



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 12:33 PM EDT

PDB ID : 9MXZ / pdb_00009mxz
EMDB ID : EMD-48724
Title : Lecithin:Cholesterol Acyltransferase Bound to Apolipoprotein A-I dimer in HDL
Authors : Coleman, B.; Bedi, S.; Hill, J.H.; Morris, J.; Manthei, K.A.; Hart, R.C.; He, Y.; Shah, A.S.; Jerome, W.G.; Vaisar, T.; Bornfeldt, K.E.; Song, H.; Segrest, J.P.; Heinecke, J.W.; Aller, S.G.; Tesmer, J.J.G.; Davidson, S.
Deposited on : 2025-01-21
Resolution : 9.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

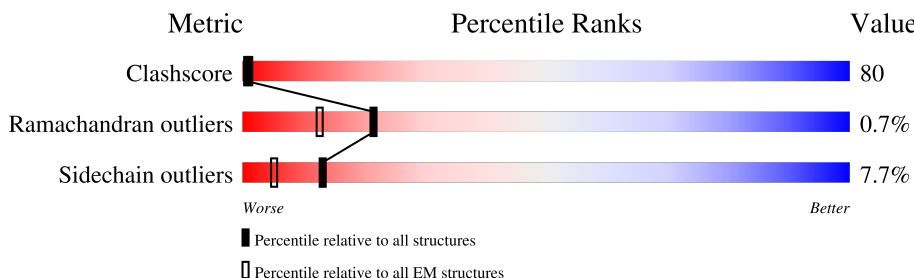
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	243	<div> <div>5%</div> <div>72%</div> <div>26%</div> <div>•</div> </div>
1	E	243	<div> <div>14%</div> <div>66%</div> <div>32%</div> <div>•</div> </div>
2	B	396	<div> <div>•</div> <div>72%</div> <div>20%</div> <div>•</div> <div>7%</div> </div>
2	C	396	<div> <div>12%</div> <div>71%</div> <div>21%</div> <div>•</div> <div>7%</div> </div>

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
3	6PL	A	502	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	6PL	A	503	-	-	X	-
3	6PL	A	504	-	-	X	-
3	6PL	A	505	-	-	X	-
3	6PL	A	506	-	-	X	-
3	6PL	A	508	-	-	X	-
3	6PL	A	509	-	-	X	-
3	6PL	A	510	-	-	X	-
3	6PL	A	511	-	-	X	-
3	6PL	A	512	-	-	X	-
3	6PL	A	513	-	-	X	-
3	6PL	A	515	-	-	X	-
3	6PL	A	516	-	-	X	-
3	6PL	A	517	-	-	X	-
3	6PL	A	518	-	-	X	-
3	6PL	A	519	-	-	X	-
3	6PL	A	520	-	-	X	-
3	6PL	A	521	-	-	X	-
3	6PL	A	522	-	-	X	-
3	6PL	A	523	-	-	X	-
3	6PL	A	524	-	-	X	-
3	6PL	A	525	-	-	X	-
3	6PL	A	526	-	-	X	-
3	6PL	A	527	-	-	X	-
3	6PL	A	528	-	-	X	-
3	6PL	A	529	-	-	X	-
3	6PL	A	530	-	-	X	-
3	6PL	A	531	-	-	X	-
3	6PL	A	532	-	-	X	-
3	6PL	A	533	-	-	X	-
3	6PL	A	534	-	-	X	-
3	6PL	A	535	-	-	X	-
3	6PL	A	536	-	-	X	-
3	6PL	A	537	-	-	X	-
3	6PL	A	538	-	-	X	-
3	6PL	A	539	-	-	X	-
3	6PL	A	540	-	-	X	-
3	6PL	A	541	-	-	X	-
3	6PL	A	542	-	-	X	-
3	6PL	A	543	-	-	X	-
3	6PL	A	544	-	-	X	-
3	6PL	A	546	-	-	X	-
3	6PL	A	548	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	6PL	A	549	-	-	X	-
3	6PL	A	550	-	-	X	-
3	6PL	A	552	-	-	X	-
3	6PL	A	554	-	-	X	-
3	6PL	A	555	-	-	X	-
3	6PL	A	556	-	-	X	-
3	6PL	A	557	-	-	X	-
3	6PL	A	558	-	-	X	-
3	6PL	A	559	-	-	X	-
3	6PL	A	560	-	-	X	-
3	6PL	A	562	-	-	X	-
3	6PL	A	563	-	-	X	-
3	6PL	A	564	-	-	X	-
3	6PL	A	565	-	-	X	-
3	6PL	A	566	-	-	X	-
3	6PL	A	567	-	-	X	-
3	6PL	A	570	-	-	X	-
3	6PL	A	571	-	-	X	-
3	6PL	A	572	-	-	X	-
3	6PL	A	573	-	-	X	-
3	6PL	A	574	-	-	X	-
3	6PL	A	575	-	-	X	-
3	6PL	A	576	-	-	X	-
3	6PL	A	578	-	-	X	-
3	6PL	A	579	-	-	X	-
3	6PL	A	580	-	-	X	-
3	6PL	A	581	-	-	X	-
3	6PL	A	582	-	-	X	-
3	6PL	A	584	-	-	X	-
3	6PL	A	587	-	-	X	-
3	6PL	A	588	-	-	X	-
3	6PL	C	501	-	-	X	-
3	6PL	E	301	-	-	X	-
3	6PL	E	302	-	-	X	-
3	6PL	E	304	-	-	X	-
3	6PL	E	306	-	-	X	-
3	6PL	E	308	-	-	X	-
3	6PL	E	309	-	-	X	-
3	6PL	E	310	-	-	X	-
3	6PL	E	312	-	-	X	-
3	6PL	E	315	-	-	X	-
3	6PL	E	317	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	6PL	E	318	-	-	X	-
3	6PL	E	320	-	-	X	-
3	6PL	E	321	-	-	X	-
3	6PL	E	322	-	-	X	-
3	6PL	E	323	-	-	X	-
3	6PL	E	324	-	-	X	-
3	6PL	E	325	-	-	X	-
3	6PL	E	326	-	-	X	-
3	6PL	E	328	-	-	X	-
3	6PL	E	329	-	-	X	-
3	6PL	E	330	-	-	X	-
3	6PL	E	331	-	-	X	-
3	6PL	E	332	-	-	X	-
3	6PL	E	333	-	-	X	-
3	6PL	E	335	-	-	X	-
3	6PL	E	337	-	-	X	-
3	6PL	E	339	-	-	X	-
3	6PL	E	340	-	-	X	-
3	6PL	E	341	-	-	X	-
3	6PL	E	344	-	-	X	-
3	6PL	E	345	-	-	X	-
3	6PL	E	346	-	-	X	-
3	6PL	E	347	-	-	X	-
3	6PL	E	348	-	-	X	-
3	6PL	E	350	-	-	X	-
3	6PL	E	351	-	-	X	-
3	6PL	E	353	-	-	X	-
3	6PL	E	355	-	-	X	-
3	6PL	E	356	-	-	X	-
3	6PL	E	357	-	-	X	-
3	6PL	E	358	-	-	X	-
3	6PL	E	359	-	-	X	-
3	6PL	E	360	-	-	X	-
3	6PL	E	361	-	-	X	-
3	6PL	E	362	-	-	X	-
3	6PL	E	363	-	-	X	-
3	6PL	E	364	-	-	X	-
3	6PL	E	365	-	-	X	-
3	6PL	E	366	-	-	X	-
3	6PL	E	367	-	-	X	-
3	6PL	E	368	-	-	X	-
3	6PL	E	369	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20264 atoms, of which 2138 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 Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	E	243	Total	C	H	N	O	S	0	0
			2438	1241	459	347	388	3		
1	A	243	Total	C	H	N	O	S	0	0
			2438	1241	459	347	388	3		

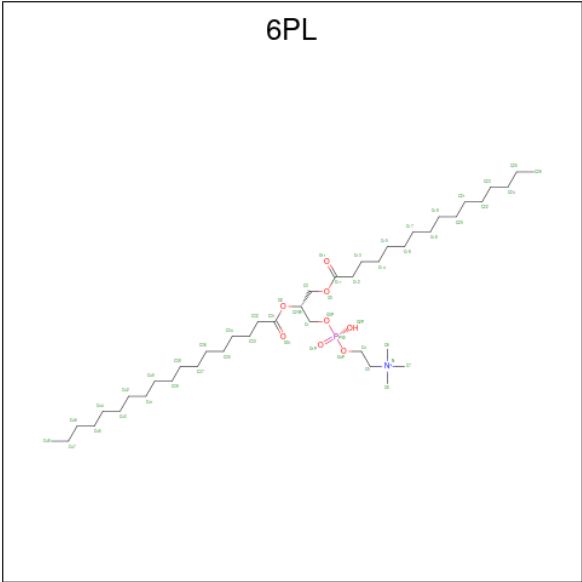
- Molecule 2 is a protein called Phosphatidylcholine-sterol acyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	369	Total	C	H	N	O	S	0	0
			3586	1930	610	501	532	13		
2	C	369	Total	C	H	N	O	S	0	0
			3586	1930	610	501	532	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	31	TYR	CYS	conflict	UNP P04180
C	31	TYR	CYS	conflict	UNP P04180

- Molecule 3 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
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			52	42	1	8	1	

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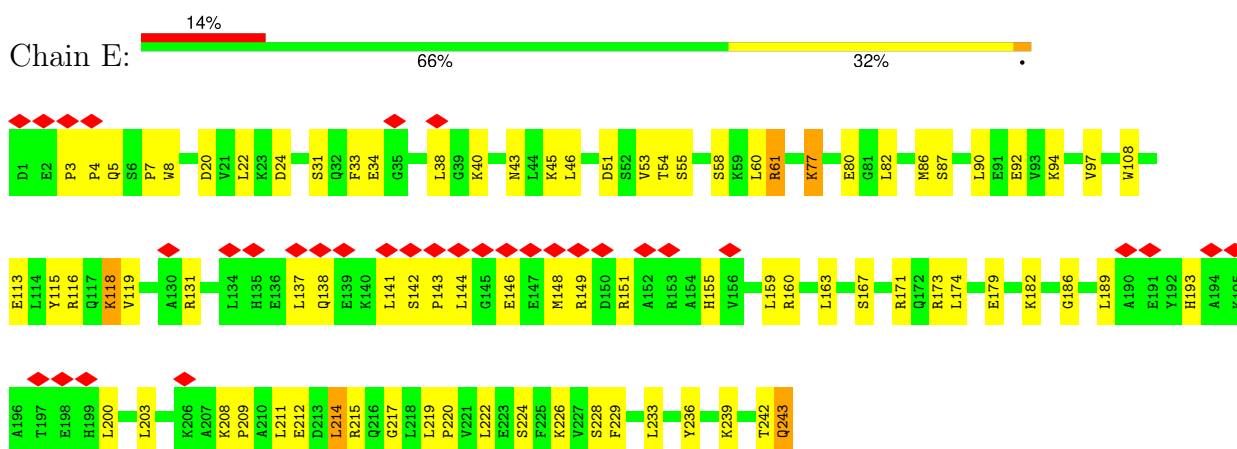
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Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	

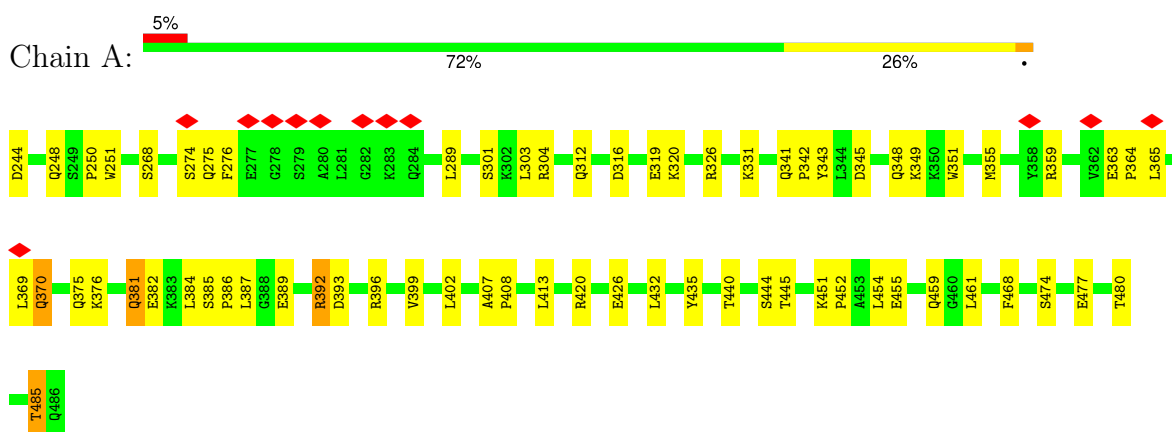
3 Residue-property plots

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.

