



Full wwPDB EM Validation Report ⓘ

Nov 11, 2025 – 09:42 PM JST

PDB ID : 8ZSM / pdb_00008zsm
EMDB ID : EMD-60420
Title : Complex I from respirasome closed state 1 bound by metformin (SC-MetC1-iii)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-06-05
Resolution : 3.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

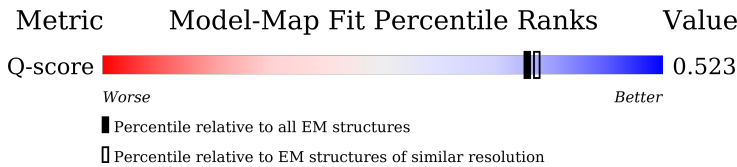
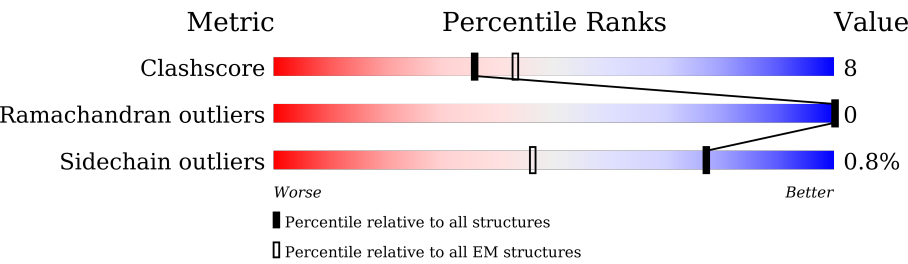
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14599 (2.75 - 3.75)

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

Mol	Chain	Length	Quality of chain
1	4L	98	<div><div>5%</div><div>72%</div><div>28%</div></div>
2	A1	70	<div><div>19%</div><div>86%</div><div>14%</div></div>
3	A2	85	<div><div>31%</div><div>78%</div><div>22%</div></div>
4	A3	83	<div><div>39%</div><div>92%</div><div>8%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A5	112	<div> <div>29%</div> <div>86%</div> <div>13%</div> </div>
6	A6	114	<div> <div>26%</div> <div>81%</div> <div>19%</div> </div>
7	A7	112	<div> <div>45%</div> <div>71%</div> <div>15%</div> <div>13%</div> </div>
8	A8	171	<div> <div>28%</div> <div>81%</div> <div>19%</div> </div>
9	A9	341	<div> <div>16%</div> <div>81%</div> <div>19%</div> </div>
10	AB	87	<div> <div>71%</div> <div>75%</div> <div>14%</div> <div>11%</div> </div>
10	AC	87	<div> <div>22%</div> <div>89%</div> <div>10%</div> </div>
11	AK	321	<div> <div>36%</div> <div>83%</div> <div>17%</div> </div>
12	AL	140	<div> <div>46%</div> <div>87%</div> <div>13%</div> </div>
13	AM	144	<div> <div>85%</div> <div>88%</div> <div>12%</div> </div>
14	AN	142	<div> <div>28%</div> <div>81%</div> <div>19%</div> </div>
15	B1	56	<div> <div>45%</div> <div>79%</div> <div>21%</div> </div>
16	B2	67	<div> <div>40%</div> <div>81%</div> <div>19%</div> </div>
17	B3	80	<div> <div>36%</div> <div>84%</div> <div>16%</div> </div>
18	B4	128	<div> <div>30%</div> <div>88%</div> <div>12%</div> </div>
19	B5	138	<div> <div>9%</div> <div>90%</div> <div>10%</div> </div>
20	B6	126	<div> <div>28%</div> <div>63%</div> <div>17%</div> <div>18%</div> </div>
21	B7	125	<div> <div>34%</div> <div>86%</div> <div>14%</div> </div>
22	B8	156	<div> <div>21%</div> <div>82%</div> <div>18%</div> </div>
23	B9	178	<div> <div>22%</div> <div>89%</div> <div>11%</div> </div>
24	BK	176	<div> <div>22%</div> <div>81%</div> <div>18%</div> </div>
25	BL	102	<div> <div>32%</div> <div>80%</div> <div>17%</div> </div>
26	CA	49	<div> <div>49%</div> <div>90%</div> <div>10%</div> </div>
27	CB	121	<div> <div>21%</div> <div>83%</div> <div>17%</div> </div>
28	N1	318	<div> <div>11%</div> <div>75%</div> <div>25%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	N2	347	
30	N3	115	
31	N4	459	
32	N5	603	
33	N6	174	
34	S1	689	
35	S2	430	
36	S3	208	
37	S4	124	
38	S5	105	
39	S6	96	
40	S7	156	
41	S8	176	
42	V1	431	
43	V2	217	
44	V3	42	

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
53	SF4	S8	302	-	-	X	-
53	SF4	V1	501	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 68795 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

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

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

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

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

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

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

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

- Molecule 7 is a protein called Complex I-B14.5a.

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

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

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

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

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

- Molecule 10 is a protein called Acyl carrier protein.

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

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

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

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

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

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B6	103	Total	C	N	O	S	0	0
			882	577	156	148	1		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

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

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

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase chain 3.

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

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S2	430	Total	C	N	O	S	0	0
			3459	2212	594	629	24		

- Molecule 36 is a protein called Complex I-30kD.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	S4	124	Total	C	N	O	S	0	0
			1007	637	179	188	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

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

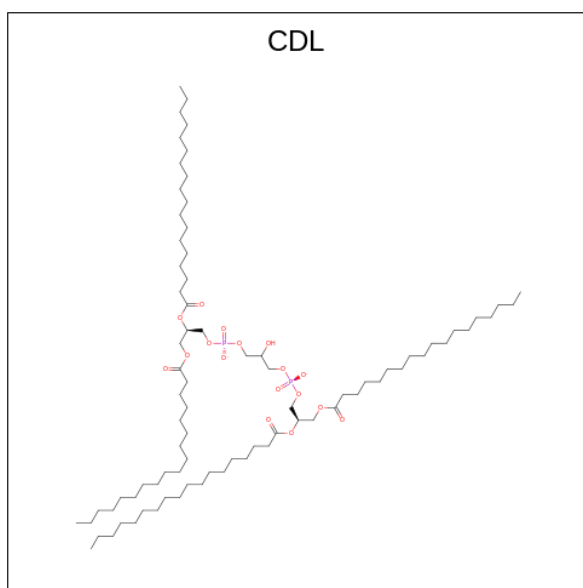
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 44 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

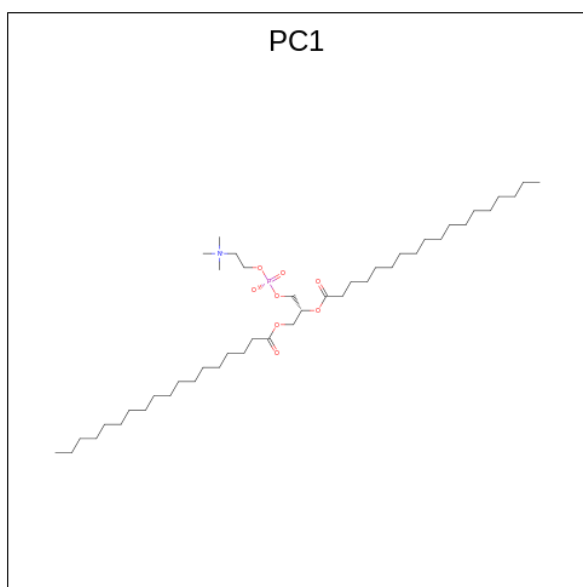
Mol	Chain	Residues	Atoms					AltConf	Trace
44	V3	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



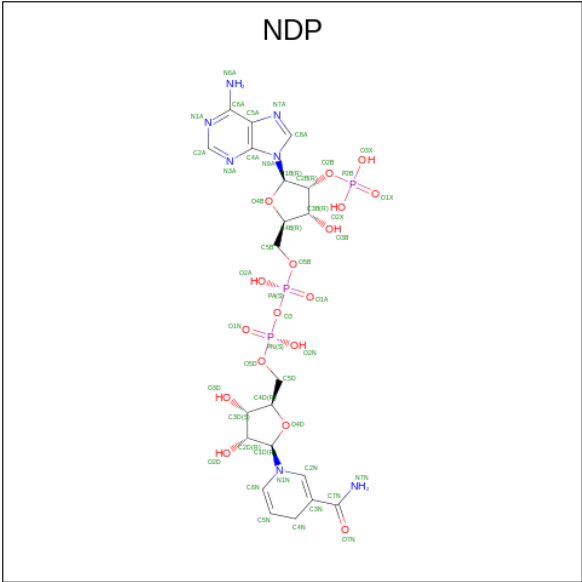
Mol	Chain	Residues	Atoms				AltConf
45	4L	1	Total	C	O	P	0
			92	73	17	2	
45	A1	1	Total	C	O	P	0
			94	75	17	2	
45	AL	1	Total	C	O	P	0
			94	75	17	2	
45	AL	1	Total	C	O	P	0
			71	52	17	2	
45	B5	1	Total	C	O	P	0
			100	81	17	2	
45	CB	1	Total	C	O	P	0
			83	64	17	2	
45	N1	1	Total	C	O	P	0
			78	59	17	2	
45	N2	1	Total	C	O	P	0
			68	49	17	2	
45	N4	1	Total	C	O	P	0
			100	81	17	2	
45	N5	1	Total	C	O	P	0
			89	70	17	2	
45	N5	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



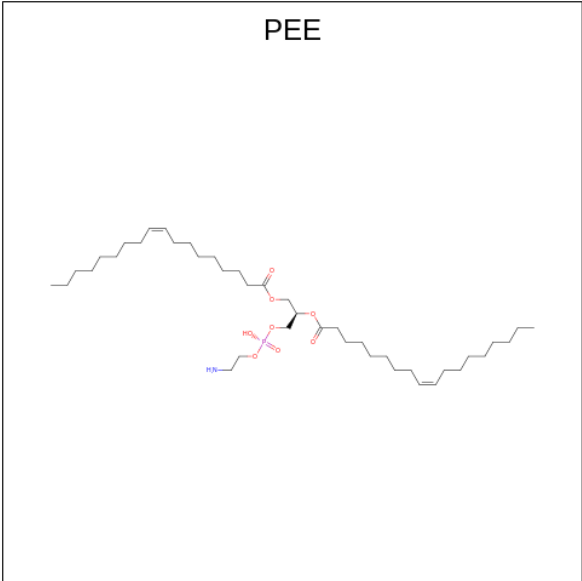
Mol	Chain	Residues	Atoms					AltConf
46	A3	1	Total	C	N	O	P	0
			50	40	1	8	1	
46	A3	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	AN	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	B8	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 47 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



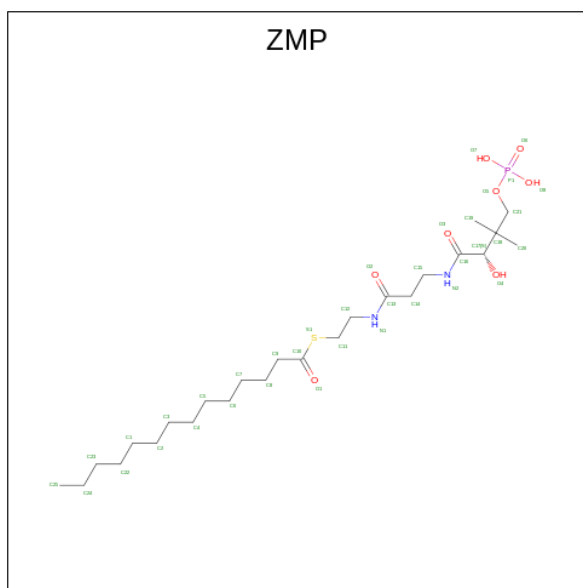
Mol	Chain	Residues	Atoms					AltConf
48	A9	1	Total	C	N	O	P	0
			39	29	1	8	1	
48	AK	1	Total	C	N	O	P	0
			40	30	1	8	1	

Continued on next page...

Continued from previous page...

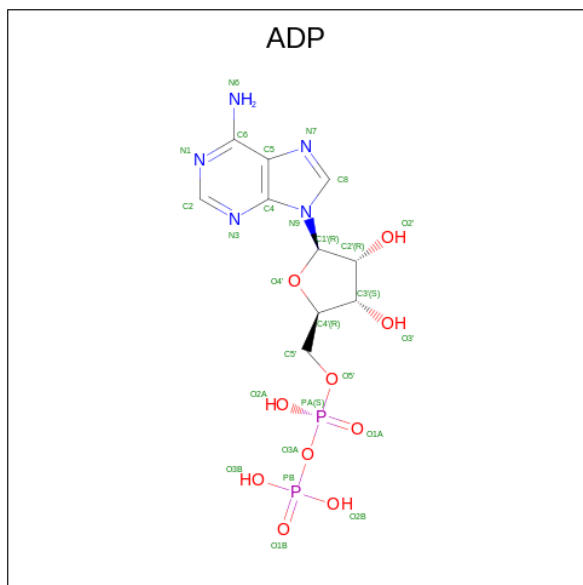
Mol	Chain	Residues	Atoms					AltConf
48	AL	1	Total	C	N	O	P	0
			36	26	1	8	1	
48	AL	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	AN	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	B6	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	N1	1	Total	C	N	O	P	0
			31	21	1	8	1	
48	N2	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	N2	1	Total	C	N	O	P	0
			48	38	1	8	1	
48	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
48	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 50 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

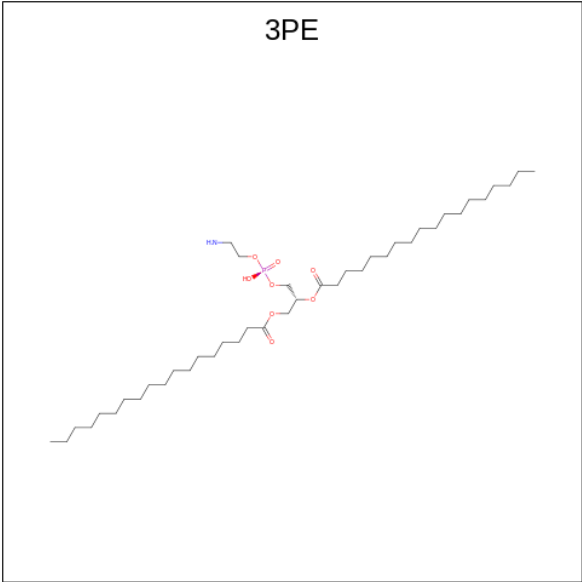


Mol	Chain	Residues	Atoms					AltConf
50	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 51 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).

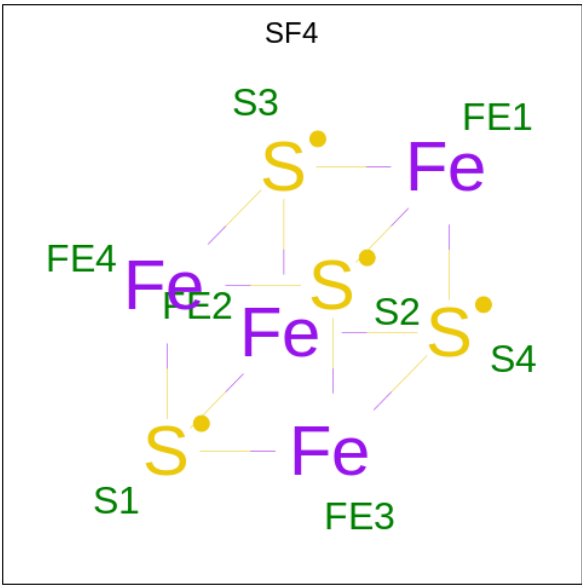


- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
52	B4	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	CB	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	N4	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 53 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



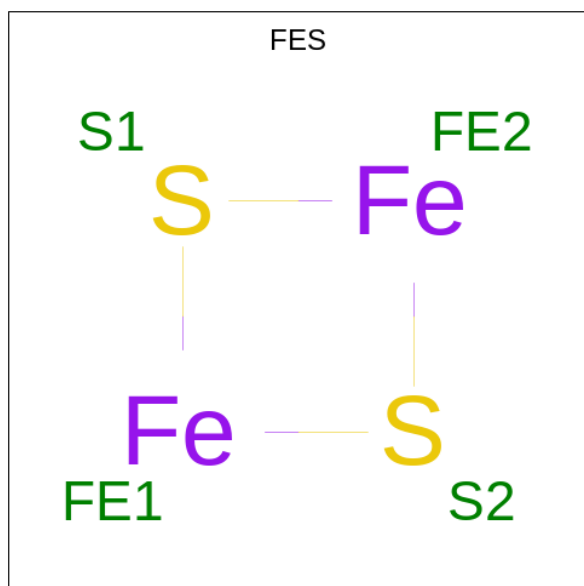
Mol	Chain	Residues	Atoms			AltConf
53	S1	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

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

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

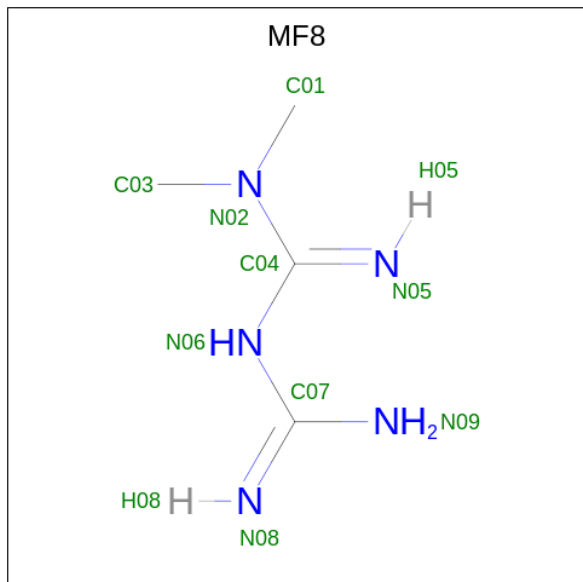


Mol	Chain	Residues	Atoms			AltConf
54	S1	1	Total	Fe	S	0
			4	2	2	
54	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	S1	1	Total	Mg	0
			1	1	

- Molecule 56 is Metformin (CCD ID: MF8) (formula: $C_4H_{11}N_5$) (labeled as "Ligand of Interest" by depositor).

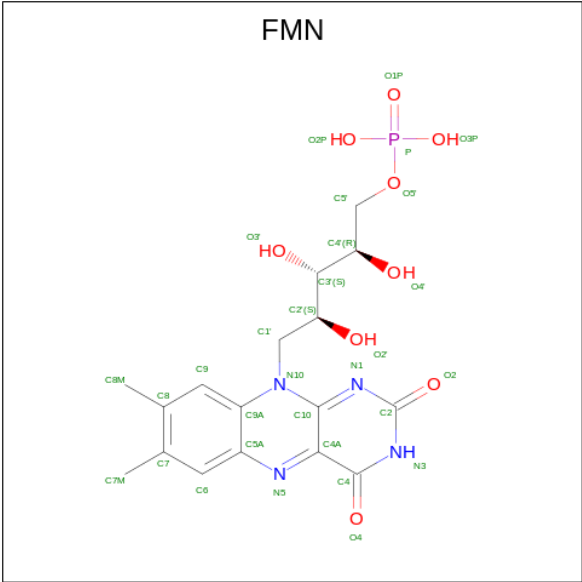


Mol	Chain	Residues	Atoms			AltConf
56	S2	1	Total	C	N	0
			9	4	5	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 58 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

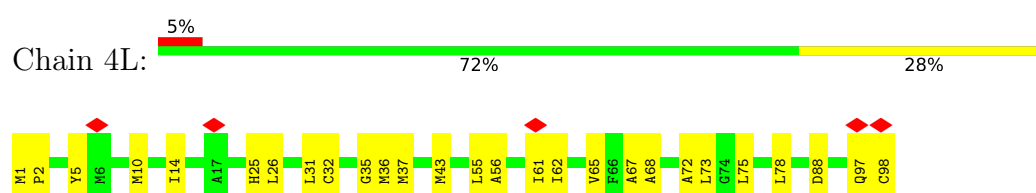


Mol	Chain	Residues	Atoms					AltConf
58	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

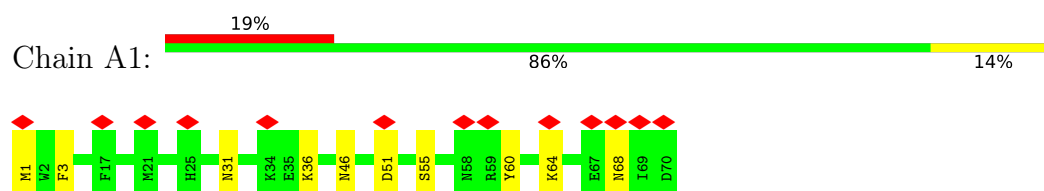
3 Residue-property plots

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

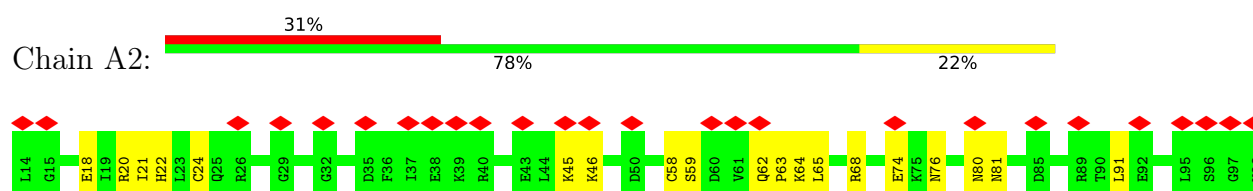
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



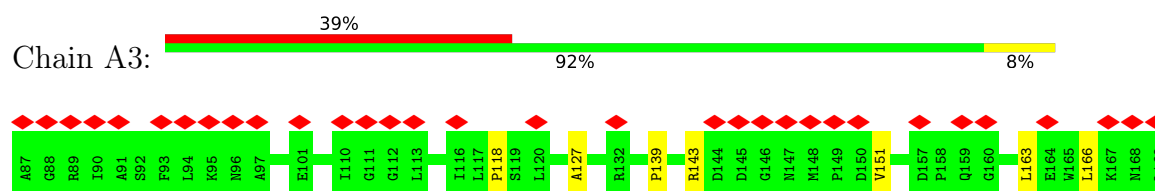
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



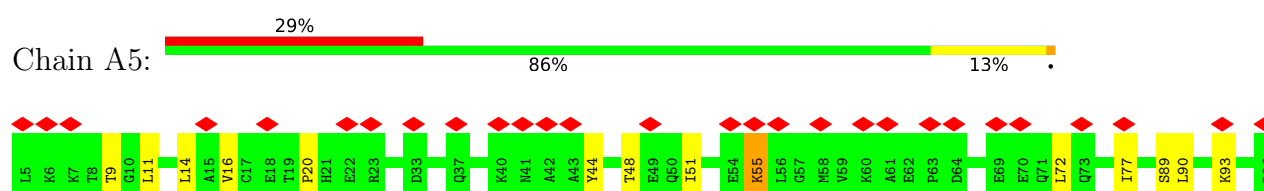
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

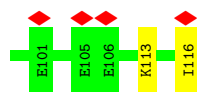


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

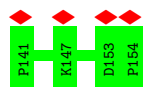
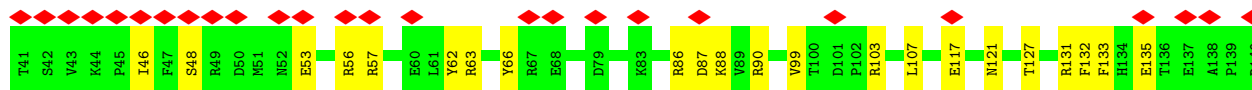
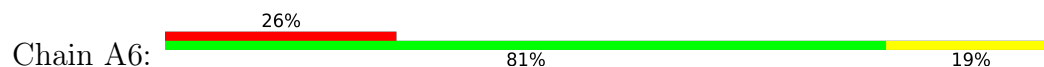


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

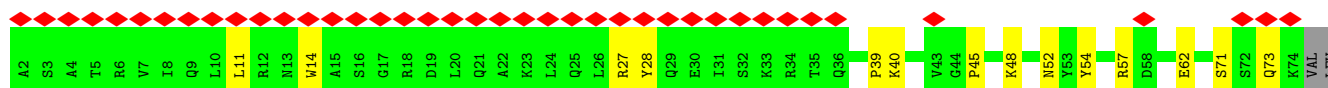
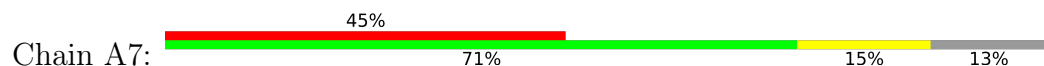




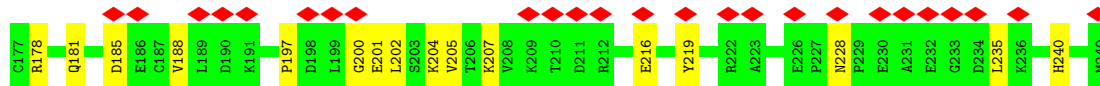
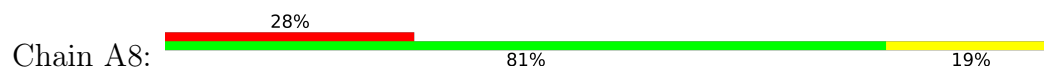
- Molecule 6: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



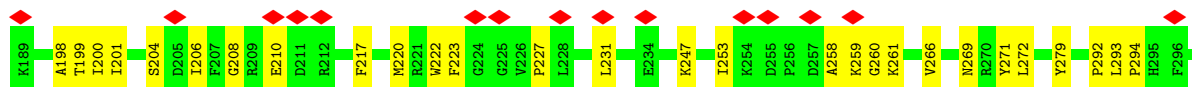
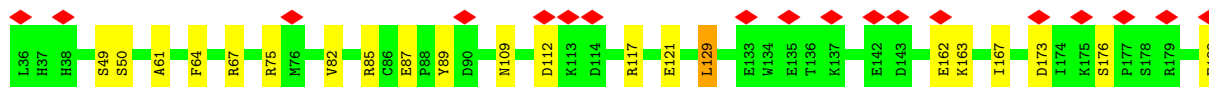
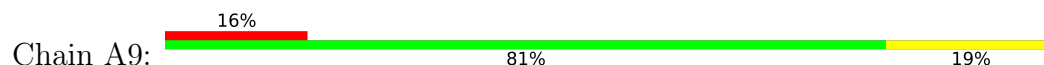
- Molecule 7: Complex I-B14.5a

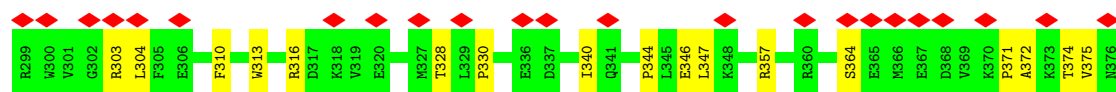


- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

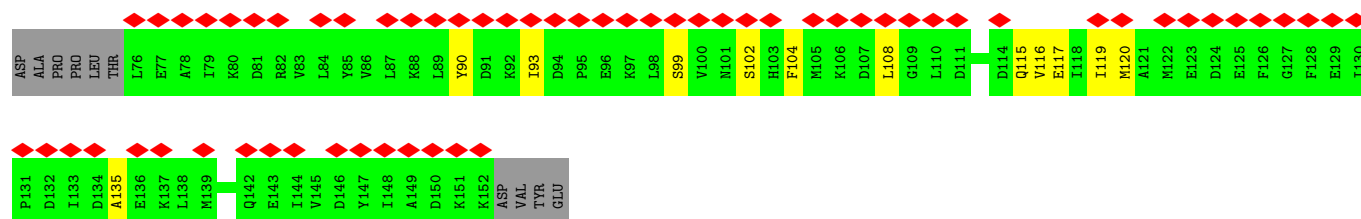
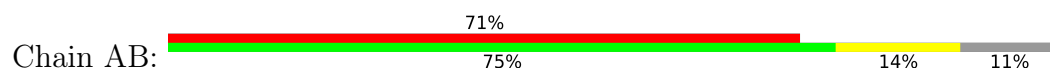


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

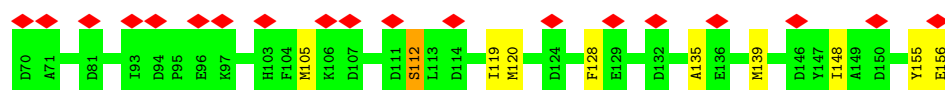
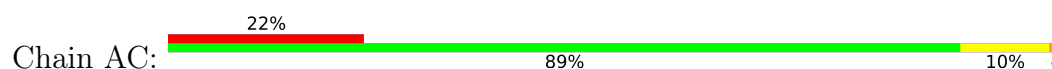




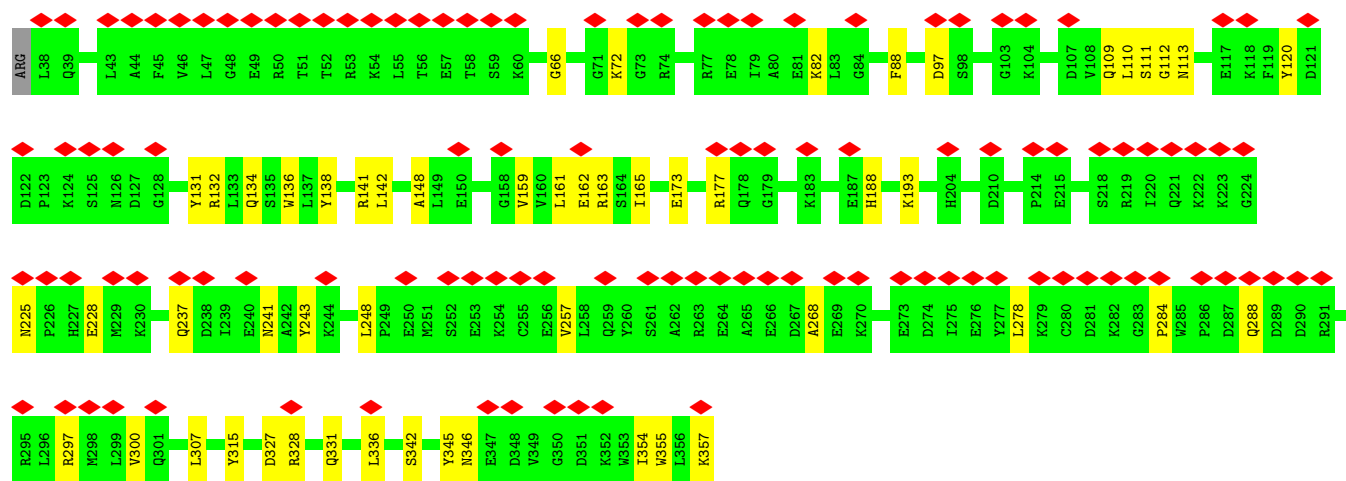
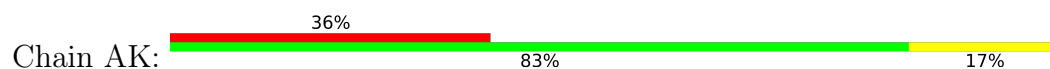
• Molecule 10: Acyl carrier protein



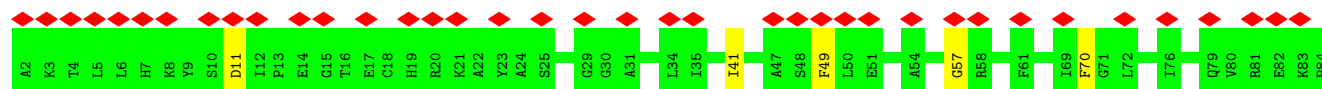
• Molecule 10: Acyl carrier protein

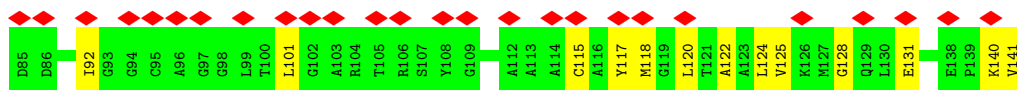


• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

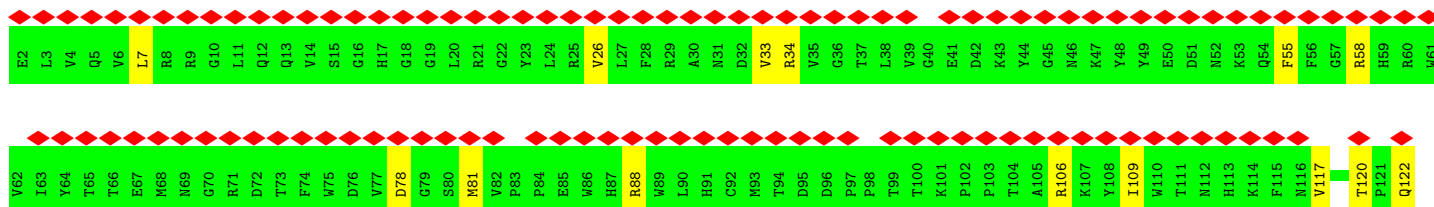
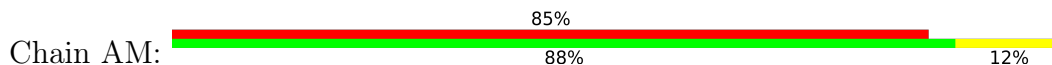


• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

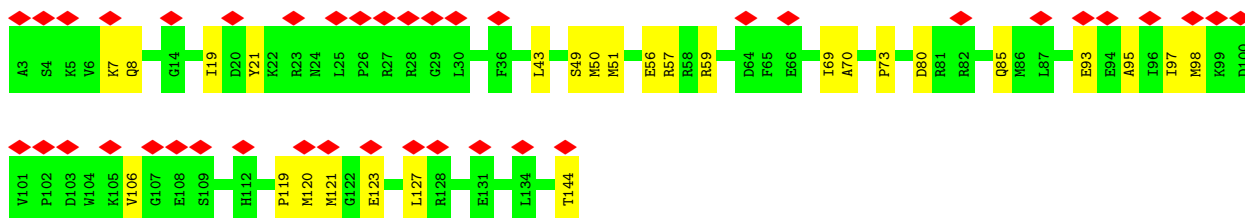
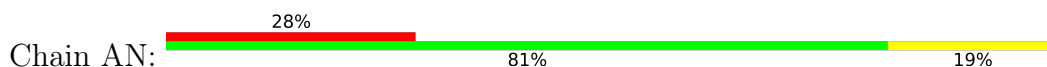




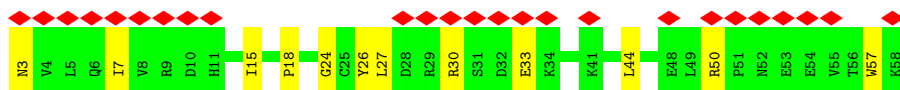
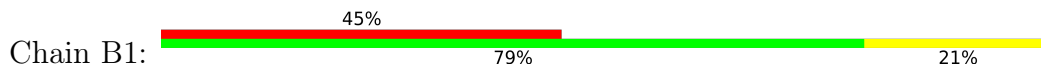
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



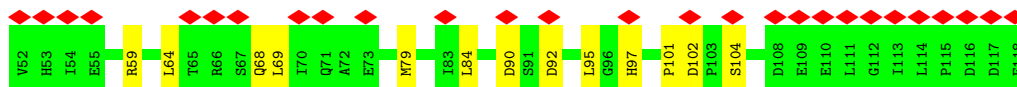
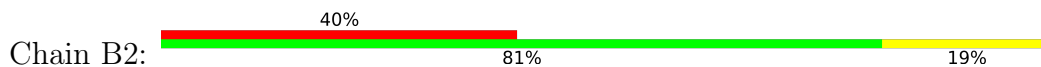
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



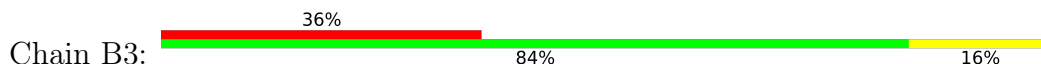
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

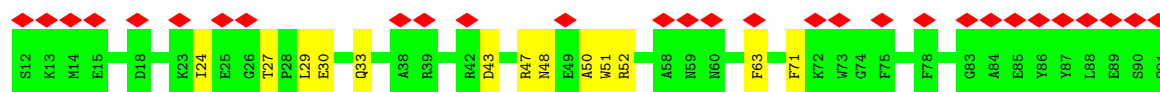


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

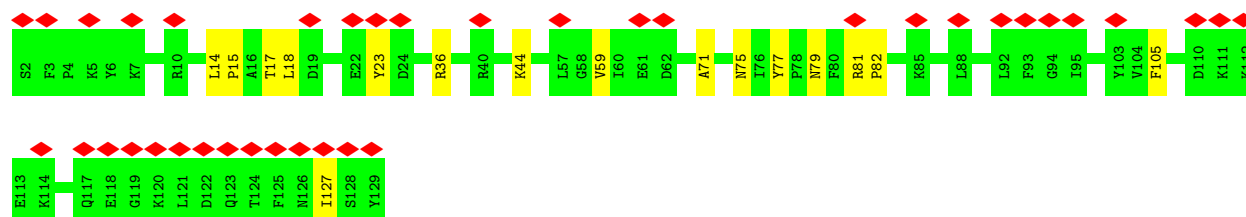
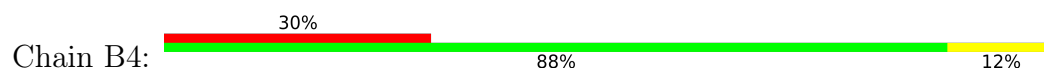


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3





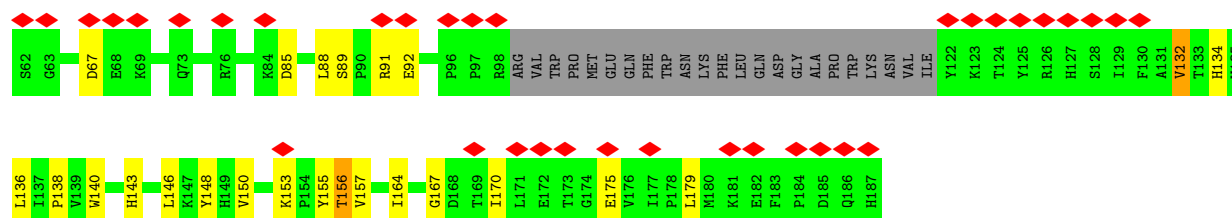
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



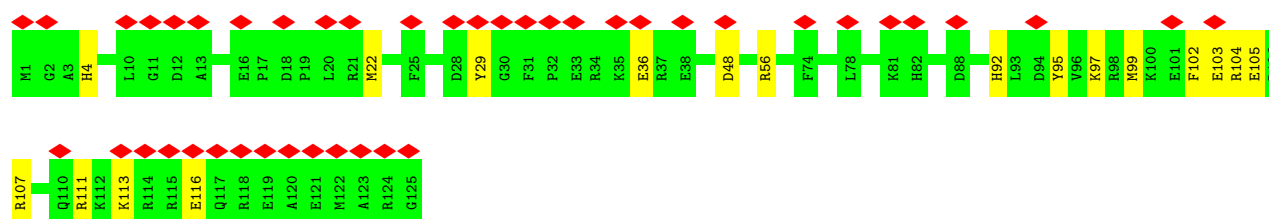
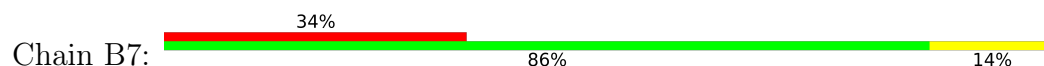
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



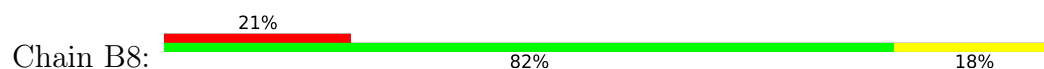
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

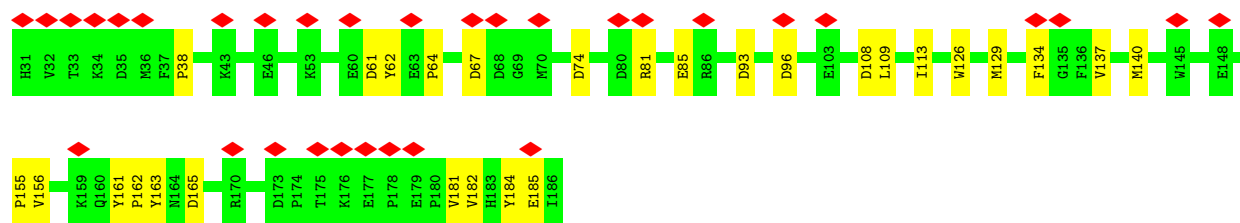


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

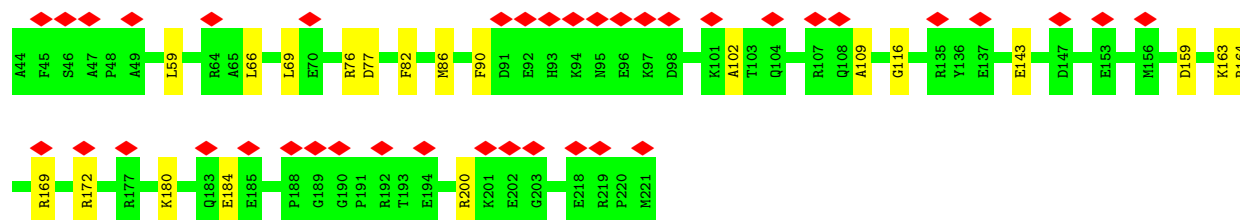
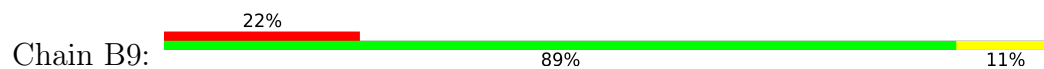


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

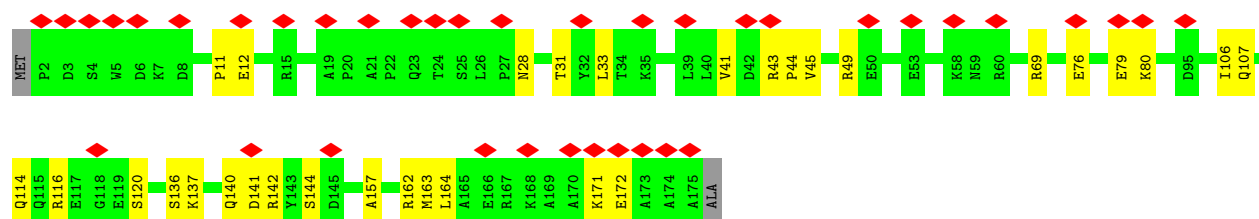
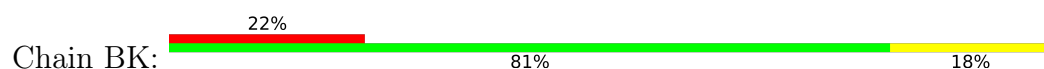




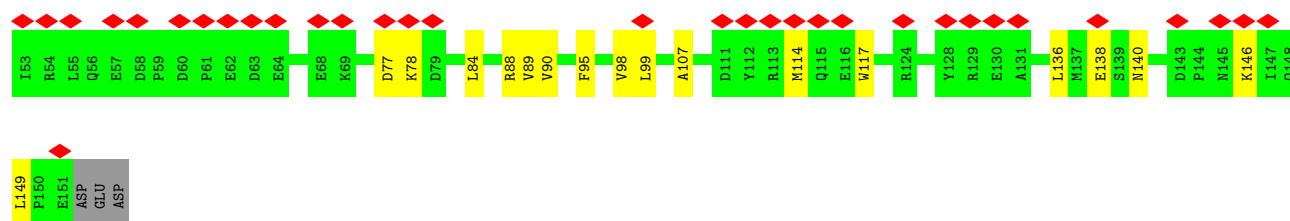
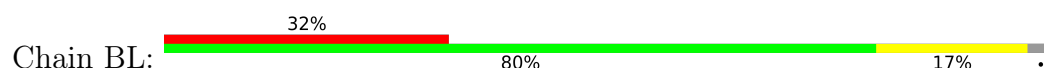
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



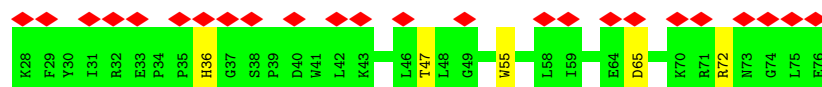
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



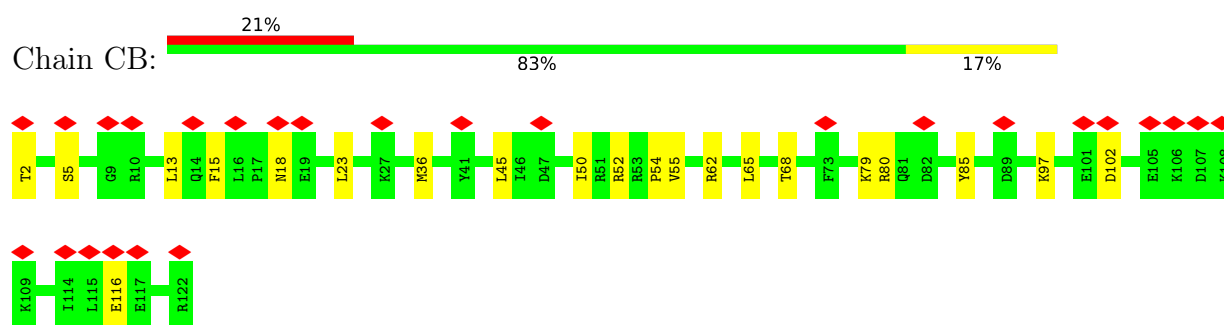
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



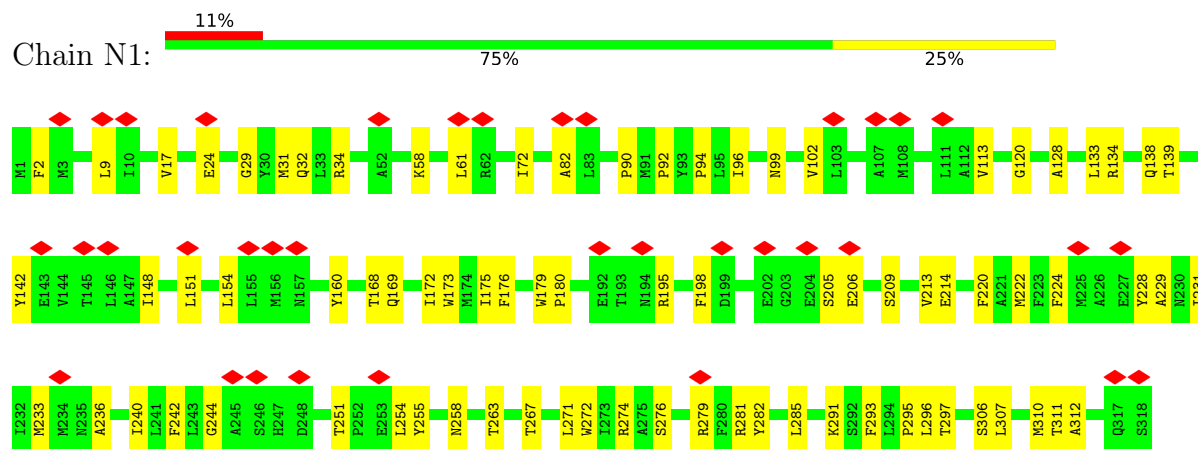
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



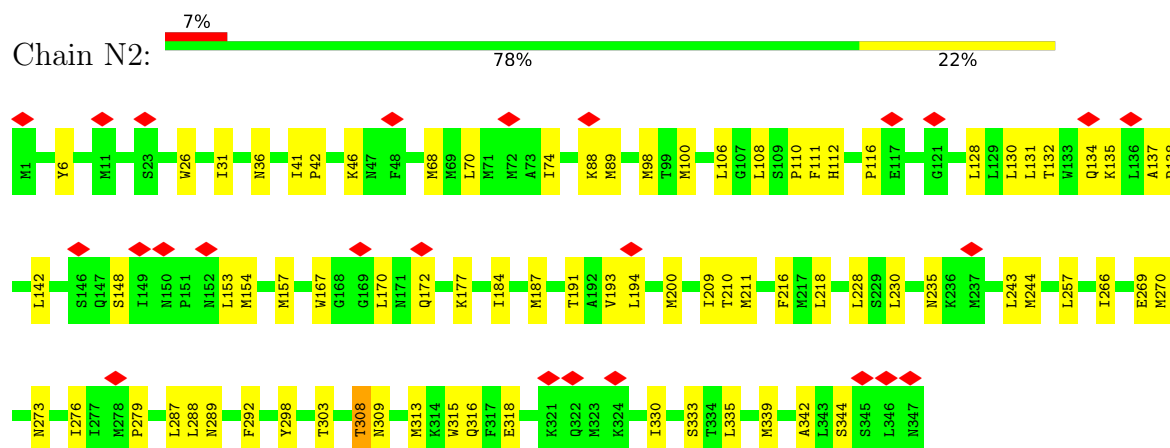
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2



