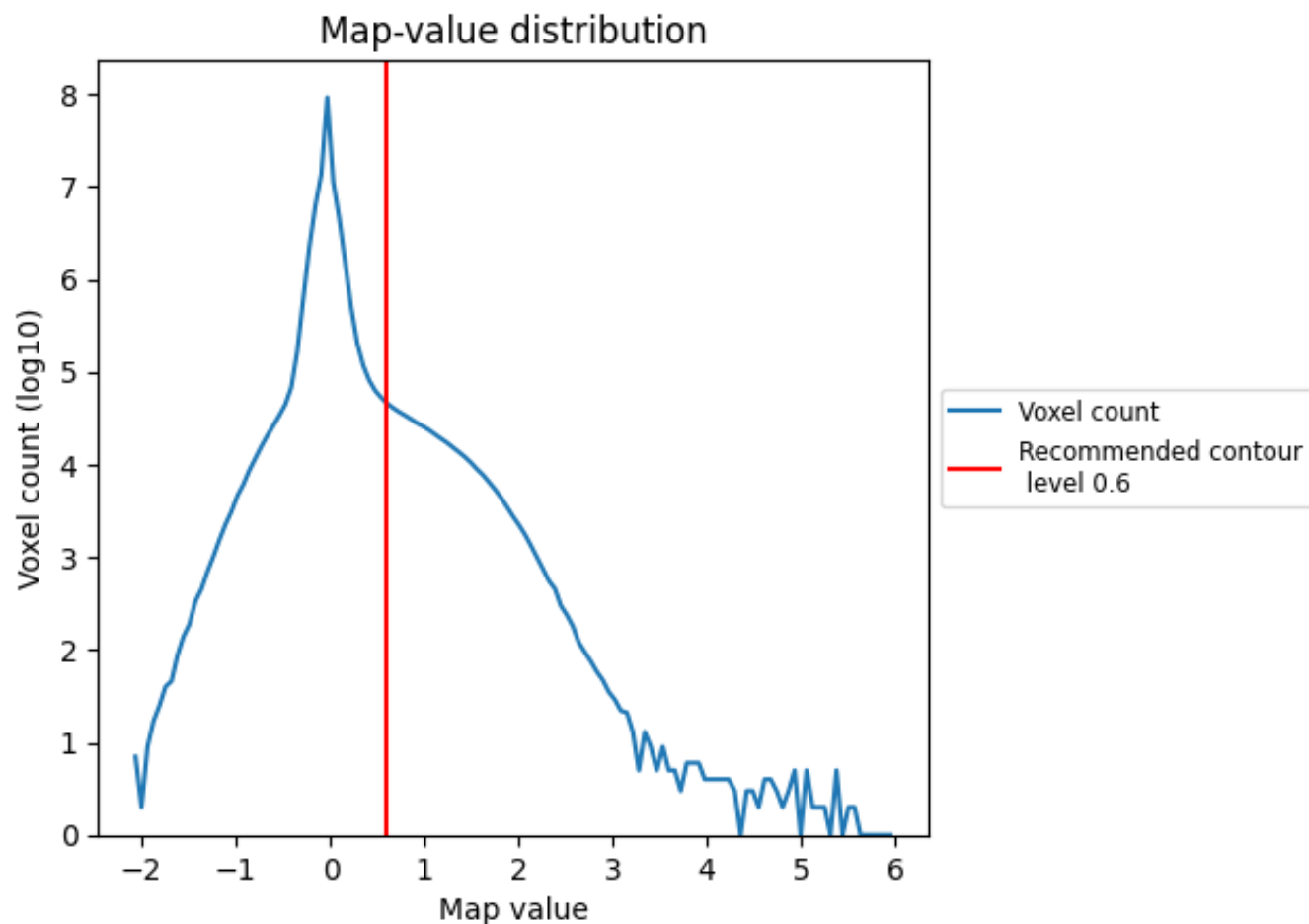
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