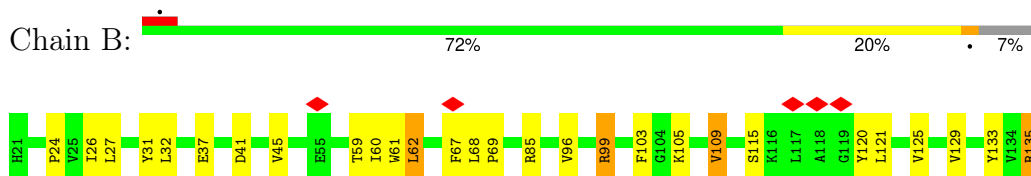
• Molecule 1: Apolipoprotein A-I

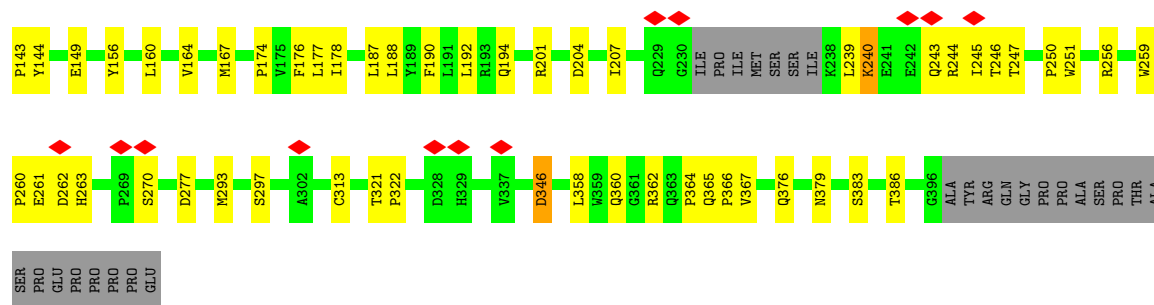


• Molecule 1: Apolipoprotein A-I

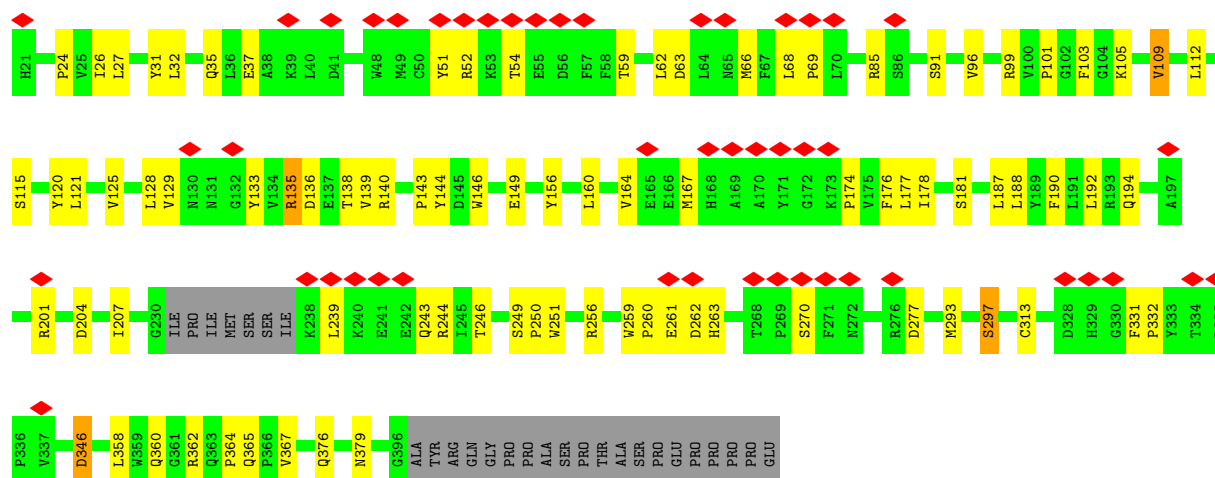


• Molecule 2: Phosphatidylcholine-sterol acyltransferase





• Molecule 2: Phosphatidylcholine-sterol acyltransferase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.599	Depositor
Minimum map value	-0.233	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	246.96, 246.96, 246.96	wwPDB
Map dimensions	126, 126, 126	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.96, 1.96, 1.96	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6PL

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	A	0.29	0/2014	0.41	0/2714
1	E	0.29	0/2014	0.43	0/2714
2	B	0.30	0/3070	0.46	0/4187
2	C	0.30	0/3070	0.47	0/4187
All	All	0.30	0/10168	0.45	0/13802

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	1	0
2	B	2	0
2	C	1	0
All	All	4	0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	38	LEU	CA
2	B	61	TRP	CA
2	B	62	LEU	CA
2	C	62	LEU	CA

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	A	1979	459	1965	80	0
1	E	1979	459	1968	97	0
2	B	2976	610	2884	45	0
2	C	2976	610	2884	43	0
3	A	4576	0	7392	1947	0
3	C	52	0	84	45	0
3	E	3588	0	5796	1433	0
All	All	18126	2138	22973	3278	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 80.