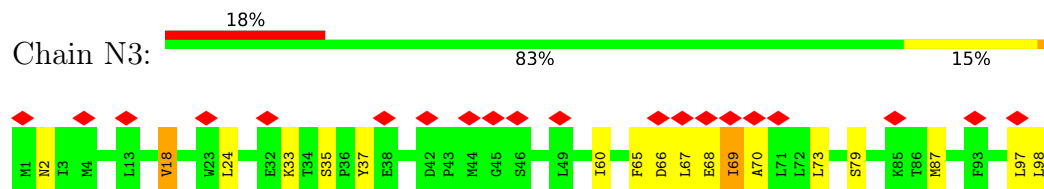
• Molecule 28: NADH-ubiquinone oxidoreductase chain 1



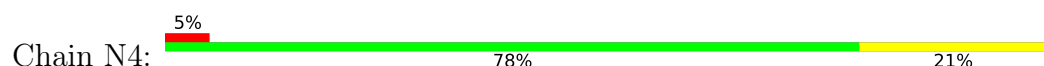
• Molecule 29: NADH-ubiquinone oxidoreductase chain 2

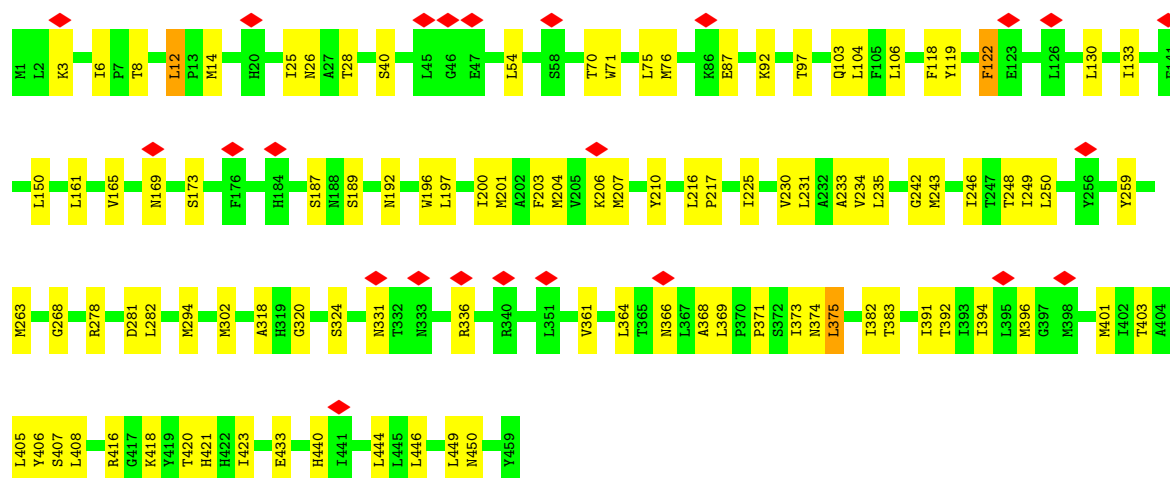


• Molecule 30: NADH-ubiquinone oxidoreductase chain 3

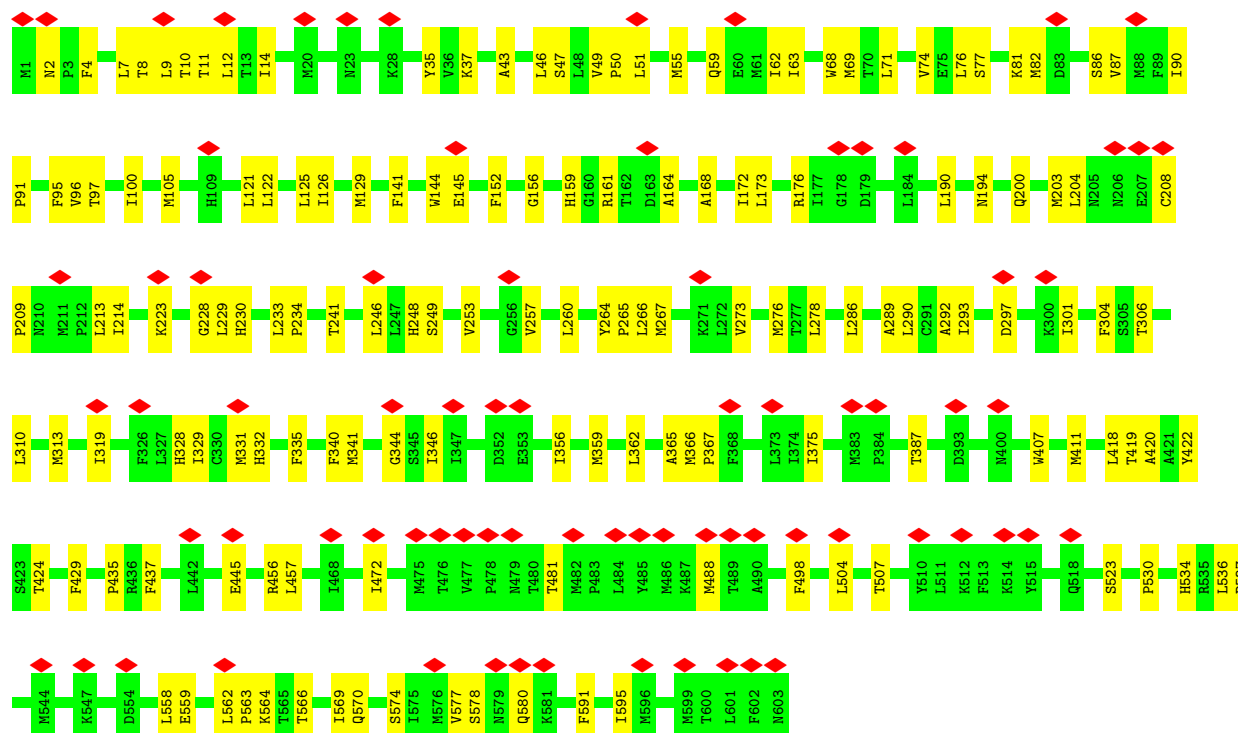
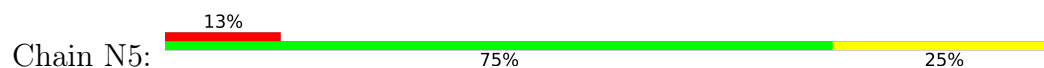


• Molecule 31: NADH-ubiquinone oxidoreductase chain 4

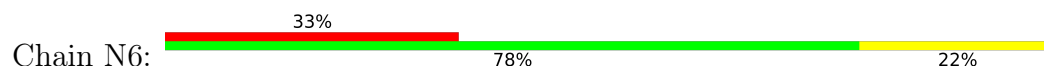




• Molecule 32: NADH-ubiquinone oxidoreductase chain 5

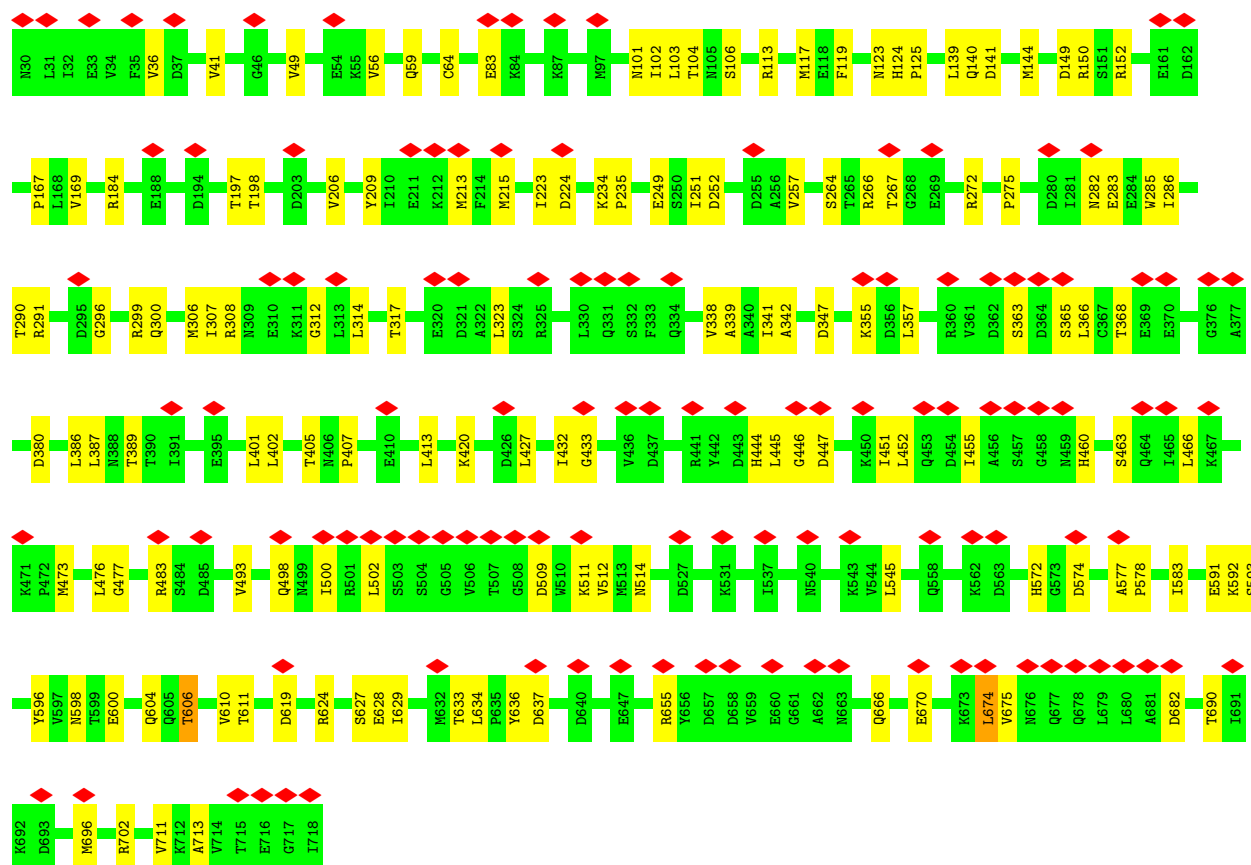
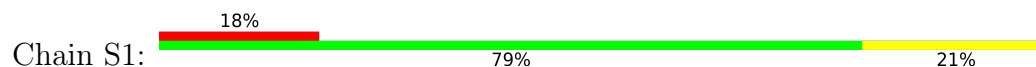


• Molecule 33: NADH-ubiquinone oxidoreductase chain 6

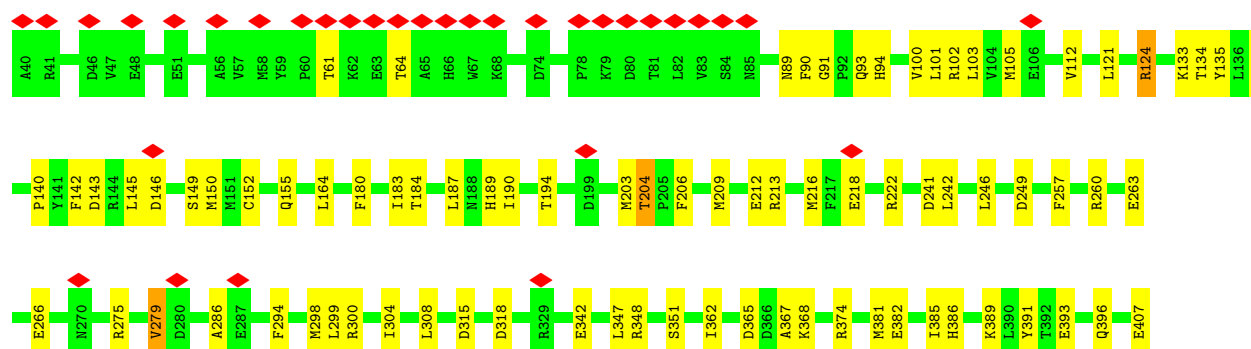
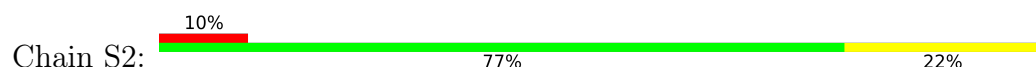


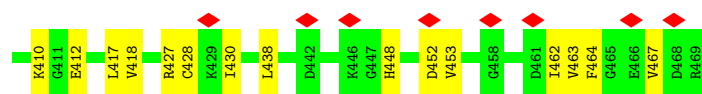


- Molecule 34: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

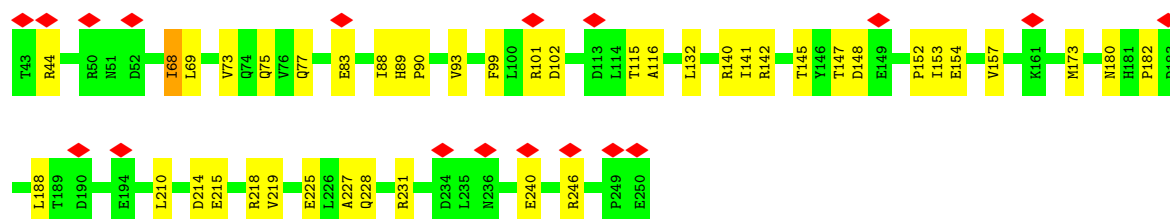
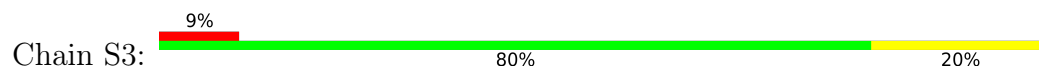


- Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

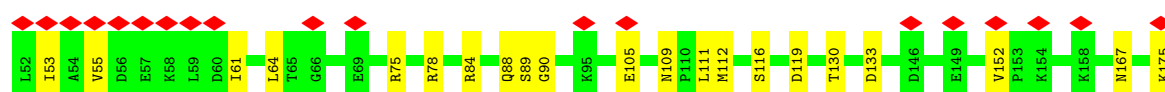
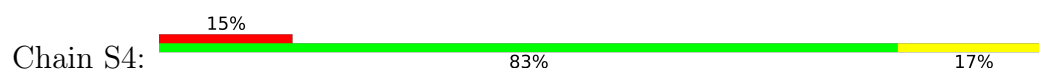




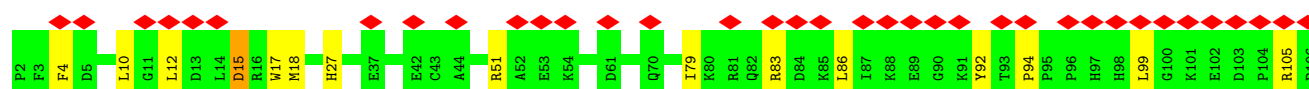
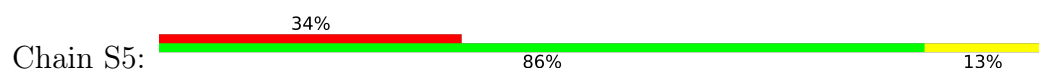
• Molecule 36: Complex I-30kD



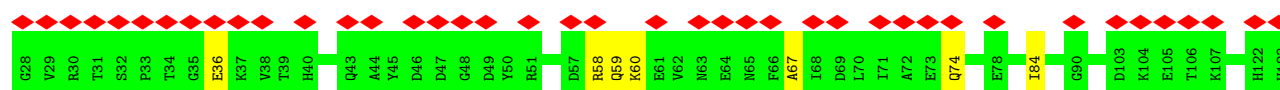
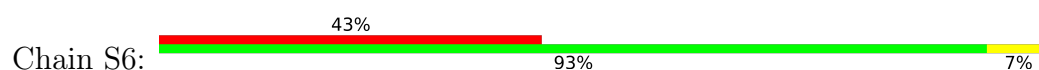
• Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



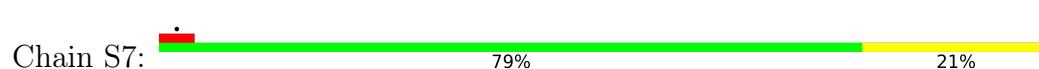
• Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



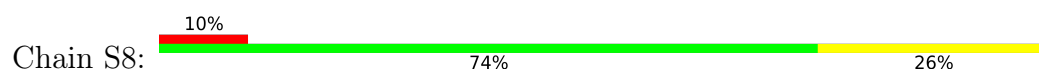
• Molecule 39: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

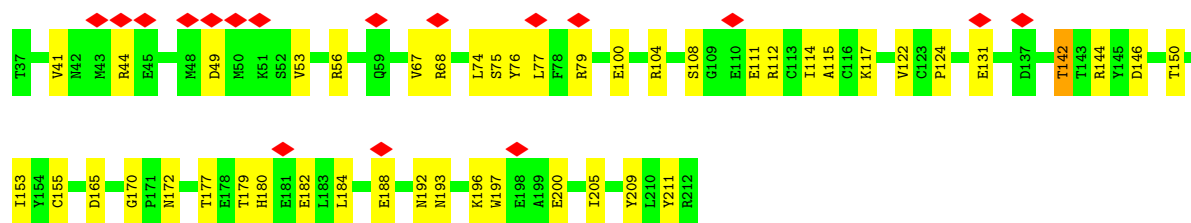


• Molecule 40: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

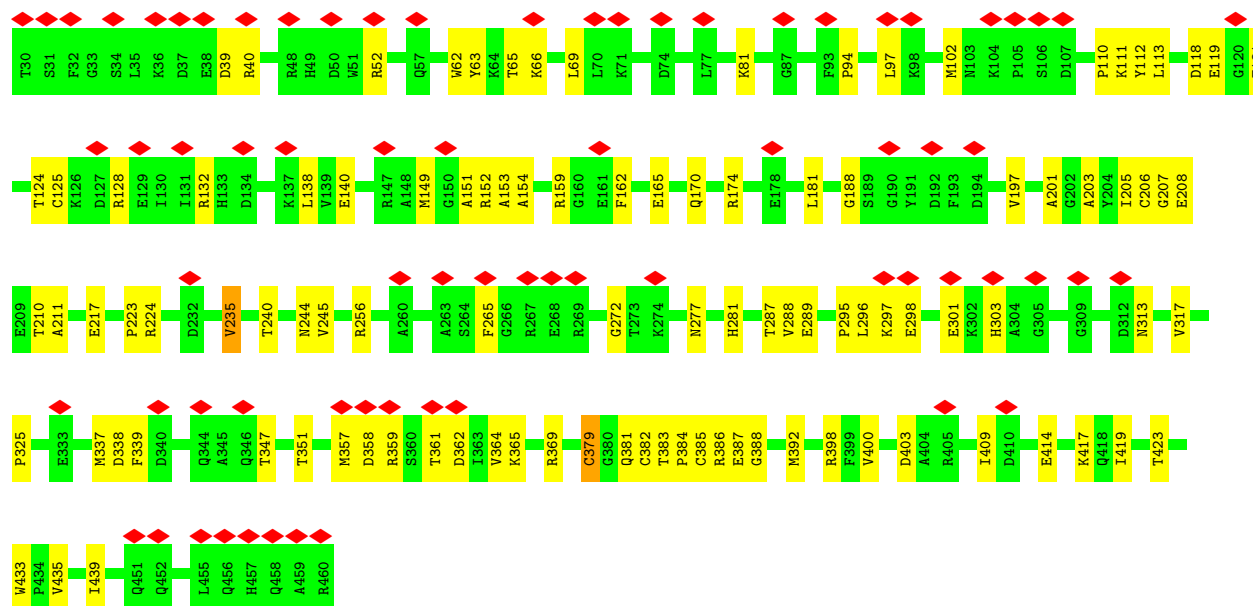
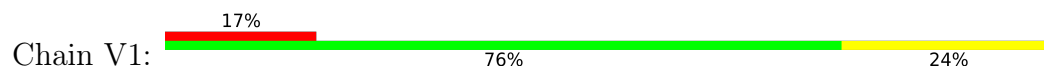


• Molecule 41: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

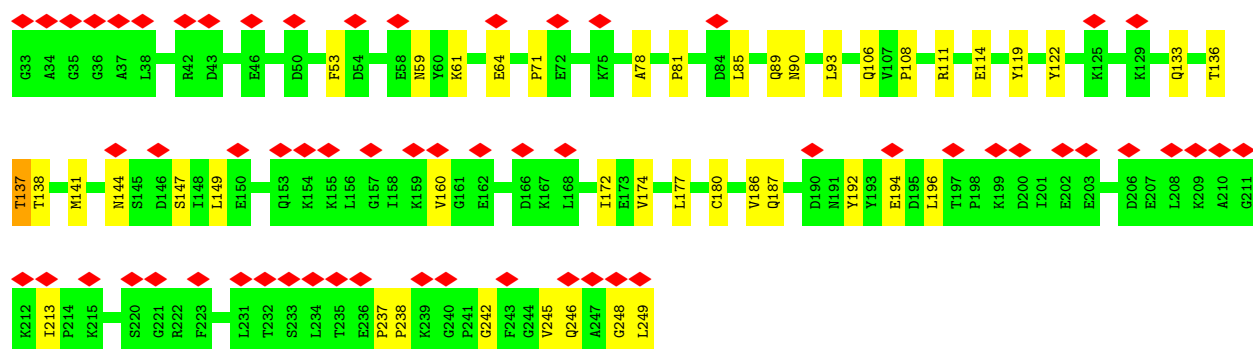
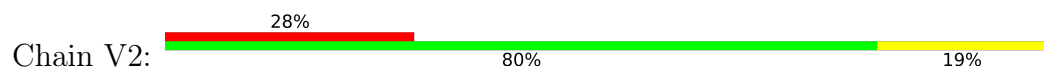




- Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

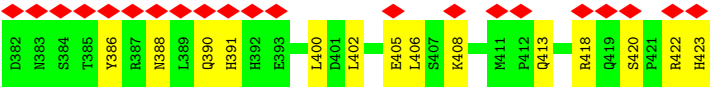


- Molecule 43: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 44: NADH:ubiquinone oxidoreductase subunit V3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20004	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	42.429	Depositor
Minimum map value	-13.805	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.014	Depositor
Recommended contour level	7	Depositor
Map size (Å)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, MF8, PC1, SF4, NDP, 2MR, FMN, FES, 3PE, ZN, PLX, CDL, ZMP, PEE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	4L	0.13	0/759	0.26	0/1029
2	A1	0.11	0/577	0.23	0/777
3	A2	0.09	0/697	0.24	0/938
4	A3	0.09	0/664	0.21	0/912
5	A5	0.10	0/929	0.21	0/1258
6	A6	0.11	0/991	0.26	0/1335
7	A7	0.10	0/798	0.25	0/1079
8	A8	0.10	0/1436	0.23	0/1938
9	A9	0.11	0/2820	0.23	0/3823
10	AB	0.07	0/633	0.19	0/851
10	AC	0.10	0/714	0.20	0/965
11	AK	0.10	0/2650	0.24	0/3588
12	AL	0.11	0/1042	0.21	0/1411
13	AM	0.08	0/1245	0.21	0/1694
14	AN	0.12	0/1204	0.24	0/1624
15	B1	0.10	0/491	0.23	0/663
16	B2	0.11	0/610	0.25	0/836
17	B3	0.10	0/660	0.21	0/892
18	B4	0.11	0/1092	0.22	0/1481
19	B5	0.11	0/1184	0.23	0/1603
20	B6	0.12	0/910	0.28	0/1237
21	B7	0.10	0/1092	0.22	0/1459
22	B8	0.10	0/1371	0.23	0/1875
23	B9	0.11	0/1590	0.23	0/2155
24	BK	0.11	0/1489	0.23	0/2008
25	BL	0.11	0/851	0.25	0/1155
26	CA	0.09	0/430	0.20	0/581
27	CB	0.11	0/1031	0.22	0/1394
28	N1	0.16	0/2581	0.33	2/3529 (0.1%)
29	N2	0.15	0/2773	0.29	0/3768
30	N3	0.13	0/938	0.25	0/1281
31	N4	0.14	0/3723	0.28	0/5078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	N5	0.14	0/4914	0.31	0/6683
33	N6	0.12	0/1364	0.27	0/1850
34	S1	0.12	0/5378	0.27	0/7287
35	S2	0.14	0/3538	0.26	0/4796
36	S3	0.12	0/1789	0.26	0/2436
37	S4	0.11	0/1030	0.27	0/1391
38	S5	0.09	0/889	0.21	0/1190
39	S6	0.10	0/755	0.25	0/1018
40	S7	0.13	0/1279	0.25	0/1730
41	S8	0.13	0/1443	0.25	0/1952
42	V1	0.13	0/3391	0.27	0/4583
43	V2	0.11	0/1711	0.26	0/2328
44	V3	0.09	0/365	0.25	0/493
All	All	0.12	0/67821	0.26	2/91954 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N1	276	SER	CA-C-N	-5.24	111.47	123.15
28	N1	276	SER	C-N-CA	-5.24	111.47	123.15

There are no chirality outliers.

There are no planarity outliers.

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	4L	748	0	799	27	0
2	A1	562	0	557	9	0
3	A2	686	0	699	13	0
4	A3	643	0	642	7	0
5	A5	910	0	950	11	0
6	A6	967	0	972	18	0
7	A7	780	0	808	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A8	1398	0	1372	25	0
9	A9	2743	0	2762	43	0
10	AB	624	0	625	11	0
10	AC	702	0	694	6	0
11	AK	2590	0	2553	31	0
12	AL	1021	0	1025	20	0
13	AM	1204	0	1162	11	0
14	AN	1173	0	1166	26	0
15	B1	479	0	486	11	0
16	B2	584	0	529	11	0
17	B3	641	0	620	9	0
18	B4	1062	0	1072	12	0
19	B5	1151	0	1164	14	0
20	B6	882	0	899	22	0
21	B7	1068	0	1043	15	0
22	B8	1315	0	1208	19	0
23	B9	1534	0	1470	17	0
24	BK	1456	0	1424	26	0
25	BL	828	0	788	14	0
26	CA	417	0	422	5	0
27	CB	1000	0	994	20	0
28	N1	2508	0	2607	58	0
29	N2	2710	0	2874	62	0
30	N3	914	0	951	21	0
31	N4	3631	0	3839	71	0
32	N5	4785	0	4933	106	0
33	N6	1329	0	1326	36	0
34	S1	5290	0	5321	90	0
35	S2	3459	0	3396	75	0
36	S3	1738	0	1693	28	0
37	S4	1007	0	1008	18	0
38	S5	867	0	871	13	0
39	S6	741	0	701	6	0
40	S7	1248	0	1254	28	0
41	S8	1412	0	1363	35	0
42	V1	3316	0	3272	69	0
43	V2	1671	0	1673	28	0
44	V3	355	0	329	10	0
45	4L	92	0	137	6	0
45	A1	94	0	141	6	0
45	AL	165	0	224	16	0
45	B5	100	0	156	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	CB	83	0	113	2	0
45	N1	78	0	103	6	0
45	N2	68	0	80	2	0
45	N4	100	0	156	8	0
45	N5	189	0	284	7	0
46	A3	104	0	165	2	0
46	AN	54	0	88	4	0
46	B5	54	0	88	1	0
46	B8	41	0	59	0	0
46	N3	108	0	176	4	0
47	A9	48	0	26	1	0
48	A9	39	0	52	6	0
48	AK	40	0	57	2	0
48	AL	76	0	103	7	0
48	AN	51	0	82	2	0
48	B6	46	0	69	3	0
48	N1	31	0	36	2	0
48	N2	83	0	117	5	0
48	N3	51	0	82	3	0
48	N4	49	0	75	3	0
48	N5	51	0	82	3	0
48	S8	51	0	82	1	0
49	AB	36	0	47	2	0
49	AC	36	0	47	5	0
50	AK	27	0	12	3	0
51	AL	47	0	75	7	0
51	B5	52	0	88	3	0
51	CB	52	0	88	3	0
51	N1	52	0	88	4	0
51	N3	52	0	88	3	0
51	N4	43	0	67	5	0
51	S7	52	0	88	3	0
52	B4	51	0	82	2	0
52	CB	51	0	82	5	0
52	N4	51	0	82	3	0
53	S1	16	0	0	1	0
53	S7	8	0	0	0	0
53	S8	16	0	0	3	0
53	V1	8	0	0	4	0
54	S1	4	0	0	0	0
54	V2	4	0	0	0	0
55	S1	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	S2	9	0	0	0	0
57	S6	1	0	0	0	0
58	V1	31	0	19	1	0
All	All	68795	0	70102	1055	0