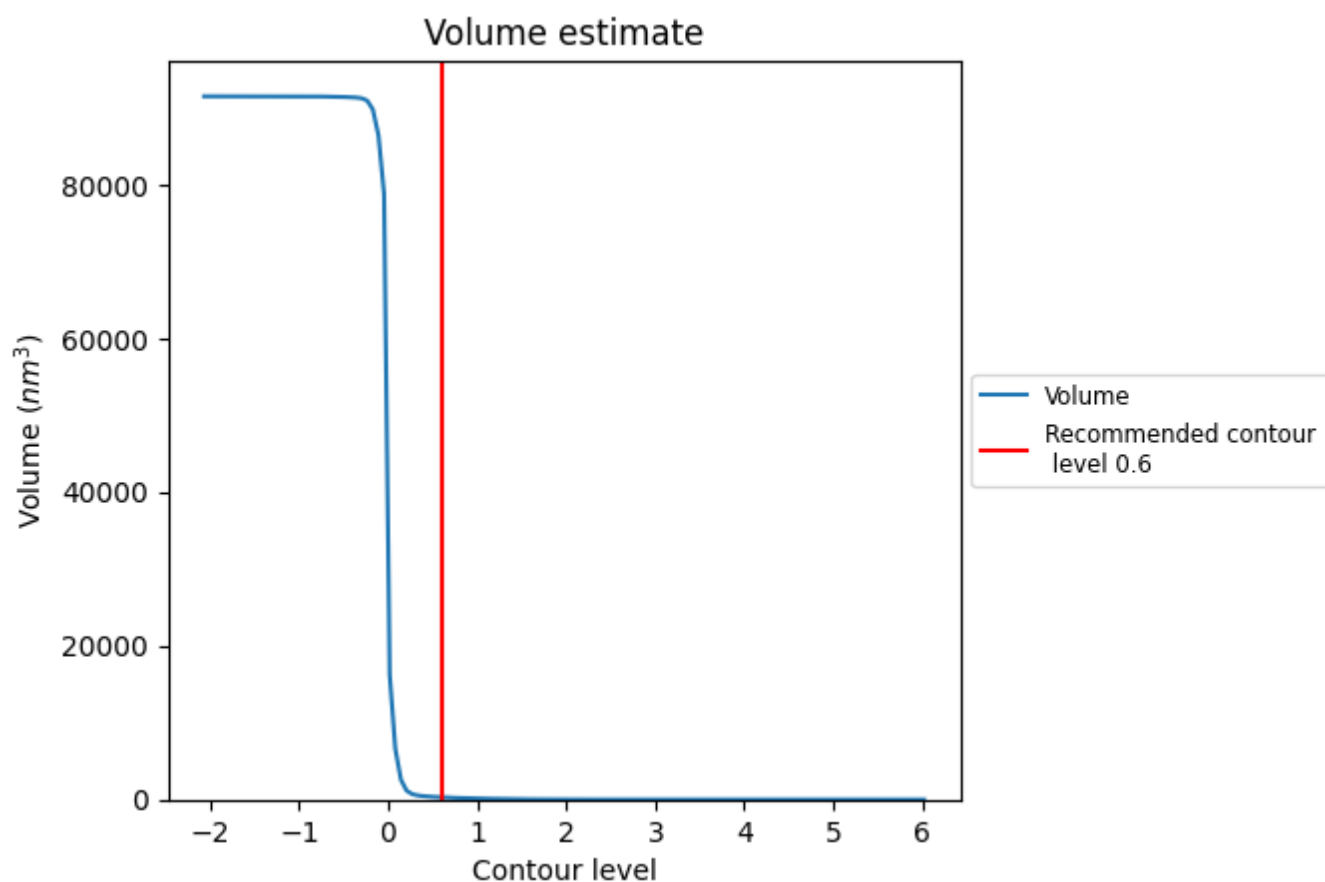
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