All (3278) 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)
3:E:306:6PL:H351	3:E:306:6PL:C16	1.60	1.31
3:E:306:6PL:H162	3:E:306:6PL:C35	1.59	1.30
3:A:525:6PL:H51	3:A:583:6PL:H321	1.21	1.19
3:A:549:6PL:C41	3:A:555:6PL:H262	1.71	1.19
3:A:541:6PL:H402	3:A:541:6PL:H441	1.23	1.18
3:A:506:6PL:H441	3:A:506:6PL:H482	1.18	1.18
3:A:502:6PL:O11	3:A:505:6PL:H142	1.39	1.17
3:E:367:6PL:H142	3:A:526:6PL:H381	1.17	1.16
3:A:535:6PL:H172	3:A:564:6PL:H461	1.25	1.16
3:A:550:6PL:H263	3:A:550:6PL:H221	1.19	1.16
3:E:346:6PL:H382	3:A:553:6PL:H471	1.20	1.16
3:A:527:6PL:H331	3:A:564:6PL:H202	1.28	1.15
3:A:588:6PL:H482	3:A:588:6PL:H441	1.26	1.15
3:A:532:6PL:H462	3:A:562:6PL:H432	1.18	1.15
3:E:304:6PL:H161	3:E:331:6PL:H32	1.29	1.15
3:A:520:6PL:H483	3:A:542:6PL:H422	1.25	1.15
3:E:324:6PL:H342	3:A:503:6PL:C3	1.77	1.14
3:E:332:6PL:H421	3:E:357:6PL:H241	1.26	1.14
3:E:357:6PL:H122	3:E:357:6PL:H352	1.29	1.14
3:A:542:6PL:H151	3:A:581:6PL:H182	1.21	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:359:6PL:H402	3:A:586:6PL:H432	1.17	1.13
3:A:543:6PL:H412	3:A:566:6PL:H441	1.28	1.13
3:A:572:6PL:C40	3:A:576:6PL:H172	1.78	1.13
3:E:320:6PL:H181	3:E:369:6PL:H462	1.30	1.13
3:E:350:6PL:H122	3:E:360:6PL:H181	1.31	1.12
3:A:507:6PL:H361	3:A:507:6PL:H322	1.26	1.12
3:A:512:6PL:H2	3:A:587:6PL:H71	1.20	1.12
3:A:512:6PL:H52	3:A:524:6PL:C12	1.80	1.12
3:A:579:6PL:H142	3:A:583:6PL:H192	1.15	1.12
3:E:336:6PL:H392	3:E:336:6PL:H432	1.31	1.12
3:E:333:6PL:H421	3:E:363:6PL:H121	1.22	1.11
3:A:573:6PL:C34	3:A:575:6PL:H202	1.81	1.11
3:E:324:6PL:H342	3:A:503:6PL:H32	1.14	1.11
3:A:549:6PL:H411	3:A:555:6PL:H262	1.12	1.11
3:E:332:6PL:H11	3:E:332:6PL:H82	1.24	1.11
3:A:546:6PL:H342	3:A:554:6PL:H32	1.30	1.11
3:E:306:6PL:H391	3:E:350:6PL:H121	1.11	1.10
3:A:503:6PL:H322	3:A:504:6PL:H121	1.29	1.10
3:A:515:6PL:H432	3:A:515:6PL:H472	1.13	1.10
3:A:540:6PL:H352	3:A:550:6PL:H141	1.14	1.10
1:E:167:SER:HB2	3:E:346:6PL:H121	1.32	1.10
3:A:539:6PL:H412	3:A:571:6PL:H391	1.18	1.10
3:A:542:6PL:C21	3:A:542:6PL:H421	1.81	1.10
3:A:578:6PL:H421	3:A:578:6PL:H461	1.31	1.10
3:E:301:6PL:H482	3:E:317:6PL:H222	1.24	1.10
3:E:310:6PL:H132	3:E:331:6PL:H161	1.27	1.10
3:E:325:6PL:H181	3:E:325:6PL:H221	1.31	1.10
3:E:346:6PL:H382	3:A:553:6PL:C47	1.80	1.10
3:A:552:6PL:H372	3:A:570:6PL:H241	1.31	1.10
3:A:523:6PL:H362	3:A:544:6PL:H12	1.30	1.09
3:A:512:6PL:H182	3:A:585:6PL:H231	1.31	1.09
3:E:328:6PL:H451	3:A:549:6PL:C26	1.82	1.09
3:C:501:6PL:H142	3:C:501:6PL:H372	1.29	1.09
3:A:505:6PL:H12	3:A:506:6PL:H83	1.35	1.09
3:A:540:6PL:H391	3:A:540:6PL:H132	1.26	1.09
3:E:319:6PL:H251	3:E:363:6PL:H221	1.17	1.08
3:A:518:6PL:H451	3:A:560:6PL:H432	1.11	1.08
3:E:352:6PL:H121	3:E:352:6PL:H161	1.26	1.08
3:E:346:6PL:H422	3:E:346:6PL:H381	1.26	1.08
3:E:353:6PL:H262	3:A:566:6PL:H481	1.31	1.08
3:A:534:6PL:H362	3:A:534:6PL:H161	1.30	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:515:6PL:H252	3:A:555:6PL:H472	1.36	1.08
3:E:324:6PL:H341	3:E:358:6PL:H442	1.36	1.07
3:A:522:6PL:C15	3:A:522:6PL:H342	1.85	1.07
3:A:542:6PL:C15	3:A:581:6PL:H182	1.83	1.07
3:E:333:6PL:H192	3:A:511:6PL:H411	1.12	1.07
3:A:566:6PL:C1	3:A:578:6PL:H52	1.84	1.07
3:A:528:6PL:H192	3:A:528:6PL:H232	1.30	1.07
3:A:549:6PL:H321	3:A:555:6PL:H162	1.32	1.06
3:A:573:6PL:H342	3:A:575:6PL:H202	1.11	1.06
3:E:317:6PL:H172	3:A:508:6PL:H251	1.26	1.06
3:A:541:6PL:H361	3:A:557:6PL:H381	1.12	1.06
3:E:318:6PL:H242	3:A:518:6PL:C46	1.85	1.06
3:A:526:6PL:H231	3:A:550:6PL:H192	1.32	1.06
3:A:525:6PL:H171	3:A:583:6PL:H251	1.30	1.06
3:A:534:6PL:H152	3:A:534:6PL:H192	1.33	1.06
3:A:526:6PL:H131	3:A:575:6PL:H161	1.32	1.05
3:E:321:6PL:H2	3:E:344:6PL:H81	1.38	1.05
3:E:310:6PL:H263	3:E:357:6PL:H211	1.09	1.05
3:E:317:6PL:H331	3:A:508:6PL:C20	1.85	1.05
3:E:340:6PL:H361	3:E:340:6PL:H401	1.34	1.05
3:E:337:6PL:H122	3:E:337:6PL:H341	1.35	1.04
3:A:549:6PL:H341	3:A:555:6PL:H171	1.09	1.04
3:A:503:6PL:H412	3:A:560:6PL:H263	1.39	1.04
3:A:530:6PL:H171	3:A:535:6PL:H361	1.07	1.04
3:A:548:6PL:H402	3:A:548:6PL:H172	1.35	1.04
3:A:565:6PL:H332	3:A:580:6PL:H31	1.35	1.04
3:A:570:6PL:H481	3:A:582:6PL:C13	1.86	1.04
3:A:541:6PL:C3	3:A:557:6PL:H431	1.86	1.04
3:A:520:6PL:H351	3:A:542:6PL:H332	1.40	1.04
3:A:529:6PL:H41	3:A:529:6PL:H2	1.37	1.04
3:E:330:6PL:H191	3:A:537:6PL:H232	1.37	1.03
3:E:348:6PL:H73	3:E:355:6PL:H131	1.35	1.03
3:E:322:6PL:C12	3:E:365:6PL:H391	1.88	1.03
3:E:335:6PL:H221	3:E:356:6PL:H231	1.08	1.03
3:E:357:6PL:H82	3:E:357:6PL:H2	1.41	1.03
3:A:584:6PL:H362	3:A:584:6PL:H412	1.35	1.03
3:E:362:6PL:H381	3:E:362:6PL:H422	1.41	1.02
3:A:587:6PL:H402	3:A:587:6PL:H162	1.39	1.02
3:A:552:6PL:H361	3:A:552:6PL:H481	1.41	1.02
1:E:148:MET:HG2	3:C:501:6PL:H252	1.38	1.02
3:E:316:6PL:H321	3:E:327:6PL:H331	1.36	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:340:6PL:H451	3:E:350:6PL:H441	1.39	1.02
3:A:543:6PL:H341	3:A:581:6PL:H152	1.39	1.02
3:E:318:6PL:H222	3:E:331:6PL:H252	1.41	1.02
3:A:519:6PL:H421	3:A:519:6PL:H263	1.40	1.02
3:A:548:6PL:H12	3:A:548:6PL:H52	1.42	1.02
3:A:546:6PL:H431	3:A:554:6PL:H381	1.37	1.01
3:A:558:6PL:O31	3:A:558:6PL:H12	1.58	1.01
3:A:520:6PL:H141	3:A:542:6PL:H352	1.43	1.01
3:E:353:6PL:O4P	3:E:353:6PL:H63	1.55	1.01
3:A:518:6PL:H431	3:A:558:6PL:H451	1.43	1.01
3:E:317:6PL:H331	3:A:508:6PL:H202	1.36	1.01
3:E:329:6PL:C5	3:E:366:6PL:H131	1.90	1.00
3:E:333:6PL:H372	3:E:363:6PL:H132	1.43	1.00
3:A:508:6PL:H452	3:A:510:6PL:H371	1.39	1.00
3:A:541:6PL:H402	3:A:541:6PL:C44	1.90	1.00
3:E:333:6PL:C37	3:E:363:6PL:H132	1.90	1.00
3:E:335:6PL:C22	3:E:356:6PL:H231	1.91	1.00
3:A:509:6PL:H62	3:A:509:6PL:O4P	1.61	1.00
3:E:321:6PL:H11	3:E:365:6PL:H31	1.44	1.00
3:A:516:6PL:H261	3:A:563:6PL:H231	1.42	1.00
3:E:309:6PL:H131	3:E:344:6PL:H63	1.37	1.00
3:E:321:6PL:H142	3:E:365:6PL:H142	1.44	1.00
3:E:346:6PL:C38	3:A:553:6PL:H471	1.90	1.00
3:A:535:6PL:H42	3:A:564:6PL:O1P	1.61	1.00
3:A:523:6PL:H382	3:A:572:6PL:H142	1.41	1.00
3:E:322:6PL:H121	3:E:365:6PL:H391	1.00	0.99
3:E:369:6PL:H362	3:E:369:6PL:H402	1.44	0.99
3:A:543:6PL:H441	3:A:580:6PL:H261	1.43	0.99
3:A:513:6PL:H421	3:A:552:6PL:H411	1.42	0.99
3:A:518:6PL:H341	3:A:532:6PL:H391	1.43	0.99
3:A:532:6PL:H191	3:A:541:6PL:H372	1.44	0.99
3:A:546:6PL:H392	3:A:568:6PL:H132	1.40	0.99
3:E:369:6PL:H152	3:A:533:6PL:H321	1.40	0.99
3:A:520:6PL:H451	3:A:542:6PL:H422	1.43	0.99
3:A:535:6PL:H351	3:A:564:6PL:H392	1.40	0.99
3:A:542:6PL:C41	3:A:556:6PL:H211	1.92	0.99
3:E:319:6PL:C25	3:E:363:6PL:H221	1.93	0.99
3:E:320:6PL:H202	3:E:369:6PL:H441	1.42	0.99
3:E:304:6PL:H191	3:E:355:6PL:H481	1.44	0.99
3:A:531:6PL:H331	3:A:555:6PL:O2	1.61	0.99
3:A:533:6PL:H141	3:A:579:6PL:H202	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:528:6PL:H422	3:A:528:6PL:H221	1.44	0.98
3:A:541:6PL:H31	3:A:557:6PL:H431	1.42	0.98
3:A:549:6PL:C34	3:A:555:6PL:H171	1.91	0.98
3:A:530:6PL:C17	3:A:535:6PL:H361	1.93	0.98
3:E:336:6PL:H382	3:E:362:6PL:H382	1.42	0.98
3:E:309:6PL:H131	3:E:344:6PL:C6	1.94	0.98
3:E:320:6PL:H381	3:E:338:6PL:H392	1.43	0.98
3:A:505:6PL:H62	3:A:505:6PL:O4P	1.63	0.98
3:A:511:6PL:H401	3:A:511:6PL:H362	1.42	0.98
3:A:520:6PL:C48	3:A:542:6PL:H441	1.91	0.98
3:A:537:6PL:H162	3:A:549:6PL:C24	1.93	0.98
3:E:341:6PL:H472	3:E:360:6PL:H261	1.43	0.98
3:A:532:6PL:H82	3:A:551:6PL:O11	1.64	0.98
3:A:542:6PL:H421	3:A:542:6PL:H212	1.42	0.98
3:A:512:6PL:C5	3:A:524:6PL:H122	1.93	0.97
3:A:518:6PL:H182	3:A:529:6PL:H181	1.46	0.97
3:E:310:6PL:C26	3:E:357:6PL:H211	1.92	0.97
3:A:570:6PL:H481	3:A:582:6PL:H132	1.45	0.97
3:E:363:6PL:H412	3:E:364:6PL:H392	1.45	0.97
3:E:324:6PL:H341	3:E:358:6PL:C44	1.94	0.97
3:A:521:6PL:H231	3:A:557:6PL:H251	1.47	0.97
3:A:541:6PL:C36	3:A:557:6PL:H381	1.95	0.97
3:E:304:6PL:H341	3:E:355:6PL:H382	1.44	0.97