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

All (1055) 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)
24:BK:140:GLN:O	24:BK:144:SER:HB2	1.58	1.03
21:B7:92:HIS:HD1	32:N5:481:THR:HG1	1.16	0.89
34:S1:338:VAL:O	34:S1:365:SER:HB2	1.75	0.87
5:A5:20:PRO:HB3	5:A5:77:ILE:HG21	1.59	0.85
1:4L:37:MET:HG2	1:4L:67:ALA:HB2	1.59	0.84
20:B6:132:VAL:O	20:B6:136:LEU:HB3	1.81	0.80
34:S1:251:ILE:HG12	34:S1:606:THR:HG22	1.66	0.76
24:BK:79:GLU:HG2	24:BK:80:LYS:HG2	1.70	0.73
20:B6:143:HIS:HD2	24:BK:45:VAL:HG21	1.55	0.72
34:S1:149:ASP:HB2	35:S2:367:ALA:HB3	1.69	0.72
29:N2:108:LEU:HD11	29:N2:191:THR:HG21	1.72	0.71
5:A5:90:LEU:HD11	36:S3:99:PHE:HA	1.71	0.71
42:V1:111:LYS:HB2	42:V1:151:ALA:HA	1.71	0.71
40:S7:188:LYS:HB2	40:S7:191:ARG:HB2	1.73	0.70
42:V1:94:PRO:HB2	42:V1:97:LEU:HB2	1.73	0.70
1:4L:61:ILE:HG12	33:N6:55:MET:HE1	1.73	0.70
45:N4:503:CDL:H262	45:N4:503:CDL:H742	1.73	0.70
34:S1:83:GLU:HB2	34:S1:101:ASN:HB3	1.74	0.70
20:B6:88:LEU:HD22	20:B6:92:GLU:HG2	1.72	0.70
29:N2:132:THR:HG21	45:N2:402:CDL:H391	1.73	0.70
3:A2:24:CYS:N	3:A2:58:CYS:SG	2.64	0.69
49:AC:201:ZMP:H14	23:B9:102:ALA:HB1	1.74	0.69
41:S8:177:THR:HG21	41:S8:182:GLU:HB2	1.72	0.69
28:N1:295:PRO:HB3	48:N3:201:PEE:H29	1.73	0.69
7:A7:11:LEU:HD12	7:A7:14:TRP:HE1	1.57	0.69
35:S2:209:MET:HE1	35:S2:260:ARG:HB3	1.75	0.69
32:N5:97:THR:HG21	32:N5:125:LEU:HD22	1.75	0.68
15:B1:57:TRP:NE1	19:B5:134:GLU:OE1	2.26	0.68
35:S2:124:2MR:O	40:S7:146:SER:OG	2.10	0.68
11:AK:354:ILE:HD11	27:CB:54:PRO:HG2	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AN:144:THR:HB	28:N1:96:ILE:HG23	1.74	0.68
29:N2:88:LYS:HG3	29:N2:148:SER:HB3	1.75	0.68
42:V1:52:ARG:HH21	44:V3:390:GLN:HG2	1.59	0.68
42:V1:112:TYR:HB2	42:V1:240:THR:HG22	1.74	0.68
1:4L:68:ALA:HB3	30:N3:67:LEU:HD11	1.75	0.67
34:S1:124:HIS:HD2	35:S2:381:MET:HE2	1.57	0.67
42:V1:110:PRO:HB3	42:V1:152:ARG:HD3	1.76	0.67
17:B3:27:THR:HG22	17:B3:29:LEU:H	1.60	0.67
42:V1:409:ILE:HG23	42:V1:439:ILE:HD12	1.77	0.67
3:A2:64:LYS:HD3	3:A2:76:ASN:HD22	1.59	0.67
9:A9:188:GLU:HG3	9:A9:200:ILE:HD13	1.77	0.66
9:A9:198:ALA:O	9:A9:260:GLY:HA2	1.95	0.66
30:N3:37:TYR:OH	35:S2:93:GLN:NE2	2.28	0.66
13:AM:88:ARG:HD3	41:S8:200:GLU:HG3	1.78	0.66
33:N6:34:ILE:HD12	33:N6:61:LEU:HD23	1.77	0.66
34:S1:49:VAL:HG13	34:S1:102:ILE:HD13	1.77	0.66
35:S2:222:ARG:NH1	35:S2:249:ASP:OD2	2.25	0.65
42:V1:205:ILE:HG12	42:V1:379:CYS:HB3	1.77	0.65
45:A1:101:CDL:H531	45:A1:101:CDL:H112	1.77	0.65
14:AN:119:PRO:HB3	14:AN:123:GLU:HB2	1.79	0.65
11:AK:141:ARG:NH2	50:AK:401:ADP:N7	2.45	0.64
8:A8:107:HIS:HB3	8:A8:197:PRO:HD2	1.78	0.64
42:V1:40:ARG:NH1	42:V1:289:GLU:O	2.30	0.64
42:V1:211:ALA:HB2	42:V1:223:PRO:HG3	1.78	0.64
34:S1:150:ARG:NH2	35:S2:365:ASP:OD1	2.30	0.64
19:B5:163:ARG:NH1	27:CB:102:ASP:OD2	2.29	0.64
34:S1:123:ASN:ND2	42:V1:387:GLU:OE1	2.30	0.64
19:B5:95:GLU:OE1	19:B5:114:LYS:NZ	2.31	0.64
51:CB:201:PLX:H332	29:N2:342:ALA:HB3	1.78	0.64
30:N3:70:ALA:HB2	33:N6:59:ILE:HD11	1.80	0.64
42:V1:118:ASP:HB3	42:V1:207:GLY:HA2	1.80	0.64
8:A8:121:MET:HE2	14:AN:73:PRO:HA	1.79	0.64
40:S7:55:ASN:ND2	40:S7:187:GLU:O	2.31	0.64
27:CB:36:MET:HE2	29:N2:339:MET:HE2	1.80	0.64
35:S2:308:LEU:HB2	35:S2:407:GLU:HB2	1.79	0.64
44:V3:405:GLU:O	44:V3:408:LYS:NZ	2.31	0.64
32:N5:362:LEU:HA	32:N5:365:ALA:HB3	1.80	0.63
35:S2:374:ARG:NH2	41:S8:165:ASP:OD1	2.31	0.63
42:V1:235:VAL:HG12	42:V1:240:THR:HG21	1.81	0.63
32:N5:90:ILE:HG23	32:N5:129:MET:HE1	1.79	0.63
34:S1:140:GLN:NE2	53:S1:801:SF4:S3	2.71	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A9:357:ARG:NH1	9:A9:364:SER:OG	2.32	0.63
31:N4:165:VAL:O	31:N4:169:ASN:ND2	2.31	0.63
32:N5:100:ILE:HG21	32:N5:246:LEU:HB2	1.80	0.63
3:A2:62:GLN:HE21	3:A2:80:ASN:HD22	1.46	0.63
43:V2:246:GLN:HG2	43:V2:248:GLY:H	1.62	0.63
42:V1:66:LYS:NZ	42:V1:188:GLY:O	2.31	0.63
7:A7:40:LYS:HB2	14:AN:7:LYS:H	1.64	0.62
14:AN:19:ILE:HD11	35:S2:351:SER:HB2	1.81	0.62
45:B5:202:CDL:H791	45:B5:202:CDL:H182	1.81	0.62
34:S1:433:GLY:HA2	34:S1:447:ASP:HA	1.80	0.62
34:S1:433:GLY:O	34:S1:444:HIS:NE2	2.22	0.62
20:B6:85:ASP:O	23:B9:163:LYS:NZ	2.32	0.62
12:AL:140:LYS:H	29:N2:273:ASN:HD22	1.46	0.62
34:S1:405:THR:HB	34:S1:477:GLY:HA3	1.82	0.62
45:N1:401:CDL:H822	33:N6:35:VAL:HG11	1.81	0.62
9:A9:173:ASP:HB3	9:A9:176:SER:HB2	1.82	0.62
9:A9:313:TRP:HB3	48:A9:402:PEE:H13	1.81	0.62
35:S2:190:ILE:HG23	35:S2:209:MET:HB3	1.82	0.62
36:S3:228:GLN:OE1	36:S3:231:ARG:NH1	2.33	0.61
7:A7:62:GLU:OE2	36:S3:44:ARG:NH2	2.33	0.61
9:A9:67:ARG:NH2	36:S3:214:ASP:OD2	2.32	0.61
37:S4:75:ARG:NH1	37:S4:119:ASP:OD1	2.28	0.61
14:AN:56:GLU:OE1	14:AN:59:ARG:NH2	2.32	0.61
9:A9:61:ALA:HB3	9:A9:82:VAL:HG13	1.83	0.61
14:AN:98:MET:HE2	38:S5:79:ILE:HA	1.82	0.61
27:CB:62:ARG:HG3	52:CB:202:3PE:H222	1.82	0.61
5:A5:11:LEU:HD12	5:A5:14:LEU:HD22	1.81	0.61
6:A6:135:GLU:OE1	36:S3:218:ARG:NH2	2.31	0.61
27:CB:2:THR:HB	27:CB:5:SER:HB3	1.81	0.61
29:N2:289:ASN:HA	29:N2:292:PHE:CE2	2.36	0.61
31:N4:361:VAL:HG13	45:N5:701:CDL:H332	1.81	0.61
9:A9:279:TYR:HB2	9:A9:372:ALA:HB2	1.82	0.61
34:S1:611:THR:HG21	37:S4:105:GLU:HA	1.83	0.61
37:S4:84:ARG:NH1	37:S4:88:GLN:O	2.34	0.60
34:S1:224:ASP:OD2	34:S1:291:ARG:NH2	2.32	0.60
34:S1:628:GLU:HA	34:S1:633:THR:HG22	1.81	0.60
34:S1:674:LEU:HD12	34:S1:675:VAL:HG23	1.82	0.60
31:N4:368:ALA:HB1	31:N4:375:LEU:HD12	1.83	0.60
31:N4:403:THR:HA	31:N4:406:TYR:CE2	2.37	0.60
40:S7:62:LEU:HB2	40:S7:91:VAL:HG22	1.81	0.60
45:N5:701:CDL:H592	45:N5:701:CDL:H212	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:59:GLN:HE22	37:S4:90:GLY:HA2	1.66	0.60
34:S1:282:ASN:ND2	34:S1:285:TRP:O	2.34	0.60
40:S7:53:LEU:HD22	51:S7:302:PLX:H341	1.83	0.60
29:N2:42:PRO:HG2	33:N6:167:VAL:HG22	1.84	0.60
1:4L:26:LEU:HD23	1:4L:78:LEU:HD23	1.84	0.59
35:S2:155:GLN:NE2	35:S2:315:ASP:OD2	2.35	0.59
10:AB:116:VAL:HG12	10:AB:120:MET:HE2	1.83	0.59
11:AK:82:LYS:HZ2	11:AK:268:ALA:HB3	1.65	0.59
1:4L:65:VAL:HA	30:N3:67:LEU:HD22	1.83	0.59
29:N2:142:LEU:HB3	29:N2:194:LEU:HD21	1.84	0.59
12:AL:140:LYS:O	29:N2:273:ASN:ND2	2.35	0.59
16:B2:68:GLN:NE2	32:N5:445:GLU:OE2	2.35	0.59
34:S1:141:ASP:OD2	37:S4:88:GLN:NE2	2.33	0.59
41:S8:100:GLU:OE2	41:S8:193:ASN:ND2	2.36	0.59
29:N2:26:TRP:HB3	29:N2:74:ILE:HD13	1.85	0.59
32:N5:8:THR:HG21	32:N5:82:MET:HG2	1.85	0.59
1:4L:78:LEU:HD21	1:4L:88:ASP:HB2	1.83	0.59
45:4L:201:CDL:H381	45:4L:201:CDL:H421	1.83	0.59
12:AL:140:LYS:H	29:N2:273:ASN:ND2	2.01	0.59
34:S1:323:LEU:HB3	34:S1:629:ILE:HD12	1.85	0.59
15:B1:50:ARG:NH2	19:B5:106:VAL:O	2.35	0.58
34:S1:266:ARG:HD2	34:S1:267:THR:HG23	1.85	0.58
35:S2:135:TYR:HE1	35:S2:417:LEU:HD21	1.67	0.58
43:V2:108:PRO:HB2	43:V2:111:ARG:HG2	1.85	0.58
34:S1:198:THR:HG21	34:S1:209:TYR:HB2	1.84	0.58
35:S2:391:TYR:HD1	41:S8:122:VAL:HG21	1.68	0.58
36:S3:157:VAL:HG21	36:S3:182:PRO:HD3	1.84	0.58
42:V1:281:HIS:ND1	42:V1:358:ASP:OD1	2.36	0.58
7:A7:45:PRO:O	7:A7:48:LYS:NZ	2.35	0.58
19:B5:95:GLU:OE2	45:B5:202:CDL:O1	2.19	0.58
25:BL:89:VAL:HG21	31:N4:25:ILE:HG23	1.83	0.58
31:N4:8:THR:HG21	31:N4:104:LEU:HB2	1.84	0.58
34:S1:299:ARG:HG2	34:S1:300:GLN:HG2	1.85	0.58
5:A5:55:LYS:HG2	5:A5:72:LEU:HD22	1.85	0.58
42:V1:288:VAL:HG21	42:V1:303:HIS:HD2	1.67	0.58
32:N5:419:THR:HA	32:N5:422:TYR:CE2	2.39	0.58
43:V2:85:LEU:HD13	44:V3:400:LEU:HD22	1.84	0.58
43:V2:133:GLN:OE1	43:V2:187:GLN:NE2	2.36	0.58
45:N1:401:CDL:H832	33:N6:12:ILE:HG23	1.85	0.58
48:N4:501:PEE:H65	48:N4:501:PEE:H32	1.86	0.58
34:S1:483:ARG:HH22	34:S1:682:ASP:HB2	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B7:29:TYR:O	21:B7:104:ARG:NH2	2.37	0.58
35:S2:90:PHE:HB2	35:S2:105:MET:HE2	1.86	0.58
11:AK:66:GLY:O	11:AK:163:ARG:NH2	2.33	0.58
42:V1:138:LEU:HD13	42:V1:245:VAL:HG13	1.86	0.58
1:4L:98:CYS:HB3	32:N5:580:GLN:HB2	1.86	0.58
21:B7:36:GLU:HA	22:B8:184:TYR:HA	1.84	0.58
34:S1:592:LYS:NZ	34:S1:619:ASP:OD2	2.36	0.58
35:S2:393:GLU:OE2	35:S2:396:GLN:NE2	2.36	0.58
3:A2:18:GLU:HG2	3:A2:68:ARG:HB3	1.85	0.57
3:A2:59:SER:HB2	34:S1:655:ARG:HE	1.68	0.57
14:AN:51:MET:HE2	28:N1:311:THR:HB	1.85	0.57
46:AN:202:PC1:H372	46:AN:202:PC1:H262	1.85	0.57
9:A9:129:LEU:HD23	9:A9:167:ILE:HG13	1.85	0.57
28:N1:173:TRP:HB2	28:N1:176:PHE:HD1	1.68	0.57
31:N4:12:LEU:HD21	31:N4:97:THR:HG23	1.86	0.57
13:AM:106:ARG:HB2	13:AM:109:ILE:HG13	1.86	0.57
32:N5:208:CYS:HB2	32:N5:266:LEU:HD22	1.85	0.57
32:N5:346:ILE:HG21	32:N5:359:MET:HE3	1.87	0.57
34:S1:466:LEU:HD13	34:S1:500:ILE:HD11	1.87	0.57
20:B6:153:LYS:HE2	48:B6:201:PEE:H10	1.85	0.57
45:A1:101:CDL:H851	13:AM:7:LEU:HD11	1.86	0.57
28:N1:134:ARG:NH1	28:N1:206:GLU:OE1	2.35	0.57
11:AK:237:GLN:NE2	11:AK:241:ASN:OD1	2.38	0.57
49:AC:201:ZMP:H5A	23:B9:109:ALA:HB1	1.86	0.56
14:AN:8:GLN:NE2	35:S2:241:ASP:OD2	2.32	0.56
35:S2:382:GLU:O	35:S2:386:HIS:ND1	2.36	0.56
31:N4:122:PHE:CE1	31:N4:206:LYS:HG3	2.40	0.56
35:S2:464:PHE:HA	35:S2:467:VAL:HB	1.85	0.56
8:A8:124:ARG:NE	14:AN:80:ASP:OD2	2.39	0.56
31:N4:375:LEU:HD11	32:N5:141:PHE:HE2	1.70	0.56
45:N5:701:CDL:HB62	45:N5:701:CDL:HA22	1.87	0.56
1:4L:73:LEU:HD21	29:N2:41:ILE:HG13	1.87	0.56
36:S3:68:ILE:HG22	36:S3:69:LEU:HG	1.86	0.56
35:S2:412:GLU:OE2	36:S3:140:ARG:NH2	2.37	0.56
43:V2:59:ASN:ND2	43:V2:89:GLN:OE1	2.39	0.56
1:4L:56:ALA:HA	38:S5:18:MET:HE3	1.88	0.56
8:A8:174:PHE:HB3	8:A8:178:ARG:HH12	1.70	0.56
28:N1:173:TRP:HB3	28:N1:175:ILE:HG22	1.88	0.56
7:A7:27:ARG:NH1	35:S2:218:GLU:OE1	2.28	0.56
9:A9:50:SER:OG	36:S3:225:GLU:OE2	2.21	0.56
9:A9:117:ARG:NH1	9:A9:121:GLU:OE2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:B5:201:PLX:H91	31:N4:40:SER:HB3	1.87	0.56
28:N1:72:ILE:HD13	48:N1:403:PEE:H14	1.88	0.56
28:N1:291:LYS:NZ	30:N3:112:GLU:OE2	2.39	0.56
35:S2:286:ALA:HB1	35:S2:304:ILE:HD11	1.88	0.56
42:V1:338:ASP:OD1	42:V1:339:PHE:N	2.38	0.56
15:B1:26:TYR:OH	15:B1:30:ARG:NH1	2.38	0.56
21:B7:29:TYR:OH	21:B7:111:ARG:NH2	2.38	0.56
24:BK:114:GLN:HG3	32:N5:203:MET:HG2	1.88	0.56
42:V1:392:MET:HE3	42:V1:435:VAL:HG21	1.88	0.56
10:AB:93:ILE:HD12	10:AB:108:LEU:HD13	1.88	0.56
34:S1:64:CYS:O	34:S1:184:ARG:NH2	2.31	0.56
29:N2:167:TRP:O	32:N5:574:SER:OG	2.20	0.56
31:N4:248:THR:HG23	31:N4:249:ILE:HG23	1.87	0.56
42:V1:112:TYR:O	42:V1:240:THR:HA	2.06	0.56
15:B1:50:ARG:HH21	19:B5:106:VAL:HB	1.72	0.55
27:CB:15:PHE:O	27:CB:80:ARG:NH1	2.37	0.55
29:N2:298:TYR:O	29:N2:303:THR:OG1	2.24	0.55
40:S7:59:ARG:HG3	40:S7:181:GLN:HB3	1.86	0.55
12:AL:128:GLY:HA3	45:AL:202:CDL:H711	1.88	0.55
51:AL:204:PLX:H141	52:N4:504:3PE:H2A2	1.87	0.55
16:B2:101:PRO:HD2	21:B7:99:MET:HE1	1.87	0.55
52:N4:504:3PE:H2B2	52:N4:504:3PE:H3D2	1.88	0.55
35:S2:257:PHE:HD2	35:S2:347:LEU:HD11	1.72	0.55
32:N5:125:LEU:O	32:N5:129:MET:HG2	2.07	0.55
33:N6:129:ASP:OD1	33:N6:130:THR:N	2.39	0.55
9:A9:85:ARG:HH12	40:S7:196:ARG:HA	1.72	0.55
31:N4:87:GLU:O	31:N4:92:LYS:NZ	2.30	0.55
41:S8:188:GLU:O	41:S8:192:ASN:ND2	2.28	0.55
33:N6:111:GLU:HG3	33:N6:121:GLY:H	1.71	0.55
35:S2:133:LYS:NZ	41:S8:124:PRO:O	2.39	0.55
39:S6:36:GLU:OE2	39:S6:60:LYS:NZ	2.36	0.55
40:S7:139:GLY:O	40:S7:152:GLY:N	2.39	0.55
42:V1:296:LEU:HD13	42:V1:337:MET:HE3	1.87	0.55
3:A2:18:GLU:OE2	3:A2:20:ARG:NH1	2.38	0.55
31:N4:122:PHE:HE1	31:N4:206:LYS:HG3	1.72	0.55
31:N4:366:ASN:ND2	31:N4:407:SER:OG	2.39	0.55
32:N5:362:LEU:HD22	32:N5:366:MET:HE2	1.88	0.55
2:A1:1:MET:HE2	45:A1:101:CDL:HA22	1.89	0.55
6:A6:48:SER:HB3	6:A6:53:GLU:HB2	1.88	0.55
12:AL:120:LEU:HD21	48:N4:501:PEE:H68	1.89	0.55
24:BK:171:LYS:NZ	24:BK:172:GLU:OE2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BL:95:PHE:O	25:BL:99:LEU:HB2	2.07	0.55
2:A1:64:LYS:HB3	2:A1:68:ASN:HB2	1.89	0.55
16:B2:68:GLN:NE2	32:N5:367:PRO:HD2	2.21	0.55
18:B4:71:ALA:HB2	22:B8:38:PRO:HG2	1.88	0.55
48:B6:201:PEE:H27	51:N4:502:PLX:H111	1.88	0.55
31:N4:392:THR:O	31:N4:396:MET:HG2	2.07	0.55
25:BL:77:ASP:OD1	25:BL:78:LYS:N	2.40	0.55
27:CB:50:ILE:HD11	29:N2:243:LEU:HD12	1.89	0.55
42:V1:295:PRO:HG2	42:V1:298:GLU:HB3	1.89	0.55
8:A8:201:GLU:HA	8:A8:204:LYS:HD3	1.88	0.54
36:S3:132:LEU:HB2	36:S3:141:ILE:HG22	1.89	0.54
45:4L:201:CDL:H452	12:AL:57:GLY:HA2	1.90	0.54
45:4L:201:CDL:H521	33:N6:88:THR:HG23	1.89	0.54
24:BK:33:LEU:HD13	32:N5:49:VAL:HG13	1.89	0.54
34:S1:117:MET:HE1	34:S1:139:LEU:HD12	1.88	0.54
35:S2:145:LEU:HD13	35:S2:430:ILE:HG21	1.90	0.54
41:S8:53:VAL:HG22	41:S8:56:ARG:HH21	1.72	0.54
19:B5:123:ARG:NH2	46:B5:203:PC1:O14	2.41	0.54
20:B6:143:HIS:CD2	24:BK:45:VAL:HG21	2.41	0.54
31:N4:231:LEU:HD23	31:N4:235:LEU:HD12	1.88	0.54
32:N5:121:LEU:HD22	32:N5:246:LEU:HD23	1.90	0.54
42:V1:381:GLN:N	53:V1:501:SF4:S4	2.81	0.54
3:A2:46:LYS:HE2	34:S1:674:LEU:HD22	1.90	0.54
12:AL:125:VAL:HG12	45:AL:202:CDL:H731	1.90	0.54
18:B4:75:ASN:OD1	18:B4:79:ASN:ND2	2.40	0.54
28:N1:31:MET:HG2	41:S8:77:LEU:HB2	1.90	0.54
28:N1:102:VAL:HG11	28:N1:154:LEU:HD11	1.90	0.54
5:A5:90:LEU:HD12	36:S3:102:ASP:HB2	1.89	0.54
9:A9:87:GLU:HG3	9:A9:89:TYR:H	1.73	0.54
1:4L:31:LEU:HD21	33:N6:67:VAL:HG11	1.88	0.54
31:N4:383:THR:HG21	32:N5:190:LEU:HD22	1.89	0.54
32:N5:292:ALA:HB2	32:N5:304:PHE:HB3	1.90	0.54
35:S2:448:HIS:HB3	35:S2:452:ASP:HB2	1.89	0.54
42:V1:369:ARG:NE	43:V2:136:THR:O	2.40	0.54
6:A6:66:TYR:O	6:A6:86:ARG:NH1	2.39	0.54
45:AL:201:CDL:H391	48:AL:205:PEE:H32	1.89	0.54
32:N5:278:LEU:HD13	32:N5:319:ILE:HD11	1.90	0.54
9:A9:303:ARG:HB2	9:A9:316:ARG:HD3	1.90	0.54
35:S2:140:PRO:HB2	40:S7:142:TYR:CE2	2.43	0.54
11:AK:342:SER:O	11:AK:346:ASN:ND2	2.41	0.54
16:B2:64:LEU:HD23	16:B2:69:LEU:HD21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N2:132:THR:HG23	29:N2:209:ILE:HD12	1.88	0.54
35:S2:194:THR:HG21	35:S2:209:MET:HB2	1.90	0.54
42:V1:113:LEU:O	42:V1:154:ALA:HA	2.07	0.54
42:V1:203:ALA:HB3	42:V1:206:CYS:HB2	1.89	0.54
22:B8:140:MET:HE1	32:N5:411:MET:HE3	1.90	0.53
34:S1:387:LEU:HD12	34:S1:514:ASN:HB3	1.90	0.53
34:S1:593:SER:HA	34:S1:606:THR:O	2.07	0.53
29:N2:235:ASN:O	29:N2:315:TRP:NE1	2.39	0.53
1:4L:75:LEU:HB3	33:N6:70:TYR:HE2	1.74	0.53
28:N1:293:PHE:O	28:N1:297:THR:OG1	2.23	0.53
29:N2:270:MET:HE3	29:N2:279:PRO:HG3	1.90	0.53
8:A8:95:VAL:HG12	8:A8:97:VAL:HG22	1.89	0.53
8:A8:160:THR:HA	8:A8:163:TRP:CD1	2.42	0.53
18:B4:44:LYS:NZ	22:B8:93:ASP:OD1	2.42	0.53
29:N2:335:LEU:HD21	45:N4:503:CDL:H402	1.91	0.53
32:N5:214:ILE:HG12	32:N5:276:MET:HE1	1.91	0.53
35:S2:241:ASP:OD1	35:S2:242:LEU:N	2.41	0.53
5:A5:89:SER:OG	5:A5:93:LYS:NZ	2.41	0.53
8:A8:202:LEU:HD13	14:AN:70:ALA:HB2	1.89	0.53
19:B5:90:ASN:ND2	45:B5:202:CDL:OA7	2.33	0.53
28:N1:148:ILE:HD11	30:N3:69:ILE:HG22	1.91	0.53
31:N4:187:SER:O	31:N4:192:ASN:ND2	2.35	0.53
34:S1:197:THR:HG22	34:S1:206:VAL:HG22	1.90	0.53
34:S1:446:GLY:HA3	34:S1:451:ILE:HD12	1.90	0.53
34:S1:666:GLN:NE2	34:S1:670:GLU:OE2	2.41	0.53
12:AL:141:VAL:HG22	19:B5:158:ARG:HB2	1.89	0.53
20:B6:146:LEU:HA	20:B6:150:VAL:HB	1.90	0.53
34:S1:167:PRO:HD2	34:S1:215:MET:HE1	1.90	0.53
45:AL:201:CDL:H531	32:N5:577:VAL:HG22	1.91	0.53
45:AL:202:CDL:H181	48:N2:401:PEE:H10	1.91	0.53
43:V2:93:LEU:HD12	43:V2:122:TYR:HB3	1.91	0.53
24:BK:162:ARG:NH1	25:BL:140:ASN:OD1	2.42	0.53
38:S5:15:ASP:OD1	38:S5:15:ASP:N	2.40	0.53
32:N5:530:PRO:O	32:N5:534:HIS:HB2	2.08	0.53
34:S1:338:VAL:HB	34:S1:363:SER:HB2	1.90	0.53
2:A1:55:SER:O	2:A1:64:LYS:NZ	2.41	0.52
3:A2:20:ARG:NH2	3:A2:74:GLU:OE1	2.42	0.52
31:N4:119:TYR:CZ	31:N4:161:LEU:HB2	2.44	0.52
28:N1:32:GLN:HE22	35:S2:203:MET:HE2	1.75	0.52
28:N1:113:VAL:HG13	28:N1:139:THR:HG21	1.91	0.52
30:N3:68:GLU:HG3	30:N3:98:LEU:HD13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:90:PHE:HB3	35:S2:103:LEU:HB3	1.91	0.52
42:V1:140:GLU:OE2	42:V1:256:ARG:NH1	2.41	0.52
11:AK:342:SER:HB2	11:AK:345:TYR:HD1	1.74	0.52
18:B4:82:PRO:HB2	52:B4:201:3PE:H32	1.91	0.52
22:B8:62:TYR:OH	22:B8:74:ASP:O	2.20	0.52
26:CA:72:ARG:NH2	27:CB:18:ASN:OD1	2.38	0.52
32:N5:562:LEU:HB2	32:N5:563:PRO:HD3	1.91	0.52
35:S2:187:LEU:HD21	35:S2:216:MET:HB2	1.90	0.52
8:A8:228:ASN:OD1	38:S5:51:ARG:NH1	2.42	0.52
28:N1:24:GLU:HA	28:N1:271:LEU:HD13	1.90	0.52
28:N1:205:SER:OG	28:N1:279:ARG:NH2	2.37	0.52
29:N2:172:GLN:OE1	32:N5:578:SER:OG	2.28	0.52
45:B5:202:CDL:H781	51:N4:502:PLX:H92	1.92	0.52
31:N4:70:THR:HA	31:N4:103:GLN:HE21	1.75	0.52
35:S2:242:LEU:HD22	35:S2:246:LEU:HD23	1.92	0.52
36:S3:101:ARG:NE	36:S3:102:ASP:OD1	2.37	0.52
6:A6:107:LEU:HD23	37:S4:64:LEU:HD13	1.91	0.52
36:S3:240:GLU:OE1	36:S3:246:ARG:NH2	2.42	0.52
9:A9:49:SER:HB2	36:S3:225:GLU:HG2	1.90	0.52
12:AL:118:MET:HE2	45:AL:201:CDL:H382	1.91	0.52
12:AL:124:LEU:HD23	45:AL:202:CDL:H762	1.92	0.52
14:AN:43:LEU:HG	28:N1:179:TRP:HE1	1.74	0.52
28:N1:139:THR:HA	28:N1:142:TYR:CE2	2.44	0.52
28:N1:310:MET:HG3	28:N1:311:THR:HG23	1.92	0.52
30:N3:79:SER:HA	30:N3:87:MET:HE2	1.91	0.52
35:S2:140:PRO:HB2	40:S7:142:TYR:HE2	1.75	0.52
10:AC:128:PHE:HZ	10:AC:148:ILE:HG12	1.75	0.52
45:AL:201:CDL:H791	45:AL:202:CDL:H171	1.91	0.52
16:B2:102:ASP:OD2	16:B2:104:SER:OG	2.25	0.52
31:N4:216:LEU:HB3	31:N4:217:PRO:HD3	1.92	0.52
46:A3:202:PC1:H272	46:A3:202:PC1:H232	1.92	0.52
34:S1:152:ARG:NH1	42:V1:414:GLU:OE1	2.43	0.52
34:S1:355:LYS:HA	34:S1:366:LEU:HD21	1.91	0.52
34:S1:389:THR:OG1	34:S1:511:LYS:O	2.27	0.52
3:A2:80:ASN:OD1	3:A2:81:ASN:ND2	2.43	0.51
7:A7:113:LEU:O	41:S8:44:ARG:NH1	2.42	0.51
20:B6:91:ARG:NH2	23:B9:159:ASP:OD1	2.42	0.51
34:S1:308:ARG:NH1	34:S1:312:GLY:O	2.41	0.51
36:S3:73:VAL:HA	36:S3:88:ILE:HG22	1.93	0.51
42:V1:217:GLU:OE2	42:V1:224:ARG:NH2	2.44	0.51
9:A9:206:ILE:HG12	47:A9:401:NDP:H42N	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AL:201:CDL:H442	45:AL:202:CDL:H361	1.92	0.51
18:B4:14:LEU:HD12	18:B4:15:PRO:HD2	1.92	0.51
32:N5:290:LEU:O	32:N5:523:SER:OG	2.27	0.51
33:N6:82:VAL:HG13	33:N6:84:VAL:H	1.75	0.51
34:S1:251:ILE:HD13	34:S1:604:GLN:HB2	1.93	0.51
34:S1:389:THR:HG21	34:S1:473:MET:HE2	1.92	0.51
28:N1:307:LEU:HA	28:N1:310:MET:HG2	1.92	0.51
29:N2:287:LEU:HD12	48:N2:403:PEE:H65	1.92	0.51
34:S1:401:LEU:HD11	34:S1:432:ILE:HG13	1.91	0.51
41:S8:74:LEU:HD12	41:S8:77:LEU:HD23	1.92	0.51
43:V2:137:THR:O	43:V2:141:MET:N	2.41	0.51
13:AM:122:GLN:O	39:S6:59:GLN:NE2	2.43	0.51
33:N6:2:THR:HG22	33:N6:4:TYR:H	1.76	0.51
33:N6:17:PHE:HA	33:N6:20:PHE:CD2	2.46	0.51
1:4L:1:MET:HG2	1:4L:2:PRO:HD2	1.92	0.51
9:A9:109:ASN:HB3	9:A9:112:ASP:HB2	1.92	0.51
11:AK:148:ALA:HB1	11:AK:159:VAL:HG21	1.93	0.51
29:N2:154:MET:HE3	29:N2:191:THR:HB	1.91	0.51
34:S1:104:THR:O	34:S1:113:ARG:NH2	2.43	0.51
34:S1:342:ALA:HB3	34:S1:368:THR:HG22	1.92	0.51
35:S2:410:LYS:HE2	35:S2:463:VAL:HG23	1.92	0.51
37:S4:130:THR:HG23	37:S4:133:ASP:H	1.76	0.51
42:V1:362:ASP:HB3	42:V1:365:LYS:HB3	1.92	0.51
8:A8:178:ARG:NH1	8:A8:181:GLN:OE1	2.43	0.51
11:AK:111:SER:OG	29:N2:316:GLN:NE2	2.44	0.51
16:B2:84:LEU:HD11	17:B3:71:PHE:HE1	1.74	0.51
35:S2:418:VAL:HB	35:S2:427:ARG:HB3	1.93	0.51
36:S3:83:GLU:OE1	36:S3:142:ARG:NH2	2.34	0.51
1:4L:55:LEU:HD13	38:S5:17:TRP:HE3	1.75	0.51
9:A9:344:PRO:HG2	9:A9:347:LEU:HD13	1.93	0.51
24:BK:76:GLU:OE2	25:BL:146:LYS:NZ	2.35	0.51
26:CA:55:TRP:NE1	27:CB:68:THR:OG1	2.43	0.51
28:N1:160:TYR:OH	30:N3:73:LEU:O	2.28	0.51
34:S1:213:MET:HE1	34:S1:713:ALA:HB1	1.93	0.51
16:B2:90:ASP:N	16:B2:90:ASP:OD1	2.42	0.51
45:B5:202:CDL:H661	32:N5:12:LEU:HB3	1.92	0.51
34:S1:283:GLU:OE2	34:S1:420:LYS:NZ	2.37	0.51
35:S2:266:GLU:OE2	41:S8:68:ARG:NH2	2.44	0.51
43:V2:149:LEU:HD11	43:V2:160:VAL:HG23	1.91	0.51
7:A7:113:LEU:HD12	41:S8:41:VAL:HA	1.92	0.51
9:A9:222:TRP:CD1	48:A9:402:PEE:H7	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N2:112:HIS:O	29:N2:116:PRO:HD2	2.11	0.51
34:S1:498:GLN:HG3	34:S1:502:LEU:HD23	1.93	0.51
4:A3:127:ALA:HB2	28:N1:312:ALA:HA	1.92	0.50
28:N1:254:LEU:O	28:N1:258:ASN:ND2	2.35	0.50
21:B7:56:ARG:HH22	24:BK:120:SER:HB3	1.75	0.50
31:N4:371:PRO:HD2	45:N5:701:CDL:H382	1.94	0.50
36:S3:154:GLU:OE2	36:S3:180:ASN:ND2	2.43	0.50
31:N4:408:LEU:HD12	32:N5:172:ILE:HG21	1.93	0.50
41:S8:153:ILE:HG12	53:S8:302:SF4:S1	2.51	0.50
11:AK:131:TYR:OH	11:AK:188:HIS:ND1	2.38	0.50
27:CB:45:LEU:HD22	27:CB:55:VAL:HG12	1.92	0.50
31:N4:133:ILE:HD11	31:N4:231:LEU:HD11	1.92	0.50
29:N2:211:MET:HG2	29:N2:333:SER:HB2	1.94	0.50
31:N4:97:THR:HG21	45:N4:503:CDL:H232	1.94	0.50
32:N5:260:LEU:HD22	32:N5:267:MET:HE3	1.92	0.50
35:S2:187:LEU:HD23	35:S2:213:ARG:HG2	1.94	0.50
2:A1:31:ASN:OD1	2:A1:60:TYR:OH	2.20	0.50
9:A9:269:ASN:HD22	9:A9:374:THR:HG21	1.77	0.50
14:AN:127:LEU:HD22	38:S5:83:ARG:HD3	1.94	0.50
17:B3:33:GLN:NE2	17:B3:43:ASP:OD1	2.45	0.50
45:N2:402:CDL:H352	45:N2:402:CDL:H121	1.92	0.50
31:N4:449:LEU:HG	45:N5:701:CDL:H441	1.92	0.50
32:N5:69:MET:HE3	32:N5:76:LEU:HD12	1.93	0.50
35:S2:101:LEU:HB2	35:S2:464:PHE:CZ	2.47	0.50
35:S2:183:ILE:HG23	35:S2:216:MET:HE2	1.93	0.50
42:V1:121:GLU:HG3	42:V1:351:THR:HG21	1.93	0.50
9:A9:162:GLU:O	9:A9:259:LYS:NZ	2.44	0.50
19:B5:139:ILE:HG23	31:N4:54:LEU:HD23	1.93	0.50
32:N5:504:LEU:O	32:N5:507:THR:OG1	2.29	0.50
34:S1:512:VAL:O	34:S1:514:ASN:ND2	2.45	0.50
41:S8:100:GLU:OE1	41:S8:172:ASN:ND2	2.34	0.50
42:V1:124:THR:HA	42:V1:277:ASN:HD22	1.76	0.50
42:V1:174:ARG:HD3	44:V3:402:LEU:HD11	1.94	0.50
8:A8:235:LEU:HB3	27:CB:23:LEU:HD21	1.94	0.50
9:A9:222:TRP:HB3	48:A9:402:PEE:H56	1.93	0.50
37:S4:109:ASN:ND2	37:S4:111:LEU:O	2.44	0.50
20:B6:155:TYR:OH	24:BK:11:PRO:O	2.22	0.49
43:V2:106:GLN:O	44:V3:422:ARG:NH2	2.45	0.49
6:A6:117:GLU:O	6:A6:121:ASN:ND2	2.36	0.49
28:N1:236:ALA:HA	28:N1:263:THR:HG22	1.92	0.49
34:S1:306:MET:HB2	34:S1:583:ILE:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A7:52:ASN:OD1	7:A7:57:ARG:NE	2.40	0.49
9:A9:223:PHE:HE2	48:A9:402:PEE:H14	1.76	0.49
15:B1:24:GLY:HA2	31:N4:6:ILE:HD12	1.94	0.49
17:B3:48:ASN:O	17:B3:51:TRP:HD1	1.96	0.49
27:CB:52:ARG:NH1	29:N2:318:GLU:OE1	2.45	0.49
18:B4:127:ILE:HD11	24:BK:136:SER:HB2	1.94	0.49
31:N4:225:ILE:HD13	31:N4:331:ASN:HB2	1.95	0.49
34:S1:103:LEU:HB3	34:S1:106:SER:HB2	1.94	0.49
36:S3:89:HIS:CG	36:S3:90:PRO:HD2	2.47	0.49
11:AK:72:LYS:HZ2	11:AK:162:GLU:HG2	1.76	0.49
34:S1:624:ARG:NH2	34:S1:637:ASP:OD1	2.43	0.49
42:V1:118:ASP:HA	42:V1:159:ARG:HB3	1.94	0.49
42:V1:423:THR:HB	53:V1:501:SF4:S2	2.52	0.49
43:V2:137:THR:OG1	43:V2:138:THR:N	2.44	0.49
11:AK:248:LEU:HD22	11:AK:257:VAL:HG11	1.93	0.49
46:AN:202:PC1:H3B1	33:N6:39:VAL:HG22	1.93	0.49
32:N5:407:TRP:CE2	32:N5:411:MET:HE2	2.47	0.49
36:S3:115:THR:OG1	36:S3:116:ALA:N	2.45	0.49
43:V2:111:ARG:NH1	43:V2:114:GLU:OE2	2.45	0.49
31:N4:369:LEU:HD23	45:N5:701:CDL:H352	1.94	0.49
28:N1:120:GLY:HA2	28:N1:128:ALA:HB1	1.94	0.49
29:N2:111:PHE:HA	32:N5:591:PHE:CE1	2.48	0.49
19:B5:147:ALA:HB2	31:N4:173:SER:HB2	1.94	0.49
5:A5:44:TYR:O	5:A5:48:THR:HG22	2.13	0.49
6:A6:63:ARG:HG2	10:AB:120:MET:SD	2.52	0.49
29:N2:112:HIS:HB2	29:N2:184:ILE:HD13	1.95	0.49
34:S1:574:ASP:OD2	34:S1:702:ARG:NE	2.46	0.49
48:AK:402:PEE:H48	48:AK:402:PEE:H26	1.95	0.48
14:AN:120:MET:HG3	14:AN:121:MET:H	1.78	0.48
29:N2:106:LEU:HD22	29:N2:187:MET:HE2	1.93	0.48
34:S1:306:MET:HE2	34:S1:314:LEU:HB3	1.94	0.48
42:V1:296:LEU:HD21	42:V1:317:VAL:HG21	1.95	0.48
10:AB:99:SER:OG	10:AB:102:SER:OG	2.18	0.48
31:N4:14:MET:HE3	31:N4:26:ASN:HB3	1.94	0.48
34:S1:476:LEU:HD22	34:S1:493:VAL:HG21	1.94	0.48
1:4L:65:VAL:HG11	33:N6:157:THR:HG23	1.94	0.48
12:AL:117:TYR:HD2	48:AL:205:PEE:H26	1.78	0.48
23:B9:77:ASP:OD1	23:B9:77:ASP:N	2.47	0.48
31:N4:318:ALA:HB2	31:N4:373:ILE:HG13	1.96	0.48
40:S7:51:ASP:HB3	40:S7:190:LEU:HB2	1.96	0.48
1:4L:35:GLY:HA3	33:N6:20:PHE:HZ	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A9:204:SER:HB2	9:A9:266:VAL:HG12	1.94	0.48
22:B8:108:ASP:OD1	31:N4:278:ARG:NH2	2.45	0.48
52:CB:202:3PE:H381	52:CB:202:3PE:H3C2	1.95	0.48
2:A1:46:ASN:ND2	33:N6:132:ASP:OD2	2.36	0.48
10:AC:120:MET:HE1	23:B9:66:LEU:HD12	1.95	0.48
31:N4:382:ILE:HG12	31:N4:396:MET:HG3	1.94	0.48
35:S2:275:ARG:O	35:S2:279:VAL:HB	2.14	0.48
35:S2:438:LEU:HD13	35:S2:462:ILE:HG13	1.95	0.48
42:V1:383:THR:HG22	42:V1:386:ARG:HH22	1.77	0.48
43:V2:133:GLN:HG2	43:V2:172:ILE:HD11	1.95	0.48
6:A6:53:GLU:O	6:A6:57:ARG:HG2	2.13	0.48
10:AC:119:ILE:HG21	10:AC:135:ALA:HB1	1.95	0.48
13:AM:26:VAL:HG13	13:AM:33:VAL:HG12	1.95	0.48
13:AM:78:ASP:H	13:AM:81:MET:HE3	1.78	0.48
22:B8:81:ARG:NH2	22:B8:85:GLU:OE2	2.47	0.48
1:4L:36:MET:HE3	29:N2:68:MET:HG3	1.96	0.48
32:N5:144:TRP:CZ2	32:N5:223:LYS:HB2	2.49	0.48
32:N5:536:LEU:HB3	32:N5:537:PRO:HD3	1.96	0.48
38:S5:10:LEU:HB3	38:S5:12:LEU:HD23	1.94	0.48
5:A5:48:THR:HA	5:A5:51:ILE:HG12	1.95	0.48
17:B3:47:ARG:HA	17:B3:50:ALA:HB3	1.94	0.48
22:B8:96:ASP:OD1	22:B8:96:ASP:N	2.46	0.48
52:CB:202:3PE:H351	52:CB:202:3PE:H392	1.95	0.48
28:N1:175:ILE:HB	28:N1:242:PHE:HB3	1.96	0.48
30:N3:66:ASP:O	30:N3:69:ILE:HG13	2.14	0.48
43:V2:61:LYS:O	43:V2:64:GLU:HG3	2.13	0.48
31:N4:203:PHE:CE1	31:N4:242:GLY:HA3	2.48	0.48
31:N4:243:MET:HE3	31:N4:302:MET:HE3	1.96	0.48
32:N5:346:ILE:HG12	32:N5:366:MET:HE1	1.95	0.48
34:S1:307:ILE:HG23	34:S1:317:THR:HG21	1.96	0.48
42:V1:62:TRP:CD2	42:V1:181:LEU:HD13	2.49	0.48
3:A2:22:HIS:O	3:A2:63:PRO:HA	2.13	0.48
6:A6:46:ILE:HG12	36:S3:152:PRO:HG3	1.96	0.48
31:N4:405:LEU:HD13	48:N5:703:PEE:H57	1.95	0.48
32:N5:257:VAL:HG21	32:N5:313:MET:HE2	1.96	0.48
32:N5:566:THR:O	32:N5:570:GLN:HG2	2.13	0.48
22:B8:134:PHE:HA	22:B8:137:VAL:HG12	1.95	0.47
45:N1:401:CDL:H112	48:N1:403:PEE:H7	1.96	0.47
39:S6:74:GLN:HG3	41:S8:108:SER:HB2	1.95	0.47
6:A6:88:LYS:NZ	6:A6:133:PHE:HA	2.29	0.47
12:AL:125:VAL:HA	45:AL:202:CDL:H712	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A7:54:TYR:CZ	35:S2:368:LYS:HD2	2.49	0.47
9:A9:247:LYS:HE2	9:A9:340:ILE:HD12	1.95	0.47
45:B5:202:CDL:H581	48:B6:201:PEE:H22	1.96	0.47
34:S1:249:GLU:OE1	37:S4:78:ARG:NH1	2.39	0.47
43:V2:133:GLN:HB3	43:V2:174:VAL:HG21	1.96	0.47
4:A3:163:LEU:HD23	4:A3:166:LEU:HD23	1.96	0.47
11:AK:142:LEU:HA	11:AK:165:ILE:HD11	1.95	0.47
42:V1:112:TYR:CD1	42:V1:153:ALA:HB3	2.49	0.47
10:AB:115:GLN:NE2	10:AB:135:ALA:O	2.39	0.47
21:B7:103:GLU:O	21:B7:107:ARG:HG2	2.15	0.47
51:N3:202:PLX:H102	51:N3:202:PLX:H131	1.71	0.47
32:N5:229:LEU:HD21	48:N5:703:PEE:H34	1.97	0.47
22:B8:126:TRP:HA	22:B8:129:MET:HE2	1.95	0.47
31:N4:76:MET:SD	31:N4:230:VAL:HB	2.54	0.47
48:N4:501:PEE:H31	48:N4:501:PEE:H38	1.59	0.47
45:N4:503:CDL:O1	45:N4:503:CDL:OB9	2.32	0.47
34:S1:432:ILE:HG12	34:S1:445:LEU:HB2	1.96	0.47
6:A6:53:GLU:HG2	6:A6:56:ARG:HH21	1.79	0.47
7:A7:11:LEU:HA	7:A7:14:TRP:CD1	2.49	0.47
9:A9:328:THR:HG22	9:A9:330:PRO:HD3	1.96	0.47
12:AL:92:ILE:HG23	48:AL:203:PEE:H78	1.95	0.47
17:B3:63:PHE:CZ	32:N5:424:THR:HG22	2.49	0.47
18:B4:15:PRO:HG2	18:B4:18:LEU:HB2	1.97	0.47
52:B4:201:3PE:H3I3	32:N5:558:LEU:HD21	1.97	0.47
20:B6:67:ASP:OD2	23:B9:200:ARG:NH2	2.46	0.47
20:B6:153:LYS:O	20:B6:156:THR:OG1	2.32	0.47
45:N1:401:CDL:H801	33:N6:16:GLY:HA2	1.96	0.47
33:N6:82:VAL:HG22	33:N6:83:TRP:H	1.80	0.47
34:S1:389:THR:N	34:S1:514:ASN:OD1	2.34	0.47
34:S1:402:LEU:HD13	34:S1:407:PRO:HG2	1.97	0.47
41:S8:177:THR:HG22	41:S8:179:THR:H	1.80	0.47
4:A3:163:LEU:HD13	8:A8:200:GLY:HA3	1.96	0.47
32:N5:200:GLN:HE21	32:N5:204:LEU:HD11	1.80	0.47
35:S2:180:PHE:O	35:S2:184:THR:OG1	2.33	0.47
43:V2:53:PHE:HE1	43:V2:90:ASN:HB2	1.79	0.47
4:A3:151:VAL:O	8:A8:207:LYS:NZ	2.36	0.47
6:A6:107:LEU:HD12	6:A6:107:LEU:HA	1.82	0.47
45:AL:201:CDL:H562	29:N2:110:PRO:HB3	1.97	0.47
31:N4:196:TRP:CD1	31:N4:250:LEU:HB3	2.50	0.47
32:N5:55:MET:HE1	32:N5:472:ILE:HG22	1.96	0.47
32:N5:62:ILE:HG22	32:N5:81:LYS:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:208:GLU:OE1	42:V1:210:THR:N	2.48	0.47
4:A3:143:ARG:NH2	8:A8:126:GLU:OE1	2.34	0.47
8:A8:216:GLU:OE1	8:A8:216:GLU:N	2.38	0.47
11:AK:315:TYR:HE2	29:N2:228:LEU:HD13	1.80	0.47
27:CB:65:LEU:HD23	52:CB:202:3PE:H221	1.97	0.47
28:N1:220:PHE:HZ	40:S7:94:ARG:HH12	1.63	0.47
32:N5:293:ILE:HG21	32:N5:418:LEU:HD22	1.97	0.47
34:S1:144:MET:HG3	35:S2:389:LYS:HG3	1.97	0.47
42:V1:65:THR:O	42:V1:69:LEU:HG	2.14	0.47
28:N1:213:VAL:HG13	28:N1:214:GLU:HG3	1.96	0.46
22:B8:161:TYR:HB2	22:B8:165:ASP:HA	1.96	0.46
32:N5:161:ARG:HG2	32:N5:164:ALA:H	1.80	0.46
34:S1:264:SER:HB2	34:S1:272:ARG:HB3	1.97	0.46
35:S2:149:SER:HA	35:S2:184:THR:HG22	1.96	0.46
6:A6:90:ARG:NH2	10:AB:117:GLU:OE2	2.47	0.46
8:A8:219:TYR:OH	19:B5:189:ASN:ND2	2.44	0.46
10:AB:117:GLU:HA	10:AB:120:MET:HE3	1.97	0.46
25:BL:90:VAL:HG22	31:N4:28:THR:HG21	1.97	0.46
31:N4:391:ILE:HG23	31:N4:394:ILE:HD12	1.97	0.46
32:N5:122:LEU:O	32:N5:126:ILE:HG12	2.16	0.46
32:N5:249:SER:HA	32:N5:306:THR:HG21	1.96	0.46
9:A9:271:TYR:OH	9:A9:346:GLU:OE2	2.28	0.46
28:N1:169:GLN:HB3	28:N1:244:GLY:HA3	1.97	0.46
29:N2:200:MET:HG3	29:N2:269:GLU:HG3	1.98	0.46
31:N4:420:THR:HG21	31:N4:423:ILE:HD12	1.97	0.46
32:N5:435:PRO:HB3	32:N5:437:PHE:CE2	2.51	0.46
20:B6:89:SER:HB3	20:B6:92:GLU:HB2	1.96	0.46
28:N1:61:LEU:HD11	40:S7:98:ARG:HD2	1.97	0.46
34:S1:591:GLU:HG2	34:S1:610:VAL:HG23	1.97	0.46
35:S2:212:GLU:O	35:S2:216:MET:HG3	2.15	0.46
35:S2:318:ASP:OD1	35:S2:318:ASP:N	2.46	0.46
1:4L:62:ILE:HG21	29:N2:31:ILE:HD11	1.98	0.46
9:A9:304:LEU:HD21	46:N3:203:PC1:H2C2	1.98	0.46
20:B6:148:TYR:CE1	24:BK:49:ARG:HG2	2.50	0.46
25:BL:84:LEU:HD21	25:BL:88:ARG:HH21	1.81	0.46
28:N1:179:TRP:CG	28:N1:180:PRO:HD3	2.50	0.46
29:N2:130:LEU:HD12	29:N2:134:GLN:HG3	1.97	0.46
33:N6:7:PHE:CZ	33:N6:104:VAL:HG23	2.51	0.46
34:S1:339:ALA:HA	34:S1:365:SER:O	2.15	0.46
42:V1:132:ARG:HB2	42:V1:165:GLU:HG3	1.97	0.46
42:V1:325:PRO:HG3	42:V1:433:TRP:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4L:35:GLY:HA3	33:N6:20:PHE:CZ	2.50	0.46
2:A1:51:ASP:OD2	8:A8:99:SER:OG	2.29	0.46
11:AK:357:LYS:HD3	26:CA:36:HIS:O	2.16	0.46
24:BK:163:MET:HE2	25:BL:149:LEU:HD11	1.97	0.46
51:N1:402:PLX:H281	51:S7:302:PLX:H141	1.98	0.46
35:S2:189:HIS:NE2	35:S2:342:GLU:OE1	2.43	0.46
42:V1:364:VAL:HG12	42:V1:400:VAL:HG12	1.98	0.46
6:A6:62:TYR:OH	10:AB:117:GLU:OE2	2.30	0.46
49:AC:201:ZMP:H2	23:B9:86:MET:HE1	1.98	0.46
29:N2:230:LEU:HD11	29:N2:244:MET:HE1	1.97	0.46
30:N3:65:PHE:O	30:N3:69:ILE:HG23	2.16	0.46
34:S1:341:ILE:HG13	34:S1:545:LEU:HD11	1.98	0.46
41:S8:115:ALA:HB2	41:S8:142:THR:HG23	1.98	0.46
2:A1:3:PHE:CZ	45:A1:101:CDL:HB31	2.51	0.46
7:A7:39:PRO:HG3	41:S8:211:TYR:CZ	2.51	0.46
9:A9:227:PRO:HG3	48:A9:402:PEE:H30	1.97	0.46
10:AB:90:TYR:OH	10:AB:117:GLU:OE1	2.29	0.46
12:AL:125:VAL:HG21	45:AL:201:CDL:H462	1.97	0.46
24:BK:106:ILE:HD11	25:BL:136:LEU:HD22	1.97	0.46
29:N2:193:VAL:HG21	29:N2:266:ILE:HG12	1.98	0.46
32:N5:213:LEU:HD23	32:N5:213:LEU:HA	1.77	0.46
32:N5:248:HIS:O	32:N5:253:VAL:HG22	2.16	0.46
33:N6:24:PRO:HG3	33:N6:83:TRP:CE2	2.51	0.46
34:S1:455:ILE:O	34:S1:463:SER:OG	2.32	0.46
42:V1:128:ARG:NH2	43:V2:194:GLU:OE2	2.48	0.46
42:V1:297:LYS:NZ	42:V1:301:GLU:OE2	2.37	0.46
1:4L:75:LEU:HB3	33:N6:70:TYR:CE2	2.50	0.46
9:A9:272:LEU:HG	9:A9:375:VAL:HG21	1.98	0.46
31:N4:197:LEU:O	31:N4:201:MET:HB2	2.17	0.46
31:N4:200:ILE:O	31:N4:204:MET:HG2	2.16	0.46
40:S7:48:ALA:HA	40:S7:191:ARG:HH11	1.81	0.46
11:AK:134:GLN:HE22	50:AK:401:ADP:HN62	1.62	0.45
48:AL:205:PEE:H50	48:AL:205:PEE:H57	1.79	0.45
34:S1:257:VAL:HG11	34:S1:413:LEU:HB2	1.98	0.45
2:A1:68:ASN:ND2	8:A8:96:LYS:HB3	2.32	0.45
29:N2:170:LEU:HD11	29:N2:288:LEU:HG	1.98	0.45
32:N5:8:THR:O	32:N5:11:THR:OG1	2.28	0.45
8:A8:129:ASP:HB3	8:A8:132:ARG:HG3	1.98	0.45
45:AL:201:CDL:H551	29:N2:112:HIS:HE1	1.82	0.45
21:B7:22:MET:HE2	21:B7:105:GLU:HG2	1.98	0.45
27:CB:97:LYS:HB3	27:CB:97:LYS:HE3	1.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:N6:86:ASN:OD1	33:N6:87:LYS:N	2.48	0.45
42:V1:119:GLU:O	42:V1:159:ARG:NH1	2.50	0.45
16:B2:79:MET:SD	32:N5:375:ILE:HG12	2.56	0.45
20:B6:132:VAL:O	20:B6:136:LEU:CB	2.58	0.45
45:N4:503:CDL:H852	45:N4:503:CDL:H251	1.99	0.45
32:N5:96:VAL:O	32:N5:100:ILE:HG12	2.16	0.45
32:N5:241:THR:HG21	32:N5:344:GLY:HA3	1.97	0.45
34:S1:275:PRO:HG3	34:S1:286:ILE:HG12	1.98	0.45
16:B2:95:LEU:HD23	32:N5:488:MET:HE1	1.97	0.45
28:N1:92:PRO:HB3	28:N1:255:TYR:CD1	2.51	0.45
34:S1:455:ILE:HD13	34:S1:460:HIS:HB3	1.99	0.45
35:S2:61:THR:H	35:S2:64:THR:HG1	1.59	0.45
40:S7:62:LEU:O	40:S7:91:VAL:HA	2.16	0.45
13:AM:34:ARG:NH1	13:AM:58:ARG:O	2.49	0.45
46:AN:202:PC1:H3A1	46:AN:202:PC1:H3F1	1.98	0.45
28:N1:195:ARG:HD3	28:N1:231:ILE:HD11	1.98	0.45
51:N1:402:PLX:H261	51:N1:402:PLX:H291	1.70	0.45
32:N5:2:ASN:ND2	32:N5:59:GLN:OE1	2.50	0.45
32:N5:49:VAL:HB	32:N5:50:PRO:HD3	1.99	0.45
42:V1:244:ASN:OD1	42:V1:245:VAL:N	2.50	0.45
1:4L:75:LEU:HD22	33:N6:70:TYR:HD2	1.82	0.45
24:BK:12:GLU:OE1	24:BK:116:ARG:NH2	2.50	0.45
29:N2:42:PRO:HG3	33:N6:167:VAL:HG13	1.97	0.45
29:N2:266:ILE:HG22	29:N2:270:MET:HE2	1.99	0.45
31:N4:281:ASP:OD1	31:N4:282:LEU:N	2.49	0.45
32:N5:213:LEU:HB3	32:N5:273:VAL:HG11	1.99	0.45
32:N5:264:TYR:CG	32:N5:265:PRO:HD3	2.51	0.45
32:N5:313:MET:HG3	32:N5:328:HIS:HD2	1.81	0.45
38:S5:94:PRO:HB2	38:S5:99:LEU:HG	1.99	0.45
12:AL:122:ALA:HA	12:AL:125:VAL:HG22	1.99	0.45
20:B6:146:LEU:HD21	32:N5:9:LEU:HD12	1.97	0.45
28:N1:151:LEU:HD12	30:N3:73:LEU:HD23	1.98	0.45
29:N2:131:LEU:O	29:N2:135:LYS:HG2	2.17	0.45
29:N2:137:ALA:HB3	29:N2:138:PRO:HD3	1.98	0.45
37:S4:111:LEU:HG	37:S4:112:MET:HG2	1.98	0.45
40:S7:98:ARG:HA	40:S7:125:PRO:HD3	1.99	0.45
7:A7:90:THR:OG1	7:A7:91:GLU:N	2.50	0.45
28:N1:58:LYS:HG2	40:S7:127:PRO:HD2	1.98	0.45
31:N4:416:ARG:HG3	32:N5:159:HIS:HB3	1.97	0.45
45:N4:503:CDL:H791	45:N4:503:CDL:H401	1.99	0.45
32:N5:356:ILE:HB	32:N5:429:PHE:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:381:MET:HE3	35:S2:385:ILE:HD11	1.98	0.45
41:S8:75:SER:O	41:S8:79:ARG:HG3	2.17	0.45
42:V1:113:LEU:HD13	42:V1:149:MET:HE1	1.98	0.45
1:4L:10:MET:HE3	1:4L:14:ILE:HD11	1.99	0.45
6:A6:99:VAL:HB	49:AB:201:ZMP:H14A	1.98	0.44
11:AK:297:ARG:HA	11:AK:300:VAL:HG22	1.99	0.44
12:AL:70:PHE:CZ	45:AL:201:CDL:H461	2.52	0.44
51:AL:204:PLX:H301	51:AL:204:PLX:H372	1.98	0.44
14:AN:85:GLN:OE1	38:S5:105:ARG:NH1	2.43	0.44
15:B1:27:LEU:HD12	31:N4:6:ILE:HD11	1.99	0.44
28:N1:72:ILE:HD12	45:N1:401:CDL:H151	1.99	0.44
51:N3:202:PLX:H361	51:N3:202:PLX:H302	1.98	0.44
31:N4:75:LEU:HD13	31:N4:440:HIS:CE1	2.52	0.44
33:N6:17:PHE:HA	33:N6:20:PHE:CE2	2.52	0.44
35:S2:89:ASN:HD22	35:S2:102:ARG:HE	1.65	0.44
37:S4:61:ILE:HG22	37:S4:64:LEU:HB2	1.98	0.44
42:V1:398:ARG:NH1	42:V1:403:ASP:O	2.50	0.44
2:A1:36:LYS:NZ	14:AN:144:THR:O	2.40	0.44
9:A9:64:PHE:O	9:A9:67:ARG:HG2	2.18	0.44
9:A9:217:PHE:HA	9:A9:220:MET:HE2	1.99	0.44
10:AB:115:GLN:O	10:AB:119:ILE:HG12	2.18	0.44
48:N3:201:PEE:H30	48:N3:201:PEE:H24	1.74	0.44
36:S3:75:GLN:NE2	36:S3:77:GLN:HE21	2.15	0.44
42:V1:357:MET:HB3	42:V1:361:THR:HG21	1.99	0.44
44:V3:388:ASN:O	44:V3:391:HIS:ND1	2.51	0.44
9:A9:64:PHE:HZ	9:A9:208:GLY:HA3	1.82	0.44
12:AL:131:GLU:OE2	31:N4:189:SER:OG	2.34	0.44
48:AN:201:PEE:H48	41:S8:67:VAL:HG21	1.99	0.44
21:B7:113:LYS:O	21:B7:116:GLU:HG3	2.17	0.44
24:BK:140:GLN:O	24:BK:144:SER:CB	2.48	0.44
25:BL:107:ALA:HB2	51:N4:502:PLX:H24	1.99	0.44
29:N2:153:LEU:O	29:N2:157:MET:HG3	2.18	0.44
42:V1:383:THR:HG22	42:V1:386:ARG:NH2	2.32	0.44
5:A5:113:LYS:HE2	5:A5:113:LYS:HB3	1.81	0.44
11:AK:327:ASP:O	11:AK:331:GLN:HG2	2.17	0.44
26:CA:65:ASP:OD2	27:CB:79:LYS:NZ	2.51	0.44
28:N1:2:PHE:CZ	30:N3:2:ASN:HB3	2.53	0.44
30:N3:24:LEU:HD11	46:N3:204:PC1:H341	1.99	0.44
32:N5:559:GLU:O	32:N5:564:LYS:HB2	2.17	0.44
41:S8:117:LYS:N	53:S8:301:SF4:S1	2.83	0.44
27:CB:13:LEU:HD21	38:S5:4:PHE:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:CB:36:MET:HE1	51:CB:201:PLX:H372	1.99	0.44
48:N2:403:PEE:H49	48:N2:403:PEE:H55	1.62	0.44
32:N5:332:HIS:HA	32:N5:335:PHE:CZ	2.53	0.44
6:A6:103:ARG:HH11	37:S4:53:ILE:HD11	1.82	0.44
48:N5:703:PEE:H49	48:N5:703:PEE:H54	1.61	0.44
22:B8:162:PRO:HB2	22:B8:163:TYR:CD2	2.52	0.44
28:N1:293:PHE:C	28:N1:297:THR:HG1	2.23	0.44
32:N5:264:TYR:CD1	32:N5:265:PRO:HD3	2.52	0.44
34:S1:36:VAL:HG11	34:S1:56:VAL:HG21	1.99	0.44
34:S1:252:ASP:OD2	34:S1:290:THR:OG1	2.28	0.44
35:S2:203:MET:O	35:S2:206:PHE:HB3	2.18	0.44
42:V1:170:GLN:HE21	42:V1:197:VAL:HB	1.83	0.44
51:AL:204:PLX:H91	51:AL:204:PLX:H281	2.00	0.44
46:AN:202:PC1:H122	28:N1:99:ASN:HB2	2.00	0.44
24:BK:164:LEU:HD23	25:BL:149:LEU:HD13	1.99	0.44
31:N4:336:ARG:NH1	31:N4:433:GLU:OE2	2.48	0.44
32:N5:152:PHE:CD1	32:N5:168:ALA:HB1	2.53	0.44
32:N5:313:MET:HE3	32:N5:329:ILE:HG12	1.99	0.44
34:S1:296:GLY:O	34:S1:572:HIS:NE2	2.43	0.44
11:AK:88:PHE:HB2	11:AK:161:LEU:HD23	2.00	0.44
26:CA:47:THR:HG23	27:CB:65:LEU:HD22	2.00	0.44
31:N4:106:LEU:HD13	31:N4:234:VAL:HG11	2.00	0.44
31:N4:233:ALA:HA	31:N4:320:GLY:HA2	1.99	0.44
32:N5:228:GLY:H	32:N5:230:HIS:HD2	1.64	0.44
34:S1:59:GLN:NE2	37:S4:89:SER:O	2.51	0.44
34:S1:696:MET:HG2	34:S1:711:VAL:HG21	1.99	0.44
39:S6:67:ALA:HB2	41:S8:111:GLU:HG3	1.99	0.44
42:V1:140:GLU:CD	42:V1:256:ARG:HH12	2.26	0.44
8:A8:160:THR:HA	8:A8:163:TRP:NE1	2.33	0.43
9:A9:231:LEU:HD13	9:A9:292:PRO:HG3	2.00	0.43
21:B7:4:HIS:NE2	22:B8:155:PRO:HD3	2.33	0.43
21:B7:22:MET:HE1	21:B7:102:PHE:CD2	2.53	0.43
23:B9:169:ARG:HG2	23:B9:172:ARG:HH21	1.83	0.43
24:BK:43:ARG:HB3	24:BK:44:PRO:HD3	2.00	0.43
35:S2:462:ILE:HG23	35:S2:467:VAL:HG21	1.99	0.43
41:S8:131:GLU:HB2	41:S8:144:ARG:HB3	1.99	0.43
45:B5:202:CDL:H372	20:B6:140:TRP:CE3	2.53	0.43
29:N2:167:TRP:HB3	32:N5:574:SER:HA	1.99	0.43
40:S7:94:ARG:NH2	40:S7:99:GLN:OE1	2.51	0.43
20:B6:164:ILE:HB	21:B7:48:ASP:HB3	1.99	0.43
28:N1:222:MET:SD	30:N3:18:VAL:HG23	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N1:233:MET:HE3	28:N1:233:MET:HB3	1.86	0.43
29:N2:210:THR:HG22	29:N2:333:SER:HB3	2.00	0.43
34:S1:169:VAL:HG22	34:S1:223:ILE:HD11	1.99	0.43
42:V1:102:MET:HG3	42:V1:149:MET:HB3	2.00	0.43
1:4L:25:HIS:HD1	1:4L:88:ASP:CG	2.26	0.43
11:AK:110:LEU:HD13	11:AK:336:LEU:HD11	2.00	0.43
14:AN:50:MET:HA	14:AN:50:MET:HE2	1.99	0.43
23:B9:69:LEU:HD11	23:B9:82:PHE:HB3	1.99	0.43
28:N1:90:PRO:HB3	28:N1:94:PRO:HD3	1.99	0.43
29:N2:36:ASN:OD1	29:N2:134:GLN:NE2	2.30	0.43
35:S2:121:LEU:O	40:S7:110:THR:OG1	2.26	0.43
35:S2:300:ARG:NH2	35:S2:407:GLU:OE2	2.51	0.43
43:V2:242:GLY:HA2	43:V2:245:VAL:HG23	2.00	0.43
1:4L:72:ALA:HB1	30:N3:60:ILE:HG23	2.01	0.43
45:A1:101:CDL:H552	45:A1:101:CDL:H731	2.00	0.43
12:AL:101:LEU:HD21	45:AL:201:CDL:H311	2.00	0.43
28:N1:29:GLY:O	28:N1:34:ARG:N	2.48	0.43
40:S7:124:MET:HE3	40:S7:128:ARG:HB2	2.00	0.43
8:A8:111:ALA:HB2	8:A8:197:PRO:HG3	1.99	0.43
9:A9:64:PHE:CD1	9:A9:210:GLU:HB2	2.54	0.43
9:A9:163:LYS:NZ	9:A9:253:ILE:O	2.31	0.43
9:A9:167:ILE:HD13	9:A9:201:ILE:HB	2.00	0.43
11:AK:109:GLN:OE1	11:AK:328:ARG:NH1	2.35	0.43
48:AL:205:PEE:H17	32:N5:569:ILE:HG12	1.99	0.43
31:N4:418:LYS:HE2	31:N4:421:HIS:HE1	1.83	0.43
35:S2:145:LEU:HD11	35:S2:430:ILE:HD13	2.00	0.43
36:S3:210:LEU:HD12	36:S3:219:VAL:HG12	2.00	0.43
42:V1:388:GLY:HA3	42:V1:419:ILE:HD11	1.99	0.43
43:V2:237:PRO:HA	43:V2:238:PRO:HD3	1.95	0.43
45:4L:201:CDL:H311	12:AL:41:ILE:HD13	2.01	0.43
8:A8:143:CYS:HA	8:A8:146:ASP:OD2	2.18	0.43
28:N1:82:ALA:HB1	28:N1:229:ALA:HB3	2.00	0.43
32:N5:457:LEU:HD23	32:N5:457:LEU:HA	1.85	0.43
35:S2:263:GLU:OE2	41:S8:79:ARG:NH2	2.38	0.43
8:A8:235:LEU:HD23	8:A8:235:LEU:HA	1.92	0.43
9:A9:199:THR:OG1	9:A9:258:ALA:O	2.35	0.43
9:A9:258:ALA:HA	9:A9:261:LYS:HD2	2.00	0.43
11:AK:173:GLU:O	11:AK:177:ARG:HG2	2.19	0.43
48:AN:201:PEE:H65	48:AN:201:PEE:H33	2.01	0.43
25:BL:114:MET:HB3	25:BL:117:TRP:HB3	2.00	0.43
45:CB:203:CDL:H192	45:CB:203:CDL:H401	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:N1:402:PLX:H1B2	51:N1:402:PLX:H22	1.72	0.43
29:N2:154:MET:HE2	29:N2:194:LEU:HD23	2.01	0.43
29:N2:308:THR:HG22	29:N2:309:ASN:H	1.83	0.43
33:N6:170:GLU:OE2	33:N6:173:ARG:NH2	2.51	0.43
45:B5:202:CDL:H571	45:B5:202:CDL:H531	2.01	0.43
20:B6:140:TRP:HD1	24:BK:41:VAL:HG13	1.84	0.43
24:BK:107:GLN:HE22	32:N5:194:ASN:ND2	2.17	0.43
30:N3:97:LEU:HD23	30:N3:97:LEU:HA	1.87	0.43
35:S2:149:SER:HB2	35:S2:152:CYS:HB2	2.00	0.43
41:S8:150:THR:HG21	41:S8:180:HIS:CD2	2.54	0.43
43:V2:186:VAL:HG22	43:V2:196:LEU:HD11	2.01	0.43
7:A7:71:SER:HB3	7:A7:73:GLN:HG3	2.00	0.43
23:B9:143:GLU:O	23:B9:164:ARG:NH2	2.52	0.43
24:BK:28:ASN:OD1	24:BK:31:THR:N	2.47	0.43
10:AB:104:PHE:HD1	10:AB:108:LEU:HD12	1.83	0.42
10:AC:112:SER:HB2	23:B9:59:LEU:HD21	2.00	0.42
14:AN:49:SER:HB3	28:N1:172:ILE:HD13	2.01	0.42
28:N1:209:SER:HB2	28:N1:213:VAL:HA	2.00	0.42
34:S1:509:ASP:OD1	34:S1:509:ASP:N	2.50	0.42
36:S3:93:VAL:HG22	36:S3:145:THR:HG21	2.00	0.42
42:V1:162:PHE:HB3	42:V1:165:GLU:HB2	2.01	0.42
49:AC:201:ZMP:H24	23:B9:116:GLY:O	2.20	0.42
51:AL:204:PLX:H1A2	51:AL:204:PLX:H22	1.70	0.42
45:N5:701:CDL:H161	45:N5:701:CDL:H601	2.01	0.42
34:S1:124:HIS:CG	34:S1:125:PRO:HD2	2.54	0.42
37:S4:75:ARG:HA	37:S4:75:ARG:HD2	1.79	0.42
41:S8:49:ASP:OD1	41:S8:49:ASP:N	2.52	0.42
3:A2:45:LYS:NZ	34:S1:380:ASP:OD2	2.33	0.42
11:AK:284:PRO:O	11:AK:288:GLN:HG2	2.19	0.42
14:AN:97:ILE:HG23	38:S5:86:LEU:HD12	2.01	0.42
22:B8:62:TYR:CE2	22:B8:64:PRO:HG3	2.54	0.42
29:N2:89:MET:SD	29:N2:98:MET:HG3	2.59	0.42
29:N2:128:LEU:HD12	29:N2:216:PHE:HB3	2.02	0.42
31:N4:259:TYR:O	31:N4:263:MET:HG2	2.19	0.42
31:N4:450:ASN:HB2	51:N4:502:PLX:H251	2.02	0.42
43:V2:177:LEU:O	43:V2:192:TYR:OH	2.29	0.42
48:AK:402:PEE:H49	48:AK:402:PEE:H54	1.87	0.42
14:AN:95:ALA:HA	14:AN:106:VAL:HG11	2.01	0.42
22:B8:109:LEU:O	22:B8:113:ILE:HG23	2.19	0.42
30:N3:35:SER:O	40:S7:98:ARG:NH2	2.52	0.42
35:S2:299:LEU:HB3	35:S2:304:ILE:HB	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:382:CYS:N	53:V1:501:SF4:S4	2.82	0.42
5:A5:116:ILE:HD12	5:A5:116:ILE:HA	1.94	0.42
14:AN:21:TYR:CZ	35:S2:348:ARG:HD2	2.54	0.42
20:B6:134:HIS:NE2	32:N5:35:TYR:OH	2.37	0.42
31:N4:203:PHE:HE2	31:N4:246:ILE:HG13	1.85	0.42
33:N6:122:LEU:HG	33:N6:123:GLY:H	1.85	0.42
35:S2:190:ILE:HG21	35:S2:213:ARG:HG3	2.01	0.42
45:4L:201:CDL:HA61	12:AL:49:PHE:HA	2.02	0.42
5:A5:9:THR:HG23	5:A5:16:VAL:HG22	2.00	0.42
7:A7:11:LEU:HD12	7:A7:14:TRP:NE1	2.27	0.42
14:AN:120:MET:O	33:N6:130:THR:OG1	2.29	0.42
34:S1:577:ALA:HB3	34:S1:578:PRO:HD3	2.01	0.42
43:V2:144:ASN:HB3	43:V2:147:SER:OG	2.20	0.42
44:V3:420:SER:HB3	44:V3:423:HIS:ND1	2.34	0.42
9:A9:346:GLU:HG2	9:A9:371:PRO:HB3	2.01	0.42
11:AK:307:LEU:HD13	29:N2:313:MET:HE3	2.01	0.42
25:BL:98:VAL:HG11	31:N4:71:TRP:CZ3	2.54	0.42
31:N4:207:MET:HE3	31:N4:294:MET:HE3	2.01	0.42
33:N6:113:VAL:HG13	33:N6:118:LYS:HB3	2.01	0.42
42:V1:39:ASP:HB3	42:V1:265:PHE:HE2	1.84	0.42
9:A9:310:PHE:HE1	46:N3:204:PC1:H232	1.84	0.42
11:AK:97:ASP:OD1	29:N2:316:GLN:NE2	2.41	0.42
32:N5:286:LEU:HG	32:N5:411:MET:SD	2.60	0.42
48:S8:303:PEE:H33	48:S8:303:PEE:H39	1.94	0.42
42:V1:63:TYR:CE2	43:V2:245:VAL:HG21	2.54	0.42
42:V1:265:PHE:O	42:V1:272:GLY:N	2.42	0.42
42:V1:313:ASN:O	42:V1:359:ARG:HG2	2.19	0.42
14:AN:21:TYR:CE2	35:S2:348:ARG:HD2	2.55	0.42
28:N1:138:GLN:HG3	28:N1:285:LEU:HD21	2.00	0.42
28:N1:198:PHE:CD1	28:N1:285:LEU:HD13	2.55	0.42
29:N2:276:ILE:C	29:N2:279:PRO:HD2	2.44	0.42
31:N4:405:LEU:HD21	32:N5:173:LEU:HD12	2.02	0.42
32:N5:297:ASP:O	32:N5:301:ILE:HG13	2.20	0.42
34:S1:386:LEU:HD23	34:S1:386:LEU:HA	1.90	0.42
35:S2:146:ASP:OD2	35:S2:149:SER:OG	2.38	0.42
40:S7:53:LEU:HB2	51:S7:302:PLX:H301	2.02	0.42
3:A2:21:ILE:HG12	3:A2:65:LEU:HD23	2.02	0.42
6:A6:127:THR:O	6:A6:131:ARG:HG3	2.20	0.42
14:AN:93:GLU:OE1	38:S5:92:TYR:OH	2.32	0.42
19:B5:109:HIS:HD2	19:B5:122:ALA:HB1	1.84	0.42
23:B9:66:LEU:HD23	23:B9:66:LEU:HA	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:210:TYR:CG	31:N4:268:GLY:HA3	2.55	0.42
35:S2:143:ASP:OD1	35:S2:150:MET:HB3	2.19	0.42
3:A2:65:LEU:HD21	3:A2:91:LEU:HD21	2.01	0.41
18:B4:81:ARG:NH1	22:B8:67:ASP:OD1	2.53	0.41
45:CB:203:CDL:H552	45:CB:203:CDL:H581	1.95	0.41
37:S4:112:MET:HG3	41:S8:184:LEU:HD23	2.00	0.41
37:S4:175:LYS:NZ	42:V1:223:PRO:O	2.53	0.41
4:A3:118:PRO:HG3	28:N1:306:SER:OG	2.19	0.41
8:A8:185:ASP:HA	8:A8:188:VAL:HG22	2.02	0.41
48:AL:203:PEE:H49	48:AL:203:PEE:H54	1.81	0.41
32:N5:51:LEU:HD22	32:N5:91:PRO:HG3	2.01	0.41
32:N5:289:ALA:O	32:N5:293:ILE:HG23	2.20	0.41
33:N6:141:MET:HE2	38:S5:27:HIS:CD2	2.55	0.41
34:S1:119:PHE:CD2	42:V1:384:PRO:HA	2.55	0.41
11:AK:138:TYR:OH	11:AK:193:LYS:HA	2.20	0.41
31:N4:318:ALA:HB1	31:N4:374:ASN:CG	2.45	0.41
32:N5:341:MET:HE2	32:N5:457:LEU:HD12	2.03	0.41
39:S6:84:ILE:HD12	39:S6:84:ILE:HA	1.91	0.41
1:4L:68:ALA:HB3	30:N3:67:LEU:HD21	2.03	0.41
45:AL:202:CDL:H191	48:N2:401:PEE:H2	2.02	0.41
17:B3:52:ARG:HD2	23:B9:76:ARG:HG3	2.02	0.41
18:B4:17:THR:O	18:B4:23:TYR:OH	2.31	0.41
27:CB:85:TYR:CZ	29:N2:344:SER:HB3	2.55	0.41
32:N5:90:ILE:HD12	32:N5:129:MET:SD	2.60	0.41
32:N5:420:ALA:HB1	32:N5:498:PHE:CD1	2.55	0.41
34:S1:338:VAL:HB	34:S1:363:SER:CB	2.50	0.41
34:S1:347:ASP:OD1	34:S1:347:ASP:N	2.46	0.41
34:S1:598:ASN:ND2	34:S1:600:GLU:HG2	2.36	0.41
1:4L:5:TYR:HB3	1:4L:43:MET:HE1	2.01	0.41
8:A8:240:HIS:NE2	19:B5:145:GLU:OE1	2.38	0.41
51:AL:204:PLX:H111	52:N4:504:3PE:H372	2.02	0.41
15:B1:3:ASN:O	15:B1:7:ILE:HG12	2.21	0.41
15:B1:30:ARG:NE	15:B1:33:GLU:OE2	2.53	0.41
18:B4:77:TYR:CZ	32:N5:564:LYS:HG2	2.55	0.41
24:BK:142:ARG:HD2	25:BL:138:GLU:O	2.20	0.41
28:N1:267:THR:O	28:N1:271:LEU:HG	2.21	0.41
28:N1:281:ARG:NH1	35:S2:452:ASP:OD1	2.48	0.41
45:N1:401:CDL:OB9	33:N6:83:TRP:HB2	2.20	0.41
29:N2:70:LEU:HG	29:N2:98:MET:SD	2.61	0.41
32:N5:71:LEU:N	32:N5:74:VAL:O	2.52	0.41
40:S7:154:ASP:OD1	40:S7:154:ASP:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:S7:161:ILE:HG13	40:S7:180:LEU:HB2	2.03	0.41
42:V1:119:GLU:HA	58:V1:502:FMN:HM71	2.03	0.41
10:AC:155:TYR:CD2	10:AC:156:GLU:HG3	2.55	0.41
18:B4:105:PHE:CD2	31:N4:263:MET:HE1	2.55	0.41
51:B5:201:PLX:H32	31:N4:3:LYS:HE2	2.03	0.41
32:N5:68:TRP:H	32:N5:77:SER:HA	1.85	0.41
32:N5:95:PHE:CZ	32:N5:456:ARG:HG2	2.55	0.41
37:S4:167:ASN:O	44:V3:418:ARG:NE	2.52	0.41
40:S7:41:SER:OG	40:S7:42:ARG:N	2.54	0.41
41:S8:155:CYS:N	53:S8:302:SF4:S4	2.92	0.41
6:A6:132:PHE:CD1	49:AB:201:ZMP:H1	2.55	0.41
21:B7:95:TYR:CZ	22:B8:156:VAL:HG11	2.55	0.41
28:N1:17:VAL:HG13	28:N1:228:TYR:HB2	2.02	0.41
31:N4:130:LEU:HD22	31:N4:150:LEU:HD22	2.03	0.41
31:N4:364:LEU:HB3	31:N4:369:LEU:HD22	2.03	0.41
45:N4:503:CDL:H231	45:N4:503:CDL:H832	2.02	0.41
32:N5:37:LYS:HD3	32:N5:105:MET:HE2	2.03	0.41
35:S2:294:PHE:HB3	35:S2:298:MET:HB3	2.02	0.41
42:V1:125:CYS:H	42:V1:277:ASN:ND2	2.19	0.41
42:V1:201:ALA:HB3	43:V2:119:TYR:CD1	2.55	0.41
42:V1:223:PRO:HD2	53:V1:501:SF4:S3	2.60	0.41
1:4L:97:GLN:O	29:N2:177:LYS:NZ	2.48	0.41
11:AK:225:ASN:HB3	11:AK:228:GLU:HG2	2.02	0.41
11:AK:355:TRP:H	11:AK:355:TRP:CD1	2.39	0.41
29:N2:6:TYR:CE1	29:N2:46:LYS:HD2	2.56	0.41
51:N3:202:PLX:H131	51:N3:202:PLX:H161	1.87	0.41
32:N5:208:CYS:HA	32:N5:209:PRO:HD3	1.82	0.41
35:S2:91:GLY:HA2	35:S2:94:HIS:H	1.86	0.41
36:S3:148:ASP:OD1	36:S3:148:ASP:N	2.54	0.41
4:A3:139:PRO:HD3	14:AN:69:ILE:HD13	2.03	0.41
9:A9:75:ARG:NH2	36:S3:215:GLU:OE1	2.37	0.41
9:A9:293:LEU:HD12	9:A9:294:PRO:HD2	2.02	0.41
48:A9:402:PEE:H48	48:A9:402:PEE:H8	1.94	0.41
49:AC:201:ZMP:H6	23:B9:90:PHE:CE1	2.56	0.41
11:AK:113:ASN:O	11:AK:132:ARG:NH1	2.53	0.41
51:AL:204:PLX:H131	51:AL:204:PLX:H102	1.90	0.41
13:AM:123:GLN:NE2	39:S6:58:ARG:HE	2.19	0.41
15:B1:15:ILE:C	15:B1:18:PRO:HD2	2.46	0.41
17:B3:24:ILE:O	17:B3:30:GLU:HB3	2.21	0.41
20:B6:170:ILE:HB	20:B6:175:GLU:HB3	2.03	0.41
24:BK:137:LYS:NZ	24:BK:141:ASP:OD2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:CB:201:PLX:H1A3	51:CB:201:PLX:H22	1.78	0.41
28:N1:32:GLN:HG2	35:S2:204:THR:HG23	2.01	0.41
30:N3:37:TYR:HD1	40:S7:123:GLN:HE22	1.68	0.41
48:N3:201:PEE:H57	48:N3:201:PEE:H63	1.38	0.41
46:N3:204:PC1:H382	46:N3:204:PC1:H2A1	2.03	0.41
31:N4:373:ILE:HD11	31:N4:444:LEU:HD23	2.03	0.41
32:N5:10:THR:O	32:N5:14:ILE:HG23	2.21	0.41
32:N5:86:SER:O	32:N5:90:ILE:HG12	2.20	0.41
32:N5:156:GLY:HA2	32:N5:164:ALA:HB1	2.03	0.41
34:S1:234:LYS:HB3	34:S1:235:PRO:HD3	2.03	0.41
35:S2:142:PHE:HZ	35:S2:428:CYS:SG	2.44	0.41
36:S3:147:THR:HB	36:S3:153:ILE:HD11	2.01	0.41
41:S8:100:GLU:O	41:S8:170:GLY:N	2.50	0.41
42:V1:81:LYS:HE3	42:V1:81:LYS:HB2	1.85	0.41
42:V1:417:LYS:HD2	42:V1:417:LYS:HA	1.91	0.41
43:V2:71:PRO:HA	44:V3:413:GLN:HB3	2.03	0.41
44:V3:386:TYR:CZ	44:V3:388:ASN:HB2	2.56	0.41
45:A1:101:CDL:H782	45:A1:101:CDL:H591	2.03	0.41
51:AL:204:PLX:H301	51:AL:204:PLX:H351	2.03	0.41
16:B2:59:ARG:HD2	17:B3:51:TRP:CG	2.56	0.41
20:B6:167:GLY:HA3	20:B6:179:LEU:HG	2.03	0.41
23:B9:180:LYS:O	23:B9:184:GLU:HG2	2.21	0.41
28:N1:24:GLU:OE2	28:N1:274:ARG:NH1	2.43	0.41
29:N2:100:MET:HE1	32:N5:595:ILE:HG23	2.02	0.41
31:N4:324:SER:OG	31:N4:440:HIS:NE2	2.42	0.41
32:N5:4:PHE:HZ	32:N5:87:VAL:HG11	1.85	0.41
34:S1:251:ILE:HD11	34:S1:596:TYR:HB2	2.02	0.41
34:S1:251:ILE:HG21	34:S1:604:GLN:HB3	2.03	0.41
35:S2:137:GLN:O	40:S7:142:TYR:OH	2.39	0.41
41:S8:104:ARG:HB2	41:S8:112:ARG:HD2	2.03	0.41
1:4L:32:CYS:HA	33:N6:20:PHE:HE1	1.86	0.40
7:A7:28:TYR:CZ	13:AM:55:PHE:HB3	2.55	0.40
48:AL:205:PEE:H25	48:N2:401:PEE:H23	2.03	0.40
13:AM:137:TRP:CZ2	13:AM:140:PRO:HD3	2.56	0.40
16:B2:92:ASP:HB3	16:B2:97:HIS:HB2	2.03	0.40
51:B5:201:PLX:H1A3	51:B5:201:PLX:H22	1.80	0.40
21:B7:92:HIS:ND1	32:N5:481:THR:OG1	2.26	0.40
52:CB:202:3PE:H351	52:CB:202:3PE:H322	1.97	0.40
28:N1:272:TRP:CZ2	41:S8:74:LEU:HB2	2.56	0.40
51:N1:402:PLX:H51	51:N1:402:PLX:H91	2.04	0.40
32:N5:145:GLU:OE2	32:N5:176:ARG:NH1	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:233:LEU:HB3	32:N5:234:PRO:HD3	2.03	0.40
33:N6:39:VAL:O	33:N6:43:ILE:HG13	2.21	0.40
41:S8:205:ILE:O	41:S8:209:TYR:HB3	2.21	0.40
10:AC:105:MET:HE3	10:AC:139:MET:HE1	2.04	0.40
24:BK:157:ALA:HB2	27:CB:116:GLU:HG3	2.02	0.40
28:N1:169:GLN:NE2	28:N1:240:ILE:O	2.48	0.40
29:N2:218:LEU:HD21	29:N2:330:ILE:HD11	2.04	0.40
29:N2:257:LEU:HD21	45:N4:503:CDL:H432	2.03	0.40
32:N5:47:SER:C	32:N5:50:PRO:HD2	2.46	0.40
43:V2:78:ALA:C	43:V2:81:PRO:HD2	2.46	0.40
43:V2:249:LEU:H	43:V2:249:LEU:HD23	1.85	0.40
11:AK:112:GLY:HA2	11:AK:136:TRP:CD2	2.56	0.40
13:AM:117:VAL:O	13:AM:120:THR:OG1	2.32	0.40
15:B1:30:ARG:O	15:B1:33:GLU:HG2	2.22	0.40
18:B4:36:ARG:NH2	22:B8:61:ASP:OD1	2.52	0.40
20:B6:138:PRO:HG2	32:N5:14:ILE:HG22	2.03	0.40
32:N5:7:LEU:HD22	32:N5:46:LEU:HD11	2.03	0.40
35:S2:218:GLU:OE2	40:S7:83:ARG:NH1	2.30	0.40
36:S3:173:MET:HE3	36:S3:188:LEU:HB2	2.03	0.40
36:S3:227:ALA:O	37:S4:116:SER:OG	2.32	0.40
41:S8:196:LYS:HE3	41:S8:197:TRP:NE1	2.36	0.40
46:A3:202:PC1:H111	46:A3:202:PC1:H152	1.89	0.40
11:AK:120:TYR:OH	50:AK:401:ADP:O2'	2.22	0.40
14:AN:57:ARG:NH1	28:N1:168:THR:OG1	2.55	0.40
15:B1:44:LEU:HD12	24:BK:69:ARG:HG2	2.03	0.40
30:N3:33:LYS:HE2	30:N3:33:LYS:HB2	1.92	0.40
31:N4:446:LEU:HB3	51:N4:502:PLX:H272	2.03	0.40
32:N5:14:ILE:HD11	32:N5:43:ALA:HA	2.03	0.40
32:N5:331:MET:HB3	32:N5:387:THR:HG22	2.02	0.40
34:S1:357:LEU:HD13	34:S1:627:SER:HB3	2.03	0.40
43:V2:141:MET:HE3	43:V2:141:MET:HB3	1.99	0.40
45:4L:201:CDL:H231	45:4L:201:CDL:H202	1.92	0.40
6:A6:66:TYR:CE2	6:A6:86:ARG:HD3	2.56	0.40
21:B7:97:LYS:NZ	22:B8:185:GLU:OE1	2.46	0.40
28:N1:24:GLU:HG3	28:N1:271:LEU:HD22	2.03	0.40
31:N4:118:PHE:O	31:N4:122:PHE:HB3	2.22	0.40
31:N4:401:MET:HA	32:N5:176:ARG:HG2	2.03	0.40
34:S1:124:HIS:CD2	35:S2:381:MET:HE2	2.46	0.40
35:S2:112:VAL:HG21	35:S2:453:VAL:HG21	2.02	0.40
35:S2:164:LEU:HD12	35:S2:417:LEU:HD23	2.03	0.40
41:S8:144:ARG:NH1	41:S8:146:ASP:OD2	2.53	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	4L	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
2	A1	68/70 (97%)	68 (100%)	0	0	100	100
3	A2	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
4	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
5	A5	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
6	A6	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
7	A7	93/112 (83%)	91 (98%)	2 (2%)	0	100	100
8	A8	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
9	A9	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
10	AB	75/87 (86%)	73 (97%)	2 (3%)	0	100	100
10	AC	85/87 (98%)	85 (100%)	0	0	100	100
11	AK	318/321 (99%)	309 (97%)	9 (3%)	0	100	100
12	AL	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
13	AM	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
14	AN	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
15	B1	54/56 (96%)	54 (100%)	0	0	100	100
16	B2	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
17	B3	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
18	B4	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
19	B5	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
20	B6	99/126 (79%)	95 (96%)	4 (4%)	0	100	100
21	B7	123/125 (98%)	120 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	B8	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
23	B9	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
24	BK	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
25	BL	97/102 (95%)	90 (93%)	7 (7%)	0	100	100
26	CA	47/49 (96%)	47 (100%)	0	0	100	100
27	CB	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
28	N1	316/318 (99%)	308 (98%)	8 (2%)	0	100	100
29	N2	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
30	N3	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
31	N4	457/459 (100%)	454 (99%)	3 (1%)	0	100	100
32	N5	601/603 (100%)	577 (96%)	24 (4%)	0	100	100
33	N6	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
34	S1	687/689 (100%)	661 (96%)	26 (4%)	0	100	100
35	S2	427/430 (99%)	411 (96%)	16 (4%)	0	100	100
36	S3	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
37	S4	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
38	S5	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
39	S6	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
40	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
41	S8	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
42	V1	429/431 (100%)	406 (95%)	23 (5%)	0	100	100
43	V2	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
44	V3	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
All	All	8150/8299 (98%)	7906 (97%)	244 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4L	85/85 (100%)	85 (100%)	0	100	100
2	A1	58/58 (100%)	58 (100%)	0	100	100
3	A2	76/76 (100%)	76 (100%)	0	100	100
4	A3	69/69 (100%)	69 (100%)	0	100	100
5	A5	99/99 (100%)	98 (99%)	1 (1%)	73	82
6	A6	107/107 (100%)	106 (99%)	1 (1%)	75	84
7	A7	87/97 (90%)	87 (100%)	0	100	100
8	A8	153/153 (100%)	152 (99%)	1 (1%)	81	87
9	A9	295/295 (100%)	294 (100%)	1 (0%)	91	94
10	AB	71/80 (89%)	71 (100%)	0	100	100
10	AC	80/80 (100%)	79 (99%)	1 (1%)	65	78
11	AK	283/284 (100%)	281 (99%)	2 (1%)	81	87
12	AL	101/101 (100%)	99 (98%)	2 (2%)	50	70
13	AM	130/130 (100%)	130 (100%)	0	100	100
14	AN	123/123 (100%)	123 (100%)	0	100	100
15	B1	53/53 (100%)	53 (100%)	0	100	100
16	B2	62/62 (100%)	62 (100%)	0	100	100
17	B3	62/62 (100%)	62 (100%)	0	100	100
18	B4	113/113 (100%)	112 (99%)	1 (1%)	75	84
19	B5	121/121 (100%)	121 (100%)	0	100	100
20	B6	98/119 (82%)	95 (97%)	3 (3%)	35	59
21	B7	112/112 (100%)	112 (100%)	0	100	100
22	B8	141/141 (100%)	139 (99%)	2 (1%)	62	77
23	B9	159/159 (100%)	159 (100%)	0	100	100
24	BK	155/156 (99%)	155 (100%)	0	100	100
25	BL	91/94 (97%)	91 (100%)	0	100	100
26	CA	45/45 (100%)	45 (100%)	0	100	100
27	CB	108/108 (100%)	108 (100%)	0	100	100
28	N1	275/275 (100%)	269 (98%)	6 (2%)	47	68
29	N2	311/311 (100%)	310 (100%)	1 (0%)	91	94
30	N3	100/100 (100%)	98 (98%)	2 (2%)	50	70
31	N4	410/410 (100%)	407 (99%)	3 (1%)	81	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	N5	537/537 (100%)	534 (99%)	3 (1%)	84	89
33	N6	140/140 (100%)	140 (100%)	0	100	100
34	S1	579/579 (100%)	571 (99%)	8 (1%)	62	77
35	S2	370/370 (100%)	365 (99%)	5 (1%)	62	77
36	S3	190/190 (100%)	189 (100%)	1 (0%)	86	90
37	S4	112/112 (100%)	110 (98%)	2 (2%)	54	72
38	S5	93/93 (100%)	92 (99%)	1 (1%)	70	81
39	S6	79/79 (100%)	79 (100%)	0	100	100
40	S7	132/132 (100%)	131 (99%)	1 (1%)	79	86
41	S8	151/151 (100%)	148 (98%)	3 (2%)	50	70
42	V1	344/344 (100%)	339 (98%)	5 (2%)	60	75
43	V2	183/183 (100%)	180 (98%)	3 (2%)	58	74
44	V3	41/41 (100%)	40 (98%)	1 (2%)	44	66
All	All	7184/7229 (99%)	7124 (99%)	60 (1%)	77	86