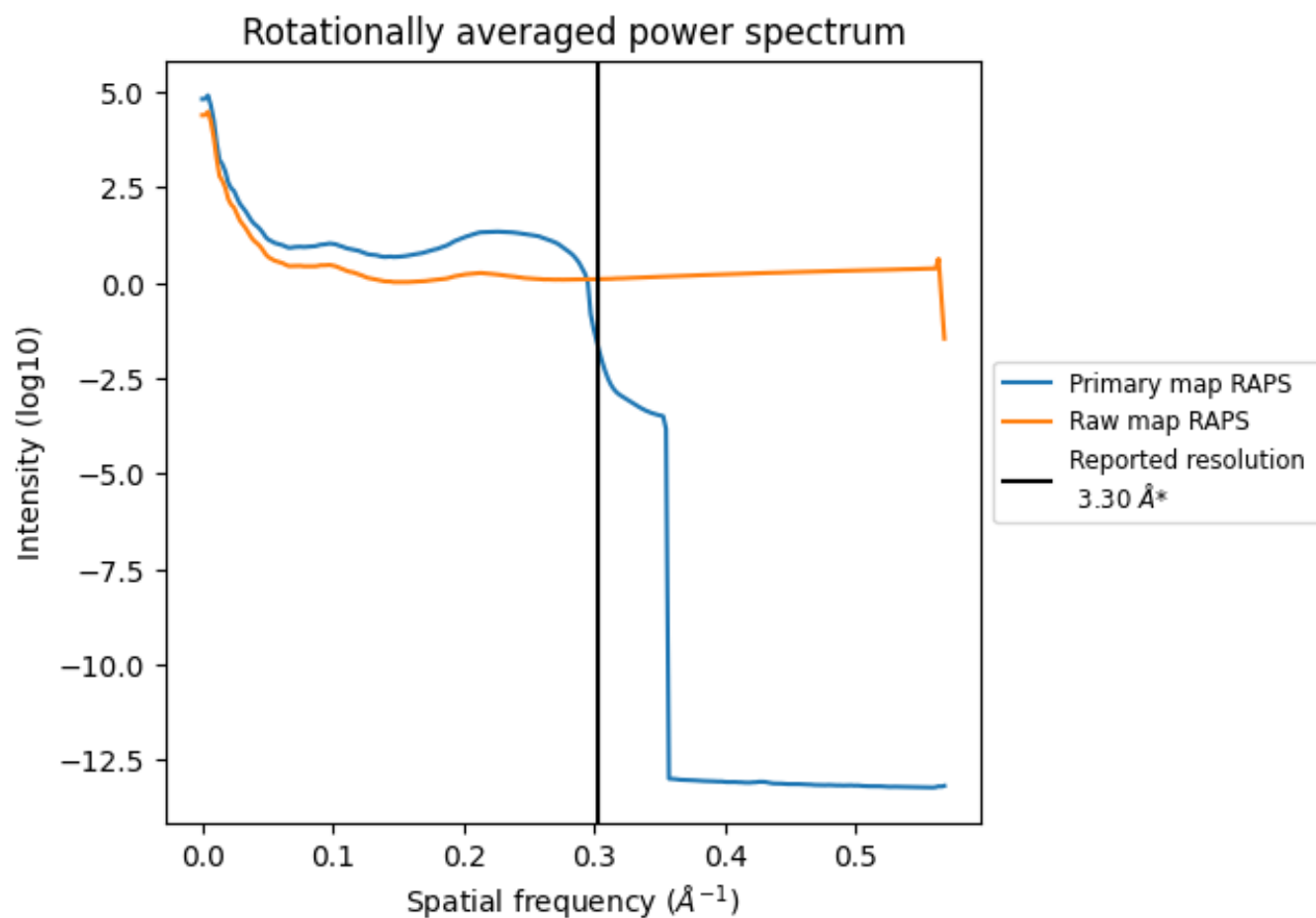


The volume at the recommended contour level is 293 nm<sup>3</sup>; this corresponds to an approximate mass of 265 kDa.