3:A:506:6PL:H63	3:A:506:6PL:P	2.05	0.97
3:E:302:6PL:H201	3:E:308:6PL:H211	1.45	0.97
3:E:344:6PL:H461	3:E:367:6PL:H231	1.47	0.97
3:E:353:6PL:H32	3:E:353:6PL:O31	1.65	0.97
3:A:520:6PL:H442	3:A:556:6PL:H242	1.46	0.97
3:A:515:6PL:H472	3:A:515:6PL:C43	1.95	0.97
3:A:537:6PL:H162	3:A:549:6PL:H241	0.98	0.97
3:A:544:6PL:H401	3:A:551:6PL:H261	1.43	0.97
3:E:325:6PL:H221	3:E:325:6PL:C18	1.95	0.96
3:E:333:6PL:H402	3:E:363:6PL:H141	1.44	0.96
3:A:512:6PL:H52	3:A:524:6PL:H122	0.99	0.96
3:E:321:6PL:H261	3:E:365:6PL:H241	1.45	0.96
3:E:322:6PL:H121	3:E:365:6PL:C39	1.94	0.96
3:A:506:6PL:H481	3:A:508:6PL:H482	1.42	0.96
3:A:572:6PL:C39	3:A:576:6PL:H172	1.94	0.96
3:E:338:6PL:H472	3:A:522:6PL:H231	1.47	0.96
3:E:340:6PL:H471	3:E:350:6PL:H421	1.47	0.96
3:E:324:6PL:C34	3:E:358:6PL:H442	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:520:6PL:H221	3:A:557:6PL:H182	1.46	0.96
3:A:529:6PL:H152	3:A:574:6PL:H331	1.45	0.96
3:A:505:6PL:H351	3:A:506:6PL:H382	1.45	0.96
3:A:520:6PL:H483	3:A:542:6PL:C42	1.96	0.96
3:A:532:6PL:C46	3:A:562:6PL:H432	1.94	0.96
3:E:309:6PL:H461	3:E:363:6PL:H251	1.46	0.96
3:A:502:6PL:H341	3:A:511:6PL:H142	1.47	0.96
3:A:502:6PL:H422	3:A:502:6PL:H192	1.44	0.96
3:E:355:6PL:H41	3:E:355:6PL:O2	1.66	0.95
3:A:533:6PL:H472	3:A:574:6PL:H141	1.47	0.95
3:A:552:6PL:O4P	3:A:552:6PL:H63	1.64	0.95
3:E:353:6PL:H481	3:A:542:6PL:H452	1.49	0.95
3:A:539:6PL:H412	3:A:571:6PL:C39	1.96	0.95
3:E:369:6PL:H402	3:E:369:6PL:C36	1.96	0.95
3:E:307:6PL:H73	3:E:311:6PL:O11	1.66	0.95
3:A:512:6PL:H2	3:A:587:6PL:C7	1.97	0.95
3:A:562:6PL:H11	3:A:562:6PL:C7	1.95	0.95
3:E:332:6PL:H262	3:E:357:6PL:H231	1.46	0.95
3:E:359:6PL:H342	3:A:537:6PL:H442	1.44	0.95
3:A:537:6PL:O4P	3:A:537:6PL:H62	1.66	0.95
3:A:545:6PL:H62	3:A:545:6PL:O4P	1.64	0.95
3:E:306:6PL:C39	3:E:350:6PL:H121	1.97	0.95
3:E:350:6PL:H122	3:E:360:6PL:C18	1.96	0.95
3:A:520:6PL:H62	3:A:520:6PL:O4P	1.66	0.95
3:E:333:6PL:C19	3:A:511:6PL:H411	1.97	0.94
3:A:542:6PL:O2P	3:A:581:6PL:H2	1.66	0.94
3:E:328:6PL:H202	3:A:537:6PL:H261	1.47	0.94
3:A:537:6PL:C16	3:A:549:6PL:H241	1.95	0.94
3:E:309:6PL:H122	3:E:326:6PL:H142	1.49	0.94
3:E:324:6PL:O4P	3:E:324:6PL:H63	1.67	0.94
3:E:369:6PL:H262	3:A:533:6PL:C45	1.97	0.94
3:E:306:6PL:H391	3:E:350:6PL:C12	1.96	0.94
3:E:317:6PL:H141	3:E:366:6PL:H382	1.50	0.94
3:A:506:6PL:H482	3:A:506:6PL:C44	1.96	0.94
3:E:309:6PL:H251	3:E:344:6PL:H192	1.50	0.94
3:E:303:6PL:O4P	3:E:303:6PL:H63	1.63	0.94
3:E:319:6PL:H251	3:E:363:6PL:C22	1.98	0.94
3:E:320:6PL:H401	3:A:533:6PL:H252	1.49	0.94
3:E:317:6PL:H152	3:A:508:6PL:H231	1.49	0.93
3:A:502:6PL:H372	3:A:505:6PL:H441	1.50	0.93
3:A:517:6PL:O4P	3:A:517:6PL:H63	1.65	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:566:6PL:H11	3:A:578:6PL:H52	1.48	0.93
3:E:321:6PL:H263	3:E:326:6PL:H262	1.50	0.93
3:A:530:6PL:H62	3:A:530:6PL:O4P	1.66	0.93
3:A:535:6PL:C16	3:A:564:6PL:H441	1.98	0.93
3:A:584:6PL:H62	3:A:584:6PL:O4P	1.64	0.93
3:E:367:6PL:H262	3:A:526:6PL:H451	1.49	0.93
3:E:343:6PL:H261	3:A:513:6PL:H482	1.48	0.93
3:A:541:6PL:H242	3:A:580:6PL:H391	1.51	0.93
3:E:326:6PL:H402	3:E:364:6PL:H12	1.50	0.93
3:A:516:6PL:O31	3:A:516:6PL:H12	1.66	0.93
3:A:505:6PL:H141	3:A:510:6PL:H122	1.49	0.93
3:A:523:6PL:O1P	3:A:559:6PL:H71	1.68	0.93
3:A:575:6PL:H12	3:A:575:6PL:O31	1.64	0.93
3:A:525:6PL:H83	3:A:556:6PL:H2	1.51	0.93
3:A:584:6PL:H412	3:A:584:6PL:C36	1.98	0.92
3:E:328:6PL:H451	3:A:549:6PL:H262	1.48	0.92
3:A:522:6PL:H371	3:A:536:6PL:H382	1.50	0.92
3:E:305:6PL:H62	3:E:305:6PL:O4P	1.66	0.92
3:A:505:6PL:H221	3:A:510:6PL:C20	1.98	0.92
3:A:580:6PL:H372	3:A:588:6PL:H202	1.52	0.92
3:E:348:6PL:O4P	3:E:348:6PL:H63	1.69	0.92
3:E:322:6PL:H331	3:E:365:6PL:H402	1.48	0.92
3:E:337:6PL:H12	3:E:337:6PL:C5	1.99	0.92
3:E:368:6PL:H141	3:A:513:6PL:C44	2.00	0.92
3:A:505:6PL:H331	3:A:506:6PL:H391	1.52	0.92
3:E:318:6PL:H331	3:E:324:6PL:H451	1.49	0.92
3:E:333:6PL:H192	3:A:511:6PL:C41	1.99	0.92
3:E:333:6PL:C41	3:E:363:6PL:H352	2.00	0.92
3:A:518:6PL:H451	3:A:560:6PL:C43	2.00	0.92
3:E:301:6PL:H72	3:E:307:6PL:O2P	1.69	0.91
3:E:358:6PL:H431	3:E:358:6PL:H392	1.50	0.91
3:A:547:6PL:H391	3:A:555:6PL:H452	1.51	0.91
3:E:369:6PL:H62	3:E:369:6PL:C1	2.00	0.91
3:A:540:6PL:H372	3:A:540:6PL:H131	1.51	0.91
3:E:337:6PL:H392	3:E:337:6PL:H162	1.52	0.91
3:E:357:6PL:H122	3:E:357:6PL:C35	2.00	0.91
3:A:524:6PL:H472	3:A:585:6PL:H212	1.51	0.91
3:A:588:6PL:H32	3:A:588:6PL:O2P	1.70	0.91
3:E:304:6PL:H161	3:E:331:6PL:C3	2.00	0.91
3:A:539:6PL:C41	3:A:571:6PL:H391	1.99	0.91
3:A:552:6PL:H372	3:A:570:6PL:C24	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:565:6PL:C33	3:A:580:6PL:H31	2.00	0.91
3:A:526:6PL:H242	3:A:575:6PL:H262	1.51	0.91
3:E:329:6PL:H41	3:E:340:6PL:O11	1.71	0.91
1:E:226:LYS:HG3	3:E:327:6PL:H151	1.52	0.91
3:A:519:6PL:H251	3:A:549:6PL:H442	1.53	0.91
3:E:304:6PL:C47	3:E:308:6PL:H241	2.00	0.91
3:E:318:6PL:H242	3:A:518:6PL:H461	1.51	0.91
3:A:518:6PL:H332	3:A:532:6PL:H371	1.51	0.91
3:A:549:6PL:H321	3:A:555:6PL:C16	2.00	0.91
3:A:510:6PL:C4	3:A:510:6PL:H2	2.01	0.90
3:A:520:6PL:H152	3:A:542:6PL:C38	2.01	0.90
3:A:527:6PL:H352	3:A:530:6PL:H361	1.53	0.90
3:A:540:6PL:H371	3:A:550:6PL:C16	2.01	0.90
3:A:524:6PL:H231	3:A:540:6PL:H362	1.51	0.90
3:A:557:6PL:O11	3:A:565:6PL:H82	1.70	0.90
3:A:535:6PL:H83	3:A:564:6PL:O1P	1.71	0.90
3:E:335:6PL:H221	3:E:356:6PL:C23	1.98	0.90
3:A:503:6PL:H41	3:A:504:6PL:H31	1.53	0.90
3:A:532:6PL:H122	3:A:560:6PL:H351	1.51	0.90
3:E:310:6PL:H32	3:E:331:6PL:C13	2.02	0.90
3:E:358:6PL:H232	3:A:509:6PL:H152	1.54	0.90
3:A:502:6PL:O3	3:A:511:6PL:H122	1.71	0.90
3:E:358:6PL:H172	3:A:509:6PL:O2	1.71	0.90
3:E:302:6PL:C20	3:E:308:6PL:H211	2.01	0.90
3:E:304:6PL:H472	3:E:308:6PL:H241	1.51	0.90
3:E:309:6PL:H241	3:E:344:6PL:H171	1.54	0.90
1:E:163:LEU:HD13	3:A:554:6PL:H472	1.53	0.90
3:A:524:6PL:H471	3:A:528:6PL:H252	1.53	0.90
3:A:558:6PL:H483	3:A:574:6PL:H222	1.51	0.90
3:A:512:6PL:O31	3:A:587:6PL:H81	1.72	0.89
3:A:515:6PL:H432	3:A:515:6PL:C47	2.01	0.89
3:E:329:6PL:H51	3:E:366:6PL:H131	1.53	0.89
3:A:519:6PL:H421	3:A:519:6PL:C26	2.00	0.89
3:A:538:6PL:H442	3:A:542:6PL:H221	1.51	0.89
3:A:543:6PL:H412	3:A:566:6PL:C44	2.02	0.89
3:E:304:6PL:H452	3:E:308:6PL:H221	1.53	0.89
3:E:310:6PL:H131	3:E:318:6PL:H342	1.55	0.89
3:E:328:6PL:O11	3:E:330:6PL:H172	1.72	0.89
3:A:526:6PL:H162	3:A:575:6PL:H172	1.53	0.89
3:A:566:6PL:H242	3:A:578:6PL:H422	1.55	0.89
3:A:512:6PL:H263	3:A:587:6PL:H231	1.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:574:6PL:H72	3:A:574:6PL:O1P	1.72	0.89
3:E:340:6PL:H331	3:E:342:6PL:H181	1.53	0.89
3:A:580:6PL:H392	3:A:588:6PL:H202	1.55	0.89
3:E:358:6PL:H221	3:A:509:6PL:H182	1.55	0.88
3:E:367:6PL:C14	3:A:526:6PL:H381	2.01	0.88
3:E:332:6PL:O4P	3:E:332:6PL:H63	1.72	0.88
3:A:532:6PL:H172	3:A:557:6PL:H422	1.52	0.88
3:E:328:6PL:H451	3:A:549:6PL:H261	1.56	0.88
1:A:426:GLU:OE2	3:A:519:6PL:H52	1.73	0.88
3:A:515:6PL:O31	3:A:515:6PL:H12	1.70	0.88
3:A:548:6PL:H52	3:A:548:6PL:C1	2.03	0.88
3:A:550:6PL:H221	3:A:550:6PL:C26	2.03	0.88
3:E:315:6PL:H182	3:E:323:6PL:H372	1.55	0.88
3:E:317:6PL:C17	3:A:508:6PL:H251	2.03	0.88
3:E:324:6PL:H361	3:E:358:6PL:H432	1.52	0.88
3:E:353:6PL:H382	3:E:353:6PL:H172	1.55	0.88
3:A:527:6PL:O3	3:A:564:6PL:H181	1.73	0.88
3:E:333:6PL:H412	3:E:363:6PL:H352	1.55	0.88
3:A:503:6PL:H412	3:A:560:6PL:C26	2.02	0.88
3:E:368:6PL:H162	3:A:554:6PL:H231	1.56	0.88
3:A:505:6PL:H352	3:A:506:6PL:H321	1.56	0.88
3:A:527:6PL:H151	3:A:571:6PL:O2	1.74	0.88
3:E:344:6PL:H202	3:E:344:6PL:H462	1.56	0.88
3:A:520:6PL:H442	3:A:556:6PL:C24	2.03	0.88
3:A:531:6PL:H131	3:A:547:6PL:H361	1.56	0.88
3:A:510:6PL:H2	3:A:510:6PL:O4P	1.74	0.87
3:A:524:6PL:H441	3:A:528:6PL:H181	1.55	0.87
1:E:90:LEU:HD22	3:E:349:6PL:H192	1.56	0.87
