



## Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 06:40 PM JST

PDB ID : 8ZSR / pdb\_00008zsr  
EMDB ID : EMD-60425  
Title : Complex I form respirasome open state bound by proguanil (SC-ProgO)  
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.  
Deposited on : 2024-06-05  
Resolution : 3.10 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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) : 2.47



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Mol	Chain	Length	Quality of chain
5	A5	112	
6	A6	114	
7	A7	112	
8	A8	171	
9	A9	341	
10	AB	87	
10	AC	87	
11	AK	321	
12	AL	140	
13	AM	144	
14	AN	142	
15	B1	56	
16	B2	67	
17	B3	80	
18	B4	128	
19	B5	138	
20	B6	126	
21	B7	125	
22	B8	156	
23	B9	178	
24	BK	176	
25	BL	102	
26	CA	49	
27	CB	121	
28	N1	318	

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Mol	Chain	Length	Quality of chain
29	N2	347	 78%22%
30	N3	115	 70%11%18%
31	N4	459	 80%20%
32	N5	603	 76%23%
33	N6	174	 78%17%5%
34	S1	689	 79%21%.
35	S2	430	 76%21%..
36	S3	208	 84%16%
37	S4	124	 88%12%
38	S5	105	 83%17%
39	S6	96	 93%7%
40	S7	156	 83%15%.
41	S8	176	 81%19%
42	V1	431	 81%18%
43	V2	217	 88%12%
44	V3	42	 76%24%

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	XEW	N1	403	-	X	-	-
53	XEW	S2	501	-	X	-	-

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 68306 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	337	Total	C	N	O	S	0	0
			2703	1750	472	472	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	102	Total	C	N	O	S	0	0
			870	568	155	146	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	309	Total	C	N	O	S	0	0
			2440	1636	375	408	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	94	Total	C	N	O	S	0	0
			752	513	109	125	5		

- 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	166	Total	C	N	O	S	0	0
			1259	844	180	224	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S1	685	Total	C	N	O	S	0	0
			5266	3303	918	1006	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S2	420	Total	C	N	O	S	0	0
			3385	2166	579	616	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		

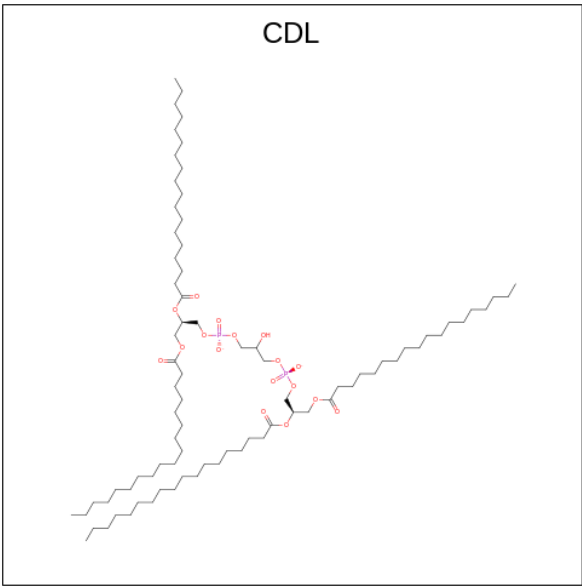
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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		

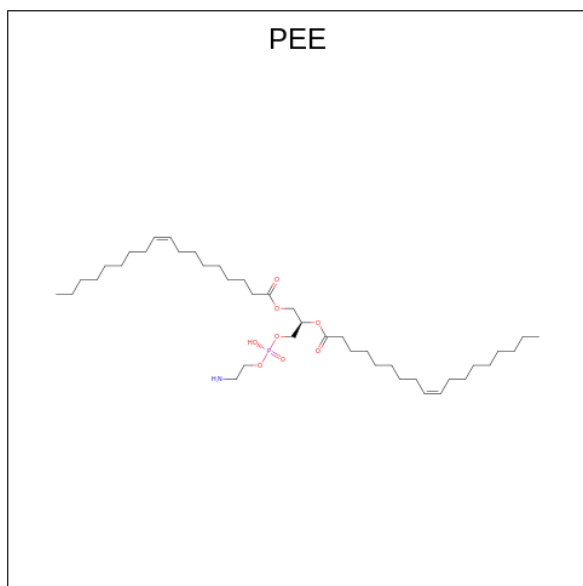
- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
45	4L	1	Total	C	O	P	0
			92	73	17	2	
45	A7	1	Total	C	O	P	0
			94	75	17	2	
45	A8	1	Total	C	O	P	0
			77	58	17	2	
45	AL	1	Total	C	O	P	0
			94	75	17	2	
45	AL	1	Total	C	O	P	0
			90	71	17	2	
45	B4	1	Total	C	O	P	0
			62	43	17	2	
45	B5	1	Total	C	O	P	0
			98	79	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
			82	63	17	2	
45	N5	1	Total	C	O	P	0
			100	81	17	2	
45	S8	1	Total	C	O	P	0
			100	81	17	2	

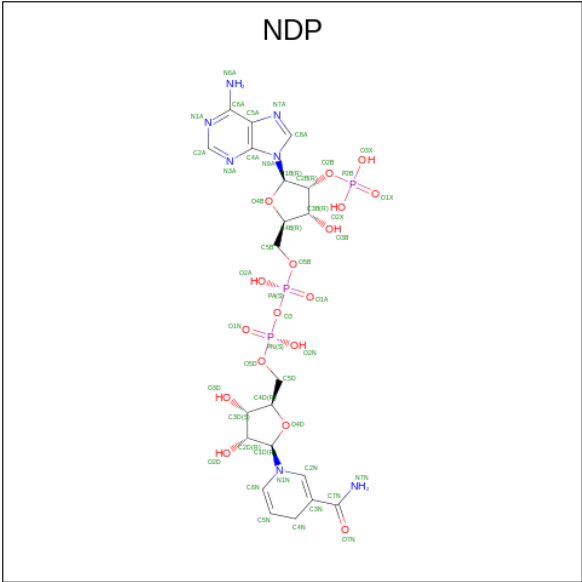
- Molecule 46 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:

C<sub>41</sub>H<sub>78</sub>NO<sub>8</sub>P).



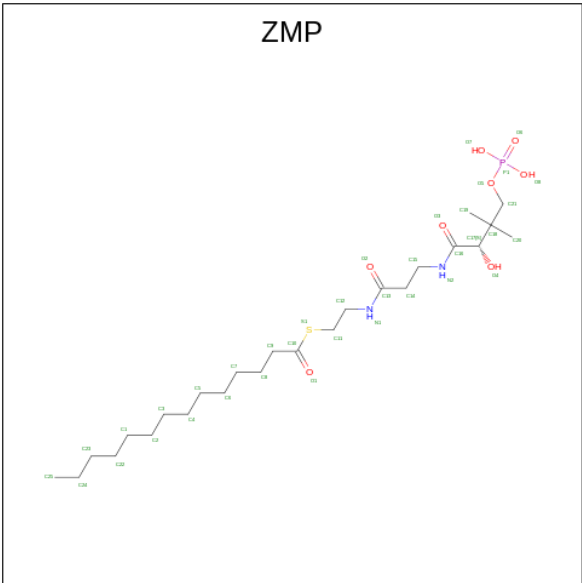
Mol	Chain	Residues	Atoms					AltConf
46	A3	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	AL	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	B4	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	N1	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	N1	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	N2	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	N5	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 47 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



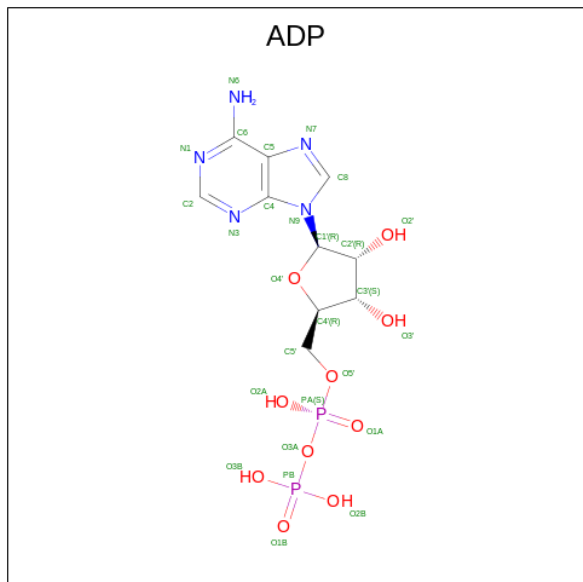
Mol	Chain	Residues	Atoms					AltConf
47	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 48 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS) (labeled as "Ligand of Interest" by depositor).



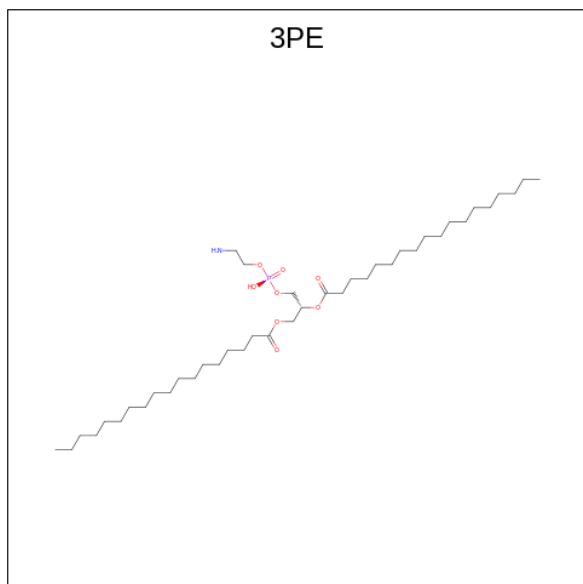
Mol	Chain	Residues	Atoms						AltConf
48	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
48	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 49 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



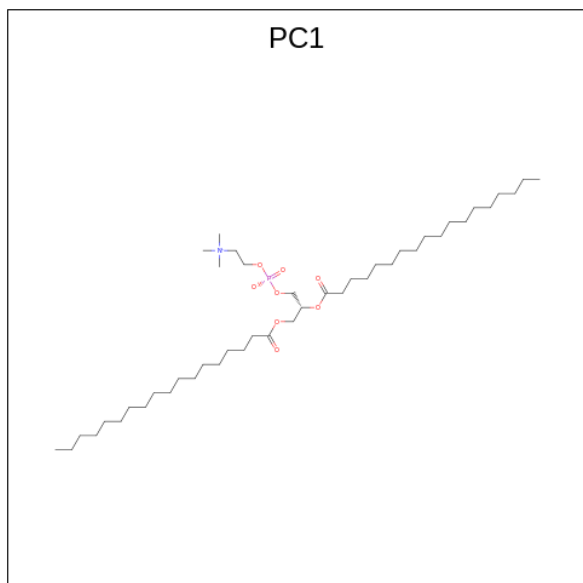
Mol	Chain	Residues	Atoms					AltConf
50	AL	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
50	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
50	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	

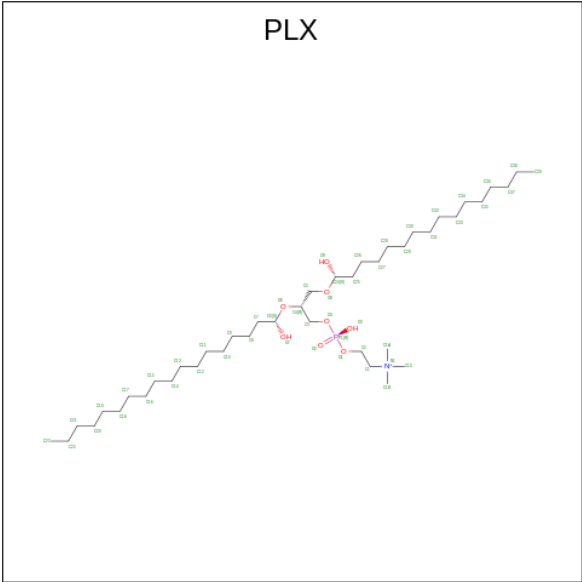
- Molecule 51 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
51	AL	1	Total	C	N	O	P	0
			31	21	1	8	1	
51	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	B7	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	N1	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	N1	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	S7	1	Total	C	N	O	P	0
			54	44	1	8	1	

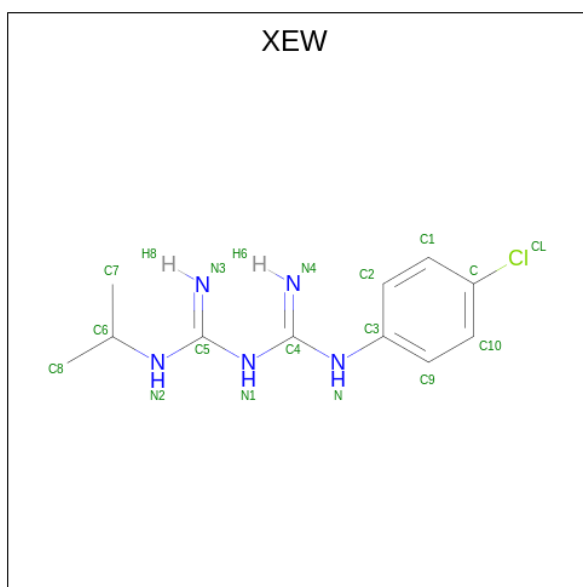
- Molecule 52 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula:  $C_{42}H_{89}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).





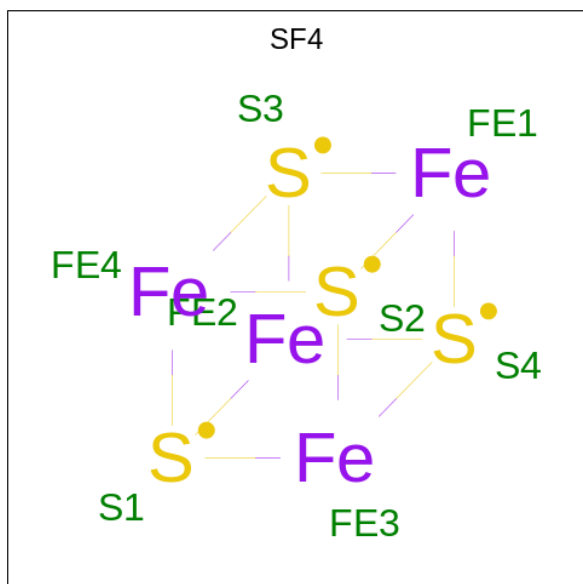
Mol	Chain	Residues	Atoms					AltConf
52	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	B5	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	N3	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	N4	1	Total	C	N	O	P	0
			47	37	1	8	1	
52	N4	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 53 is N-(4-chlorophenyl)-N'-(propan-2-yl)triimidodicarbonic diamide (CCD ID: XEW) (formula: C<sub>11</sub>H<sub>16</sub>ClN<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
53	N1	1	Total	C	Cl	N	0
			17	11	1	5	
53	S2	1	Total	C	Cl	N	0
			17	11	1	5	

- Molecule 54 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



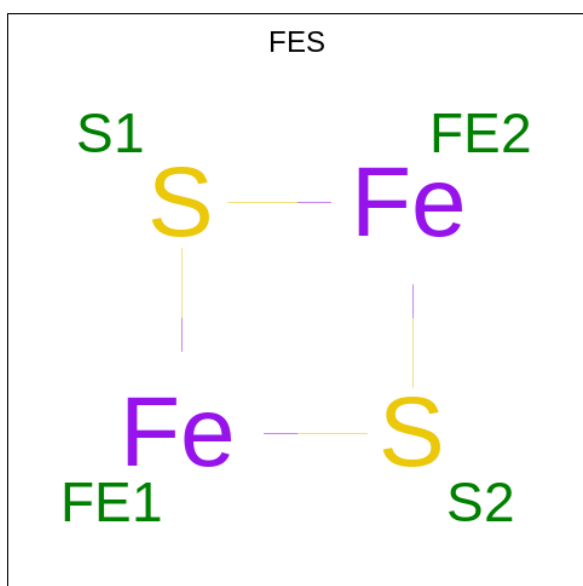
Mol	Chain	Residues	Atoms			AltConf
54	S1	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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

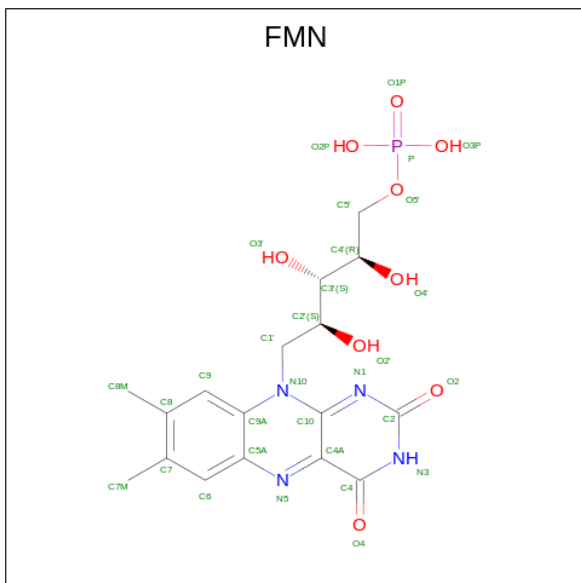
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- 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:  $C_{17}H_{21}N_4O_9P$ ).

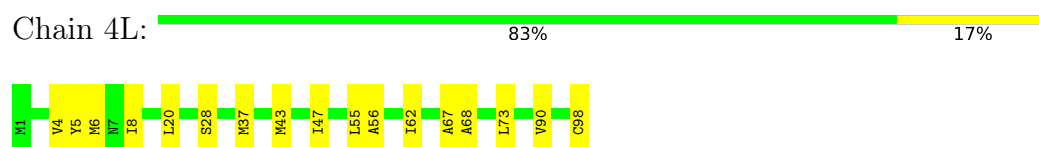


Mol	Chain	Residues	Atoms					AltConf
58	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

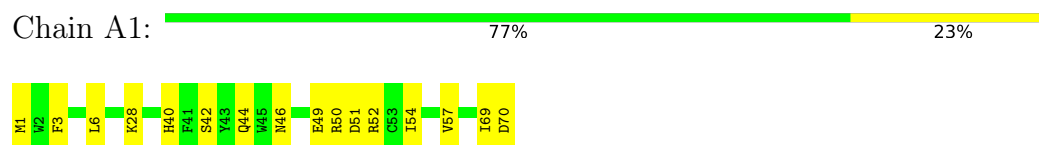
### 3 Residue-property plots

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.

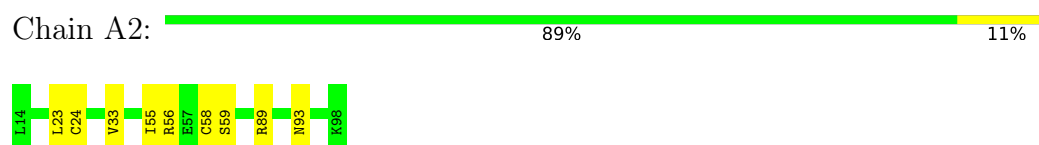
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



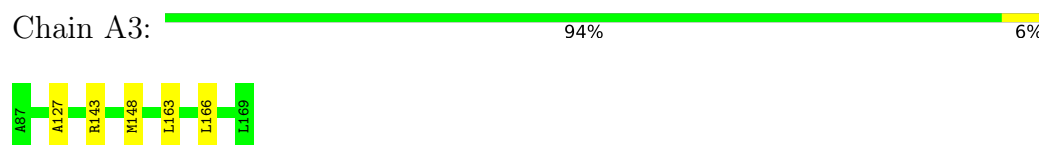
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



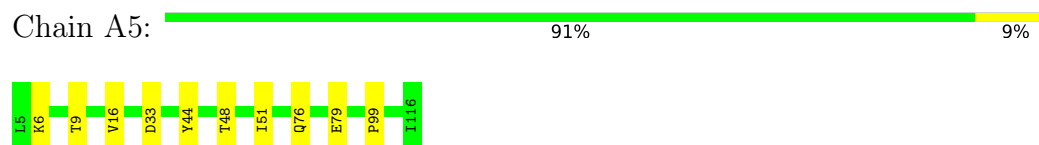
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



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

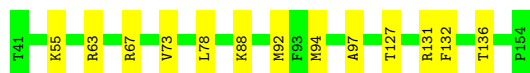


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5




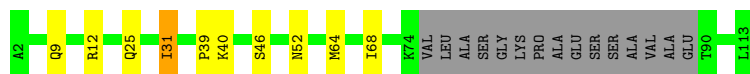
- Molecule 6: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:  89% 11%




- Molecule 7: Complex I-B14.5a

Chain A7:  78% 8% 13%




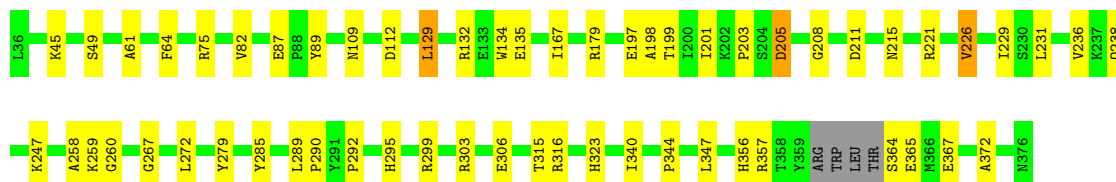
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:  80% 20%



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

Chain A9:  82% 16% ..




- Molecule 10: Acyl carrier protein

Chain AB:  61% 28% 11%




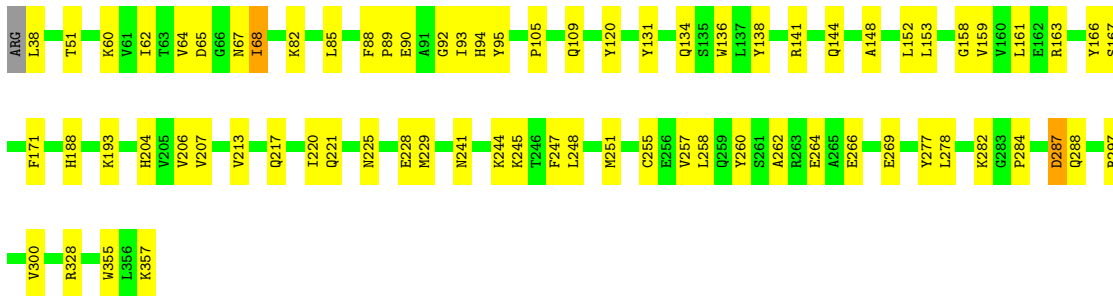
- Molecule 10: Acyl carrier protein

Chain AC:  80% 18% .




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

Chain AK:  77% 22%



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

Chain AL:  88% 12%




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

Chain AM:  88% 12%



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

Chain AN:  85% 15%




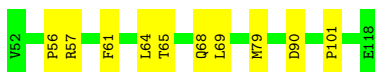
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain B1:  93% 7%



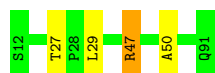
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain B2:  85% 15%



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

Chain B3:  95% ..



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

Chain B4:  92% 8%



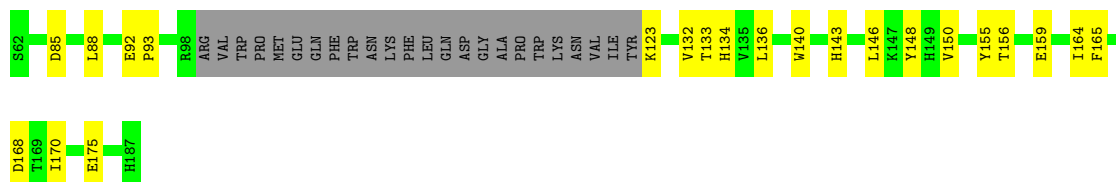
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:  93% 7%




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

Chain B6:  63% 17% 19%



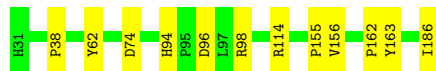
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:  83% 17%




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

Chain B8:  92% 8%



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

Chain B9:  86% 14%





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

Chain BK: 82% 16%



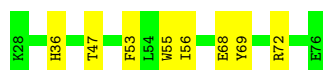
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BL: 86% 11%



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

Chain CA: 84% 16%



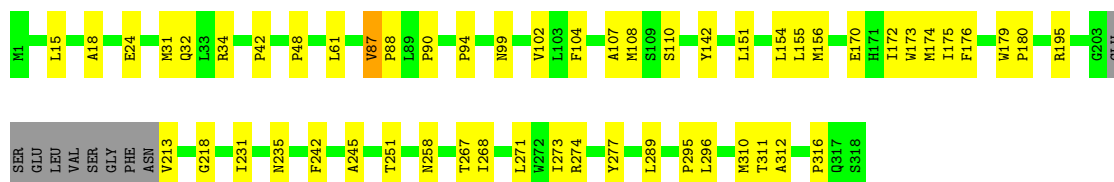
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain CB: 88% 12%



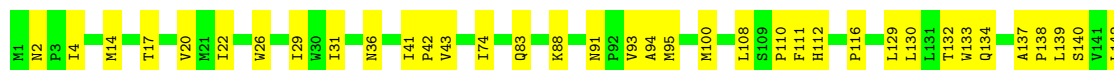
- Molecule 28: NADH-ubiquinone oxidoreductase chain 1

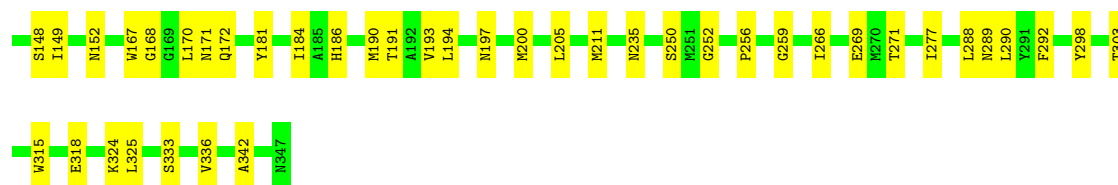
Chain N1: 80% 17%



- Molecule 29: NADH-ubiquinone oxidoreductase chain 2

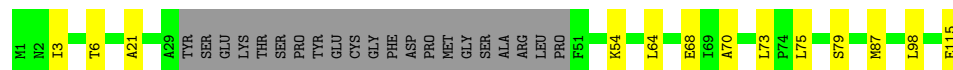
Chain N2: 78% 22%





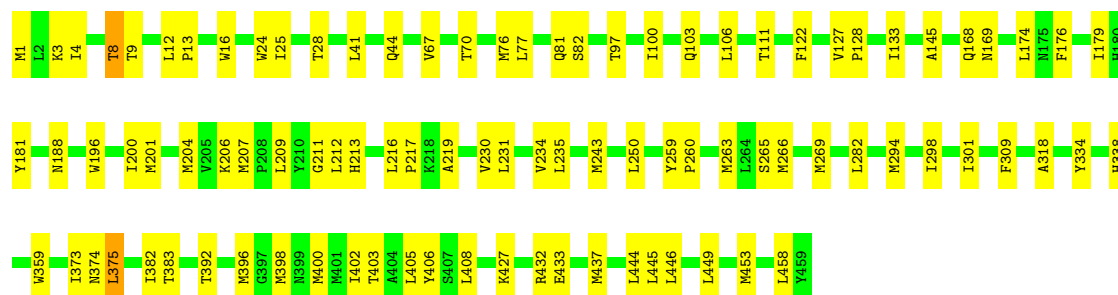
• Molecule 30: NADH-ubiquinone oxidoreductase chain 3

Chain N3: 70% 11% 18%



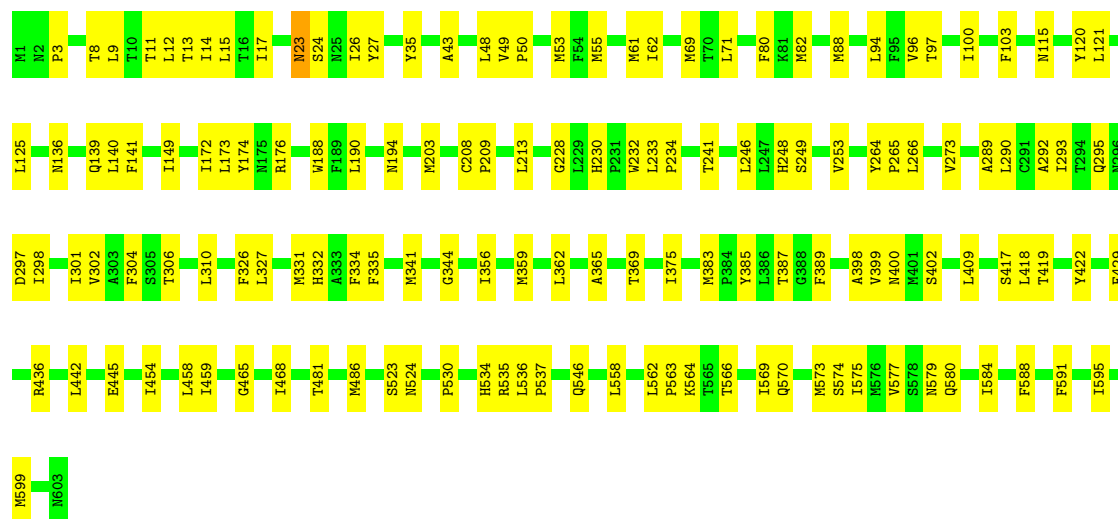
• Molecule 31: NADH-ubiquinone oxidoreductase chain 4

Chain N4: 80% 20%



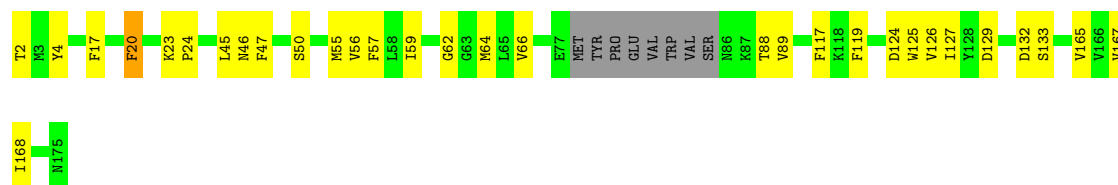
• Molecule 32: NADH-ubiquinone oxidoreductase chain 5

Chain N5: 76% 23%



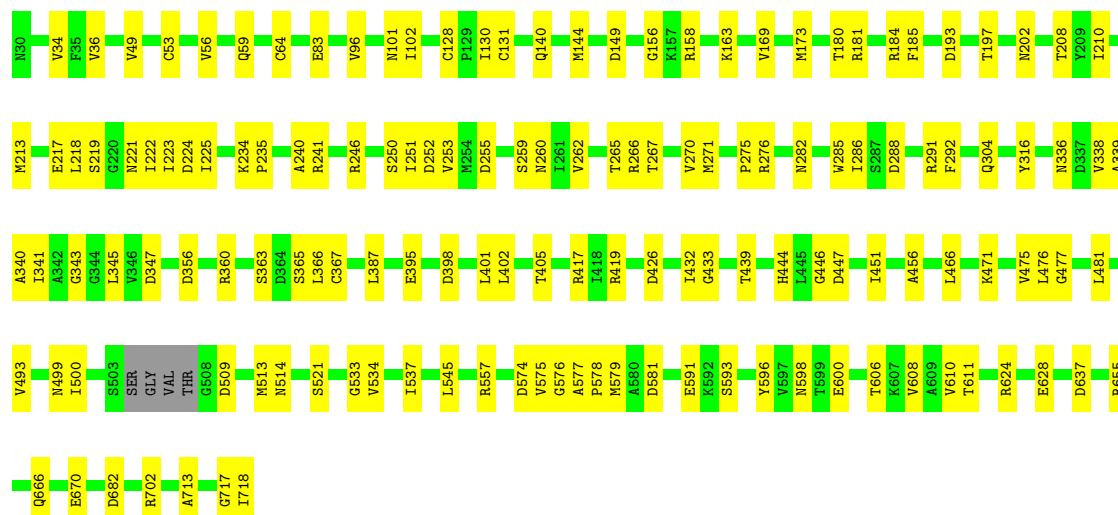
• Molecule 33: NADH-ubiquinone oxidoreductase chain 6

Chain N6: 78% 17% 5%



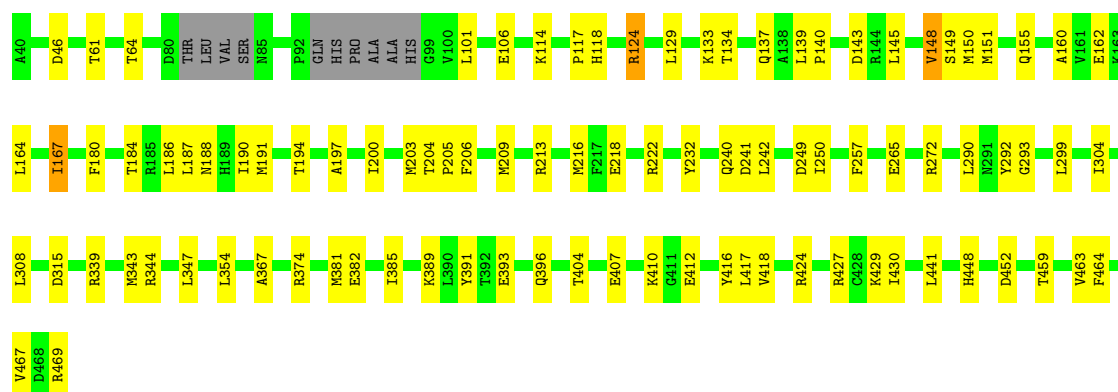
- Molecule 34: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain S1: 79% 21% .



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

Chain S2: 76% 21% ..




- Molecule 36: Complex I-30kD


Chain S3: 84% 16%




E250

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

Chain S4:  88% 12%



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

Chain S5:  83% 17%




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

Chain S6:  93% 7%






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

Chain S7:  83% 15%




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

Chain S8:  81% 19%

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

Chain V1:  81% 18%





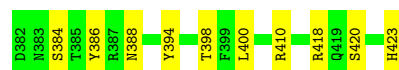
- Molecule 43: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2: 88% 12%



- Molecule 44: NADH:ubiquinone oxidoreductase subunit V3

Chain V3: 76% 24%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133663	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	58.499	Depositor
Minimum map value	-23.662	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.002	Depositor
Recommended contour level	0.05	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: XEW, PC1, 3PE, CDL, SF4, MG, ADP, PEE, FES, 2MR, FMN, ZN, NDP, ZMP, PLX

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	0.10	0/759	0.23	0/1029
2	A1	0.10	0/577	0.31	1/777 (0.1%)
3	A2	0.09	0/697	0.24	0/938
4	A3	0.09	0/664	0.22	0/912
5	A5	0.08	0/929	0.19	0/1258
6	A6	0.09	0/991	0.21	0/1335
7	A7	0.08	0/798	0.21	0/1079
8	A8	0.09	0/1436	0.23	0/1938
9	A9	0.10	0/2777	0.25	0/3762
10	AB	0.07	0/633	0.21	0/851
10	AC	0.10	0/714	0.22	0/965
11	AK	0.11	0/2650	0.27	0/3588
12	AL	0.10	0/1042	0.21	0/1411
13	AM	0.09	0/1245	0.22	0/1694
14	AN	0.11	0/1204	0.23	0/1624
15	B1	0.10	0/491	0.23	0/663
16	B2	0.10	0/610	0.23	0/836
17	B3	0.10	0/660	0.24	0/892
18	B4	0.12	0/1092	0.24	0/1481
19	B5	0.12	0/1184	0.26	0/1603
20	B6	0.13	0/897	0.28	0/1219
21	B7	0.10	0/1092	0.23	0/1459
22	B8	0.10	0/1371	0.23	0/1875
23	B9	0.11	0/1590	0.24	0/2155
24	BK	0.11	0/1489	0.25	0/2008
25	BL	0.12	0/851	0.26	0/1155
26	CA	0.08	0/430	0.19	0/581
27	CB	0.11	0/1031	0.25	0/1394
28	N1	0.13	0/2511	0.29	0/3433
29	N2	0.14	0/2773	0.30	0/3768
30	N3	0.11	0/769	0.25	0/1050
31	N4	0.15	0/3723	0.31	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	0.10	0/1289	0.26	0/1744
34	S1	0.12	0/5353	0.29	0/7251
35	S2	0.13	0/3459	0.27	0/4683
36	S3	0.11	0/1789	0.26	0/2436
37	S4	0.10	0/1030	0.24	0/1391
38	S5	0.09	0/889	0.23	0/1190
39	S6	0.10	0/755	0.26	0/1018
40	S7	0.12	0/1279	0.24	0/1730
41	S8	0.12	0/1443	0.27	0/1952
42	V1	0.12	0/3391	0.28	0/4583
43	V2	0.11	0/1711	0.26	0/2328
44	V3	0.07	0/365	0.19	0/493
All	All	0.12	0/67347	0.26	1/91293 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A1	57	VAL	N-CA-C	-5.08	107.51	112.29

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	14	0
2	A1	562	0	557	11	0
3	A2	686	0	699	5	0
4	A3	643	0	642	5	0
5	A5	910	0	950	6	0
6	A6	967	0	972	13	0
7	A7	780	0	808	8	0
8	A8	1398	0	1372	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A9	2703	0	2720	33	0
10	AB	624	0	625	17	0
10	AC	702	0	694	12	0
11	AK	2590	0	2553	45	0
12	AL	1021	0	1025	13	0
13	AM	1204	0	1162	11	0
14	AN	1173	0	1166	20	0
15	B1	479	0	486	2	0
16	B2	584	0	529	8	0
17	B3	641	0	620	3	0
18	B4	1062	0	1072	9	0
19	B5	1151	0	1164	8	0
20	B6	870	0	890	18	0
21	B7	1068	0	1041	18	0
22	B8	1315	0	1208	10	0
23	B9	1534	0	1470	20	0
24	BK	1456	0	1426	26	0
25	BL	828	0	788	8	0
26	CA	417	0	422	6	0
27	CB	1000	0	994	11	0
28	N1	2440	0	2546	47	0
29	N2	2710	0	2874	59	0
30	N3	752	0	802	11	0
31	N4	3631	0	3839	67	0
32	N5	4785	0	4933	104	0
33	N6	1259	0	1261	24	0
34	S1	5266	0	5296	88	0
35	S2	3385	0	3323	68	0
36	S3	1738	0	1693	24	0
37	S4	1007	0	1008	12	0
38	S5	867	0	871	15	0
39	S6	741	0	701	5	0
40	S7	1248	0	1254	19	0
41	S8	1412	0	1363	31	0
42	V1	3316	0	3272	51	0
43	V2	1671	0	1673	18	0
44	V3	355	0	329	9	0
45	4L	92	0	137	2	0
45	A7	94	0	141	3	0
45	A8	77	0	98	5	0
45	AL	184	0	268	17	0
45	B4	62	0	68	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B5	98	0	149	2	0
45	N2	68	0	80	4	0
45	N4	100	0	156	3	0
45	N5	182	0	270	10	0
45	S8	100	0	156	11	0
46	A3	51	0	82	3	0
46	AL	46	0	69	1	0
46	B4	51	0	82	0	0
46	N1	102	0	164	10	0
46	N2	48	0	73	1	0
46	N5	188	0	287	13	0
47	A9	48	0	26	1	0
48	AB	36	0	47	4	0
48	AC	36	0	47	4	0
49	AK	27	0	12	3	0
50	AL	51	0	82	3	0
50	B8	32	0	38	0	0
50	CA	51	0	82	3	0
51	AL	31	0	36	4	0
51	B5	54	0	88	4	0
51	B7	54	0	88	3	0
51	N1	108	0	176	9	0
51	S7	54	0	88	2	0
52	AM	104	0	176	8	0
52	B5	52	0	88	2	0
52	CB	52	0	88	5	0
52	N3	52	0	88	3	0
52	N4	99	0	163	8	0
53	N1	17	0	0	0	0
53	S2	17	0	0	0	0
54	S1	16	0	0	1	0
54	S7	8	0	0	0	0
54	S8	16	0	0	2	0
54	V1	8	0	0	0	0
55	S1	4	0	0	0	0
55	V2	4	0	0	0	0
56	S1	1	0	0	0	0
57	S6	1	0	0	0	0
58	V1	31	0	19	0	0
All	All	68306	0	69604	926	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 7.