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 ⓘ

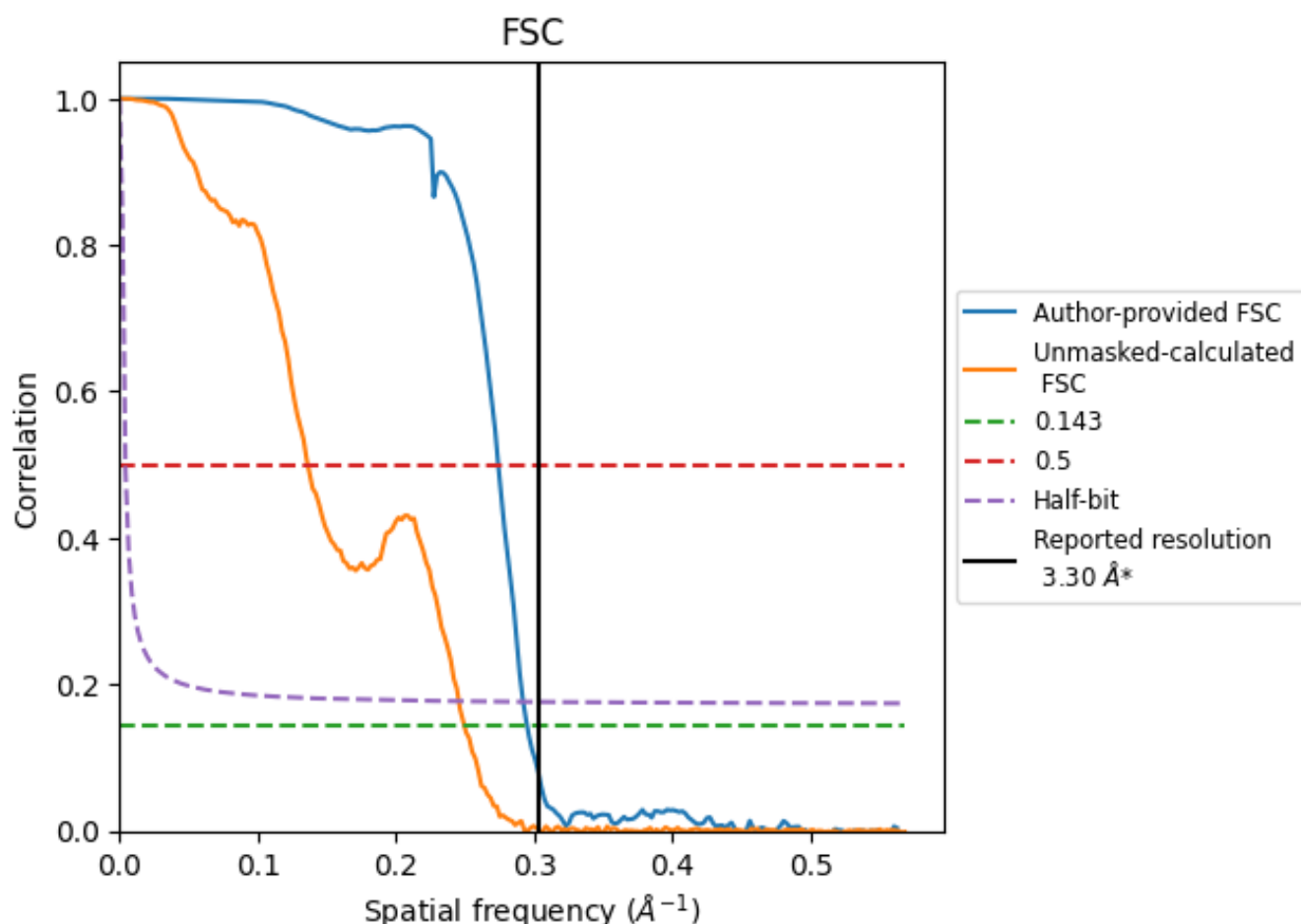


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

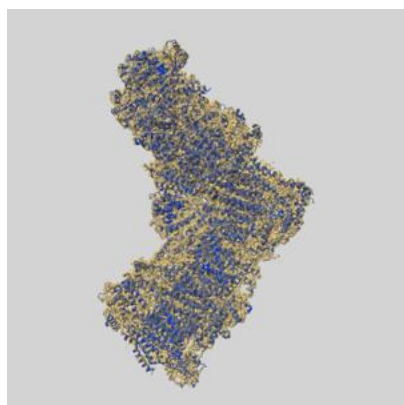
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.39	3.65	3.42
Unmasked-calculated*	4.01	7.34	4.07

\*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 4.01 differs from the reported value 3.3 by more than 10 %

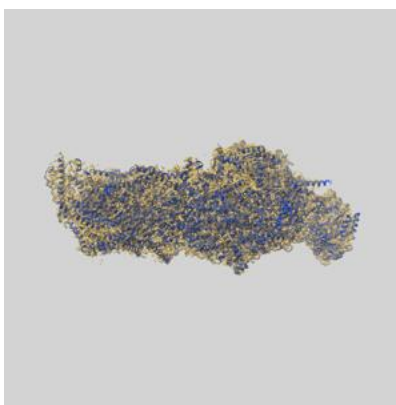
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28581 and PDB model 8ESW. Per-residue inclusion information can be found in section [3](#) on page [19](#).

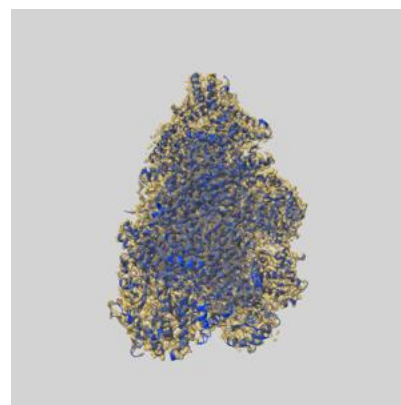
### 9.1 Map-model overlay [i](#)