3:A:541:6PL:H241	3:A:580:6PL:H401	1.54	0.87
3:E:340:6PL:H262	3:A:513:6PL:H252	1.54	0.87
3:A:559:6PL:O2P	3:A:559:6PL:H52	1.75	0.87
3:A:513:6PL:H2	3:A:513:6PL:O11	1.74	0.87
3:A:524:6PL:H452	3:A:528:6PL:H263	1.55	0.87
3:E:359:6PL:O4P	3:E:359:6PL:H63	1.73	0.87
3:E:368:6PL:H141	3:A:513:6PL:C43	2.04	0.87
3:A:542:6PL:H412	3:A:556:6PL:H211	1.56	0.87
3:A:535:6PL:H161	3:A:564:6PL:H441	1.54	0.87
3:A:541:6PL:H31	3:A:557:6PL:C43	2.04	0.87
3:A:572:6PL:H401	3:A:576:6PL:H172	1.57	0.87
3:E:309:6PL:H322	3:E:325:6PL:H122	1.56	0.87
3:E:331:6PL:O4P	3:E:331:6PL:H63	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:359:6PL:H331	3:A:537:6PL:H462	1.57	0.87
3:A:511:6PL:O1P	3:A:511:6PL:H52	1.72	0.87
3:A:531:6PL:H142	3:A:531:6PL:H361	1.56	0.87
3:A:543:6PL:H172	3:A:566:6PL:H351	1.56	0.87
3:A:520:6PL:H351	3:A:542:6PL:C33	2.03	0.87
3:A:512:6PL:H31	3:A:524:6PL:H412	1.56	0.86
3:A:580:6PL:H152	3:A:581:6PL:H421	1.57	0.86
3:E:311:6PL:H321	3:E:342:6PL:H83	1.55	0.86
3:A:505:6PL:C22	3:A:510:6PL:H201	2.05	0.86
3:A:530:6PL:H171	3:A:535:6PL:C36	2.02	0.86
3:E:314:6PL:H431	3:A:508:6PL:H421	1.57	0.86
3:E:324:6PL:H122	3:E:349:6PL:H211	1.57	0.86
3:A:540:6PL:H371	3:A:550:6PL:H151	1.56	0.86
3:A:572:6PL:H391	3:A:576:6PL:H151	1.55	0.86
3:A:577:6PL:O4P	3:A:577:6PL:H63	1.73	0.86
3:E:309:6PL:H242	3:E:309:6PL:H462	1.57	0.86
3:E:310:6PL:H32	3:E:331:6PL:H132	1.58	0.86
3:E:321:6PL:H142	3:E:365:6PL:C14	2.05	0.86
3:A:502:6PL:C37	3:A:505:6PL:H441	2.04	0.86
3:A:546:6PL:C34	3:A:554:6PL:H32	2.05	0.86
3:E:348:6PL:H73	3:E:355:6PL:C13	2.05	0.86
3:A:536:6PL:O4P	3:A:536:6PL:H83	1.74	0.86
3:E:318:6PL:H371	3:E:331:6PL:H172	1.58	0.86
3:A:517:6PL:H361	3:A:533:6PL:O2P	1.76	0.86
3:A:578:6PL:H461	3:A:578:6PL:C42	2.05	0.86
3:E:309:6PL:H51	3:E:325:6PL:O11	1.76	0.86
3:E:319:6PL:H222	3:E:363:6PL:H232	1.57	0.86
3:A:520:6PL:H483	3:A:542:6PL:H441	1.58	0.86
3:A:566:6PL:H12	3:A:578:6PL:H52	1.57	0.86
3:E:321:6PL:H11	3:E:365:6PL:C3	2.06	0.85
3:A:503:6PL:C4	3:A:504:6PL:H31	2.06	0.85
3:A:516:6PL:H391	3:A:586:6PL:O3P	1.76	0.85
3:E:304:6PL:H341	3:E:355:6PL:C38	2.05	0.85
3:E:306:6PL:H482	3:A:513:6PL:H222	1.57	0.85
3:A:525:6PL:H83	3:A:556:6PL:O11	1.76	0.85
3:A:548:6PL:H32	3:A:548:6PL:O31	1.75	0.85
3:E:330:6PL:H452	3:A:537:6PL:H242	1.57	0.85
3:A:518:6PL:H402	3:A:518:6PL:H441	1.57	0.85
3:A:518:6PL:O31	3:A:560:6PL:H321	1.76	0.85
3:E:302:6PL:H212	3:E:308:6PL:H231	1.58	0.85
3:E:308:6PL:H371	3:E:326:6PL:H441	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:540:6PL:H391	3:A:540:6PL:C13	2.06	0.85
3:E:304:6PL:H392	3:E:357:6PL:H362	1.58	0.85
3:A:527:6PL:H263	3:A:535:6PL:H483	1.56	0.85
3:E:322:6PL:H263	3:E:339:6PL:H402	1.56	0.85
3:A:513:6PL:H421	3:A:552:6PL:C41	2.07	0.85
3:E:306:6PL:H471	3:A:582:6PL:H483	1.59	0.84
3:E:323:6PL:H432	3:E:355:6PL:H262	1.59	0.84
3:E:325:6PL:H262	3:E:363:6PL:C20	2.07	0.84
3:A:510:6PL:O4P	3:A:510:6PL:H62	1.77	0.84
3:A:540:6PL:H371	3:A:550:6PL:C15	2.06	0.84
3:A:512:6PL:O11	3:A:585:6PL:H171	1.76	0.84
3:A:565:6PL:H162	3:A:580:6PL:C41	2.08	0.84
3:E:337:6PL:H52	3:E:337:6PL:C1	2.06	0.84
3:E:345:6PL:H51	3:C:501:6PL:H362	1.57	0.84
3:A:521:6PL:O3	3:A:562:6PL:H142	1.76	0.84
3:A:521:6PL:H121	3:A:562:6PL:H151	1.58	0.84
3:A:533:6PL:H441	3:A:574:6PL:H141	1.59	0.84
3:A:572:6PL:H72	3:A:572:6PL:O1P	1.77	0.84
3:E:303:6PL:H122	3:E:362:6PL:H52	1.57	0.84
3:E:337:6PL:H12	3:E:337:6PL:C4	2.06	0.84
3:E:357:6PL:H12	3:E:357:6PL:O31	1.75	0.84
3:A:503:6PL:H322	3:A:504:6PL:C12	2.06	0.84
3:A:573:6PL:C46	3:A:575:6PL:H171	2.06	0.84
1:A:326:ARG:HG3	3:A:545:6PL:H151	1.59	0.84
3:E:344:6PL:H32	3:E:344:6PL:O31	1.77	0.84
3:A:514:6PL:H222	3:A:567:6PL:H172	1.59	0.84
3:A:514:6PL:H462	3:A:567:6PL:C20	2.07	0.84
3:A:517:6PL:H63	3:A:517:6PL:P	2.17	0.84
3:E:306:6PL:H2	3:E:306:6PL:O1P	1.74	0.84
3:A:541:6PL:H382	3:A:557:6PL:H391	1.58	0.84
3:A:563:6PL:H261	3:A:567:6PL:H471	1.58	0.84
3:E:306:6PL:H252	3:A:545:6PL:H422	1.59	0.84
3:E:346:6PL:H381	3:E:346:6PL:C42	2.06	0.84
3:A:505:6PL:H352	3:A:506:6PL:H352	1.59	0.84
3:E:308:6PL:C37	3:E:326:6PL:H441	2.08	0.84
3:E:309:6PL:H362	3:E:325:6PL:H172	1.59	0.84
3:E:312:6PL:H192	3:E:315:6PL:H412	1.59	0.84
3:E:330:6PL:H262	3:A:537:6PL:H171	1.57	0.84
3:A:505:6PL:H332	3:A:506:6PL:H341	1.60	0.84
3:E:353:6PL:H262	3:A:566:6PL:C48	2.06	0.83
3:A:529:6PL:H431	3:A:534:6PL:H142	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:326:6PL:H422	3:E:364:6PL:H11	1.60	0.83
3:A:515:6PL:H263	3:A:531:6PL:H212	1.60	0.83
3:A:518:6PL:H402	3:A:518:6PL:C44	2.08	0.83
3:A:520:6PL:H202	3:A:556:6PL:C48	2.07	0.83
3:A:538:6PL:C44	3:A:542:6PL:H221	2.08	0.83
3:A:566:6PL:O2P	3:A:578:6PL:H72	1.78	0.83
3:A:582:6PL:O4P	3:A:582:6PL:H62	1.76	0.83
3:E:317:6PL:C15	3:A:508:6PL:H231	2.07	0.83
3:E:318:6PL:H222	3:E:331:6PL:C25	2.09	0.83
3:E:335:6PL:H371	3:E:353:6PL:H352	1.58	0.83
3:A:541:6PL:H361	3:A:557:6PL:C38	2.05	0.83
3:E:317:6PL:H411	3:E:353:6PL:H402	1.61	0.83
3:E:332:6PL:H261	3:E:357:6PL:H242	1.58	0.83
3:A:549:6PL:H341	3:A:555:6PL:C17	2.02	0.83
3:E:344:6PL:H232	3:E:344:6PL:H483	1.59	0.83
3:E:346:6PL:H431	3:A:553:6PL:C24	2.07	0.83
3:E:315:6PL:O3	3:E:326:6PL:H321	1.78	0.83
3:A:503:6PL:C32	3:A:504:6PL:H121	2.08	0.83
3:A:522:6PL:H472	3:A:536:6PL:H351	1.61	0.83
3:A:538:6PL:H451	3:A:542:6PL:H232	1.59	0.83
3:A:543:6PL:H161	3:A:566:6PL:H152	1.58	0.83
3:E:321:6PL:O4P	3:E:321:6PL:H63	1.78	0.82
3:A:540:6PL:H352	3:A:550:6PL:C14	2.03	0.82
3:A:550:6PL:H263	3:A:550:6PL:C22	2.08	0.82
3:E:324:6PL:C34	3:A:503:6PL:H32	2.04	0.82
3:E:327:6PL:H152	3:E:350:6PL:H381	1.60	0.82
3:A:584:6PL:H483	3:A:584:6PL:H162	1.61	0.82
3:A:522:6PL:H342	3:A:522:6PL:H152	1.58	0.82
3:A:528:6PL:H192	3:A:528:6PL:C23	2.10	0.82
3:A:577:6PL:H381	3:A:577:6PL:H151	1.62	0.82
3:E:321:6PL:O1P	3:E:344:6PL:H71	1.80	0.82
3:A:543:6PL:H441	3:A:580:6PL:C26	2.08	0.82
3:A:573:6PL:H461	3:A:575:6PL:H171	1.61	0.82
3:E:340:6PL:H401	3:E:340:6PL:C36	2.09	0.82
3:A:525:6PL:C8	3:A:556:6PL:H2	2.10	0.82
3:A:514:6PL:H72	3:A:514:6PL:P	2.18	0.82
3:A:527:6PL:H32	3:A:564:6PL:H172	1.60	0.82
3:E:341:6PL:H252	3:E:341:6PL:H211	1.60	0.82
3:A:517:6PL:O31	3:A:517:6PL:H11	1.78	0.82
3:A:529:6PL:H2	3:A:529:6PL:C4	2.10	0.82
3:A:534:6PL:H362	3:A:534:6PL:C16	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:548:6PL:O4P	3:A:548:6PL:H83	1.80	0.82
3:A:512:6PL:C2	3:A:587:6PL:H71	2.09	0.81
3:A:527:6PL:H331	3:A:564:6PL:C20	2.09	0.81
3:E:335:6PL:H202	3:E:347:6PL:H221	1.60	0.81
3:E:340:6PL:H432	3:E:340:6PL:H242	1.61	0.81
3:E:358:6PL:H422	3:E:358:6PL:H462	1.62	0.81
3:A:580:6PL:H172	3:A:581:6PL:H412	1.60	0.81
3:E:317:6PL:H182	3:E:343:6PL:H401	1.61	0.81
3:E:333:6PL:H182	3:E:364:6PL:H382	1.62	0.81
3:E:356:6PL:H372	3:E:362:6PL:H151	1.62	0.81
3:A:556:6PL:H241	3:A:577:6PL:H242	1.61	0.81
3:A:532:6PL:C12	3:A:560:6PL:H351	2.11	0.81
3:E:325:6PL:C23	3:E:344:6PL:H321	2.10	0.81
3:E:355:6PL:O31	3:E:355:6PL:H12	1.80	0.81
3:A:527:6PL:H162	3:A:571:6PL:H331	1.61	0.81
3:C:501:6PL:H142	3:C:501:6PL:C37	2.10	0.81
3:E:354:6PL:H252	3:A:561:6PL:H252	1.62	0.81
3:A:502:6PL:O31	3:A:502:6PL:H31	1.78	0.81
3:A:520:6PL:O31	3:A:520:6PL:H32	1.78	0.81
3:A:529:6PL:H432	3:A:534:6PL:H381	1.63	0.81
3:C:501:6PL:H132	3:C:501:6PL:H352	1.63	0.81
1:E:131:ARG:NH1	3:E:320:6PL:H2	1.96	0.81
1:E:239:LYS:HD2	3:E:313:6PL:H331	1.63	0.81
3:E:362:6PL:H381	3:E:362:6PL:C42	2.09	0.81
3:A:520:6PL:H152	3:A:542:6PL:H381	1.63	0.81
3:E:369:6PL:H212	3:A:574:6PL:H2	1.63	0.81
3:A:528:6PL:H371	3:A:584:6PL:H351	1.61	0.81
3:E:304:6PL:H263	3:E:331:6PL:H222	1.60	0.81
3:A:505:6PL:H221	3:A:510:6PL:H201	1.60	0.81
1:E:94:LYS:HB3	3:E:349:6PL:H212	1.63	0.80
3:E:368:6PL:H362	3:A:546:6PL:H252	1.62	0.80
1:A:454:LEU:HD11	3:A:586:6PL:H362	1.63	0.80
3:A:527:6PL:H202	3:A:571:6PL:H402	1.63	0.80
3:A:502:6PL:H442	3:A:510:6PL:H241	1.62	0.80