All (926) 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)
44:V3:420:SER:HG	44:V3:423:HIS:HD1	1.14	0.95
20:B6:88:LEU:HD22	20:B6:92:GLU:HG2	1.62	0.81
21:B7:92:HIS:HD1	32:N5:481:THR:HG1	1.29	0.79
9:A9:198:ALA:O	9:A9:260:GLY:HA2	1.84	0.77
42:V1:110:PRO:HB3	42:V1:152:ARG:HD3	1.67	0.76
43:V2:182:ASN:HB3	43:V2:194:GLU:HB3	1.68	0.75
34:S1:149:ASP:HB2	35:S2:367:ALA:HB3	1.69	0.74
11:AK:141:ARG:NH2	49:AK:401:ADP:N7	2.34	0.74
12:AL:128:GLY:HA3	45:AL:202:CDL:H722	1.69	0.74
32:N5:3:PRO:HB2	32:N5:53:MET:HE1	1.69	0.73
29:N2:132:THR:HG21	45:N2:401:CDL:H381	1.70	0.73
35:S2:410:LYS:HE2	35:S2:463:VAL:HG23	1.71	0.73
3:A2:24:CYS:N	3:A2:58:CYS:SG	2.63	0.71
34:S1:338:VAL:O	34:S1:365:SER:HB2	1.91	0.71
45:B4:202:CDL:HB22	31:N4:260:PRO:HG3	1.73	0.70
46:N5:706:PEE:H34	46:N5:706:PEE:H64	1.73	0.70
37:S4:62:THR:HG23	37:S4:72:ILE:HD13	1.73	0.70
42:V1:112:TYR:HB2	42:V1:240:THR:HG22	1.73	0.70
34:S1:433:GLY:O	34:S1:444:HIS:NE2	2.24	0.69
28:N1:258:ASN:HD21	51:N1:402:PC1:H122	1.57	0.69
1:4L:28:SER:HB3	33:N6:23:LYS:HD2	1.72	0.69
50:CA:101:3PE:H381	29:N2:324:LYS:HA	1.74	0.69
35:S2:188:ASN:OD1	35:S2:410:LYS:NZ	2.26	0.69
9:A9:129:LEU:HD23	9:A9:167:ILE:HG13	1.74	0.68
29:N2:93:VAL:HG13	32:N5:599:MET:HE1	1.76	0.68
50:AL:203:3PE:H32	18:B4:82:PRO:HB2	1.75	0.67
50:CA:101:3PE:H3F1	29:N2:325:LEU:HD21	1.76	0.67
28:N1:173:TRP:HB2	28:N1:176:PHE:HD2	1.59	0.66
45:AL:202:CDL:H122	29:N2:152:ASN:HD22	1.59	0.66
11:AK:82:LYS:HZ3	11:AK:269:GLU:HG2	1.59	0.66
51:AL:205:PC1:H332	32:N5:569:ILE:HG23	1.78	0.66
32:N5:100:ILE:HG21	32:N5:246:LEU:HB2	1.77	0.66
31:N4:445:LEU:HB3	45:N5:703:CDL:H452	1.77	0.65
10:AB:93:ILE:HD12	10:AB:108:LEU:HD13	1.78	0.65
32:N5:530:PRO:O	32:N5:534:HIS:HB2	1.95	0.65
35:S2:374:ARG:NH2	41:S8:162:CYS:O	2.26	0.65
35:S2:222:ARG:NH1	35:S2:249:ASP:OD2	2.29	0.65
41:S8:205:ILE:O	41:S8:209:TYR:HB3	1.96	0.65
28:N1:24:GLU:OE2	28:N1:274:ARG:NH1	2.30	0.65
6:A6:67:ARG:NH2	10:AB:123:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:55:MET:HE1	46:N5:706:PEE:H74	1.78	0.64
35:S2:290:LEU:O	35:S2:293:GLY:N	2.30	0.64
11:AK:244:LYS:HA	11:AK:248:LEU:HD12	1.79	0.64
52:AM:201:PLX:H372	52:AM:202:PLX:H212	1.78	0.64
25:BL:150:PRO:HG2	27:CB:115:LEU:HD22	1.80	0.64
42:V1:94:PRO:HB2	42:V1:97:LEU:HB2	1.79	0.64
34:S1:128:CYS:SG	34:S1:140:GLN:NE2	2.70	0.64
38:S5:103:ASP:O	38:S5:105:ARG:NH1	2.31	0.64
21:B7:29:TYR:O	21:B7:104:ARG:NH2	2.31	0.64
29:N2:42:PRO:HG2	33:N6:167:VAL:HG22	1.81	0.63
9:A9:285:TYR:OH	9:A9:367:GLU:O	2.14	0.63
24:BK:171:LYS:O	24:BK:175:ALA:HB3	1.99	0.63
29:N2:108:LEU:HD11	29:N2:191:THR:HG21	1.79	0.63
10:AC:91:ASP:OD1	17:B3:47:ARG:NH2	2.31	0.63
11:AK:92:GLY:H	11:AK:95:TYR:HB3	1.63	0.63
28:N1:156:MET:HB3	28:N1:174:MET:HE1	1.81	0.63
35:S2:308:LEU:HB2	35:S2:407:GLU:HB2	1.80	0.63
3:A2:89:ARG:O	3:A2:93:ASN:ND2	2.32	0.63
43:V2:108:PRO:HB2	43:V2:111:ARG:HG2	1.80	0.63
46:N1:405:PEE:H79	45:S8:303:CDL:H821	1.81	0.63
29:N2:170:LEU:HD11	29:N2:288:LEU:HD22	1.80	0.62
34:S1:433:GLY:HA2	34:S1:447:ASP:HA	1.81	0.62
31:N4:211:GLY:H	31:N4:213:HIS:HD2	1.47	0.62
32:N5:387:THR:HG22	32:N5:465:GLY:H	1.64	0.62
10:AB:93:ILE:HD11	10:AB:110:LEU:HD11	1.80	0.62
48:AC:201:ZMP:H5A	23:B9:109:ALA:HB1	1.80	0.62
9:A9:132:ARG:NH2	47:A9:401:NDP:O3X	2.31	0.62
14:AN:122:GLY:HA3	33:N6:126:VAL:HG13	1.82	0.62
34:S1:246:ARG:HH22	37:S4:123:ASN:HD21	1.47	0.62
35:S2:292:TYR:HA	36:S3:161:LYS:HB2	1.80	0.62
3:A2:59:SER:HB2	34:S1:655:ARG:HD3	1.82	0.62
11:AK:65:ASP:HB2	11:AK:206:VAL:HA	1.80	0.62
35:S2:155:GLN:NE2	35:S2:315:ASP:OD2	2.33	0.62
17:B3:27:THR:HG22	17:B3:29:LEU:H	1.63	0.62
10:AC:94:ASP:HB3	10:AC:97:LYS:HG2	1.82	0.62
36:S3:211:ARG:NH2	36:S3:222:GLU:OE2	2.33	0.61
28:N1:34:ARG:HG2	40:S7:82:PRO:HA	1.80	0.61
43:V2:59:ASN:ND2	43:V2:89:GLN:OE1	2.33	0.61
34:S1:250:SER:HB2	34:S1:606:THR:HG23	1.82	0.61
42:V1:40:ARG:NH1	42:V1:289:GLU:O	2.34	0.61
12:AL:129:GLN:HG2	45:AL:202:CDL:HB32	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N2:88:LYS:HG3	29:N2:148:SER:HB3	1.82	0.61
29:N2:289:ASN:HA	29:N2:292:PHE:CE2	2.36	0.61
36:S3:89:HIS:ND1	36:S3:91:ASP:OD1	2.34	0.61
9:A9:221:ARG:HH12	9:A9:356:HIS:HB3	1.65	0.61
34:S1:224:ASP:OD2	34:S1:291:ARG:NH2	2.33	0.60
12:AL:67:GLY:HA2	45:AL:201:CDL:H221	1.83	0.60
45:S8:303:CDL:H622	45:S8:303:CDL:H172	1.82	0.60
8:A8:107:HIS:HB3	8:A8:197:PRO:HD2	1.83	0.60
9:A9:87:GLU:HG3	9:A9:89:TYR:H	1.66	0.60
29:N2:142:LEU:HB3	29:N2:194:LEU:HD21	1.84	0.60
13:AM:106:ARG:HB2	13:AM:109:ILE:HG13	1.83	0.60
20:B6:143:HIS:HD2	24:BK:45:VAL:HG21	1.67	0.60
24:BK:140:GLN:O	24:BK:144:SER:HB2	2.02	0.60
32:N5:362:LEU:HA	32:N5:365:ALA:HB3	1.82	0.60
45:N5:703:CDL:HB31	45:N5:703:CDL:HA22	1.82	0.60
34:S1:266:ARG:HG2	34:S1:267:THR:HG23	1.84	0.60
42:V1:102:MET:HE3	42:V1:111:LYS:HD2	1.84	0.60
14:AN:51:MET:HE2	28:N1:311:THR:HB	1.84	0.60
34:S1:260:ASN:N	34:S1:282:ASN:OD1	2.35	0.60
5:A5:99:PRO:HA	36:S3:71:LYS:HE2	1.84	0.59
45:N2:401:CDL:H741	45:N2:401:CDL:H522	1.84	0.59
31:N4:403:THR:HA	31:N4:406:TYR:CE2	2.37	0.59
37:S4:112:MET:O	41:S8:144:ARG:NH1	2.32	0.59
10:AC:114:ASP:OD1	23:B9:87:ARG:NH2	2.35	0.59
43:V2:38:LEU:O	43:V2:124:ARG:NH2	2.31	0.59
2:A1:6:LEU:HD12	45:A7:201:CDL:H562	1.84	0.59
9:A9:344:PRO:HG2	9:A9:347:LEU:HD13	1.85	0.59
34:S1:217:GLU:HG2	34:S1:218:LEU:HG	1.83	0.59
20:B6:134:HIS:NE2	32:N5:35:TYR:OH	2.28	0.59
32:N5:375:ILE:HD12	32:N5:458:LEU:HD11	1.84	0.59
35:S2:412:GLU:OE2	36:S3:140:ARG:NH2	2.35	0.59
31:N4:383:THR:HG21	32:N5:190:LEU:HD22	1.84	0.59
34:S1:493:VAL:HG23	34:S1:513:MET:HE1	1.84	0.59
7:A7:25:GLN:NE2	41:S8:76:TYR:OH	2.36	0.59
21:B7:15:LYS:HG2	21:B7:113:LYS:HG3	1.85	0.59
34:S1:144:MET:HG3	35:S2:389:LYS:HG3	1.85	0.59
28:N1:296:LEU:HD13	46:N1:405:PEE:H19	1.85	0.59
33:N6:2:THR:HG22	33:N6:4:TYR:H	1.67	0.59
34:S1:83:GLU:HB2	34:S1:101:ASN:HB3	1.83	0.59
34:S1:275:PRO:HG3	34:S1:286:ILE:HG12	1.84	0.58
28:N1:231:ILE:O	28:N1:235:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:205:ILE:HG12	42:V1:379:CYS:HB3	1.85	0.58
34:S1:405:THR:HB	34:S1:477:GLY:HA3	1.84	0.58
34:S1:476:LEU:HD21	34:S1:481:LEU:HD21	1.85	0.58
8:A8:146:ASP:OD1	8:A8:149:ARG:NH2	2.36	0.58
8:A8:174:PHE:HB3	8:A8:178:ARG:HH12	1.67	0.58
11:AK:90:GLU:OE2	11:AK:163:ARG:NH1	2.36	0.58
45:AL:202:CDL:H742	29:N2:277:ILE:HD13	1.84	0.58
20:B6:132:VAL:O	20:B6:136:LEU:HB3	2.03	0.58
34:S1:131:CYS:O	34:S1:241:ARG:NH1	2.36	0.58
9:A9:135:GLU:OE2	9:A9:179:ARG:NH1	2.37	0.58
51:B7:201:PC1:H362	24:BK:27:PRO:HB2	1.84	0.58
21:B7:19:PRO:HA	21:B7:22:MET:HE3	1.86	0.58
42:V1:325:PRO:HG3	42:V1:433:TRP:HB3	1.84	0.58
23:B9:87:ARG:NH1	23:B9:91:ASP:OD2	2.37	0.58
31:N4:408:LEU:HD12	32:N5:172:ILE:HG21	1.85	0.58
35:S2:374:ARG:NH2	41:S8:165:ASP:OD1	2.35	0.58
24:BK:33:LEU:HD13	32:N5:49:VAL:HG13	1.86	0.58
29:N2:17:THR:HG1	29:N2:133:TRP:CD1	2.22	0.58
32:N5:103:PHE:HB2	32:N5:341:MET:HE3	1.85	0.58
45:AL:201:CDL:H532	32:N5:577:VAL:HA	1.85	0.57
11:AK:62:ILE:HA	11:AK:204:HIS:HB2	1.86	0.57
29:N2:91:ASN:HD22	29:N2:94:ALA:H	1.51	0.57
45:A8:301:CDL:H592	31:N4:9:THR:HG21	1.86	0.57
19:B5:119:ARG:HH21	51:B5:203:PC1:H11	1.70	0.57
14:AN:29:GLY:HA2	45:S8:303:CDL:HB62	1.85	0.57
21:B7:92:HIS:ND1	32:N5:481:THR:OG1	2.28	0.57
29:N2:26:TRP:HB3	29:N2:74:ILE:HD13	1.86	0.57
32:N5:359:MET:O	32:N5:436:ARG:NH2	2.38	0.57
2:A1:46:ASN:ND2	33:N6:132:ASP:OD2	2.36	0.57
11:AK:213:VAL:HG12	11:AK:217:GLN:HE21	1.69	0.57
1:4L:98:CYS:HB3	32:N5:580:GLN:HB2	1.87	0.57
6:A6:88:LYS:HE2	6:A6:92:MET:HE2	1.87	0.57
37:S4:109:ASN:ND2	37:S4:111:LEU:O	2.37	0.57
9:A9:64:PHE:HZ	9:A9:208:GLY:HA3	1.70	0.57
34:S1:265:THR:HG22	34:S1:270:VAL:HA	1.86	0.57
28:N1:173:TRP:HB3	28:N1:175:ILE:HG22	1.87	0.56
35:S2:257:PHE:HD2	35:S2:347:LEU:HD11	1.69	0.56
48:AC:201:ZMP:H14	23:B9:102:ALA:HB1	1.86	0.56
45:A8:301:CDL:H381	29:N2:256:PRO:HB2	1.87	0.56
9:A9:306:GLU:HG2	9:A9:315:THR:HG22	1.88	0.56
28:N1:24:GLU:HA	28:N1:271:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:N1:401:PC1:H362	51:N1:401:PC1:H261	1.88	0.56
29:N2:14:MET:HA	29:N2:133:TRP:HE1	1.70	0.56
29:N2:197:ASN:HD22	29:N2:200:MET:HG2	1.69	0.56
11:AK:94:HIS:HB3	11:AK:105:PRO:HB3	1.88	0.56
28:N1:218:GLY:HA3	30:N3:21:ALA:HB1	1.87	0.56
29:N2:252:GLY:HA3	29:N2:290:LEU:HD13	1.88	0.56
32:N5:88:MET:HE2	32:N5:468:ILE:HG23	1.88	0.56
35:S2:194:THR:HG21	35:S2:209:MET:HB2	1.88	0.56
16:B2:90:ASP:O	32:N5:385:TYR:OH	2.23	0.56
29:N2:235:ASN:O	29:N2:315:TRP:NE1	2.38	0.56
34:S1:340:ALA:HB3	34:S1:366:LEU:HD23	1.88	0.56
8:A8:239:LYS:HD3	19:B5:149:LEU:HD11	1.87	0.56
29:N2:298:TYR:O	29:N2:303:THR:OG1	2.22	0.56
42:V1:119:GLU:O	42:V1:159:ARG:NH1	2.39	0.56
32:N5:419:THR:HA	32:N5:422:TYR:CE2	2.40	0.56
39:S6:74:GLN:HG3	41:S8:108:SER:HB2	1.87	0.56
10:AB:116:VAL:HG12	10:AB:120:MET:HE2	1.87	0.56
45:AL:202:CDL:H332	45:AL:202:CDL:HB62	1.86	0.56
21:B7:34:ARG:HH21	22:B8:186:ILE:HB	1.70	0.56
7:A7:46:SER:O	7:A7:52:ASN:ND2	2.38	0.56
18:B4:15:PRO:HG2	18:B4:18:LEU:HB2	1.87	0.56
32:N5:575:ILE:O	32:N5:579:ASN:HB2	2.05	0.56
36:S3:132:LEU:HB2	36:S3:141:ILE:HG22	1.88	0.56
5:A5:6:LYS:NZ	5:A5:76:GLN:OE1	2.38	0.56
52:AM:201:PLX:H72	52:AM:201:PLX:H252	1.88	0.56
34:S1:259:SER:HB3	34:S1:282:ASN:HD21	1.71	0.56
37:S4:112:MET:HG3	41:S8:184:LEU:HD23	1.88	0.56
10:AB:106:LYS:NZ	10:AB:107:ASP:OD1	2.37	0.55
50:AL:203:3PE:H3G1	32:N5:558:LEU:HD21	1.88	0.55
29:N2:112:HIS:O	29:N2:116:PRO:HD2	2.07	0.55
52:CB:201:PLX:H332	29:N2:342:ALA:HB3	1.88	0.55
43:V2:111:ARG:NH1	43:V2:114:GLU:OE2	2.39	0.55
35:S2:140:PRO:HB2	40:S7:142:TYR:CE2	2.41	0.55
42:V1:235:VAL:HG12	42:V1:240:THR:HG21	1.88	0.55
4:A3:143:ARG:NH2	8:A8:126:GLU:OE1	2.39	0.55
9:A9:205:ASP:N	9:A9:205:ASP:OD1	2.37	0.55
12:AL:108:TYR:HB2	50:AL:203:3PE:H11	1.88	0.55
32:N5:69:MET:HE3	32:N5:71:LEU:HD21	1.87	0.55
31:N4:266:MET:HA	31:N4:269:MET:HE2	1.89	0.55
40:S7:190:LEU:HD21	51:S7:302:PC1:H331	1.88	0.55
11:AK:206:VAL:HB	11:AK:257:VAL:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:446:LEU:HB3	52:N4:502:PLX:H272	1.88	0.55
42:V1:296:LEU:HD21	42:V1:317:VAL:HG11	1.88	0.55
23:B9:52:LEU:O	23:B9:57:LYS:NZ	2.40	0.55
24:BK:171:LYS:O	24:BK:175:ALA:CB	2.54	0.55
34:S1:557:ARG:NH2	34:S1:581:ASP:OD1	2.38	0.55
8:A8:228:ASN:OD1	38:S5:51:ARG:NH1	2.38	0.55
31:N4:133:ILE:HD11	31:N4:231:LEU:HD11	1.89	0.55
31:N4:392:THR:O	31:N4:396:MET:HG2	2.07	0.55
33:N6:17:PHE:HA	33:N6:20:PHE:HD1	1.72	0.54
11:AK:120:TYR:OH	49:AK:401:ADP:O2'	2.20	0.54
13:AM:88:ARG:HD3	41:S8:200:GLU:HG3	1.90	0.54
24:BK:107:GLN:HE22	32:N5:194:ASN:ND2	2.05	0.54
32:N5:400:ASN:HB3	32:N5:486:MET:HE3	1.89	0.54
11:AK:134:GLN:NE2	49:AK:401:ADP:N1	2.54	0.54
45:AL:201:CDL:H751	45:AL:201:CDL:H392	1.90	0.54
35:S2:137:GLN:O	40:S7:142:TYR:OH	2.25	0.54
15:B1:47:ARG:HH11	19:B5:106:VAL:HG11	1.72	0.54
42:V1:118:ASP:HB3	42:V1:207:GLY:HA2	1.89	0.54
1:4L:56:ALA:HA	38:S5:18:MET:HE3	1.90	0.54
1:4L:68:ALA:HB2	33:N6:64:MET:HE2	1.89	0.54
11:AK:93:ILE:HA	11:AK:136:TRP:HE1	1.71	0.54
31:N4:375:LEU:HD11	32:N5:141:PHE:HE2	1.73	0.54
34:S1:275:PRO:O	37:S4:86:ASN:ND2	2.40	0.54
42:V1:48:ARG:HH21	44:V3:384:SER:HA	1.72	0.54
11:AK:109:GLN:HE22	11:AK:328:ARG:HH12	1.56	0.54
19:B5:152:LYS:HD3	27:CB:96:VAL:HG21	1.89	0.54
23:B9:143:GLU:O	23:B9:164:ARG:NH2	2.41	0.54
8:A8:160:THR:HA	8:A8:163:TRP:CD1	2.42	0.54
34:S1:341:ILE:HG13	34:S1:545:LEU:HD11	1.90	0.54
34:S1:466:LEU:HD13	34:S1:500:ILE:HD11	1.90	0.54
25:BL:95:PHE:O	25:BL:99:LEU:HB2	2.07	0.54
28:N1:195:ARG:HH11	28:N1:231:ILE:HD13	1.73	0.54
34:S1:158:ARG:NH1	34:S1:202:ASN:OD1	2.41	0.54
36:S3:103:HIS:HB3	36:S3:106:ALA:HB3	1.90	0.54
42:V1:325:PRO:HB2	42:V1:347:THR:HG22	1.90	0.54
9:A9:201:ILE:HG22	9:A9:203:PRO:HD3	1.90	0.54
32:N5:97:THR:HG21	32:N5:125:LEU:HD22	1.89	0.54
34:S1:49:VAL:HG13	34:S1:102:ILE:HD13	1.90	0.54
31:N4:405:LEU:HD21	32:N5:173:LEU:HD12	1.89	0.53
35:S2:299:LEU:HD22	35:S2:304:ILE:HD12	1.89	0.53
37:S4:111:LEU:HG	37:S4:112:MET:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AN:98:MET:HE3	14:AN:101:VAL:HG21	1.91	0.53
21:B7:103:GLU:O	21:B7:107:ARG:HG2	2.08	0.53
24:BK:12:GLU:OE2	24:BK:15:ARG:NH2	2.40	0.53
38:S5:97:HIS:HA	38:S5:102:GLU:HB2	1.90	0.53
32:N5:459:ILE:HD12	46:N5:706:PEE:H21	1.91	0.53
20:B6:155:TYR:OH	24:BK:11:PRO:O	2.23	0.53
28:N1:102:VAL:HG21	28:N1:154:LEU:HD11	1.90	0.53
32:N5:417:SER:HB2	45:N5:704:CDL:H572	1.91	0.53
42:V1:203:ALA:HB3	42:V1:206:CYS:HB2	1.91	0.53
45:A7:201:CDL:H532	45:A7:201:CDL:H742	1.91	0.53
20:B6:85:ASP:OD2	23:B9:167:TRP:NE1	2.32	0.53
20:B6:159:GLU:HG2	32:N5:61:MET:HG2	1.89	0.53
24:BK:114:GLN:HG3	32:N5:203:MET:HG2	1.91	0.53
35:S2:265:GLU:OE1	35:S2:344:ARG:NH2	2.38	0.53
11:AK:89:PRO:O	11:AK:144:GLN:NE2	2.37	0.53
40:S7:75:GLU:HG3	40:S7:167:PRO:HB2	1.90	0.53
35:S2:197:ALA:O	35:S2:200:ILE:C	2.52	0.53
30:N3:70:ALA:HB2	33:N6:59:ILE:HD11	1.90	0.53
31:N4:204:MET:HE3	31:N4:209:LEU:HD22	1.90	0.53
40:S7:96:SER:OG	40:S7:99:GLN:OE1	2.27	0.53
34:S1:219:SER:OG	34:S1:288:ASP:OD2	2.19	0.52
48:AC:201:ZMP:H1	23:B9:113:PHE:HA	1.91	0.52
45:A7:201:CDL:H521	45:A7:201:CDL:H121	1.90	0.52
18:B4:71:ALA:HB2	22:B8:38:PRO:HG2	1.91	0.52
42:V1:162:PHE:HB3	42:V1:165:GLU:HB2	1.90	0.52
8:A8:196:ARG:NH2	14:AN:63:GLU:OE2	2.42	0.52
11:AK:241:ASN:HB3	11:AK:245:LYS:HE2	1.90	0.52
25:BL:89:VAL:HG21	31:N4:25:ILE:HG23	1.90	0.52
36:S3:44:ARG:HD2	36:S3:47:ILE:HD12	1.91	0.52
48:AC:201:ZMP:H24	23:B9:116:GLY:O	2.09	0.52
51:N1:401:PC1:H132	51:N1:401:PC1:H12	1.90	0.52
13:AM:34:ARG:HH21	13:AM:54:GLN:HG3	1.74	0.52
35:S2:232:TYR:OH	35:S2:240:GLN:O	2.28	0.52
42:V1:138:LEU:HD13	42:V1:245:VAL:HG13	1.91	0.52
23:B9:181:GLN:NE2	23:B9:198:PRO:O	2.40	0.52
34:S1:624:ARG:NH2	34:S1:637:ASP:OD1	2.41	0.52
9:A9:61:ALA:HB3	9:A9:82:VAL:HG13	1.91	0.52
30:N3:68:GLU:HG3	30:N3:98:LEU:HD13	1.91	0.52
39:S6:100:ILE:HD11	39:S6:111:CYS:HB2	1.91	0.52
34:S1:339:ALA:HA	34:S1:365:SER:HB2	1.92	0.52
22:B8:96:ASP:O	22:B8:114:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:262:VAL:HG23	34:S1:276:ARG:HB2	1.92	0.52
31:N4:216:LEU:HB3	31:N4:217:PRO:HD3	1.91	0.51
11:AK:355:TRP:H	11:AK:355:TRP:CD1	2.28	0.51
29:N2:197:ASN:HB2	29:N2:269:GLU:HG2	1.92	0.51
34:S1:446:GLY:HA3	34:S1:451:ILE:HD12	1.92	0.51
9:A9:211:ASP:O	9:A9:215:ASN:ND2	2.43	0.51
14:AN:26:PRO:O	41:S8:68:ARG:NH2	2.43	0.51
35:S2:391:TYR:HD1	41:S8:122:VAL:HG21	1.76	0.51
11:AK:60:LYS:HG3	11:AK:62:ILE:HG13	1.91	0.51
11:AK:131:TYR:OH	11:AK:188:HIS:ND1	2.33	0.51
28:N1:110:SER:HB2	33:N6:62:GLY:HA3	1.92	0.51
34:S1:456:ALA:O	34:S1:499:ASN:ND2	2.43	0.51
41:S8:131:GLU:HB2	41:S8:144:ARG:HB3	1.92	0.51
28:N1:195:ARG:HH21	28:N1:274:ARG:HD2	1.74	0.51
36:S3:157:VAL:HG21	36:S3:182:PRO:HD3	1.92	0.51
37:S4:98:LYS:NZ	37:S4:127:THR:OG1	2.37	0.51
9:A9:238:GLN:NE2	9:A9:267:GLY:O	2.44	0.51
24:BK:153:ARG:NH1	31:N4:181:TYR:O	2.44	0.51
52:CB:201:PLX:H372	29:N2:336:VAL:HB	1.91	0.51
28:N1:18:ALA:HB1	28:N1:48:PRO:HB3	1.92	0.51
28:N1:31:MET:HG2	41:S8:77:LEU:HB2	1.92	0.51
35:S2:418:VAL:HB	35:S2:427:ARG:HB3	1.92	0.51
42:V1:140:GLU:OE2	42:V1:256:ARG:NH1	2.40	0.51
8:A8:246:PHE:HE2	45:A8:301:CDL:H341	1.75	0.51
12:AL:35:ILE:HD12	45:AL:201:CDL:H811	1.92	0.51
34:S1:387:LEU:HD12	34:S1:514:ASN:HB3	1.93	0.51
35:S2:381:MET:HE2	35:S2:385:ILE:HG13	1.93	0.51
41:S8:150:THR:HG21	41:S8:180:HIS:CD2	2.46	0.51
42:V1:113:LEU:O	42:V1:154:ALA:HA	2.10	0.51
9:A9:226:VAL:HG13	9:A9:290:PRO:HA	1.93	0.51
35:S2:148:VAL:HG11	35:S2:191:MET:HG2	1.91	0.51
30:N3:79:SER:HA	30:N3:87:MET:HE2	1.92	0.51
9:A9:75:ARG:NH1	36:S3:215:GLU:OE1	2.44	0.51
35:S2:143:ASP:OD1	35:S2:150:MET:HB3	2.10	0.51
40:S7:47:VAL:HG12	51:S7:302:PC1:H282	1.92	0.51
52:B5:201:PLX:H232	51:B5:203:PC1:H2B1	1.93	0.50
34:S1:591:GLU:HG2	34:S1:610:VAL:HG23	1.93	0.50
35:S2:61:THR:H	35:S2:64:THR:HG1	1.53	0.50
16:B2:57:ARG:NH1	16:B2:61:PHE:O	2.43	0.50
24:BK:97:LYS:NZ	25:BL:113:ARG:O	2.45	0.50
31:N4:122:PHE:HE1	31:N4:206:LYS:HG2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:V2:93:LEU:HD12	43:V2:122:TYR:HB3	1.94	0.50
31:N4:41:LEU:O	31:N4:44:GLN:NE2	2.42	0.50
32:N5:208:CYS:HB2	32:N5:266:LEU:HD22	1.92	0.50
42:V1:364:VAL:HG12	42:V1:400:VAL:HG12	1.94	0.50
34:S1:64:CYS:O	34:S1:184:ARG:NH2	2.35	0.50
45:S8:303:CDL:H602	45:S8:303:CDL:H801	1.93	0.50
35:S2:118:HIS:HD1	36:S3:191:TYR:HH	1.59	0.50
40:S7:85:ASP:O	40:S7:88:ARG:HG2	2.11	0.50
34:S1:347:ASP:OD1	34:S1:347:ASP:N	2.42	0.50
34:S1:401:LEU:HD11	34:S1:432:ILE:HG13	1.94	0.50
34:S1:666:GLN:NE2	34:S1:670:GLU:OE2	2.44	0.50
29:N2:133:TRP:HZ3	45:N2:401:CDL:H392	1.77	0.50
42:V1:112:TYR:CD1	42:V1:153:ALA:HB3	2.47	0.50
2:A1:49:GLU:OE1	2:A1:52:ARG:NH2	2.38	0.49
6:A6:55:LYS:NZ	48:AB:201:ZMP:O6	2.37	0.49
45:AL:201:CDL:H571	29:N2:110:PRO:HB3	1.92	0.49
20:B6:150:VAL:O	20:B6:156:THR:OG1	2.28	0.49
5:A5:76:GLN:HB2	5:A5:79:GLU:HG3	1.94	0.49
20:B6:165:PHE:O	20:B6:168:ASP:HB2	2.12	0.49
6:A6:127:THR:HG22	6:A6:131:ARG:HE	1.77	0.49
14:AN:93:GLU:HG3	38:S5:98:HIS:CD2	2.46	0.49
13:AM:55:PHE:CZ	13:AM:58:ARG:HG3	2.47	0.49
27:CB:52:ARG:NH1	29:N2:318:GLU:OE1	2.44	0.49
31:N4:8:THR:HG22	31:N4:100:ILE:HG23	1.93	0.49
34:S1:197:THR:O	42:V1:220:GLN:NE2	2.43	0.49
42:V1:295:PRO:HG2	42:V1:298:GLU:HB3	1.93	0.49
1:4L:43:MET:HE3	1:4L:47:ILE:HD11	1.93	0.49
45:4L:201:CDL:H532	33:N6:88:THR:HG23	1.94	0.49
32:N5:48:LEU:HD11	46:N5:706:PEE:H65	1.95	0.49
32:N5:399:VAL:HG12	32:N5:409:LEU:HD13	1.92	0.49
32:N5:562:LEU:HB2	32:N5:563:PRO:HD3	1.94	0.49
34:S1:624:ARG:NH1	34:S1:628:GLU:OE1	2.40	0.49
8:A8:95:VAL:HG12	8:A8:97:VAL:HG22	1.93	0.49
16:B2:101:PRO:HD2	21:B7:99:MET:HE1	1.94	0.49
20:B6:170:ILE:HB	20:B6:175:GLU:HB3	1.95	0.49
28:N1:87:VAL:HG22	28:N1:88:PRO:HD3	1.95	0.49
51:N1:401:PC1:H222	30:N3:3:ILE:HG12	1.93	0.49
31:N4:24:TRP:CD2	31:N4:81:GLN:HG2	2.47	0.49
32:N5:149:ILE:HD11	45:N5:703:CDL:H161	1.93	0.49
33:N6:45:LEU:HD23	33:N6:50:SER:HA	1.94	0.49
42:V1:102:MET:HE2	42:V1:149:MET:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:V3:418:ARG:NH1	44:V3:423:HIS:O	2.45	0.49
6:A6:88:LYS:NZ	6:A6:132:PHE:O	2.41	0.49
13:AM:127:TYR:OH	39:S6:61:GLU:O	2.23	0.49
30:N3:64:LEU:HD13	33:N6:165:VAL:HG22	1.94	0.49
31:N4:76:MET:SD	31:N4:230:VAL:HB	2.52	0.49
31:N4:196:TRP:CD1	31:N4:250:LEU:HB3	2.47	0.49
31:N4:449:LEU:HG	45:N5:703:CDL:H441	1.95	0.49
32:N5:295:GLN:HB2	32:N5:301:ILE:HG12	1.95	0.49
41:S8:63:TRP:HZ3	45:S8:303:CDL:H871	1.77	0.49
46:A3:201:PEE:H29	28:N1:295:PRO:HB3	1.95	0.49
32:N5:228:GLY:H	32:N5:230:HIS:HD2	1.61	0.49
34:S1:130:ILE:HG23	41:S8:114:ILE:HD12	1.95	0.49
16:B2:65:THR:HB	16:B2:68:GLN:HG2	1.94	0.49
28:N1:108:MET:HE1	51:N1:401:PC1:H2A1	1.93	0.49
28:N1:173:TRP:HE1	51:N1:402:PC1:H152	1.77	0.49
32:N5:174:TYR:CD2	32:N5:232:TRP:HB3	2.48	0.49
35:S2:145:LEU:HD13	35:S2:430:ILE:HG21	1.95	0.49
35:S2:190:ILE:HG23	35:S2:209:MET:HB3	1.95	0.49
16:B2:65:THR:H	16:B2:68:GLN:HE21	1.61	0.49
28:N1:142:TYR:CE1	28:N1:289:LEU:HD13	2.48	0.49
31:N4:204:MET:HE1	31:N4:298:ILE:HG21	1.94	0.49
42:V1:366:ALA:HA	43:V2:141:MET:HE1	1.94	0.49
29:N2:190:MET:HE1	29:N2:205:LEU:HB2	1.94	0.48
8:A8:175:ARG:NH1	28:N1:170:GLU:OE1	2.46	0.48
9:A9:49:SER:HB2	36:S3:225:GLU:HG2	1.96	0.48
11:AK:287:ASP:OD1	11:AK:287:ASP:N	2.45	0.48
11:AK:225:ASN:HB3	11:AK:228:GLU:HG2	1.95	0.48
35:S2:101:LEU:HB2	35:S2:464:PHE:CZ	2.48	0.48
35:S2:430:ILE:HB	35:S2:469:ARG:HD2	1.94	0.48
42:V1:195:VAL:O	44:V3:410:ARG:NH1	2.46	0.48
35:S2:250:ILE:HG22	35:S2:354:LEU:HD11	1.95	0.48
5:A5:44:TYR:O	5:A5:48:THR:HG22	2.13	0.48
14:AN:43:LEU:HG	28:N1:179:TRP:HE1	1.79	0.48
43:V2:85:LEU:HD13	44:V3:400:LEU:HD22	1.95	0.48
7:A7:68:ILE:HD12	36:S3:75:GLN:HE21	1.79	0.48
9:A9:247:LYS:HE2	9:A9:340:ILE:HD12	1.95	0.48
32:N5:536:LEU:HB3	32:N5:537:PRO:HD3	1.96	0.48
42:V1:64:LYS:HD2	43:V2:249:LEU:HD23	1.96	0.48
42:V1:326:LEU:HD23	42:V1:326:LEU:H	1.78	0.48
52:AM:201:PLX:H231	28:N1:15:LEU:HD13	1.96	0.48
45:B5:202:CDL:H672	32:N5:12:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:176:ARG:HD3	32:N5:176:ARG:HA	1.67	0.48
2:A1:50:ARG:NH2	8:A8:95:VAL:O	2.47	0.48
8:A8:224:ARG:NH2	38:S5:42:GLU:OE1	2.47	0.48
52:AM:201:PLX:H131	28:N1:42:PRO:HG3	1.96	0.48
17:B3:47:ARG:HA	17:B3:50:ALA:HB3	1.95	0.48
19:B5:71:MET:HE3	45:N5:703:CDL:H551	1.96	0.48
24:BK:107:GLN:HE22	32:N5:194:ASN:HD22	1.62	0.48
31:N4:309:PHE:HB2	31:N4:458:LEU:HD12	1.96	0.48
35:S2:190:ILE:HD11	35:S2:257:PHE:CZ	2.49	0.48
5:A5:48:THR:HA	5:A5:51:ILE:HG12	1.94	0.48
11:AK:67:ASN:OD1	11:AK:68:ILE:N	2.34	0.48
12:AL:109:GLY:HA3	46:N5:702:PEE:H8	1.96	0.48
46:N1:405:PEE:H59	41:S8:66:LEU:HD13	1.96	0.48
34:S1:163:LYS:HD3	34:S1:173:MET:HG3	1.95	0.48
28:N1:99:ASN:N	51:N1:401:PC1:O12	2.47	0.48
29:N2:130:LEU:HD12	29:N2:134:GLN:HG3	1.96	0.48
35:S2:129:LEU:O	35:S2:133:LYS:HG2	2.14	0.48
36:S3:89:HIS:HD1	36:S3:91:ASP:H	1.60	0.48
31:N4:82:SER:HB2	31:N4:432:ARG:NH1	2.29	0.47
34:S1:59:GLN:HE22	37:S4:90:GLY:HA2	1.78	0.47
46:N1:404:PEE:H50	46:N1:404:PEE:H56	1.59	0.47
22:B8:62:TYR:OH	22:B8:74:ASP:O	2.26	0.47
46:N2:402:PEE:H13	46:N2:402:PEE:H1	1.70	0.47
31:N4:3:LYS:HG3	31:N4:4:ILE:HD12	1.96	0.47
35:S2:464:PHE:HA	35:S2:467:VAL:HB	1.96	0.47
4:A3:148:MET:O	8:A8:207:LYS:NZ	2.47	0.47
30:N3:54:LYS:HE2	30:N3:115:GLU:H	1.78	0.47
31:N4:67:VAL:HG12	52:N4:502:PLX:H362	1.97	0.47
32:N5:356:ILE:HB	32:N5:429:PHE:HB3	1.95	0.47
46:N5:706:PEE:H60	46:N5:706:PEE:H66	1.63	0.47
28:N1:107:ALA:HB1	33:N6:57:PHE:HD2	1.78	0.47
30:N3:73:LEU:HD12	33:N6:55:MET:HE1	1.95	0.47
34:S1:575:VAL:HG12	34:S1:579:MET:HE3	1.97	0.47
40:S7:108:THR:HA	40:S7:136:CYS:HB3	1.97	0.47
2:A1:40:HIS:N	2:A1:44:GLN:OE1	2.46	0.47
18:B4:11:LEU:O	32:N5:535:ARG:NH1	2.46	0.47
32:N5:23:ASN:CG	45:N5:703:CDL:H512	2.40	0.47
34:S1:338:VAL:HB	34:S1:363:SER:HB2	1.96	0.47
35:S2:140:PRO:HB2	40:S7:142:TYR:HE2	1.78	0.47
9:A9:198:ALA:O	9:A9:260:GLY:CA	2.59	0.47
9:A9:303:ARG:HB2	9:A9:316:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N2:271:THR:HG23	31:N4:169:ASN:ND2	2.29	0.47
31:N4:334:TYR:O	31:N4:338:HIS:N	2.43	0.47
34:S1:185:PHE:CZ	34:S1:221:ASN:HB2	2.50	0.47
42:V1:113:LEU:HD13	42:V1:149:MET:HE1	1.95	0.47
1:4L:37:MET:HG3	1:4L:67:ALA:CB	2.44	0.47
34:S1:36:VAL:HG11	34:S1:56:VAL:HG21	1.95	0.47
35:S2:197:ALA:O	35:S2:200:ILE:O	2.33	0.47
6:A6:94:MET:HE2	10:AB:113:LEU:HD12	1.96	0.47
8:A8:174:PHE:O	8:A8:178:ARG:NH1	2.47	0.47
45:AL:202:CDL:H461	45:AL:202:CDL:H201	1.97	0.47
42:V1:217:GLU:OE2	42:V1:224:ARG:NH2	2.47	0.47
5:A5:9:THR:HG23	5:A5:16:VAL:HG22	1.97	0.46
10:AB:115:GLN:NE2	10:AB:135:ALA:O	2.48	0.46
11:AK:148:ALA:HB1	11:AK:159:VAL:HG21	1.96	0.46
29:N2:36:ASN:OD1	29:N2:134:GLN:NE2	2.32	0.46
32:N5:121:LEU:HD22	32:N5:246:LEU:HD23	1.97	0.46
32:N5:327:LEU:O	32:N5:331:MET:HG2	2.15	0.46
33:N6:117:PHE:HB2	33:N6:119:PHE:CZ	2.50	0.46
14:AN:85:GLN:HE22	38:S5:105:ARG:HH21	1.63	0.46
31:N4:318:ALA:HB2	31:N4:373:ILE:HG13	1.96	0.46
35:S2:190:ILE:HD11	35:S2:257:PHE:HZ	1.81	0.46
42:V1:111:LYS:HB2	42:V1:151:ALA:HA	1.97	0.46
21:B7:99:MET:HG3	22:B8:156:VAL:HG12	1.97	0.46
1:4L:90:VAL:HB	32:N5:584:ILE:HD11	1.96	0.46
14:AN:103:ASP:OD1	14:AN:103:ASP:N	2.46	0.46
51:B7:201:PC1:H382	51:B7:201:PC1:H3D2	1.98	0.46
32:N5:88:MET:HE3	46:N5:706:PEE:H45	1.98	0.46
35:S2:160:ALA:HA	35:S2:404:THR:HG21	1.97	0.46
45:A8:301:CDL:H331	45:A8:301:CDL:H171	1.97	0.46
52:AM:201:PLX:H201	52:AM:201:PLX:H332	1.98	0.46
32:N5:253:VAL:HG23	32:N5:310:LEU:HD21	1.97	0.46
32:N5:566:THR:O	32:N5:570:GLN:HG2	2.16	0.46
34:S1:402:LEU:HD23	34:S1:475:VAL:HB	1.96	0.46
34:S1:574:ASP:OD2	34:S1:702:ARG:NE	2.46	0.46
35:S2:241:ASP:OD1	35:S2:242:LEU:N	2.48	0.46
7:A7:39:PRO:HG3	41:S8:211:TYR:CZ	2.50	0.46
9:A9:229:ILE:HB	9:A9:323:HIS:CD2	2.50	0.46
9:A9:295:HIS:CE1	9:A9:299:ARG:HD2	2.50	0.46
45:AL:201:CDL:H782	45:AL:201:CDL:H432	1.97	0.46
13:AM:75:TRP:NE1	52:AM:201:PLX:O2	2.48	0.46
21:B7:107:ARG:HA	21:B7:110:GLN:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N1:87:VAL:HG11	30:N3:6:THR:HG21	1.98	0.46
46:N1:405:PEE:H81	45:S8:303:CDL:H842	1.96	0.46
32:N5:249:SER:HA	32:N5:306:THR:HG21	1.98	0.46
35:S2:145:LEU:HD11	35:S2:430:ILE:HD13	1.98	0.46
7:A7:40:LYS:HB3	14:AN:7:LYS:H	1.79	0.46
16:B2:79:MET:SD	32:N5:375:ILE:HG12	2.56	0.46
20:B6:140:TRP:HD1	24:BK:41:VAL:HG13	1.80	0.46
29:N2:100:MET:HE3	32:N5:595:ILE:HG12	1.96	0.46
32:N5:297:ASP:O	32:N5:301:ILE:HG13	2.15	0.46
34:S1:213:MET:HE1	34:S1:713:ALA:HB1	1.98	0.46
36:S3:89:HIS:CG	36:S3:90:PRO:HD2	2.51	0.46
46:A3:201:PEE:H27	46:A3:201:PEE:H22	1.60	0.46
28:N1:61:LEU:HD13	40:S7:98:ARG:HH11	1.79	0.46
33:N6:24:PRO:HA	33:N6:89:VAL:HG21	1.97	0.46
34:S1:180:THR:N	54:S1:802:SF4:S4	2.85	0.46
34:S1:282:ASN:ND2	34:S1:285:TRP:O	2.41	0.46
35:S2:382:GLU:OE1	35:S2:382:GLU:N	2.47	0.46
41:S8:119:CYS:SG	41:S8:145:TYR:OH	2.71	0.46