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A5	55	LYS
6	A6	87	ASP
8	A8	205	VAL
9	A9	129	LEU
10	AC	112	SER
11	AK	243	TYR
11	AK	278	LEU
12	AL	11	ASP
12	AL	115	CYS
18	B4	59	VAL
20	B6	132	VAL
20	B6	156	THR
20	B6	157	VAL
22	B8	181	VAL
22	B8	182	VAL
28	N1	9	LEU
28	N1	133	LEU
28	N1	224	PHE
28	N1	251	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	N1	282	TYR
28	N1	296	LEU
29	N2	308	THR
30	N3	18	VAL
30	N3	69	ILE
31	N4	12	LEU
31	N4	122	PHE
31	N4	375	LEU
32	N5	63	ILE
32	N5	310	LEU
32	N5	340	PHE
34	S1	41	VAL
34	S1	427	LEU
34	S1	452	LEU
34	S1	606	THR
34	S1	634	LEU
34	S1	636	TYR
34	S1	674	LEU
34	S1	690	THR
35	S2	100	VAL
35	S2	134	THR
35	S2	204	THR
35	S2	279	VAL
35	S2	362	ILE
36	S3	68	ILE
37	S4	55	VAL
37	S4	152	VAL
38	S5	15	ASP
40	S7	71	CYS
41	S8	76	TYR
41	S8	114	ILE
41	S8	142	THR
42	V1	235	VAL
42	V1	287	THR
42	V1	347	THR
42	V1	379	CYS
42	V1	385	CYS
43	V2	137	THR
43	V2	180	CYS
43	V2	213	ILE
44	V3	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95)

such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	83	ASN
3	A2	48	ASN
3	A2	62	GLN
3	A2	73	GLN
3	A2	81	ASN
4	A3	131	ASN
4	A3	147	ASN
4	A3	156	GLN
5	A5	21	HIS
5	A5	50	GLN
5	A5	86	ASN
6	A6	152	HIS
7	A7	25	GLN
8	A8	142	GLN
9	A9	102	GLN
11	AK	134	GLN
11	AK	217	GLN
11	AK	225	ASN
11	AK	324	HIS
13	AM	13	GLN
13	AM	31	ASN
13	AM	116	ASN
13	AM	122	GLN
13	AM	123	GLN
14	AN	61	GLN
19	B5	109	HIS
19	B5	181	HIS
19	B5	189	ASN
20	B6	73	GLN
20	B6	143	HIS
21	B7	47	ASN
21	B7	54	GLN
21	B7	55	GLN
21	B7	85	HIS
21	B7	110	GLN
22	B8	83	GLN
22	B8	164	ASN
23	B9	117	GLN
24	BK	104	ASN
24	BK	107	GLN
24	BK	124	ASN
25	BL	70	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	BL	115	GLN
27	CB	81	GLN
29	N2	112	HIS
29	N2	144	GLN
29	N2	273	ASN
29	N2	316	GLN
31	N4	44	GLN
31	N4	138	ASN
31	N4	251	ASN
31	N4	304	GLN
31	N4	366	ASN
31	N4	399	ASN
31	N4	415	GLN
31	N4	421	HIS
32	N5	2	ASN
32	N5	59	GLN
32	N5	72	GLN
32	N5	226	GLN
32	N5	230	HIS
32	N5	248	HIS
32	N5	274	GLN
34	S1	51	GLN
34	S1	140	GLN
34	S1	282	ASN
34	S1	336	ASN
34	S1	384	ASN
34	S1	453	GLN
35	S2	85	ASN
35	S2	89	ASN
35	S2	93	GLN
35	S2	229	HIS
35	S2	239	HIS
35	S2	240	GLN
36	S3	55	HIS
36	S3	77	GLN
36	S3	107	GLN
36	S3	131	ASN
37	S4	86	ASN
37	S4	141	ASN
38	S5	45	HIS
39	S6	120	GLN
40	S7	123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	S7	138	ASN
41	S8	42	ASN
41	S8	85	ASN
42	V1	49	HIS
42	V1	277	ASN
42	V1	303	HIS
42	V1	344	GLN
42	V1	436	GLN
43	V2	90	ASN
43	V2	187	GLN
44	V3	383	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
35	2MR	S2	124	35	10,12,13	2.44	2 (20%)	5,13,15	0.97	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
35	2MR	S2	124	35	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	124	2MR	CZ-NE	5.20	1.45	1.34
35	S2	124	2MR	CZ-NH2	5.06	1.44	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 2 are monoatomic - leaving 55 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
51	PLX	S7	302	-	51,51,51	1.11	4 (7%)	55,59,59	0.89	2 (3%)
51	PLX	N3	202	-	51,51,51	1.10	4 (7%)	55,59,59	0.88	1 (1%)
50	ADP	AK	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.43	4 (13%)
53	SF4	S8	302	41	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PEE	N2	403	-	47,47,50	1.35	5 (10%)	50,52,55	1.21	4 (8%)
52	3PE	N4	504	-	50,50,50	0.30	0	53,55,55	0.28	0
53	SF4	V1	501	42	0,12,12	-	-	-		
53	SF4	S8	301	41	0,12,12	-	-	-		
45	CDL	A1	101	-	93,93,99	0.31	0	99,105,111	0.28	0
45	CDL	N1	401	-	77,77,99	0.34	0	83,89,111	0.33	0
53	SF4	S1	801	34	0,12,12	-	-	-		
51	PLX	CB	201	-	51,51,51	1.10	3 (5%)	55,59,59	0.91	1 (1%)
45	CDL	CB	203	-	82,82,99	0.33	0	88,94,111	0.29	0
46	PC1	A3	201	-	49,49,53	0.32	0	55,57,61	0.42	0
48	PEE	S8	303	-	50,50,50	1.32	5 (10%)	53,55,55	1.13	2 (3%)
45	CDL	N5	702	-	99,99,99	0.30	0	105,111,111	0.27	0
52	3PE	B4	201	-	50,50,50	0.31	0	53,55,55	0.29	0
51	PLX	N1	402	-	51,51,51	1.11	4 (7%)	55,59,59	0.86	1 (1%)
48	PEE	AL	205	-	39,39,50	1.48	5 (12%)	41,44,55	1.23	3 (7%)
47	NDP	A9	401	-	45,52,52	0.52	0	53,80,80	0.53	1 (1%)
52	3PE	CB	202	-	50,50,50	0.31	0	53,55,55	0.28	0
45	CDL	AL	202	-	70,70,99	0.34	0	76,82,111	0.31	0
45	CDL	4L	201	-	91,91,99	0.32	0	97,103,111	0.36	0
53	SF4	S1	802	34	0,12,12	-	-	-		
45	CDL	N5	701	-	88,88,99	0.31	0	94,100,111	0.28	0
46	PC1	A3	202	-	53,53,53	0.30	0	59,61,61	0.26	0
48	PEE	N4	501	-	48,48,50	1.35	5 (10%)	51,53,55	1.18	3 (5%)
48	PEE	AN	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.17	3 (5%)
48	PEE	N3	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.15	2 (3%)
53	SF4	S7	301	40	0,12,12	-	-	-		
54	FES	S1	803	34	0,4,4	-	-	-		
45	CDL	N2	402	-	67,67,99	0.35	0	73,79,111	0.28	0
46	PC1	B5	203	-	53,53,53	0.29	0	59,61,61	0.26	0
56	MF8	S2	501	-	7,8,8	0.99	0	7,10,10	1.48	1 (14%)
49	ZMP	AC	201	10	29,35,36	0.66	1 (3%)	34,42,45	0.77	0
58	FMN	V1	502	-	33,33,33	0.22	0	48,50,50	0.44	0
46	PC1	N3	204	-	53,53,53	0.29	0	59,61,61	0.29	0
46	PC1	B8	201	-	40,40,53	0.33	0	46,48,61	0.37	0
45	CDL	B5	202	-	99,99,99	0.31	0	105,111,111	0.27	0
51	PLX	AL	204	-	46,46,51	1.16	4 (8%)	50,54,59	0.87	1 (2%)
48	PEE	B6	201	-	45,45,50	1.39	5 (11%)	48,50,55	1.20	2 (4%)
51	PLX	B5	201	-	51,51,51	1.10	4 (7%)	55,59,59	0.88	1 (1%)
48	PEE	AL	203	-	35,35,50	1.37	4 (11%)	38,40,55	1.15	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.31	0
48	PEE	N2	401	-	34,34,50	1.41	5 (14%)	37,39,55	1.23	2 (5%)
48	PEE	N5	703	-	50,50,50	1.32	5 (10%)	53,55,55	1.16	3 (5%)
54	FES	V2	301	43	0,4,4	-	-	-	-	-
45	CDL	N4	503	-	99,99,99	0.30	0	105,111,111	0.26	0
46	PC1	N3	203	-	53,53,53	0.29	0	59,61,61	0.26	0
46	PC1	AN	202	-	53,53,53	0.29	0	59,61,61	0.31	0
48	PEE	N1	403	-	30,30,50	1.28	3 (10%)	33,35,55	1.16	2 (6%)
48	PEE	A9	402	-	38,38,50	1.49	5 (13%)	41,43,55	1.22	3 (7%)
51	PLX	N4	502	-	42,42,51	1.18	3 (7%)	46,50,59	0.89	2 (4%)
49	ZMP	AB	201	10	29,35,36	0.64	1 (3%)	34,42,45	0.73	0
48	PEE	AK	402	-	39,39,50	1.33	4 (10%)	42,44,55	1.17	4 (9%)

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
51	PLX	S7	302	-	-	20/55/55/55	-
51	PLX	N3	202	-	-	21/55/55/55	-
50	ADP	AK	401	-	-	1/12/32/32	0/3/3/3
53	SF4	S8	302	41	-	-	0/6/5/5
48	PEE	N2	403	-	-	26/51/51/54	-
52	3PE	N4	504	-	-	17/54/54/54	-
53	SF4	V1	501	42	-	-	0/6/5/5
53	SF4	S8	301	41	-	-	0/6/5/5
45	CDL	A1	101	-	-	19/104/104/110	-
45	CDL	N1	401	-	-	22/88/88/110	-
53	SF4	S1	801	34	-	-	0/6/5/5
51	PLX	CB	201	-	-	16/55/55/55	-
45	CDL	CB	203	-	-	16/93/93/110	-
46	PC1	A3	201	-	-	19/53/53/57	-
48	PEE	S8	303	-	-	24/54/54/54	-
45	CDL	N5	702	-	-	18/110/110/110	-
52	3PE	B4	201	-	-	16/54/54/54	-
51	PLX	N1	402	-	-	23/55/55/55	-
48	PEE	AL	205	-	-	23/43/43/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	NDP	A9	401	-	-	6/30/77/77	0/5/5/5
52	3PE	CB	202	-	-	11/54/54/54	-
45	CDL	AL	202	-	-	18/81/81/110	-
45	CDL	4L	201	-	-	25/102/102/110	-
53	SF4	S1	802	34	-	-	0/6/5/5
45	CDL	N5	701	-	-	17/99/99/110	-
46	PC1	A3	202	-	-	11/57/57/57	-
48	PEE	N4	501	-	-	26/52/52/54	-
48	PEE	AN	201	-	-	24/54/54/54	-
48	PEE	N3	201	-	-	30/54/54/54	-
53	SF4	S7	301	40	-	-	0/6/5/5
54	FES	S1	803	34	-	-	0/1/1/1
45	CDL	N2	402	-	-	14/78/78/110	-
46	PC1	B5	203	-	-	5/57/57/57	-
56	MF8	S2	501	-	-	5/8/8/8	-
49	ZMP	AC	201	10	-	19/40/42/43	-
58	FMN	V1	502	-	-	4/18/18/18	0/3/3/3
46	PC1	N3	204	-	-	11/57/57/57	-
46	PC1	B8	201	-	-	15/44/44/57	-
45	CDL	B5	202	-	-	18/110/110/110	-
51	PLX	AL	204	-	-	23/50/50/55	-
48	PEE	B6	201	-	-	28/49/49/54	-
51	PLX	B5	201	-	-	19/55/55/55	-
48	PEE	AL	203	-	-	17/39/39/54	-
45	CDL	AL	201	-	-	13/104/104/110	-
48	PEE	N2	401	-	-	19/38/38/54	-
48	PEE	N5	703	-	-	26/54/54/54	-
54	FES	V2	301	43	-	-	0/1/1/1
45	CDL	N4	503	-	-	23/110/110/110	-
46	PC1	N3	203	-	-	14/57/57/57	-
46	PC1	AN	202	-	-	11/57/57/57	-
48	PEE	N1	403	-	-	16/34/34/54	-
48	PEE	A9	402	-	-	20/42/42/54	-
51	PLX	N4	502	-	-	13/46/46/55	-
49	ZMP	AB	201	10	-	13/40/42/43	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	AK	402	-	-	27/43/43/54	-

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S8	303	PEE	C18-C19	4.06	1.55	1.31
48	N2	401	PEE	C18-C19	4.05	1.55	1.31
48	A9	402	PEE	C18-C19	4.05	1.55	1.31
48	AL	205	PEE	C18-C19	4.05	1.55	1.31
48	AK	402	PEE	C18-C19	4.05	1.55	1.31
48	B6	201	PEE	C18-C19	4.04	1.55	1.31
48	N5	703	PEE	C18-C19	4.04	1.55	1.31
48	AN	201	PEE	C18-C19	4.04	1.55	1.31
48	N3	201	PEE	C18-C19	4.03	1.55	1.31
48	N2	403	PEE	C18-C19	4.03	1.55	1.31
48	N4	501	PEE	C18-C19	4.03	1.55	1.31
48	AN	201	PEE	C39-C38	3.96	1.54	1.31
48	N4	501	PEE	C39-C38	3.95	1.54	1.31
48	B6	201	PEE	C39-C38	3.95	1.54	1.31
48	AL	203	PEE	C39-C38	3.94	1.54	1.31
48	S8	303	PEE	C39-C38	3.94	1.54	1.31
48	AL	205	PEE	C39-C38	3.94	1.54	1.31
48	N5	703	PEE	C39-C38	3.94	1.54	1.31
48	N3	201	PEE	C39-C38	3.93	1.54	1.31
48	N2	403	PEE	C39-C38	3.91	1.54	1.31
48	A9	402	PEE	C39-C38	3.87	1.54	1.28
48	N1	403	PEE	O3-C30	3.27	1.42	1.33
48	N5	703	PEE	O3-C30	3.26	1.42	1.33
48	AL	203	PEE	O3-C30	3.26	1.42	1.33
48	AN	201	PEE	O3-C30	3.24	1.42	1.33
48	A9	402	PEE	O3-C30	3.24	1.42	1.33
48	AK	402	PEE	O3-C30	3.22	1.42	1.33
48	N2	401	PEE	O3-C30	3.22	1.42	1.33
48	S8	303	PEE	O3-C30	3.22	1.42	1.33
48	B6	201	PEE	O3-C30	3.22	1.42	1.33
48	AL	205	PEE	O3-C30	3.20	1.42	1.33
48	N3	201	PEE	O3-C30	3.20	1.42	1.33
48	N4	501	PEE	O3-C30	3.18	1.42	1.33
48	N2	403	PEE	O3-C30	3.17	1.42	1.33
51	S7	302	PLX	O6-C4	-3.06	1.40	1.44
51	AL	204	PLX	O6-C4	-2.95	1.40	1.44
51	N4	502	PLX	O6-C4	-2.95	1.40	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	B5	201	PLX	O6-C4	-2.87	1.40	1.44
51	CB	201	PLX	O6-C4	-2.87	1.40	1.44
51	N1	402	PLX	O6-C4	-2.86	1.40	1.44
51	N3	202	PLX	O6-C4	-2.82	1.40	1.44
48	N2	401	PEE	O2-C10	2.77	1.42	1.34
48	S8	303	PEE	O2-C10	2.75	1.42	1.34
48	AL	205	PEE	O2-C10	2.72	1.42	1.34
48	N2	403	PEE	O2-C10	2.70	1.41	1.34
48	AK	402	PEE	O2-C10	2.67	1.41	1.34
48	B6	201	PEE	O2-C10	2.67	1.41	1.34
48	A9	402	PEE	O2-C10	2.66	1.41	1.34
48	N5	703	PEE	O2-C10	2.64	1.41	1.34
48	N3	201	PEE	O2-C10	2.63	1.41	1.34
48	AN	201	PEE	O2-C10	2.62	1.41	1.34
48	N4	501	PEE	O2-C10	2.61	1.41	1.34
48	N1	403	PEE	O2-C10	2.59	1.41	1.34
48	AL	203	PEE	O2-C10	2.59	1.41	1.34
48	N4	501	PEE	O2-C2	-2.52	1.40	1.46
48	N3	201	PEE	O2-C2	-2.50	1.40	1.46
48	A9	402	PEE	O2-C2	-2.50	1.40	1.46
48	AL	203	PEE	O2-C2	-2.49	1.40	1.46
48	N1	403	PEE	O2-C2	-2.49	1.40	1.46
49	AC	201	ZMP	C9-C10	-2.48	1.48	1.50
48	N2	403	PEE	O2-C2	-2.48	1.40	1.46
48	N5	703	PEE	O2-C2	-2.48	1.40	1.46
48	AN	201	PEE	O2-C2	-2.46	1.40	1.46
50	AK	401	ADP	C5-C4	2.44	1.47	1.40
48	B6	201	PEE	O2-C2	-2.42	1.40	1.46
48	AK	402	PEE	O2-C2	-2.41	1.40	1.46
49	AB	201	ZMP	C9-C10	-2.39	1.48	1.50
48	AL	205	PEE	O2-C2	-2.36	1.40	1.46
48	N2	401	PEE	O2-C2	-2.30	1.40	1.46
48	S8	303	PEE	O2-C2	-2.23	1.41	1.46
51	AL	204	PLX	C1B-N1	-2.16	1.43	1.50
51	B5	201	PLX	C1B-N1	-2.16	1.43	1.50
51	N4	502	PLX	C1B-N1	-2.15	1.43	1.50
51	N3	202	PLX	C1B-N1	-2.14	1.43	1.50
51	CB	201	PLX	C1B-N1	-2.13	1.43	1.50
51	S7	302	PLX	C1B-N1	-2.12	1.43	1.50
51	N1	402	PLX	C1B-N1	-2.10	1.43	1.50
51	AL	204	PLX	C1A-N1	-2.05	1.44	1.50
51	S7	302	PLX	C1A-N1	-2.04	1.44	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	N1	402	PLX	P1-O4	2.03	1.67	1.59
51	N3	202	PLX	P1-O4	2.03	1.67	1.59
51	B5	201	PLX	P1-O4	2.03	1.67	1.59
51	N3	202	PLX	C1A-N1	-2.03	1.44	1.50
51	N4	502	PLX	P1-O4	2.02	1.67	1.59
51	N1	402	PLX	C1A-N1	-2.02	1.44	1.50
51	CB	201	PLX	C1A-N1	-2.02	1.44	1.50
51	B5	201	PLX	C1A-N1	-2.01	1.44	1.50
51	AL	204	PLX	P1-O4	2.01	1.67	1.59
51	S7	302	PLX	P1-O4	2.00	1.67	1.59
48	N2	401	PEE	C11-C10	2.00	1.56	1.50

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N2	403	PEE	O2-C10-C11	4.40	120.99	111.50
48	N2	401	PEE	O2-C10-C11	4.38	120.95	111.50
48	AK	402	PEE	O2-C10-C11	4.27	120.71	111.50
48	AL	205	PEE	O2-C10-C11	4.08	120.28	111.50
48	B6	201	PEE	O2-C10-C11	4.01	120.15	111.50
48	N5	703	PEE	O2-C10-C11	4.00	120.11	111.50
48	N1	403	PEE	O2-C10-C11	3.96	120.03	111.50
48	N4	501	PEE	O2-C10-C11	3.93	119.97	111.50
48	S8	303	PEE	O2-C10-C11	3.93	119.97	111.50
48	AN	201	PEE	O2-C10-C11	3.90	119.92	111.50
48	N3	201	PEE	O2-C10-C11	3.82	119.72	111.50
48	A9	402	PEE	O2-C10-C11	3.78	119.66	111.50
56	S2	501	MF8	C07-N06-C04	3.55	132.32	124.55
50	AK	401	ADP	PA-O3A-PB	-3.36	121.29	132.83
48	AL	203	PEE	O2-C10-C11	3.35	120.14	110.80
50	AK	401	ADP	N3-C2-N1	-3.19	123.69	128.68
50	AK	401	ADP	C3'-C2'-C1'	3.16	105.74	100.98
48	B6	201	PEE	O3-C30-C31	2.67	120.29	111.91
50	AK	401	ADP	C4-C5-N7	-2.63	106.66	109.40
48	AL	203	PEE	O3-C30-C31	2.63	120.15	111.91
48	N1	403	PEE	O3-C30-C31	2.59	120.05	111.91
48	N4	501	PEE	O3-C30-C31	2.59	120.03	111.91
48	S8	303	PEE	O3-C30-C31	2.56	119.93	111.91
48	N2	401	PEE	O3-C30-C31	2.55	119.92	111.91
48	N5	703	PEE	O3-C30-C31	2.55	119.92	111.91
48	A9	402	PEE	C37-C38-C39	-2.55	109.50	126.84
48	AN	201	PEE	O3-C30-C31	2.54	119.89	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N3	201	PEE	O3-C30-C31	2.53	119.85	111.91
48	AL	205	PEE	O3-C30-C31	2.50	119.75	111.91
48	A9	402	PEE	O3-C30-C31	2.48	119.70	111.91
48	N2	403	PEE	O3-C30-C31	2.43	119.53	111.91
48	AK	402	PEE	O3-C30-C31	2.41	119.47	111.91
47	A9	401	NDP	C5A-C6A-N6A	2.29	123.84	120.35
51	CB	201	PLX	O3-P1-O2	-2.25	101.10	112.24
51	N1	402	PLX	O3-P1-O2	-2.24	101.18	112.24
51	B5	201	PLX	O3-P1-O2	-2.23	101.24	112.24
51	S7	302	PLX	O3-P1-O2	-2.22	101.26	112.24
51	N4	502	PLX	O3-P1-O2	-2.20	101.35	112.24
51	N3	202	PLX	O3-P1-O2	-2.20	101.39	112.24
51	AL	204	PLX	O3-P1-O2	-2.19	101.39	112.24
51	S7	302	PLX	C8-C7-C6	-2.10	108.53	113.38
51	N4	502	PLX	C26-C25-C24	-2.09	108.55	113.38
48	N2	403	PEE	C37-C38-C39	-2.05	109.01	124.73
48	N5	703	PEE	C17-C18-C19	-2.04	109.08	124.73
48	N4	501	PEE	C17-C18-C19	-2.03	109.18	124.73
48	AN	201	PEE	C20-C19-C18	-2.02	109.19	124.73
48	N2	403	PEE	C20-C19-C18	-2.02	109.23	124.73
48	AL	205	PEE	C17-C18-C19	-2.02	109.24	124.73
48	AK	402	PEE	C20-C19-C18	-2.01	109.27	124.73
48	AK	402	PEE	C17-C18-C19	-2.00	109.35	124.73

There are no chirality outliers.