3:A:519:6PL:H191	3:A:549:6PL:H391	1.63	0.80
3:A:552:6PL:H361	3:A:552:6PL:C48	2.11	0.80
3:A:559:6PL:O31	3:A:559:6PL:O3	1.99	0.80
3:E:307:6PL:H471	3:E:351:6PL:H182	1.62	0.80
3:A:515:6PL:C26	3:A:531:6PL:H232	2.12	0.80
3:E:325:6PL:H232	3:E:344:6PL:H321	1.63	0.80
3:A:519:6PL:H252	3:A:549:6PL:H431	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:541:6PL:H382	3:A:557:6PL:C39	2.10	0.80
3:A:562:6PL:H11	3:A:562:6PL:H73	1.62	0.80
3:E:352:6PL:H121	3:E:352:6PL:C16	2.08	0.80
3:A:527:6PL:H212	3:A:571:6PL:H431	1.64	0.80
3:E:309:6PL:O11	3:E:344:6PL:H62	1.81	0.80
3:E:337:6PL:H12	3:E:337:6PL:H52	1.64	0.80
3:E:368:6PL:H141	3:A:513:6PL:H431	1.63	0.80
3:A:515:6PL:H451	3:A:535:6PL:C23	2.11	0.80
3:A:518:6PL:H441	3:A:518:6PL:C40	2.11	0.80
3:A:580:6PL:H382	3:A:588:6PL:H381	1.62	0.80
3:E:314:6PL:H351	3:A:508:6PL:H332	1.62	0.80
3:E:344:6PL:H441	3:E:367:6PL:H222	1.62	0.80
3:E:358:6PL:H431	3:E:358:6PL:C39	2.11	0.80
3:A:518:6PL:H31	3:A:560:6PL:H321	1.64	0.80
3:A:566:6PL:C1	3:A:566:6PL:O31	2.25	0.80
3:A:520:6PL:C14	3:A:542:6PL:H352	2.12	0.79
3:A:520:6PL:H421	3:A:538:6PL:H263	1.64	0.79
3:A:526:6PL:O31	3:A:526:6PL:H11	1.80	0.79
3:A:573:6PL:C45	3:A:575:6PL:H171	2.13	0.79
3:E:320:6PL:C38	3:E:338:6PL:H392	2.11	0.79
3:E:321:6PL:H263	3:E:326:6PL:C26	2.11	0.79
3:E:328:6PL:H202	3:A:537:6PL:C26	2.12	0.79
3:E:329:6PL:H31	3:E:366:6PL:H162	1.62	0.79
3:E:368:6PL:H141	3:A:513:6PL:H442	1.64	0.79
3:A:518:6PL:C33	3:A:532:6PL:H371	2.11	0.79
3:E:359:6PL:H402	3:A:586:6PL:C43	2.05	0.79
3:A:576:6PL:O1P	3:A:576:6PL:H52	1.79	0.79
3:E:333:6PL:H371	3:E:363:6PL:H132	1.64	0.79
3:A:505:6PL:H141	3:A:510:6PL:C12	2.11	0.79
3:A:525:6PL:H171	3:A:583:6PL:C25	2.12	0.79
3:A:537:6PL:H192	3:A:549:6PL:H263	1.64	0.79
3:A:549:6PL:H411	3:A:555:6PL:C26	2.05	0.79
3:A:567:6PL:O1P	3:A:567:6PL:H63	1.82	0.79
3:A:575:6PL:O4P	3:A:575:6PL:H73	1.80	0.79
3:E:323:6PL:C40	3:E:326:6PL:H212	2.13	0.79
3:A:507:6PL:O4P	3:A:507:6PL:H63	1.83	0.79
3:A:532:6PL:H2	3:A:532:6PL:O11	1.80	0.79
3:A:565:6PL:H83	3:A:565:6PL:O4P	1.81	0.79
3:E:326:6PL:H402	3:E:364:6PL:C1	2.13	0.79
3:E:327:6PL:H62	3:E:327:6PL:O4P	1.83	0.79
3:E:346:6PL:H431	3:A:553:6PL:H242	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:351:6PL:H63	3:E:351:6PL:O4P	1.82	0.79
3:E:357:6PL:H352	3:E:357:6PL:C12	2.09	0.79
3:A:505:6PL:H41	3:A:508:6PL:O2	1.83	0.79
3:E:321:6PL:H191	3:E:359:6PL:H121	1.65	0.79
3:E:348:6PL:H12	3:E:348:6PL:O31	1.83	0.79
2:B:68:LEU:HG	2:B:69:PRO:HD2	1.62	0.79
3:E:355:6PL:H41	3:E:355:6PL:C31	2.13	0.79
3:A:537:6PL:H181	3:A:549:6PL:H252	1.65	0.79
3:A:563:6PL:H262	3:A:567:6PL:H451	1.65	0.79
3:A:529:6PL:H412	3:A:534:6PL:H361	1.64	0.79
3:A:540:6PL:C35	3:A:550:6PL:H141	2.05	0.79
3:A:581:6PL:H32	3:A:581:6PL:O31	1.82	0.79
3:E:304:6PL:C34	3:E:355:6PL:H382	2.12	0.79
3:A:527:6PL:H341	3:A:530:6PL:O31	1.83	0.78
3:E:302:6PL:H162	3:E:355:6PL:H432	1.63	0.78
3:E:311:6PL:C32	3:E:342:6PL:H83	2.12	0.78
3:E:316:6PL:H202	3:E:327:6PL:H471	1.65	0.78
3:E:350:6PL:H11	3:E:350:6PL:H42	1.65	0.78
3:A:502:6PL:C34	3:A:511:6PL:H142	2.12	0.78
3:A:524:6PL:O1P	3:A:524:6PL:H51	1.83	0.78
3:E:333:6PL:O3	3:E:363:6PL:H11	1.82	0.78
3:A:532:6PL:O31	3:A:532:6PL:H11	1.83	0.78
3:A:571:6PL:H32	3:A:571:6PL:O31	1.81	0.78
1:E:61:ARG:HD3	3:E:330:6PL:H181	1.62	0.78
3:A:535:6PL:C17	3:A:564:6PL:H461	2.11	0.78
3:E:317:6PL:H141	3:E:366:6PL:C38	2.13	0.78
3:E:323:6PL:H131	3:E:330:6PL:H362	1.64	0.78
3:E:330:6PL:C26	3:A:537:6PL:H171	2.14	0.78
3:E:369:6PL:H262	3:A:533:6PL:H451	1.65	0.78
3:A:558:6PL:O4P	3:A:558:6PL:H82	1.82	0.78
3:E:367:6PL:C26	3:A:526:6PL:H451	2.13	0.78
3:E:369:6PL:H262	3:A:533:6PL:H452	1.66	0.78
3:A:535:6PL:H62	3:A:535:6PL:O4P	1.82	0.78
3:A:534:6PL:H152	3:A:534:6PL:C19	2.13	0.78
3:A:572:6PL:O1P	3:A:572:6PL:H52	1.81	0.78
3:E:359:6PL:H221	3:A:516:6PL:H222	1.66	0.78
3:A:580:6PL:O4P	3:A:580:6PL:H2	1.83	0.78
3:E:360:6PL:H11	3:E:360:6PL:O31	1.84	0.78
3:A:506:6PL:H441	3:A:506:6PL:C48	2.06	0.78
3:A:532:6PL:H212	3:A:541:6PL:H372	1.66	0.78
3:E:329:6PL:H421	3:A:548:6PL:C21	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:359:6PL:H422	3:A:586:6PL:H441	1.65	0.78
3:A:518:6PL:H51	3:A:518:6PL:O2P	1.84	0.78
3:A:546:6PL:C19	3:A:554:6PL:H121	2.13	0.78
3:A:558:6PL:O31	3:A:558:6PL:C1	2.31	0.78
3:E:318:6PL:C37	3:E:331:6PL:H172	2.14	0.77
3:E:359:6PL:C40	3:A:586:6PL:H432	2.07	0.77
3:E:369:6PL:H152	3:A:533:6PL:C32	2.14	0.77
3:A:558:6PL:C4	3:A:558:6PL:H11	2.13	0.77
3:E:315:6PL:H162	3:E:323:6PL:H351	1.65	0.77
3:A:506:6PL:H63	3:A:506:6PL:O4P	1.83	0.77
3:A:507:6PL:H322	3:A:507:6PL:C36	2.11	0.77
3:E:302:6PL:H162	3:E:355:6PL:C43	2.14	0.77
3:E:318:6PL:C36	3:E:331:6PL:H172	2.14	0.77
3:E:348:6PL:C7	3:E:355:6PL:H131	2.13	0.77
3:E:369:6PL:C21	3:A:574:6PL:H2	2.14	0.77
3:E:346:6PL:H422	3:E:346:6PL:C38	2.12	0.77
3:A:523:6PL:C38	3:A:572:6PL:H142	2.12	0.77
3:A:527:6PL:O2P	3:A:555:6PL:H82	1.84	0.77
3:E:333:6PL:C42	3:E:363:6PL:H121	2.11	0.77
3:E:343:6PL:O3P	3:E:343:6PL:O31	2.02	0.77
3:A:569:6PL:H32	3:A:569:6PL:O31	1.81	0.77
3:A:584:6PL:H362	3:A:584:6PL:C41	2.15	0.77
3:A:588:6PL:H482	3:A:588:6PL:C44	2.09	0.77
3:E:345:6PL:H421	3:E:351:6PL:H191	1.66	0.77
3:A:511:6PL:O4P	3:A:511:6PL:H83	1.83	0.77
3:A:544:6PL:H351	3:A:559:6PL:H131	1.67	0.77
3:A:582:6PL:O31	3:A:582:6PL:H12	1.85	0.77
3:A:540:6PL:H41	3:A:550:6PL:H2	1.66	0.77
3:E:309:6PL:C36	3:E:325:6PL:H172	2.15	0.77
3:E:345:6PL:O4P	3:E:345:6PL:H82	1.83	0.77
3:A:527:6PL:H52	3:A:530:6PL:O2P	1.85	0.77
3:A:528:6PL:O4P	3:A:528:6PL:H82	1.84	0.77
3:A:587:6PL:H402	3:A:587:6PL:C16	2.14	0.77
3:E:307:6PL:H231	3:E:307:6PL:H451	1.64	0.77
3:A:506:6PL:H402	3:A:508:6PL:H401	1.66	0.77
3:E:321:6PL:C26	3:E:365:6PL:H241	2.15	0.77
3:A:513:6PL:O31	3:A:513:6PL:H12	1.84	0.77
3:A:515:6PL:H263	3:A:531:6PL:H232	1.67	0.77
3:A:527:6PL:H42	3:A:527:6PL:O2	1.85	0.77
3:A:528:6PL:C48	3:A:582:6PL:H442	2.15	0.77
3:E:313:6PL:H483	3:E:368:6PL:H261	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:323:6PL:H401	3:E:326:6PL:H212	1.65	0.76
3:A:526:6PL:H171	3:A:573:6PL:H472	1.67	0.76
3:E:314:6PL:H12	3:E:314:6PL:O31	1.85	0.76
1:A:432:LEU:HD23	3:A:519:6PL:H32	1.67	0.76
3:A:523:6PL:H332	3:A:544:6PL:H52	1.66	0.76
3:A:529:6PL:H73	3:A:529:6PL:O4P	1.84	0.76
3:E:332:6PL:C42	3:E:357:6PL:H241	2.11	0.76
3:E:369:6PL:H62	3:E:369:6PL:O3P	1.85	0.76
3:A:503:6PL:H2	3:A:503:6PL:O11	1.85	0.76
3:A:532:6PL:H132	3:A:560:6PL:H371	1.68	0.76
3:E:324:6PL:H372	3:E:358:6PL:H392	1.68	0.76
3:E:353:6PL:O3	3:E:353:6PL:H142	1.86	0.76
3:E:364:6PL:H162	3:E:364:6PL:H342	1.66	0.76
3:A:524:6PL:C47	3:A:585:6PL:H212	2.15	0.76
3:A:525:6PL:H52	3:A:525:6PL:O1P	1.84	0.76
3:A:531:6PL:H442	3:A:555:6PL:C24	2.15	0.76
3:A:539:6PL:H472	3:A:571:6PL:H472	1.66	0.76
3:A:570:6PL:H482	3:A:582:6PL:H352	1.67	0.76
3:A:520:6PL:H152	3:A:542:6PL:H382	1.65	0.76
3:A:585:6PL:O4P	3:A:585:6PL:H63	1.85	0.76
3:E:369:6PL:H131	3:A:517:6PL:C43	2.16	0.76
3:A:522:6PL:H342	3:A:522:6PL:H151	1.65	0.76
3:E:317:6PL:H331	3:A:508:6PL:H201	1.67	0.76
3:E:329:6PL:H72	3:E:340:6PL:O11	1.86	0.76
3:E:357:6PL:H142	3:E:357:6PL:H372	1.68	0.76
3:E:304:6PL:H362	3:E:308:6PL:H142	1.66	0.76
3:E:304:6PL:C16	3:E:331:6PL:H32	2.14	0.76
3:E:326:6PL:H32	3:E:326:6PL:O31	1.85	0.76
3:E:354:6PL:H32	3:E:354:6PL:O31	1.84	0.76
3:E:355:6PL:O2	3:E:355:6PL:C4	2.32	0.76
3:E:360:6PL:O4P	3:E:360:6PL:H73	1.85	0.76
1:A:477:GLU:OE2	3:A:514:6PL:H82	1.86	0.76
3:A:540:6PL:H131	3:A:540:6PL:C37	2.14	0.76
3:A:579:6PL:H162	3:A:583:6PL:H212	1.66	0.76
3:E:302:6PL:H181	3:E:308:6PL:H191	1.67	0.76
3:A:514:6PL:H332	3:A:567:6PL:H322	1.68	0.76
3:A:549:6PL:H412	3:A:555:6PL:H262	1.65	0.76
3:A:560:6PL:H51	3:A:560:6PL:O2P	1.86	0.76
1:E:113:GLU:OE2	3:E:334:6PL:H63	1.86	0.76
3:E:320:6PL:H2	3:E:320:6PL:O11	1.84	0.76