29:N2:43:VAL:HG11	29:N2:129:LEU:HD23	1.97	0.46
31:N4:122:PHE:CE1	31:N4:206:LYS:HE3	2.51	0.46
40:S7:62:LEU:O	40:S7:91:VAL:HA	2.15	0.46
42:V1:210:THR:HB	42:V1:224:ARG:H	1.81	0.46
8:A8:126:GLU:OE1	8:A8:212:ARG:NH1	2.39	0.46
19:B5:74:TYR:O	25:BL:96:SER:OG	2.31	0.46
20:B6:143:HIS:CD2	24:BK:45:VAL:HG21	2.49	0.46
29:N2:42:PRO:HG3	33:N6:167:VAL:HG13	1.98	0.46
31:N4:12:LEU:HB2	31:N4:13:PRO:HD3	1.97	0.46
34:S1:219:SER:O	34:S1:222:ILE:HG12	2.15	0.46
36:S3:187:ILE:HG23	36:S3:188:LEU:HG	1.97	0.46
1:4L:73:LEU:HD21	29:N2:41:ILE:HG13	1.98	0.45
11:AK:65:ASP:HB2	11:AK:206:VAL:HG13	1.98	0.45
11:AK:167:SER:HB3	11:AK:247:PHE:CZ	2.51	0.45
24:BK:43:ARG:HB3	24:BK:44:PRO:HD3	1.97	0.45
50:CA:101:3PE:H372	29:N2:325:LEU:H	1.80	0.45
32:N5:213:LEU:HB3	32:N5:273:VAL:HG11	1.98	0.45
34:S1:611:THR:HG21	37:S4:105:GLU:HA	1.97	0.45
42:V1:412:LEU:HD12	42:V1:415:ILE:HD11	1.97	0.45
23:B9:120:GLN:HB2	32:N5:524:ASN:HD21	1.81	0.45
34:S1:156:GLY:O	42:V1:394:LYS:NZ	2.49	0.45
35:S2:162:GLU:HG2	35:S2:167:ILE:HD11	1.99	0.45
8:A8:117:ASN:O	8:A8:121:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AC:140:CYS:HB2	10:AC:143:GLU:HG3	1.98	0.45
20:B6:164:ILE:HB	21:B7:48:ASP:HB3	1.99	0.45
11:AK:260:TYR:HB3	11:AK:264:GLU:HB2	1.98	0.45
26:CA:47:THR:HG23	27:CB:65:LEU:HD22	1.98	0.45
32:N5:24:SER:HB2	32:N5:26:ILE:HG22	1.98	0.45
41:S8:63:TRP:HB3	41:S8:66:LEU:HD12	1.98	0.45
1:4L:5:TYR:HB3	1:4L:43:MET:HE1	1.98	0.45
20:B6:148:TYR:CE1	24:BK:49:ARG:HG2	2.51	0.45
29:N2:111:PHE:HA	32:N5:591:PHE:CE1	2.51	0.45
45:S8:303:CDL:H1	45:S8:303:CDL:HB61	1.99	0.45
9:A9:199:THR:OG1	9:A9:258:ALA:O	2.33	0.45
32:N5:334:PHE:HZ	46:N5:706:PEE:H36	1.81	0.45
35:S2:448:HIS:HB3	35:S2:452:ASP:HB2	1.99	0.45
40:S7:59:ARG:HG3	40:S7:181:GLN:HB3	1.98	0.45
42:V1:160:GLY:N	42:V1:200:GLY:O	2.50	0.45
4:A3:127:ALA:HB2	28:N1:312:ALA:HA	1.98	0.45
4:A3:163:LEU:HD13	8:A8:200:GLY:HA3	1.98	0.45
8:A8:84:LEU:O	14:AN:88:ARG:NH1	2.50	0.45
26:CA:68:GLU:OE2	26:CA:72:ARG:NE	2.50	0.45
31:N4:16:TRP:CE2	45:N4:503:CDL:H272	2.52	0.45
32:N5:398:ALA:O	32:N5:402:SER:OG	2.28	0.45
34:S1:575:VAL:C	34:S1:578:PRO:HD2	2.42	0.45
27:CB:3:MET:HE3	27:CB:4:MET:HE2	1.99	0.45
29:N2:171:ASN:HB2	32:N5:574:SER:HB2	1.99	0.45
31:N4:373:ILE:HD11	31:N4:444:LEU:HD23	1.99	0.45
32:N5:15:LEU:HD11	32:N5:94:LEU:HD21	1.99	0.45
41:S8:53:VAL:HG22	41:S8:56:ARG:HH21	1.81	0.45
2:A1:42:SER:OG	33:N6:133:SER:O	2.35	0.45
8:A8:201:GLU:HA	8:A8:204:LYS:HD3	1.99	0.45
9:A9:45:LYS:HE2	37:S4:118:ALA:HB1	1.99	0.45
11:AK:85:LEU:HD22	11:AK:158:GLY:HA3	1.98	0.45
12:AL:118:MET:HA	12:AL:121:THR:HG22	1.99	0.45
14:AN:49:SER:HB3	28:N1:172:ILE:HD13	1.99	0.45
28:N1:267:THR:O	28:N1:271:LEU:HG	2.17	0.45
34:S1:169:VAL:HG22	34:S1:223:ILE:HD11	1.98	0.45
42:V1:383:THR:HG23	42:V1:387:GLU:HG3	1.99	0.45
29:N2:83:GLN:HE22	38:S5:20:ILE:HG22	1.83	0.45
31:N4:70:THR:HA	31:N4:103:GLN:HE21	1.81	0.45
37:S4:55:VAL:HG22	37:S4:57:GLU:HG2	1.99	0.45
40:S7:67:PHE:CE1	40:S7:120:VAL:HG21	2.51	0.45
43:V2:133:GLN:HE21	43:V2:174:VAL:HG11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AC:112:SER:HB2	23:B9:59:LEU:HD21	1.98	0.44
51:AL:205:PC1:H331	32:N5:573:MET:HE2	1.98	0.44
28:N1:174:MET:HB2	28:N1:242:PHE:HA	1.99	0.44
43:V2:188:ILE:HD13	43:V2:208:LEU:HD11	2.00	0.44
10:AC:119:ILE:HG21	10:AC:135:ALA:HB1	1.98	0.44
29:N2:2:ASN:HD22	29:N2:4:ILE:H	1.65	0.44
34:S1:395:GLU:OE2	34:S1:417:ARG:NH1	2.50	0.44
35:S2:218:GLU:OE2	40:S7:83:ARG:NH1	2.46	0.44
41:S8:162:CYS:HA	54:S8:301:SF4:S3	2.57	0.44
45:S8:303:CDL:H822	45:S8:303:CDL:H782	1.99	0.44
42:V1:288:VAL:HG21	42:V1:303:HIS:CD2	2.52	0.44
11:AK:220:ILE:HG23	11:AK:228:GLU:HG3	1.99	0.44
14:AN:68:ARG:O	14:AN:72:MET:HG3	2.17	0.44
28:N1:155:LEU:HD21	30:N3:75:LEU:HB3	1.99	0.44
28:N1:273:ILE:HD11	46:N1:405:PEE:H65	1.98	0.44
46:N1:405:PEE:H76	45:S8:303:CDL:H851	1.99	0.44
32:N5:383:MET:O	32:N5:389:PHE:HB2	2.17	0.44
34:S1:598:ASN:HD21	34:S1:600:GLU:HG2	1.83	0.44
35:S2:194:THR:HB	35:S2:206:PHE:HA	1.99	0.44
42:V1:112:TYR:O	42:V1:240:THR:HA	2.17	0.44
25:BL:90:VAL:HG22	31:N4:28:THR:HG21	1.98	0.44
52:N4:502:PLX:H181	45:N5:703:CDL:H432	2.00	0.44
32:N5:248:HIS:O	32:N5:253:VAL:HG22	2.17	0.44
34:S1:251:ILE:HD11	34:S1:596:TYR:HB2	2.00	0.44
34:S1:253:VAL:HG12	34:S1:345:LEU:HD22	2.00	0.44
1:4L:55:LEU:HD13	38:S5:17:TRP:HE3	1.82	0.44
10:AC:88:LYS:HG3	10:AC:98:LEU:HD23	1.99	0.44
34:S1:367:CYS:HB3	34:S1:533:GLY:O	2.17	0.44
35:S2:106:GLU:HB2	35:S2:114:LYS:HB3	2.00	0.44
35:S2:203:MET:O	35:S2:206:PHE:HB3	2.16	0.44
41:S8:75:SER:O	41:S8:79:ARG:HG3	2.18	0.44
11:AK:255:CYS:HA	11:AK:282:LYS:HD2	1.99	0.44
20:B6:146:LEU:HD23	20:B6:150:VAL:HG21	1.99	0.44
51:B7:201:PC1:H221	46:N5:706:PEE:H78	1.99	0.44
29:N2:211:MET:HG2	29:N2:333:SER:HB2	2.00	0.44
52:N3:201:PLX:H351	52:N3:201:PLX:H382	1.79	0.44
31:N4:168:GLN:HB2	31:N4:174:LEU:HG	1.99	0.44
32:N5:292:ALA:HB2	32:N5:304:PHE:HB3	2.00	0.44
38:S5:21:GLN:HG3	38:S5:37:GLU:OE1	2.17	0.44
41:S8:168:VAL:HG21	41:S8:201:ILE:HG21	1.99	0.44
6:A6:97:ALA:HA	48:AB:201:ZMP:H15	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:357:LYS:O	27:CB:62:ARG:NH1	2.50	0.44
21:B7:92:HIS:O	21:B7:96:VAL:HG13	2.18	0.44
34:S1:34:VAL:HG11	34:S1:96:VAL:HB	2.00	0.44
34:S1:336:ASN:OD1	34:S1:336:ASN:N	2.50	0.44
35:S2:187:LEU:HD23	35:S2:213:ARG:HG2	2.00	0.44
9:A9:132:ARG:HD2	9:A9:134:TRP:CZ2	2.53	0.44
9:A9:279:TYR:HB2	9:A9:372:ALA:HB2	1.98	0.44
15:B1:30:ARG:O	15:B1:33:GLU:HG2	2.17	0.44
32:N5:49:VAL:HB	32:N5:50:PRO:HD3	1.99	0.44
32:N5:208:CYS:HA	32:N5:209:PRO:HD3	1.76	0.44
32:N5:241:THR:HG21	32:N5:344:GLY:HA3	1.99	0.44
46:N5:701:PEE:H35	46:N5:701:PEE:H29	1.73	0.44
35:S2:393:GLU:OE2	35:S2:396:GLN:NE2	2.51	0.44
3:A2:55:ILE:O	3:A2:56:ARG:NH1	2.49	0.44
8:A8:115:LYS:HB3	8:A8:116:PRO:HD3	1.99	0.44
10:AB:82:ARG:HH21	10:AB:125:GLU:HG3	1.82	0.44
10:AB:87:LEU:HD13	10:AB:98:LEU:HD11	2.00	0.44
23:B9:77:ASP:OD1	23:B9:77:ASP:N	2.51	0.44
29:N2:137:ALA:HB3	29:N2:138:PRO:HD3	2.00	0.44
29:N2:167:TRP:HB3	32:N5:574:SER:HA	1.99	0.44
32:N5:298:ILE:O	32:N5:302:VAL:HG23	2.18	0.44
34:S1:576:GLY:HA2	34:S1:579:MET:HG2	1.99	0.44
45:A8:301:CDL:H582	45:A8:301:CDL:H531	2.00	0.43
10:AB:117:GLU:HA	10:AB:120:MET:HE3	1.99	0.43
10:AB:138:LEU:HD23	10:AB:144:ILE:HG12	1.99	0.43
52:AM:201:PLX:H261	52:AM:202:PLX:H111	2.00	0.43
52:N4:502:PLX:H22	52:N4:502:PLX:H1A3	1.70	0.43
35:S2:134:THR:HG22	35:S2:424:ARG:HG2	2.00	0.43
35:S2:416:TYR:HB3	35:S2:429:LYS:HB3	2.00	0.43
42:V1:65:THR:O	42:V1:69:LEU:HG	2.18	0.43
21:B7:12:ASP:OD1	21:B7:14:SER:OG	2.34	0.43
34:S1:398:ASP:H	34:S1:471:LYS:HB2	1.82	0.43
18:B4:77:TYR:CZ	32:N5:564:LYS:HG2	2.53	0.43
24:BK:144:SER:HB3	24:BK:158:LYS:HE3	1.99	0.43
29:N2:190:MET:HE2	29:N2:190:MET:HB3	1.72	0.43
29:N2:250:SER:O	29:N2:259:GLY:HA3	2.18	0.43
31:N4:211:GLY:H	31:N4:213:HIS:CD2	2.31	0.43
46:N5:706:PEE:H42	46:N5:706:PEE:H35	1.57	0.43
33:N6:2:THR:OG1	33:N6:125:TRP:NE1	2.51	0.43
29:N2:112:HIS:HB2	29:N2:184:ILE:HD13	2.00	0.43
31:N4:188:ASN:HD22	52:N4:501:PLX:H1A2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:96:VAL:O	32:N5:100:ILE:HG12	2.19	0.43
42:V1:146:GLY:HA3	42:V1:193:PHE:CE1	2.54	0.43
6:A6:88:LYS:HD2	6:A6:88:LYS:HA	1.80	0.43
8:A8:160:THR:HA	8:A8:163:TRP:NE1	2.34	0.43
11:AK:88:PHE:HB2	11:AK:161:LEU:HD23	2.00	0.43
20:B6:92:GLU:HB3	20:B6:93:PRO:HD3	2.00	0.43
23:B9:91:ASP:HA	23:B9:94:LYS:HB2	2.00	0.43
23:B9:144:TRP:HA	23:B9:147:ASP:OD2	2.18	0.43
24:BK:73:ASP:OD1	24:BK:73:ASP:N	2.39	0.43
52:CB:201:PLX:H4	52:CB:201:PLX:H72	1.58	0.43
31:N4:207:MET:HG2	31:N4:298:ILE:CG1	2.49	0.43
35:S2:149:SER:HA	35:S2:184:THR:HG22	2.00	0.43
35:S2:339:ARG:NH2	35:S2:459:THR:O	2.47	0.43
24:BK:115:GLN:HG2	32:N5:62:ILE:HG12	1.99	0.43
31:N4:145:ALA:HB1	31:N4:219:ALA:HA	2.01	0.43
31:N4:382:ILE:HG12	31:N4:396:MET:HG3	2.00	0.43
34:S1:593:SER:HB2	34:S1:608:VAL:HG23	2.00	0.43
35:S2:46:ASP:OD1	35:S2:46:ASP:N	2.50	0.43
42:V1:384:PRO:HB2	42:V1:423:THR:HG22	2.01	0.43
6:A6:63:ARG:HG2	10:AB:120:MET:SD	2.59	0.43
7:A7:64:MET:HB2	36:S3:80:CYS:SG	2.59	0.43
11:AK:284:PRO:O	11:AK:288:GLN:HG2	2.19	0.43
18:B4:129:TYR:CZ	24:BK:145:ASP:HA	2.53	0.43
25:BL:77:ASP:OD1	25:BL:78:LYS:N	2.50	0.43
26:CA:69:TYR:CZ	27:CB:24:PRO:HG3	2.53	0.43
28:N1:90:PRO:HB3	28:N1:94:PRO:HD3	2.01	0.43
31:N4:259:TYR:O	31:N4:263:MET:HG2	2.18	0.43
32:N5:213:LEU:HD23	32:N5:213:LEU:HA	1.78	0.43
36:S3:126:PHE:HB2	36:S3:147:THR:O	2.18	0.43
1:4L:6:MET:HB2	33:N6:119:PHE:CD1	2.54	0.43
45:AL:201:CDL:HA61	51:AL:205:PC1:H221	2.01	0.43
26:CA:53:PHE:O	26:CA:56:ILE:HG13	2.19	0.43
27:CB:13:LEU:HD21	38:S5:4:PHE:HB3	2.01	0.43
28:N1:245:ALA:HA	51:N1:402:PC1:H153	2.00	0.43
29:N2:133:TRP:CZ3	45:N2:401:CDL:H392	2.53	0.43
29:N2:186:HIS:O	29:N2:190:MET:HG3	2.18	0.43
32:N5:8:THR:O	32:N5:11:THR:OG1	2.30	0.43
32:N5:289:ALA:O	32:N5:293:ILE:HG23	2.19	0.43
39:S6:116:LEU:HD23	39:S6:116:LEU:HA	1.91	0.43
21:B7:56:ARG:HH22	24:BK:120:SER:HB3	1.84	0.43
24:BK:74:ILE:HG23	24:BK:156:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N2:193:VAL:HG21	29:N2:266:ILE:HG12	2.01	0.43
31:N4:282:LEU:HD21	31:N4:359:TRP:HH2	1.83	0.43
32:N5:369:THR:OG1	32:N5:445:GLU:OE1	2.30	0.43
33:N6:165:VAL:O	33:N6:168:ILE:HG13	2.19	0.43
34:S1:255:ASP:OD1	34:S1:255:ASP:N	2.51	0.43
42:V1:36:LYS:O	42:V1:40:ARG:HG3	2.19	0.43
9:A9:236:VAL:HG22	9:A9:272:LEU:HD23	2.00	0.43
11:AK:262:ALA:O	11:AK:266:GLU:HG2	2.19	0.43
19:B5:78:THR:C	19:B5:81:PRO:HD2	2.44	0.43
20:B6:146:LEU:HD11	32:N5:9:LEU:HD12	2.00	0.43
31:N4:176:PHE:HA	31:N4:179:ILE:HG12	2.00	0.43
32:N5:13:THR:O	32:N5:17:ILE:HG13	2.18	0.43
34:S1:208:THR:O	34:S1:210:ILE:N	2.52	0.43
36:S3:71:LYS:HE3	36:S3:72:TYR:CZ	2.54	0.43
11:AK:60:LYS:HE2	11:AK:62:ILE:HD11	2.01	0.42
11:AK:68:ILE:HD11	11:AK:171:PHE:HE1	1.83	0.42
21:B7:95:TYR:CZ	22:B8:156:VAL:HG11	2.54	0.42
28:N1:180:PRO:HB3	46:N1:405:PEE:H24	2.00	0.42
29:N2:20:VAL:HG13	29:N2:29:ILE:HG23	2.01	0.42
31:N4:97:THR:HG21	45:N4:503:CDL:H232	2.01	0.42
31:N4:127:VAL:HB	31:N4:128:PRO:HD3	2.01	0.42
32:N5:290:LEU:O	32:N5:523:SER:OG	2.37	0.42
32:N5:341:MET:HE2	32:N5:454:ILE:HG12	2.01	0.42
34:S1:534:VAL:HG23	34:S1:537:ILE:HD12	2.01	0.42
43:V2:66:ILE:HD11	44:V3:400:LEU:HD23	2.00	0.42
28:N1:179:TRP:CG	28:N1:180:PRO:HD3	2.54	0.42
52:N3:201:PLX:H22	52:N3:201:PLX:H1C2	1.77	0.42
34:S1:181:ARG:HB3	34:S1:225:ILE:HD12	2.00	0.42
1:4L:20:LEU:HD23	32:N5:588:PHE:HD2	1.84	0.42
6:A6:136:THR:HG21	36:S3:220:VAL:HG11	2.01	0.42
8:A8:117:ASN:HB3	14:AN:73:PRO:HG2	2.02	0.42
18:B4:14:LEU:HD12	18:B4:15:PRO:HD2	2.01	0.42
24:BK:144:SER:O	24:BK:146:LEU:N	2.52	0.42
28:N1:32:GLN:HG2	35:S2:204:THR:HG22	2.01	0.42
29:N2:139:LEU:HD13	29:N2:190:MET:HE1	2.01	0.42
29:N2:140:SER:HB3	38:S5:2:PRO:HA	2.01	0.42
32:N5:332:HIS:HA	32:N5:335:PHE:CZ	2.54	0.42
35:S2:272:ARG:NH2	41:S8:59:GLN:O	2.52	0.42
2:A1:28:LYS:NZ	8:A8:168:TYR:OH	2.39	0.42
9:A9:109:ASN:HB3	9:A9:112:ASP:HB2	2.01	0.42
10:AC:155:TYR:CD2	10:AC:156:GLU:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:4:THR:O	12:AL:8:LYS:HG2	2.19	0.42
52:B5:201:PLX:H352	52:B5:201:PLX:H321	1.80	0.42
34:S1:598:ASN:ND2	34:S1:600:GLU:HG2	2.35	0.42
42:V1:281:HIS:ND1	42:V1:358:ASP:OD1	2.52	0.42
8:A8:111:ALA:HB2	8:A8:197:PRO:HG3	2.01	0.42
9:A9:357:ARG:HH11	9:A9:364:SER:N	2.17	0.42
11:AK:51:THR:HG21	11:AK:153:LEU:HD22	2.02	0.42
13:AM:25:ARG:O	13:AM:29:ARG:HG2	2.19	0.42
31:N4:1:MET:HE2	31:N4:111:THR:HG21	2.02	0.42
33:N6:129:ASP:HB2	38:S5:32:ARG:NH1	2.35	0.42
34:S1:291:ARG:HD2	34:S1:292:PHE:CE2	2.54	0.42
10:AC:112:SER:HB3	23:B9:59:LEU:HD11	2.02	0.42
10:AC:133:ILE:HG13	23:B9:46:SER:HB2	2.01	0.42
52:CB:201:PLX:H22	52:CB:201:PLX:H1C2	1.77	0.42
34:S1:304:GLN:HB2	34:S1:316:TYR:CD1	2.54	0.42
34:S1:717:GLY:O	34:S1:718:ILE:HG13	2.19	0.42
42:V1:75:TRP:O	42:V1:79:GLU:HG2	2.20	0.42
8:A8:157:GLU:HB3	8:A8:158:PRO:HD3	2.01	0.42
21:B7:22:MET:HE1	21:B7:102:PHE:CD2	2.55	0.42
22:B8:162:PRO:HB2	22:B8:163:TYR:CD2	2.54	0.42
31:N4:16:TRP:HB3	45:N4:503:CDL:H511	2.01	0.42
32:N5:233:LEU:HB3	32:N5:234:PRO:HD3	2.01	0.42
36:S3:190:ASP:OD1	36:S3:191:TYR:N	2.53	0.42
41:S8:168:VAL:HG11	41:S8:205:ILE:HD11	2.02	0.42
42:V1:55:GLY:O	42:V1:58:SER:OG	2.26	0.42
42:V1:141:GLY:HA3	42:V1:248:VAL:O	2.19	0.42
43:V2:92:TRP:CE2	43:V2:126:PRO:HG3	2.54	0.42
2:A1:50:ARG:NH1	8:A8:97:VAL:O	2.38	0.42
12:AL:81:ARG:NH1	12:AL:89:ASN:HD21	2.18	0.42
26:CA:55:TRP:NE1	27:CB:68:THR:OG1	2.52	0.42
31:N4:200:ILE:O	31:N4:204:MET:HG2	2.20	0.42
35:S2:164:LEU:HD12	35:S2:417:LEU:HD23	2.01	0.42
43:V2:48:ASN:OD1	43:V2:51:THR:OG1	2.24	0.42
1:4L:62:ILE:HG21	29:N2:31:ILE:HD11	2.02	0.42
8:A8:202:LEU:HD13	14:AN:70:ALA:HB2	2.01	0.42
11:AK:64:VAL:HG13	11:AK:207:VAL:HB	2.02	0.42
12:AL:32:THR:HG23	45:AL:201:CDL:H781	2.02	0.42
13:AM:88:ARG:HB2	41:S8:200:GLU:HG3	2.01	0.42
31:N4:318:ALA:HB1	31:N4:374:ASN:CG	2.45	0.42
8:A8:87:LEU:HD22	14:AN:85:GLN:HG3	2.02	0.42
11:AK:109:GLN:NE2	11:AK:328:ARG:HH12	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AL:205:PC1:H122	46:N5:702:PEE:H1	2.01	0.42
14:AN:120:MET:HB3	14:AN:123:GLU:HG3	2.02	0.42
18:B4:109:ARG:HH22	27:CB:122:ARG:C	2.28	0.42
46:N1:405:PEE:H14	46:N1:405:PEE:H1	1.74	0.42
31:N4:106:LEU:HD21	31:N4:235:LEU:HD23	2.00	0.42
41:S8:153:ILE:HG12	54:S8:302:SF4:S1	2.60	0.42
42:V1:256:ARG:HA	43:V2:249:LEU:HD13	2.01	0.42
44:V3:386:TYR:CE2	44:V3:388:ASN:HB3	2.55	0.42
2:A1:51:ASP:O	2:A1:54:ILE:HG13	2.20	0.41
2:A1:69:ILE:HD12	2:A1:70:ASP:HB2	2.02	0.41
7:A7:31:ILE:H	7:A7:31:ILE:HG13	1.58	0.41
9:A9:167:ILE:HD13	9:A9:201:ILE:HB	2.02	0.41
13:AM:85:GLU:CD	13:AM:85:GLU:H	2.27	0.41
52:AM:202:PLX:H21	52:AM:202:PLX:H1A3	1.87	0.41
14:AN:97:ILE:HG23	38:S5:86:LEU:HD12	2.01	0.41
16:B2:64:LEU:HD13	16:B2:69:LEU:HD21	2.01	0.41
52:CB:201:PLX:H151	52:CB:201:PLX:H182	1.89	0.41
46:N1:405:PEE:H73	45:S8:303:CDL:H851	2.02	0.41
29:N2:168:GLY:O	29:N2:172:GLN:HG2	2.19	0.41
31:N4:400:MET:HG2	32:N5:176:ARG:NH1	2.35	0.41
34:S1:193:ASP:OD1	43:V2:111:ARG:NH2	2.42	0.41
42:V1:115:VAL:HG21	42:V1:142:CYS:SG	2.60	0.41
43:V2:207:GLU:HB2	43:V2:214:PRO:HG3	2.00	0.41
10:AC:104:PHE:HD1	10:AC:108:LEU:HD12	1.85	0.41
51:B5:203:PC1:H112	24:BK:61:TYR:HB3	2.03	0.41
28:N1:277:TYR:OH	41:S8:70:LEU:HG	2.20	0.41
31:N4:77:LEU:O	31:N4:81:GLN:HG3	2.20	0.41
32:N5:264:TYR:CG	32:N5:265:PRO:HD3	2.55	0.41
33:N6:124:ASP:HA	33:N6:127:ILE:HG12	2.02	0.41
34:S1:240:ALA:HB2	34:S1:271:MET:HE2	2.02	0.41
28:N1:273:ILE:HG23	28:N1:277:TYR:CD2	2.55	0.41
36:S3:85:GLU:HG2	36:S3:142:ARG:HH11	1.85	0.41
45:S8:303:CDL:H801	45:S8:303:CDL:C60	2.49	0.41
2:A1:1:MET:HB2	2:A1:3:PHE:CE2	2.55	0.41
4:A3:163:LEU:HD23	4:A3:166:LEU:HD23	2.02	0.41
6:A6:92:MET:HB3	48:AB:201:ZMP:H5A	2.02	0.41
51:B5:203:PC1:H2I2	51:B5:203:PC1:H382	2.02	0.41
52:N3:201:PLX:H311	52:N3:201:PLX:H281	1.70	0.41
31:N4:398:MET:O	31:N4:402:ILE:HG13	2.20	0.41
32:N5:27:TYR:O	32:N5:115:ASN:ND2	2.49	0.41
32:N5:264:TYR:CD2	32:N5:265:PRO:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N5:702:PEE:H52	46:N5:702:PEE:H58	1.74	0.41
45:N5:704:CDL:H212	45:N5:704:CDL:H251	2.01	0.41
35:S2:124:2MR:HG3	40:S7:108:THR:HG21	2.03	0.41
43:V2:137:THR:HG22	43:V2:138:THR:H	1.86	0.41
9:A9:197:GLU:HB3	9:A9:259:LYS:HG3	2.03	0.41
12:AL:36:VAL:HG22	45:AL:201:CDL:H742	2.02	0.41
24:BK:59:ASN:O	24:BK:59:ASN:ND2	2.54	0.41
27:CB:45:LEU:HD22	27:CB:55:VAL:HG12	2.03	0.41
29:N2:22:ILE:HD12	38:S5:6:VAL:HG21	2.01	0.41
31:N4:201:MET:HE1	31:N4:212:LEU:HD11	2.02	0.41
31:N4:265:SER:O	31:N4:269:MET:HG3	2.21	0.41
32:N5:120:TYR:OH	45:N5:703:CDL:OA4	2.36	0.41
34:S1:53:CYS:HA	34:S1:56:VAL:HG22	2.03	0.41
34:S1:234:LYS:HB3	34:S1:235:PRO:HD3	2.02	0.41
35:S2:410:LYS:HE2	35:S2:463:VAL:CG2	2.46	0.41
40:S7:130:VAL:HB	40:S7:159:VAL:HA	2.03	0.41
7:A7:9:GLN:HA	7:A7:12:ARG:HG2	2.02	0.41
10:AB:140:CYS:HB2	10:AB:143:GLU:OE1	2.21	0.41
18:B4:72:ARG:NH2	32:N5:546:GLN:OE1	2.52	0.41
29:N2:91:ASN:HD21	29:N2:93:VAL:HB	1.86	0.41
31:N4:243:MET:HB3	31:N4:301:ILE:HG21	2.01	0.41
31:N4:427:LYS:HA	31:N4:427:LYS:HD3	1.94	0.41
31:N4:433:GLU:O	31:N4:437:MET:HG2	2.20	0.41
52:N4:501:PLX:H72	52:N4:501:PLX:H4	1.67	0.41
34:S1:222:ILE:HA	34:S1:225:ILE:HG12	2.02	0.41
34:S1:343:GLY:O	34:S1:521:SER:OG	2.36	0.41
41:S8:153:ILE:HG13	41:S8:155:CYS:HB3	2.01	0.41
42:V1:244:ASN:OD1	42:V1:245:VAL:N	2.53	0.41
6:A6:127:THR:O	6:A6:131:ARG:HG3	2.21	0.41
45:B5:202:CDL:H511	45:B5:202:CDL:H162	2.03	0.41
35:S2:117:PRO:HG3	35:S2:441:LEU:HD23	2.02	0.41
35:S2:190:ILE:HG21	35:S2:213:ARG:HG3	2.03	0.41
36:S3:119:VAL:HG12	36:S3:121:THR:HG22	2.03	0.41
40:S7:118:ARG:HA	40:S7:118:ARG:HD2	1.89	0.41
45:4L:201:CDL:H181	45:4L:201:CDL:H212	1.84	0.41
3:A2:23:LEU:HD22	3:A2:33:VAL:HG12	2.02	0.41
9:A9:231:LEU:HD13	9:A9:292:PRO:HG3	2.02	0.41
48:AB:201:ZMP:H24	48:AB:201:ZMP:H1	1.75	0.41
11:AK:93:ILE:HG12	11:AK:136:TRP:CD1	2.55	0.41
11:AK:297:ARG:HA	11:AK:300:VAL:HG22	2.02	0.41
22:B8:94:HIS:O	22:B8:98:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:360:ARG:HD3	34:S1:360:ARG:HA	1.92	0.41
34:S1:419:ARG:NH1	34:S1:439:THR:O	2.53	0.41
40:S7:108:THR:OG1	40:S7:136:CYS:SG	2.75	0.41
10:AB:78:ALA:HA	10:AB:81:ASP:OD2	2.20	0.41
11:AK:357:LYS:HD3	26:CA:36:HIS:O	2.21	0.41
45:AL:201:CDL:H761	45:AL:202:CDL:H211	2.02	0.41
23:B9:212:ILE:O	23:B9:215:ARG:NH1	2.53	0.41
25:BL:106:VAL:HG13	31:N4:453:MET:HE3	2.03	0.41
29:N2:95:MET:HE2	29:N2:149:ILE:HA	2.02	0.41
32:N5:188:TRP:CZ2	32:N5:209:PRO:HG2	2.56	0.41
34:S1:356:ASP:O	34:S1:360:ARG:HG2	2.21	0.41
34:S1:426:ASP:OD2	44:V3:418:ARG:NH2	2.54	0.41
35:S2:186:LEU:HD23	35:S2:343:MET:HG2	2.02	0.41
35:S2:204:THR:N	35:S2:205:PRO:HD2	2.35	0.41
42:V1:116:ASN:O	42:V1:245:VAL:HG23	2.21	0.41
42:V1:314:LEU:HD11	42:V1:317:VAL:HG23	2.03	0.41
10:AB:77:GLU:CD	10:AB:77:GLU:H	2.29	0.41
13:AM:44:TYR:OH	13:AM:113:HIS:N	2.47	0.41
16:B2:56:PRO:HB3	32:N5:442:LEU:HD23	2.03	0.41
21:B7:4:HIS:NE2	22:B8:155:PRO:HD3	2.35	0.41
28:N1:310:MET:HG3	28:N1:311:THR:HG23	2.03	0.41
32:N5:136:ASN:ND2	32:N5:139:GLN:H	2.19	0.41
33:N6:17:PHE:HA	33:N6:20:PHE:CD1	2.55	0.41
35:S2:469:ARG:NH2	36:S3:169:GLU:OE2	2.54	0.41
1:4L:4:VAL:O	1:4L:8:ILE:HG12	2.21	0.40
10:AB:143:GLU:OE1	10:AB:143:GLU:N	2.54	0.40
45:AL:201:CDL:H342	45:AL:201:CDL:H311	1.95	0.40
22:B8:96:ASP:OD1	22:B8:96:ASP:N	2.54	0.40
31:N4:12:LEU:HD22	31:N4:97:THR:HG23	2.03	0.40
31:N4:106:LEU:HD13	31:N4:234:VAL:HG11	2.03	0.40
52:N4:502:PLX:H151	52:N4:502:PLX:H182	1.83	0.40
35:S2:190:ILE:HD12	35:S2:216:MET:HE1	2.03	0.40
46:A3:201:PEE:H67	46:A3:201:PEE:H72	1.84	0.40
12:AL:120:LEU:O	12:AL:124:LEU:HG	2.21	0.40
19:B5:113:PHE:O	19:B5:119:ARG:NH1	2.54	0.40
29:N2:168:GLY:HA3	29:N2:181:TYR:CE1	2.55	0.40
31:N4:282:LEU:HD21	31:N4:359:TRP:CH2	2.56	0.40
32:N5:14:ILE:HD11	32:N5:43:ALA:HA	2.03	0.40
32:N5:80:PHE:HB3	32:N5:82:MET:HE2	2.04	0.40
11:AK:166:TYR:HB3	11:AK:251:MET:HE3	2.03	0.40
11:AK:221:GLN:HE22	11:AK:229:MET:HE3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B7:44:GLN:NE2	21:B7:48:ASP:OD1	2.55	0.40
28:N1:151:LEU:HD21	30:N3:75:LEU:HD12	2.04	0.40
32:N5:253:VAL:HB	32:N5:310:LEU:HD11	2.04	0.40
42:V1:367:ILE:O	42:V1:371:ILE:HG12	2.22	0.40
10:AB:104:PHE:HD1	10:AB:108:LEU:HD12	1.86	0.40
10:AC:123:GLU:OE2	23:B9:63:LYS:NZ	2.48	0.40
12:AL:120:LEU:HD21	46:AL:204:PEE:H69	2.02	0.40
13:AM:130:THR:HG23	41:S8:144:ARG:HB2	2.02	0.40
14:AN:57:ARG:HB3	28:N1:316:PRO:HG3	2.03	0.40
23:B9:171:ARG:HD2	23:B9:210:TRP:CD2	2.56	0.40
31:N4:207:MET:HE3	31:N4:294:MET:HE3	2.02	0.40
52:N4:502:PLX:H362	52:N4:502:PLX:H392	1.93	0.40
32:N5:88:MET:HB3	32:N5:326:PHE:CE2	2.57	0.40
34:S1:577:ALA:HB3	34:S1:578:PRO:HD3	2.03	0.40
39:S6:38:VAL:HG22	39:S6:44:ALA:HB2	2.02	0.40
44:V3:394:TYR:CD1	44:V3:398:THR:HG21	2.56	0.40
6:A6:73:VAL:HA	6:A6:78:LEU:HD12	2.03	0.40
11:AK:138:TYR:OH	11:AK:193:LYS:HA	2.21	0.40
11:AK:207:VAL:HA	11:AK:258:LEU:O	2.21	0.40
20:B6:133:THR:OG1	20:B6:134:HIS:N	2.55	0.40
28:N1:104:PHE:CE1	51:N1:401:PC1:H232	2.57	0.40
32:N5:293:ILE:HD13	32:N5:418:LEU:HD22	2.02	0.40
35:S2:139:LEU:HB3	35:S2:140:PRO:HD3	2.04	0.40
35:S2:151:MET:SD	35:S2:180:PHE:HB3	2.62	0.40
41:S8:142:THR:O	41:S8:187:LYS:NZ	2.54	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%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A1	68/70 (97%)	68 (100%)	0	0	100	100
3	A2	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
4	A3	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
5	A5	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
6	A6	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
7	A7	93/112 (83%)	93 (100%)	0	0	100	100
8	A8	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
9	A9	333/341 (98%)	325 (98%)	8 (2%)	0	100	100
10	AB	75/87 (86%)	72 (96%)	3 (4%)	0	100	100
10	AC	85/87 (98%)	85 (100%)	0	0	100	100
11	AK	318/321 (99%)	307 (96%)	11 (4%)	0	100	100
12	AL	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
13	AM	142/144 (99%)	142 (100%)	0	0	100	100
14	AN	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
15	B1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
16	B2	65/67 (97%)	65 (100%)	0	0	100	100
17	B3	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
18	B4	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
19	B5	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
20	B6	98/126 (78%)	96 (98%)	2 (2%)	0	100	100
21	B7	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
22	B8	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
23	B9	176/178 (99%)	176 (100%)	0	0	100	100
24	BK	172/176 (98%)	165 (96%)	7 (4%)	0	100	100
25	BL	97/102 (95%)	89 (92%)	8 (8%)	0	100	100
26	CA	47/49 (96%)	47 (100%)	0	0	100	100
27	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
28	N1	305/318 (96%)	293 (96%)	12 (4%)	0	100	100
29	N2	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
30	N3	90/115 (78%)	88 (98%)	2 (2%)	0	100	100
31	N4	457/459 (100%)	453 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	N5	601/603 (100%)	576 (96%)	25 (4%)	0	100	100
33	N6	162/174 (93%)	152 (94%)	10 (6%)	0	100	100
34	S1	681/689 (99%)	650 (95%)	31 (5%)	0	100	100
35	S2	413/430 (96%)	399 (97%)	14 (3%)	0	100	100
36	S3	206/208 (99%)	201 (98%)	5 (2%)	0	100	100
37	S4	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
38	S5	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
39	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
40	S7	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
41	S8	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
42	V1	429/431 (100%)	413 (96%)	16 (4%)	0	100	100
43	V2	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
44	V3	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
All	All	8079/8299 (97%)	7848 (97%)	231 (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	86
6	A6	107/107 (100%)	107 (100%)	0	100	100
7	A7	87/97 (90%)	86 (99%)	1 (1%)	70	84
8	A8	153/153 (100%)	152 (99%)	1 (1%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	A9	291/295 (99%)	286 (98%)	5 (2%)	56	78
10	AB	71/80 (89%)	71 (100%)	0	100	100
10	AC	80/80 (100%)	79 (99%)	1 (1%)	65	82
11	AK	283/284 (100%)	277 (98%)	6 (2%)	48	72
12	AL	101/101 (100%)	100 (99%)	1 (1%)	73	86
13	AM	130/130 (100%)	128 (98%)	2 (2%)	60	80
14	AN	123/123 (100%)	123 (100%)	0	100	100
15	B1	53/53 (100%)	52 (98%)	1 (2%)	52	75
16	B2	62/62 (100%)	62 (100%)	0	100	100
17	B3	62/62 (100%)	61 (98%)	1 (2%)	58	79
18	B4	113/113 (100%)	113 (100%)	0	100	100
19	B5	121/121 (100%)	121 (100%)	0	100	100
20	B6	97/119 (82%)	96 (99%)	1 (1%)	73	86
21	B7	112/112 (100%)	112 (100%)	0	100	100
22	B8	141/141 (100%)	141 (100%)	0	100	100
23	B9	159/159 (100%)	159 (100%)	0	100	100
24	BK	155/156 (99%)	154 (99%)	1 (1%)	84	91
25	BL	91/94 (97%)	90 (99%)	1 (1%)	70	84
26	CA	45/45 (100%)	45 (100%)	0	100	100
27	CB	108/108 (100%)	107 (99%)	1 (1%)	75	88
28	N1	267/275 (97%)	263 (98%)	4 (2%)	60	80
29	N2	311/311 (100%)	311 (100%)	0	100	100
30	N3	82/100 (82%)	82 (100%)	0	100	100
31	N4	410/410 (100%)	408 (100%)	2 (0%)	86	92
32	N5	537/537 (100%)	535 (100%)	2 (0%)	89	94
33	N6	132/140 (94%)	127 (96%)	5 (4%)	28	59
34	S1	576/579 (100%)	573 (100%)	3 (0%)	86	92
35	S2	362/370 (98%)	360 (99%)	2 (1%)	84	91
36	S3	190/190 (100%)	190 (100%)	0	100	100
37	S4	112/112 (100%)	111 (99%)	1 (1%)	75	88
38	S5	93/93 (100%)	92 (99%)	1 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	S6	79/79 (100%)	79 (100%)	0	100	100
40	S7	132/132 (100%)	127 (96%)	5 (4%)	28	59
41	S8	151/151 (100%)	150 (99%)	1 (1%)	81	90
42	V1	344/344 (100%)	340 (99%)	4 (1%)	67	83
43	V2	183/183 (100%)	182 (100%)	1 (0%)	86	92
44	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	7134/7229 (99%)	7079 (99%)	55 (1%)	77	89