All (822) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	4L	201	CDL	CA2-OA2-PA1-OA3
45	4L	201	CDL	CA2-OA2-PA1-OA4
45	4L	201	CDL	CA2-OA2-PA1-OA5
45	4L	201	CDL	CA3-OA5-PA1-OA3
45	4L	201	CDL	CB2-OB2-PB2-OB3
45	4L	201	CDL	CB2-OB2-PB2-OB4
45	4L	201	CDL	CB3-OB5-PB2-OB3
45	A1	101	CDL	CA2-OA2-PA1-OA4
45	AL	201	CDL	CB2-OB2-PB2-OB5
45	AL	202	CDL	CA2-OA2-PA1-OA3
45	AL	202	CDL	CA3-OA5-PA1-OA3
45	AL	202	CDL	CA3-OA5-PA1-OA4
45	AL	202	CDL	CB2-OB2-PB2-OB3
45	AL	202	CDL	OB5-CB3-CB4-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	B5	202	CDL	CA3-OA5-PA1-OA3
45	B5	202	CDL	CA3-OA5-PA1-OA4
45	CB	203	CDL	CA3-OA5-PA1-OA3
45	N1	401	CDL	CA3-OA5-PA1-OA4
45	N1	401	CDL	CB2-OB2-PB2-OB3
45	N1	401	CDL	CB2-OB2-PB2-OB4
45	N1	401	CDL	CB2-OB2-PB2-OB5
45	N2	402	CDL	CA2-OA2-PA1-OA4
45	N2	402	CDL	CA3-OA5-PA1-OA4
45	N2	402	CDL	CA4-CA3-OA5-PA1
45	N5	701	CDL	CA2-OA2-PA1-OA3
45	N5	701	CDL	CA2-OA2-PA1-OA4
45	N5	701	CDL	CA2-OA2-PA1-OA5
45	N5	701	CDL	CA3-OA5-PA1-OA2
45	N5	701	CDL	CA3-OA5-PA1-OA3
45	N5	701	CDL	CA3-OA5-PA1-OA4
45	N5	701	CDL	CB2-OB2-PB2-OB4
45	N5	701	CDL	CB3-OB5-PB2-OB3
45	N5	702	CDL	CA2-OA2-PA1-OA4
45	N5	702	CDL	CA3-OA5-PA1-OA2
46	A3	201	PC1	C1-O11-P-O14
46	A3	201	PC1	O21-C2-C3-O31
46	A3	202	PC1	C1-O11-P-O14
46	AN	202	PC1	C11-O13-P-O12
46	AN	202	PC1	C11-O13-P-O11
46	AN	202	PC1	C1-O11-P-O14
46	B8	201	PC1	C11-O13-P-O14
46	N3	203	PC1	C11-O13-P-O12
46	N3	203	PC1	C11-O13-P-O14
46	N3	204	PC1	C11-O13-P-O12
46	N3	204	PC1	C11-O13-P-O14
46	N3	204	PC1	C11-O13-P-O11
47	A9	401	NDP	C2N-C3N-C7N-N7N
48	A9	402	PEE	C4-O4P-P-O1P
48	AK	402	PEE	O4-C10-O2-C2
48	AK	402	PEE	O4P-C4-C5-N
48	AL	205	PEE	C18-C19-C20-C21
48	AL	205	PEE	C1-O3P-P-O2P
48	AL	205	PEE	C1-O3P-P-O1P
48	AL	205	PEE	C1-O3P-P-O4P
48	AL	205	PEE	O4P-C4-C5-N
48	AN	201	PEE	C1-O3P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	AN	201	PEE	C4-O4P-P-O3P
48	AN	201	PEE	C4-O4P-P-O2P
48	AN	201	PEE	C4-O4P-P-O1P
48	B6	201	PEE	C11-C10-O2-C2
48	B6	201	PEE	C1-O3P-P-O2P
48	B6	201	PEE	C1-O3P-P-O1P
48	B6	201	PEE	C4-O4P-P-O1P
48	N1	403	PEE	C1-O3P-P-O2P
48	N2	401	PEE	C11-C10-O2-C2
48	N2	401	PEE	O4-C10-O2-C2
48	N2	401	PEE	C1-O3P-P-O1P
48	N2	403	PEE	C11-C10-O2-C2
48	N2	403	PEE	O4-C10-O2-C2
48	N3	201	PEE	C4-O4P-P-O1P
48	N3	201	PEE	O4P-C4-C5-N
48	N4	501	PEE	O3P-C1-C2-O2
48	N5	703	PEE	C1-O3P-P-O2P
48	N5	703	PEE	C1-O3P-P-O1P
48	N5	703	PEE	C4-O4P-P-O2P
48	N5	703	PEE	C4-O4P-P-O1P
48	S8	303	PEE	C17-C18-C19-C20
48	S8	303	PEE	C4-O4P-P-O3P
48	S8	303	PEE	C37-C38-C39-C40
49	AC	201	ZMP	C17-C18-C21-O5
49	AC	201	ZMP	S1-C11-C12-N1
49	AC	201	ZMP	O1-C10-S1-C11
49	AC	201	ZMP	C9-C10-S1-C11
49	AC	201	ZMP	C7-C8-C9-C10
51	AL	204	PLX	O7-C6-C7-C8
51	AL	204	PLX	O7-C6-O6-C4
51	AL	204	PLX	C3-O4-P1-O2
51	AL	204	PLX	C3-O4-P1-O3
51	AL	204	PLX	N1-C1-C2-O1
51	CB	201	PLX	O7-C6-C7-C8
51	CB	201	PLX	C7-C6-O6-C4
51	CB	201	PLX	O7-C6-O6-C4
51	CB	201	PLX	O4-C3-C4-O6
51	CB	201	PLX	C2-O1-P1-O4
51	CB	201	PLX	C2-O1-P1-O3
51	CB	201	PLX	N1-C1-C2-O1
51	N1	402	PLX	O7-C6-O6-C4
51	N1	402	PLX	C3-O4-P1-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	N1	402	PLX	N1-C1-C2-O1
51	N1	402	PLX	O9-C24-O8-C5
51	N3	202	PLX	O7-C6-O6-C4
51	N3	202	PLX	C3-O4-P1-O1
51	N3	202	PLX	C3-O4-P1-O2
51	N3	202	PLX	O9-C24-O8-C5
51	N4	502	PLX	C3-O4-P1-O2
51	N4	502	PLX	C3-O4-P1-O3
51	N4	502	PLX	O9-C24-O8-C5
51	S7	302	PLX	O7-C6-O6-C4
51	S7	302	PLX	C2-O1-P1-O3
52	B4	201	3PE	C1-O11-P-O12
52	B4	201	3PE	C1-O11-P-O14
52	B4	201	3PE	C11-O13-P-O12
52	B4	201	3PE	C11-O13-P-O14
52	B4	201	3PE	O13-C11-C12-N
52	CB	202	3PE	C11-O13-P-O12
52	N4	504	3PE	C1-O11-P-O12
52	N4	504	3PE	C1-O11-P-O13
52	N4	504	3PE	C1-O11-P-O14
52	N4	504	3PE	C11-O13-P-O12
52	N4	504	3PE	C2-C1-O11-P
52	N4	504	3PE	C12-C11-O13-P
52	N4	504	3PE	O13-C11-C12-N
58	V1	502	FMN	C5'-O5'-P-O1P
58	V1	502	FMN	C5'-O5'-P-O2P
58	V1	502	FMN	C5'-O5'-P-O3P
48	A9	402	PEE	O5-C30-O3-C3
48	A9	402	PEE	C31-C30-O3-C3
48	N3	201	PEE	O5-C30-O3-C3
48	B6	201	PEE	O4-C10-O2-C2
48	N3	201	PEE	C31-C30-O3-C3
48	AK	402	PEE	C11-C10-O2-C2
48	AL	203	PEE	O5-C30-O3-C3
48	AL	203	PEE	C31-C30-O3-C3
48	AK	402	PEE	C17-C18-C19-C20
48	N2	403	PEE	C17-C18-C19-C20
48	S8	303	PEE	O4-C10-O2-C2
48	S8	303	PEE	C11-C10-O2-C2
45	CB	203	CDL	C52-C53-C54-C55
46	N3	203	PC1	C11-C12-N-C13
48	N3	201	PEE	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	N5	701	CDL	CA5-C11-C12-C13
48	N5	703	PEE	C10-C11-C12-C13
48	N3	201	PEE	C37-C38-C39-C40
48	N5	703	PEE	C37-C38-C39-C40
48	AN	201	PEE	C10-C11-C12-C13
48	AN	201	PEE	C30-C31-C32-C33
48	N1	403	PEE	C10-C11-C12-C13
45	N4	503	CDL	C74-C75-C76-C77
48	AK	402	PEE	C10-C11-C12-C13
48	N4	501	PEE	C10-C11-C12-C13
45	4L	201	CDL	CB2-OB2-PB2-OB5
45	4L	201	CDL	CB3-OB5-PB2-OB2
45	A1	101	CDL	CA2-OA2-PA1-OA5
45	A1	101	CDL	CB3-OB5-PB2-OB2
45	AL	202	CDL	CA3-OA5-PA1-OA2
45	B5	202	CDL	CA3-OA5-PA1-OA2
45	B5	202	CDL	CB2-OB2-PB2-OB5
45	CB	203	CDL	CA2-OA2-PA1-OA5
45	N2	402	CDL	CA2-OA2-PA1-OA5
45	N2	402	CDL	CB2-OB2-PB2-OB5
45	N5	701	CDL	CB2-OB2-PB2-OB5
45	N5	701	CDL	CB3-OB5-PB2-OB2
45	N5	702	CDL	CA2-OA2-PA1-OA5
46	A3	201	PC1	C11-O13-P-O11
46	B5	203	PC1	C11-O13-P-O11
46	N3	203	PC1	C11-O13-P-O11
48	AK	402	PEE	C4-O4P-P-O3P
48	AL	203	PEE	C4-O4P-P-O3P
48	N1	403	PEE	C1-O3P-P-O4P
48	N1	403	PEE	C4-O4P-P-O3P
48	N5	703	PEE	C1-O3P-P-O4P
48	N5	703	PEE	C4-O4P-P-O3P
51	AL	204	PLX	C3-O4-P1-O1
51	AL	204	PLX	C2-O1-P1-O4
51	N1	402	PLX	C3-O4-P1-O1
51	N3	202	PLX	C2-O1-P1-O4
51	N4	502	PLX	C3-O4-P1-O1
51	S7	302	PLX	C2-O1-P1-O4
52	B4	201	3PE	C1-O11-P-O13
52	B4	201	3PE	C11-O13-P-O11
52	CB	202	3PE	C1-O11-P-O13
52	CB	202	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	N4	504	3PE	C11-O13-P-O11
48	N1	403	PEE	C30-C31-C32-C33
46	N3	203	PC1	C11-C12-N-C14
48	N3	201	PEE	C11-C12-C13-C14
51	AL	204	PLX	O6-C6-C7-C8
51	N1	402	PLX	O8-C24-C25-C26
51	N3	202	PLX	O6-C6-C7-C8
48	A9	402	PEE	C11-C12-C13-C14
51	B5	201	PLX	C26-C27-C28-C29
48	N1	403	PEE	C12-C13-C14-C15
48	N1	403	PEE	C11-C12-C13-C14
48	N2	401	PEE	C11-C12-C13-C14
48	N3	201	PEE	C34-C35-C36-C37
48	N5	703	PEE	C33-C34-C35-C36
46	N3	203	PC1	C26-C27-C28-C29
48	N2	403	PEE	C32-C33-C34-C35
49	AB	201	ZMP	C1-C2-C3-C4
48	N4	501	PEE	C11-C12-C13-C14
49	AB	201	ZMP	C5-C6-C7-C8
51	AL	204	PLX	C12-C13-C14-C15
48	AL	203	PEE	C37-C38-C39-C40
48	AL	205	PEE	C37-C38-C39-C40
48	AN	201	PEE	C12-C13-C14-C15
48	N3	201	PEE	C31-C32-C33-C34
48	S8	303	PEE	C12-C13-C14-C15
45	AL	202	CDL	CA5-C11-C12-C13
48	A9	402	PEE	C30-C31-C32-C33
48	N2	403	PEE	C10-C11-C12-C13
46	N3	203	PC1	C33-C34-C35-C36
51	N4	502	PLX	C33-C34-C35-C36
48	AL	203	PEE	C34-C35-C36-C37
48	AL	205	PEE	C14-C15-C16-C17
51	CB	201	PLX	C7-C8-C9-C10
48	AL	205	PEE	C11-C12-C13-C14
48	N2	403	PEE	C12-C13-C14-C15
51	N1	402	PLX	C27-C28-C29-C30
52	CB	202	3PE	C2A-C2B-C2C-C2D
48	B6	201	PEE	C21-C22-C23-C24
48	N2	403	PEE	C35-C36-C37-C38
45	N4	503	CDL	C79-C80-C81-C82
48	AN	201	PEE	C14-C15-C16-C17
48	B6	201	PEE	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	N3	201	PEE	C33-C34-C35-C36
51	AL	204	PLX	C9-C10-C11-C12
51	AL	204	PLX	C31-C32-C33-C34
46	A3	201	PC1	C11-C12-N-C13
45	N5	702	CDL	C11-C12-C13-C14
45	N5	702	CDL	C82-C83-C84-C85
48	AK	402	PEE	C12-C13-C14-C15
48	N2	403	PEE	C31-C32-C33-C34
52	B4	201	3PE	C36-C37-C38-C39
45	N5	702	CDL	C60-C61-C62-C63
46	N3	204	PC1	C37-C38-C39-C3A
48	AK	402	PEE	C21-C22-C23-C24
48	S8	303	PEE	C22-C23-C24-C25
51	CB	201	PLX	C10-C11-C12-C13
51	S7	302	PLX	C9-C10-C11-C12
45	B5	202	CDL	CB5-C51-C52-C53
48	AL	205	PEE	C12-C13-C14-C15
51	CB	201	PLX	C16-C17-C18-C19
45	B5	202	CDL	C78-C79-C80-C81
49	AB	201	ZMP	C6-C7-C8-C9
48	S8	303	PEE	C11-C12-C13-C14
51	B5	201	PLX	C35-C36-C37-C38
45	N4	503	CDL	C42-C43-C44-C45
48	AK	402	PEE	C1-C2-C3-O3
45	A1	101	CDL	C18-C19-C20-C21
45	N5	702	CDL	C17-C18-C19-C20
52	CB	202	3PE	C31-C32-C33-C34
49	AC	201	ZMP	C6-C7-C8-C9
51	AL	204	PLX	O9-C24-C25-C26
51	B5	201	PLX	O9-C24-C25-C26
51	N1	402	PLX	O9-C24-C25-C26
51	N3	202	PLX	O9-C24-C25-C26
51	S7	302	PLX	O7-C6-C7-C8
51	S7	302	PLX	O9-C24-C25-C26
48	N2	403	PEE	C43-C44-C45-C46
49	AC	201	ZMP	C3-C4-C5-C6
51	CB	201	PLX	C31-C32-C33-C34
51	N1	402	PLX	C11-C10-C9-C8
48	AL	203	PEE	C35-C36-C37-C38
48	S8	303	PEE	C35-C36-C37-C38
48	N2	403	PEE	C14-C15-C16-C17
46	A3	201	PC1	C38-C39-C3A-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	N4	503	CDL	C81-C82-C83-C84
46	A3	201	PC1	C35-C36-C37-C38
51	AL	204	PLX	C11-C10-C9-C8
51	N1	402	PLX	C31-C32-C33-C34
46	N3	203	PC1	C11-C12-N-C15
48	AK	402	PEE	C14-C15-C16-C17
48	AN	201	PEE	C41-C42-C43-C44
48	N4	501	PEE	C12-C13-C14-C15
46	B8	201	PC1	C39-C3A-C3B-C3C
48	B6	201	PEE	C12-C13-C14-C15
48	N4	501	PEE	C30-C31-C32-C33
48	N3	201	PEE	C12-C13-C14-C15
49	AC	201	ZMP	C22-C23-C24-C25
48	AN	201	PEE	C35-C36-C37-C38
48	B6	201	PEE	C19-C20-C21-C22
48	N4	501	PEE	C35-C36-C37-C38
48	S8	303	PEE	C15-C16-C17-C18
48	AL	203	PEE	O4-C10-O2-C2
48	N4	501	PEE	O4-C10-O2-C2
48	B6	201	PEE	C30-C31-C32-C33
48	N3	201	PEE	C14-C15-C16-C17
46	N3	203	PC1	C27-C28-C29-C2A
51	B5	201	PLX	C27-C28-C29-C30
52	N4	504	3PE	C21-C22-C23-C24
49	AB	201	ZMP	C22-C23-C24-C25
45	CB	203	CDL	C56-C57-C58-C59
46	AN	202	PC1	C3C-C3D-C3E-C3F
51	S7	302	PLX	C11-C12-C13-C14
45	N5	701	CDL	C56-C57-C58-C59
46	B5	203	PC1	C38-C39-C3A-C3B
48	AL	203	PEE	C11-C10-O2-C2
48	N4	501	PEE	C11-C10-O2-C2
51	AL	204	PLX	O4-C3-C4-O6
46	A3	202	PC1	C3E-C3F-C3G-C3H
51	N1	402	PLX	C7-C8-C9-C10
51	B5	201	PLX	C16-C17-C18-C19
46	N3	204	PC1	O21-C2-C3-O31
48	AN	201	PEE	O2-C2-C3-O3
45	B5	202	CDL	C59-C60-C61-C62
51	B5	201	PLX	C7-C8-C9-C10
48	A9	402	PEE	C35-C36-C37-C38
48	AL	205	PEE	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	B6	201	PEE	C35-C36-C37-C38
48	N2	401	PEE	C15-C16-C17-C18
48	N3	201	PEE	C15-C16-C17-C18
48	N5	703	PEE	C35-C36-C37-C38
51	N3	202	PLX	C16-C17-C18-C19
48	B6	201	PEE	C37-C38-C39-C40
45	4L	201	CDL	C16-C17-C18-C19
45	CB	203	CDL	C55-C56-C57-C58
49	AB	201	ZMP	C3-C4-C5-C6
48	N3	201	PEE	C16-C17-C18-C19
46	A3	202	PC1	C1-O11-P-O13
46	AN	202	PC1	C1-O11-P-O13
46	B8	201	PC1	C11-O13-P-O11
48	AL	205	PEE	C4-O4P-P-O3P
48	AN	201	PEE	C1-O3P-P-O4P
48	B6	201	PEE	C1-O3P-P-O4P
48	B6	201	PEE	C4-O4P-P-O3P
46	AN	202	PC1	C2-C1-O11-P
45	AL	202	CDL	OB5-CB3-CB4-CB6
45	CB	203	CDL	OA5-CA3-CA4-CA6
45	N1	401	CDL	OB5-CB3-CB4-CB6
45	N4	503	CDL	OB5-CB3-CB4-CB6
48	AL	205	PEE	O3P-C1-C2-C3
48	N2	401	PEE	O3P-C1-C2-C3
48	N3	201	PEE	O3P-C1-C2-C3
48	N4	501	PEE	O3P-C1-C2-C3
51	CB	201	PLX	O4-C3-C4-C5
45	N2	402	CDL	C31-C32-C33-C34
52	CB	202	3PE	C2E-C2F-C2G-C2H
48	B6	201	PEE	C14-C15-C16-C17
49	AC	201	ZMP	C2-C3-C4-C5
48	N3	201	PEE	C35-C36-C37-C38
48	B6	201	PEE	C32-C33-C34-C35
51	AL	204	PLX	C32-C33-C34-C35
51	AL	204	PLX	C34-C35-C36-C37
46	A3	201	PC1	C11-C12-N-C14
46	A3	201	PC1	C11-C12-N-C15
46	A3	201	PC1	C1-C2-C3-O31
46	N3	204	PC1	C1-C2-C3-O31
48	N1	403	PEE	C1-C2-C3-O3
48	N2	403	PEE	C1-C2-C3-O3
51	N1	402	PLX	C3-C4-C5-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	N5	703	PEE	C12-C13-C14-C15
51	N4	502	PLX	C9-C10-C11-C12
51	B5	201	PLX	O8-C24-C25-C26
49	AB	201	ZMP	O3-C16-C17-O4
51	B5	201	PLX	C14-C15-C16-C17
48	AN	201	PEE	C19-C20-C21-C22
45	N4	503	CDL	C53-C54-C55-C56
46	A3	201	PC1	C33-C34-C35-C36
51	CB	201	PLX	C11-C12-C13-C14
48	S8	303	PEE	C3-C2-O2-C10
51	N4	502	PLX	C31-C32-C33-C34
48	N2	401	PEE	C12-C13-C14-C15
45	AL	202	CDL	OA5-CA3-CA4-OA6
46	A3	202	PC1	O11-C1-C2-O21
48	S8	303	PEE	C32-C33-C34-C35
48	B6	201	PEE	O2-C2-C3-O3
48	N1	403	PEE	O2-C2-C3-O3
48	N2	403	PEE	C21-C22-C23-C24
48	S8	303	PEE	C31-C32-C33-C34
48	N3	201	PEE	C20-C21-C22-C23
48	N4	501	PEE	C21-C22-C23-C24
48	AK	402	PEE	C22-C23-C24-C25
51	CB	201	PLX	C15-C16-C17-C18
48	N2	401	PEE	C21-C22-C23-C24
48	N1	403	PEE	C14-C15-C16-C17
48	AN	201	PEE	C17-C18-C19-C20
48	N5	703	PEE	C17-C18-C19-C20
48	A9	402	PEE	C10-C11-C12-C13
52	CB	202	3PE	C38-C39-C3A-C3B
45	B5	202	CDL	C53-C54-C55-C56
46	B8	201	PC1	O11-C1-C2-C3
46	N3	203	PC1	O11-C1-C2-C3
48	N2	403	PEE	O3P-C1-C2-C3
51	AL	204	PLX	O4-C3-C4-C5
51	N1	402	PLX	O4-C3-C4-C5
51	S7	302	PLX	O4-C3-C4-C5
48	B6	201	PEE	O4P-C4-C5-N
45	B5	202	CDL	C17-C18-C19-C20
52	N4	504	3PE	C29-C2A-C2B-C2C
46	A3	202	PC1	C22-C23-C24-C25
48	N2	403	PEE	C31-C30-O3-C3
45	N4	503	CDL	CB5-C51-C52-C53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	B8	201	PC1	C2-C1-O11-P
51	N1	402	PLX	C4-C3-O4-P1
48	N5	703	PEE	C13-C14-C15-C16
49	AB	201	ZMP	C2-C1-C22-C23
48	AN	201	PEE	C1-C2-C3-O3
48	B6	201	PEE	C1-C2-C3-O3
48	N4	501	PEE	C1-C2-C3-O3
51	B5	201	PLX	C3-C4-C5-O8
52	N4	504	3PE	C1-C2-C3-O31
48	AN	201	PEE	C37-C38-C39-C40
51	AL	204	PLX	C7-C8-C9-C10
49	AB	201	ZMP	N2-C16-C17-C18
48	N2	401	PEE	C31-C30-O3-C3
45	4L	201	CDL	CA3-OA5-PA1-OA2
45	AL	202	CDL	CA2-OA2-PA1-OA5
45	AL	202	CDL	CB2-OB2-PB2-OB5
51	N1	402	PLX	C2-O1-P1-O4
51	N3	202	PLX	C5-C4-O6-C6
51	N3	202	PLX	O7-C6-C7-C8
45	N1	401	CDL	C61-C62-C63-C64
45	4L	201	CDL	OB5-CB3-CB4-OB6
48	AL	205	PEE	O3P-C1-C2-O2
48	N2	401	PEE	O3P-C1-C2-O2
51	N3	202	PLX	O4-C3-C4-O6
51	S7	302	PLX	O4-C3-C4-O6
52	N4	504	3PE	O11-C1-C2-O21
45	N2	402	CDL	C73-C74-C75-C76
45	N5	702	CDL	C52-C53-C54-C55
48	AN	201	PEE	C22-C23-C24-C25
48	N4	501	PEE	O2-C2-C3-O3
48	N5	703	PEE	C14-C15-C16-C17
51	S7	302	PLX	C25-C26-C27-C28
45	AL	201	CDL	C1-CB2-OB2-PB2
45	CB	203	CDL	CA4-CA3-OA5-PA1
45	N1	401	CDL	C1-CA2-OA2-PA1
48	AN	201	PEE	C2-C1-O3P-P
48	N3	201	PEE	C23-C24-C25-C26
45	AL	201	CDL	CA5-C11-C12-C13
48	N2	401	PEE	C30-C31-C32-C33
48	AL	203	PEE	C31-C32-C33-C34
48	A9	402	PEE	C36-C37-C38-C39
45	B5	202	CDL	C44-C45-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	B5	202	CDL	C83-C84-C85-C86
45	A1	101	CDL	C76-C77-C78-C79
51	B5	201	PLX	C15-C16-C17-C18
49	AC	201	ZMP	S1-C10-C9-C8
48	A9	402	PEE	C14-C15-C16-C17
48	A9	402	PEE	O3P-C1-C2-C3
51	N3	202	PLX	O4-C3-C4-C5
52	B4	201	3PE	O11-C1-C2-C3
52	N4	504	3PE	O11-C1-C2-C3
45	AL	201	CDL	C40-C41-C42-C43
49	AB	201	ZMP	C4-C5-C6-C7
48	N3	201	PEE	C24-C25-C26-C27
48	N2	403	PEE	C11-C12-C13-C14
51	N4	502	PLX	C11-C10-C9-C8
51	AL	204	PLX	C30-C31-C32-C33
45	N2	402	CDL	C12-C11-CA5-OA6
45	4L	201	CDL	C15-C16-C17-C18
45	A1	101	CDL	C81-C82-C83-C84
48	N4	501	PEE	C20-C21-C22-C23
51	N4	502	PLX	C32-C33-C34-C35
48	AK	402	PEE	C3-C2-O2-C10
48	N2	401	PEE	C3-C2-O2-C10
45	N4	503	CDL	C1-CA2-OA2-PA1
48	N3	201	PEE	C2-C1-O3P-P
46	A3	202	PC1	C2E-C2F-C2G-C2H
45	CB	203	CDL	OA5-CA3-CA4-OA6
46	N3	203	PC1	O11-C1-C2-O21
48	A9	402	PEE	O3P-C1-C2-O2
48	AL	203	PEE	O3P-C1-C2-O2
51	N1	402	PLX	O4-C3-C4-O6
52	B4	201	3PE	O11-C1-C2-O21
56	S2	501	MF8	N06-C04-N02-C01
48	N2	403	PEE	O5-C30-O3-C3
48	A9	402	PEE	O2-C2-C3-O3
48	N2	403	PEE	O2-C2-C3-O3
51	B5	201	PLX	O6-C4-C5-O8
48	N2	401	PEE	O5-C30-O3-C3
45	A1	101	CDL	C52-C53-C54-C55
48	N1	403	PEE	C32-C33-C34-C35
48	N3	201	PEE	C41-C42-C43-C44
48	AK	402	PEE	C19-C20-C21-C22
45	A1	101	CDL	C53-C54-C55-C56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	N3	204	PC1	C29-C2A-C2B-C2C
48	N4	501	PEE	C14-C15-C16-C17
48	N5	703	PEE	C31-C32-C33-C34
51	B5	201	PLX	C31-C32-C33-C34
45	N1	401	CDL	C77-C78-C79-C80
48	AL	205	PEE	C34-C35-C36-C37
51	N3	202	PLX	C29-C30-C31-C32
48	N4	501	PEE	C32-C33-C34-C35
45	CB	203	CDL	CA3-OA5-PA1-OA2
46	A3	201	PC1	C1-O11-P-O13
48	N2	401	PEE	C1-O3P-P-O4P
48	N3	201	PEE	C4-O4P-P-O3P
48	N4	501	PEE	C4-O4P-P-O3P
51	S7	302	PLX	C3-O4-P1-O1
45	N4	503	CDL	C76-C77-C78-C79
45	N1	401	CDL	C1-CB2-OB2-PB2
45	N4	503	CDL	CB4-CB3-OB5-PB2
46	A3	202	PC1	C2-C1-O11-P
48	AK	402	PEE	C2-C1-O3P-P
45	4L	201	CDL	CB3-OB5-PB2-OB4
45	A1	101	CDL	CB3-OB5-PB2-OB3
45	A1	101	CDL	CB3-OB5-PB2-OB4
45	AL	201	CDL	CB2-OB2-PB2-OB4
45	B5	202	CDL	CB2-OB2-PB2-OB3
45	CB	203	CDL	CA2-OA2-PA1-OA3
45	N2	402	CDL	CB2-OB2-PB2-OB3
45	N5	701	CDL	CB2-OB2-PB2-OB3
45	N5	701	CDL	CB3-OB5-PB2-OB4
45	N5	702	CDL	CA3-OA5-PA1-OA4
46	A3	201	PC1	C11-O13-P-O14
46	A3	202	PC1	C1-O11-P-O12
46	AN	202	PC1	C11-O13-P-O14
46	AN	202	PC1	C1-O11-P-O12
46	B5	203	PC1	C11-O13-P-O14
46	B8	201	PC1	C11-O13-P-O12
48	AK	402	PEE	C4-O4P-P-O2P
48	AK	402	PEE	C4-O4P-P-O1P
48	AL	203	PEE	C4-O4P-P-O1P
48	AL	205	PEE	C4-O4P-P-O2P
48	B6	201	PEE	C4-O4P-P-O2P
48	N1	403	PEE	C1-O3P-P-O1P
48	N1	403	PEE	C4-O4P-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	N1	403	PEE	C4-O4P-P-O1P
48	N2	401	PEE	C4-O4P-P-O1P
48	N2	403	PEE	C4-O4P-P-O1P
48	S8	303	PEE	C1-O3P-P-O1P
51	AL	204	PLX	C2-O1-P1-O3
51	B5	201	PLX	C3-O4-P1-O3
51	CB	201	PLX	C2-O1-P1-O2
51	N1	402	PLX	C3-O4-P1-O2
51	N3	202	PLX	C3-O4-P1-O3
51	N3	202	PLX	C2-O1-P1-O2
51	N3	202	PLX	C2-O1-P1-O3
51	S7	302	PLX	C2-O1-P1-O2
52	CB	202	3PE	C1-O11-P-O14
48	S8	303	PEE	C30-C31-C32-C33
46	A3	202	PC1	O11-C1-C2-C3
48	AL	203	PEE	O3P-C1-C2-C3
48	N4	501	PEE	O4P-C4-C5-N
45	AL	201	CDL	C53-C54-C55-C56
48	AL	205	PEE	C17-C18-C19-C20
45	4L	201	CDL	C18-C19-C20-C21
48	AN	201	PEE	C5-C4-O4P-P
48	N3	201	PEE	C5-C4-O4P-P
51	B5	201	PLX	C25-C24-O8-C5
52	CB	202	3PE	C12-C11-O13-P
45	AL	202	CDL	C40-C41-C42-C43
48	AK	402	PEE	C13-C14-C15-C16
48	AN	201	PEE	C11-C12-C13-C14
48	AN	201	PEE	C21-C22-C23-C24
45	N1	401	CDL	OB5-CB3-CB4-OB6
45	N4	503	CDL	OB5-CB3-CB4-OB6
46	B8	201	PC1	O11-C1-C2-O21
48	N2	403	PEE	O3P-C1-C2-O2
48	N3	201	PEE	O3P-C1-C2-O2
46	A3	201	PC1	C28-C29-C2A-C2B
48	S8	303	PEE	C33-C34-C35-C36
46	AN	202	PC1	C3A-C3B-C3C-C3D
48	N2	403	PEE	C42-C43-C44-C45
45	CB	203	CDL	C32-C33-C34-C35
46	B8	201	PC1	C11-C12-N-C15
51	S7	302	PLX	C2-C1-N1-C1C
51	S7	302	PLX	C11-C10-C9-C8
45	CB	203	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	B8	201	PC1	O13-C11-C12-N
46	N3	204	PC1	O13-C11-C12-N
48	AL	203	PEE	C33-C34-C35-C36
51	N3	202	PLX	N1-C1-C2-O1
52	B4	201	3PE	C1-C2-C3-O31
45	CB	203	CDL	OB6-CB4-CB6-OB8
48	AK	402	PEE	O2-C2-C3-O3
51	N1	402	PLX	O6-C4-C5-O8
51	N3	202	PLX	C30-C31-C32-C33
45	A1	101	CDL	CA4-CA3-OA5-PA1
48	N4	501	PEE	C2-C1-O3P-P
51	N1	402	PLX	C6-C7-C8-C9
51	S7	302	PLX	C29-C30-C31-C32
45	A1	101	CDL	C14-C15-C16-C17
49	AC	201	ZMP	O3-C16-C17-O4
51	B5	201	PLX	O7-C6-C7-C8
48	AK	402	PEE	C11-C12-C13-C14
56	S2	501	MF8	N06-C04-N02-C03
48	N2	401	PEE	C14-C15-C16-C17
48	N4	501	PEE	C31-C32-C33-C34
48	S8	303	PEE	C21-C22-C23-C24
45	CB	203	CDL	C32-C31-CA7-OA8
45	N1	401	CDL	C14-C15-C16-C17
49	AB	201	ZMP	C19-C18-C21-O5
49	AC	201	ZMP	C20-C18-C21-O5
47	A9	401	NDP	C2D-C1D-N1N-C6N
45	AL	201	CDL	C36-C37-C38-C39
51	N3	202	PLX	C31-C32-C33-C34
45	AL	202	CDL	OA5-CA3-CA4-CA6
45	AL	202	CDL	C13-C14-C15-C16
45	N5	702	CDL	C73-C74-C75-C76
48	N5	703	PEE	O5-C30-O3-C3
48	N5	703	PEE	C42-C43-C44-C45
48	N3	201	PEE	C38-C39-C40-C41
48	N5	703	PEE	C18-C19-C20-C21
45	N5	702	CDL	C1-CA2-OA2-PA1
48	N5	703	PEE	C31-C30-O3-C3
48	N4	501	PEE	C37-C38-C39-C40
47	A9	401	NDP	O4D-C1D-N1N-C6N
51	N1	402	PLX	C26-C27-C28-C29
48	AL	205	PEE	O2-C2-C3-O3
52	N4	504	3PE	O21-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	A1	101	CDL	CB2-OB2-PB2-OB5
45	AL	202	CDL	CB3-OB5-PB2-OB2
45	B5	202	CDL	CA2-OA2-PA1-OA5
45	N4	503	CDL	CA2-OA2-PA1-OA5
45	N4	503	CDL	CB2-OB2-PB2-OB5
48	A9	402	PEE	C1-O3P-P-O4P
48	AK	402	PEE	C1-O3P-P-O4P
48	N3	201	PEE	C1-O3P-P-O4P
51	B5	201	PLX	C3-O4-P1-O1
51	B5	201	PLX	C2-O1-P1-O4
45	N5	701	CDL	C34-C35-C36-C37
48	AL	203	PEE	C40-C41-C42-C43
48	S8	303	PEE	C10-C11-C12-C13
48	A9	402	PEE	C12-C13-C14-C15
49	AC	201	ZMP	C14-C15-N2-C16
45	4L	201	CDL	C53-C54-C55-C56
51	N1	402	PLX	C28-C29-C30-C31
48	AL	205	PEE	C2-C1-O3P-P
52	CB	202	3PE	C2-C1-O11-P
51	AL	204	PLX	C14-C15-C16-C17
52	N4	504	3PE	C31-C32-C33-C34
48	A9	402	PEE	C34-C35-C36-C37
56	S2	501	MF8	N08-C07-N06-C04
48	AL	205	PEE	C15-C16-C17-C18
48	N3	201	PEE	C19-C20-C21-C22
45	B5	202	CDL	C39-C40-C41-C42
48	N3	201	PEE	C42-C43-C44-C45
45	N1	401	CDL	C53-C54-C55-C56
51	S7	302	PLX	C2-C1-N1-C1A
50	AK	401	ADP	O4'-C4'-C5'-O5'
49	AC	201	ZMP	C1-C2-C3-C4
45	4L	201	CDL	C20-C21-C22-C23
52	CB	202	3PE	C35-C36-C37-C38
49	AB	201	ZMP	O3-C16-C17-C18
48	N5	703	PEE	C32-C33-C34-C35
51	N4	502	PLX	C24-C25-C26-C27
45	N4	503	CDL	C58-C59-C60-C61
47	A9	401	NDP	O4B-C4B-C5B-O5B
51	B5	201	PLX	C13-C14-C15-C16
45	N2	402	CDL	CA3-CA4-CA6-OA8
45	N2	402	CDL	CB3-CB4-CB6-OB8
45	N5	702	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	AB	201	ZMP	C20-C18-C21-O5
49	AC	201	ZMP	C19-C18-C21-O5
48	N5	703	PEE	C11-C12-C13-C14
51	N3	202	PLX	C14-C15-C16-C17
49	AC	201	ZMP	N2-C16-C17-C18
48	B6	201	PEE	C31-C32-C33-C34
48	N4	501	PEE	C39-C40-C41-C42
45	4L	201	CDL	CA6-CA4-OA6-CA5
45	AL	201	CDL	CA6-CA4-OA6-CA5
46	A3	201	PC1	C1-C2-O21-C21
46	B8	201	PC1	C3-C2-O21-C21
51	S7	302	PLX	C2-C1-N1-C1B
48	N3	201	PEE	C21-C22-C23-C24
48	S8	303	PEE	C1-O3P-P-O4P
56	S2	501	MF8	N05-C04-N02-C01
45	4L	201	CDL	C12-C13-C14-C15
45	N1	401	CDL	C11-C12-C13-C14
46	B8	201	PC1	C32-C33-C34-C35
45	N1	401	CDL	CA7-C31-C32-C33
45	AL	201	CDL	C74-C75-C76-C77
51	N4	502	PLX	C30-C31-C32-C33
45	A1	101	CDL	OB6-CB4-CB6-OB8
45	AL	201	CDL	OA6-CA4-CA6-OA8
45	N5	702	CDL	OB6-CB4-CB6-OB8
52	B4	201	3PE	O21-C2-C3-O31
46	A3	202	PC1	C23-C24-C25-C26
48	N5	703	PEE	C34-C35-C36-C37
45	N5	702	CDL	C41-C42-C43-C44
45	B5	202	CDL	C77-C78-C79-C80
48	A9	402	PEE	C1-C2-C3-O3
46	B5	203	PC1	C27-C28-C29-C2A
48	N4	501	PEE	C42-C43-C44-C45
45	AL	202	CDL	C11-C12-C13-C14
52	B4	201	3PE	C21-C22-C23-C24
48	A9	402	PEE	C16-C17-C18-C19
48	AK	402	PEE	O3P-C1-C2-O2
47	A9	401	NDP	C2D-C1D-N1N-C2N
48	AK	402	PEE	C31-C32-C33-C34
49	AC	201	ZMP	O1-C10-C9-C8
48	N5	703	PEE	C21-C22-C23-C24
45	N4	503	CDL	C72-C71-CB7-OB8
46	N3	203	PC1	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	AK	402	PEE	C33-C34-C35-C36
51	S7	302	PLX	O6-C6-C7-C8
45	4L	201	CDL	OB5-CB3-CB4-CB6
45	A1	101	CDL	CA7-C31-C32-C33
46	N3	203	PC1	C2-C1-O11-P
45	N1	401	CDL	C56-C57-C58-C59
45	N1	401	CDL	C72-C71-CB7-OB8
51	AL	204	PLX	C27-C28-C29-C30
45	N5	701	CDL	C13-C14-C15-C16
48	AN	201	PEE	C18-C19-C20-C21
49	AB	201	ZMP	N2-C16-C17-O4
49	AC	201	ZMP	N2-C16-C17-O4
46	B8	201	PC1	C11-C12-N-C13
46	B8	201	PC1	C11-C12-N-C14
45	CB	203	CDL	C72-C73-C74-C75
51	S7	302	PLX	C12-C13-C14-C15
45	N4	503	CDL	C32-C31-CA7-OA8
48	B6	201	PEE	C22-C23-C24-C25
47	A9	401	NDP	O4D-C1D-N1N-C2N
45	4L	201	CDL	C32-C31-CA7-OA8
45	N4	503	CDL	C52-C51-CB5-OB6
48	N2	403	PEE	O3-C30-C31-C32
45	AL	201	CDL	C38-C39-C40-C41
48	AN	201	PEE	O2-C10-C11-C12
46	A3	202	PC1	C24-C25-C26-C27
48	N5	703	PEE	C40-C41-C42-C43
48	AK	402	PEE	C15-C16-C17-C18
48	N2	403	PEE	C39-C40-C41-C42
51	N1	402	PLX	C7-C6-O6-C4
48	B6	201	PEE	O3P-C1-C2-O2
46	A3	201	PC1	C36-C37-C38-C39
48	N2	401	PEE	O2-C10-C11-C12
45	N5	701	CDL	C59-C60-C61-C62
48	A9	402	PEE	C18-C19-C20-C21
48	AK	402	PEE	C18-C19-C20-C21
48	N4	501	PEE	C18-C19-C20-C21
51	B5	201	PLX	C10-C11-C12-C13
45	A1	101	CDL	C72-C71-CB7-OB8
45	N4	503	CDL	C21-C22-C23-C24
48	N4	501	PEE	C15-C16-C17-C18
52	B4	201	3PE	C27-C28-C29-C2A
48	AK	402	PEE	O3P-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	A3	201	PC1	O21-C21-C22-C23
48	N1	403	PEE	O2-C10-C11-C12
48	B6	201	PEE	C11-C12-C13-C14
46	AN	202	PC1	O21-C2-C3-O31
48	AL	203	PEE	O2-C2-C3-O3
48	B6	201	PEE	C36-C37-C38-C39
48	N5	703	PEE	O2-C10-C11-C12
48	S8	303	PEE	C31-C30-O3-C3
45	B5	202	CDL	C79-C80-C81-C82
48	AL	205	PEE	C36-C37-C38-C39
48	N3	201	PEE	C18-C19-C20-C21
52	N4	504	3PE	O31-C31-C32-C33
48	AL	203	PEE	O2-C10-C11-C12
48	AL	205	PEE	C33-C34-C35-C36
48	S8	303	PEE	O5-C30-O3-C3
46	A3	201	PC1	C37-C38-C39-C3A
45	4L	201	CDL	C12-C11-CA5-OA6
45	N1	401	CDL	C51-C52-C53-C54
48	N2	403	PEE	C18-C19-C20-C21
45	4L	201	CDL	C32-C31-CA7-OA9
51	CB	201	PLX	O6-C6-C7-C8
45	B5	202	CDL	C73-C74-C75-C76
48	N2	403	PEE	O5-C30-C31-C32
48	N2	401	PEE	O4-C10-C11-C12
45	B5	202	CDL	C32-C33-C34-C35
48	AN	201	PEE	O4-C10-C11-C12
48	B6	201	PEE	C20-C21-C22-C23
48	AL	203	PEE	C1-C2-C3-O3
48	AL	205	PEE	C1-C2-C3-O3
48	N2	401	PEE	C4-O4P-P-O3P
45	4L	201	CDL	C39-C40-C41-C42
45	N1	401	CDL	C72-C71-CB7-OB9
46	A3	201	PC1	O22-C21-C22-C23
46	B8	201	PC1	C38-C39-C3A-C3B
48	B6	201	PEE	C2-C1-O3P-P
48	S8	303	PEE	C2-C1-O3P-P
51	N4	502	PLX	C4-C3-O4-P1
45	N4	503	CDL	C32-C31-CA7-OA9
48	N5	703	PEE	O4-C10-C11-C12
45	A1	101	CDL	CB2-OB2-PB2-OB3
45	AL	202	CDL	CB3-OB5-PB2-OB3
45	N1	401	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	N2	402	CDL	CA3-OA5-PA1-OA3
45	N2	402	CDL	CB3-OB5-PB2-OB3
45	N4	503	CDL	CB3-OB5-PB2-OB3
48	A9	402	PEE	C1-O3P-P-O1P
48	AK	402	PEE	C1-O3P-P-O1P
48	AL	205	PEE	C4-O4P-P-O1P
48	N2	403	PEE	C1-O3P-P-O1P
48	N4	501	PEE	C4-O4P-P-O1P
51	AL	204	PLX	C2-O1-P1-O2
45	N4	503	CDL	C52-C51-CB5-OB7
52	N4	504	3PE	O32-C31-C32-C33
45	AL	202	CDL	C32-C31-CA7-OA8
45	N5	702	CDL	C55-C56-C57-C58
45	N5	702	CDL	C34-C35-C36-C37
48	S8	303	PEE	O4P-C4-C5-N
45	A1	101	CDL	C72-C71-CB7-OB9
45	A1	101	CDL	C55-C56-C57-C58
56	S2	501	MF8	N09-C07-N06-C04
52	B4	201	3PE	C26-C27-C28-C29
48	B6	201	PEE	C33-C34-C35-C36
45	AL	201	CDL	CA3-CA4-OA6-CA5
46	A3	201	PC1	C12-C11-O13-P
46	AN	202	PC1	C12-C11-O13-P
46	B8	201	PC1	C12-C11-O13-P
48	A9	402	PEE	C5-C4-O4P-P
48	S8	303	PEE	C5-C4-O4P-P
49	AC	201	ZMP	O3-C16-C17-C18
51	N1	402	PLX	C1-C2-O1-P1
51	N4	502	PLX	C25-C24-O8-C5
51	S7	302	PLX	C25-C24-O8-C5
45	N2	402	CDL	C12-C11-CA5-OA7
45	AL	201	CDL	C12-C13-C14-C15
46	B5	203	PC1	O31-C31-C32-C33
45	N4	503	CDL	C80-C81-C82-C83
45	N5	702	CDL	C76-C77-C78-C79
46	N3	204	PC1	C32-C33-C34-C35
51	N3	202	PLX	C33-C34-C35-C36
45	N5	702	CDL	C12-C11-CA5-OA6
45	N1	401	CDL	C76-C77-C78-C79
45	N4	503	CDL	C55-C56-C57-C58
48	N2	403	PEE	C40-C41-C42-C43
58	V1	502	FMN	N10-C1'-C2'-O2'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	N1	403	PEE	O4-C10-C11-C12
45	4L	201	CDL	C42-C43-C44-C45
45	N1	401	CDL	C32-C31-CA7-OA8
46	N3	204	PC1	O31-C31-C32-C33
46	N3	204	PC1	O32-C31-C32-C33
46	N3	203	PC1	C2C-C2D-C2E-C2F
45	N1	401	CDL	C32-C31-CA7-OA9
45	CB	203	CDL	C59-C60-C61-C62
48	N4	501	PEE	C40-C41-C42-C43
52	B4	201	3PE	O31-C31-C32-C33

There are no ring outliers.