3:E:337:6PL:H12	3:E:337:6PL:H42	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:524:6PL:O4P	3:A:524:6PL:H82	1.85	0.76
3:A:526:6PL:H431	3:A:573:6PL:H412	1.68	0.76
3:A:543:6PL:C17	3:A:566:6PL:H351	2.15	0.76
3:A:546:6PL:H63	3:A:546:6PL:O4P	1.85	0.76
3:A:566:6PL:O1P	3:A:566:6PL:H83	1.86	0.76
3:E:324:6PL:O2P	3:E:324:6PL:H52	1.86	0.75
3:A:512:6PL:H72	3:A:524:6PL:O11	1.86	0.75
3:A:526:6PL:C17	3:A:573:6PL:H472	2.16	0.75
3:E:309:6PL:H461	3:E:363:6PL:C25	2.13	0.75
1:E:51:ASP:OD1	3:E:365:6PL:H61	1.87	0.75
3:A:523:6PL:H41	3:A:572:6PL:H321	1.68	0.75
3:E:330:6PL:O4P	3:E:330:6PL:H72	1.86	0.75
3:E:354:6PL:H83	3:E:354:6PL:O4P	1.85	0.75
3:A:517:6PL:H52	3:A:517:6PL:O2P	1.85	0.75
3:A:525:6PL:H161	3:A:562:6PL:H481	1.68	0.75
3:E:317:6PL:H411	3:E:353:6PL:C40	2.17	0.75
3:A:506:6PL:O1P	3:A:506:6PL:H52	1.85	0.75
3:A:519:6PL:H32	3:A:519:6PL:O31	1.85	0.75
3:E:347:6PL:O31	3:E:347:6PL:H11	1.85	0.75
3:A:512:6PL:O1P	3:A:512:6PL:H51	1.86	0.75
3:A:587:6PL:H83	3:A:587:6PL:O4P	1.86	0.75
3:E:301:6PL:H392	3:E:311:6PL:H481	1.67	0.75
3:E:359:6PL:H361	3:A:537:6PL:H431	1.69	0.75
3:A:551:6PL:H51	3:A:551:6PL:O2P	1.85	0.75
3:A:557:6PL:H222	3:A:588:6PL:H481	1.69	0.75
3:A:562:6PL:H452	3:A:579:6PL:H422	1.69	0.75
3:A:565:6PL:C16	3:A:580:6PL:C41	2.65	0.75
3:E:313:6PL:C48	3:E:368:6PL:H261	2.17	0.75
3:E:329:6PL:H421	3:A:548:6PL:H212	1.69	0.75
3:E:342:6PL:O4P	3:E:342:6PL:H62	1.86	0.75
3:E:368:6PL:H161	3:A:513:6PL:H442	1.66	0.75
3:A:513:6PL:C12	3:A:548:6PL:H321	2.16	0.75
3:A:575:6PL:O31	3:A:575:6PL:C1	2.33	0.75
3:E:328:6PL:O4P	3:E:328:6PL:H72	1.87	0.75
3:E:349:6PL:H73	3:A:509:6PL:O2P	1.86	0.75
3:E:368:6PL:H31	3:E:368:6PL:O31	1.85	0.75
3:A:504:6PL:H251	3:A:561:6PL:H241	1.69	0.75
3:A:533:6PL:H82	3:A:533:6PL:O4P	1.85	0.75
3:A:557:6PL:H32	3:A:562:6PL:H221	1.69	0.75
3:E:315:6PL:O31	3:E:315:6PL:H11	1.86	0.74
3:E:324:6PL:H321	3:A:503:6PL:H31	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:338:6PL:H461	3:E:351:6PL:H221	1.68	0.74
3:E:353:6PL:H362	3:E:353:6PL:H152	1.68	0.74
3:A:530:6PL:H171	3:A:535:6PL:H332	1.69	0.74
3:A:588:6PL:H441	3:A:588:6PL:C48	2.12	0.74
3:E:350:6PL:O2	3:E:360:6PL:H321	1.87	0.74
3:E:367:6PL:O31	3:E:367:6PL:H12	1.87	0.74
3:A:519:6PL:H191	3:A:549:6PL:C39	2.17	0.74
3:A:522:6PL:H141	3:A:522:6PL:C33	2.17	0.74
3:A:523:6PL:H422	3:A:572:6PL:H472	1.68	0.74
3:A:526:6PL:O11	3:A:575:6PL:H141	1.86	0.74
3:A:580:6PL:O4P	3:A:580:6PL:H73	1.85	0.74
3:E:309:6PL:C46	3:E:363:6PL:H251	2.17	0.74
3:E:312:6PL:H242	3:E:315:6PL:H402	1.69	0.74
3:A:563:6PL:H182	3:A:567:6PL:H381	1.68	0.74
3:A:568:6PL:H63	3:A:568:6PL:O4P	1.85	0.74
3:E:341:6PL:O31	3:E:341:6PL:H11	1.86	0.74
3:A:518:6PL:H171	3:A:529:6PL:H202	1.68	0.74
3:E:310:6PL:H252	3:A:544:6PL:H481	1.70	0.74
3:E:311:6PL:O2P	3:E:311:6PL:H52	1.85	0.74
3:E:366:6PL:C35	3:E:366:6PL:C31	2.64	0.74
3:A:502:6PL:H341	3:A:511:6PL:C14	2.16	0.74
3:A:520:6PL:O2P	3:A:552:6PL:H81	1.88	0.74
3:A:533:6PL:O2P	3:A:533:6PL:H51	1.88	0.74
3:A:580:6PL:H402	3:A:588:6PL:H222	1.67	0.74
3:E:304:6PL:O4P	3:E:304:6PL:H63	1.87	0.74
3:E:351:6PL:H262	3:A:536:6PL:H451	1.68	0.74
3:A:529:6PL:H251	3:A:560:6PL:H322	1.69	0.74
3:E:310:6PL:H171	3:E:332:6PL:C11	2.17	0.74
3:E:315:6PL:H62	3:E:315:6PL:O4P	1.88	0.74
3:A:518:6PL:H182	3:A:529:6PL:C18	2.17	0.74
3:A:544:6PL:H412	3:A:559:6PL:H212	1.68	0.74
3:A:580:6PL:H172	3:A:581:6PL:C41	2.17	0.74
1:E:90:LEU:HD13	3:E:349:6PL:H151	1.70	0.74
3:E:362:6PL:H52	3:E:362:6PL:O1P	1.86	0.74
3:A:518:6PL:C18	3:A:529:6PL:H181	2.17	0.74
3:A:531:6PL:H442	3:A:555:6PL:H242	1.67	0.74
3:A:531:6PL:O31	3:A:531:6PL:H32	1.87	0.74
1:E:189:LEU:HD23	3:E:341:6PL:H2	1.70	0.74
3:E:309:6PL:H73	3:E:309:6PL:O4P	1.86	0.74
3:E:310:6PL:C13	3:E:331:6PL:H161	2.14	0.74
3:A:553:6PL:H83	3:A:553:6PL:O4P	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:333:6PL:H421	3:E:363:6PL:C12	2.12	0.73
3:E:362:6PL:H411	3:E:362:6PL:H451	1.69	0.73
3:A:526:6PL:H162	3:A:573:6PL:H472	1.70	0.73
3:E:324:6PL:O2P	3:E:324:6PL:H62	1.88	0.73
1:A:363:GLU:OE1	3:A:522:6PL:H83	1.88	0.73
3:A:526:6PL:C16	3:A:573:6PL:H472	2.18	0.73
3:A:532:6PL:O31	3:A:560:6PL:H82	1.88	0.73
3:E:304:6PL:H341	3:E:355:6PL:H391	1.70	0.73
3:E:322:6PL:H83	3:E:322:6PL:O4P	1.87	0.73
3:E:325:6PL:H12	3:E:325:6PL:O31	1.88	0.73
3:E:329:6PL:H63	3:E:329:6PL:O4P	1.86	0.73
3:E:331:6PL:H371	3:E:355:6PL:H461	1.71	0.73
3:A:518:6PL:H62	3:A:521:6PL:C6	2.18	0.73
3:A:541:6PL:C13	3:A:588:6PL:H332	2.18	0.73
3:A:543:6PL:H421	3:A:566:6PL:H483	1.69	0.73
3:A:544:6PL:H432	3:A:559:6PL:H232	1.70	0.73
3:E:310:6PL:H132	3:E:331:6PL:C16	2.15	0.73
3:E:321:6PL:C18	3:E:359:6PL:H121	2.19	0.73
3:A:516:6PL:H52	3:A:516:6PL:O1P	1.88	0.73
3:A:523:6PL:H362	3:A:544:6PL:C1	2.16	0.73
3:A:538:6PL:H411	3:A:542:6PL:C36	2.19	0.73
3:E:321:6PL:C34	3:E:339:6PL:H152	2.19	0.73
3:E:324:6PL:H151	3:E:361:6PL:H341	1.70	0.73
3:E:328:6PL:H382	3:E:348:6PL:H122	1.68	0.73
3:E:333:6PL:H392	3:E:363:6PL:C15	2.19	0.73
3:E:335:6PL:H162	3:E:356:6PL:H152	1.69	0.73
3:E:351:6PL:C26	3:A:536:6PL:H451	2.18	0.73
3:A:510:6PL:H361	3:A:510:6PL:H151	1.68	0.73
3:A:543:6PL:H372	3:A:566:6PL:H402	1.68	0.73
3:E:331:6PL:H371	3:E:355:6PL:C46	2.17	0.73
3:A:520:6PL:H462	3:A:556:6PL:H251	1.69	0.73
3:E:335:6PL:C13	3:E:356:6PL:H332	2.19	0.73
3:E:353:6PL:C26	3:A:566:6PL:H481	2.16	0.73
3:A:501:6PL:O4P	3:A:501:6PL:H82	1.88	0.73
3:A:562:6PL:H452	3:A:579:6PL:C42	2.18	0.73
3:A:571:6PL:O4P	3:A:571:6PL:H82	1.88	0.73
3:E:312:6PL:H263	3:E:315:6PL:C23	2.18	0.73
3:E:317:6PL:H361	3:E:353:6PL:H341	1.70	0.73
3:E:329:6PL:H422	3:A:548:6PL:H221	1.69	0.73
3:A:522:6PL:H141	3:A:522:6PL:H331	1.71	0.73
3:A:565:6PL:H162	3:A:580:6PL:H412	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:324:6PL:H361	3:E:358:6PL:C43	2.18	0.73
3:E:358:6PL:C23	3:A:509:6PL:H152	2.18	0.73
3:E:362:6PL:O4P	3:E:362:6PL:H83	1.89	0.73
3:A:501:6PL:O31	3:A:501:6PL:H12	1.88	0.73
3:A:517:6PL:P	3:A:517:6PL:C6	2.77	0.73
3:A:572:6PL:P	3:A:572:6PL:C7	2.77	0.73
3:E:335:6PL:H451	3:E:347:6PL:H242	1.71	0.73
3:E:340:6PL:H331	3:E:342:6PL:C18	2.19	0.73
3:A:518:6PL:H62	3:A:521:6PL:H61	1.71	0.73
3:A:528:6PL:H412	3:A:550:6PL:H352	1.70	0.73
3:A:535:6PL:H162	3:A:564:6PL:H441	1.70	0.73
3:A:551:6PL:H62	3:A:551:6PL:O4P	1.87	0.73
3:A:560:6PL:H62	3:A:560:6PL:O4P	1.87	0.73
3:E:306:6PL:C25	3:A:545:6PL:H422	2.18	0.72
3:E:333:6PL:C41	3:E:363:6PL:C35	2.67	0.72
3:E:351:6PL:O2P	3:E:351:6PL:H52	1.89	0.72
3:A:573:6PL:H451	3:A:575:6PL:H171	1.70	0.72
3:E:302:6PL:H52	3:A:509:6PL:H132	1.71	0.72
3:E:312:6PL:H222	3:E:315:6PL:H412	1.70	0.72
3:E:326:6PL:C42	3:E:364:6PL:H11	2.17	0.72
3:E:333:6PL:C17	3:E:364:6PL:H362	2.18	0.72
3:E:345:6PL:H131	3:C:501:6PL:H171	1.71	0.72
3:E:363:6PL:O4P	3:E:363:6PL:H72	1.89	0.72
3:A:514:6PL:H462	3:A:567:6PL:H202	1.70	0.72
3:A:557:6PL:O4P	3:A:557:6PL:H72	1.88	0.72
3:A:573:6PL:O4P	3:A:573:6PL:H82	1.89	0.72
3:E:328:6PL:O31	3:E:328:6PL:H12	1.89	0.72
3:A:501:6PL:H73	3:A:506:6PL:H121	1.70	0.72
3:A:512:6PL:H201	3:A:582:6PL:H221	1.71	0.72
3:A:540:6PL:H51	3:A:550:6PL:O2P	1.89	0.72
3:A:565:6PL:H32	3:A:565:6PL:O31	1.88	0.72
3:E:336:6PL:H12	3:E:336:6PL:O31	1.88	0.72
3:E:346:6PL:H62	3:E:346:6PL:O4P	1.89	0.72
3:A:525:6PL:C5	3:A:583:6PL:H321	2.12	0.72
3:A:579:6PL:C14	3:A:583:6PL:H192	2.08	0.72
3:E:302:6PL:H41	3:A:509:6PL:H141	1.70	0.72
3:A:546:6PL:H32	3:A:546:6PL:O31	1.88	0.72
3:E:319:6PL:H262	3:E:344:6PL:H472	1.71	0.72
3:E:355:6PL:H62	3:E:355:6PL:O4P	1.88	0.72
3:A:518:6PL:H431	3:A:558:6PL:C45	2.18	0.72
3:A:520:6PL:H483	3:A:542:6PL:C43	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:542:6PL:H411	3:A:556:6PL:H211	1.70	0.72
3:A:543:6PL:O4P	3:A:543:6PL:H63	1.88	0.72
3:A:567:6PL:H62	3:A:567:6PL:O4P	1.89	0.72
3:A:588:6PL:O4P	3:A:588:6PL:H72	1.88	0.72
3:E:335:6PL:H131	3:E:356:6PL:H352	1.69	0.72