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A5	33	ASP
7	A7	31	ILE
8	A8	151	ILE
9	A9	129	LEU
9	A9	205	ASP
9	A9	226	VAL
9	A9	289	LEU
9	A9	365	GLU
10	AC	112	SER
11	AK	38	LEU
11	AK	68	ILE
11	AK	152	LEU
11	AK	277	TYR
11	AK	278	LEU
11	AK	287	ASP
12	AL	115	CYS
13	AM	59	HIS
13	AM	138	VAL
15	B1	9	ARG
17	B3	47	ARG
20	B6	123	LYS
24	BK	113	CYS
25	BL	53	ILE
27	CB	2	THR
28	N1	87	VAL
28	N1	213	VAL
28	N1	251	THR
28	N1	268	ILE
31	N4	8	THR

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Mol	Chain	Res	Type
31	N4	375	LEU
32	N5	23	ASN
32	N5	140	LEU
33	N6	20	PHE
33	N6	46	ASN
33	N6	47	PHE
33	N6	56	VAL
33	N6	66	VAL
34	S1	252	ASP
34	S1	509	ASP
34	S1	682	ASP
35	S2	148	VAL
35	S2	167	ILE
37	S4	77	VAL
38	S5	89	GLU
40	S7	67	PHE
40	S7	71	CYS
40	S7	94	ARG
40	S7	101	ASP
40	S7	142	TYR
41	S8	179	THR
42	V1	235	VAL
42	V1	327	ILE
42	V1	387	GLU
42	V1	448	GLU
43	V2	137	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	7	ASN
4	A3	137	ASN
5	A5	86	ASN
6	A6	77	GLN
6	A6	84	GLN
6	A6	121	ASN
6	A6	152	HIS
7	A7	9	GLN
7	A7	21	GLN
7	A7	25	GLN
7	A7	29	GLN
8	A8	142	GLN

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Mol	Chain	Res	Type
9	A9	102	GLN
9	A9	122	HIS
9	A9	154	GLN
9	A9	295	HIS
11	AK	109	GLN
11	AK	217	GLN
11	AK	221	GLN
11	AK	288	GLN
12	AL	79	GLN
12	AL	89	ASN
14	AN	61	GLN
14	AN	90	ASN
14	AN	130	ASN
15	B1	3	ASN
16	B2	53	HIS
16	B2	63	GLN
16	B2	71	GLN
18	B4	50	GLN
18	B4	123	GLN
19	B5	181	HIS
20	B6	127	HIS
21	B7	85	HIS
21	B7	110	GLN
22	B8	56	ASN
22	B8	115	ASN
22	B8	154	GLN
23	B9	117	GLN
24	BK	59	ASN
24	BK	107	GLN
25	BL	148	GLN
27	CB	48	ASN
27	CB	63	GLN
28	N1	138	GLN
28	N1	258	ASN
28	N1	284	GLN
28	N1	287	HIS
28	N1	304	HIS
29	N2	49	ASN
29	N2	77	ASN
29	N2	83	GLN
29	N2	91	ASN
29	N2	112	HIS

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Mol	Chain	Res	Type
29	N2	152	ASN
29	N2	186	HIS
29	N2	322	GLN
30	N3	28	ASN
31	N4	81	GLN
31	N4	83	HIS
31	N4	188	ASN
31	N4	213	HIS
31	N4	366	ASN
32	N5	2	ASN
32	N5	59	GLN
32	N5	72	GLN
32	N5	139	GLN
32	N5	230	HIS
32	N5	248	HIS
32	N5	323	HIS
32	N5	332	HIS
32	N5	348	HIS
32	N5	471	ASN
32	N5	524	ASN
33	N6	86	ASN
34	S1	39	GLN
34	S1	142	GLN
34	S1	331	GLN
34	S1	453	GLN
34	S1	498	GLN
34	S1	652	ASN
34	S1	676	ASN
34	S1	678	GLN
34	S1	688	GLN
35	S2	229	HIS
36	S3	75	GLN
36	S3	82	ASN
36	S3	123	GLN
36	S3	196	HIS
37	S4	86	ASN
37	S4	92	ASN
37	S4	123	ASN
37	S4	163	ASN
39	S6	74	GLN
39	S6	117	GLN
40	S7	111	ASN

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Mol	Chain	Res	Type
41	S8	85	ASN
41	S8	180	HIS
42	V1	49	HIS
42	V1	303	HIS
42	V1	344	GLN
42	V1	376	HIS
42	V1	381	GLN
43	V2	123	ASN
43	V2	133	GLN
43	V2	182	ASN
44	V3	388	ASN
44	V3	392	HIS
44	V3	419	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
35	2MR	S2	124	35	10,12,13	2.44	2 (20%)	5,13,15	0.99	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	5.19	1.45	1.34
35	S2	124	2MR	CZ-NH2	5.10	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 55 ligands modelled in this entry, 2 are monoatomic - leaving 53 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	$\# Z  > 2$
54	SF4	V1	501	42	0,12,12	-	-	-		
54	SF4	S8	301	41	0,12,12	-	-	-		
45	CDL	B5	202	-	97,97,99	0.30	0	103,109,111	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
46	PEE	N5	705	-	50,50,50	1.32	5 (10%)	53,55,55	1.18	3 (5%)
54	SF4	S1	801	34	0,12,12	-	-	-		
49	ADP	AK	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.46	4 (13%)
58	FMN	V1	502	-	33,33,33	0.21	0	48,50,50	0.46	0
46	PEE	AL	204	-	45,45,50	1.38	5 (11%)	48,50,55	1.19	4 (8%)
52	PLX	CB	201	-	51,51,51	1.11	5 (9%)	55,59,59	0.88	1 (1%)
45	CDL	B4	202	-	61,61,99	0.37	0	67,73,111	0.36	0
45	CDL	N2	401	-	67,67,99	0.35	0	73,79,111	0.30	0
46	PEE	B4	201	-	50,50,50	1.33	5 (10%)	53,55,55	1.17	3 (5%)
52	PLX	B5	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.91	1 (1%)
51	PC1	B5	203	-	53,53,53	0.31	0	59,61,61	0.46	0
52	PLX	N3	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.88	1 (1%)
54	SF4	S7	301	40	0,12,12	-	-	-		
55	FES	V2	301	43	0,4,4	-	-	-		
53	XEW	S2	501	-	15,17,17	5.96	15 (100%)	19,22,22	2.44	4 (21%)
51	PC1	N1	401	-	53,53,53	0.29	0	59,61,61	0.27	0
46	PEE	A3	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.15	4 (7%)
45	CDL	N4	503	-	99,99,99	0.30	0	105,111,111	0.27	0
45	CDL	S8	303	-	99,99,99	0.30	0	105,111,111	0.27	0
50	3PE	AL	203	-	50,50,50	0.30	0	53,55,55	0.28	0
45	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.39	0
45	CDL	N5	703	-	81,81,99	0.32	0	87,93,111	0.31	0
46	PEE	N1	405	-	50,50,50	1.32	5 (10%)	53,55,55	1.20	3 (5%)
46	PEE	N2	402	-	47,47,50	1.36	5 (10%)	50,52,55	1.21	4 (8%)
52	PLX	AM	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.87	1 (1%)
54	SF4	S8	302	41	0,12,12	-	-	-		
46	PEE	N5	702	-	39,39,50	1.49	5 (12%)	41,44,55	1.17	2 (4%)
46	PEE	N5	706	-	50,50,50	1.32	5 (10%)	53,55,55	1.15	2 (3%)
47	NDP	A9	401	-	45,52,52	0.52	0	53,80,80	0.53	1 (1%)
45	CDL	A8	301	-	76,76,99	0.34	0	82,88,111	0.35	0
51	PC1	S7	302	-	53,53,53	0.29	0	59,61,61	0.27	0
50	3PE	B8	201	-	31,31,50	0.38	0	34,36,55	0.34	0
52	PLX	N4	502	-	51,51,51	1.11	4 (7%)	55,59,59	0.89	1 (1%)
46	PEE	N5	701	-	45,45,50	1.39	5 (11%)	48,50,55	1.18	4 (8%)
51	PC1	N1	402	-	53,53,53	0.29	0	59,61,61	0.28	0
53	XEW	N1	403	-	15,17,17	5.98	15 (100%)	19,22,22	2.32	3 (15%)
45	CDL	AL	202	-	89,89,99	0.32	0	95,101,111	0.40	0
45	CDL	A7	201	-	93,93,99	0.30	0	99,105,111	0.28	0
50	3PE	CA	101	-	50,50,50	0.31	0	53,55,55	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
52	PLX	N4	501	-	46,46,51	1.15	5 (10%)	50,54,59	0.86	1 (2%)
48	ZMP	AC	201	10	29,35,36	0.65	1 (3%)	34,42,45	0.64	0
52	PLX	AM	202	-	51,51,51	1.10	4 (7%)	55,59,59	0.89	1 (1%)
51	PC1	B7	201	-	53,53,53	0.30	0	59,61,61	0.29	0
54	SF4	S1	802	34	0,12,12	-	-	-	-	-
51	PC1	AL	205	-	30,30,53	0.37	0	36,38,61	0.33	0
48	ZMP	AB	201	10	29,35,36	0.63	1 (3%)	34,42,45	0.78	1 (2%)
45	CDL	4L	201	-	91,91,99	0.31	0	97,103,111	0.27	0
45	CDL	N5	704	-	99,99,99	0.30	0	105,111,111	0.28	0
55	FES	S1	803	34	0,4,4	-	-	-	-	-
46	PEE	N1	404	-	50,50,50	1.33	6 (12%)	53,55,55	1.18	4 (7%)

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
54	SF4	V1	501	42	-	-	0/6/5/5
54	SF4	S8	301	41	-	-	0/6/5/5
45	CDL	B5	202	-	-	19/108/108/110	-
46	PEE	N5	705	-	-	25/54/54/54	-
54	SF4	S1	801	34	-	-	0/6/5/5
49	ADP	AK	401	-	-	2/12/32/32	0/3/3/3
58	FMN	V1	502	-	-	5/18/18/18	0/3/3/3
46	PEE	AL	204	-	-	23/49/49/54	-
52	PLX	CB	201	-	-	22/55/55/55	-
45	CDL	B4	202	-	-	17/72/72/110	-
45	CDL	N2	401	-	-	17/78/78/110	-
46	PEE	B4	201	-	-	17/54/54/54	-
52	PLX	B5	201	-	-	18/55/55/55	-
51	PC1	B5	203	-	-	18/57/57/57	-
52	PLX	N3	201	-	-	17/55/55/55	-
54	SF4	S7	301	40	-	-	0/6/5/5
55	FES	V2	301	43	-	-	0/1/1/1
53	XEW	S2	501	-	-	4/12/12/12	0/1/1/1
51	PC1	N1	401	-	-	13/57/57/57	-
46	PEE	A3	201	-	-	18/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CDL	N4	503	-	-	20/110/110/110	-
45	CDL	S8	303	-	-	14/110/110/110	-
50	3PE	AL	203	-	-	9/54/54/54	-
45	CDL	AL	201	-	-	25/104/104/110	-
45	CDL	N5	703	-	-	28/92/92/110	-
46	PEE	N1	405	-	-	27/54/54/54	-
46	PEE	N2	402	-	-	20/51/51/54	-
52	PLX	AM	201	-	-	24/55/55/55	-
54	SF4	S8	302	41	-	-	0/6/5/5
46	PEE	N5	702	-	-	23/43/43/54	-
46	PEE	N5	706	-	-	23/54/54/54	-
47	NDP	A9	401	-	-	7/30/77/77	0/5/5/5
45	CDL	A8	301	-	-	23/87/87/110	-
51	PC1	S7	302	-	-	19/57/57/57	-
50	3PE	B8	201	-	-	6/35/35/54	-
52	PLX	N4	502	-	-	18/55/55/55	-
46	PEE	N5	701	-	-	19/49/49/54	-
51	PC1	N1	402	-	-	13/57/57/57	-
53	XEW	N1	403	-	-	4/12/12/12	0/1/1/1
45	CDL	AL	202	-	-	18/100/100/110	-
45	CDL	A7	201	-	-	16/104/104/110	-
50	3PE	CA	101	-	-	14/54/54/54	-
52	PLX	N4	501	-	-	26/50/50/55	-
48	ZMP	AC	201	10	-	12/40/42/43	-
52	PLX	AM	202	-	-	17/55/55/55	-
51	PC1	B7	201	-	-	9/57/57/57	-
54	SF4	S1	802	34	-	-	0/6/5/5
51	PC1	AL	205	-	-	8/34/34/57	-
48	ZMP	AB	201	10	-	18/40/42/43	-
45	CDL	4L	201	-	-	16/102/102/110	-
45	CDL	N5	704	-	-	20/110/110/110	-
55	FES	S1	803	34	-	-	0/1/1/1
46	PEE	N1	404	-	-	27/54/54/54	-

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	S2	501	XEW	C4-N	12.31	1.53	1.37
53	N1	403	XEW	C4-N	11.97	1.52	1.37
53	S2	501	XEW	C4-N4	8.41	1.52	1.29
53	S2	501	XEW	C5-N3	8.40	1.52	1.29
53	N1	403	XEW	C4-N4	8.39	1.52	1.29
53	N1	403	XEW	C5-N3	8.35	1.52	1.29
53	N1	403	XEW	C5-N2	7.53	1.52	1.34
53	S2	501	XEW	C5-N2	7.25	1.52	1.34
53	N1	403	XEW	C-CL	6.10	1.87	1.74
53	S2	501	XEW	C-CL	5.99	1.87	1.74
53	S2	501	XEW	C3-N	5.50	1.52	1.41
53	N1	403	XEW	C3-N	5.49	1.52	1.41
53	N1	403	XEW	C1-C	4.13	1.45	1.38
53	N1	403	XEW	C10-C	4.12	1.45	1.38
46	N5	705	PEE	C18-C19	4.06	1.55	1.31
46	N1	404	PEE	C18-C19	4.05	1.55	1.31
46	N5	702	PEE	C18-C19	4.05	1.55	1.31
46	B4	201	PEE	C18-C19	4.05	1.55	1.31
46	N5	701	PEE	C18-C19	4.04	1.55	1.31
46	N2	402	PEE	C18-C19	4.04	1.55	1.31
46	N5	706	PEE	C18-C19	4.04	1.55	1.31
46	N1	405	PEE	C18-C19	4.03	1.55	1.31
46	A3	201	PEE	C18-C19	4.03	1.55	1.31
53	S2	501	XEW	C10-C	4.03	1.45	1.38
46	AL	204	PEE	C18-C19	4.02	1.55	1.31
46	N5	701	PEE	C39-C38	3.95	1.54	1.31
46	N5	706	PEE	C39-C38	3.95	1.54	1.31
46	B4	201	PEE	C39-C38	3.95	1.54	1.31
46	N1	404	PEE	C39-C38	3.95	1.54	1.31
53	S2	501	XEW	C1-C	3.94	1.45	1.38
46	N5	705	PEE	C39-C38	3.94	1.54	1.31
46	N5	702	PEE	C39-C38	3.94	1.54	1.31
46	AL	204	PEE	C39-C38	3.94	1.54	1.31
46	A3	201	PEE	C39-C38	3.94	1.54	1.31
46	N2	402	PEE	C39-C38	3.92	1.54	1.31
46	N1	405	PEE	C39-C38	3.92	1.54	1.31
53	S2	501	XEW	C2-C3	3.91	1.45	1.39
53	N1	403	XEW	C9-C10	3.90	1.45	1.38
53	N1	403	XEW	C9-C3	3.87	1.45	1.39
53	N1	403	XEW	C2-C3	3.85	1.45	1.39
53	N1	403	XEW	C1-C2	3.85	1.45	1.38
53	S2	501	XEW	C9-C3	3.85	1.45	1.39
53	S2	501	XEW	C1-C2	3.83	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	S2	501	XEW	C9-C10	3.74	1.45	1.38
53	N1	403	XEW	C8-C6	3.51	1.60	1.51
53	S2	501	XEW	C8-C6	3.50	1.60	1.51
53	N1	403	XEW	C7-C6	3.49	1.60	1.51
53	S2	501	XEW	C7-C6	3.39	1.60	1.51
46	N5	702	PEE	O3-C30	3.28	1.42	1.33
46	N5	706	PEE	O3-C30	3.28	1.42	1.33
46	N5	701	PEE	O3-C30	3.25	1.42	1.33
46	A3	201	PEE	O3-C30	3.25	1.42	1.33
46	N1	404	PEE	O3-C30	3.25	1.42	1.33
46	N5	705	PEE	O3-C30	3.24	1.42	1.33
46	B4	201	PEE	O3-C30	3.24	1.42	1.33
46	N1	405	PEE	O3-C30	3.23	1.42	1.33
53	N1	403	XEW	C6-N2	3.19	1.52	1.47
46	N2	402	PEE	O3-C30	3.18	1.42	1.33
46	AL	204	PEE	O3-C30	3.17	1.42	1.33
52	N4	502	PLX	O6-C4	-2.98	1.40	1.44
52	B5	201	PLX	O6-C4	-2.97	1.40	1.44
52	AM	201	PLX	O6-C4	-2.93	1.40	1.44
52	CB	201	PLX	O6-C4	-2.91	1.40	1.44
52	AM	202	PLX	O6-C4	-2.91	1.40	1.44
46	N5	702	PEE	O2-C10	2.87	1.42	1.34
52	N3	201	PLX	O6-C4	-2.85	1.40	1.44
46	N1	404	PEE	O2-C10	2.81	1.42	1.34
53	S2	501	XEW	C6-N2	2.74	1.52	1.47
46	N5	706	PEE	O2-C10	2.70	1.41	1.34
46	N2	402	PEE	O2-C10	2.70	1.41	1.34
52	N4	501	PLX	O6-C4	-2.70	1.41	1.44
46	N1	405	PEE	O2-C10	2.68	1.41	1.34
46	B4	201	PEE	O2-C10	2.66	1.41	1.34
46	N5	701	PEE	O2-C10	2.63	1.41	1.34
46	A3	201	PEE	O2-C10	2.62	1.41	1.34
46	N5	705	PEE	O2-C10	2.60	1.41	1.34
46	AL	204	PEE	O2-C10	2.58	1.41	1.34
46	AL	204	PEE	O2-C2	-2.54	1.40	1.46
46	A3	201	PEE	O2-C2	-2.49	1.40	1.46
46	N5	705	PEE	O2-C2	-2.49	1.40	1.46
46	N1	405	PEE	O2-C2	-2.47	1.40	1.46
46	N5	701	PEE	O2-C2	-2.47	1.40	1.46
46	N2	402	PEE	O2-C2	-2.45	1.40	1.46
46	B4	201	PEE	O2-C2	-2.45	1.40	1.46
48	AC	201	ZMP	C9-C10	-2.43	1.48	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	AB	201	ZMP	C9-C10	-2.42	1.48	1.50
49	AK	401	ADP	C5-C4	2.41	1.47	1.40
46	N5	706	PEE	O2-C2	-2.41	1.40	1.46
52	CB	201	PLX	C1B-N1	-2.16	1.43	1.50
52	B5	201	PLX	C1B-N1	-2.15	1.43	1.50
46	N1	404	PEE	O2-C2	-2.14	1.41	1.46
52	N4	502	PLX	C1B-N1	-2.13	1.43	1.50
52	N4	501	PLX	C1B-N1	-2.12	1.43	1.50
52	N3	201	PLX	C1B-N1	-2.12	1.43	1.50
52	AM	202	PLX	C1B-N1	-2.11	1.43	1.50
52	AM	201	PLX	C1B-N1	-2.10	1.43	1.50
46	N5	702	PEE	O2-C2	-2.08	1.41	1.46
52	N3	201	PLX	C7-C6	2.07	1.55	1.50
52	N4	501	PLX	P1-O4	2.06	1.67	1.59
52	N4	501	PLX	C7-C6	2.06	1.55	1.50
52	CB	201	PLX	P1-O4	2.05	1.67	1.59
52	AM	201	PLX	P1-O4	2.05	1.67	1.59
52	N4	501	PLX	C1A-N1	-2.04	1.44	1.50
52	CB	201	PLX	C1A-N1	-2.03	1.44	1.50
52	AM	202	PLX	C1A-N1	-2.03	1.44	1.50
52	N3	201	PLX	P1-O4	2.02	1.67	1.59
52	B5	201	PLX	P1-O4	2.02	1.67	1.59
52	N4	502	PLX	P1-O4	2.02	1.67	1.59
52	CB	201	PLX	C7-C6	2.02	1.55	1.50
52	AM	201	PLX	C1A-N1	-2.02	1.44	1.50
46	N1	404	PEE	C11-C10	2.01	1.56	1.50
52	N4	502	PLX	C1A-N1	-2.01	1.44	1.50
52	AM	202	PLX	P1-O4	2.01	1.67	1.59
52	B5	201	PLX	C1A-N1	-2.00	1.44	1.50

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	S2	501	XEW	C5-N1-C4	-7.01	113.00	125.27
53	N1	403	XEW	C6-N2-C5	6.93	137.31	124.11
53	S2	501	XEW	C6-N2-C5	6.48	136.44	124.11
53	N1	403	XEW	C5-N1-C4	-5.18	116.21	125.27
46	N1	405	PEE	O2-C10-C11	4.31	120.79	111.50
46	N2	402	PEE	O2-C10-C11	4.25	120.66	111.50
46	N1	404	PEE	O2-C10-C11	4.24	120.64	111.50
46	N5	706	PEE	O2-C10-C11	4.01	120.15	111.50
46	N5	705	PEE	O2-C10-C11	3.97	120.06	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	B4	201	PEE	O2-C10-C11	3.96	120.05	111.50
46	AL	204	PEE	O2-C10-C11	3.85	119.80	111.50
46	A3	201	PEE	O2-C10-C11	3.82	119.74	111.50
46	N5	701	PEE	O2-C10-C11	3.80	119.70	111.50
46	N5	702	PEE	O2-C10-C11	3.74	119.57	111.50
53	N1	403	XEW	N-C4-N4	-3.62	109.13	121.58
49	AK	401	ADP	PA-O3A-PB	-3.59	120.50	132.83
53	S2	501	XEW	N-C4-N4	-3.31	110.20	121.58
49	AK	401	ADP	N3-C2-N1	-3.18	123.70	128.68
49	AK	401	ADP	C3'-C2'-C1'	3.08	105.61	100.98
46	N5	705	PEE	O3-C30-C31	2.75	120.54	111.91
46	AL	204	PEE	O3-C30-C31	2.70	120.37	111.91
46	N5	702	PEE	O3-C30-C31	2.68	120.32	111.91
46	N5	701	PEE	O3-C30-C31	2.67	120.30	111.91
49	AK	401	ADP	C4-C5-N7	-2.67	106.62	109.40
46	N1	405	PEE	O3-C30-C31	2.63	120.16	111.91
46	B4	201	PEE	O3-C30-C31	2.60	120.07	111.91
46	A3	201	PEE	O3-C30-C31	2.59	120.04	111.91
46	N1	404	PEE	O3-C30-C31	2.55	119.90	111.91
46	N2	402	PEE	O3-C30-C31	2.52	119.81	111.91
46	N5	706	PEE	O3-C30-C31	2.48	119.68	111.91
48	AB	201	ZMP	C15-C14-C13	-2.43	108.30	112.36
53	S2	501	XEW	N1-C5-N3	-2.42	113.24	121.58
47	A9	401	NDP	C5A-C6A-N6A	2.29	123.83	120.35
52	B5	201	PLX	O3-P1-O2	-2.24	101.16	112.24
52	N3	201	PLX	O3-P1-O2	-2.23	101.19	112.24
52	CB	201	PLX	O3-P1-O2	-2.23	101.20	112.24
52	AM	201	PLX	O3-P1-O2	-2.22	101.25	112.24
52	N4	501	PLX	O3-P1-O2	-2.22	101.25	112.24
52	N4	502	PLX	O3-P1-O2	-2.21	101.32	112.24
52	AM	202	PLX	O3-P1-O2	-2.17	101.51	112.24
46	N1	405	PEE	C37-C38-C39	-2.11	108.54	124.73
46	N2	402	PEE	C40-C39-C38	-2.08	108.80	124.73
46	A3	201	PEE	C40-C39-C38	-2.06	108.90	124.73
46	N1	404	PEE	C40-C39-C38	-2.06	108.93	124.73
46	AL	204	PEE	C17-C18-C19	-2.04	109.08	124.73
46	AL	204	PEE	C37-C38-C39	-2.03	109.13	124.73
46	N2	402	PEE	C17-C18-C19	-2.02	109.20	124.73
46	N1	404	PEE	C37-C38-C39	-2.02	109.22	124.73
46	N5	705	PEE	C37-C38-C39	-2.02	109.22	124.73
46	N5	701	PEE	C40-C39-C38	-2.02	109.25	124.73
46	A3	201	PEE	C20-C19-C18	-2.01	109.31	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	N5	701	PEE	C20-C19-C18	-2.00	109.36	124.73
46	B4	201	PEE	C17-C18-C19	-2.00	109.37	124.73

There are no chirality outliers.

All (758) 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	CA3-OA5-PA1-OA2
45	4L	201	CDL	CA3-OA5-PA1-OA3
45	4L	201	CDL	CA3-OA5-PA1-OA4
45	4L	201	CDL	CB2-OB2-PB2-OB3
45	A7	201	CDL	CA3-OA5-PA1-OA3
45	A7	201	CDL	CA3-OA5-PA1-OA4
45	A7	201	CDL	CB2-OB2-PB2-OB3
45	A7	201	CDL	CB3-OB5-PB2-OB2
45	A7	201	CDL	CB3-OB5-PB2-OB3
45	A8	301	CDL	CA2-OA2-PA1-OA3
45	A8	301	CDL	CA2-OA2-PA1-OA4
45	A8	301	CDL	CA2-OA2-PA1-OA5
45	A8	301	CDL	CA3-OA5-PA1-OA2
45	A8	301	CDL	CA3-OA5-PA1-OA3
45	A8	301	CDL	CA3-OA5-PA1-OA4
45	A8	301	CDL	CB2-OB2-PB2-OB3
45	A8	301	CDL	CB2-OB2-PB2-OB4
45	A8	301	CDL	CB2-OB2-PB2-OB5
45	AL	201	CDL	CA2-OA2-PA1-OA3
45	AL	201	CDL	CA3-OA5-PA1-OA3
45	AL	201	CDL	CA3-OA5-PA1-OA4
45	AL	201	CDL	CB3-OB5-PB2-OB2
45	AL	202	CDL	CA3-OA5-PA1-OA4
45	AL	202	CDL	CB3-OB5-PB2-OB2
45	AL	202	CDL	CB3-OB5-PB2-OB3
45	AL	202	CDL	CB3-OB5-PB2-OB4
45	B4	202	CDL	CA2-OA2-PA1-OA3
45	B4	202	CDL	C1-CB2-OB2-PB2
45	B4	202	CDL	CB3-OB5-PB2-OB3
45	B4	202	CDL	CB3-OB5-PB2-OB4
45	B5	202	CDL	CB2-OB2-PB2-OB3
45	B5	202	CDL	CB3-OB5-PB2-OB2
45	B5	202	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
45	B5	202	CDL	CB3-OB5-PB2-OB4
45	N2	401	CDL	CB2-OB2-PB2-OB5
45	N2	401	CDL	CB3-OB5-PB2-OB3
45	N2	401	CDL	CB3-OB5-PB2-OB4
45	N4	503	CDL	CB2-OB2-PB2-OB3
45	N4	503	CDL	CB3-OB5-PB2-OB3
45	N4	503	CDL	CB3-OB5-PB2-OB4
45	N5	703	CDL	CA2-OA2-PA1-OA3
45	N5	703	CDL	CA3-OA5-PA1-OA3
45	N5	703	CDL	CA3-OA5-PA1-OA4
45	N5	704	CDL	CA3-OA5-PA1-OA2
45	N5	704	CDL	CA3-OA5-PA1-OA3
45	N5	704	CDL	CA3-OA5-PA1-OA4
45	N5	704	CDL	CB2-OB2-PB2-OB3
45	N5	704	CDL	CB3-OB5-PB2-OB3
46	AL	204	PEE	C4-O4P-P-O1P
46	AL	204	PEE	O4P-C4-C5-N
46	B4	201	PEE	O3P-C1-C2-O2
46	B4	201	PEE	C1-O3P-P-O2P
46	B4	201	PEE	C1-O3P-P-O1P
46	N1	404	PEE	C11-C10-O2-C2
46	N1	404	PEE	C2-C1-O3P-P
46	N1	404	PEE	O4P-C4-C5-N
46	N1	405	PEE	C11-C10-O2-C2
46	N1	405	PEE	O4-C10-O2-C2
46	N1	405	PEE	C1-O3P-P-O2P
46	N1	405	PEE	C1-O3P-P-O1P
46	N1	405	PEE	C4-O4P-P-O2P
46	N2	402	PEE	C11-C10-O2-C2
46	N2	402	PEE	O4-C10-O2-C2
46	N5	701	PEE	C37-C38-C39-C40
46	N5	702	PEE	C37-C38-C39-C40
46	N5	705	PEE	C11-C10-O2-C2
46	N5	705	PEE	C1-O3P-P-O2P
46	N5	705	PEE	C1-O3P-P-O4P
46	N5	705	PEE	C4-O4P-P-O2P
46	N5	705	PEE	C4-O4P-P-O1P
46	N5	706	PEE	C11-C10-O2-C2
46	N5	706	PEE	C4-O4P-P-O2P
46	N5	706	PEE	C4-O4P-P-O1P
47	A9	401	NDP	C5D-O5D-PN-O1N
48	AB	201	ZMP	C16-C17-C18-C21

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Mol	Chain	Res	Type	Atoms
48	AB	201	ZMP	C16-C17-C18-C19
48	AB	201	ZMP	C16-C17-C18-C20
48	AB	201	ZMP	O3-C16-C17-C18
48	AB	201	ZMP	N2-C16-C17-C18
48	AB	201	ZMP	O3-C16-C17-O4
48	AB	201	ZMP	N2-C16-C17-O4
48	AB	201	ZMP	C7-C8-C9-C10
48	AC	201	ZMP	N2-C16-C17-O4
48	AC	201	ZMP	S1-C11-C12-N1
48	AC	201	ZMP	C7-C8-C9-C10
50	AL	203	3PE	C1-O11-P-O13
50	AL	203	3PE	O13-C11-C12-N
50	B8	201	3PE	O13-C11-C12-N
50	CA	101	3PE	C1-O11-P-O12
50	CA	101	3PE	C1-O11-P-O14
50	CA	101	3PE	C11-O13-P-O11
50	CA	101	3PE	C11-O13-P-O12
50	CA	101	3PE	C11-O13-P-O14
51	AL	205	PC1	C11-O13-P-O14
51	AL	205	PC1	C11-O13-P-O11
51	AL	205	PC1	C1-O11-P-O14
51	B5	203	PC1	C1-O11-P-O12
51	B5	203	PC1	C1-O11-P-O14
51	B5	203	PC1	C1-O11-P-O13
51	N1	401	PC1	C11-O13-P-O14
51	N1	401	PC1	C11-O13-P-O11
51	N1	401	PC1	C1-O11-P-O12
51	N1	401	PC1	C1-O11-P-O14
51	N1	401	PC1	C1-O11-P-O13
51	N1	402	PC1	C11-O13-P-O12
51	N1	402	PC1	C1-O11-P-O12
51	N1	402	PC1	C1-O11-P-O14
52	AM	201	PLX	O7-C6-C7-C8
52	AM	201	PLX	O7-C6-O6-C4
52	AM	201	PLX	C2-O1-P1-O2
52	AM	201	PLX	C2-O1-P1-O3
52	AM	202	PLX	C25-C24-O8-C5
52	B5	201	PLX	O7-C6-O6-C4
52	B5	201	PLX	C3-O4-P1-O2
52	B5	201	PLX	C2-O1-P1-O4
52	B5	201	PLX	O9-C24-C25-C26
52	CB	201	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
52	CB	201	PLX	O7-C6-O6-C4
52	CB	201	PLX	C3-O4-P1-O2
52	CB	201	PLX	C3-O4-P1-O3
52	CB	201	PLX	C2-O1-P1-O2
52	CB	201	PLX	C2-O1-P1-O3
52	CB	201	PLX	O9-C24-O8-C5
52	N3	201	PLX	O7-C6-C7-C8
52	N3	201	PLX	O7-C6-O6-C4
52	N3	201	PLX	C3-O4-P1-O2
52	N3	201	PLX	N1-C1-C2-O1
52	N3	201	PLX	O9-C24-O8-C5
52	N4	501	PLX	O7-C6-C7-C8
52	N4	501	PLX	C7-C6-O6-C4
52	N4	501	PLX	O7-C6-O6-C4
52	N4	501	PLX	C3-O4-P1-O1
52	N4	501	PLX	C3-O4-P1-O2
52	N4	501	PLX	C3-O4-P1-O3
52	N4	501	PLX	N1-C1-C2-O1
52	N4	502	PLX	O7-C6-O6-C4
52	N4	502	PLX	C3-O4-P1-O2
52	N4	502	PLX	C3-O4-P1-O3
52	N4	502	PLX	C2-O1-P1-O2
52	N4	502	PLX	C25-C24-O8-C5
53	N1	403	XEW	N4-C4-N-C3
53	N1	403	XEW	N1-C4-N-C3
58	V1	502	FMN	C5'-O5'-P-O2P
58	V1	502	FMN	C5'-O5'-P-O3P
46	N5	706	PEE	O5-C30-O3-C3
46	N5	706	PEE	C31-C30-O3-C3
46	A3	201	PEE	O5-C30-O3-C3
46	AL	204	PEE	O5-C30-O3-C3
46	N5	705	PEE	O5-C30-O3-C3
46	N1	404	PEE	O4-C10-O2-C2
46	N5	705	PEE	O4-C10-O2-C2
46	A3	201	PEE	C31-C30-O3-C3
46	AL	204	PEE	C31-C30-O3-C3
46	N5	702	PEE	C31-C30-O3-C3
46	N5	705	PEE	C31-C30-O3-C3
46	A3	201	PEE	C17-C18-C19-C20
46	N2	402	PEE	C37-C38-C39-C40
46	N5	705	PEE	C17-C18-C19-C20
46	N5	706	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
46	N5	702	PEE	O5-C30-O3-C3
46	N5	706	PEE	C22-C23-C24-C25
48	AB	201	ZMP	C1-C22-C23-C24
52	N4	501	PLX	O4-C3-C4-O6
45	N5	703	CDL	CB5-C51-C52-C53
50	AL	203	3PE	O21-C2-C3-O31
46	N1	404	PEE	C11-C12-C13-C14
46	N2	402	PEE	C10-C11-C12-C13
45	S8	303	CDL	C82-C83-C84-C85
45	AL	201	CDL	CA7-C31-C32-C33
46	B4	201	PEE	C10-C11-C12-C13
46	B4	201	PEE	C30-C31-C32-C33
45	B5	202	CDL	CA7-C31-C32-C33
46	N5	706	PEE	C10-C11-C12-C13
46	N5	702	PEE	C10-C11-C12-C13
45	4L	201	CDL	CA2-OA2-PA1-OA5
45	4L	201	CDL	CB2-OB2-PB2-OB5
45	A7	201	CDL	CA3-OA5-PA1-OA2
45	A7	201	CDL	CB2-OB2-PB2-OB5
45	A8	301	CDL	CB3-OB5-PB2-OB2
45	AL	201	CDL	CA3-OA5-PA1-OA2
45	AL	202	CDL	CA3-OA5-PA1-OA2
45	B4	202	CDL	CB2-OB2-PB2-OB5
45	B4	202	CDL	CB3-OB5-PB2-OB2
45	B5	202	CDL	CA3-OA5-PA1-OA2
45	N2	401	CDL	CA2-OA2-PA1-OA5
45	N2	401	CDL	CB3-OB5-PB2-OB2
45	N4	503	CDL	CA2-OA2-PA1-OA5
45	N4	503	CDL	CB3-OB5-PB2-OB2
45	N5	703	CDL	CA2-OA2-PA1-OA5
45	N5	703	CDL	CA3-OA5-PA1-OA2
45	N5	703	CDL	CB2-OB2-PB2-OB5
45	N5	703	CDL	CB3-OB5-PB2-OB2
45	N5	704	CDL	CA2-OA2-PA1-OA5
45	N5	704	CDL	CB2-OB2-PB2-OB5
45	N5	704	CDL	CB3-OB5-PB2-OB2
46	A3	201	PEE	C1-O3P-P-O4P
46	B4	201	PEE	C1-O3P-P-O4P
46	N1	404	PEE	C1-O3P-P-O4P
46	N1	405	PEE	C1-O3P-P-O4P
46	N1	405	PEE	C4-O4P-P-O3P
46	N5	701	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
46	N5	705	PEE	C4-O4P-P-O3P
50	B8	201	3PE	C11-O13-P-O11
50	CA	101	3PE	C1-O11-P-O13
51	AL	205	PC1	C1-O11-P-O13
51	B5	203	PC1	C11-O13-P-O11
51	B7	201	PC1	C1-O11-P-O13
51	N1	402	PC1	C11-O13-P-O11
51	N1	402	PC1	C1-O11-P-O13
51	S7	302	PC1	C11-O13-P-O11
52	AM	201	PLX	C2-O1-P1-O4
52	B5	201	PLX	C3-O4-P1-O1
52	CB	201	PLX	C3-O4-P1-O1
52	CB	201	PLX	C2-O1-P1-O4
52	N3	201	PLX	C3-O4-P1-O1
52	N4	501	PLX	C2-O1-P1-O4
52	N4	502	PLX	C3-O4-P1-O1
46	A3	201	PEE	C10-C11-C12-C13
46	N5	706	PEE	C30-C31-C32-C33
51	S7	302	PC1	C11-C12-N-C13
45	N5	703	CDL	C51-C52-C53-C54
48	AC	201	ZMP	C14-C15-N2-C16
48	AB	201	ZMP	C2-C3-C4-C5
52	B5	201	PLX	C13-C14-C15-C16
46	N1	405	PEE	C21-C22-C23-C24
46	N5	705	PEE	C22-C23-C24-C25
46	N5	706	PEE	C21-C22-C23-C24
48	AC	201	ZMP	C1-C2-C3-C4
52	AM	202	PLX	C14-C15-C16-C17
46	AL	204	PEE	C17-C18-C19-C20
46	N1	404	PEE	C17-C18-C19-C20
52	N4	501	PLX	C11-C10-C9-C8
46	N5	701	PEE	C14-C15-C16-C17
51	B5	203	PC1	C2A-C2B-C2C-C2D
46	B4	201	PEE	C11-C12-C13-C14
46	N1	404	PEE	C12-C13-C14-C15
46	AL	204	PEE	C14-C15-C16-C17
46	N1	404	PEE	C21-C22-C23-C24
46	N5	702	PEE	C12-C13-C14-C15
46	N1	405	PEE	C10-C11-C12-C13
46	N5	701	PEE	C33-C34-C35-C36
51	S7	302	PC1	C23-C24-C25-C26
52	N3	201	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
45	S8	303	CDL	C76-C77-C78-C79
52	N4	501	PLX	C33-C34-C35-C36
46	N5	702	PEE	O4-C10-O2-C2
46	N5	702	PEE	C11-C10-O2-C2
46	A3	201	PEE	C11-C12-C13-C14
46	N5	702	PEE	C32-C33-C34-C35
48	AB	201	ZMP	C6-C7-C8-C9
46	N2	402	PEE	C35-C36-C37-C38
46	N5	705	PEE	C39-C40-C41-C42
46	N5	702	PEE	C11-C12-C13-C14
52	AM	202	PLX	C11-C10-C9-C8
52	N4	502	PLX	C31-C32-C33-C34
46	A3	201	PEE	C33-C34-C35-C36
46	N1	405	PEE	C22-C23-C24-C25
46	N2	402	PEE	O4P-C4-C5-N
46	N5	702	PEE	O4P-C4-C5-N
46	N5	706	PEE	O4P-C4-C5-N
46	N1	404	PEE	C41-C42-C43-C44
50	CA	101	3PE	C36-C37-C38-C39
52	CB	201	PLX	C9-C10-C11-C12
46	N5	701	PEE	C21-C22-C23-C24
45	N5	704	CDL	C18-C19-C20-C21
46	B4	201	PEE	C12-C13-C14-C15
46	N2	402	PEE	C12-C13-C14-C15
46	N5	701	PEE	C12-C13-C14-C15
52	AM	202	PLX	C16-C17-C18-C19
46	N1	405	PEE	C17-C18-C19-C20
48	AC	201	ZMP	C2-C3-C4-C5
53	S2	501	XEW	N4-C4-N-C3
46	N5	705	PEE	C2-C3-O3-C30
50	CA	101	3PE	C2C-C2D-C2E-C2F
52	AM	201	PLX	O9-C24-C25-C26
53	S2	501	XEW	N3-C5-N2-C6
52	AM	201	PLX	C29-C30-C31-C32
46	AL	204	PEE	C35-C36-C37-C38
46	B4	201	PEE	C19-C20-C21-C22
46	N1	404	PEE	C35-C36-C37-C38
46	N5	705	PEE	C35-C36-C37-C38
46	N1	405	PEE	C41-C42-C43-C44
46	N5	705	PEE	C33-C34-C35-C36
45	AL	202	CDL	C36-C37-C38-C39
45	N4	503	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
46	A3	201	PEE	C21-C22-C23-C24
46	N5	705	PEE	C12-C13-C14-C15
52	AM	201	PLX	C30-C31-C32-C33
46	N5	706	PEE	C33-C34-C35-C36
46	A3	201	PEE	C35-C36-C37-C38
46	B4	201	PEE	C35-C36-C37-C38
46	N5	701	PEE	C35-C36-C37-C38
46	N1	404	PEE	C14-C15-C16-C17
46	N2	402	PEE	C14-C15-C16-C17
46	N1	404	PEE	C10-C11-C12-C13
51	S7	302	PC1	C21-C22-C23-C24
48	AC	201	ZMP	C22-C23-C24-C25
51	N1	402	PC1	C39-C3A-C3B-C3C
46	N1	404	PEE	C33-C34-C35-C36
48	AB	201	ZMP	C13-C14-C15-N2
46	N2	402	PEE	C43-C44-C45-C46
45	B5	202	CDL	C13-C14-C15-C16
46	N1	405	PEE	C43-C44-C45-C46
52	AM	202	PLX	C15-C16-C17-C18
45	N5	703	CDL	OA6-CA4-CA6-OA8
51	B7	201	PC1	O21-C2-C3-O31
45	N5	704	CDL	C13-C14-C15-C16
51	S7	302	PC1	C11-C12-N-C14
51	S7	302	PC1	C11-C12-N-C15
52	AM	202	PLX	C10-C11-C12-C13
46	N5	705	PEE	C15-C16-C17-C18
45	S8	303	CDL	CA5-C11-C12-C13
46	AL	204	PEE	C11-C12-C13-C14
46	B4	201	PEE	C17-C18-C19-C20
52	N4	502	PLX	C17-C18-C19-C20
45	B4	202	CDL	CA2-OA2-PA1-OA5
46	N5	706	PEE	C4-O4P-P-O3P
52	N4	502	PLX	C2-O1-P1-O4
46	B4	201	PEE	C22-C23-C24-C25
46	N5	702	PEE	C30-C31-C32-C33
45	N2	401	CDL	OA5-CA3-CA4-CA6
46	A3	201	PEE	C32-C33-C34-C35
51	B7	201	PC1	C3A-C3B-C3C-C3D
46	A3	201	PEE	C19-C20-C21-C22
45	N2	401	CDL	CA5-C11-C12-C13
46	N1	404	PEE	C43-C44-C45-C46
48	AC	201	ZMP	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
46	N5	701	PEE	C11-C12-C13-C14
51	B5	203	PC1	C11-C12-N-C15
45	AL	201	CDL	CB3-CB4-CB6-OB8
45	N5	703	CDL	CA3-CA4-CA6-OA8
45	N5	703	CDL	CB3-CB4-CB6-OB8
46	AL	204	PEE	C1-C2-C3-O3
50	AL	203	3PE	C1-C2-C3-O31
46	N1	404	PEE	C44-C45-C46-C47
50	CA	101	3PE	C29-C2A-C2B-C2C
45	N5	704	CDL	C12-C11-CA5-OA6
46	A3	201	PEE	C22-C23-C24-C25
52	AM	202	PLX	O8-C24-C25-C26
52	N4	501	PLX	O8-C24-C25-C26
48	AC	201	ZMP	O3-C16-C17-O4
46	N5	701	PEE	C32-C33-C34-C35
46	N5	706	PEE	C18-C19-C20-C21
46	N1	404	PEE	C39-C40-C41-C42
46	N5	706	PEE	C19-C20-C21-C22
51	B5	203	PC1	C37-C38-C39-C3A
46	N1	404	PEE	C1-C2-O2-C10
45	S8	303	CDL	CA4-CA3-OA5-PA1
58	V1	502	FMN	C5'-O5'-P-O1P
45	A8	301	CDL	C55-C56-C57-C58
52	AM	202	PLX	C25-C26-C27-C28
46	N1	405	PEE	C31-C30-O3-C3
52	AM	202	PLX	O4-C3-C4-O6
46	N5	706	PEE	C37-C38-C39-C40
46	N5	706	PEE	C12-C13-C14-C15
45	N5	704	CDL	OB6-CB4-CB6-OB8
46	N1	404	PEE	O2-C2-C3-O3
52	AM	201	PLX	C35-C36-C37-C38
48	AB	201	ZMP	O4-C17-C18-C19
48	AB	201	ZMP	O4-C17-C18-C20
45	A8	301	CDL	C53-C54-C55-C56
52	CB	201	PLX	C32-C33-C34-C35
45	B5	202	CDL	OB5-CB3-CB4-CB6
45	N5	703	CDL	OB5-CB3-CB4-CB6
46	AL	204	PEE	O3P-C1-C2-C3
46	B4	201	PEE	O3P-C1-C2-C3
46	N5	702	PEE	O3P-C1-C2-C3
52	AM	201	PLX	O4-C3-C4-C5
52	N4	501	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
46	N5	701	PEE	C30-C31-C32-C33
45	A8	301	CDL	C33-C34-C35-C36
45	A7	201	CDL	CA4-CA3-OA5-PA1
48	AB	201	ZMP	S1-C11-C12-N1
46	N2	402	PEE	C44-C45-C46-C47
46	N5	701	PEE	C22-C23-C24-C25
46	AL	204	PEE	C13-C14-C15-C16
45	N5	704	CDL	CB3-CB4-CB6-OB8
46	N1	404	PEE	C1-C2-C3-O3
52	AM	201	PLX	C3-C4-C5-O8
52	N4	501	PLX	C3-C4-C5-O8
52	N4	502	PLX	C3-C4-C5-O8
52	N3	201	PLX	C11-C10-C9-C8
46	N1	404	PEE	C37-C38-C39-C40
46	N1	405	PEE	C37-C38-C39-C40
52	N4	501	PLX	C25-C26-C27-C28
51	B5	203	PC1	C11-C12-N-C14
45	S8	303	CDL	CA2-OA2-PA1-OA5
52	AM	201	PLX	C3-O4-P1-O1
52	B5	201	PLX	C5-C4-O6-C6
52	N4	501	PLX	O9-C24-C25-C26
45	AL	201	CDL	OA5-CA3-CA4-OA6
45	N2	401	CDL	OB5-CB3-CB4-OB6
45	N4	503	CDL	OB5-CB3-CB4-OB6
46	N1	405	PEE	C35-C36-C37-C38
46	N5	702	PEE	C35-C36-C37-C38
46	N5	705	PEE	C19-C20-C21-C22
46	N1	405	PEE	O5-C30-O3-C3
46	AL	204	PEE	C33-C34-C35-C36
51	B5	203	PC1	C25-C26-C27-C28
45	AL	201	CDL	OB6-CB4-CB6-OB8
45	N5	703	CDL	OB6-CB4-CB6-OB8
46	AL	204	PEE	O2-C2-C3-O3
51	S7	302	PC1	O21-C2-C3-O31
52	AM	201	PLX	O6-C4-C5-O8
52	N4	502	PLX	O6-C4-C5-O8
51	B7	201	PC1	C38-C39-C3A-C3B
46	N2	402	PEE	C21-C22-C23-C24
52	CB	201	PLX	C33-C34-C35-C36
52	CB	201	PLX	C34-C35-C36-C37
45	4L	201	CDL	CA4-CA3-OA5-PA1
45	N2	401	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
45	N4	503	CDL	CB4-CB3-OB5-PB2
46	N5	702	PEE	C2-C1-O3P-P
50	CA	101	3PE	C2-C1-O11-P
52	N4	501	PLX	C4-C3-O4-P1
52	N4	502	PLX	C4-C3-O4-P1
46	B4	201	PEE	C14-C15-C16-C17
46	AL	204	PEE	C22-C23-C24-C25
45	4L	201	CDL	C13-C14-C15-C16
52	N4	501	PLX	C26-C27-C28-C29
47	A9	401	NDP	PN-O3-PA-O5B
45	N2	401	CDL	C73-C74-C75-C76
52	AM	201	PLX	O8-C24-C25-C26
52	N3	201	PLX	O6-C6-C7-C8
52	N4	501	PLX	O6-C6-C7-C8
45	AL	202	CDL	OB5-CB3-CB4-CB6
45	N4	503	CDL	OB5-CB3-CB4-CB6
45	A7	201	CDL	CA7-C31-C32-C33
45	S8	303	CDL	C32-C33-C34-C35
45	S8	303	CDL	C78-C79-C80-C81
46	N5	702	PEE	C1-C2-O2-C10
48	AC	201	ZMP	C9-C10-S1-C11
52	B5	201	PLX	C27-C28-C29-C30
51	N1	402	PC1	C3A-C3B-C3C-C3D
45	A8	301	CDL	CB3-CB4-CB6-OB8
45	B4	202	CDL	CA3-CA4-CA6-OA8
45	N2	401	CDL	CA4-CA3-OA5-PA1
46	N1	405	PEE	C1-C2-C3-O3
46	N2	402	PEE	C1-C2-C3-O3
52	AM	202	PLX	C3-C4-C5-O8
52	CB	201	PLX	C7-C6-O6-C4
53	S2	501	XEW	N-C4-N1-C5
52	AM	201	PLX	C16-C17-C18-C19
45	B5	202	CDL	OB5-CB3-CB4-OB6
45	N2	401	CDL	OA5-CA3-CA4-OA6
45	S8	303	CDL	OB5-CB3-CB4-OB6
46	N5	701	PEE	O3P-C1-C2-O2
46	N5	702	PEE	O3P-C1-C2-O2
45	AL	201	CDL	C72-C73-C74-C75
48	AB	201	ZMP	C3-C4-C5-C6
46	N5	706	PEE	C11-C12-C13-C14
45	A8	301	CDL	OB6-CB4-CB6-OB8
46	N1	405	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
46	N5	702	PEE	O2-C2-C3-O3
46	N5	702	PEE	O3-C30-C31-C32
47	A9	401	NDP	C5D-O5D-PN-O3
46	N5	705	PEE	C21-C22-C23-C24
52	N4	501	PLX	C29-C30-C31-C32
53	S2	501	XEW	N4-C4-N1-C5
45	A7	201	CDL	C13-C14-C15-C16
45	B5	202	CDL	CB2-OB2-PB2-OB5
45	N4	503	CDL	CB2-OB2-PB2-OB5
52	N4	502	PLX	C10-C11-C12-C13
45	AL	202	CDL	CB4-CB3-OB5-PB2
45	N5	703	CDL	CB4-CB3-OB5-PB2
45	4L	201	CDL	CB2-OB2-PB2-OB4
45	A7	201	CDL	CB2-OB2-PB2-OB4
45	A8	301	CDL	CB3-OB5-PB2-OB3
45	A8	301	CDL	CB3-OB5-PB2-OB4
45	AL	201	CDL	CB3-OB5-PB2-OB3
45	AL	202	CDL	CA3-OA5-PA1-OA3
45	B4	202	CDL	CA2-OA2-PA1-OA4
45	B4	202	CDL	CB2-OB2-PB2-OB3
45	B5	202	CDL	CA3-OA5-PA1-OA3
45	B5	202	CDL	CB2-OB2-PB2-OB4
45	N2	401	CDL	CA2-OA2-PA1-OA3
45	N2	401	CDL	CB2-OB2-PB2-OB3
45	N4	503	CDL	CA2-OA2-PA1-OA3
45	N4	503	CDL	CB2-OB2-PB2-OB4
45	N5	703	CDL	CA2-OA2-PA1-OA4
45	N5	703	CDL	CB2-OB2-PB2-OB3
45	N5	703	CDL	CB3-OB5-PB2-OB3
45	N5	703	CDL	CB3-OB5-PB2-OB4
45	N5	704	CDL	CA2-OA2-PA1-OA3
45	N5	704	CDL	CB2-OB2-PB2-OB4
45	N5	704	CDL	CB3-OB5-PB2-OB4
45	S8	303	CDL	CA2-OA2-PA1-OA4
46	A3	201	PEE	C1-O3P-P-O1P
46	N1	404	PEE	C1-O3P-P-O1P
46	N1	405	PEE	C4-O4P-P-O1P
46	N2	402	PEE	C1-O3P-P-O1P
46	N5	701	PEE	C4-O4P-P-O2P
46	N5	702	PEE	C4-O4P-P-O1P
46	N5	705	PEE	C1-O3P-P-O1P
47	A9	401	NDP	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
50	AL	203	3PE	C1-O11-P-O12
50	B8	201	3PE	C11-O13-P-O14
51	AL	205	PC1	C1-O11-P-O12
51	B5	203	PC1	C11-O13-P-O12
51	B5	203	PC1	C11-O13-P-O14
51	B7	201	PC1	C1-O11-P-O14
51	N1	402	PC1	C11-O13-P-O14
51	S7	302	PC1	C11-O13-P-O14
52	B5	201	PLX	C3-O4-P1-O3
52	N3	201	PLX	C3-O4-P1-O3
52	N4	501	PLX	C2-O1-P1-O3
45	N4	503	CDL	C21-C22-C23-C24
45	AL	201	CDL	OA5-CA3-CA4-CA6
45	N2	401	CDL	OB5-CB3-CB4-CB6
45	S8	303	CDL	OB5-CB3-CB4-CB6
45	AL	201	CDL	C13-C14-C15-C16
46	AL	204	PEE	C5-C4-O4P-P
46	N1	404	PEE	C5-C4-O4P-P
50	CA	101	3PE	C12-C11-O13-P
52	AM	201	PLX	C1-C2-O1-P1
52	AM	201	PLX	C25-C24-O8-C5
52	B5	201	PLX	C1-C2-O1-P1
52	CB	201	PLX	C1-C2-O1-P1
52	N3	201	PLX	C1-C2-O1-P1
52	N4	501	PLX	C1-C2-O1-P1
52	N4	501	PLX	C25-C24-O8-C5
52	CB	201	PLX	C20-C21-C22-C23
46	N1	404	PEE	C19-C20-C21-C22
46	N1	405	PEE	C19-C20-C21-C22
45	AL	202	CDL	OB5-CB3-CB4-OB6
45	N5	703	CDL	OB5-CB3-CB4-OB6
46	AL	204	PEE	O3P-C1-C2-O2
51	B5	203	PC1	O11-C1-C2-O21
52	AM	201	PLX	O4-C3-C4-O6
58	V1	502	FMN	N10-C1'-C2'-O2'
51	N1	401	PC1	C11-C12-N-C14
48	AB	201	ZMP	O4-C17-C18-C21
51	AL	205	PC1	O13-C11-C12-N
51	B7	201	PC1	O13-C11-C12-N
51	B7	201	PC1	C1-C2-C3-O31
51	N1	402	PC1	O13-C11-C12-N
52	AM	201	PLX	N1-C1-C2-O1