X



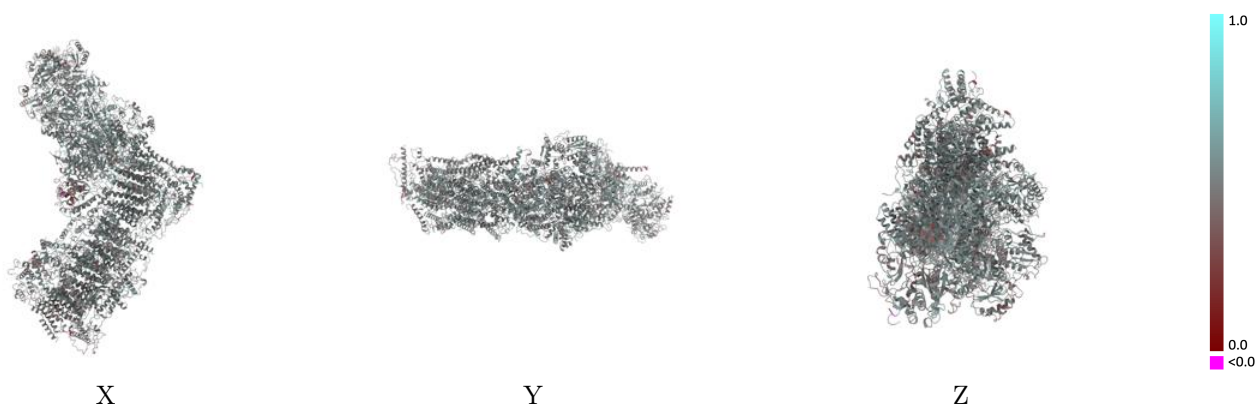
Y



Z

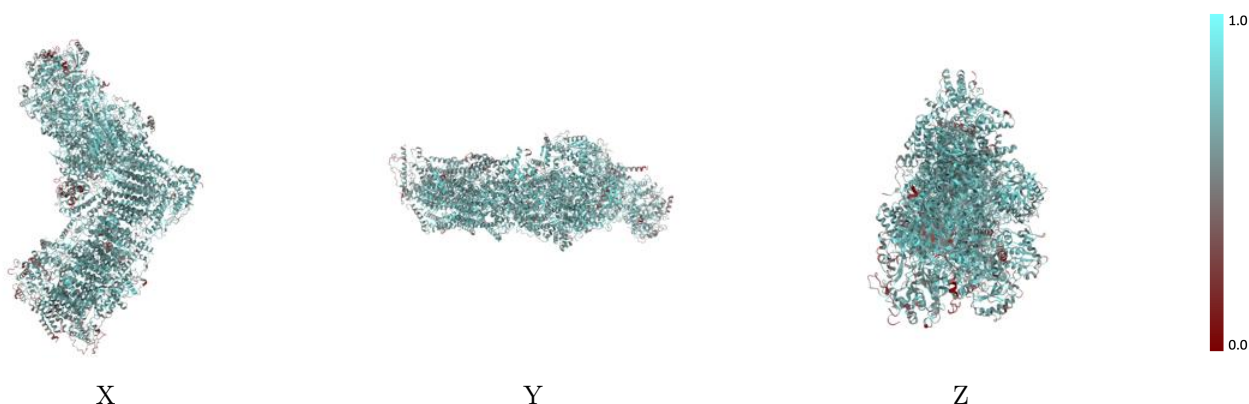
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