47 monomers are involved in 156 short contacts:

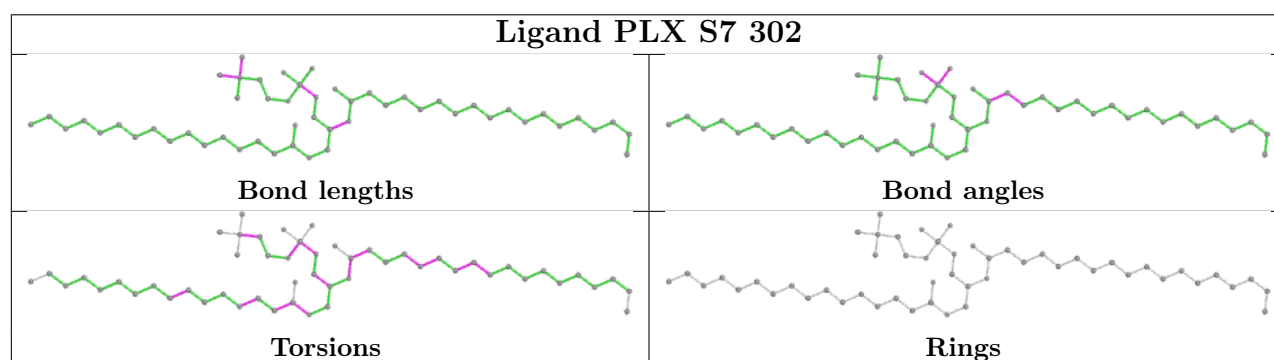
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	S7	302	PLX	3	0
51	N3	202	PLX	3	0
50	AK	401	ADP	3	0
53	S8	302	SF4	2	0
48	N2	403	PEE	2	0
52	N4	504	3PE	3	0
53	V1	501	SF4	4	0
53	S8	301	SF4	1	0
45	A1	101	CDL	6	0
45	N1	401	CDL	6	0
53	S1	801	SF4	1	0
51	CB	201	PLX	3	0
45	CB	203	CDL	2	0
48	S8	303	PEE	1	0
52	B4	201	3PE	2	0
51	N1	402	PLX	4	0
48	AL	205	PEE	5	0
47	A9	401	NDP	1	0
52	CB	202	3PE	5	0
45	AL	202	CDL	8	0
45	4L	201	CDL	6	0
45	N5	701	CDL	7	0
46	A3	202	PC1	2	0
48	N4	501	PEE	3	0
48	AN	201	PEE	2	0
48	N3	201	PEE	3	0
45	N2	402	CDL	2	0

Continued on next page...

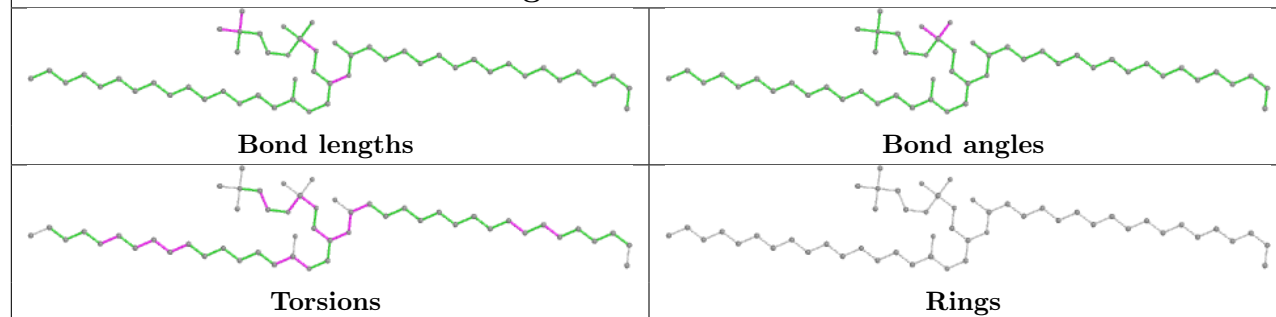
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	B5	203	PC1	1	0
49	AC	201	ZMP	5	0
58	V1	502	FMN	1	0
46	N3	204	PC1	3	0
45	B5	202	CDL	8	0
51	AL	204	PLX	7	0
48	B6	201	PEE	3	0
51	B5	201	PLX	3	0
48	AL	203	PEE	2	0
45	AL	201	CDL	10	0
48	N2	401	PEE	3	0
48	N5	703	PEE	3	0
45	N4	503	CDL	8	0
46	N3	203	PC1	1	0
46	AN	202	PC1	4	0
48	N1	403	PEE	2	0
48	A9	402	PEE	6	0
51	N4	502	PLX	5	0
49	AB	201	ZMP	2	0
48	AK	402	PEE	2	0

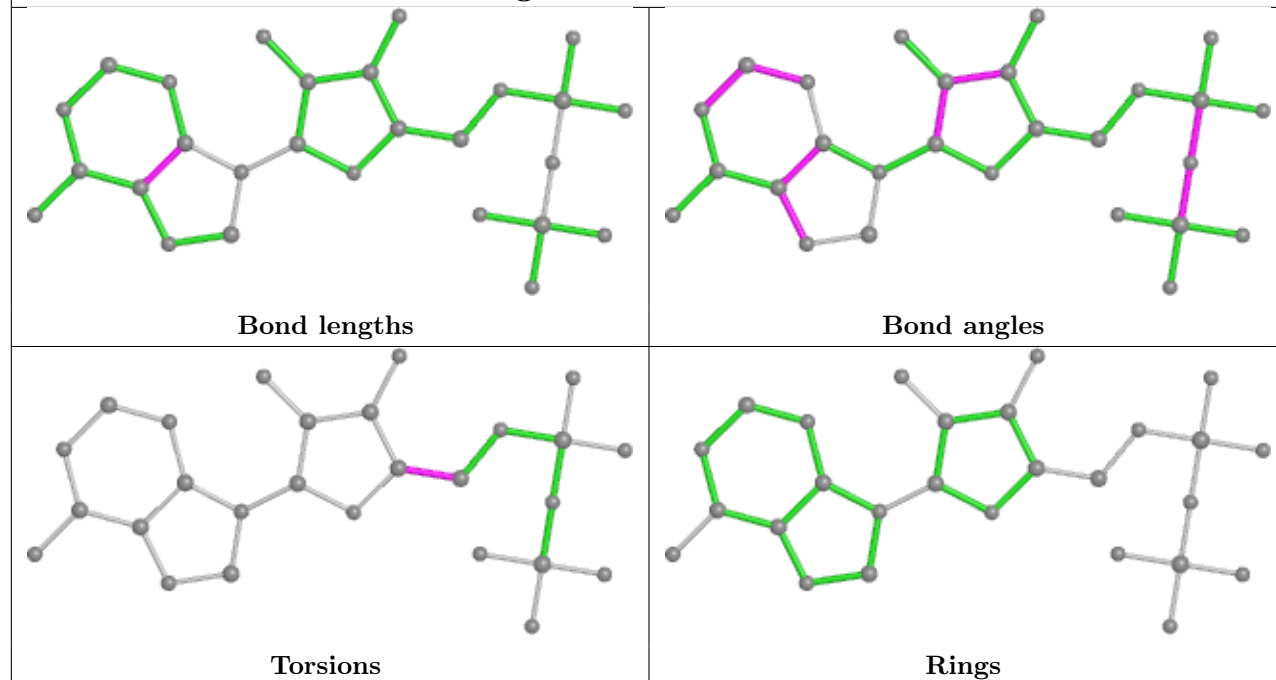
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



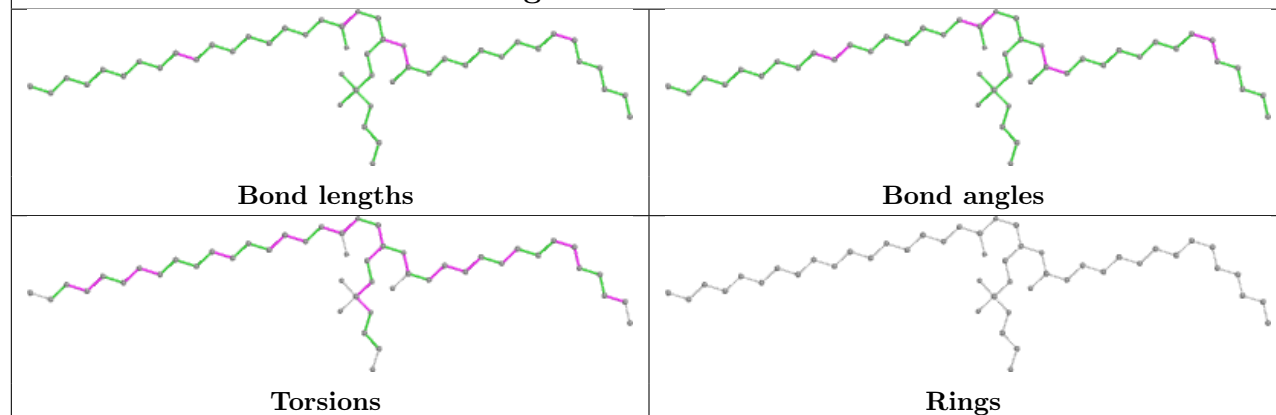
Ligand PLX N3 202

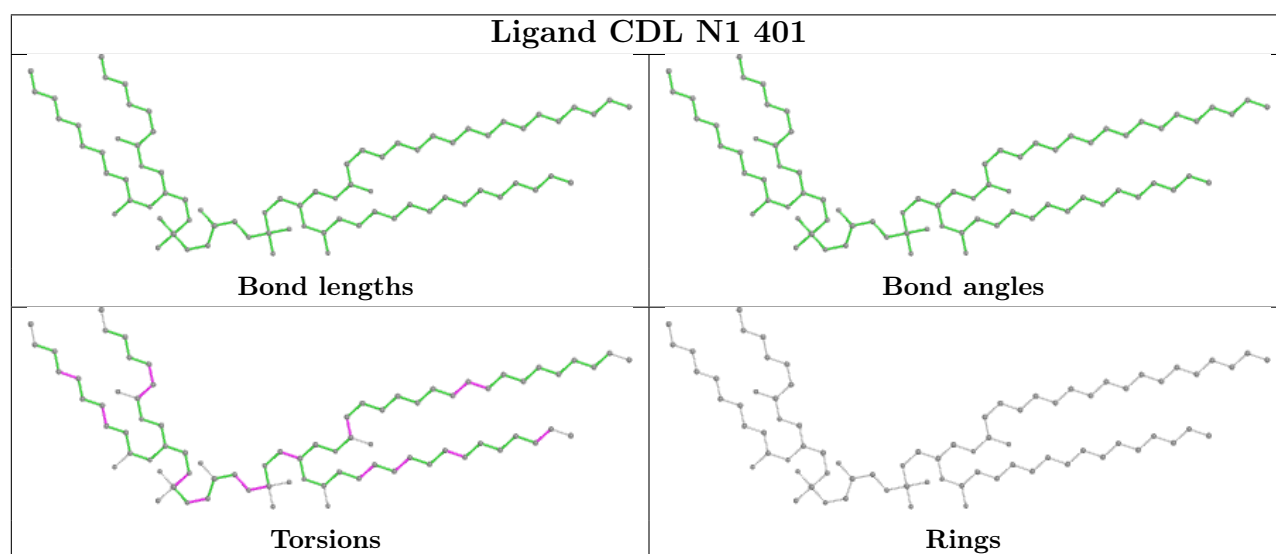
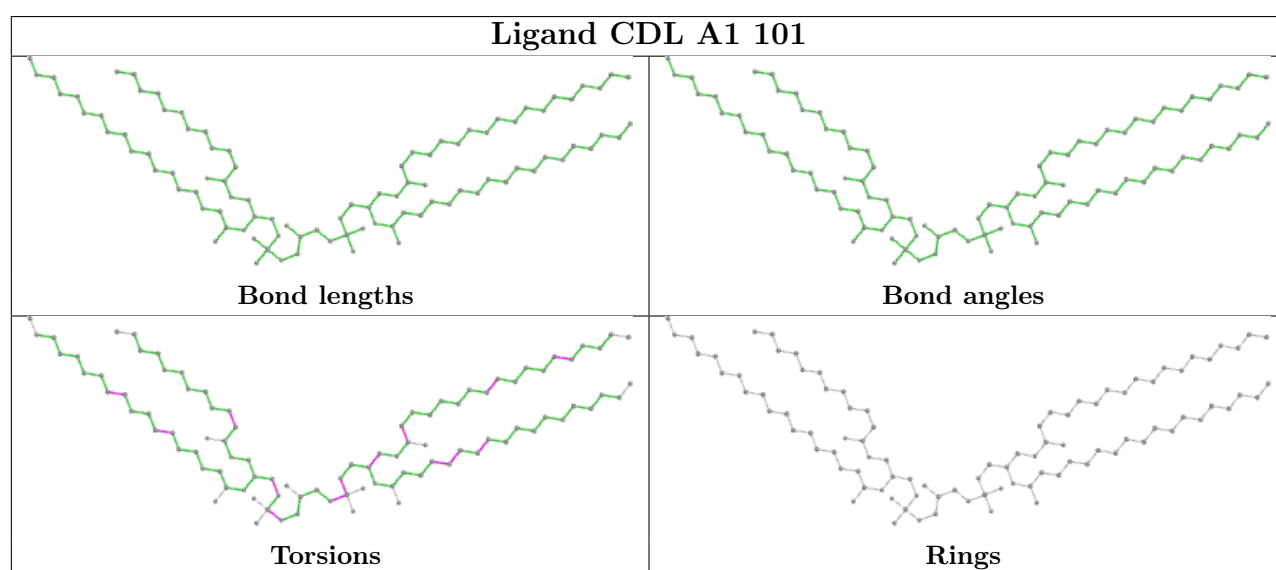
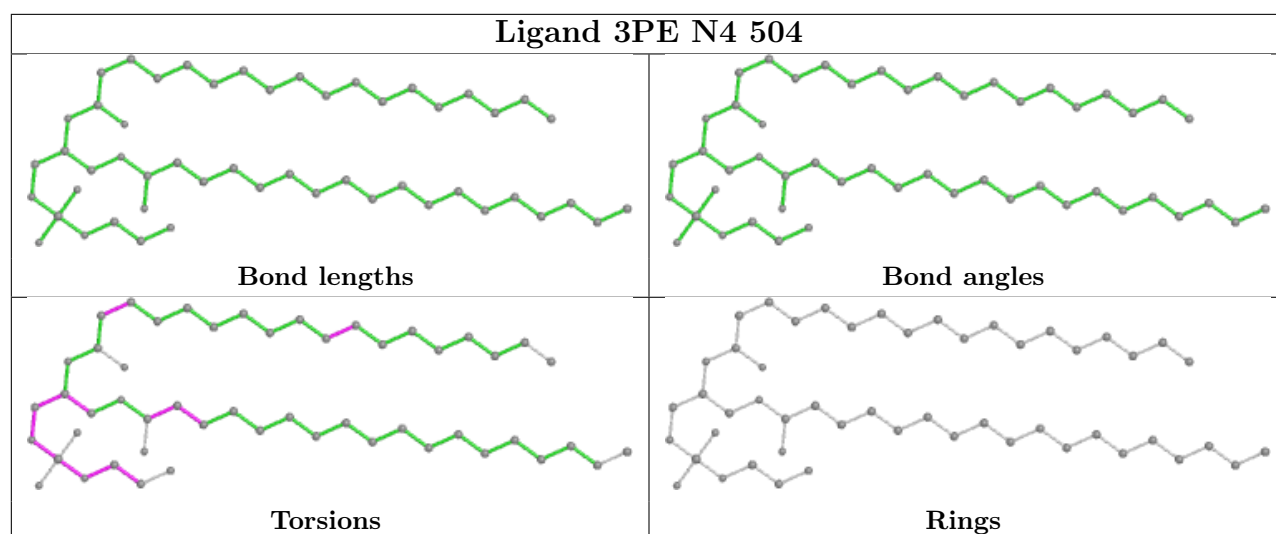


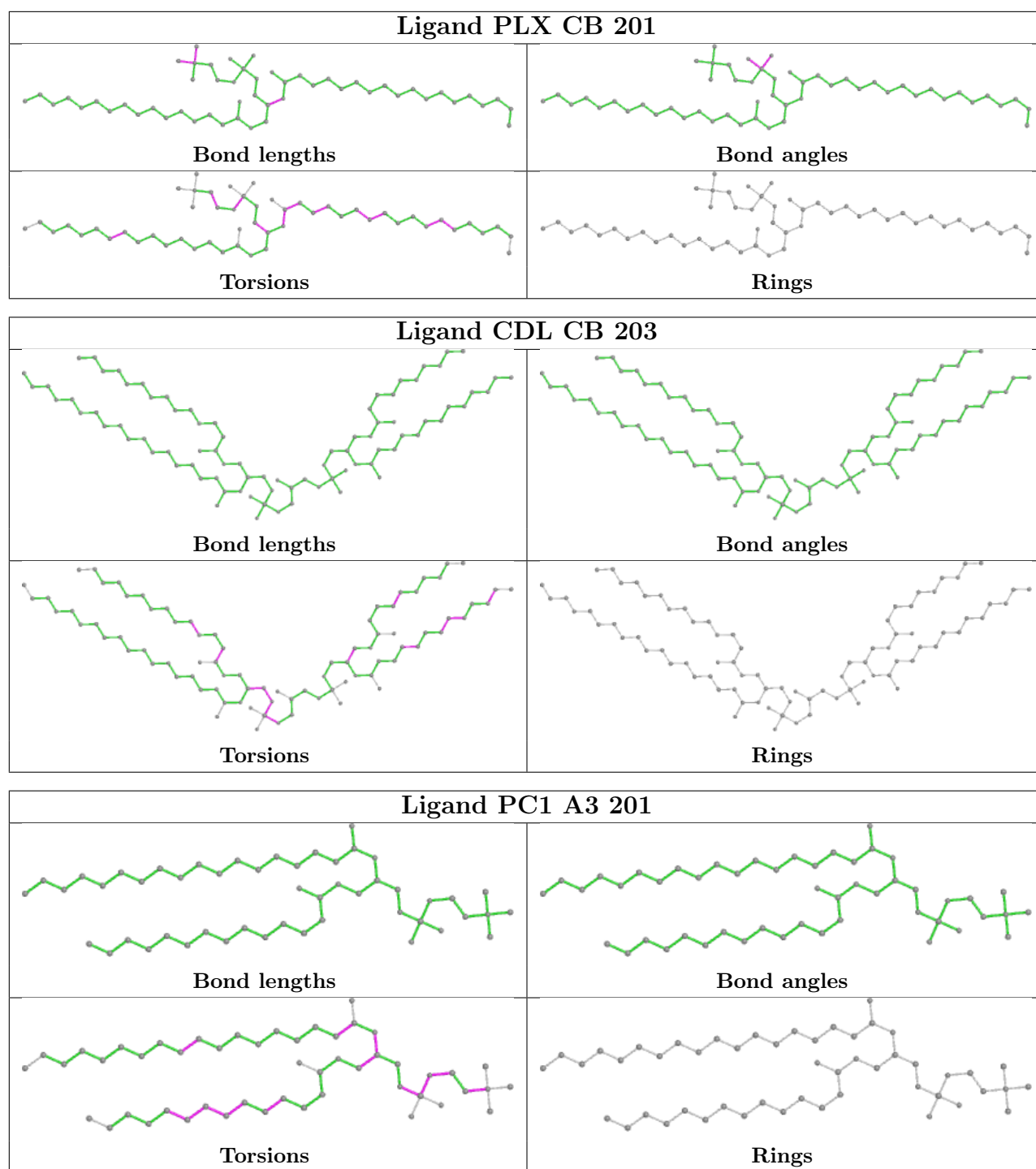
Ligand ADP AK 401

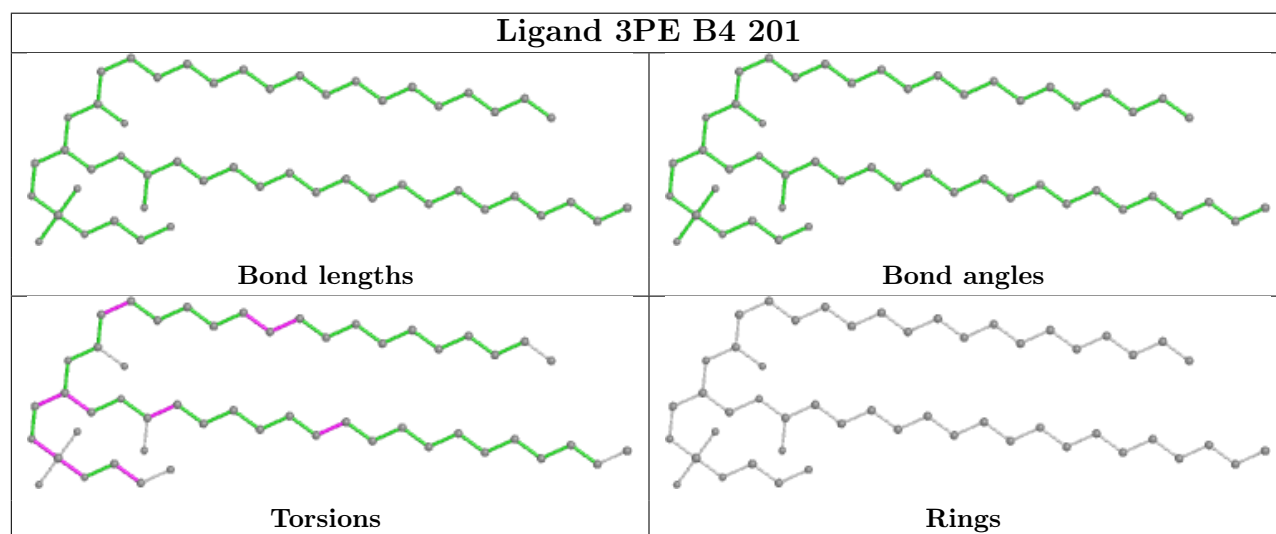
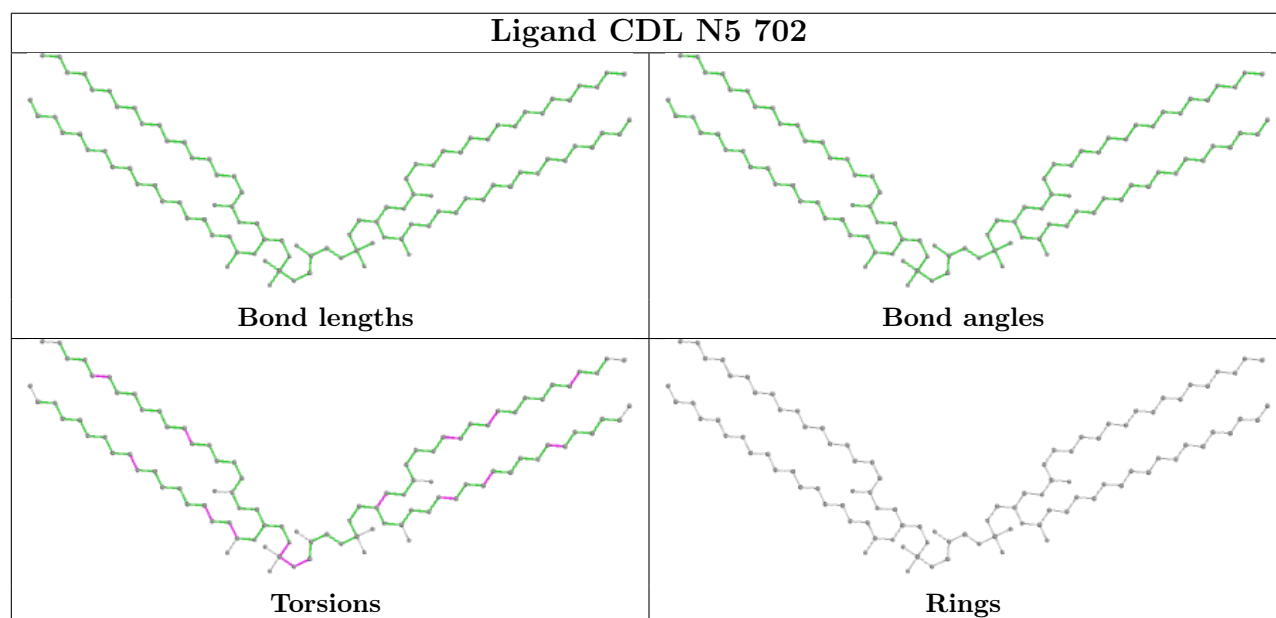
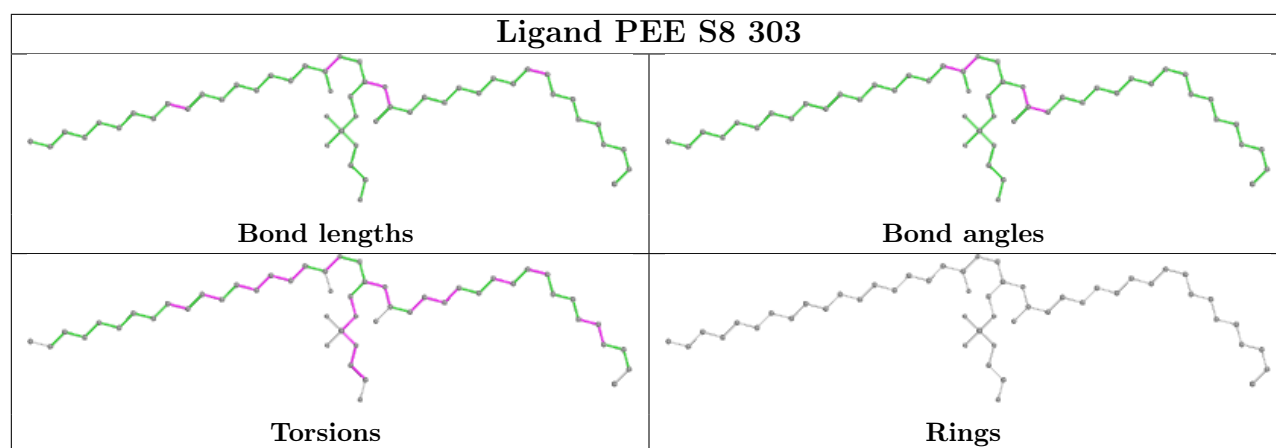


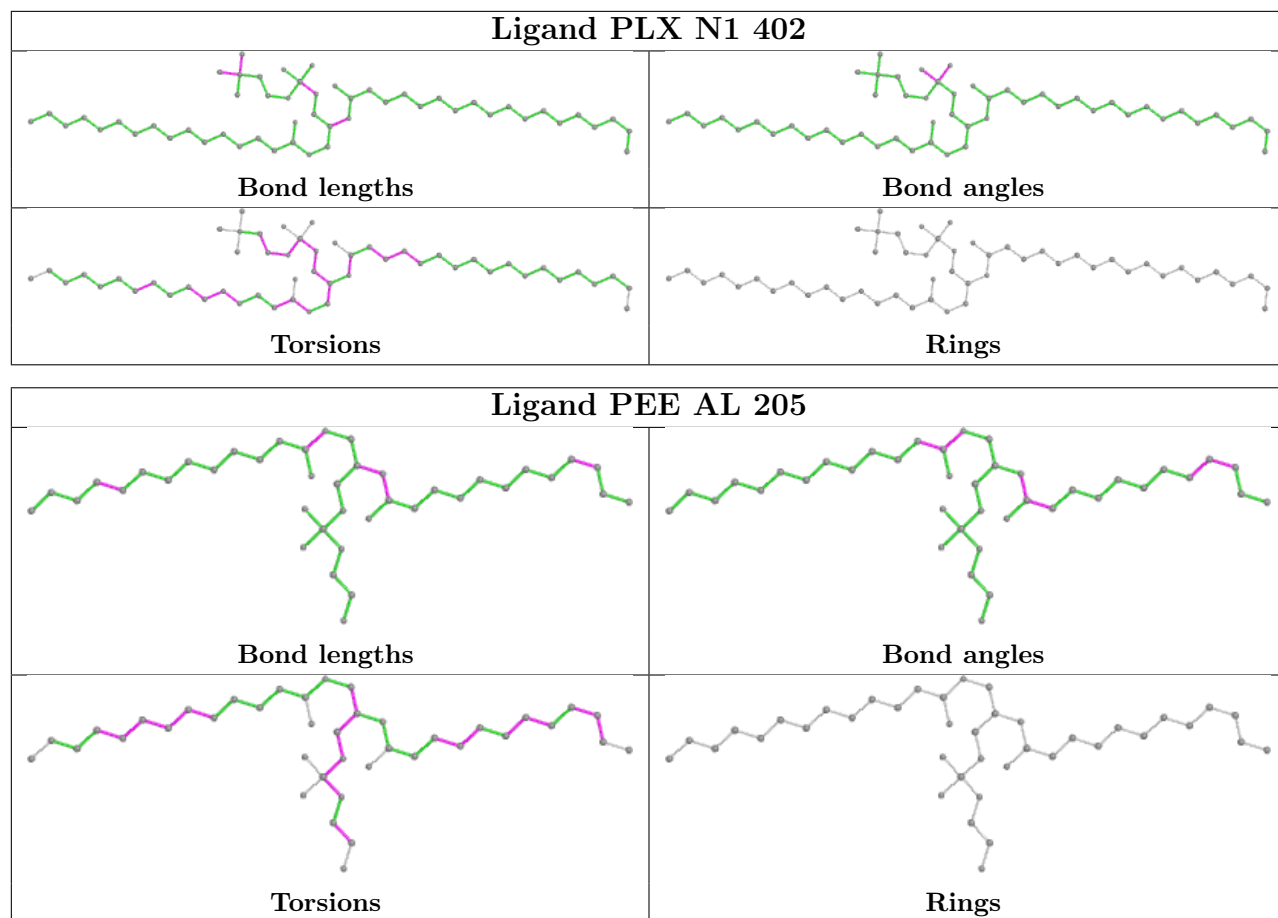
Ligand PEE N2 403

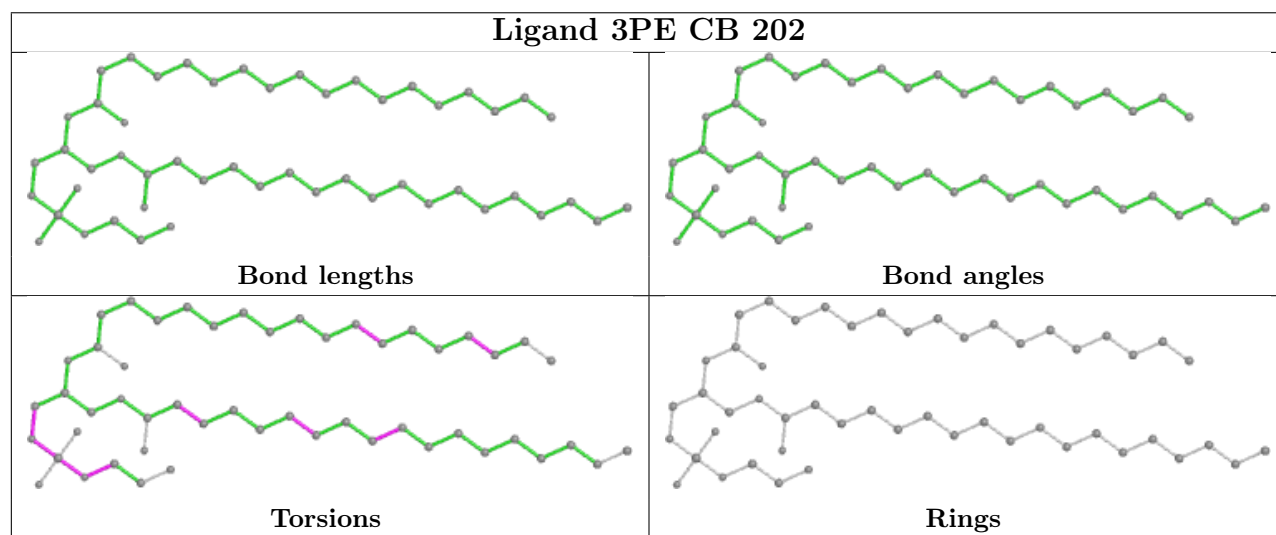
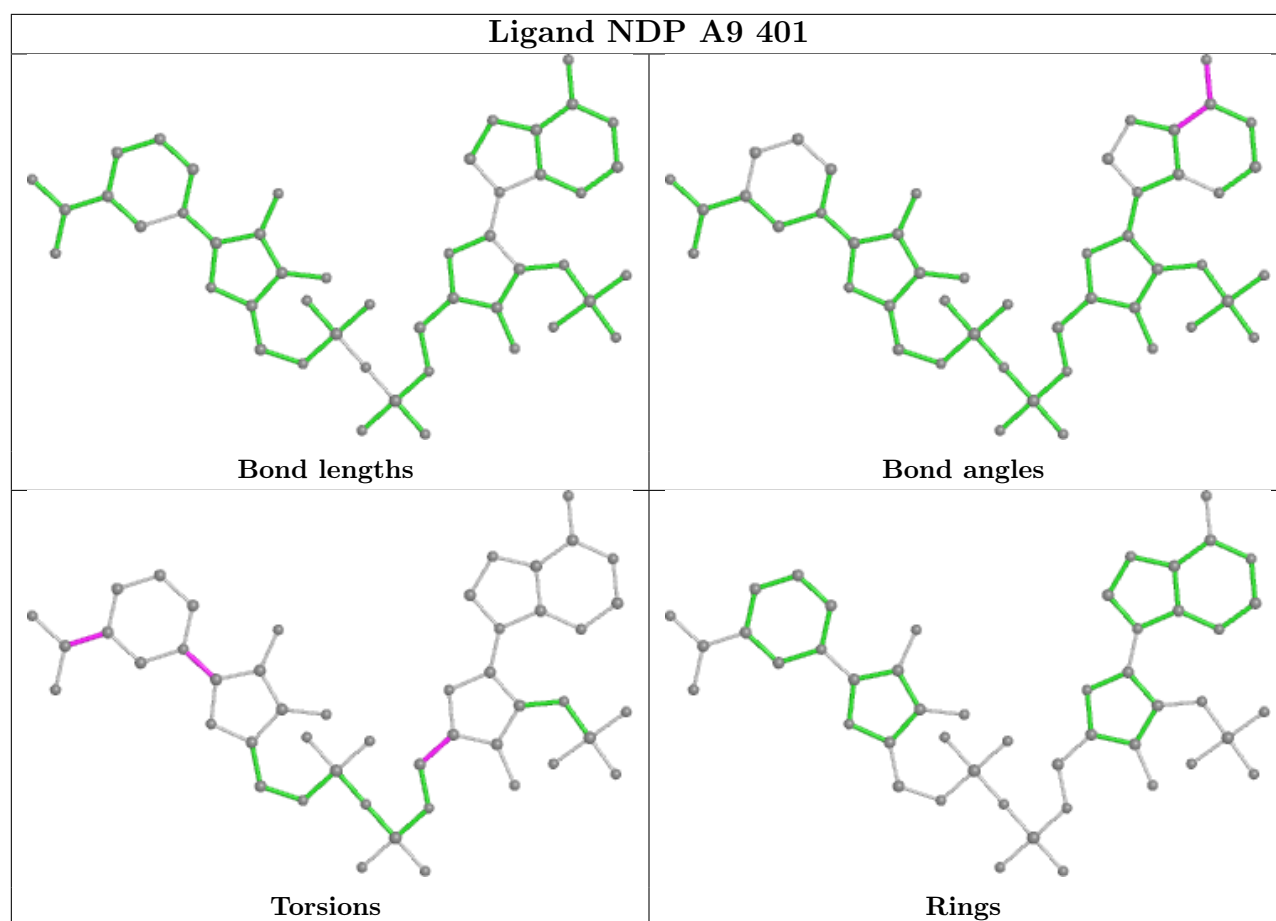


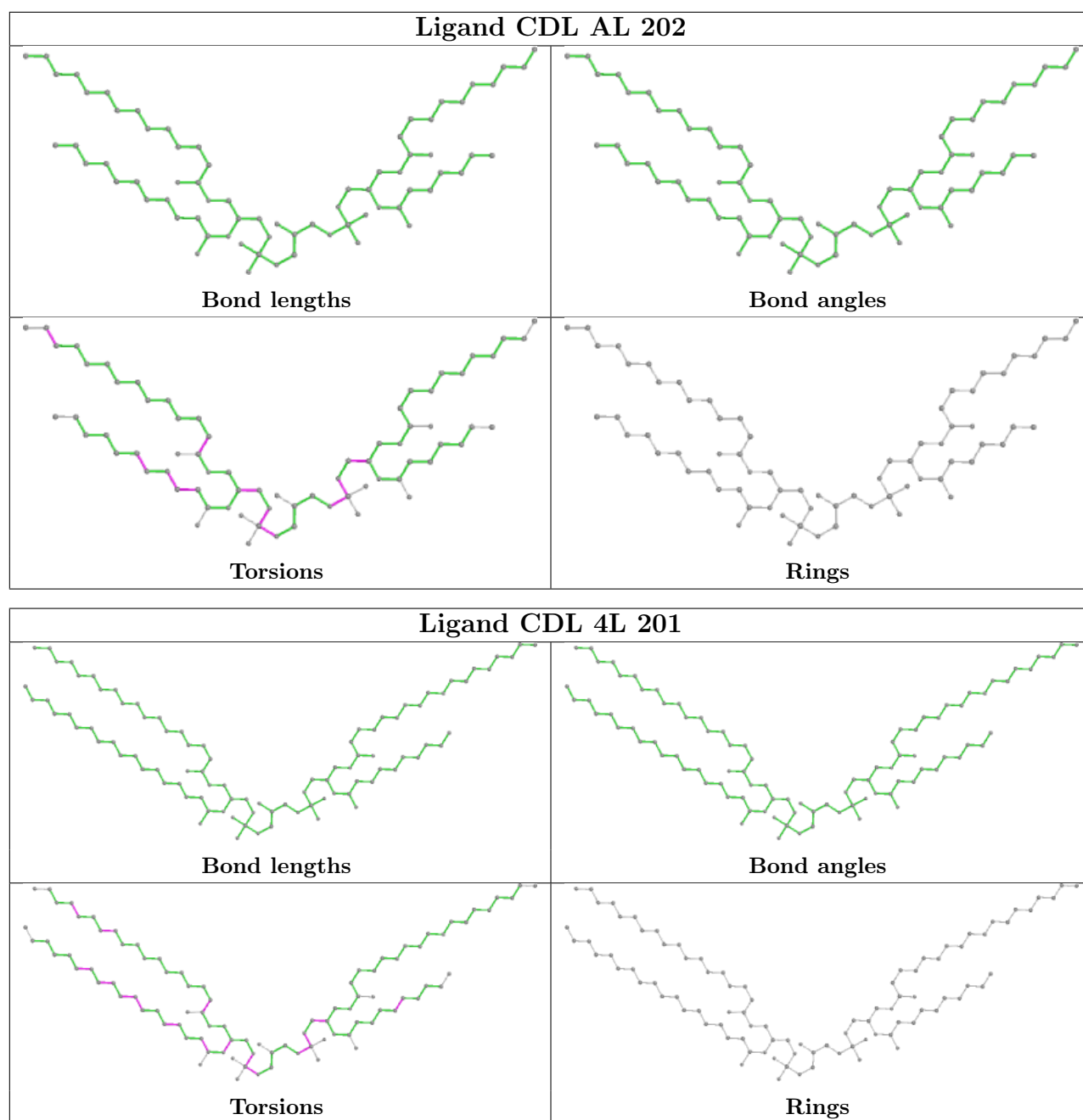


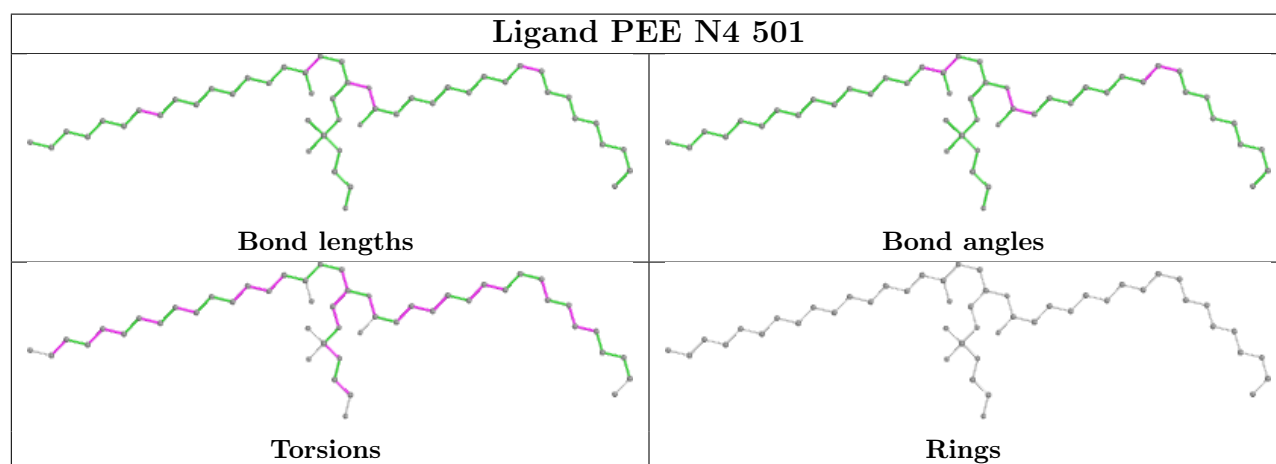
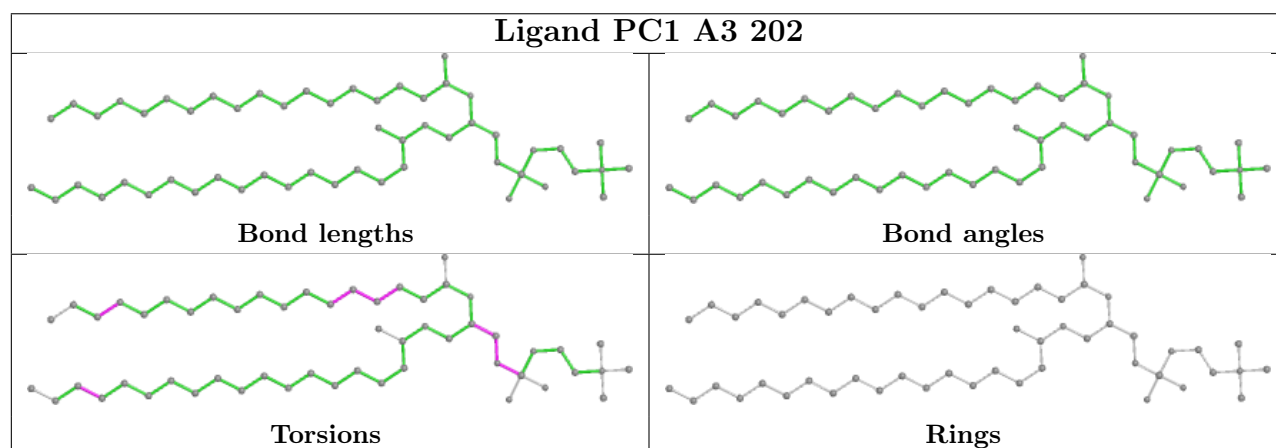
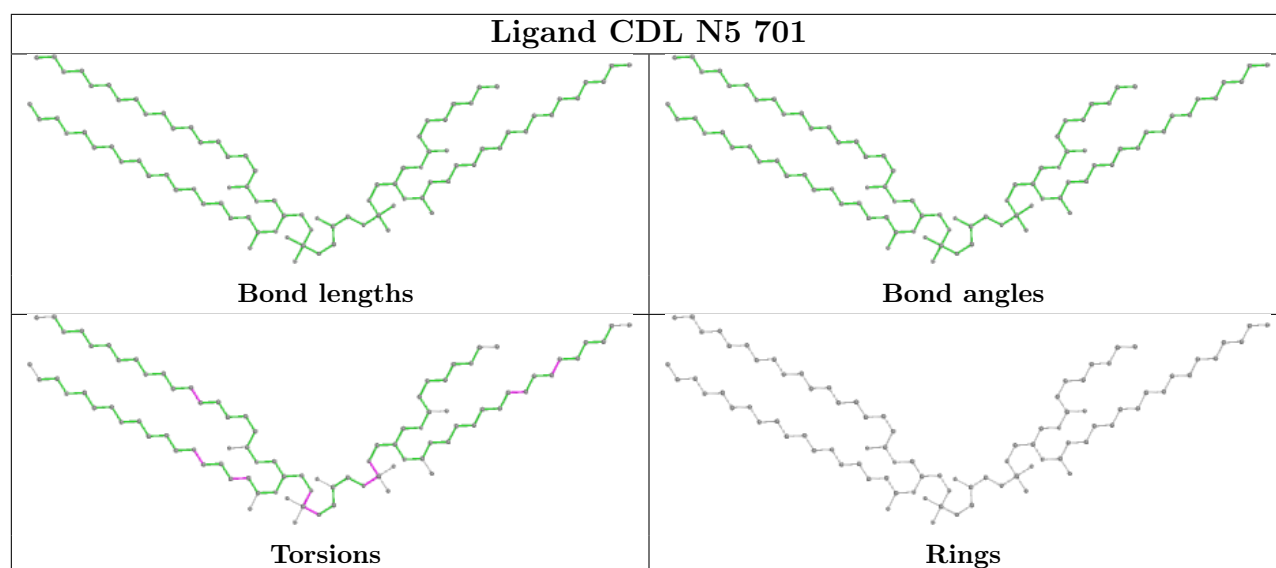