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Mol	Chain	Res	Type	Atoms
52	AM	202	PLX	N1-C1-C2-O1
52	B5	201	PLX	N1-C1-C2-O1
52	CB	201	PLX	N1-C1-C2-O1
52	N4	501	PLX	C12-C13-C14-C15
52	N4	502	PLX	C34-C35-C36-C37
52	AM	202	PLX	O6-C4-C5-O8
52	N4	501	PLX	O6-C4-C5-O8
45	AL	202	CDL	C43-C44-C45-C46
50	AL	203	3PE	C28-C29-C2A-C2B
50	B8	201	3PE	O21-C21-C22-C23
51	N1	402	PC1	C2-C1-O11-P
46	N2	402	PEE	C31-C30-O3-C3
45	AL	201	CDL	C36-C37-C38-C39
46	N1	404	PEE	C32-C33-C34-C35
46	N1	405	PEE	C31-C32-C33-C34
52	AM	201	PLX	O6-C6-C7-C8
52	B5	201	PLX	O8-C24-C25-C26
46	N2	402	PEE	O5-C30-O3-C3
52	CB	201	PLX	C16-C17-C18-C19
52	AM	202	PLX	C20-C21-C22-C23
51	B5	203	PC1	C11-C12-N-C13
46	N5	702	PEE	C14-C15-C16-C17
45	4L	201	CDL	C76-C77-C78-C79
53	N1	403	XEW	C2-C3-N-C4
50	CA	101	3PE	C3B-C3C-C3D-C3E
46	N5	701	PEE	O3P-C1-C2-C3
52	AM	202	PLX	O4-C3-C4-C5
52	N4	502	PLX	C32-C33-C34-C35
46	N5	705	PEE	C10-C11-C12-C13
46	N2	402	PEE	C18-C19-C20-C21
46	N5	701	PEE	O4-C10-O2-C2
46	N1	405	PEE	C33-C34-C35-C36
50	AL	203	3PE	C33-C34-C35-C36
51	S7	302	PC1	C3B-C3C-C3D-C3E
50	AL	203	3PE	C3D-C3E-C3F-C3G
52	B5	201	PLX	C30-C31-C32-C33
46	N5	701	PEE	C11-C10-O2-C2
45	AL	201	CDL	CA2-OA2-PA1-OA5
45	AL	201	CDL	CB2-OB2-PB2-OB5
45	AL	202	CDL	CA2-OA2-PA1-OA5
45	N4	503	CDL	CA3-OA5-PA1-OA2
45	S8	303	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
46	AL	204	PEE	C1-O3P-P-O4P
50	B8	201	3PE	C1-O11-P-O13
51	B7	201	PC1	C11-O13-P-O11
51	S7	302	PC1	C1-O11-P-O13
51	N1	401	PC1	C29-C2A-C2B-C2C
45	N4	503	CDL	CB3-CB4-CB6-OB8
45	N5	704	CDL	C22-C23-C24-C25
46	A3	201	PEE	C38-C39-C40-C41
52	N4	502	PLX	C35-C36-C37-C38
45	B4	202	CDL	C72-C71-CB7-OB8
45	N5	704	CDL	C76-C77-C78-C79
52	B5	201	PLX	C28-C29-C30-C31
52	B5	201	PLX	C32-C33-C34-C35
45	AL	201	CDL	CA4-CA3-OA5-PA1
45	B4	202	CDL	CB4-CB3-OB5-PB2
46	N5	705	PEE	C13-C14-C15-C16
47	A9	401	NDP	C2D-C1D-N1N-C6N
46	N1	405	PEE	C16-C17-C18-C19
51	N1	401	PC1	C11-C12-N-C15
51	S7	302	PC1	O11-C1-C2-C3
46	N1	405	PEE	O4P-C4-C5-N
51	B7	201	PC1	C2F-C2G-C2H-C2I
46	AL	204	PEE	C32-C33-C34-C35
45	A7	201	CDL	C15-C16-C17-C18
46	A3	201	PEE	C14-C15-C16-C17
45	N5	704	CDL	C12-C11-CA5-OA7
45	S8	303	CDL	C35-C36-C37-C38
53	N1	403	XEW	C9-C3-N-C4
45	N4	503	CDL	C13-C14-C15-C16
45	AL	201	CDL	C32-C31-CA7-OA8
46	B4	201	PEE	C13-C14-C15-C16
45	B4	202	CDL	C72-C71-CB7-OB9
45	AL	202	CDL	C12-C11-CA5-OA6
46	N2	402	PEE	C31-C32-C33-C34
51	N1	402	PC1	C33-C34-C35-C36
52	N3	201	PLX	C27-C28-C29-C30
47	A9	401	NDP	O4D-C1D-N1N-C6N
45	A8	301	CDL	C12-C13-C14-C15
45	A8	301	CDL	C38-C39-C40-C41
52	N3	201	PLX	C15-C16-C17-C18
46	AL	204	PEE	C21-C22-C23-C24
51	S7	302	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	B5	202	CDL	C73-C74-C75-C76
51	N1	401	PC1	C21-C22-C23-C24
45	AL	201	CDL	CA3-CA4-OA6-CA5
45	AL	202	CDL	CA3-CA4-OA6-CA5
51	B5	203	PC1	C1-C2-O21-C21
51	N1	401	PC1	C11-C12-N-C13
51	N1	402	PC1	C28-C29-C2A-C2B
45	N5	704	CDL	C35-C36-C37-C38
46	N5	702	PEE	C33-C34-C35-C36
51	S7	302	PC1	C34-C35-C36-C37
46	N1	405	PEE	C42-C43-C44-C45
51	N1	401	PC1	C31-C32-C33-C34
47	A9	401	NDP	O4B-C4B-C5B-O5B
49	AK	401	ADP	O4'-C4'-C5'-O5'
45	B5	202	CDL	C15-C16-C17-C18
45	AL	201	CDL	C55-C56-C57-C58
45	B4	202	CDL	C37-C38-C39-C40
52	AM	201	PLX	C18-C19-C20-C21
45	N2	401	CDL	C12-C11-CA5-OA6
46	N5	705	PEE	C31-C32-C33-C34
46	AL	204	PEE	C38-C39-C40-C41
45	A8	301	CDL	C13-C14-C15-C16
48	AC	201	ZMP	C6-C7-C8-C9
48	AC	201	ZMP	O1-C10-S1-C11
46	N5	706	PEE	C31-C32-C33-C34
45	4L	201	CDL	C18-C19-C20-C21
51	S7	302	PC1	O11-C1-C2-O21
45	AL	202	CDL	CA5-C11-C12-C13
46	N1	404	PEE	C40-C41-C42-C43
46	N5	702	PEE	C18-C19-C20-C21
52	AM	201	PLX	C13-C14-C15-C16
52	CB	201	PLX	O8-C24-C25-C26
52	AM	202	PLX	C4-C3-O4-P1
58	V1	502	FMN	C4'-C5'-O5'-P
45	B4	202	CDL	OA6-CA4-CA6-OA8
45	B5	202	CDL	OB6-CB4-CB6-OB8
52	AM	202	PLX	C24-C25-C26-C27
45	AL	201	CDL	C31-C32-C33-C34
45	4L	201	CDL	C14-C15-C16-C17
45	A7	201	CDL	C17-C18-C19-C20
46	A3	201	PEE	C12-C13-C14-C15
50	CA	101	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
52	B5	201	PLX	C31-C32-C33-C34
46	N1	405	PEE	C18-C19-C20-C21
46	N2	402	PEE	C16-C17-C18-C19
46	N5	706	PEE	C16-C17-C18-C19
45	B4	202	CDL	CB6-CB4-OB6-CB5
46	N5	701	PEE	O2-C10-C11-C12
45	N5	703	CDL	C72-C71-CB7-OB8
52	N4	501	PLX	C10-C11-C12-C13
46	N1	404	PEE	C38-C39-C40-C41
46	N5	702	PEE	C36-C37-C38-C39
46	N5	701	PEE	C2-C1-O3P-P
52	N3	201	PLX	C7-C6-O6-C4
45	B4	202	CDL	OB5-CB3-CB4-OB6
46	N5	705	PEE	C37-C38-C39-C40
45	N5	703	CDL	C12-C11-CA5-OA6
51	B5	203	PC1	C32-C33-C34-C35
51	B5	203	PC1	O11-C1-C2-C3
45	AL	202	CDL	C52-C51-CB5-OB6
51	S7	302	PC1	O31-C31-C32-C33
51	N1	402	PC1	O21-C2-C3-O31
52	CB	201	PLX	O6-C4-C5-O8
45	A8	301	CDL	CA5-C11-C12-C13
46	N2	402	PEE	C41-C42-C43-C44
51	AL	205	PC1	O21-C21-C22-C23
45	N4	503	CDL	C57-C58-C59-C60
49	AK	401	ADP	C5'-O5'-PA-O3A
52	AM	202	PLX	O7-C6-C7-C8
45	B5	202	CDL	C52-C51-CB5-OB6
51	N1	401	PC1	C2-C1-O11-P
46	N5	706	PEE	C38-C39-C40-C41
45	AL	201	CDL	C52-C51-CB5-OB6
45	S8	303	CDL	C54-C55-C56-C57
51	B5	203	PC1	C33-C34-C35-C36
52	N4	502	PLX	C9-C10-C11-C12
52	N3	201	PLX	C7-C8-C9-C10
45	4L	201	CDL	C52-C51-CB5-OB6
52	AM	201	PLX	C31-C32-C33-C34
46	A3	201	PEE	C41-C42-C43-C44
45	S8	303	CDL	C72-C73-C74-C75
46	N5	701	PEE	O4-C10-C11-C12
45	AL	201	CDL	C18-C19-C20-C21
51	S7	302	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	B4	201	PEE	O4-C10-O2-C2
45	N5	703	CDL	C33-C34-C35-C36
50	CA	101	3PE	O32-C31-C32-C33
45	AL	201	CDL	CA2-OA2-PA1-OA4
45	N4	503	CDL	CA3-OA5-PA1-OA3
46	N2	402	PEE	C4-O4P-P-O1P
50	AL	203	3PE	C11-O13-P-O14
50	B8	201	3PE	C1-O11-P-O14
52	AM	201	PLX	C3-O4-P1-O2
45	N5	703	CDL	C35-C36-C37-C38
52	B5	201	PLX	C12-C13-C14-C15
45	A7	201	CDL	C35-C36-C37-C38
45	A8	301	CDL	C15-C16-C17-C18
45	N5	703	CDL	C72-C71-CB7-OB9
51	S7	302	PC1	O32-C31-C32-C33
45	A7	201	CDL	C58-C59-C60-C61
51	N1	401	PC1	C3D-C3E-C3F-C3G
45	N4	503	CDL	C18-C19-C20-C21
51	S7	302	PC1	C12-C11-O13-P
52	N3	201	PLX	C25-C24-O8-C5
45	B5	202	CDL	C52-C51-CB5-OB7
45	N5	703	CDL	C12-C11-CA5-OA7
51	AL	205	PC1	O22-C21-C22-C23
52	CB	201	PLX	C24-C25-C26-C27
45	A8	301	CDL	C32-C31-CA7-OA8
45	B5	202	CDL	C32-C31-CA7-OA8
46	AL	204	PEE	O2-C10-C11-C12
45	N5	703	CDL	C37-C38-C39-C40
48	AB	201	ZMP	C22-C23-C24-C25
52	CB	201	PLX	C36-C37-C38-C39
46	B4	201	PEE	O2-C10-C11-C12
51	S7	302	PC1	C2A-C2B-C2C-C2D
45	AL	202	CDL	C52-C51-CB5-OB7
45	N5	703	CDL	C14-C15-C16-C17
52	B5	201	PLX	C15-C16-C17-C18
52	N3	201	PLX	C32-C33-C34-C35
45	N2	401	CDL	C52-C51-CB5-OB6
46	A3	201	PEE	O3-C30-C31-C32
46	N5	706	PEE	O3-C30-C31-C32
51	B5	203	PC1	O21-C21-C22-C23
46	AL	204	PEE	C34-C35-C36-C37
45	4L	201	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
46	AL	204	PEE	O4-C10-C11-C12
45	N4	503	CDL	C72-C71-CB7-OB8
45	B5	202	CDL	C32-C31-CA7-OA9
46	N5	706	PEE	O5-C30-C31-C32
45	AL	201	CDL	C74-C75-C76-C77
52	N4	502	PLX	C24-C25-C26-C27
45	AL	202	CDL	C32-C31-CA7-OA8
45	A7	201	CDL	C72-C71-CB7-OB8
46	N5	705	PEE	O2-C10-C11-C12

There are no ring outliers.

42 monomers are involved in 146 short contacts:

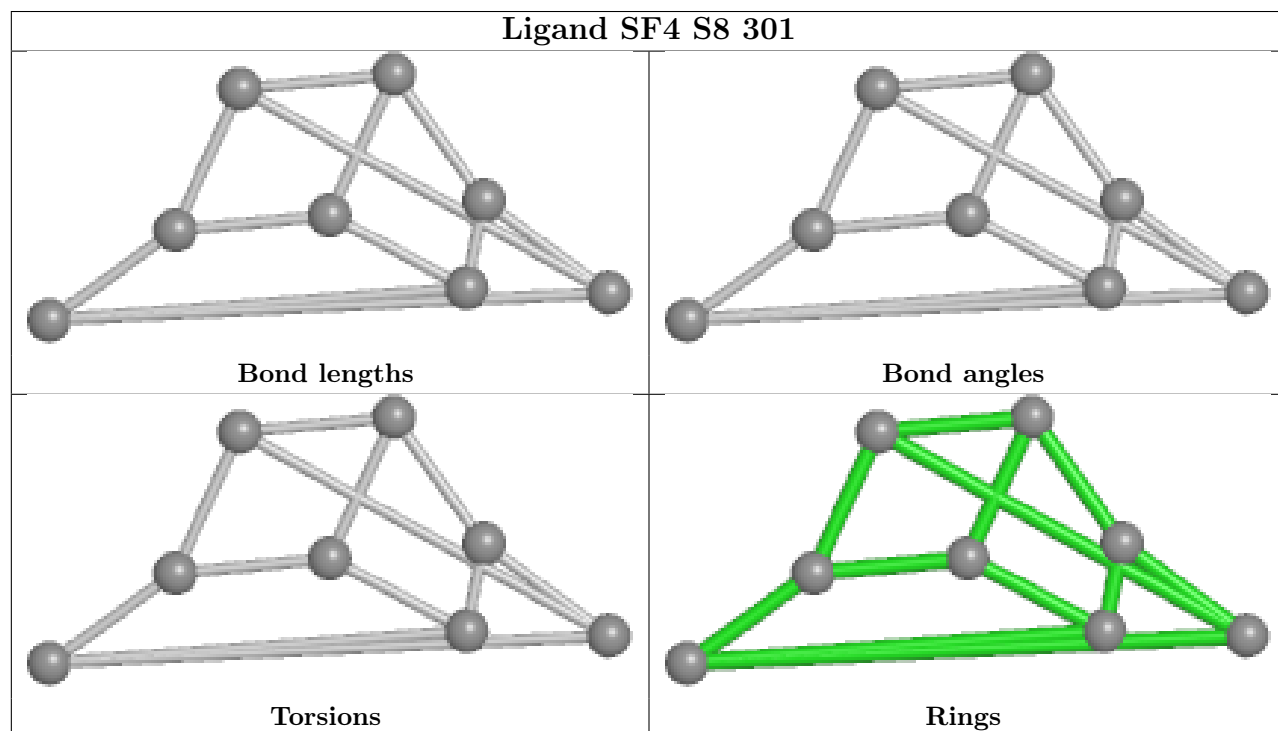
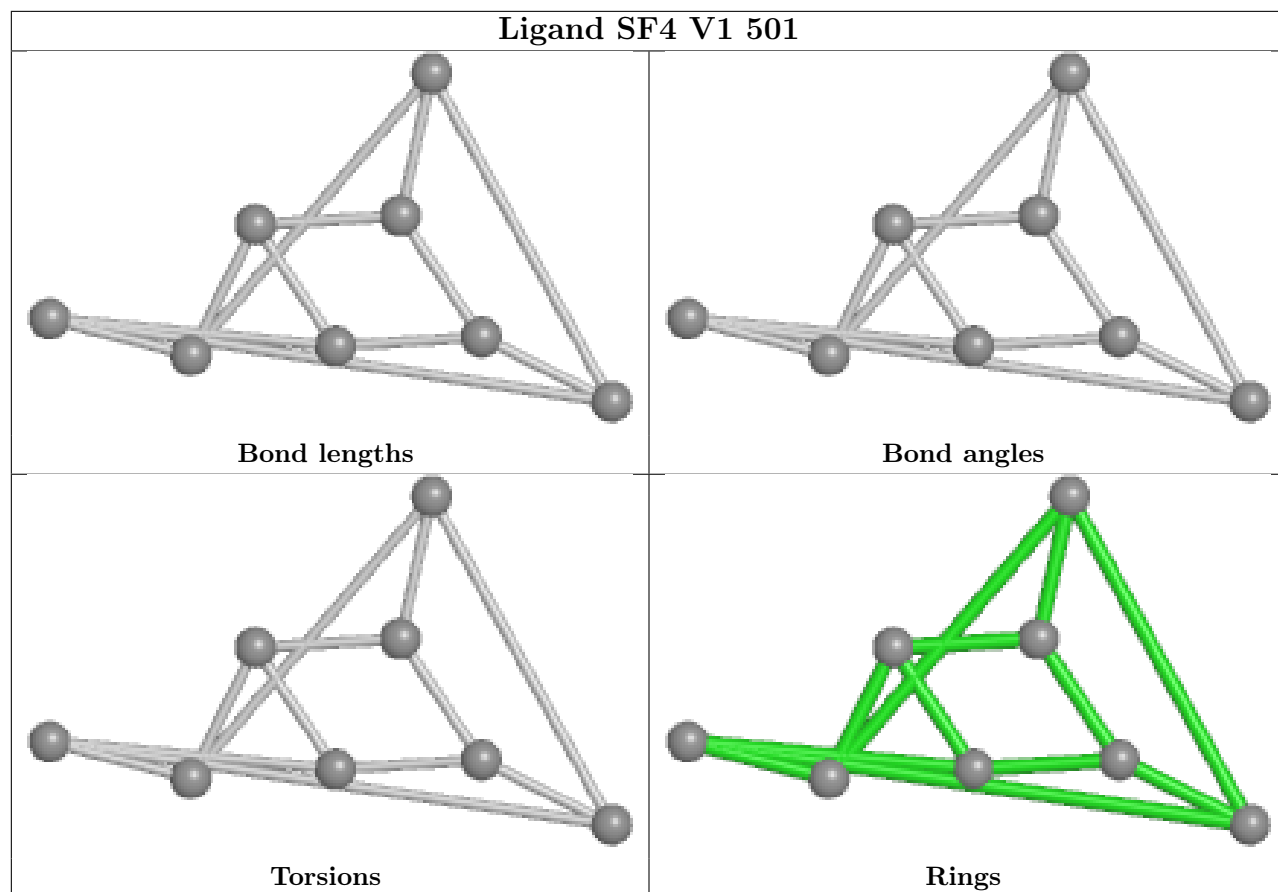
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	S8	301	SF4	1	0
45	B5	202	CDL	2	0
49	AK	401	ADP	3	0
46	AL	204	PEE	1	0
52	CB	201	PLX	5	0
45	B4	202	CDL	1	0
45	N2	401	CDL	4	0
52	B5	201	PLX	2	0
51	B5	203	PC1	4	0
52	N3	201	PLX	3	0
51	N1	401	PC1	6	0
46	A3	201	PEE	3	0
45	N4	503	CDL	3	0
45	S8	303	CDL	11	0
50	AL	203	3PE	3	0
45	AL	201	CDL	11	0
45	N5	703	CDL	8	0
46	N1	405	PEE	9	0
46	N2	402	PEE	1	0
52	AM	201	PLX	7	0
54	S8	302	SF4	1	0
46	N5	702	PEE	3	0
46	N5	706	PEE	9	0
47	A9	401	NDP	1	0
45	A8	301	CDL	5	0
51	S7	302	PC1	2	0
52	N4	502	PLX	6	0
46	N5	701	PEE	1	0

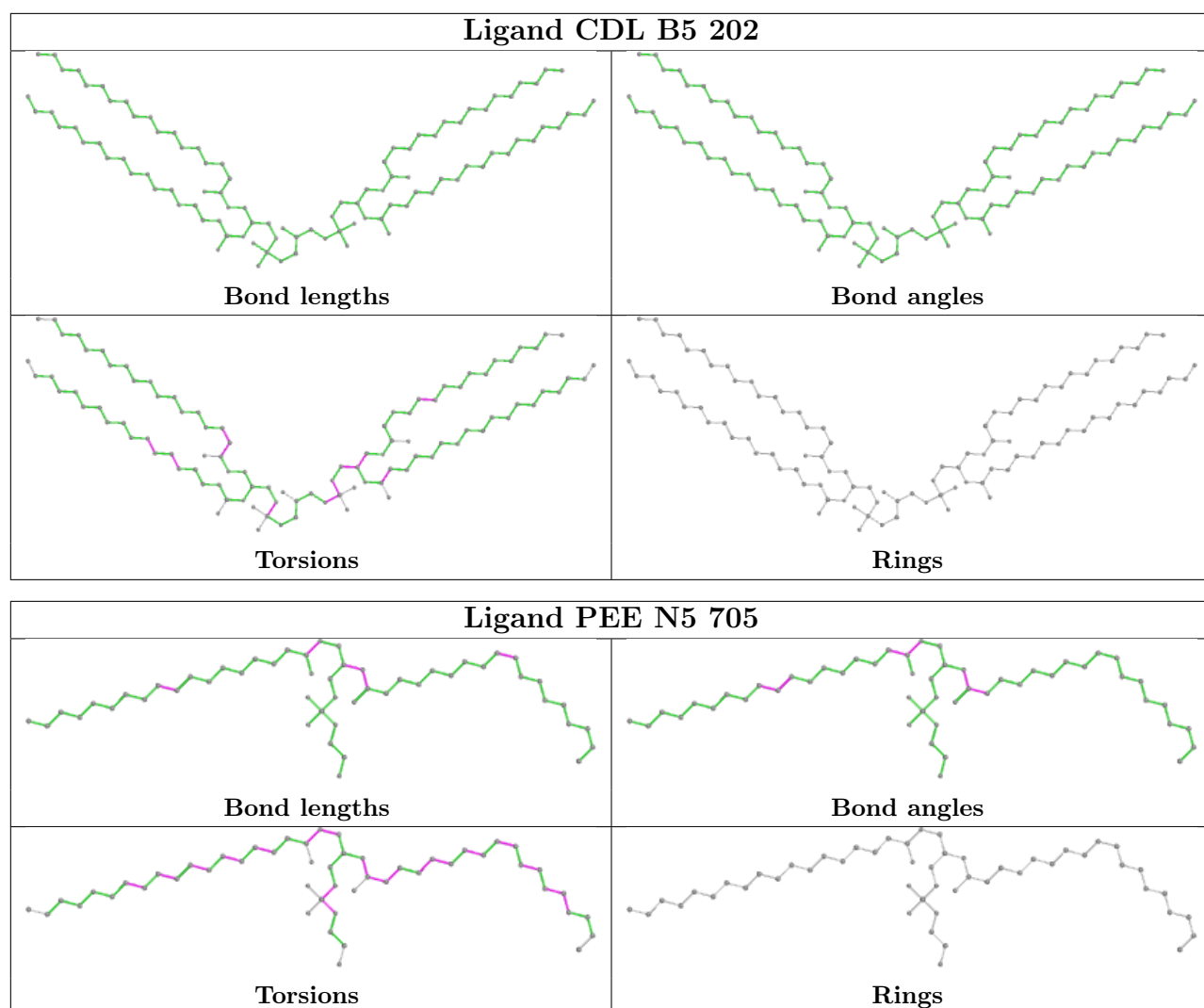
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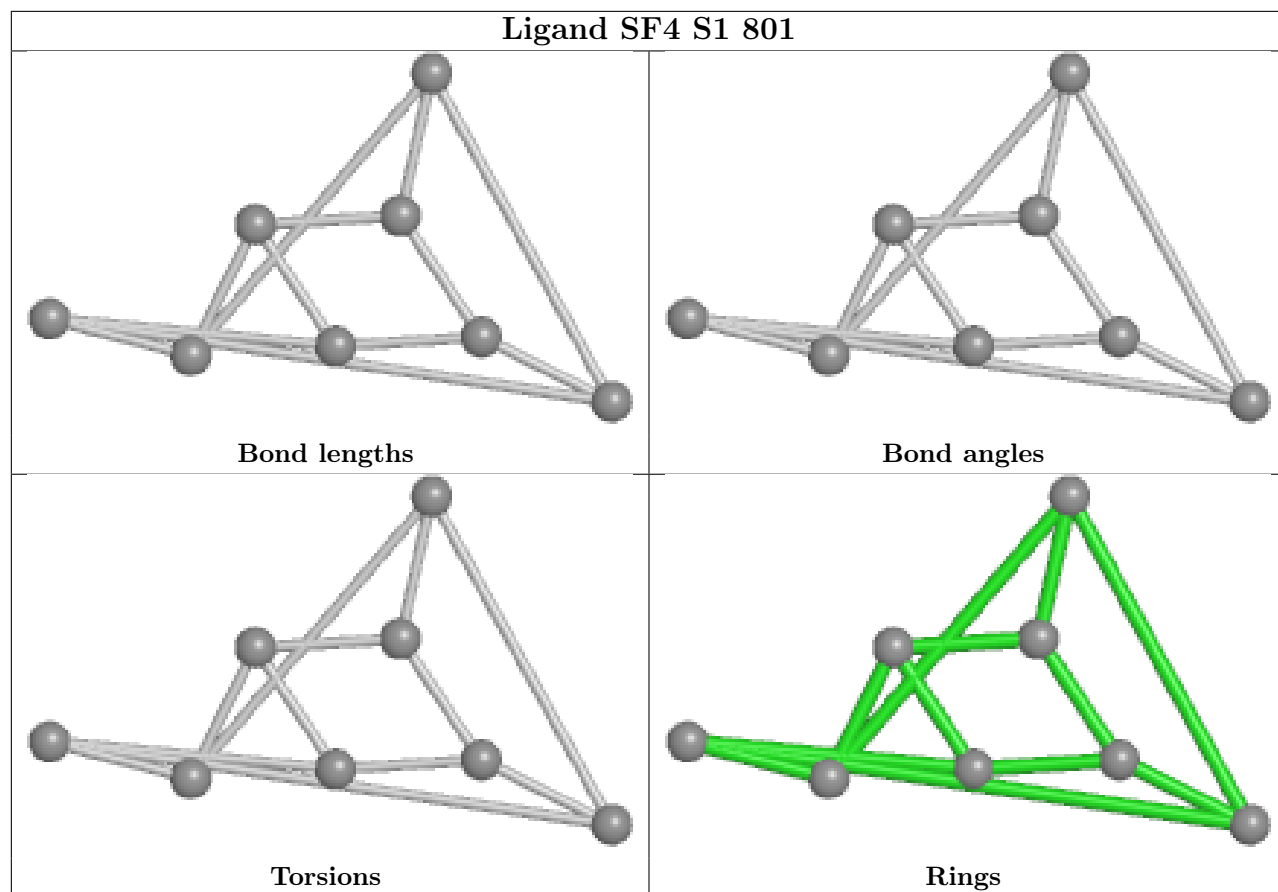
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	N1	402	PC1	3	0
45	AL	202	CDL	7	0
45	A7	201	CDL	3	0
50	CA	101	3PE	3	0
52	N4	501	PLX	2	0
48	AC	201	ZMP	4	0
52	AM	202	PLX	3	0
51	B7	201	PC1	3	0
54	S1	802	SF4	1	0
51	AL	205	PC1	4	0
48	AB	201	ZMP	4	0
45	4L	201	CDL	2	0
45	N5	704	CDL	2	0
46	N1	404	PEE	1	0

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.