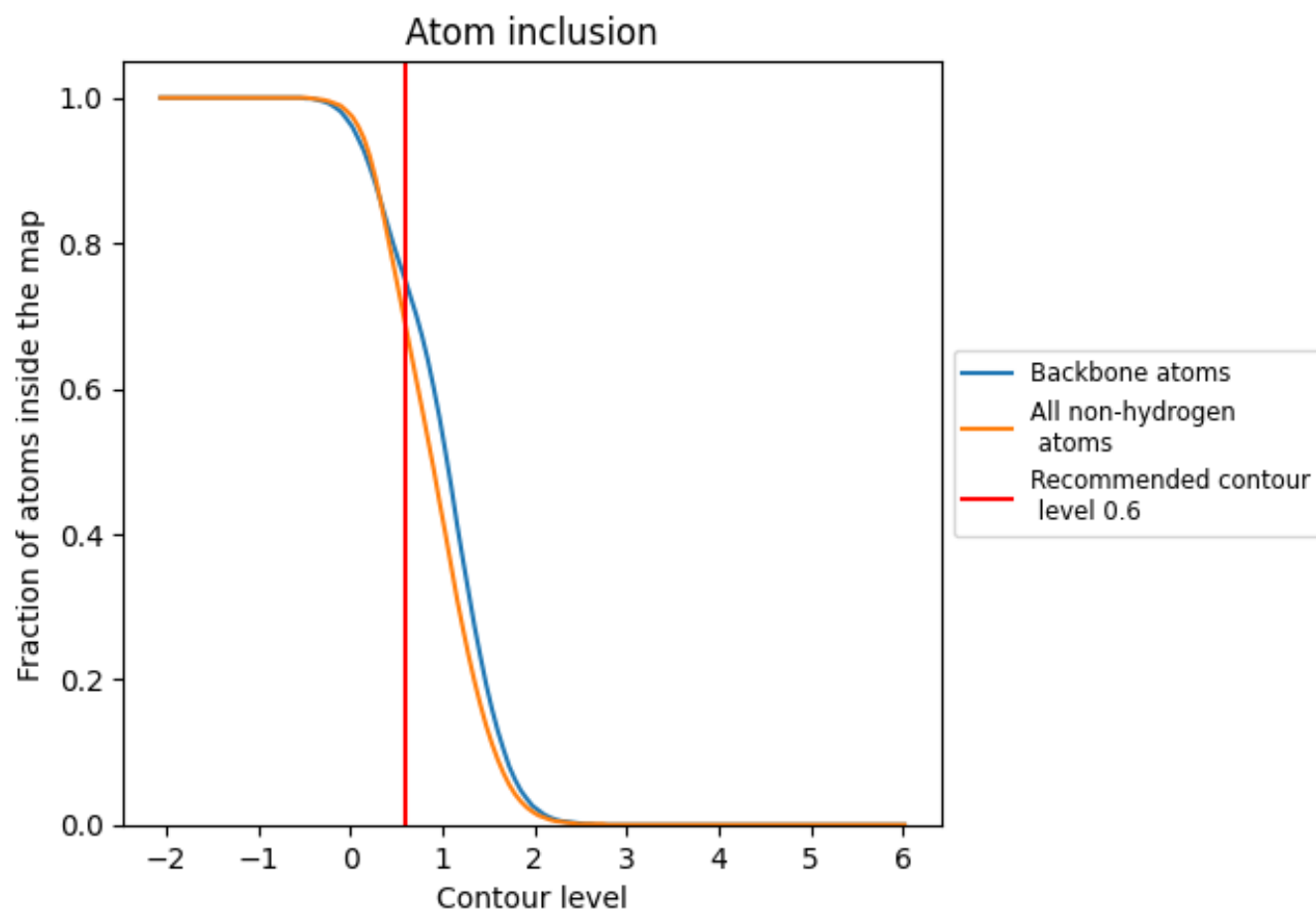
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ



















The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6850	 0.5040
1	 0.7340	 0.5070
2	 0.7330	 0.5160
3	 0.7000	 0.4960
4	 0.7420	 0.5190
4L	 0.7080	 0.5130
5	 0.6510	 0.4910
6	 0.7120	 0.5080
A1	 0.6860	 0.4920
A3	 0.6610	 0.5080
A5	 0.6960	 0.5100
A6	 0.7050	 0.5120
A7	 0.6720	 0.5060
A8	 0.6840	 0.5100
A9	 0.7290	 0.5210
AB	 0.3290	 0.3620
AC	 0.5520	 0.4780
AL	 0.7180	 0.5200
AM	 0.5900	 0.4920
AN	 0.6380	 0.5060
AO	 0.7290	 0.5150
B1	 0.5940	 0.4890
B2	 0.5180	 0.4460
B3	 0.5110	 0.4670
B4	 0.6600	 0.4990
B5	 0.7120	 0.5190
B6	 0.6140	 0.4920
B7	 0.5370	 0.4510
B8	 0.6670	 0.5000
B9	 0.6420	 0.4990
BL	 0.7300	 0.5030
BM	 0.6820	 0.5080
C2	 0.7130	 0.5170
S1	 0.6920	 0.5050
S2	 0.7450	 0.5180



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
S3	 0.7600	 0.5360
S4	 0.7060	 0.5140
S5	 0.7290	 0.5160
S6	 0.7080	 0.5360
S7	 0.7110	 0.5080
S8	 0.7560	 0.5240
V1	 0.6560	 0.4890
V2	 0.6140	 0.4810
V3	 0.1470	 0.4370