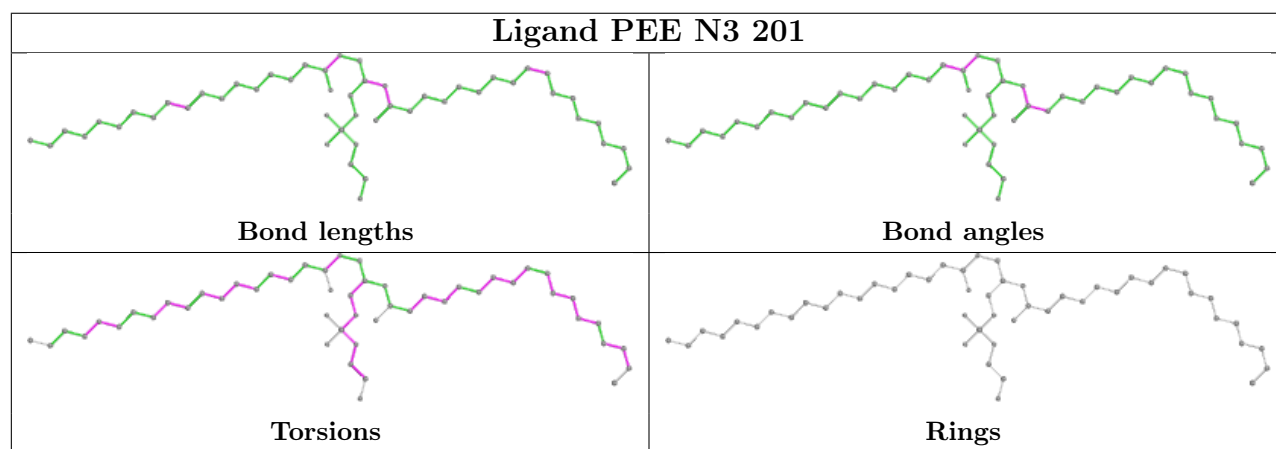
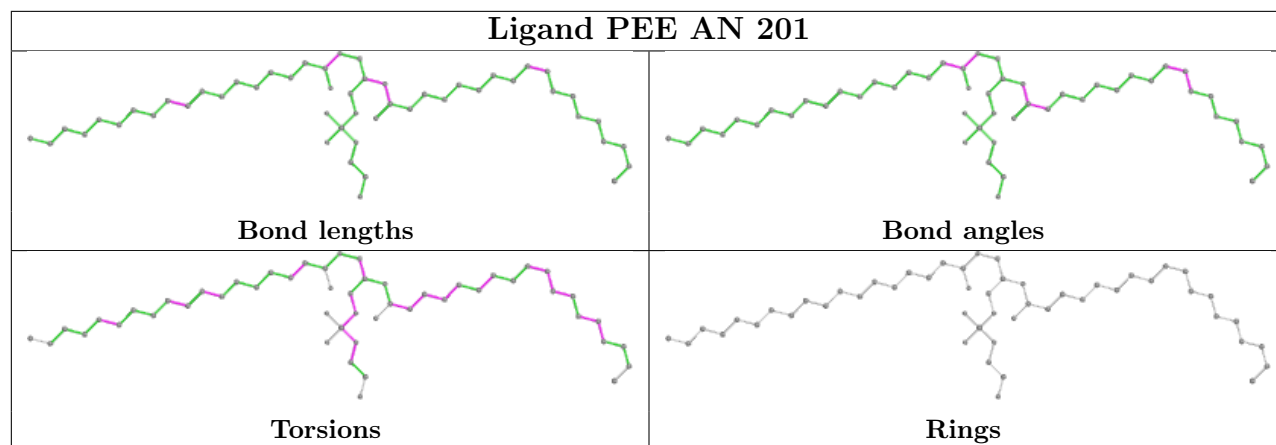


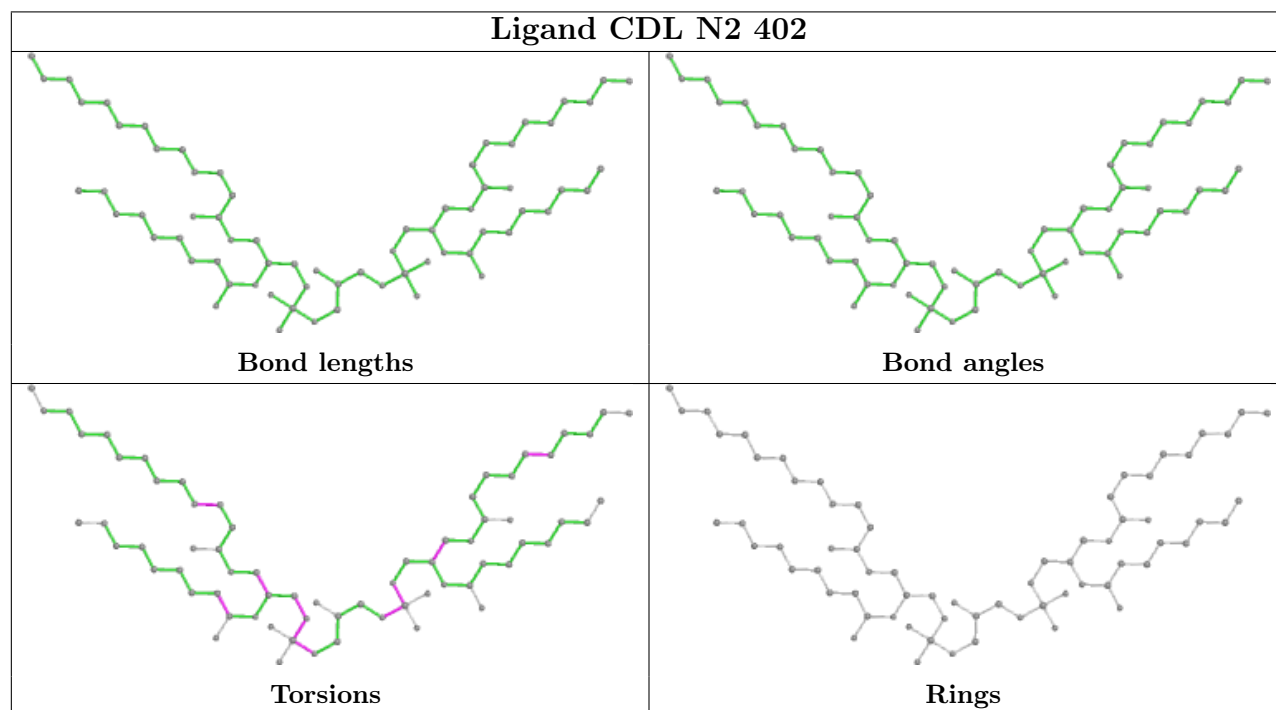
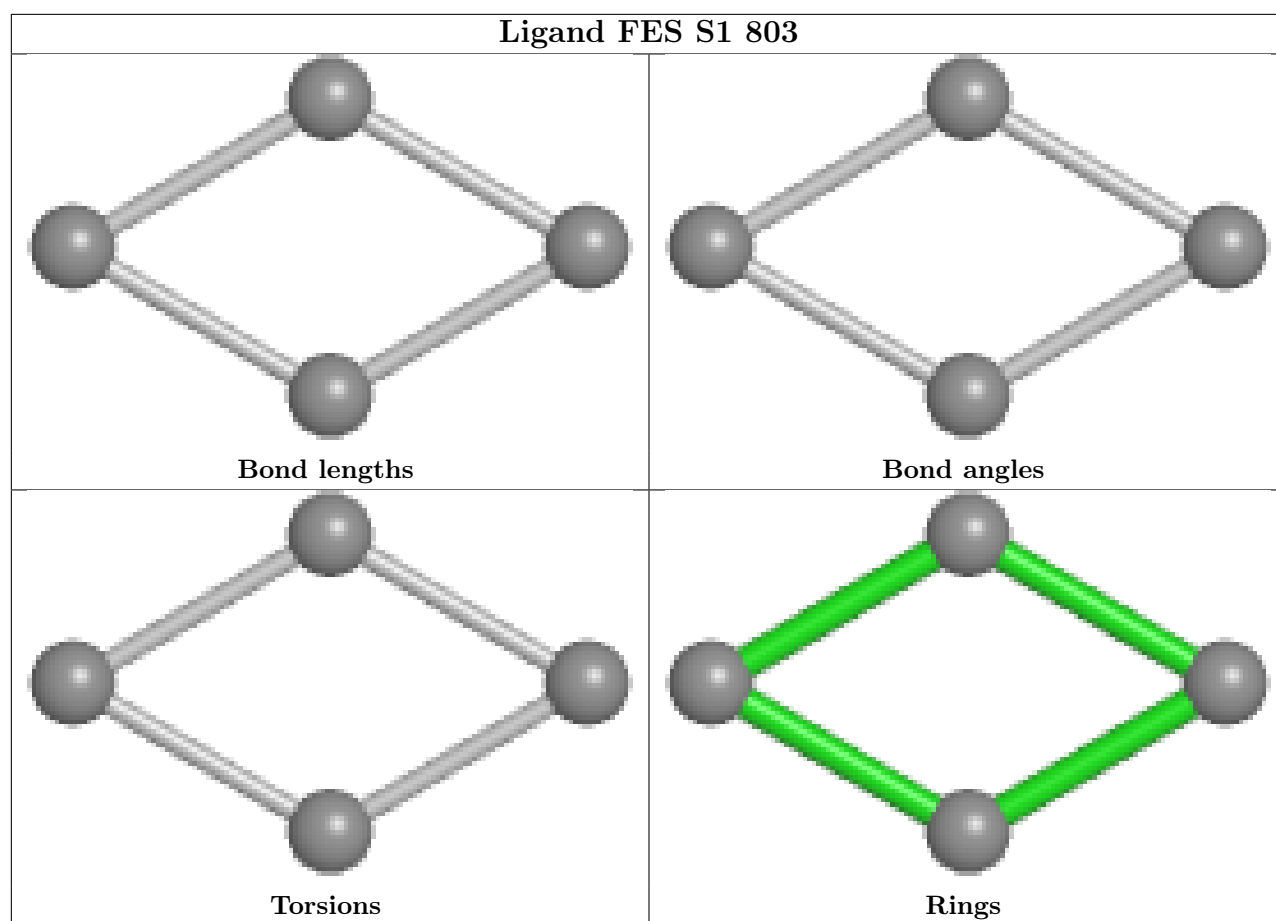


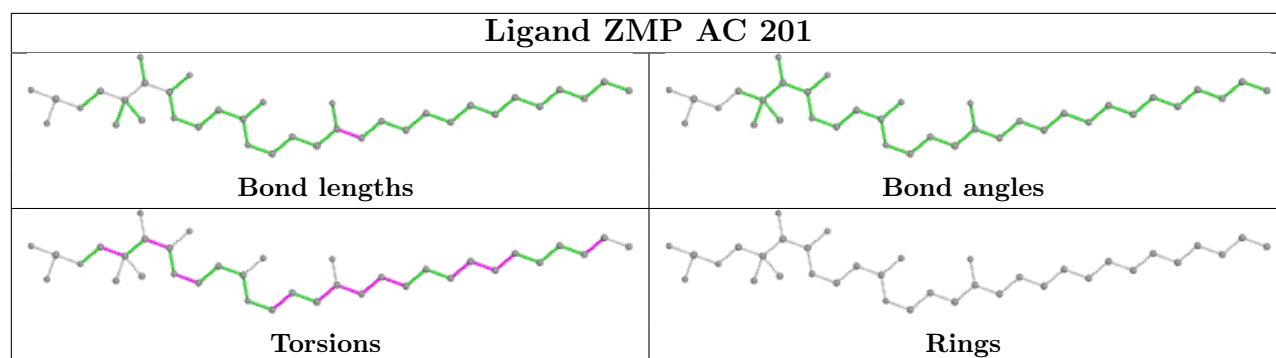
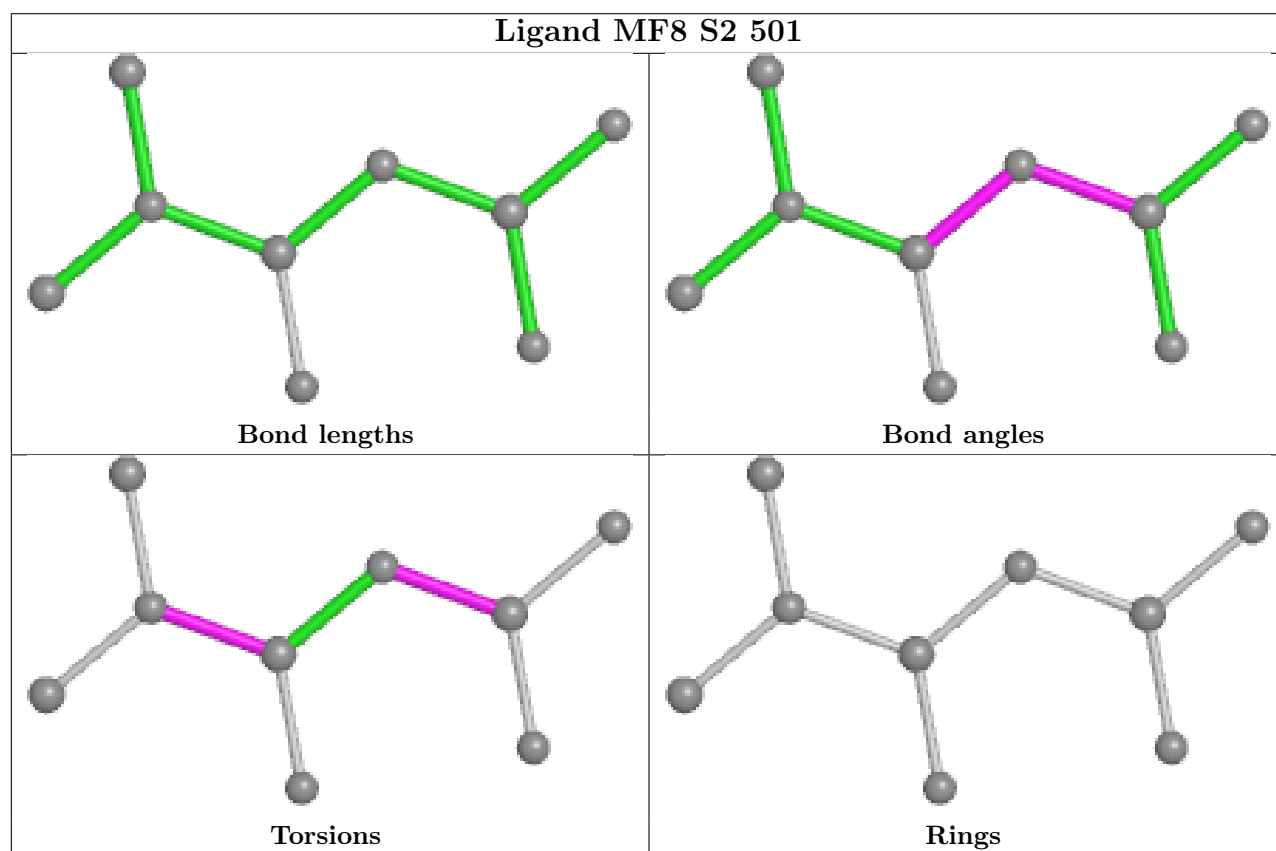
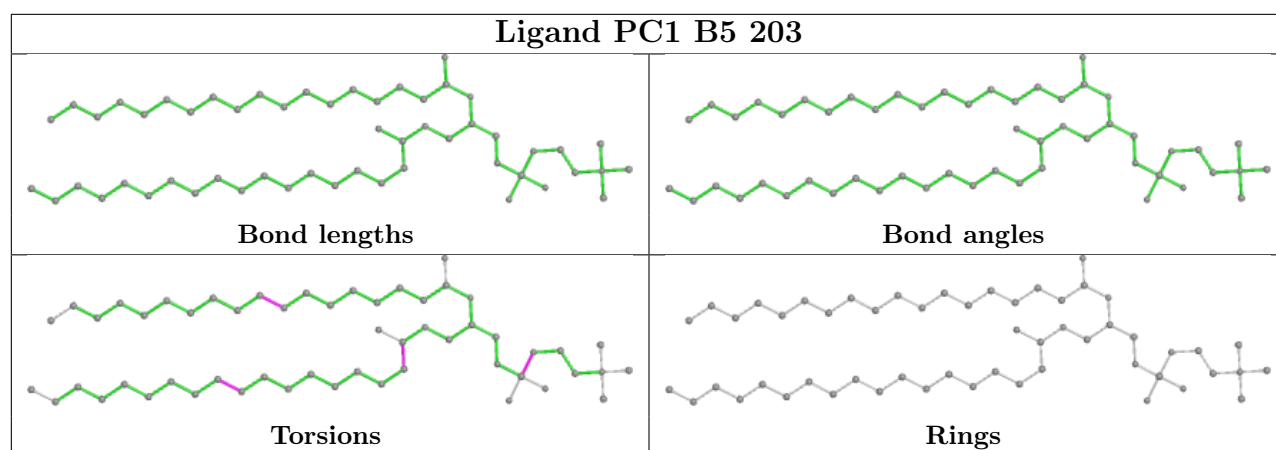




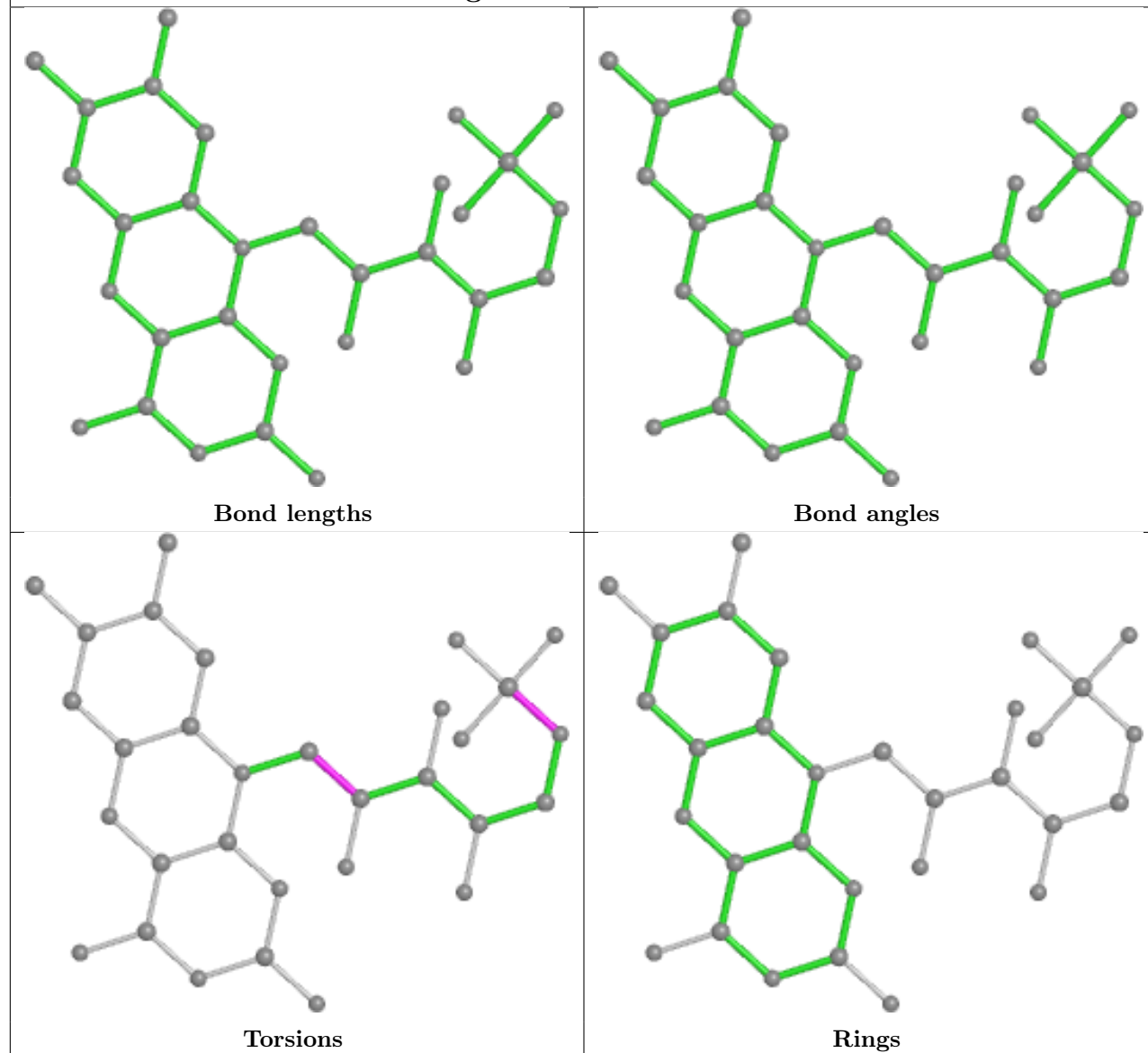




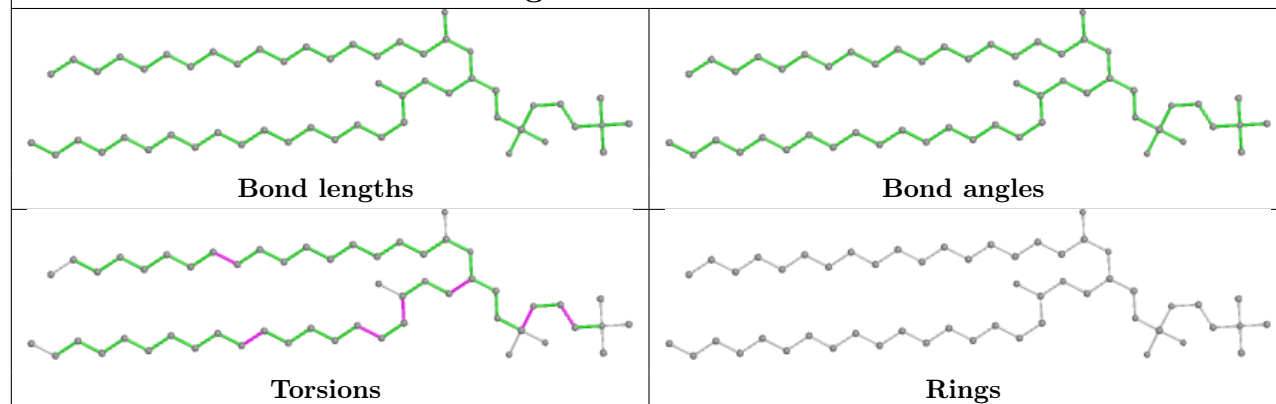


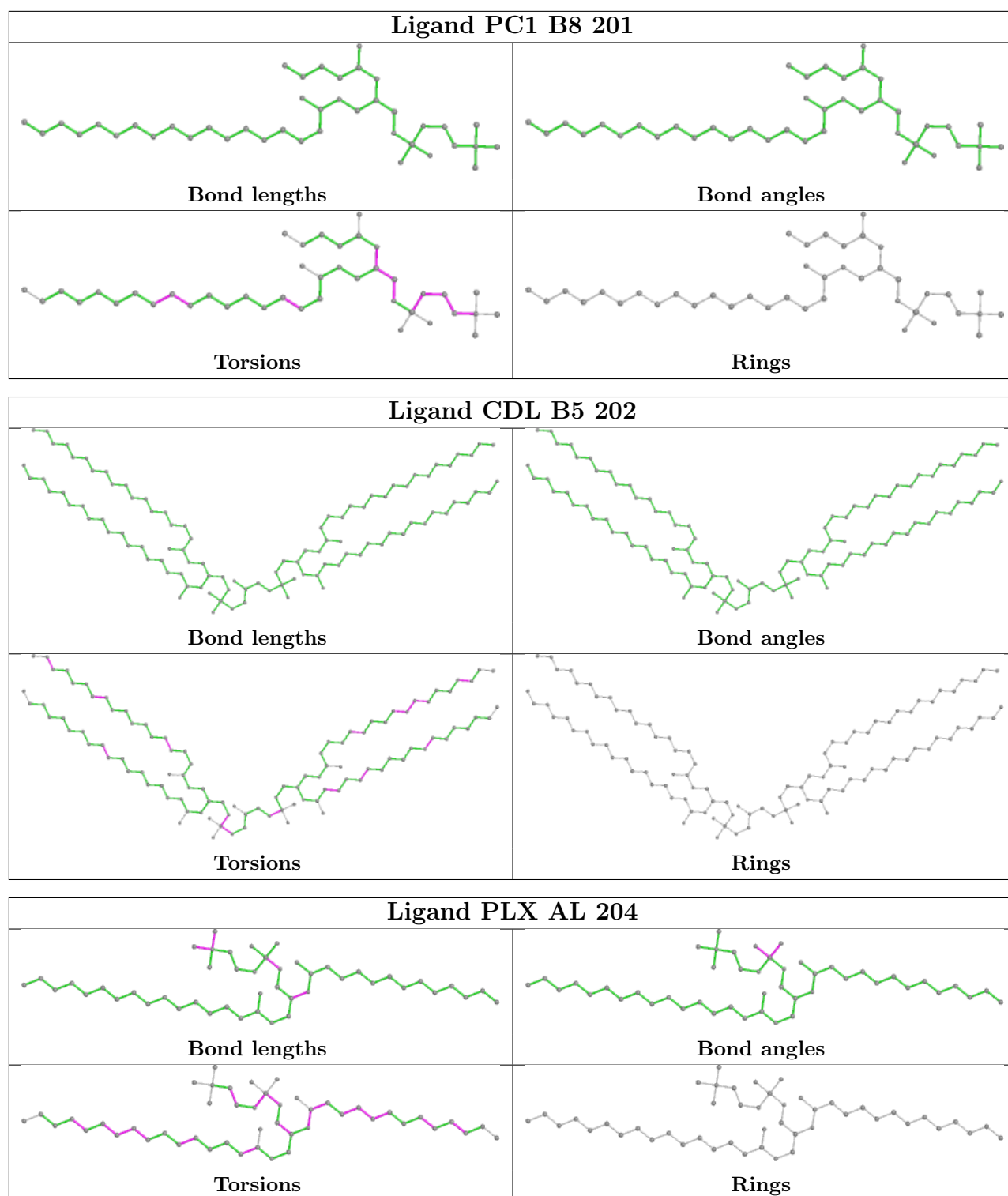


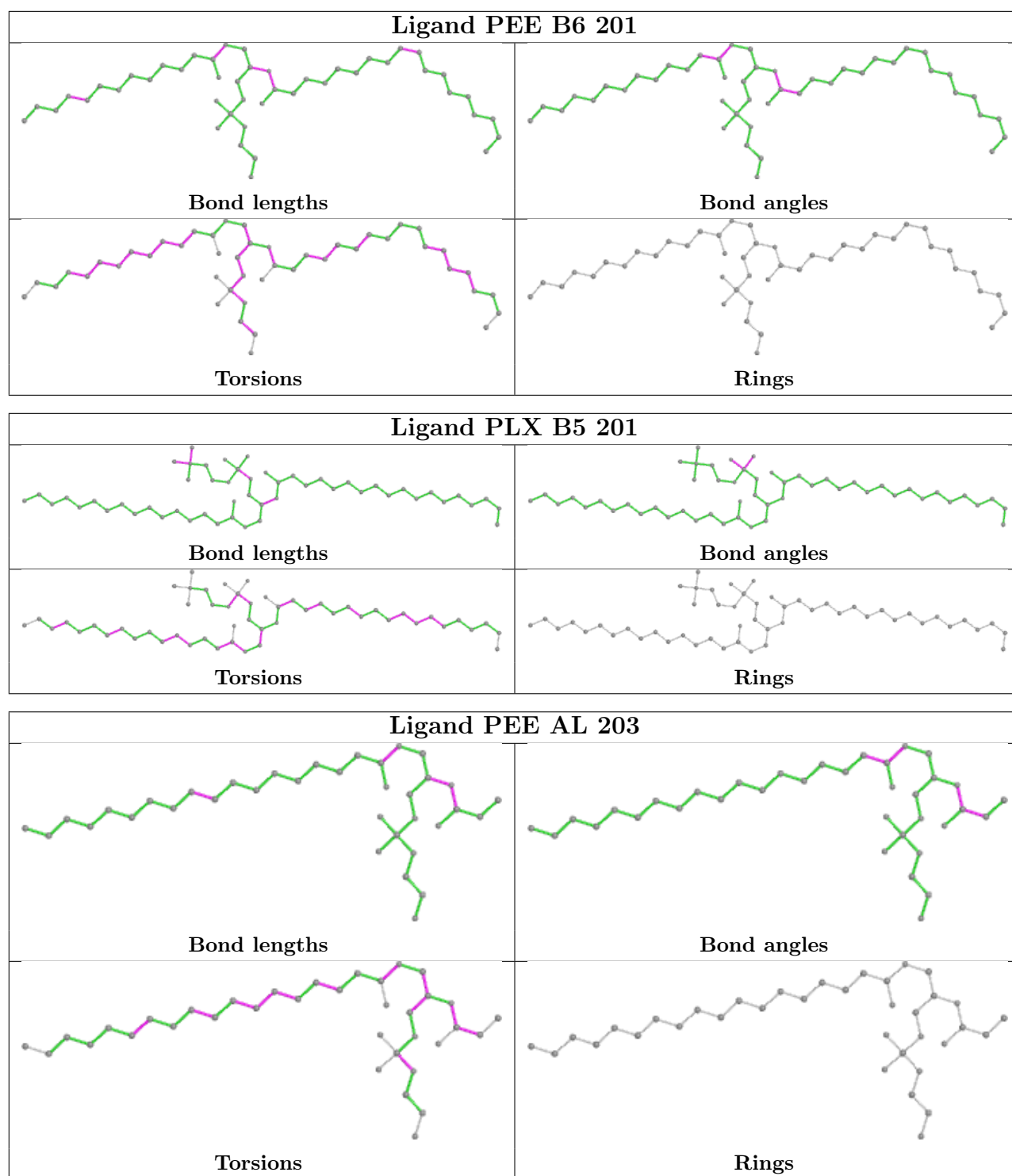
Ligand FMN V1 502

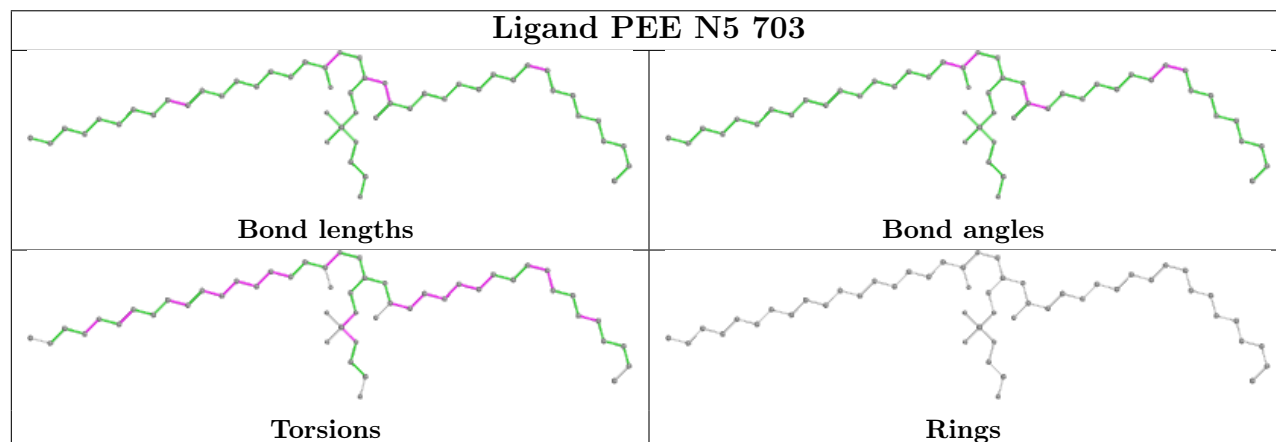
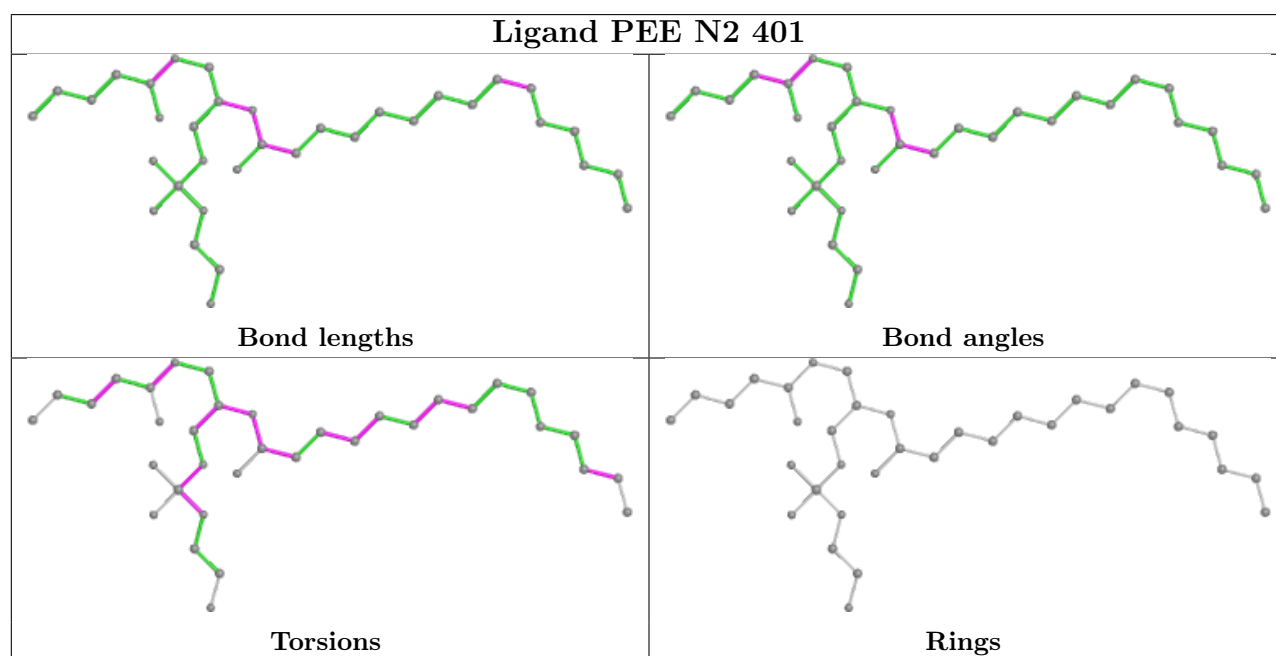
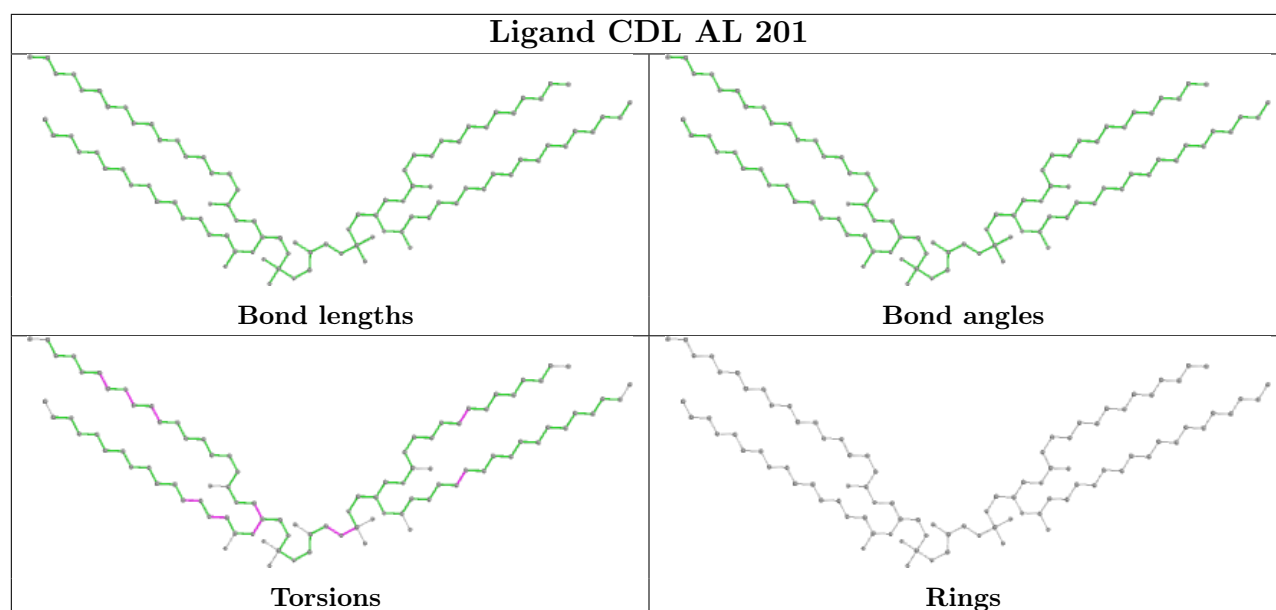


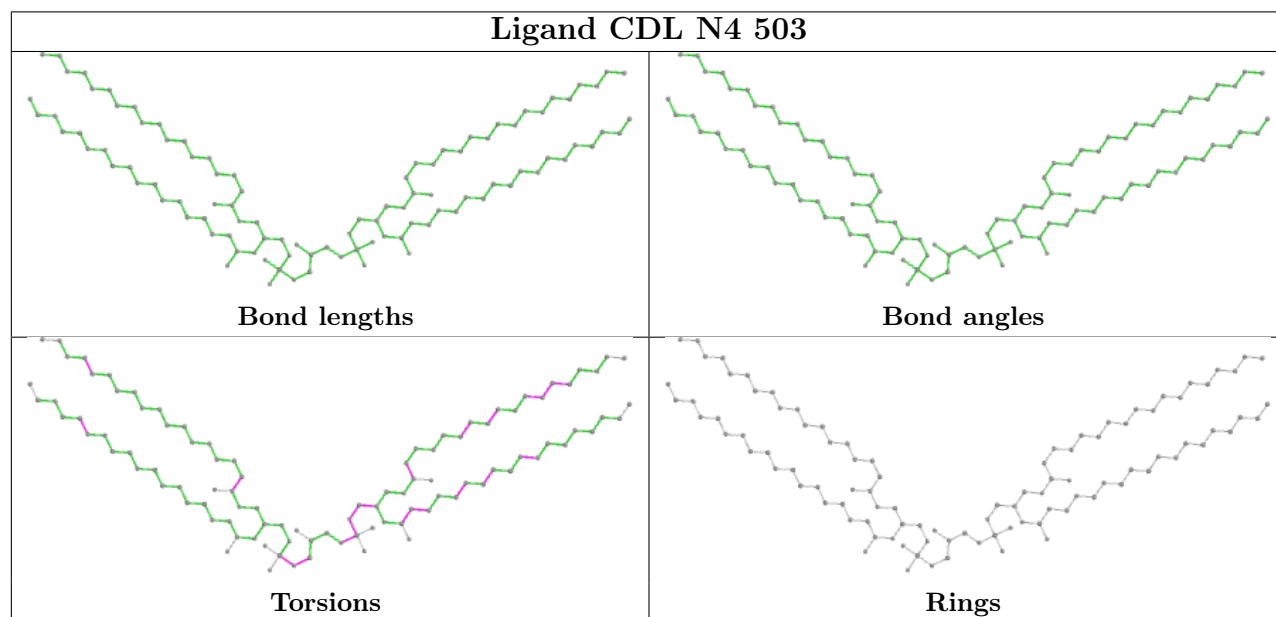
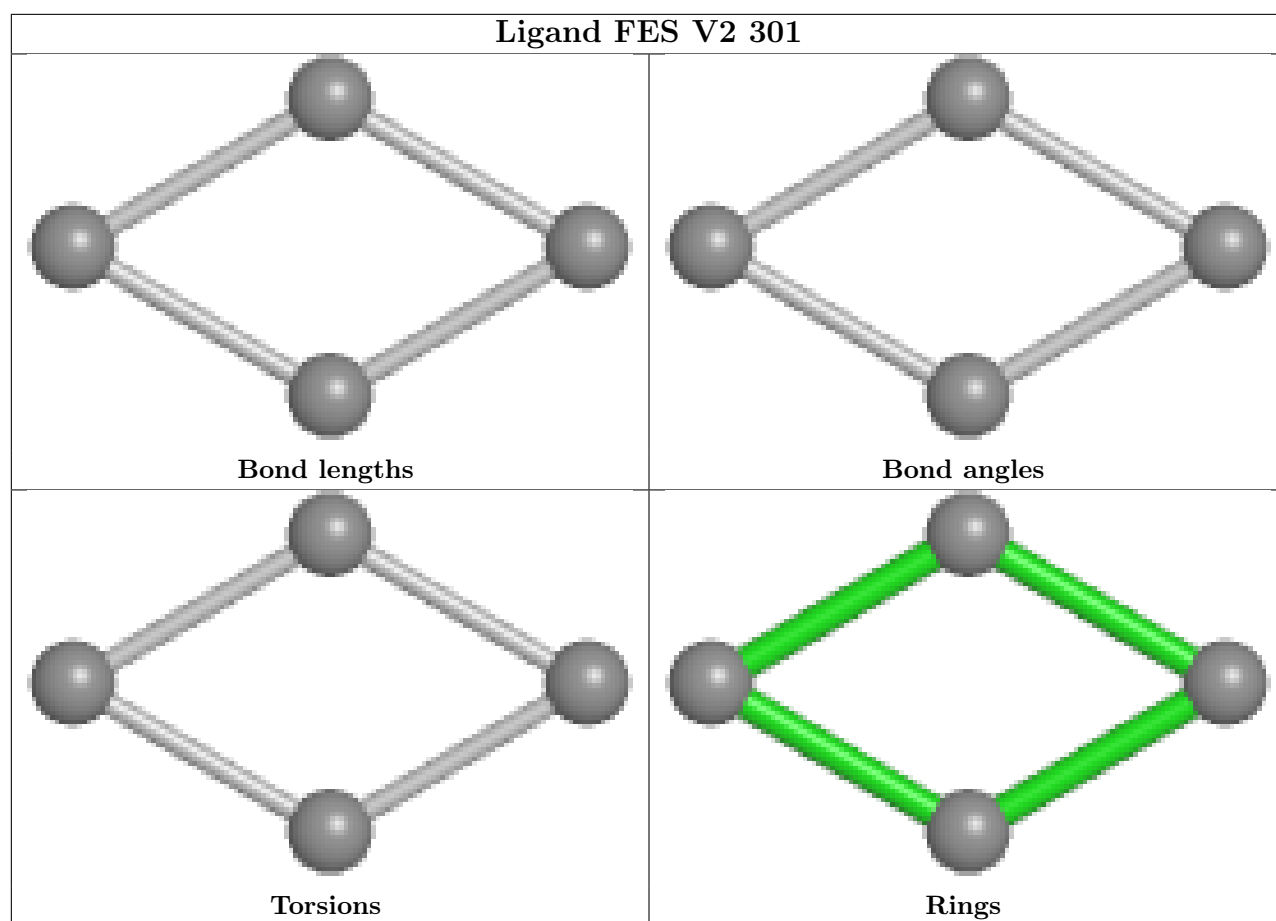
Ligand PC1 N3 204

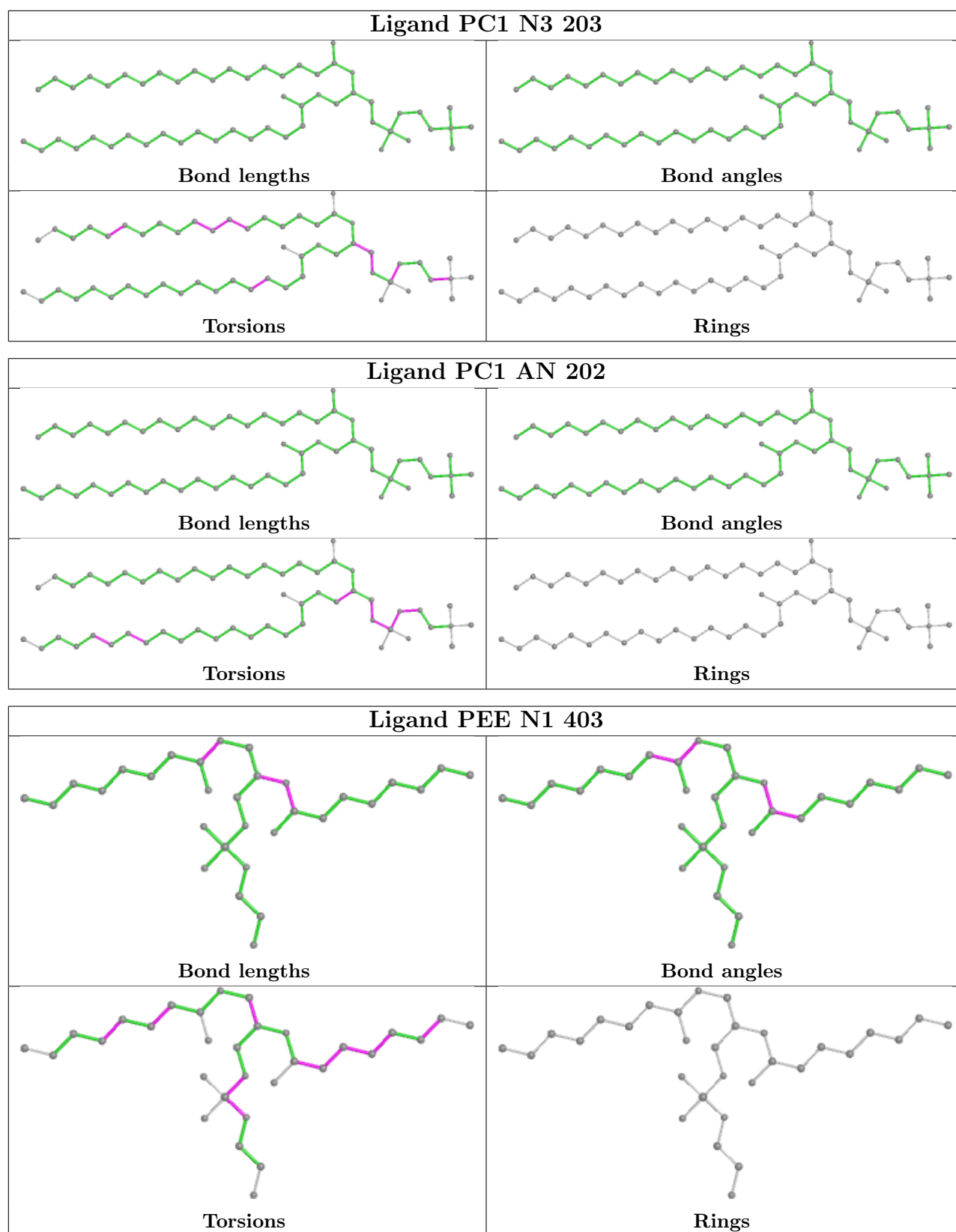


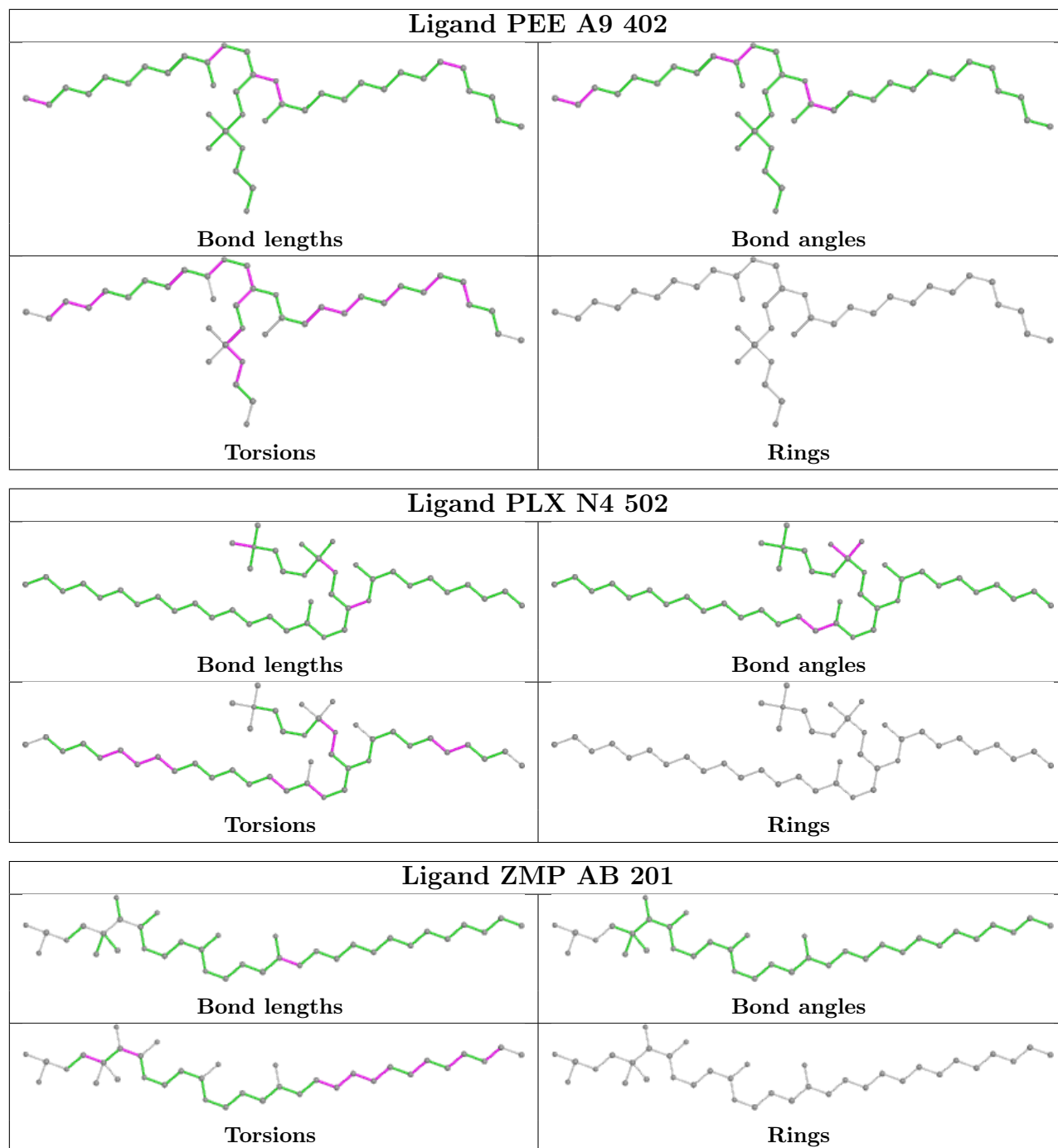


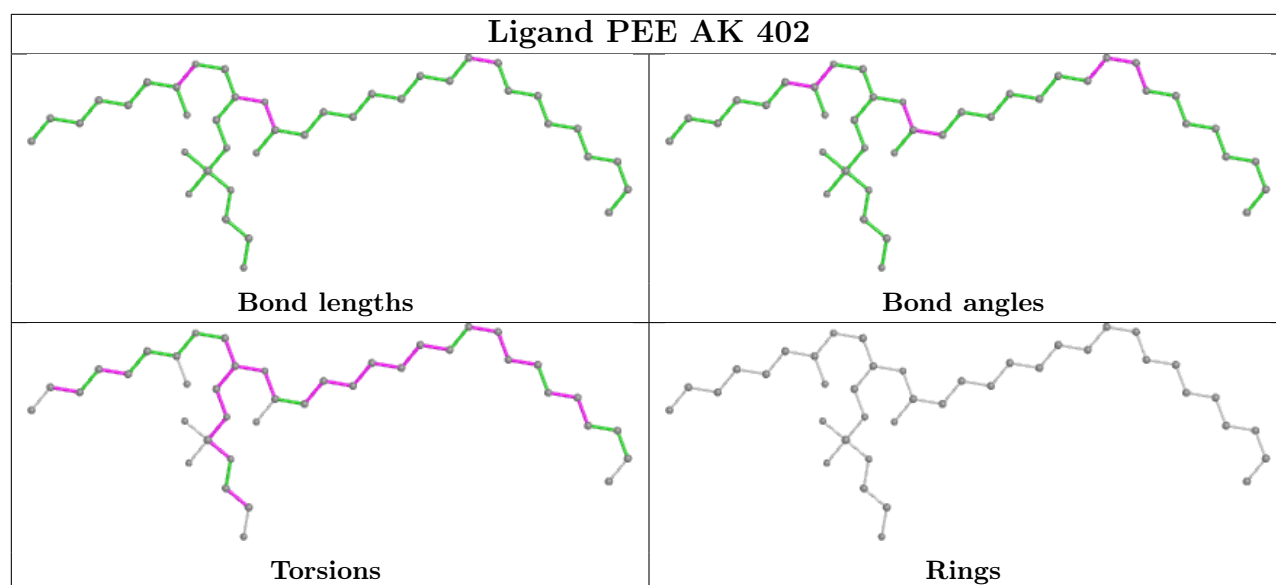












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

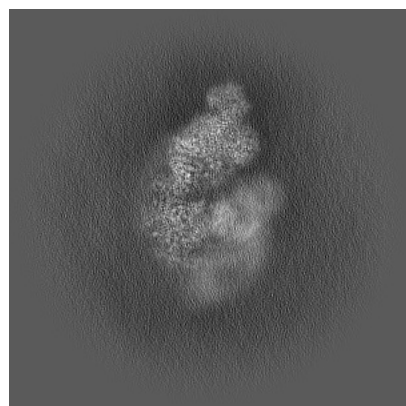
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60420. These allow visual inspection of the internal detail of the map and identification of artifacts.