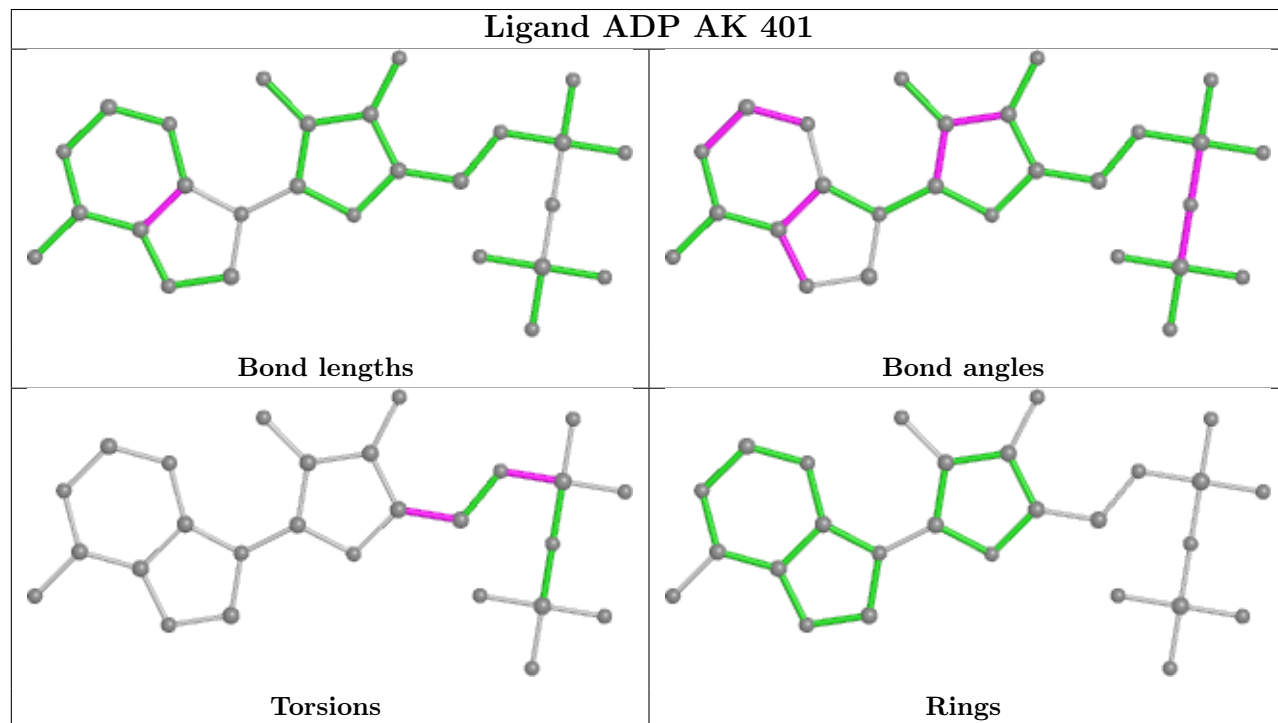




## Ligand SF4 S1 801

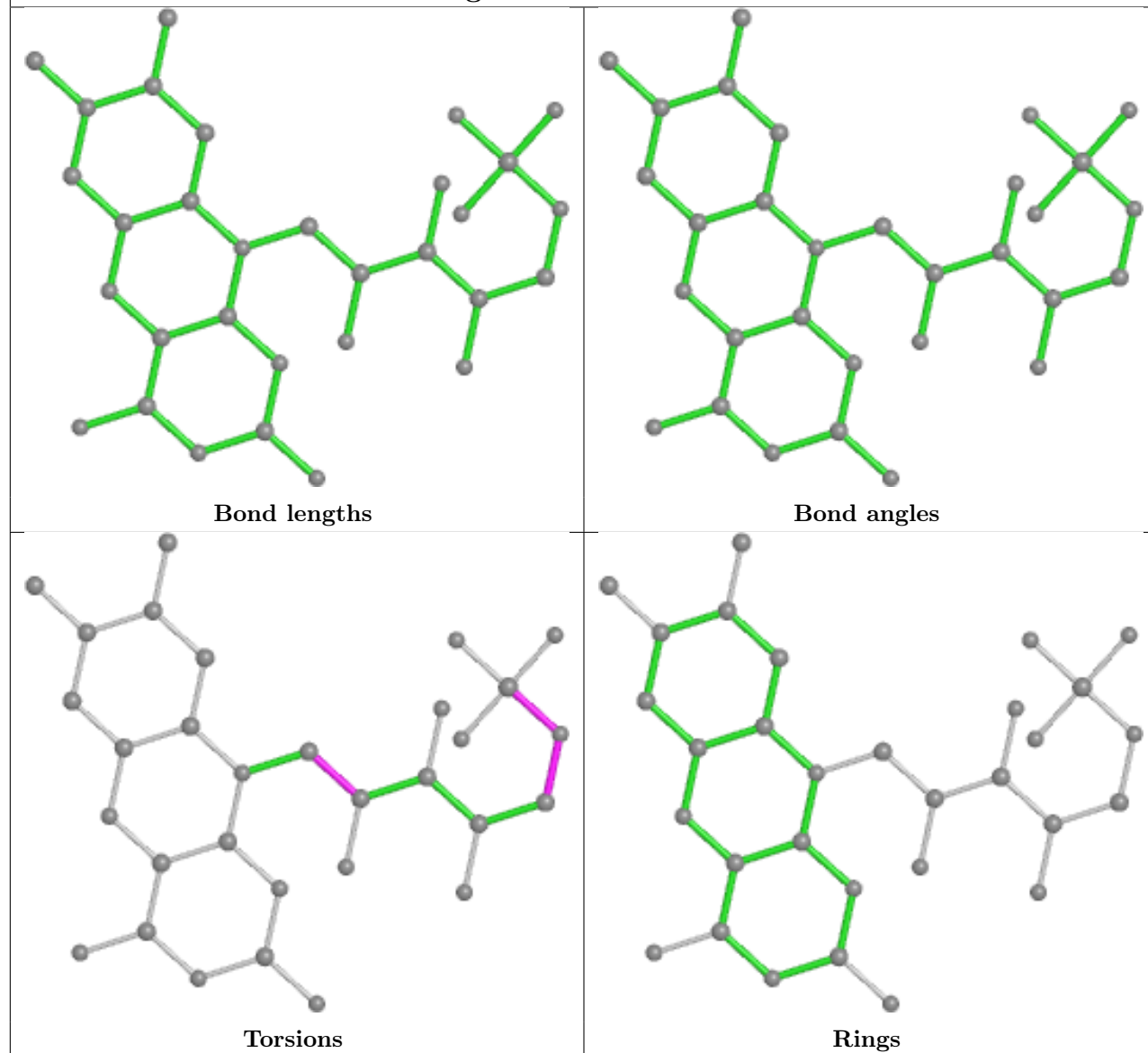


## Ligand ADP AK 401

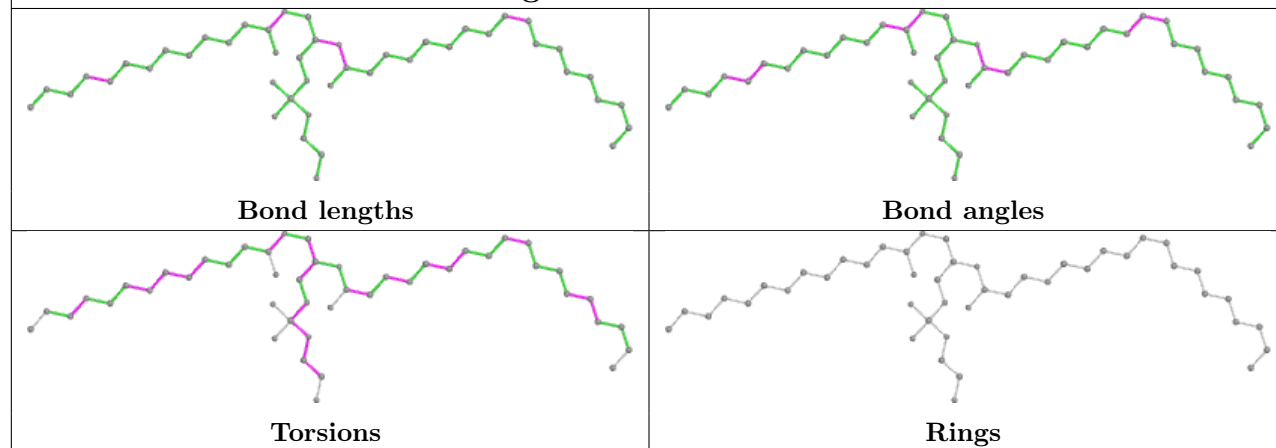


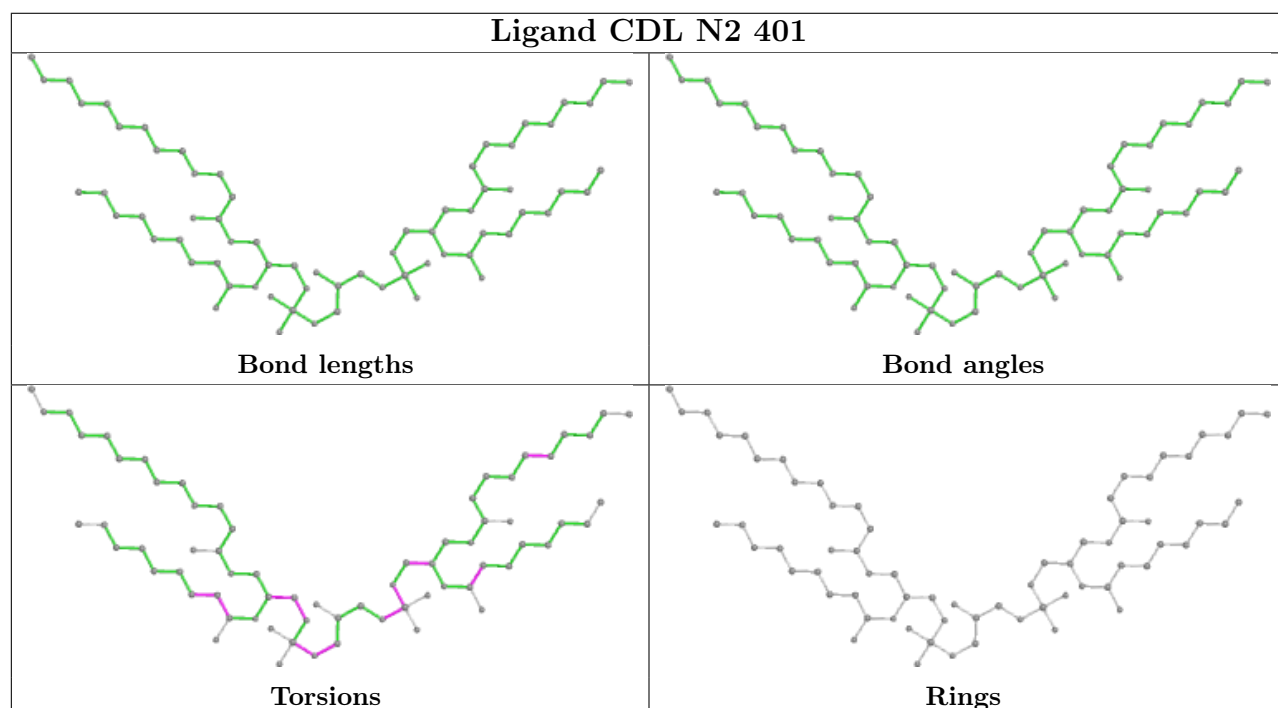
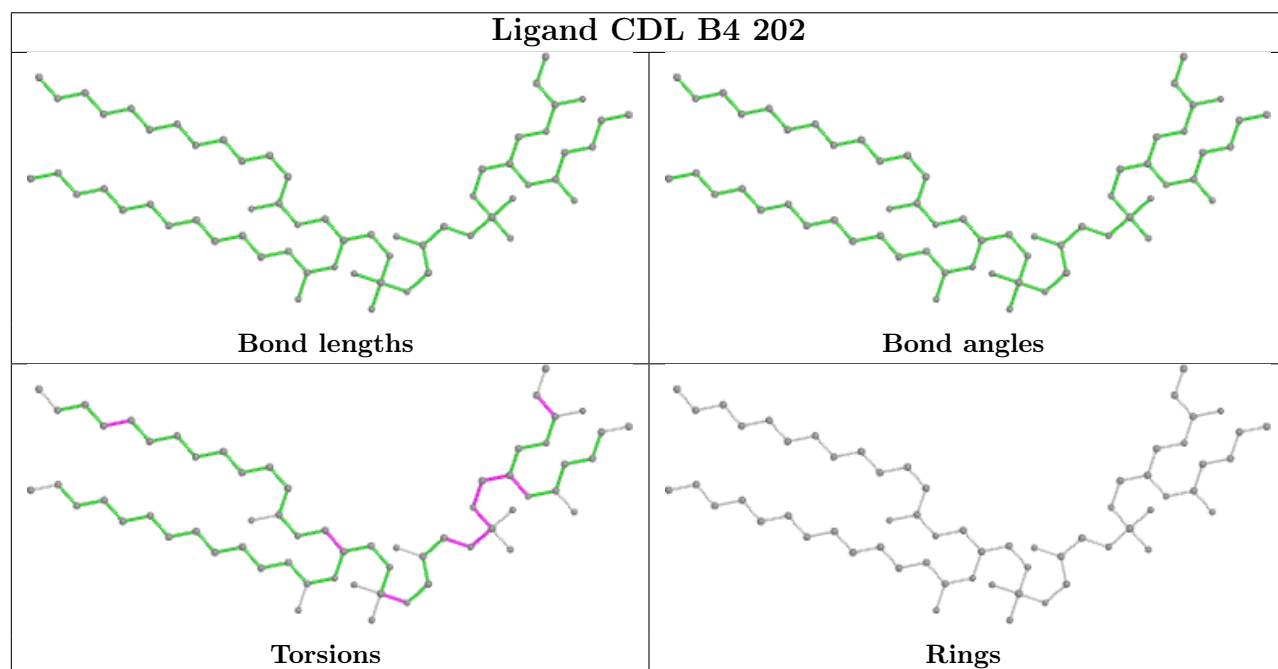
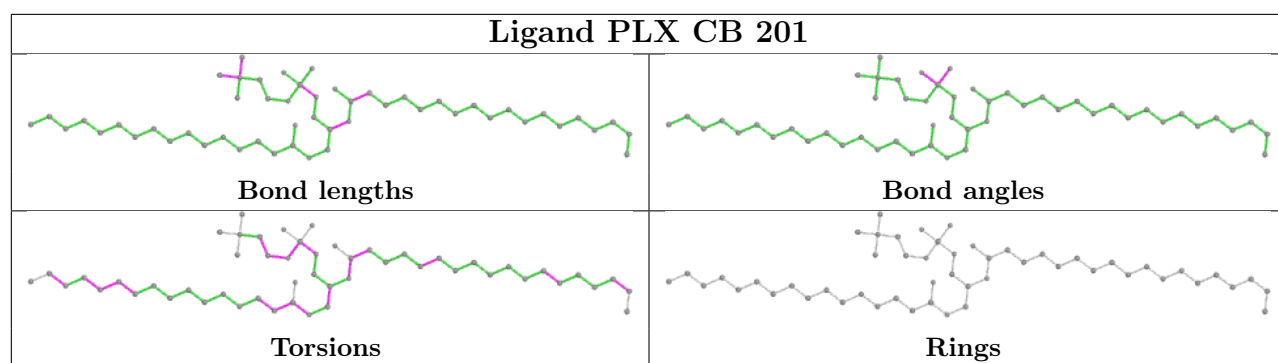


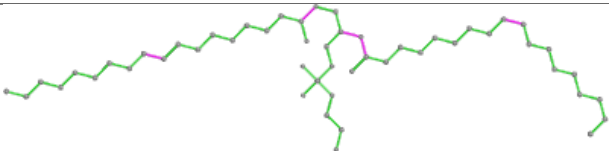
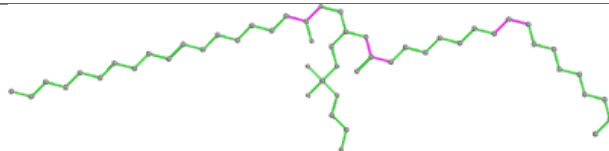
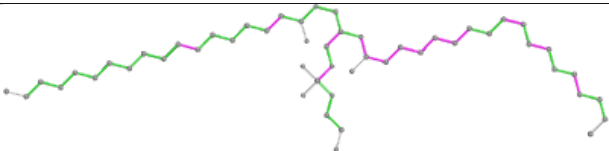
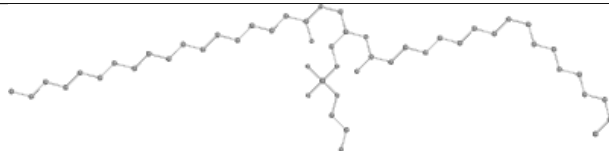
## Ligand FMN V1 502

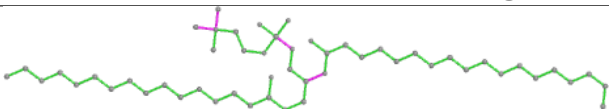
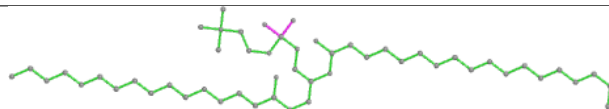
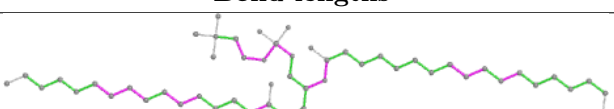
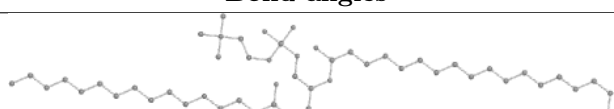


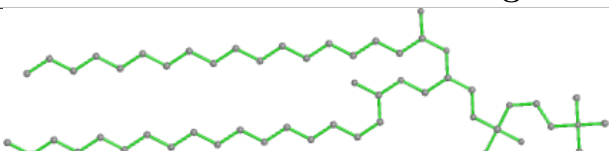
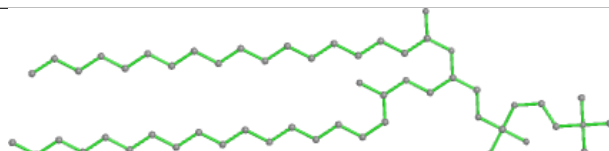
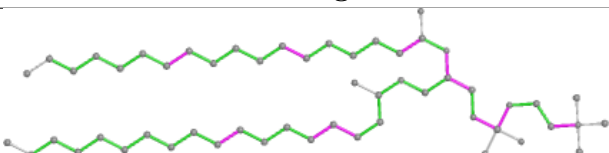
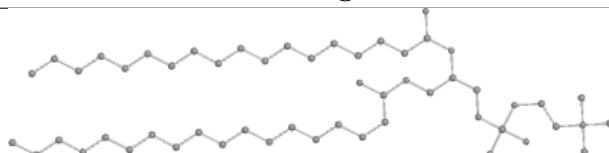
## Ligand PEE AL 204

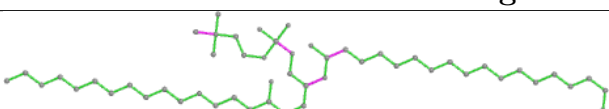
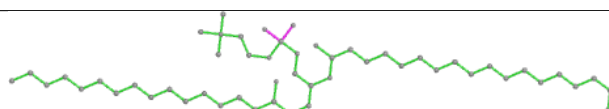
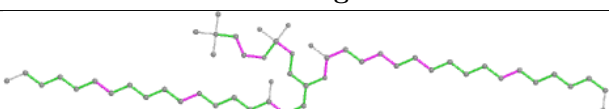
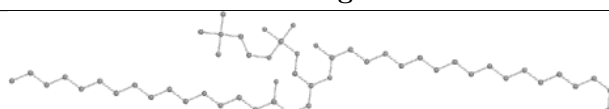


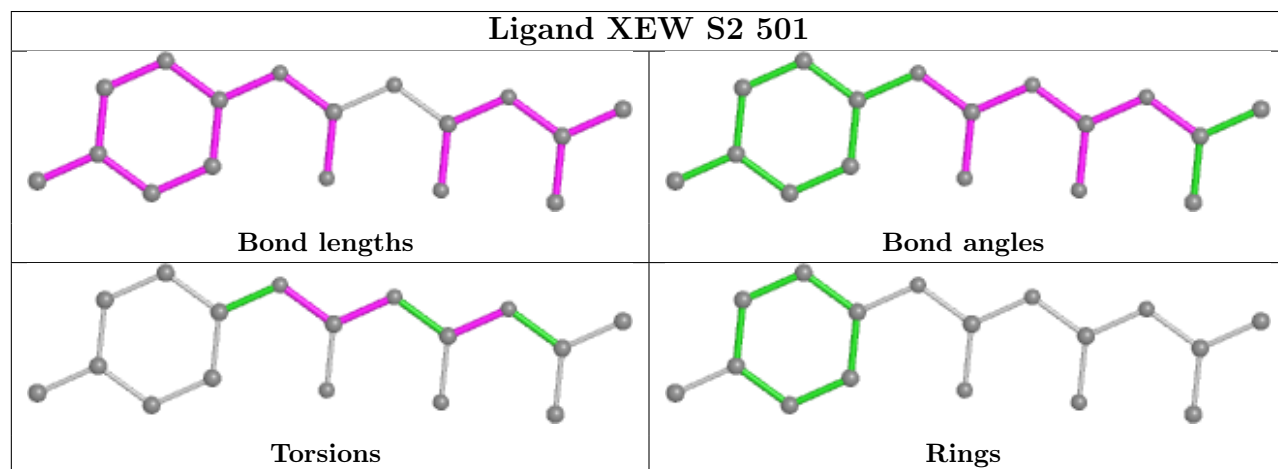
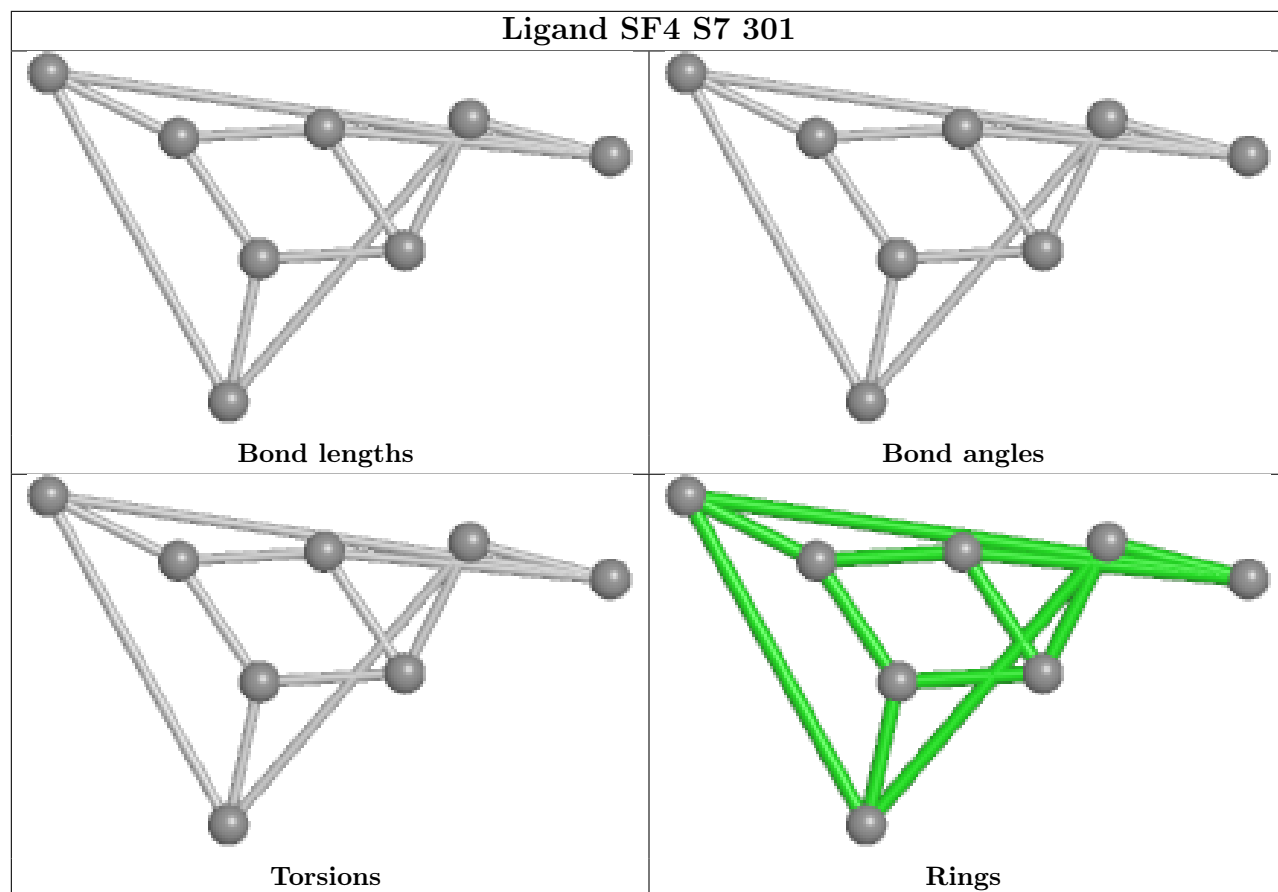


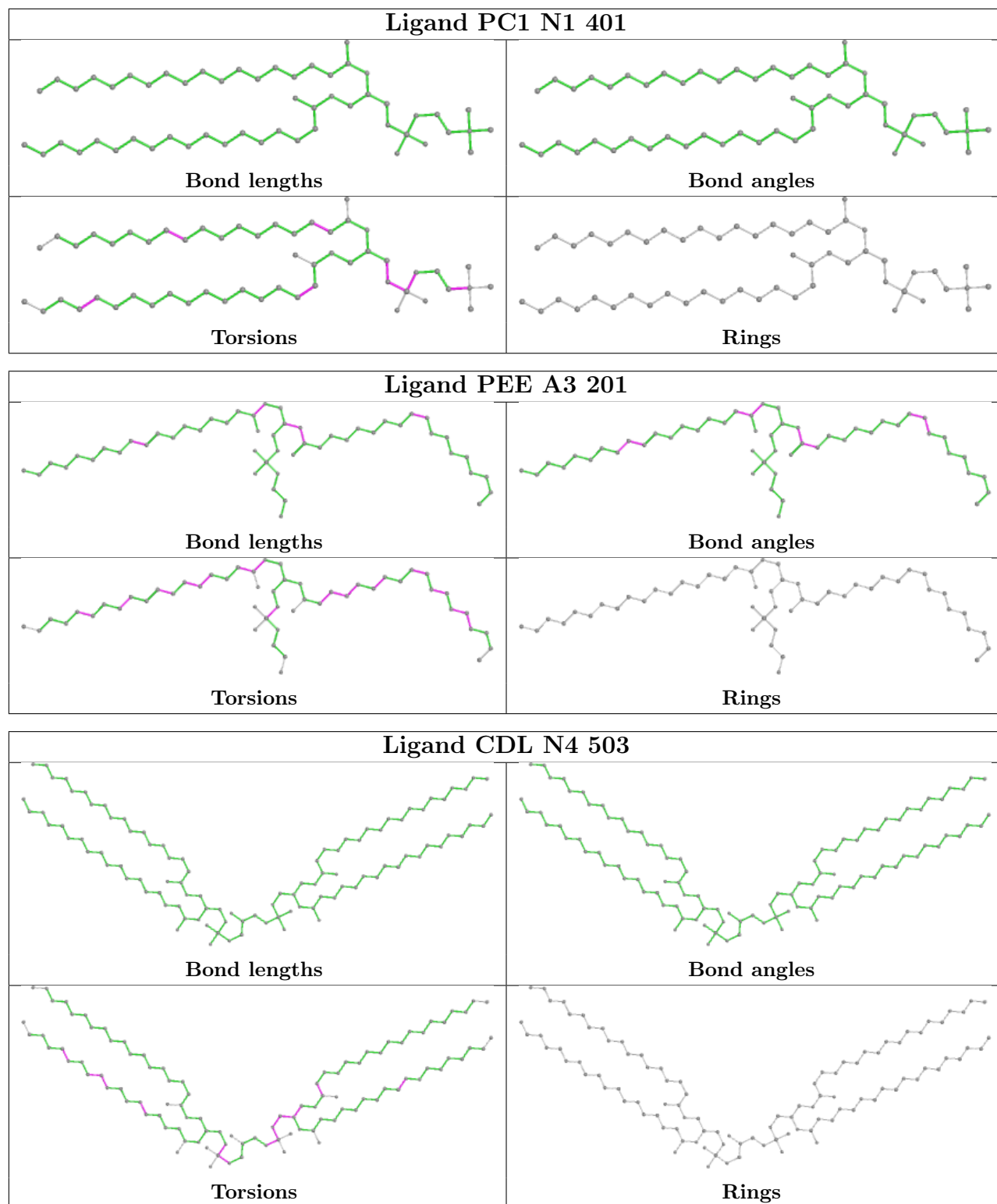
Ligand PEE B4 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

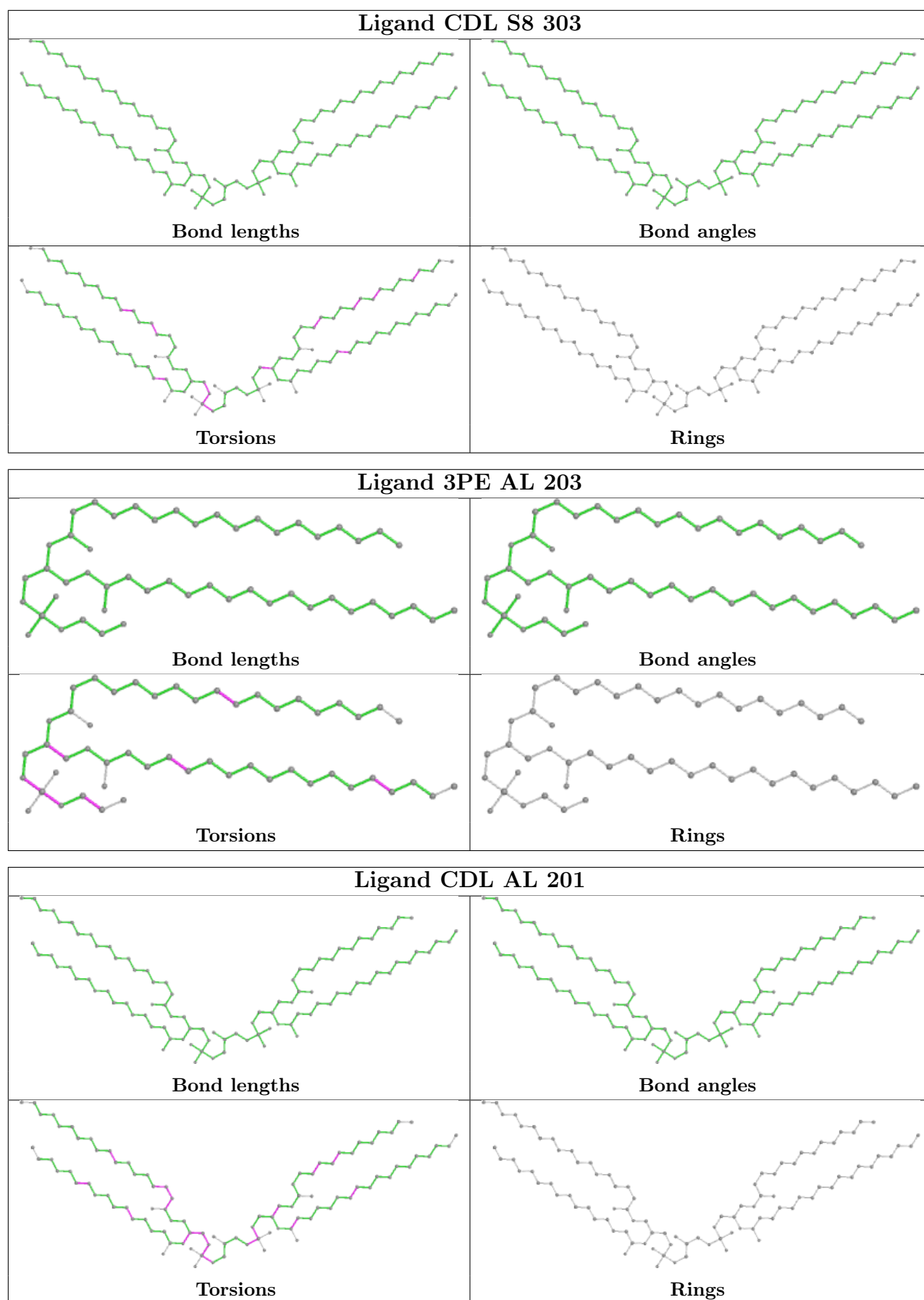
Ligand PLX B5 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

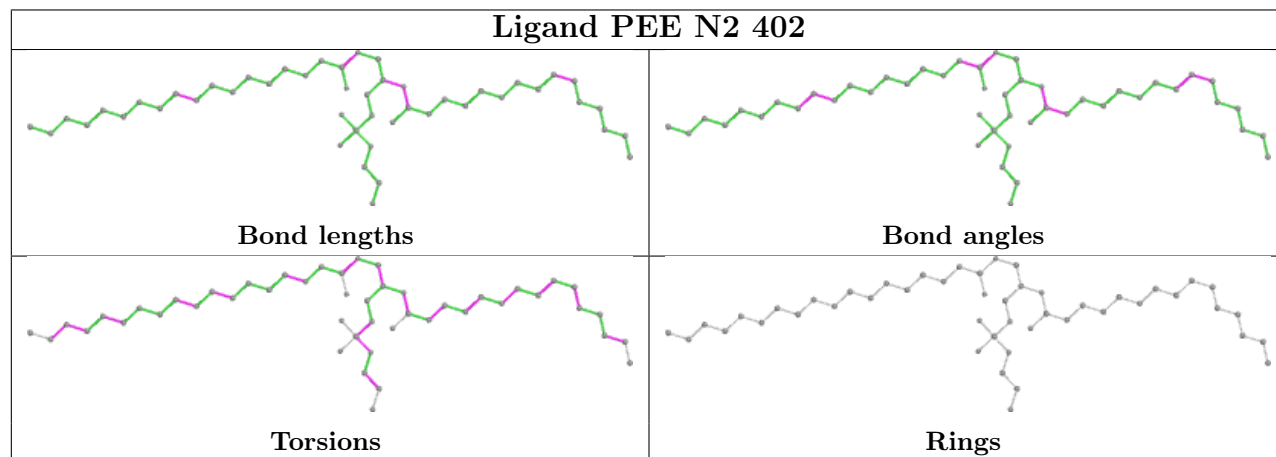
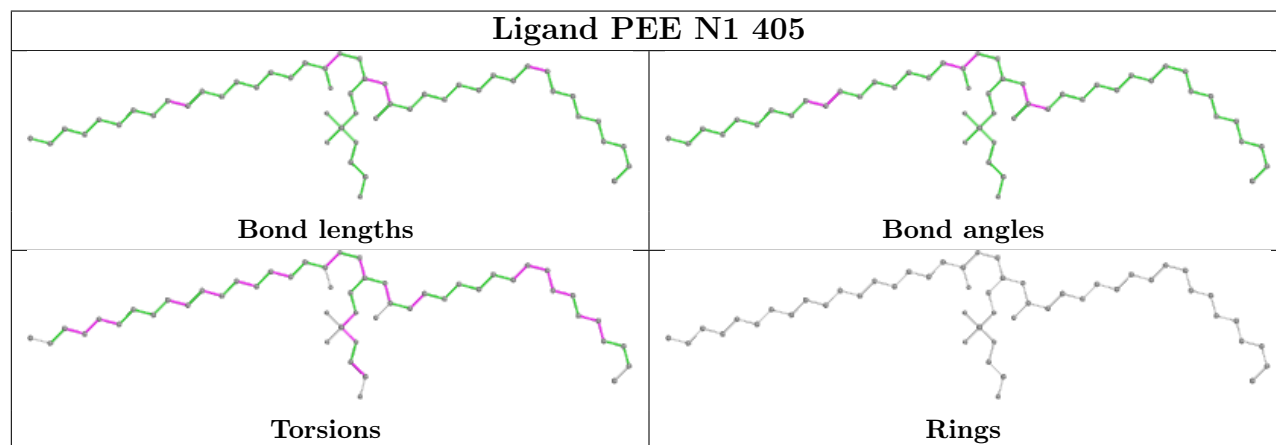
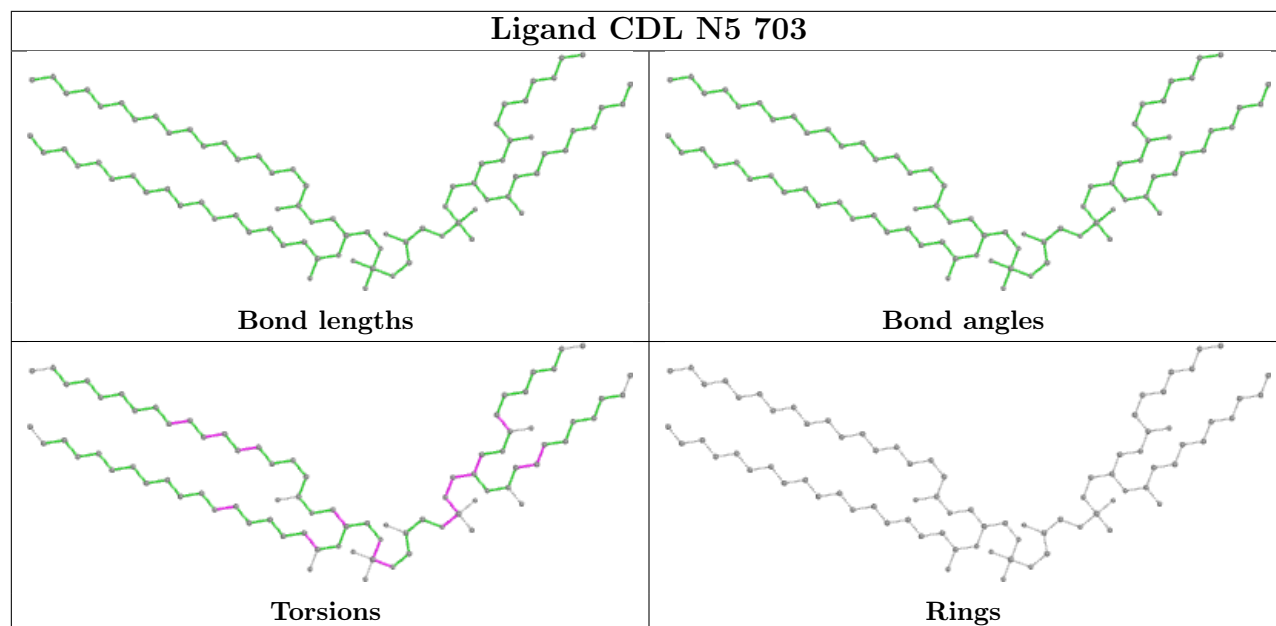
Ligand PC1 B5 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX N3 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

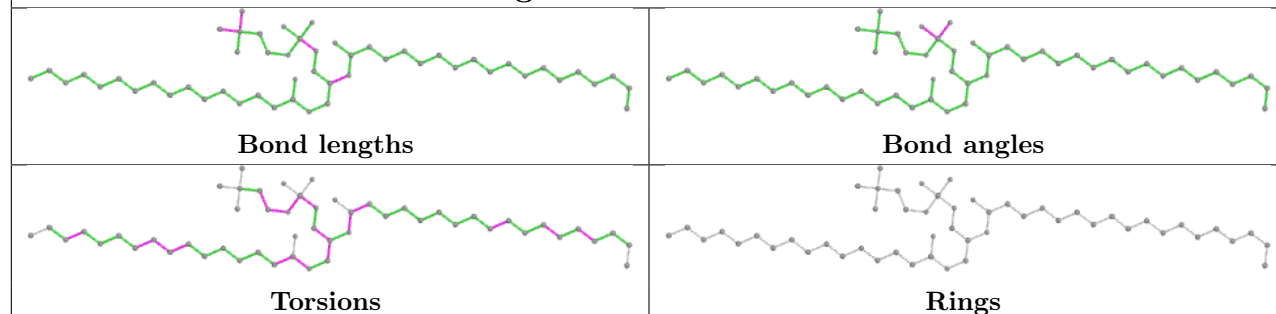




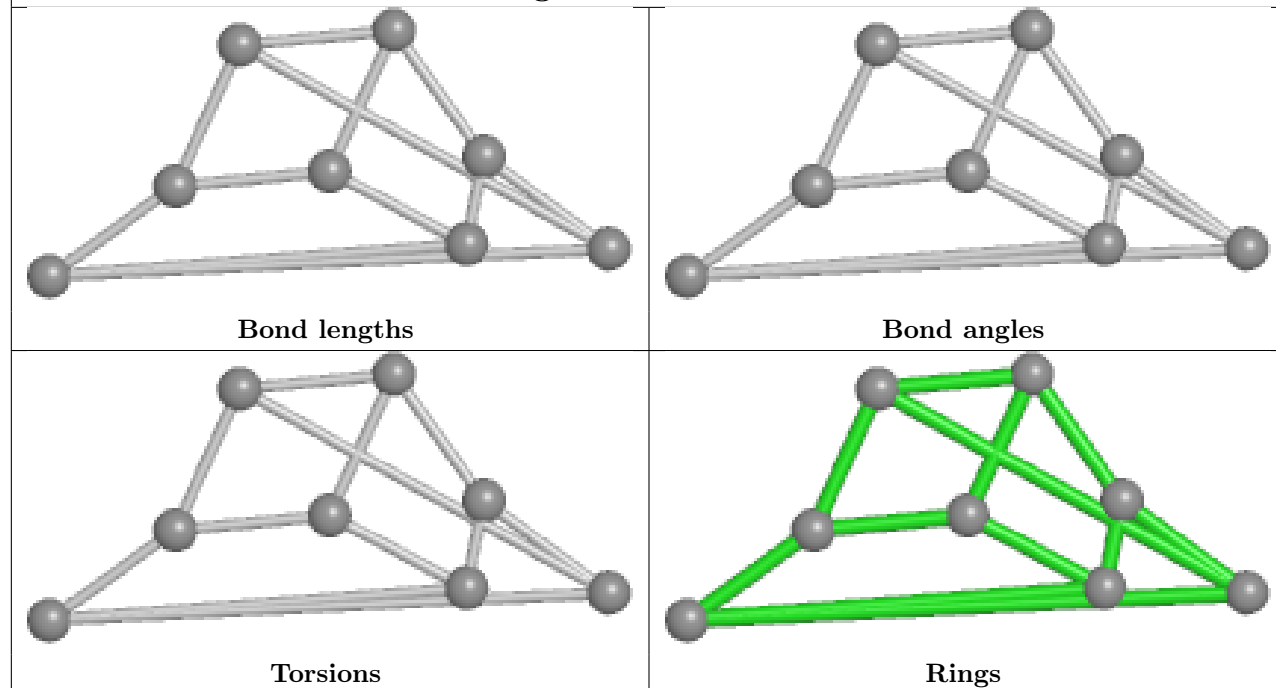




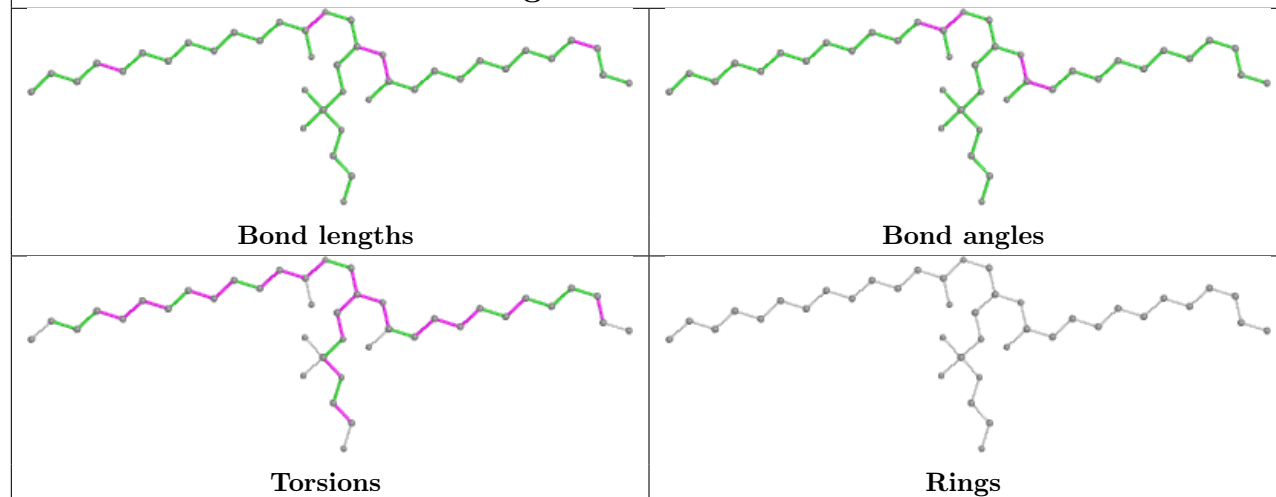
## Ligand PLX AM 201



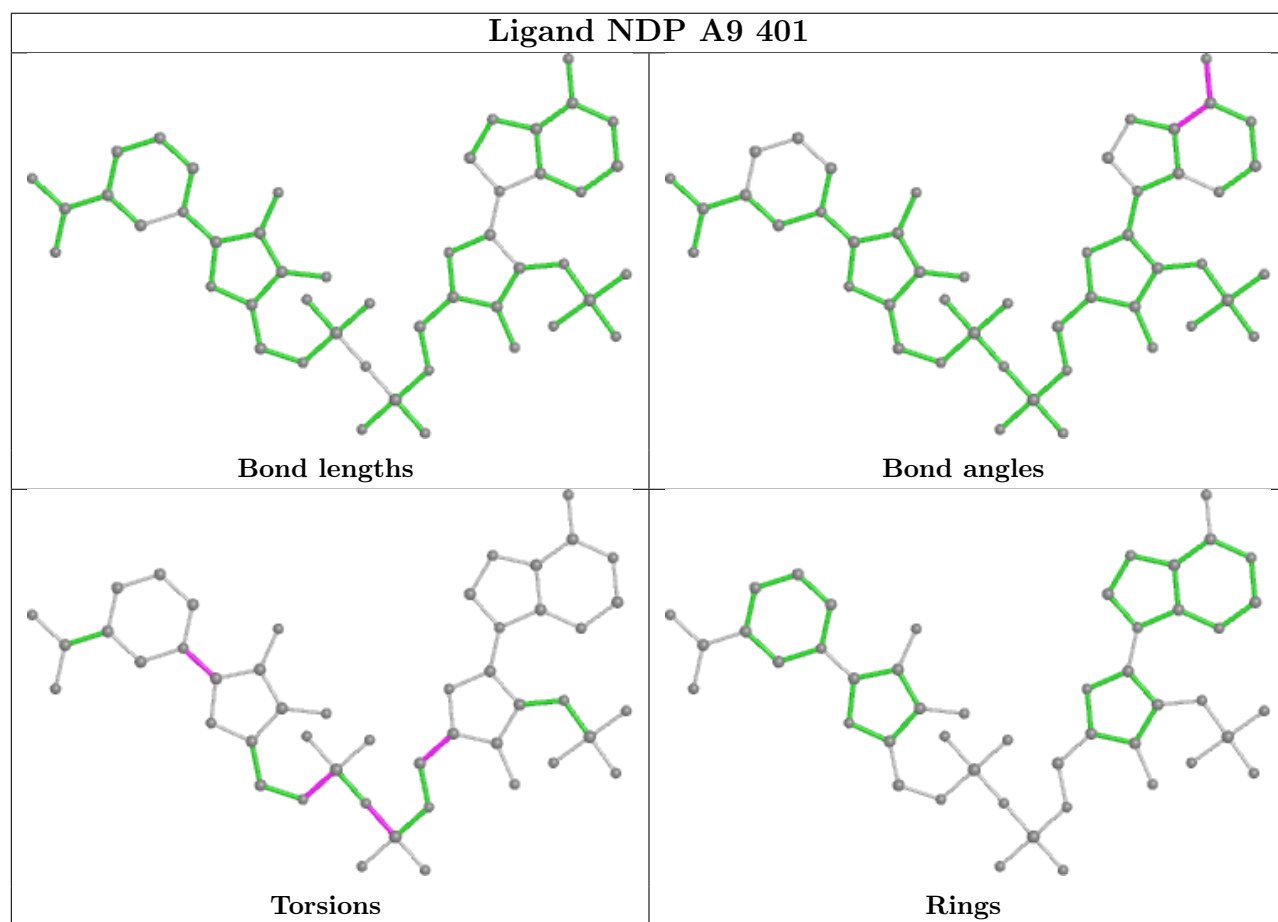
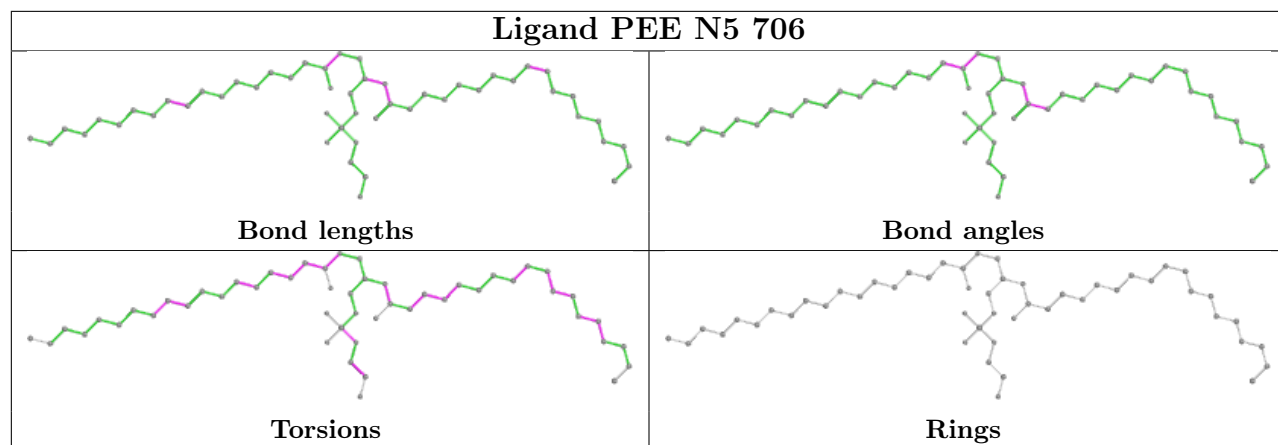
## Ligand SF4 S8 302

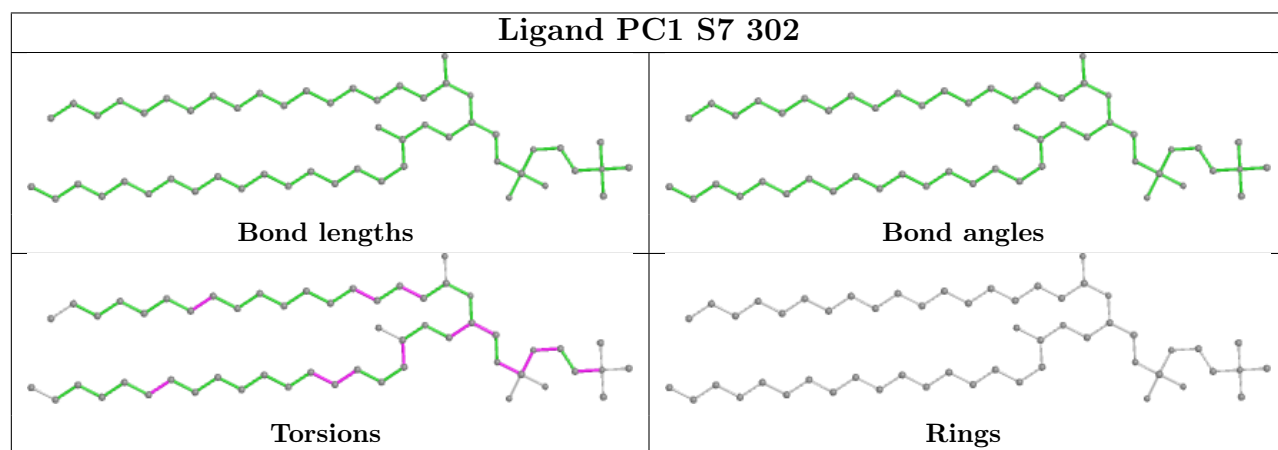
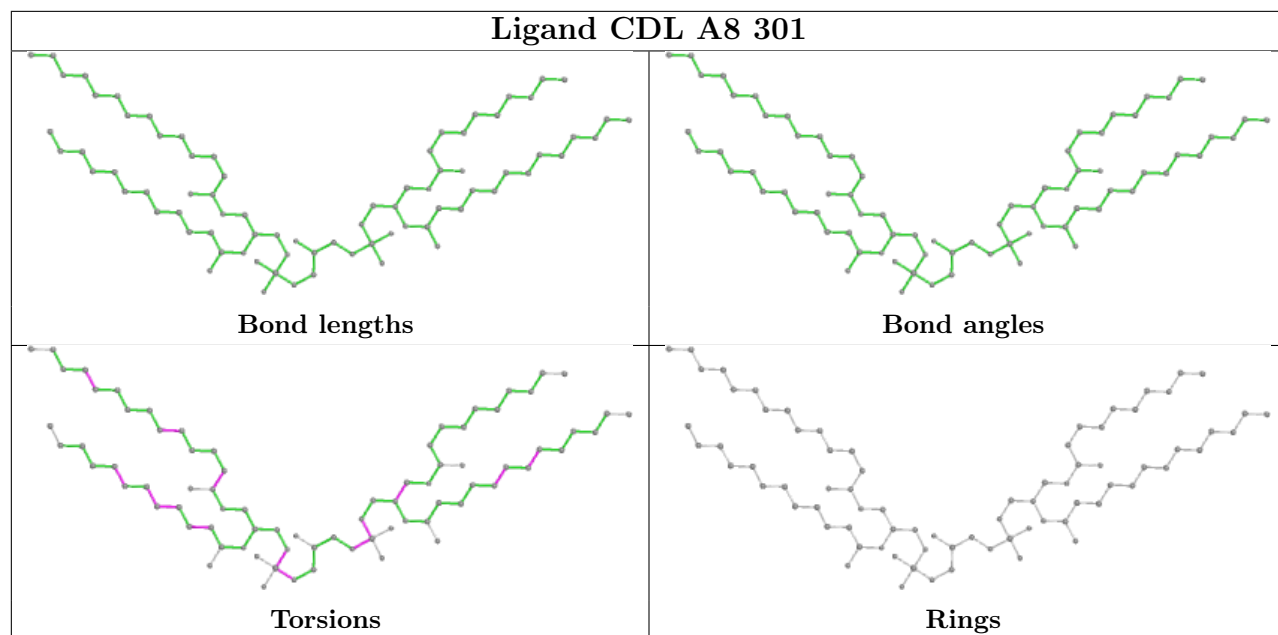


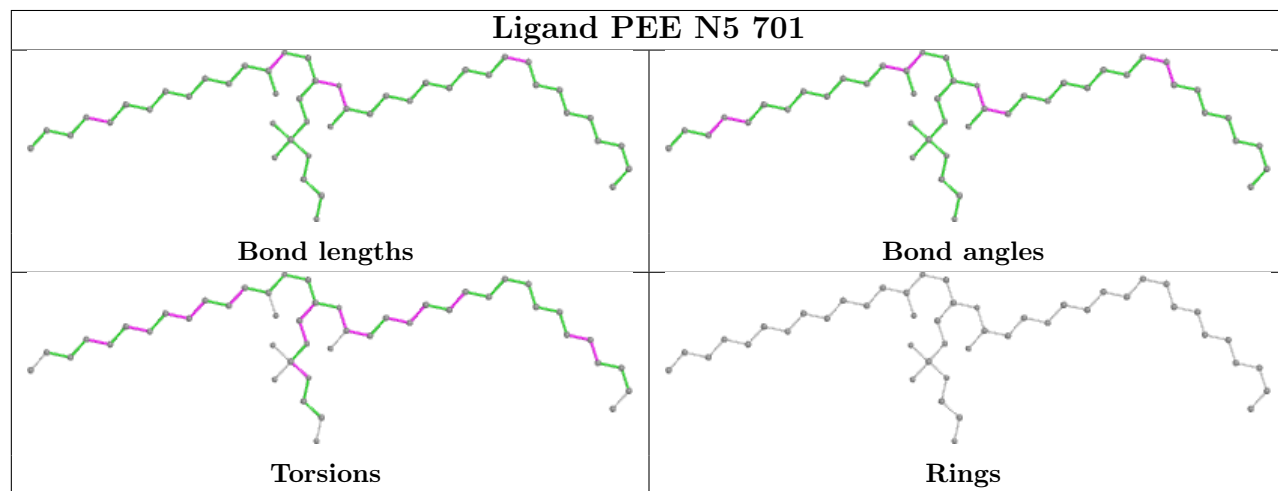
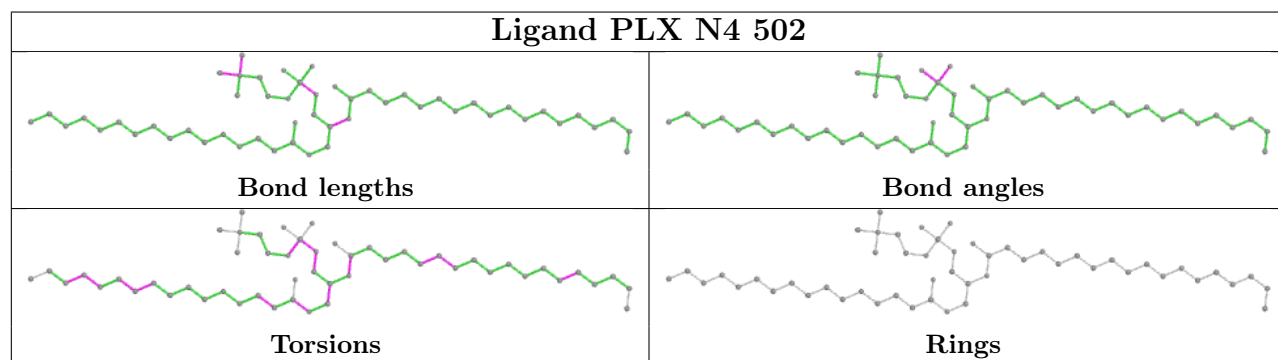
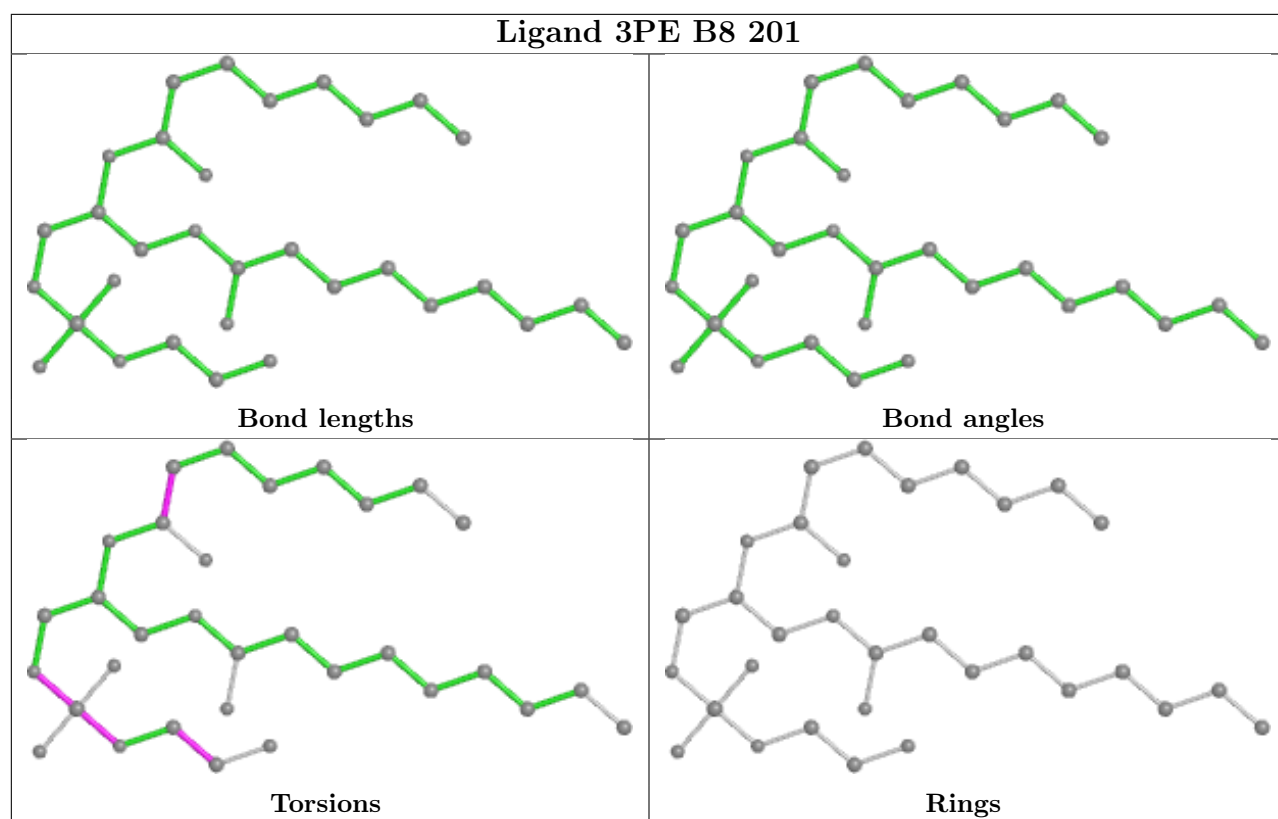
## Ligand PEE N5 702

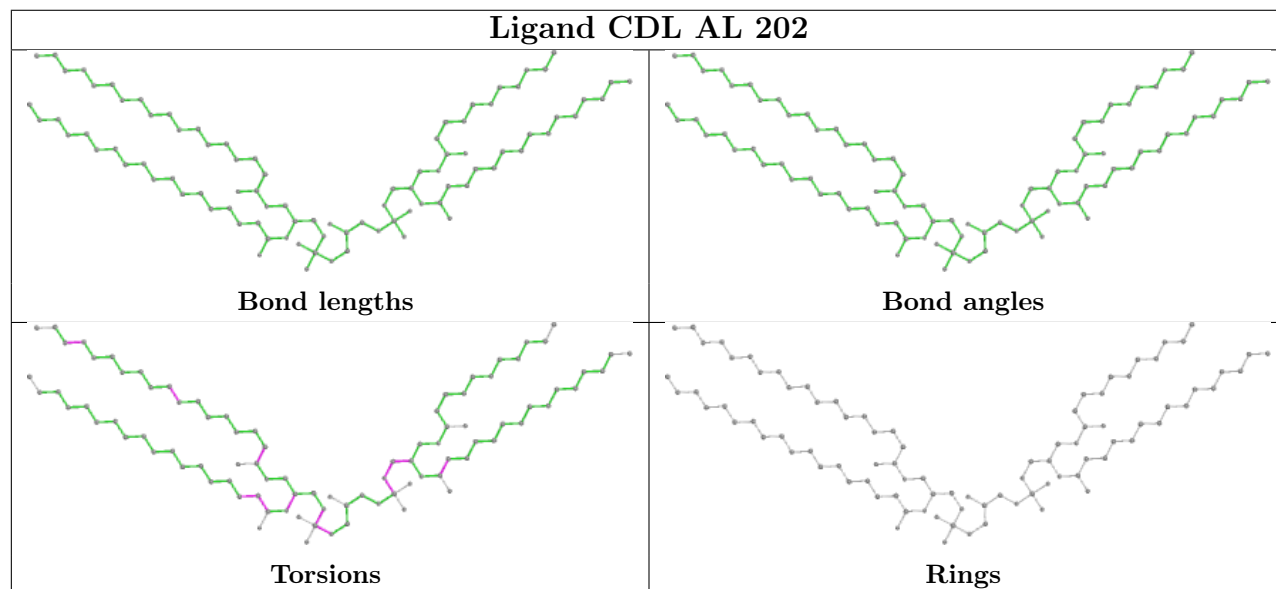
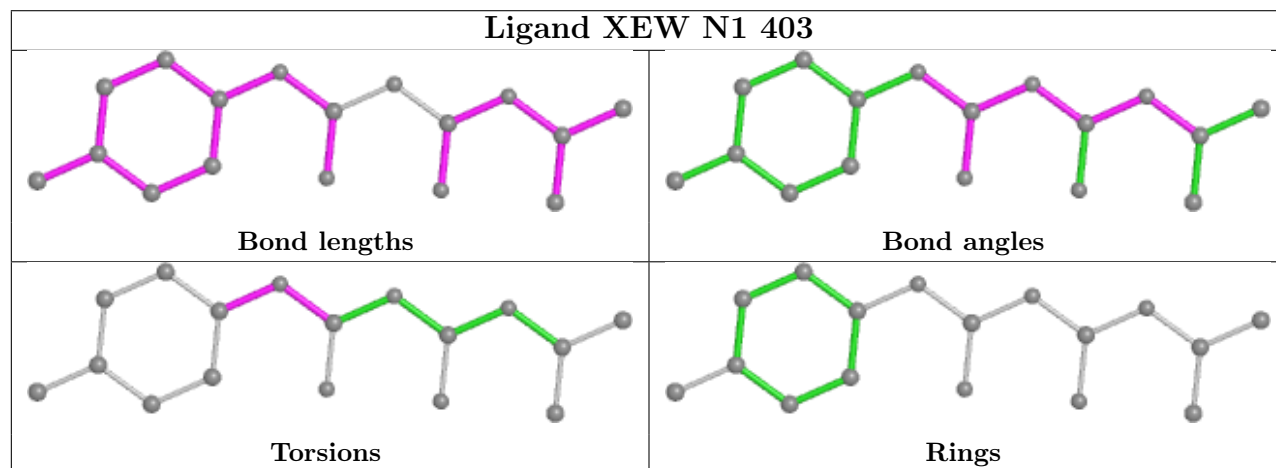
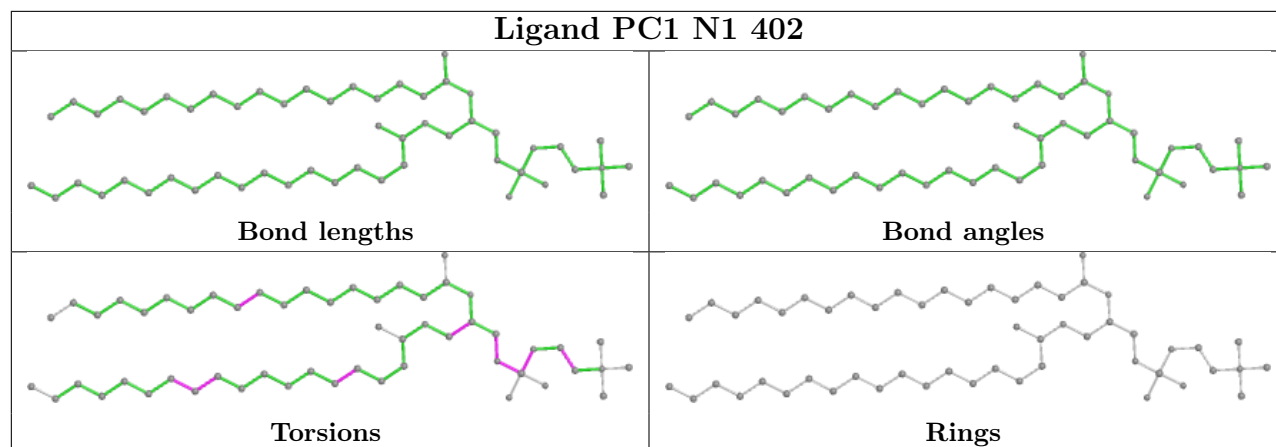


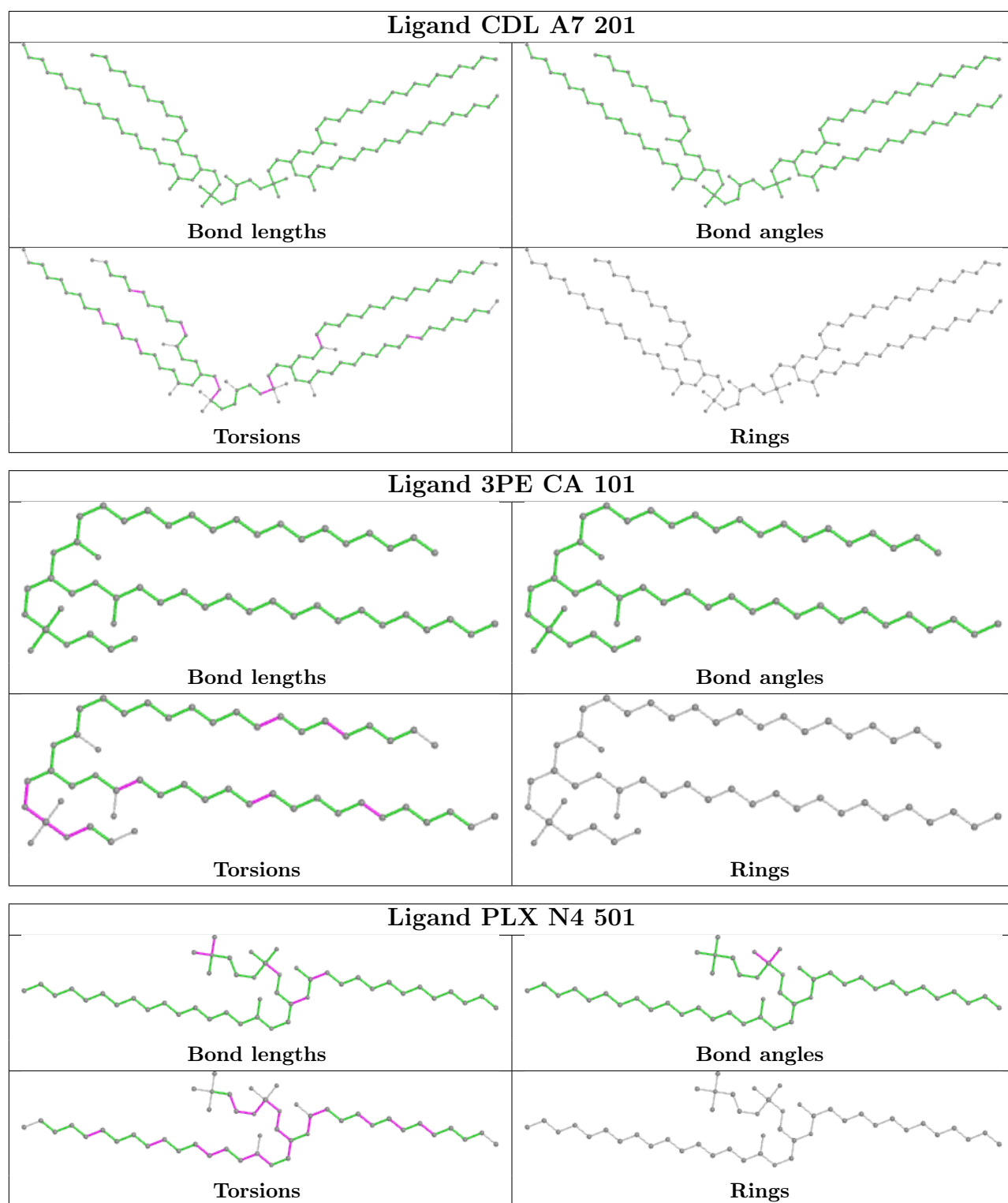


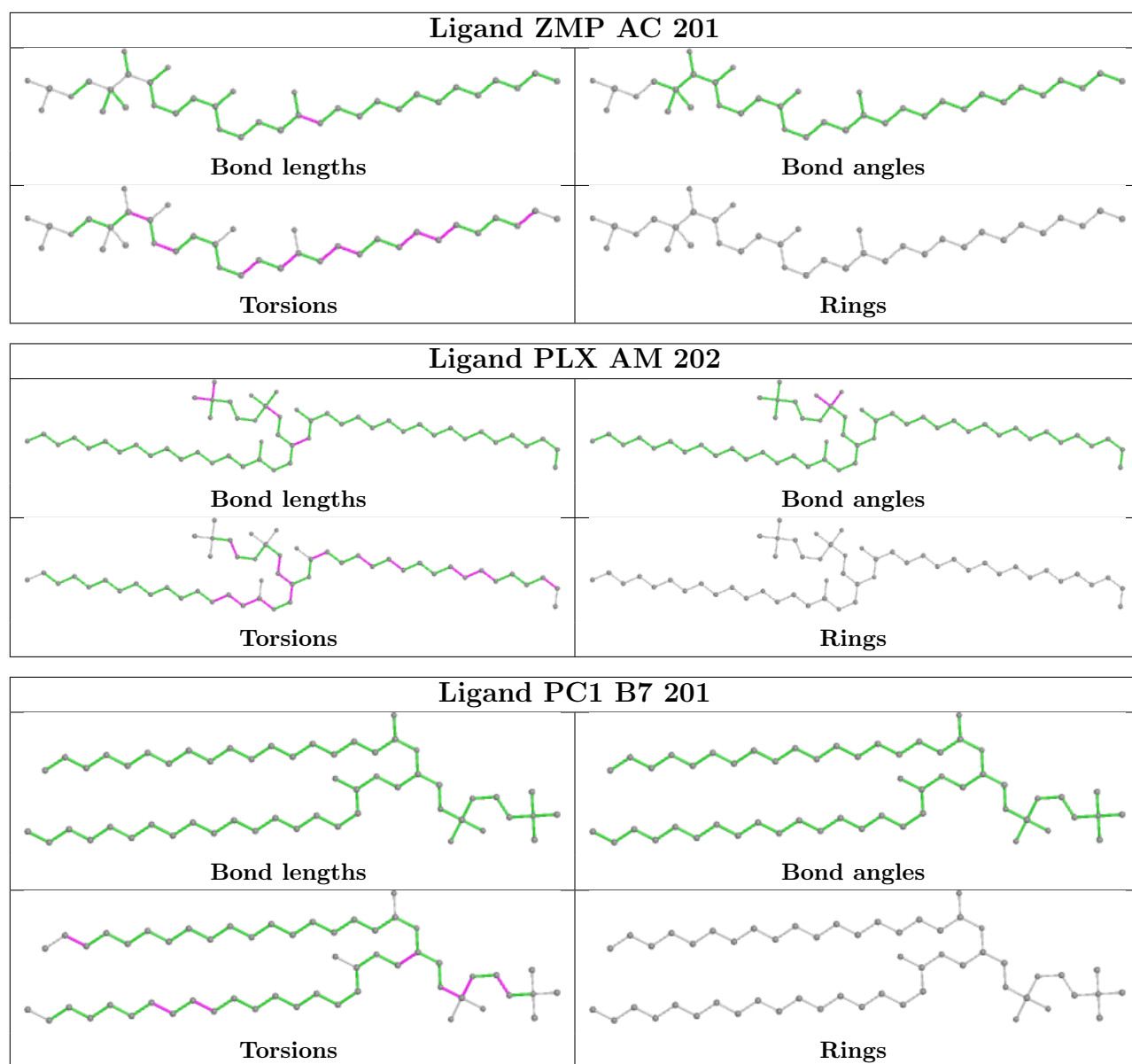


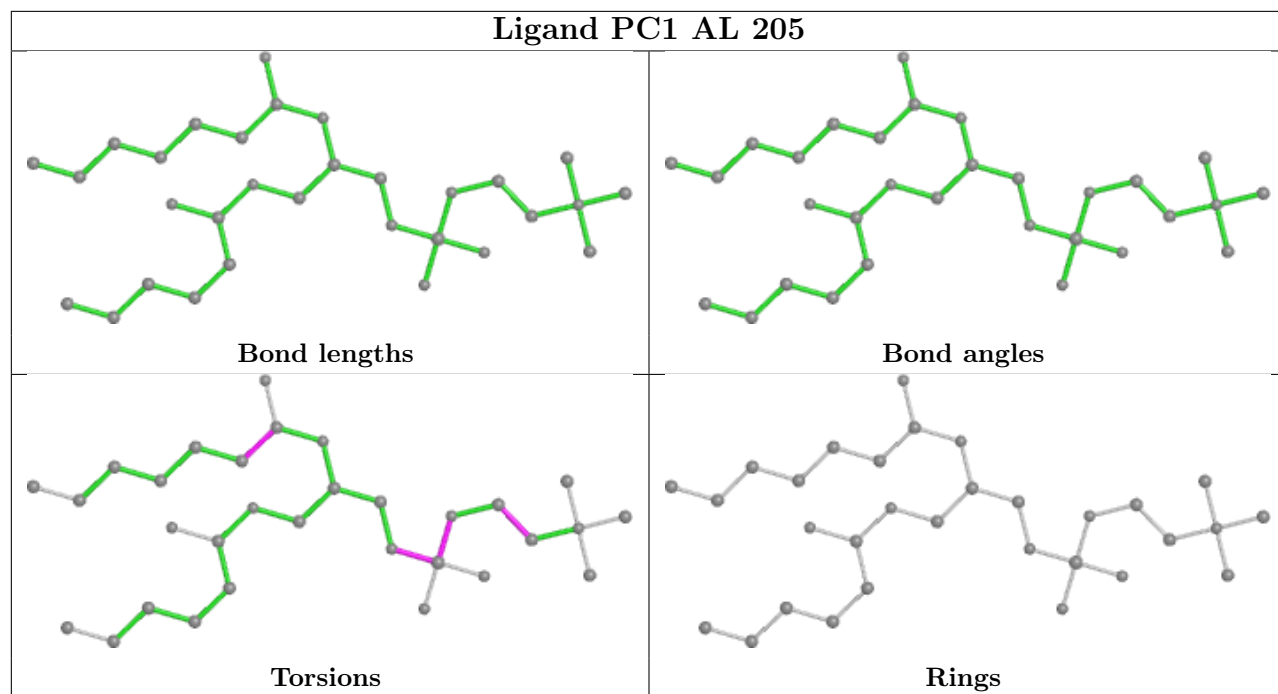
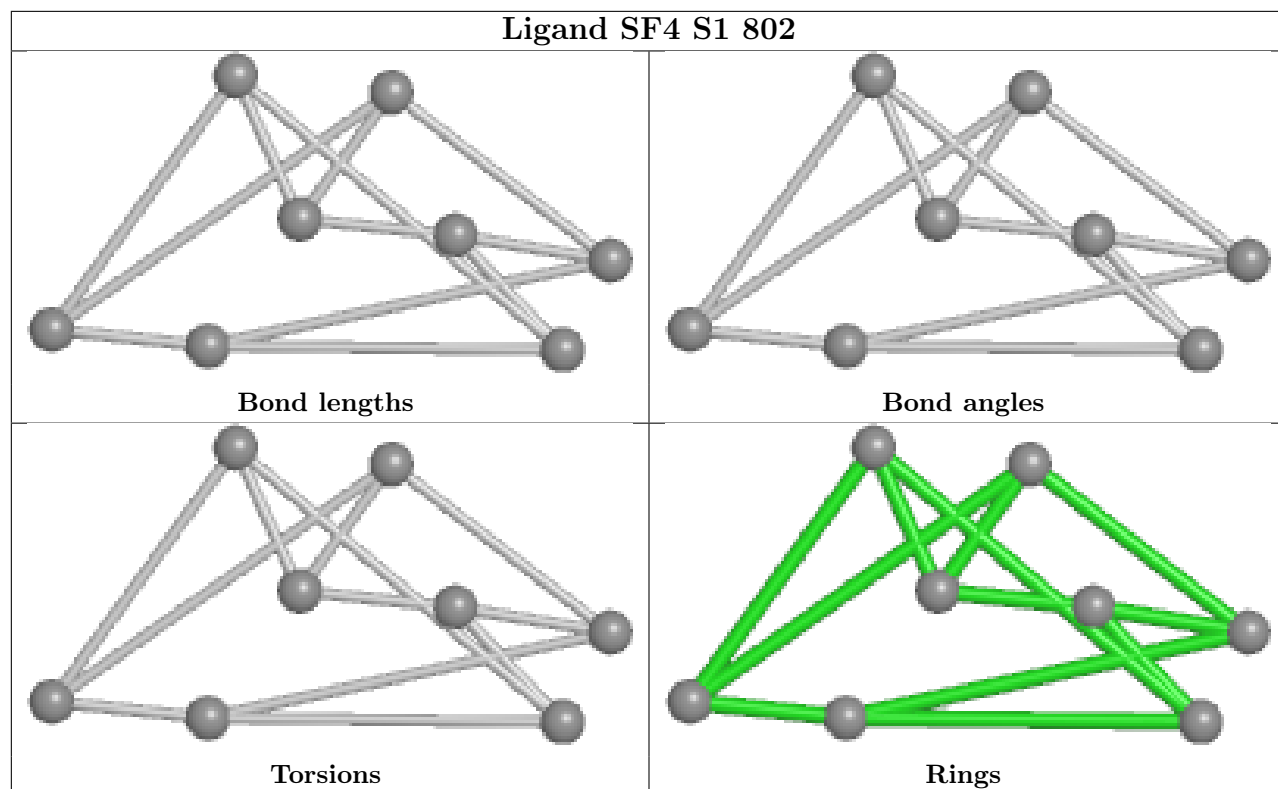


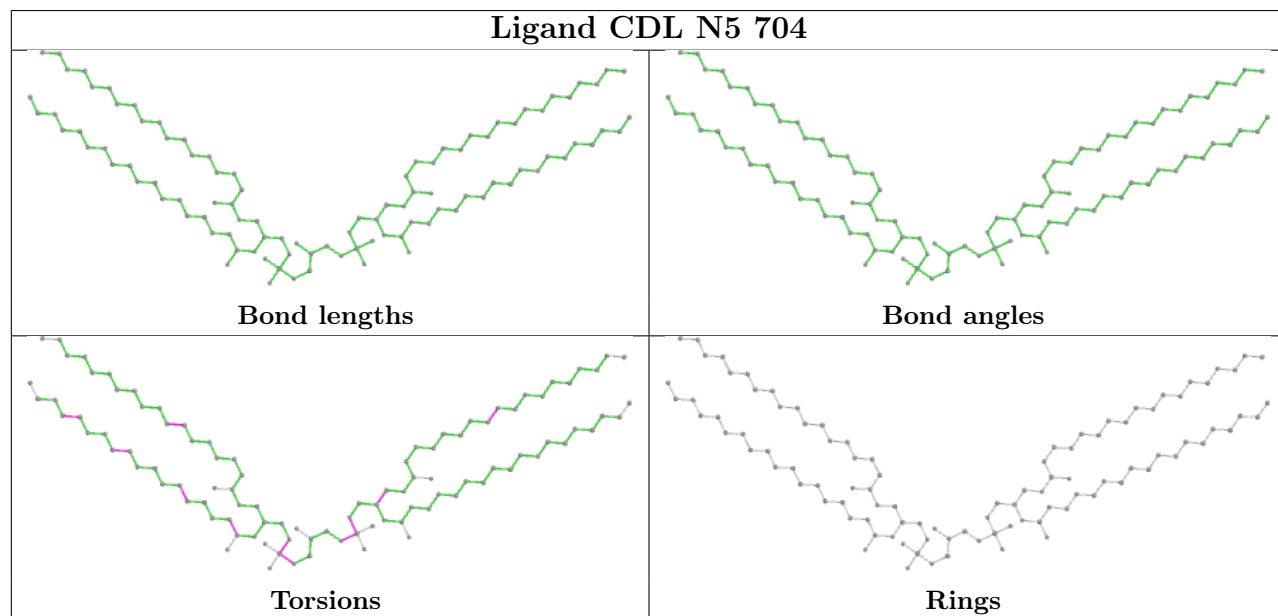
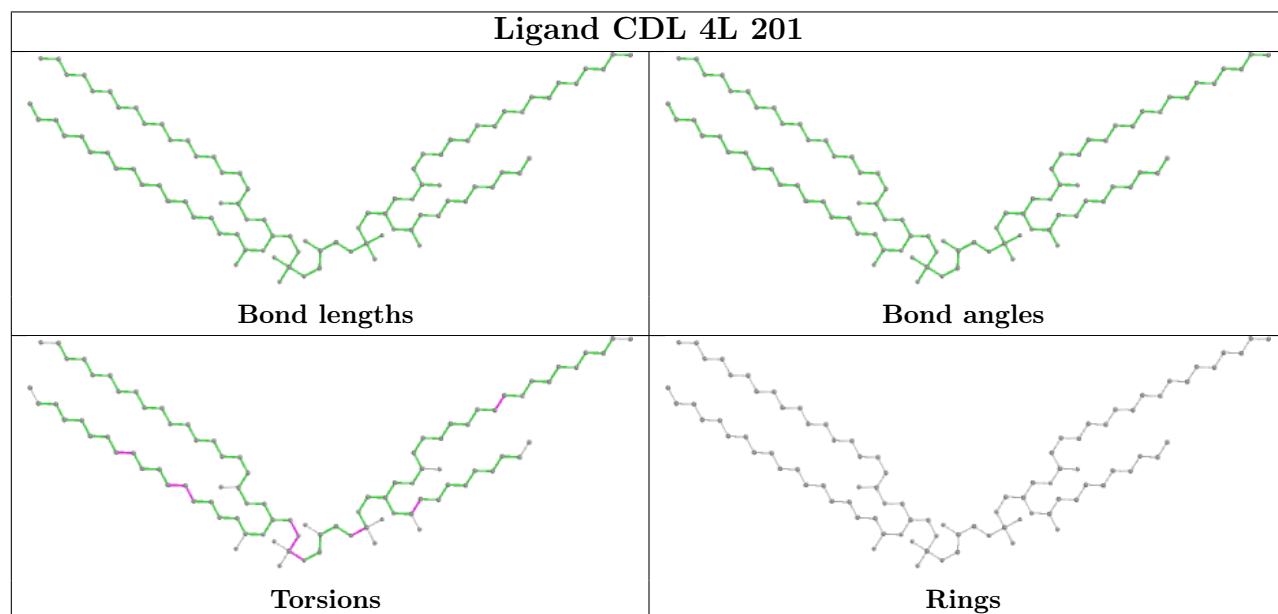
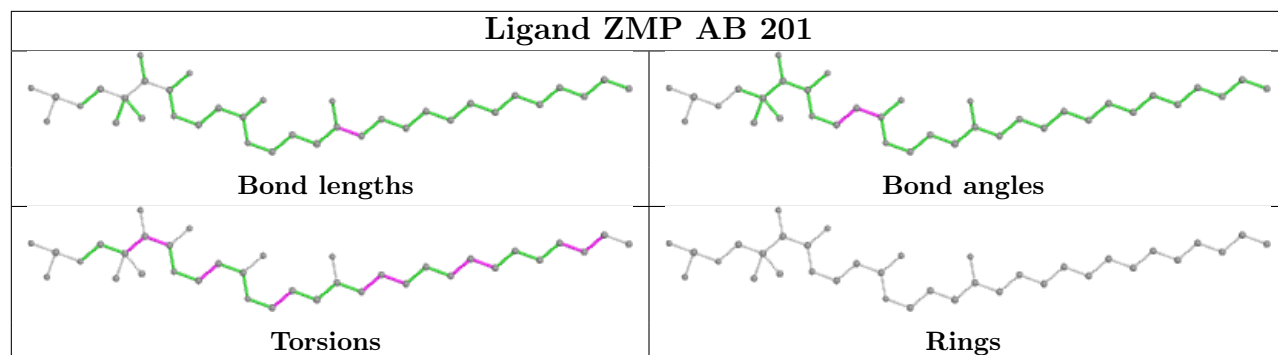




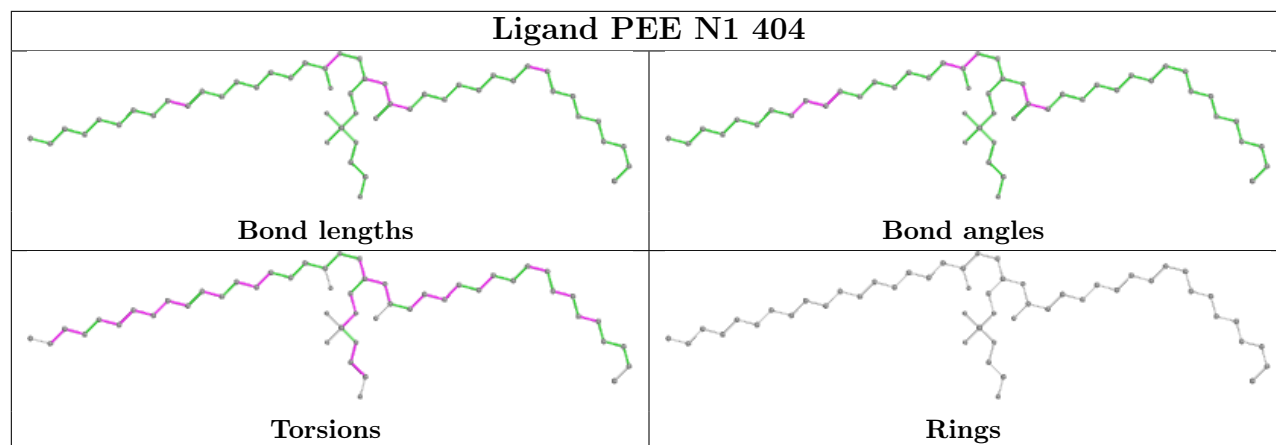












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

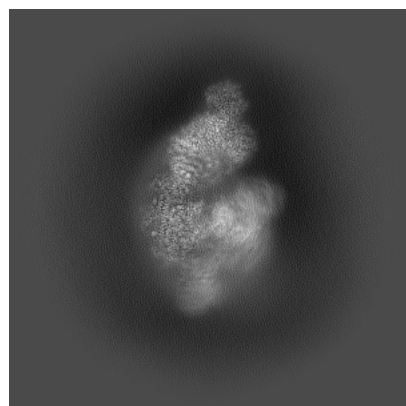
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60425. These allow visual inspection of the internal detail of the map and identification of artifacts.