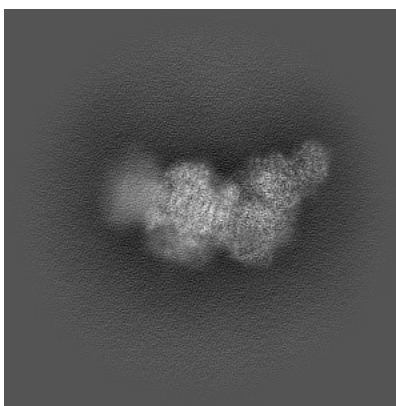
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

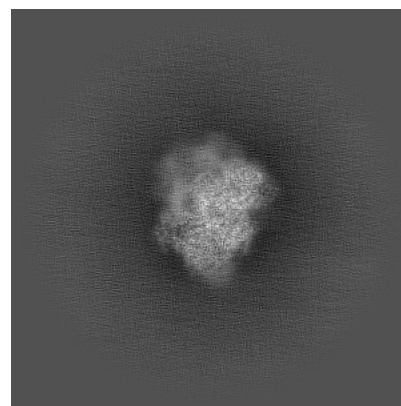
6.1.1 Primary map



X

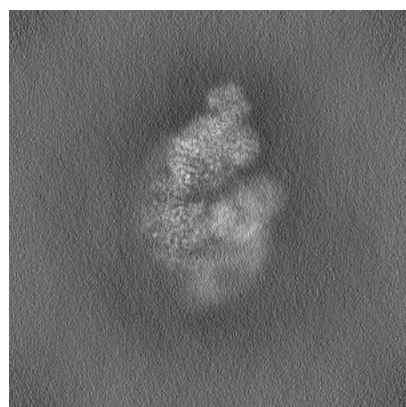


Y

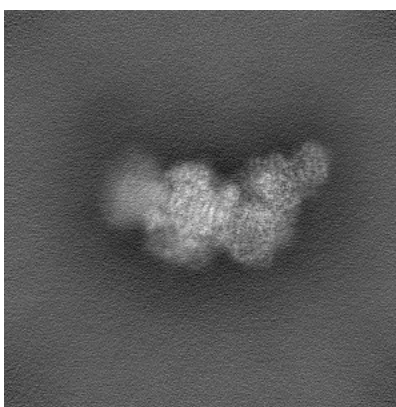


Z

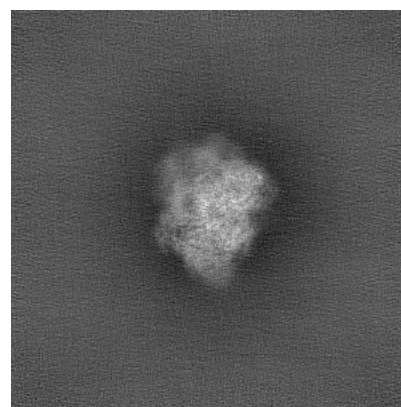
6.1.2 Raw map



X



Y

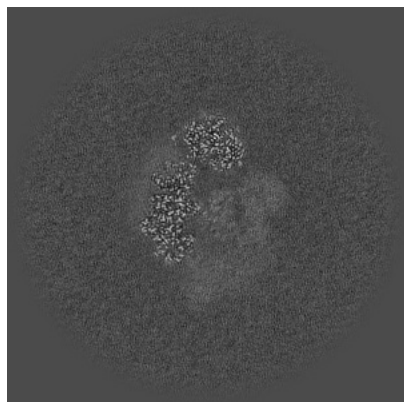


Z

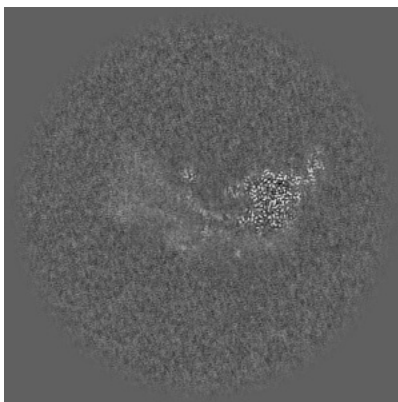
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

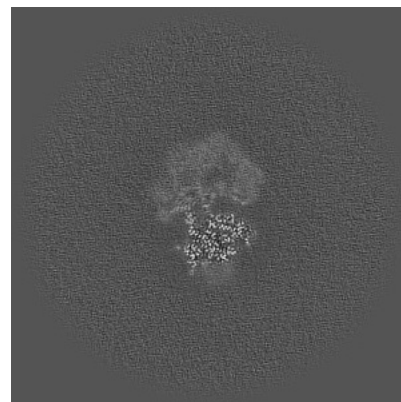
6.2.1 Primary map



X Index: 240

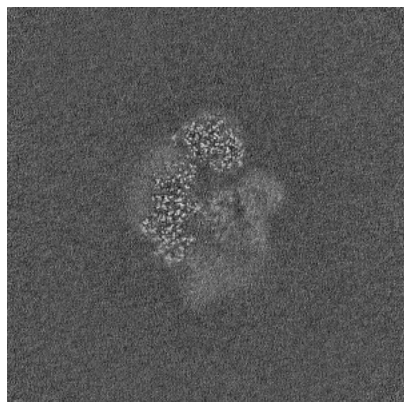


Y Index: 240

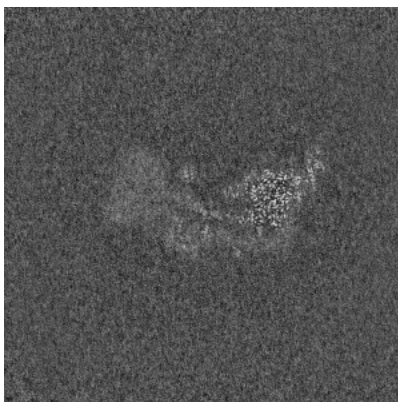


Z Index: 240

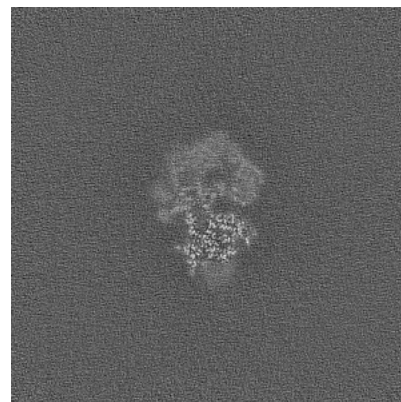
6.2.2 Raw map



X Index: 240



Y Index: 240

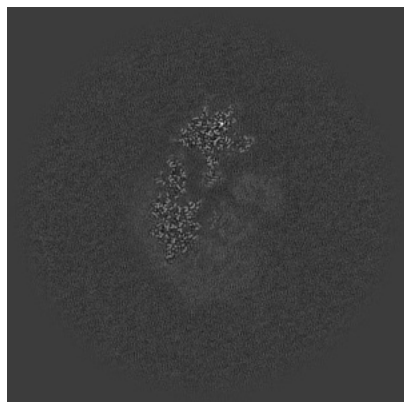


Z Index: 240

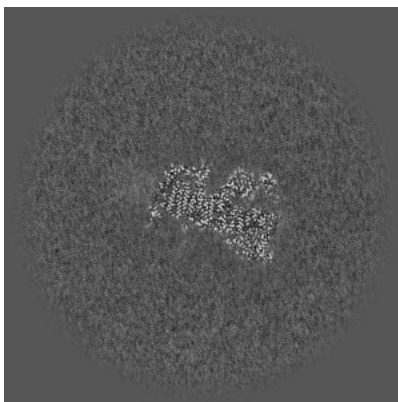
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

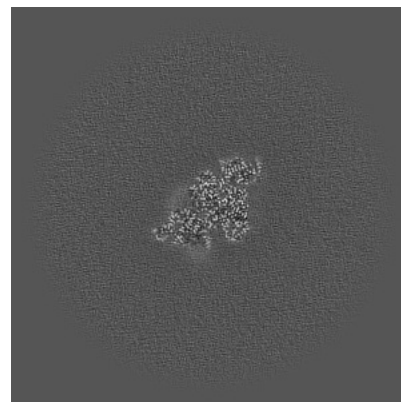
6.3.1 Primary map



X Index: 256

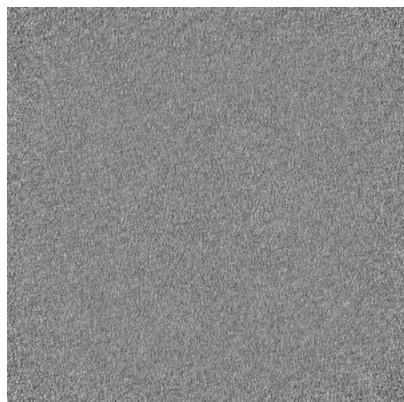


Y Index: 206

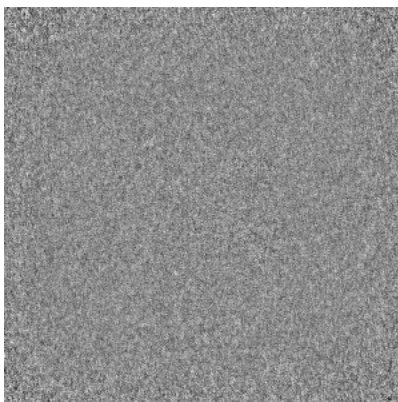


Z Index: 315

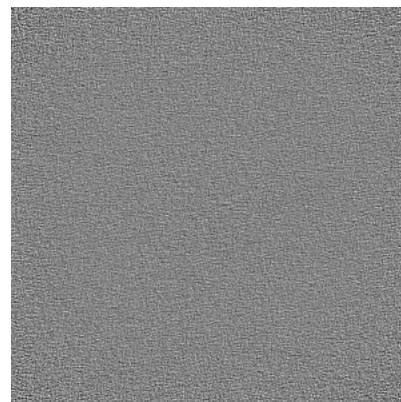
6.3.2 Raw map



X Index: 0



Y Index: 0

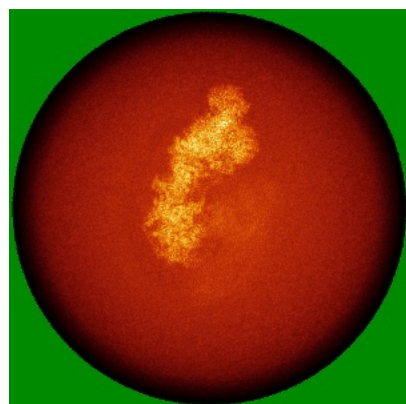


Z Index: 0

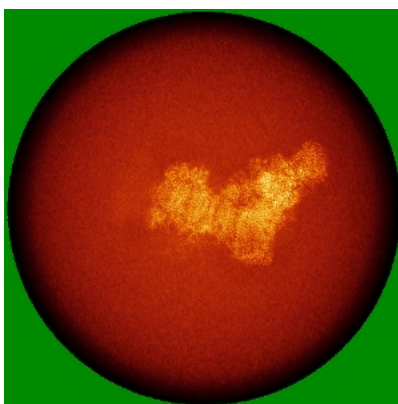
The images above show the largest variance slices of the map in three orthogonal directions.

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

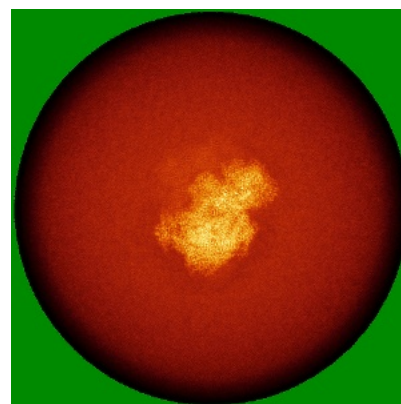
6.4.1 Primary map



X

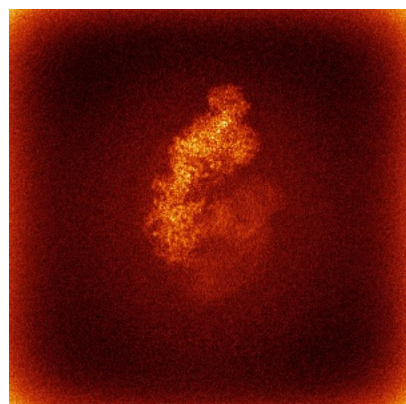


Y

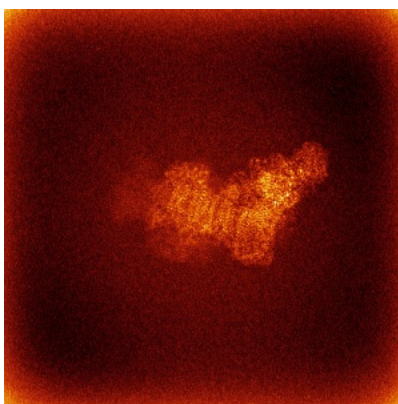


Z

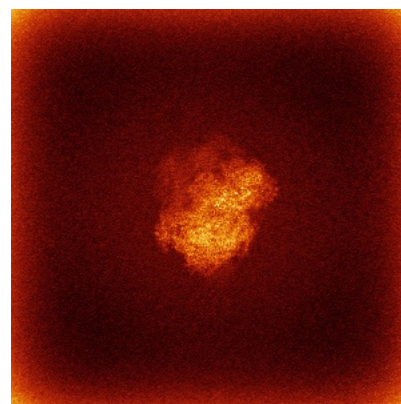
6.4.2 Raw map



X



Y

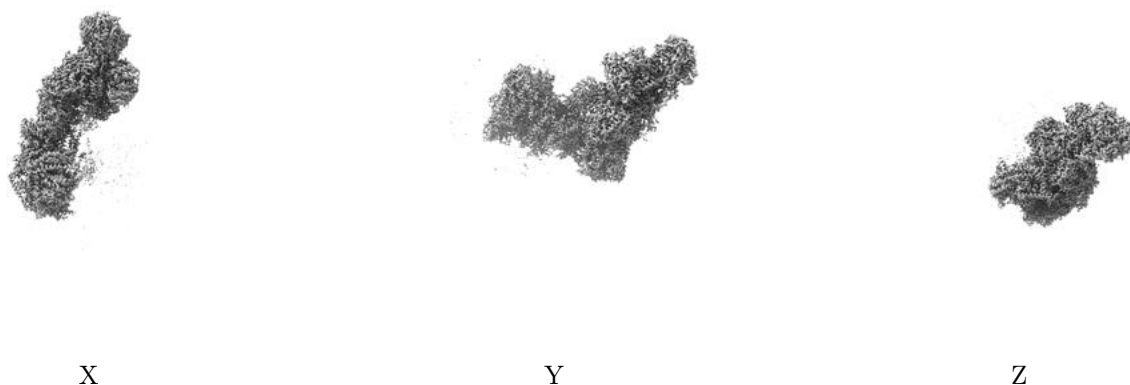


Z

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.

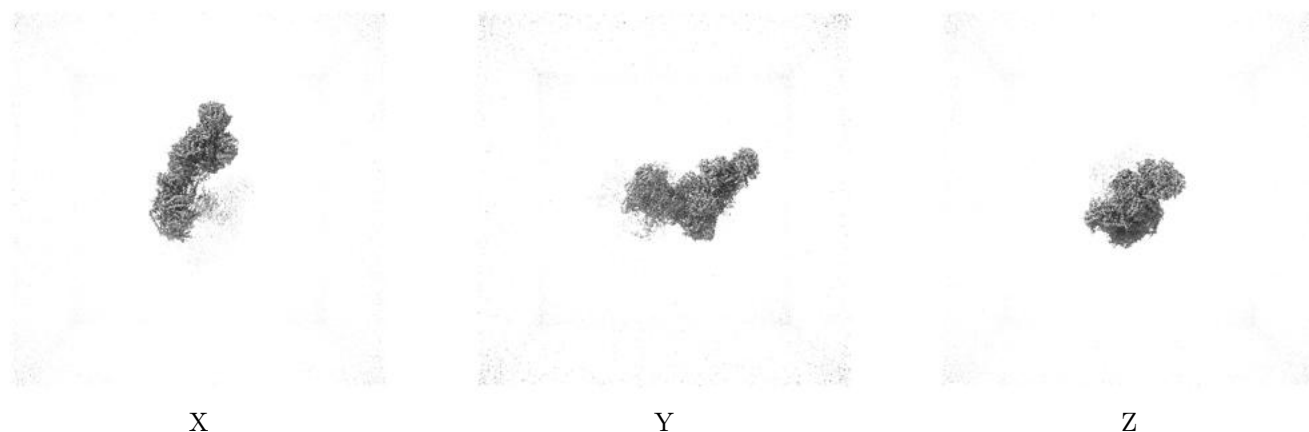
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

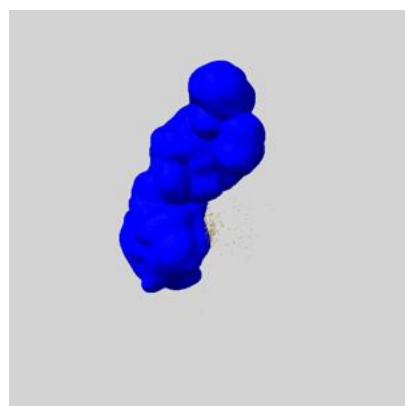
6.6 Mask visualisation [i](#)

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

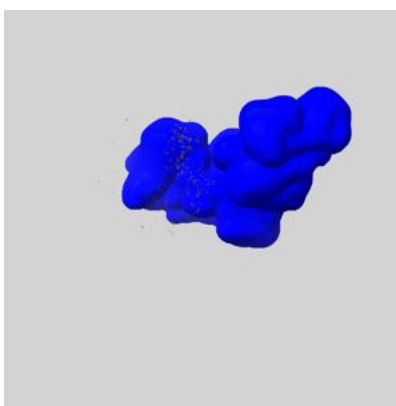
A mask typically either:

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

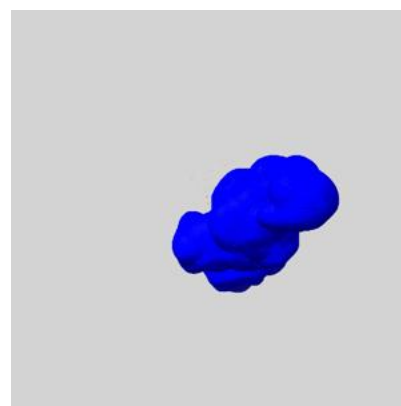
6.6.1 emd_60420_msk_1.map [i](#)



X



Y

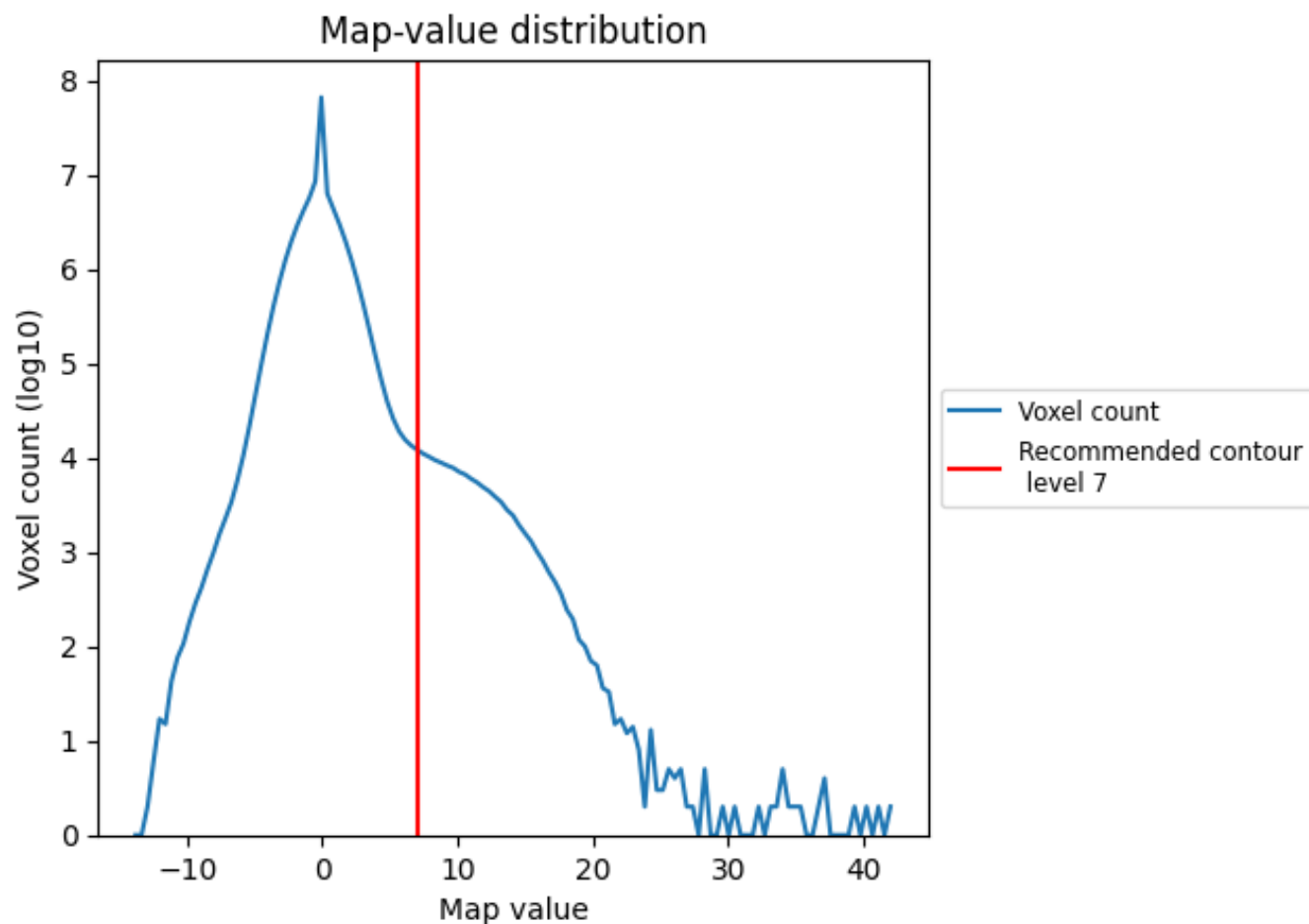


Z

7 Map analysis [i](#)

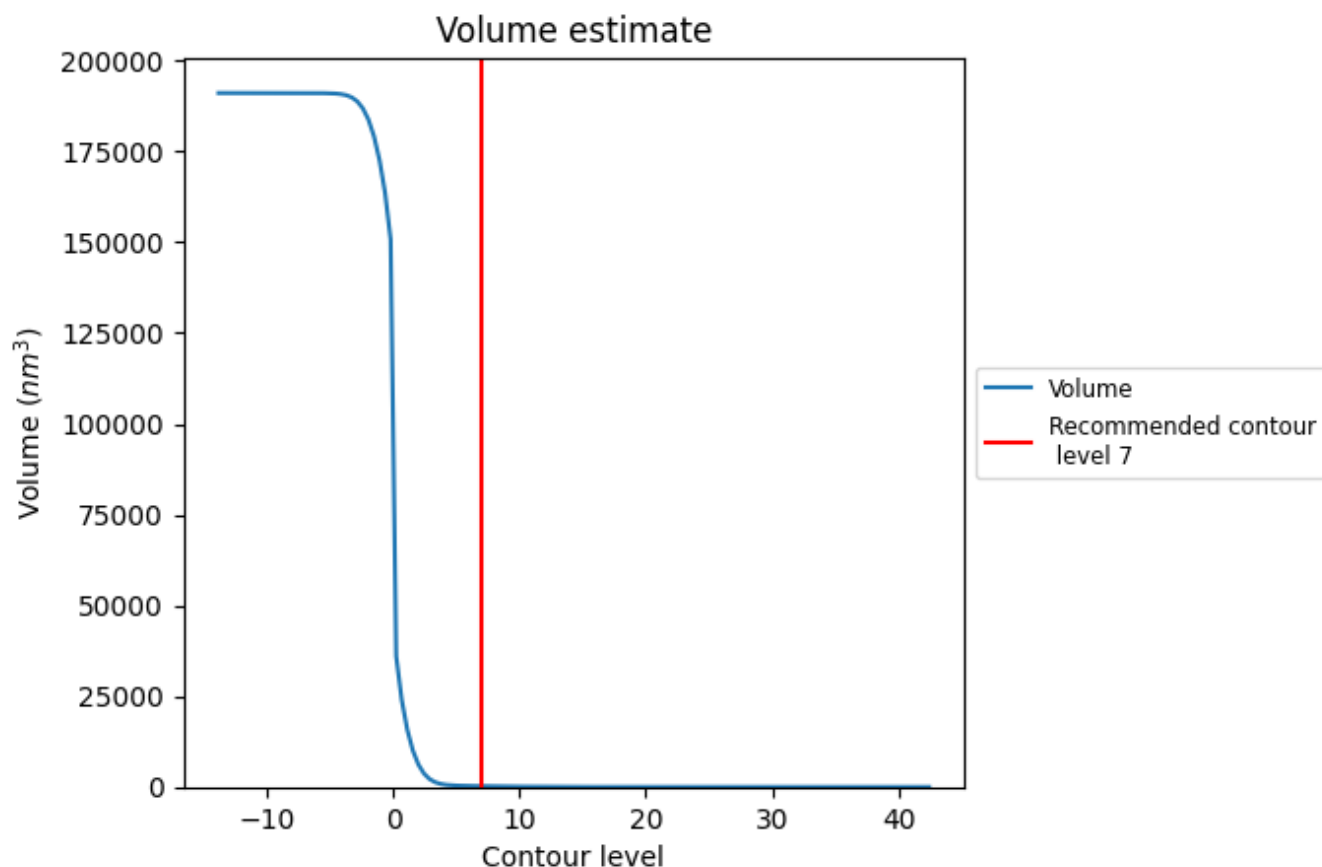
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

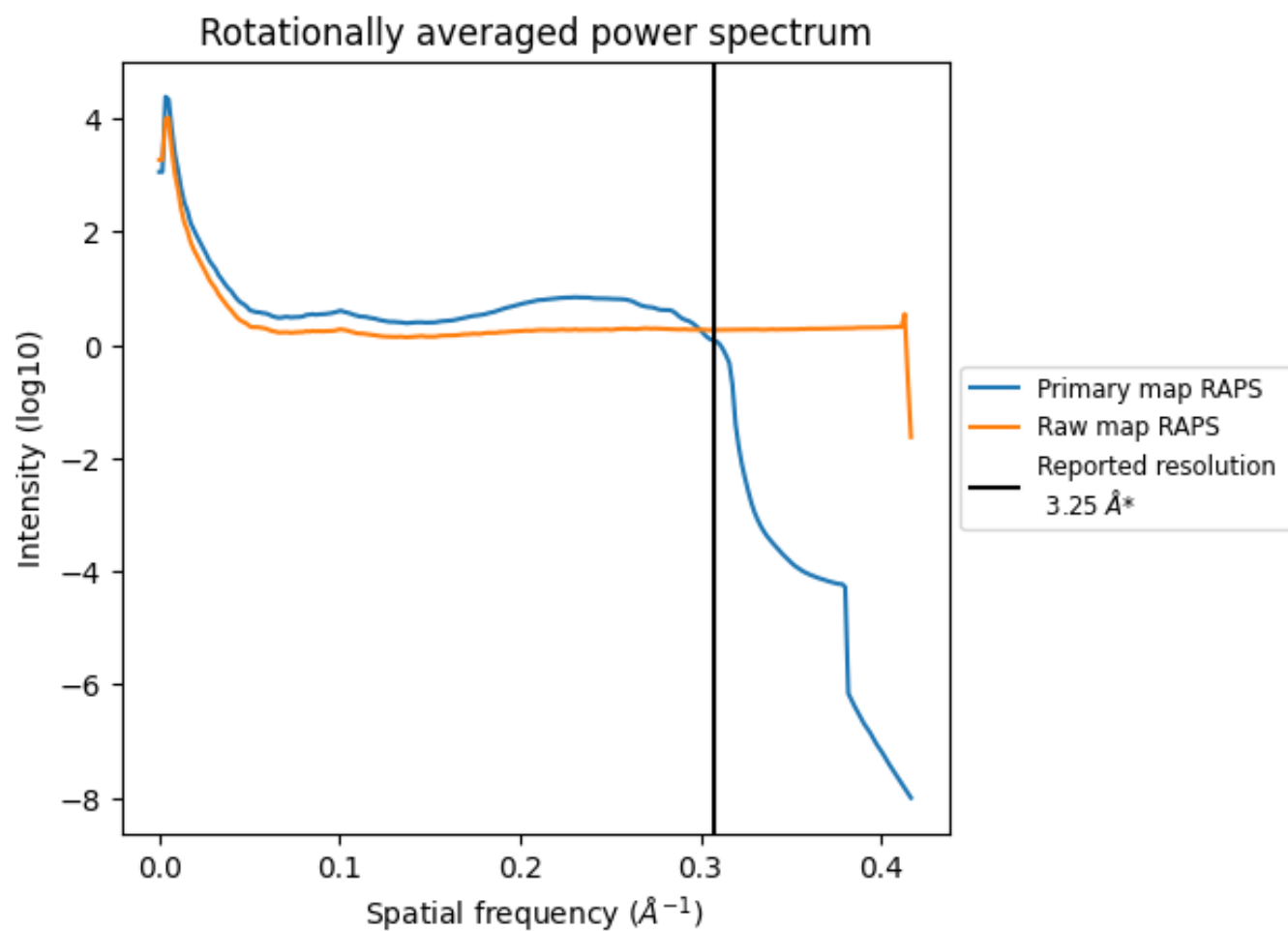
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214 nm³; this corresponds to an approximate mass of 194 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 ⓘ

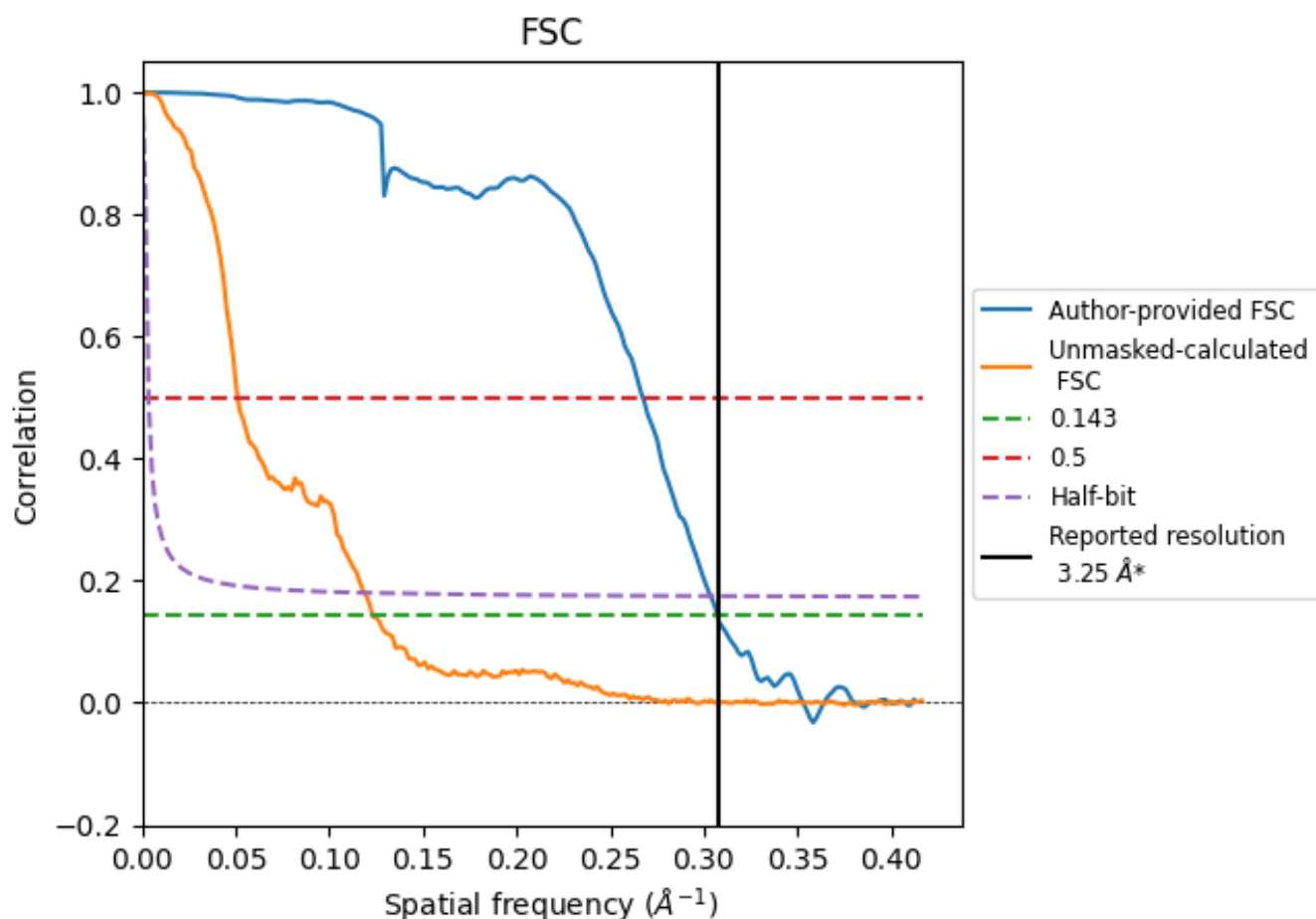


*Reported resolution corresponds to spatial frequency of 0.308 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.308 \AA^{-1}

8.2 Resolution estimates [i](#)

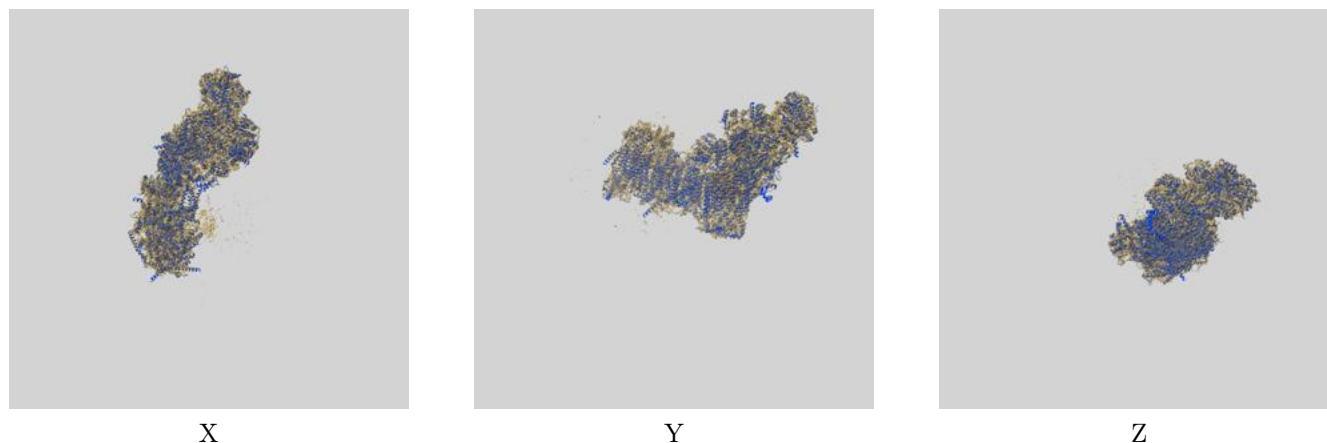
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	3.25	3.74	3.29
Unmasked-calculated*	8.12	19.57	8.42

*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 8.12 differs from the reported value 3.25 by more than 10 %

9 Map-model fit [i](#)

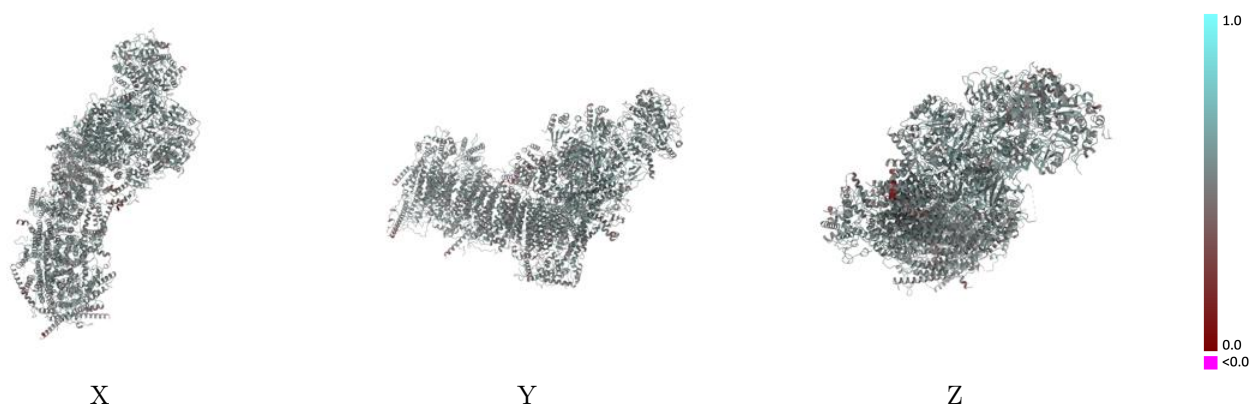
This section contains information regarding the fit between EMDB map EMD-60420 and PDB model 8ZSM. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



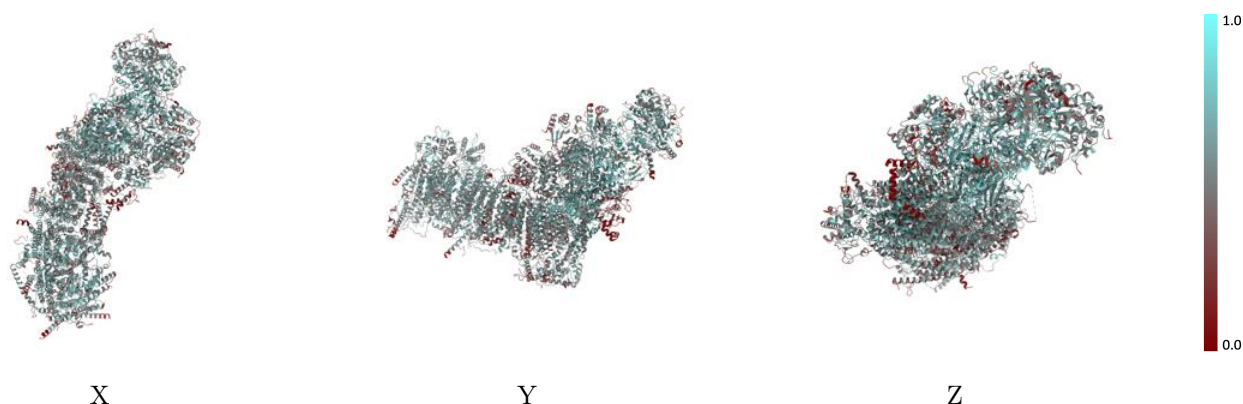
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



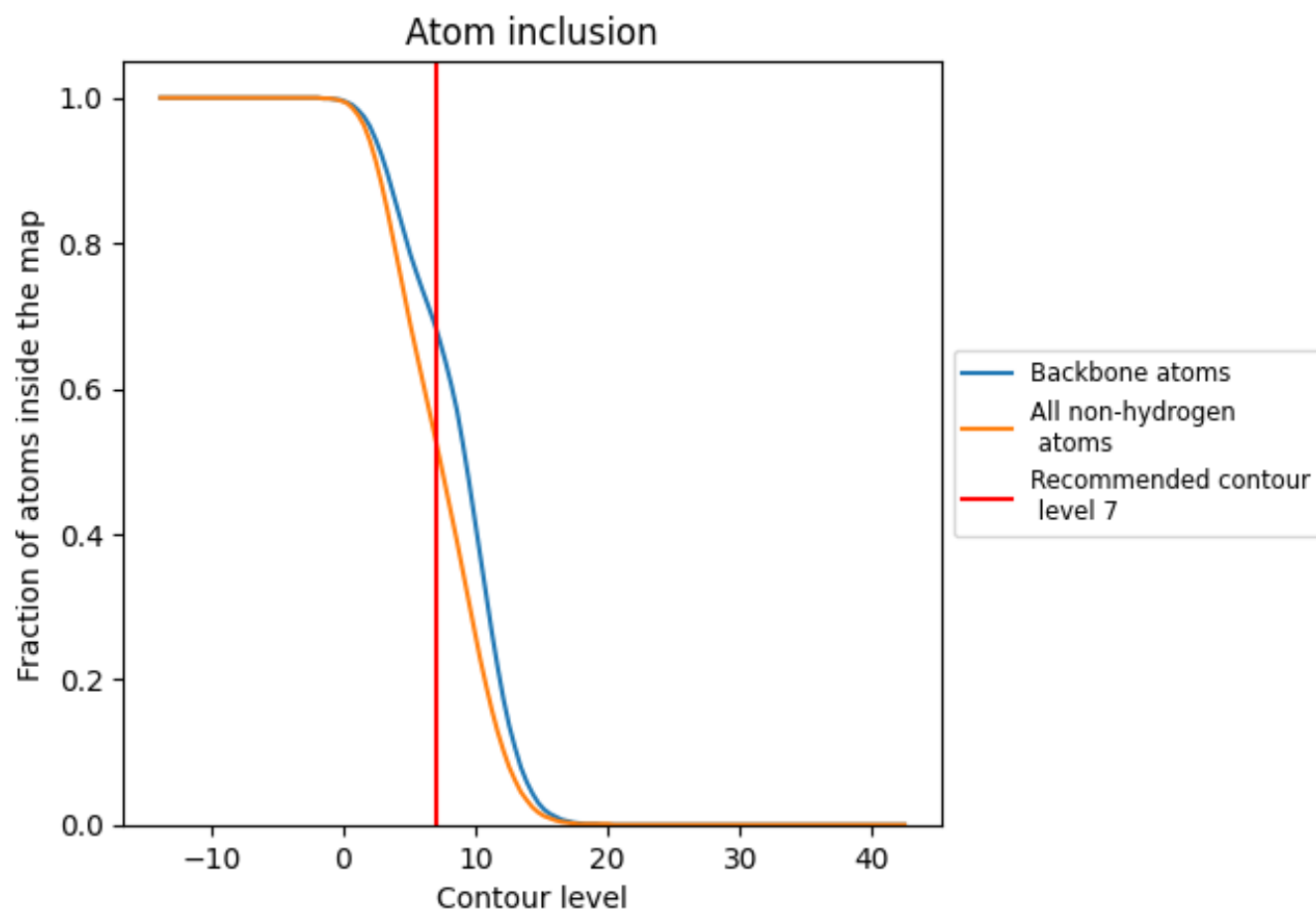
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 53% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5290	 0.5230
4L	 0.5360	 0.5310
A1	 0.4610	 0.5080
A2	 0.4810	 0.5130
A3	 0.3920	 0.5200
A5	 0.5200	 0.5220
A6	 0.5240	 0.5180
A7	 0.3470	 0.4990
A8	 0.5040	 0.5240
A9	 0.5800	 0.5350
AB	 0.2550	 0.4350
AC	 0.5340	 0.5170
AK	 0.4520	 0.4970
AL	 0.3310	 0.5120
AM	 0.1850	 0.4860
AN	 0.4750	 0.5180
B1	 0.4160	 0.5040
B2	 0.4830	 0.5010
B3	 0.4580	 0.4830
B4	 0.4750	 0.5180
B5	 0.5200	 0.5330
B6	 0.4580	 0.4930
B7	 0.4980	 0.5080
B8	 0.5450	 0.5300
B9	 0.5770	 0.5270
BK	 0.5390	 0.5090
BL	 0.5140	 0.5150
CA	 0.3940	 0.4900
CB	 0.4760	 0.5330
N1	 0.5660	 0.5290
N2	 0.5790	 0.5300
N3	 0.4660	 0.5330
N4	 0.5870	 0.5330
N5	 0.5560	 0.5290
N6	 0.4380	 0.4910



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S1	 0.5820	 0.5320
S2	 0.6400	 0.5440
S3	 0.6560	 0.5580
S4	 0.5680	 0.5390
S5	 0.4650	 0.5060
S6	 0.4450	 0.5270
S7	 0.6560	 0.5520
S8	 0.6370	 0.5520
V1	 0.5730	 0.5220
V2	 0.5210	 0.5160
V3	 0.4040	 0.5010