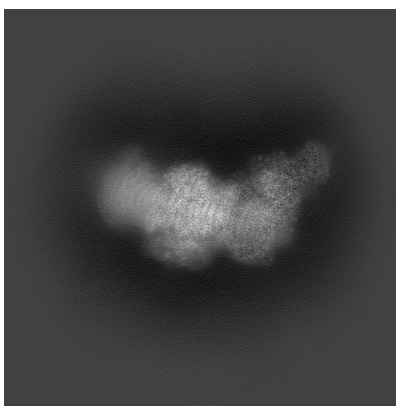
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

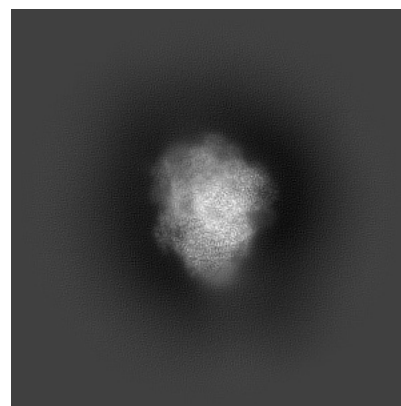
#### 6.1.1 Primary map



X

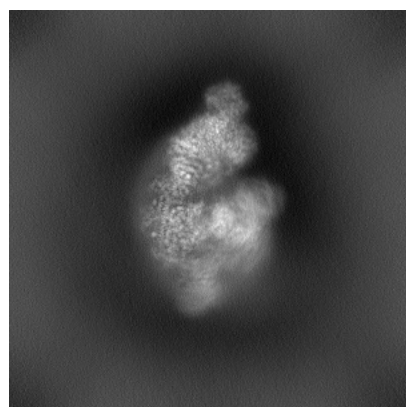


Y

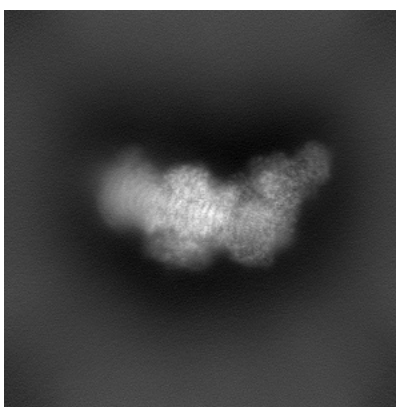


Z

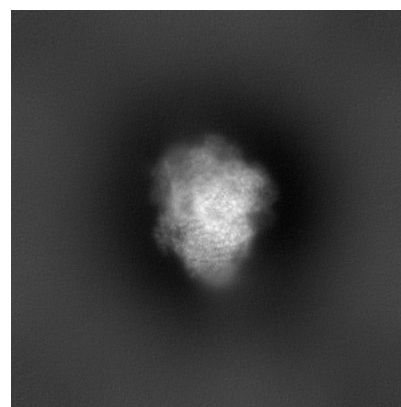
#### 6.1.2 Raw map



X



Y

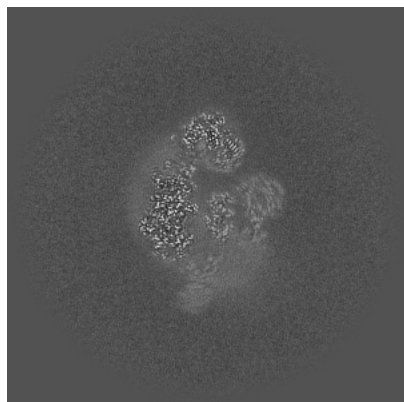


Z

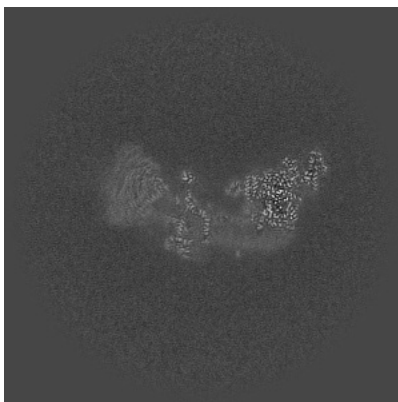
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

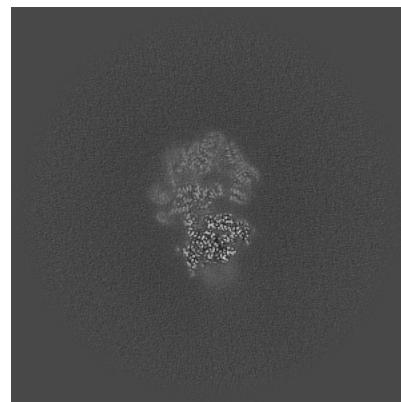
### 6.2.1 Primary map



X Index: 240

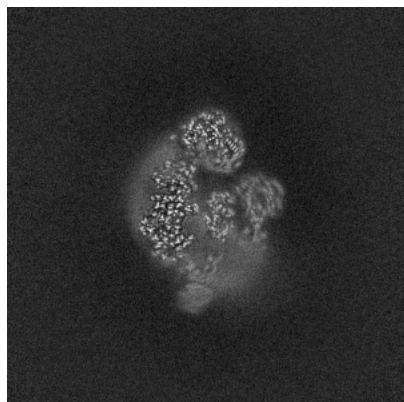


Y Index: 240



Z Index: 240

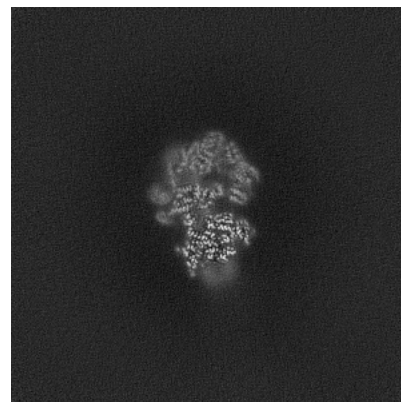
### 6.2.2 Raw map



X Index: 240



Y Index: 240

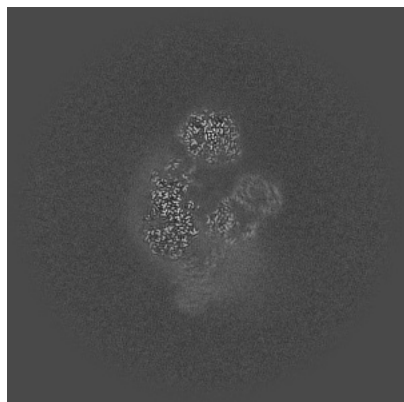


Z Index: 240

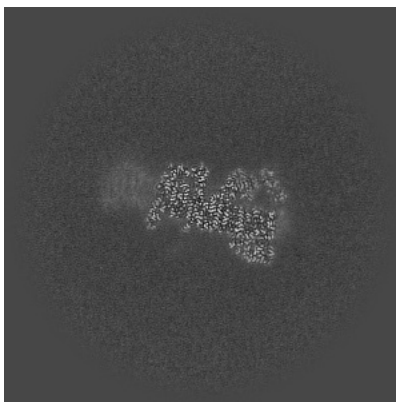
The images above show central slices of the map in three orthogonal directions.

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

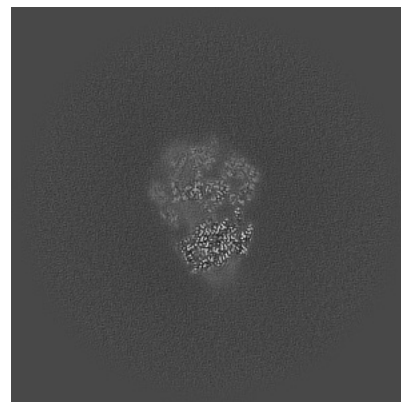
### 6.3.1 Primary map



X Index: 247

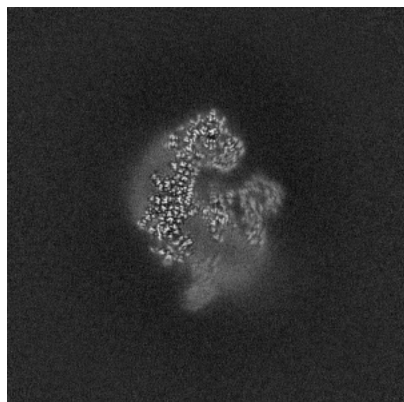


Y Index: 207

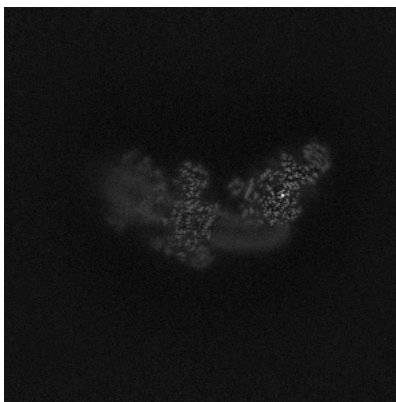


Z Index: 230

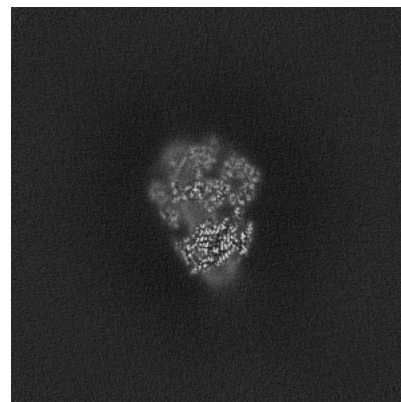
### 6.3.2 Raw map



X Index: 235



Y Index: 249

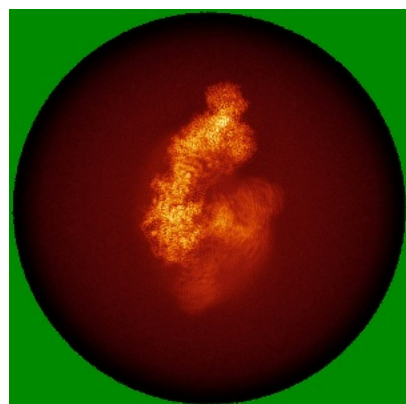


Z Index: 230

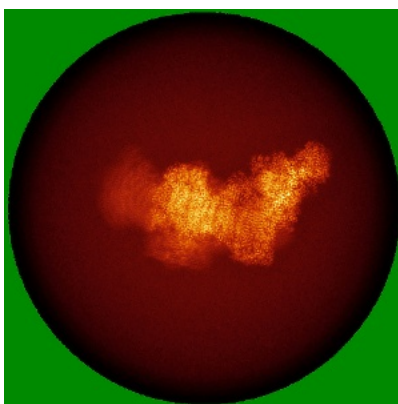
The images above show the largest variance slices of the map in three orthogonal directions.

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

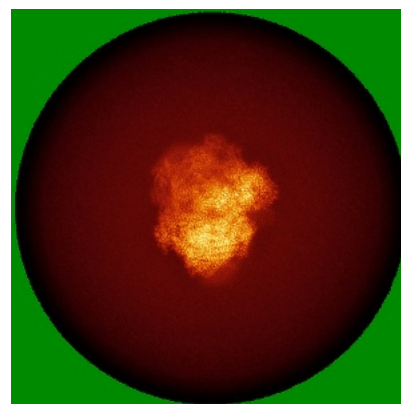
### 6.4.1 Primary map



X

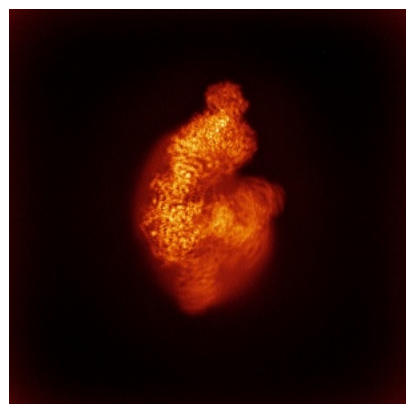


Y

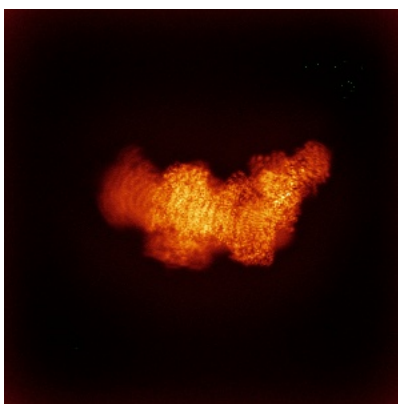


Z

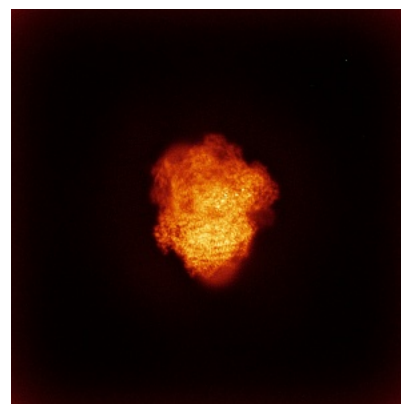
### 6.4.2 Raw map



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



X



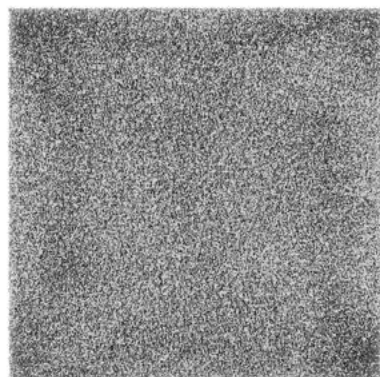
Y



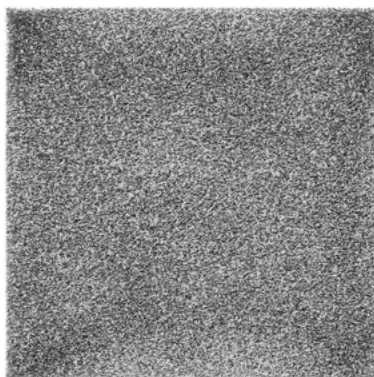
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

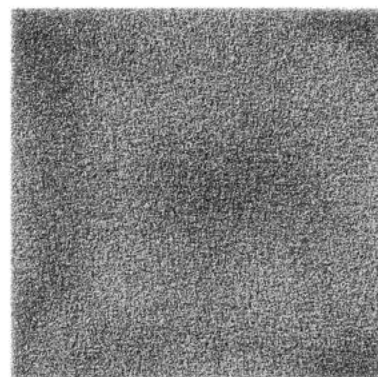
### 6.5.2 Raw map



X



Y



Z

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

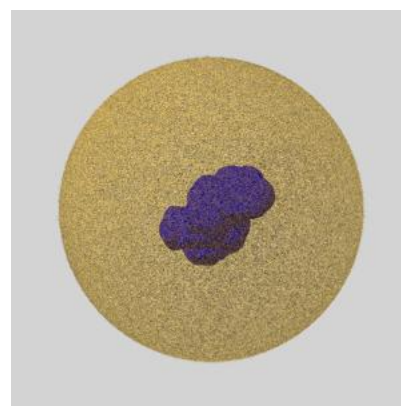
### 6.6.1 emd\_60425\_msk\_1.map [i](#)



X



Y

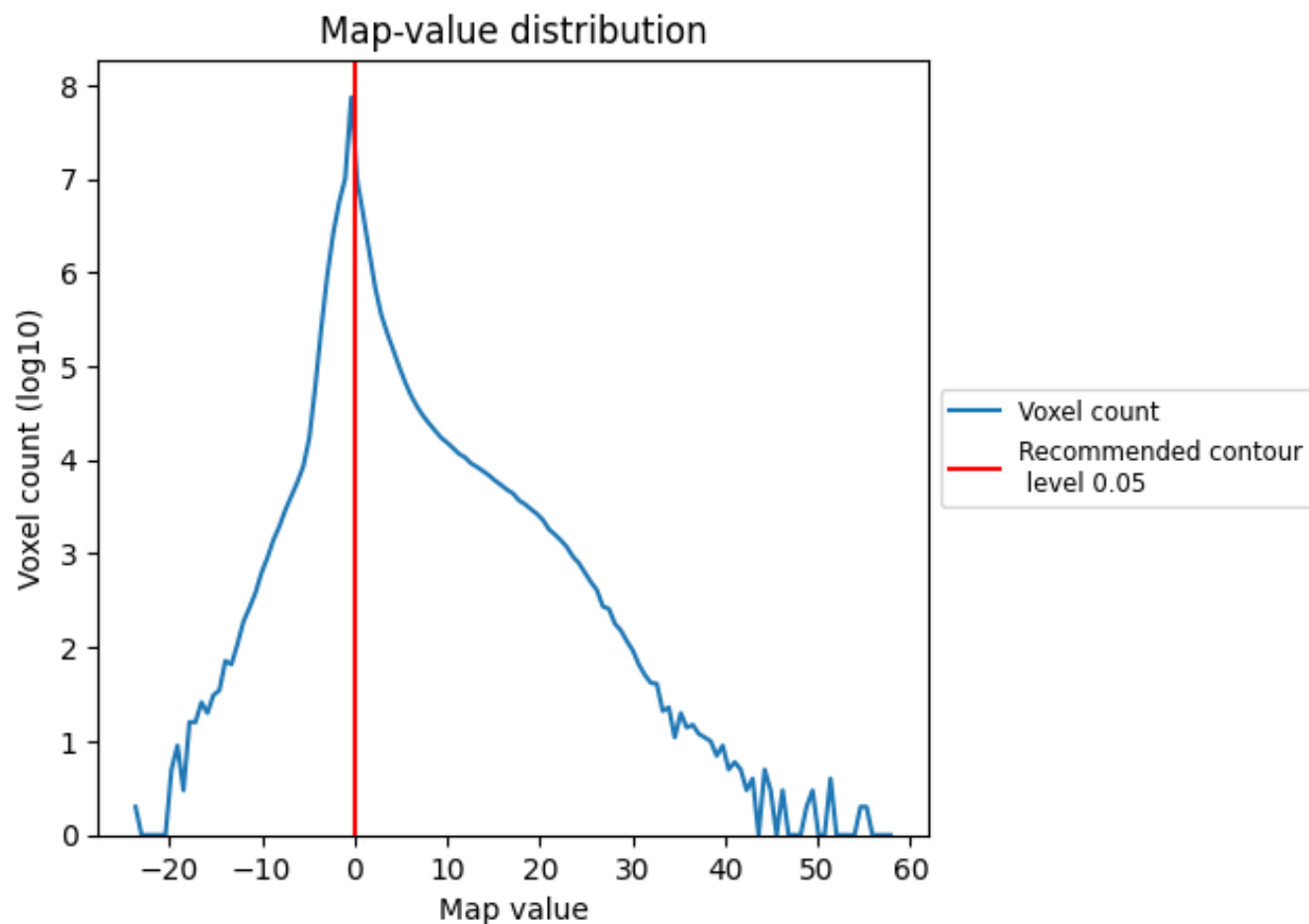


Z

## 7 Map analysis [i](#)

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

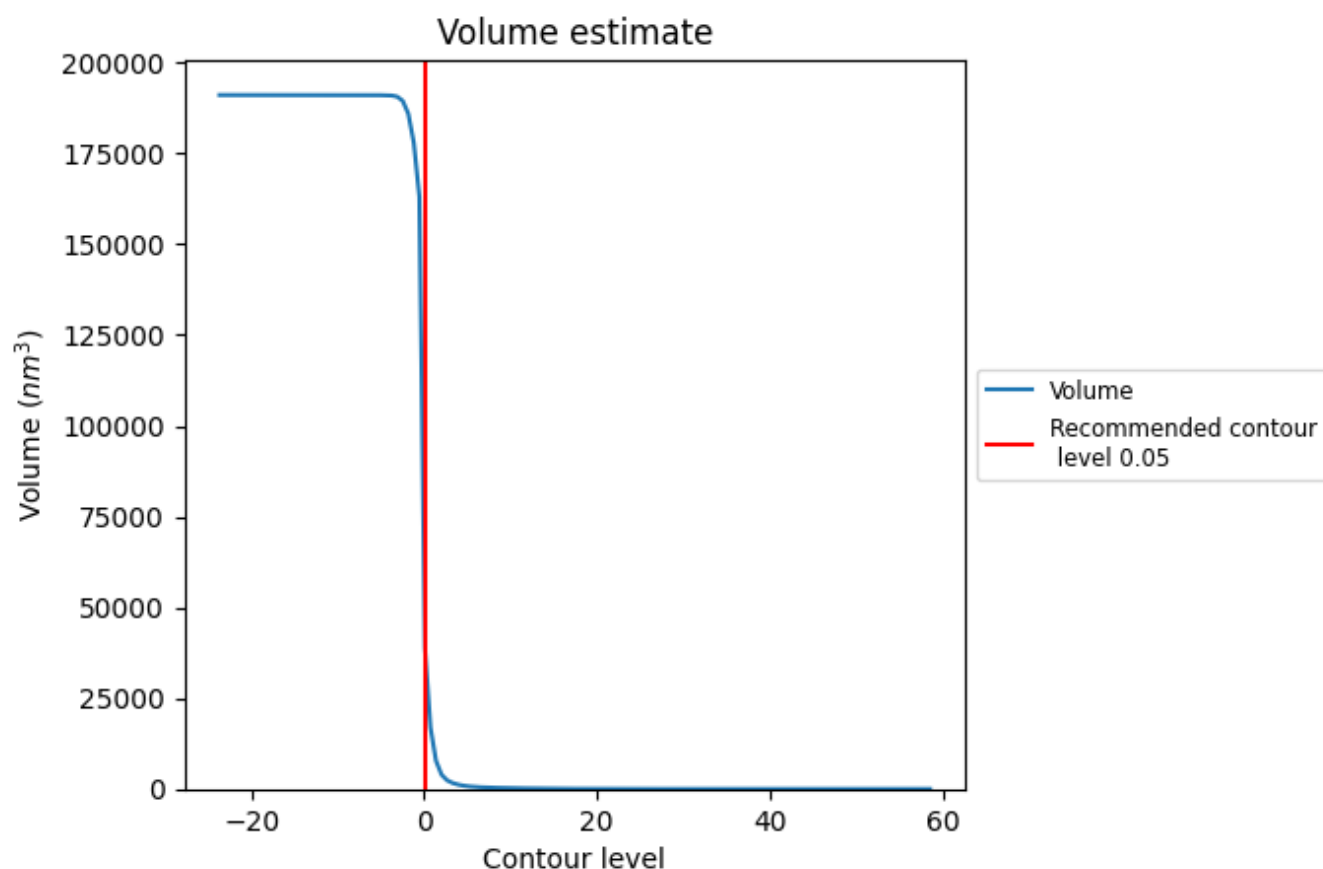
### 7.1 Map-value distribution [i](#)



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.



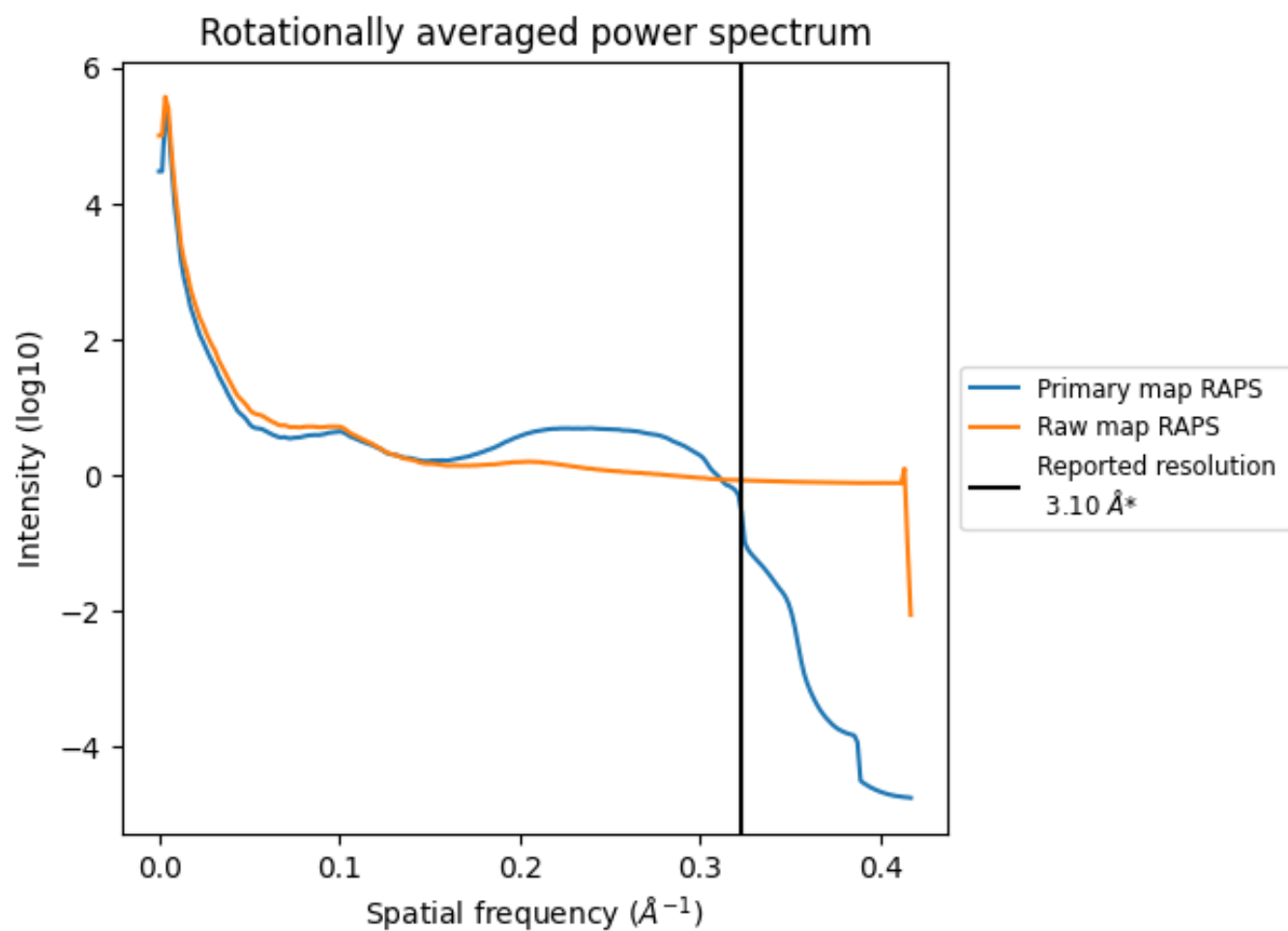
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46179  $\text{nm}^3$ ; this corresponds to an approximate mass of 41715 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 ⓘ

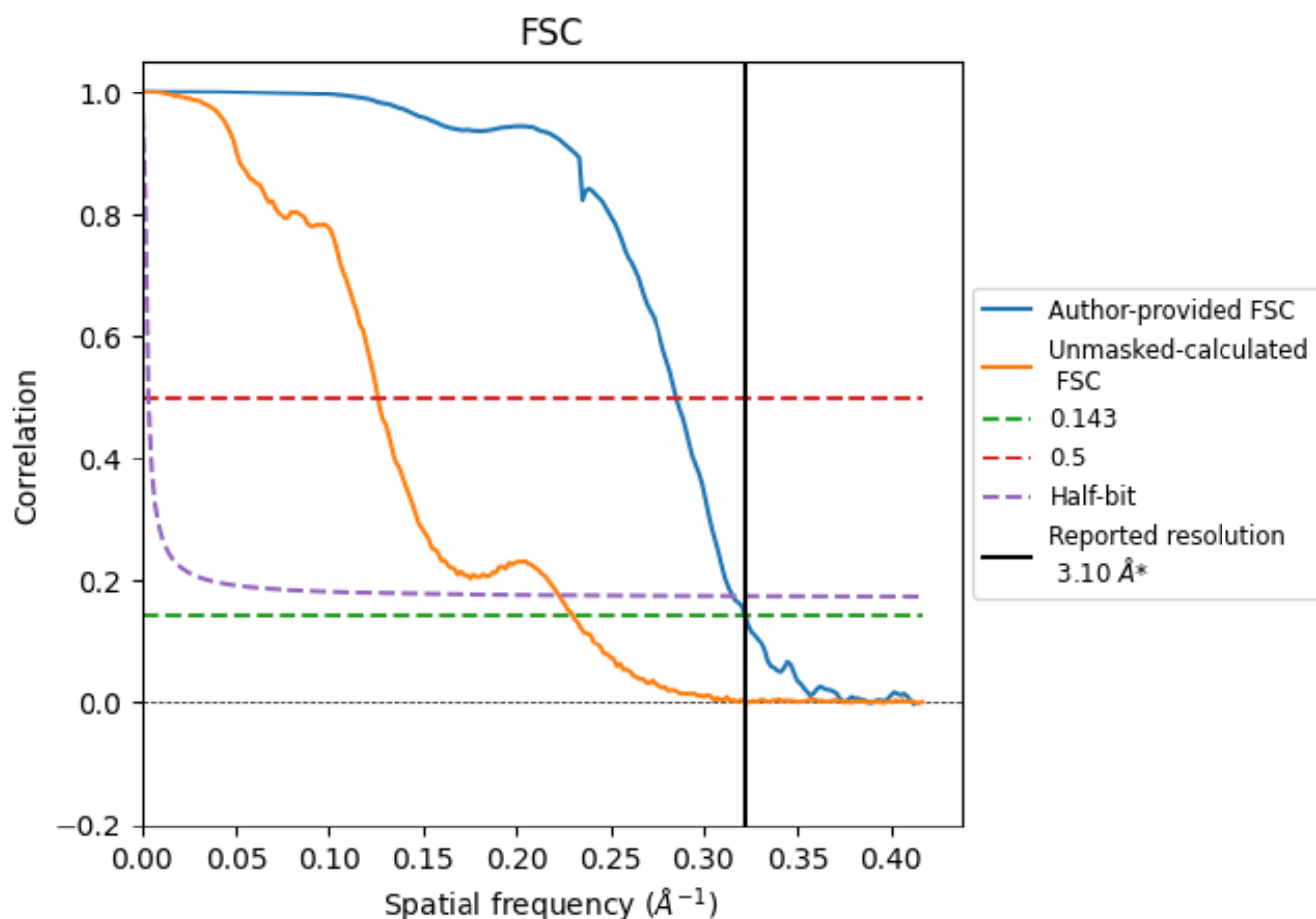


\*Reported resolution corresponds to spatial frequency of  $0.323 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.50	3.17
Unmasked-calculated*	4.35	7.94	4.49

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.1 by more than 10 %

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

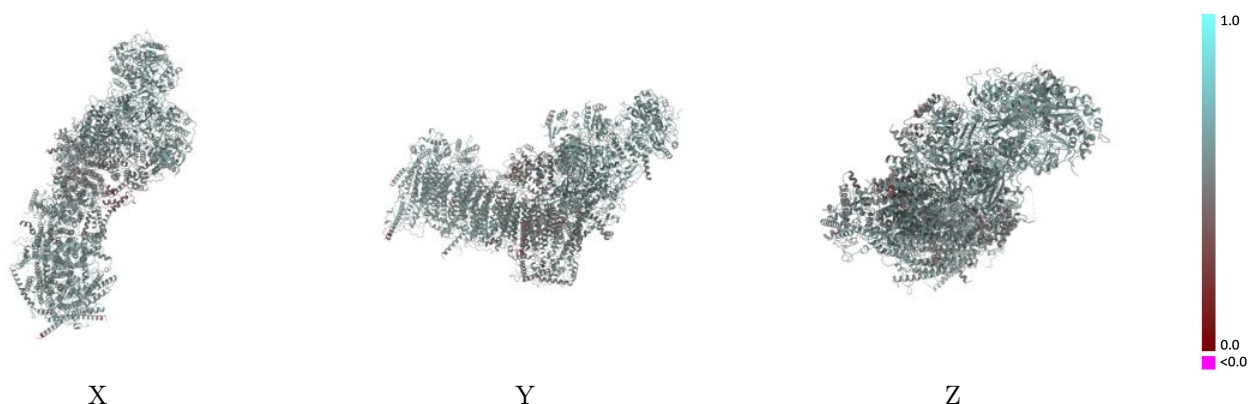
This section contains information regarding the fit between EMDB map EMD-60425 and PDB model 8ZSR. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



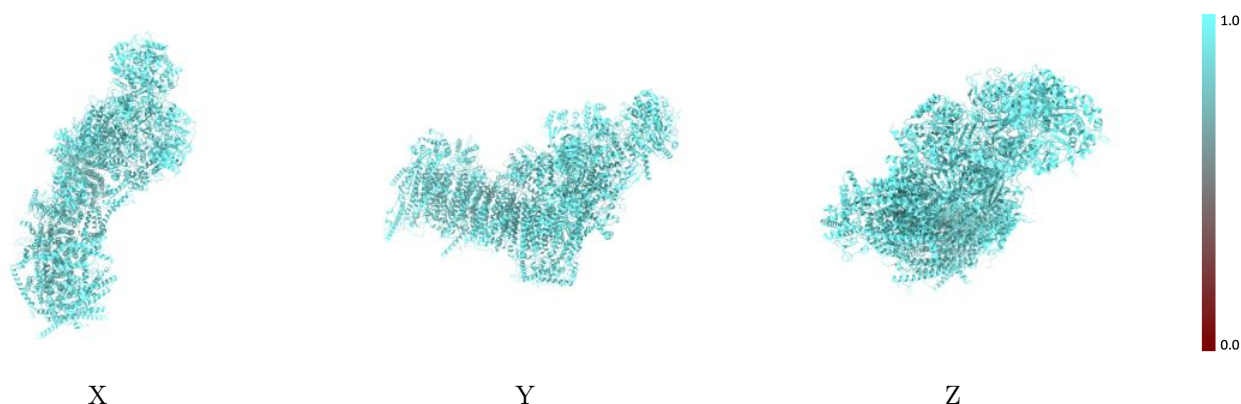
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



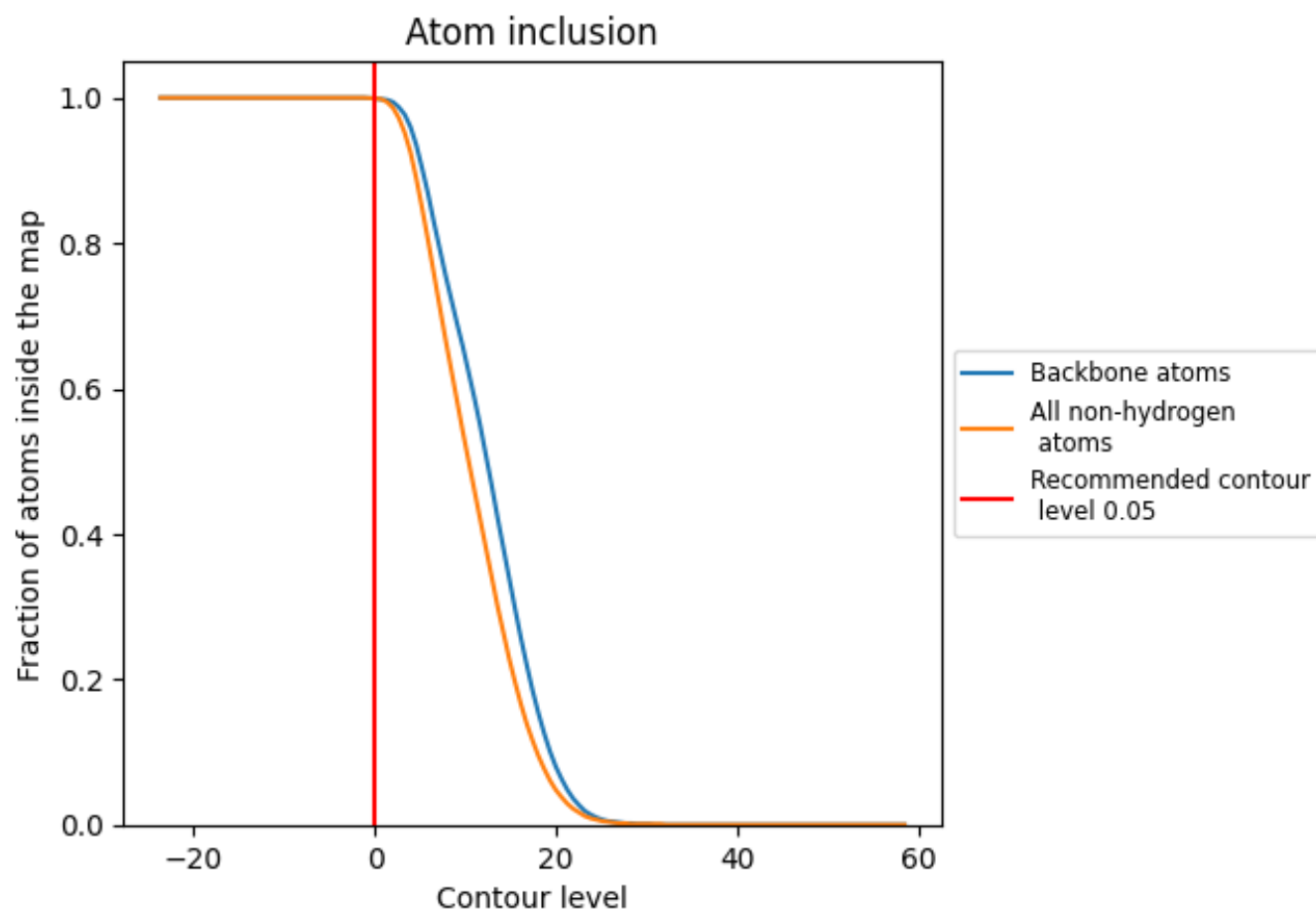
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.























Chain	Atom inclusion	Q-score
All	 0.9990	 0.5500
4L	 0.9990	 0.5330
A1	 1.0000	 0.5390
A2	 0.9970	 0.5430
A3	 1.0000	 0.5220
A5	 1.0000	 0.5030
A6	 1.0000	 0.5200
A7	 1.0000	 0.5290
A8	 0.9990	 0.5370
A9	 1.0000	 0.5060
AB	 1.0000	 0.3990
AC	 1.0000	 0.5670
AK	 0.9970	 0.5040
AL	 1.0000	 0.5380
AM	 0.9990	 0.5370
AN	 1.0000	 0.5280
B1	 1.0000	 0.5330
B2	 1.0000	 0.5560
B3	 1.0000	 0.5340
B4	 1.0000	 0.5590
B5	 0.9980	 0.5710
B6	 0.9990	 0.5370
B7	 1.0000	 0.5400
B8	 0.9990	 0.5680
B9	 0.9990	 0.5740
BK	 1.0000	 0.5500
BL	 0.9990	 0.5570
CA	 0.9980	 0.5290
CB	 1.0000	 0.5710
N1	 0.9990	 0.5400
N2	 1.0000	 0.5650
N3	 1.0000	 0.5210
N4	 0.9980	 0.5760
N5	 1.0000	 0.5730
N6	 1.0000	 0.4680



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Chain	Atom inclusion	Q-score
S1	 0.9990	 0.5810
S2	 0.9990	 0.5610
S3	 1.0000	 0.5730
S4	 1.0000	 0.5590
S5	 1.0000	 0.5230
S6	 0.9990	 0.5540
S7	 1.0000	 0.5580
S8	 0.9990	 0.5660
V1	 0.9970	 0.5730
V2	 0.9990	 0.5670
V3	 1.0000	 0.5720