3:A:505:6PL:H181	3:A:510:6PL:H141	1.69	0.72
3:A:505:6PL:H242	3:A:510:6PL:H381	1.69	0.72
3:A:532:6PL:H212	3:A:541:6PL:C37	2.20	0.72
3:A:557:6PL:H32	3:A:562:6PL:C22	2.18	0.72
3:E:322:6PL:H331	3:E:365:6PL:C40	2.19	0.72
3:E:361:6PL:H481	3:A:544:6PL:H341	1.71	0.72
3:A:505:6PL:C14	3:A:510:6PL:H122	2.20	0.72
3:A:513:6PL:H231	3:A:548:6PL:H181	1.71	0.72
3:A:526:6PL:H131	3:A:575:6PL:C16	2.16	0.72
3:A:532:6PL:H122	3:A:560:6PL:C35	2.19	0.72
3:A:561:6PL:O4P	3:A:561:6PL:H82	1.88	0.72
3:A:577:6PL:O31	3:A:577:6PL:H32	1.86	0.72
3:E:311:6PL:O4P	3:E:311:6PL:H63	1.89	0.72
3:E:347:6PL:O4P	3:E:347:6PL:H72	1.89	0.72
3:E:351:6PL:H421	3:E:351:6PL:H461	1.71	0.72
3:E:358:6PL:H212	3:A:509:6PL:H121	1.70	0.72
3:A:518:6PL:O4P	3:A:518:6PL:H82	1.89	0.72
3:A:563:6PL:C26	3:A:567:6PL:H471	2.19	0.72
3:E:326:6PL:C40	3:E:364:6PL:C1	2.68	0.71
3:E:337:6PL:O4P	3:E:337:6PL:H73	1.88	0.71
3:E:369:6PL:H192	3:A:533:6PL:H401	1.71	0.71
3:A:570:6PL:O3	3:A:570:6PL:O31	2.08	0.71
1:E:144:LEU:HD21	3:A:536:6PL:H442	1.72	0.71
3:E:314:6PL:H431	3:A:508:6PL:C42	2.19	0.71
3:A:514:6PL:H462	3:A:567:6PL:H201	1.72	0.71
3:A:572:6PL:H402	3:A:576:6PL:H172	1.70	0.71
3:A:506:6PL:P	3:A:506:6PL:C6	2.78	0.71
3:A:520:6PL:H451	3:A:542:6PL:C42	2.19	0.71
3:A:565:6PL:C16	3:A:580:6PL:H411	2.21	0.71
3:C:501:6PL:O4P	3:C:501:6PL:H72	1.90	0.71
1:A:351:TRP:CD1	3:A:536:6PL:H131	2.26	0.71
3:A:543:6PL:C42	3:A:566:6PL:H483	2.20	0.71
3:A:571:6PL:H51	3:A:571:6PL:O2P	1.90	0.71
3:A:520:6PL:H202	3:A:556:6PL:H482	1.73	0.71
3:A:531:6PL:H361	3:A:531:6PL:C14	2.21	0.71
3:A:540:6PL:H51	3:A:550:6PL:P	2.31	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:570:6PL:H322	3:A:582:6PL:C7	2.19	0.71
3:E:301:6PL:H392	3:E:311:6PL:C48	2.21	0.71
3:E:315:6PL:H332	3:E:326:6PL:H382	1.71	0.71
3:E:353:6PL:O4P	3:E:353:6PL:C6	2.35	0.71
3:E:361:6PL:H32	3:E:361:6PL:O31	1.91	0.71
3:A:518:6PL:H191	3:A:529:6PL:H202	1.72	0.71
3:A:532:6PL:H462	3:A:562:6PL:C43	2.10	0.71
3:E:360:6PL:H142	3:E:360:6PL:H332	1.72	0.71
3:A:502:6PL:H371	3:A:505:6PL:H421	1.71	0.71
3:A:526:6PL:H162	3:A:575:6PL:C17	2.19	0.71
3:A:571:6PL:O31	3:A:571:6PL:C3	2.34	0.71
3:A:572:6PL:H73	3:A:572:6PL:O4P	1.89	0.71
3:E:324:6PL:H63	3:E:324:6PL:P	2.31	0.71
3:E:333:6PL:H392	3:E:363:6PL:H152	1.73	0.71
3:A:505:6PL:H221	3:A:510:6PL:H202	1.69	0.71
3:A:529:6PL:H462	3:A:534:6PL:H382	1.70	0.71
3:A:547:6PL:O31	3:A:547:6PL:H11	1.91	0.71
3:A:557:6PL:C11	3:A:565:6PL:H73	2.21	0.71
3:A:562:6PL:O31	3:A:562:6PL:C11	2.39	0.71
3:E:317:6PL:H63	3:E:317:6PL:O4P	1.91	0.71
3:A:520:6PL:H483	3:A:542:6PL:C44	2.20	0.71
3:A:546:6PL:C34	3:A:554:6PL:C3	2.68	0.71
3:A:558:6PL:H11	3:A:558:6PL:H41	1.73	0.71
3:A:566:6PL:H222	3:A:578:6PL:H411	1.72	0.71
3:A:572:6PL:P	3:A:572:6PL:H73	2.31	0.71
3:E:329:6PL:O31	3:E:340:6PL:H152	1.91	0.71
3:E:367:6PL:H52	3:E:367:6PL:O2P	1.90	0.71
3:E:324:6PL:H192	3:E:361:6PL:H382	1.73	0.70
3:A:527:6PL:H411	3:A:530:6PL:H132	1.73	0.70
3:E:304:6PL:H472	3:E:308:6PL:C24	2.21	0.70
3:E:304:6PL:C19	3:E:355:6PL:H481	2.20	0.70
3:E:358:6PL:H152	3:A:509:6PL:H2	1.74	0.70
3:A:502:6PL:H442	3:A:510:6PL:C24	2.20	0.70
3:A:517:6PL:H171	3:A:579:6PL:C12	2.21	0.70
3:A:537:6PL:C43	3:A:586:6PL:H212	2.21	0.70
3:A:540:6PL:O4P	3:A:540:6PL:H73	1.92	0.70
3:E:326:6PL:H481	3:E:364:6PL:H322	1.72	0.70
3:E:340:6PL:H481	3:E:360:6PL:C20	2.22	0.70
3:E:364:6PL:O4P	3:E:364:6PL:H62	1.90	0.70
3:A:521:6PL:H231	3:A:557:6PL:C25	2.20	0.70
3:A:556:6PL:O2P	3:A:556:6PL:H52	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:518:6PL:H82	3:A:518:6PL:P	2.32	0.70
3:A:535:6PL:H431	3:A:564:6PL:H452	1.72	0.70
3:A:563:6PL:C26	3:A:567:6PL:H451	2.21	0.70
3:E:324:6PL:C16	3:E:361:6PL:H361	2.22	0.70
3:E:330:6PL:O11	3:E:330:6PL:H2	1.91	0.70
3:E:366:6PL:H471	3:A:508:6PL:C26	2.21	0.70
3:A:518:6PL:H171	3:A:529:6PL:C20	2.22	0.70
3:A:538:6PL:O31	3:A:542:6PL:H72	1.91	0.70
3:A:552:6PL:H432	3:A:570:6PL:H251	1.72	0.70
3:A:564:6PL:H263	3:A:564:6PL:H431	1.72	0.70
3:E:309:6PL:H362	3:E:325:6PL:C17	2.21	0.70
3:E:310:6PL:H41	3:E:331:6PL:H12	1.73	0.70
3:E:301:6PL:H472	3:E:317:6PL:H242	1.73	0.70
3:E:332:6PL:H261	3:E:357:6PL:C24	2.21	0.70
3:E:335:6PL:O4P	3:E:335:6PL:H73	1.90	0.70
3:E:357:6PL:H82	3:E:357:6PL:O4P	1.91	0.70
3:A:516:6PL:O31	3:A:516:6PL:C1	2.35	0.70
3:A:539:6PL:H202	3:A:563:6PL:H32	1.72	0.70
3:E:361:6PL:H51	3:E:361:6PL:O2P	1.91	0.70
3:A:526:6PL:H212	3:A:550:6PL:H182	1.71	0.70
3:A:559:6PL:O2P	3:A:559:6PL:H2	1.91	0.70
3:A:565:6PL:H442	3:A:580:6PL:C44	2.21	0.70
3:A:579:6PL:H172	3:A:579:6PL:H371	1.74	0.70
3:E:304:6PL:H142	3:E:331:6PL:O2	1.91	0.70
3:E:317:6PL:H161	3:E:366:6PL:H382	1.74	0.70
3:A:512:6PL:O31	3:A:587:6PL:H61	1.90	0.70
3:A:527:6PL:H151	3:A:571:6PL:C2	2.22	0.70
3:A:528:6PL:H481	3:A:582:6PL:H442	1.74	0.70
3:A:562:6PL:H11	3:A:562:6PL:H72	1.71	0.70
3:E:330:6PL:H262	3:A:537:6PL:C17	2.21	0.69
3:A:519:6PL:O31	3:A:519:6PL:C3	2.38	0.69
3:A:541:6PL:H132	3:A:588:6PL:H332	1.74	0.69
3:A:546:6PL:O2P	3:A:546:6PL:H52	1.92	0.69
3:A:549:6PL:O4P	3:A:549:6PL:H82	1.91	0.69
3:E:319:6PL:H242	3:E:325:6PL:H452	1.72	0.69
3:A:526:6PL:C23	3:A:550:6PL:H192	2.18	0.69
3:A:513:6PL:H212	3:A:548:6PL:C42	2.22	0.69
3:A:526:6PL:H212	3:A:550:6PL:C18	2.21	0.69
3:A:538:6PL:H451	3:A:542:6PL:C23	2.22	0.69
3:A:564:6PL:H83	3:A:564:6PL:O4P	1.92	0.69
3:A:565:6PL:H332	3:A:580:6PL:C3	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:332:6PL:H262	3:E:357:6PL:C23	2.21	0.69
3:E:347:6PL:H351	3:E:347:6PL:C31	2.23	0.69
3:A:511:6PL:P	3:A:511:6PL:C8	2.80	0.69
3:A:548:6PL:O31	3:A:548:6PL:C3	2.40	0.69
3:A:556:6PL:H241	3:A:577:6PL:C24	2.21	0.69
3:E:301:6PL:H451	3:E:347:6PL:H412	1.74	0.69
3:A:506:6PL:C44	3:A:506:6PL:C48	2.68	0.69
3:A:563:6PL:C18	3:A:567:6PL:H381	2.21	0.69
3:E:332:6PL:H82	3:E:332:6PL:C1	2.12	0.69
3:E:345:6PL:H41	3:C:501:6PL:H351	1.74	0.69
3:A:543:6PL:H422	3:A:581:6PL:H232	1.75	0.69
1:E:222:LEU:HD22	3:E:350:6PL:H411	1.74	0.69
3:E:308:6PL:O4P	3:E:308:6PL:H82	1.92	0.69
3:E:316:6PL:O31	3:E:316:6PL:O3	2.10	0.69
3:A:502:6PL:H62	3:A:502:6PL:O4P	1.92	0.69
3:A:508:6PL:H12	3:A:508:6PL:O31	1.90	0.69
3:A:523:6PL:H371	3:A:523:6PL:H411	1.73	0.69
3:A:557:6PL:H2	3:A:562:6PL:H172	1.75	0.69
3:E:303:6PL:H63	3:E:303:6PL:P	2.32	0.69
3:A:515:6PL:C43	3:A:515:6PL:C47	2.67	0.69
3:A:526:6PL:C16	3:A:575:6PL:H172	2.21	0.69
3:A:532:6PL:C19	3:A:541:6PL:H372	2.20	0.69
3:A:541:6PL:C24	3:A:580:6PL:H401	2.22	0.69
3:A:541:6PL:H161	3:A:588:6PL:H351	1.74	0.69
3:E:325:6PL:O4P	3:E:325:6PL:H73	1.92	0.69
3:E:345:6PL:O11	3:C:501:6PL:H151	1.93	0.69
3:E:348:6PL:H62	3:E:355:6PL:H142	1.74	0.69
3:E:356:6PL:H401	3:E:362:6PL:H191	1.75	0.69
3:A:546:6PL:H342	3:A:554:6PL:C3	2.15	0.69
3:A:546:6PL:H222	3:A:554:6PL:H141	1.75	0.69
3:C:501:6PL:O1P	3:C:501:6PL:H51	1.93	0.69
3:E:323:6PL:C11	3:E:323:6PL:O31	2.41	0.69
3:E:352:6PL:H161	3:E:352:6PL:C12	2.14	0.69
3:E:361:6PL:O31	3:E:361:6PL:C3	2.38	0.69
3:A:509:6PL:O2P	3:A:509:6PL:H31	1.92	0.69
3:A:520:6PL:H161	3:A:542:6PL:H121	1.74	0.68
3:E:333:6PL:H182	3:E:364:6PL:H362	1.75	0.68
3:A:542:6PL:O31	3:A:542:6PL:H11	1.92	0.68
3:E:355:6PL:H351	3:E:355:6PL:H122	1.76	0.68
3:A:512:6PL:H202	3:A:585:6PL:H251	1.74	0.68
3:A:516:6PL:H421	3:A:531:6PL:H421	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:524:6PL:H142	3:A:524:6PL:H391	1.75	0.68
3:A:535:6PL:H32	3:A:535:6PL:O31	1.91	0.68
3:A:536:6PL:O31	3:A:536:6PL:H12	1.91	0.68
3:A:543:6PL:C26	3:A:566:6PL:H252	2.23	0.68
3:A:547:6PL:H401	3:A:555:6PL:H461	1.74	0.68
3:A:557:6PL:H31	3:A:565:6PL:H52	1.75	0.68
3:E:362:6PL:H451	3:E:362:6PL:C41	2.23	0.68
3:A:512:6PL:H261	3:A:587:6PL:H251	1.75	0.68
3:A:580:6PL:C37	3:A:588:6PL:H202	2.23	0.68
3:E:361:6PL:O4P	3:E:361:6PL:H82	1.94	0.68
3:A:514:6PL:O3	3:A:514:6PL:O31	2.11	0.68
3:E:329:6PL:C3	3:E:366:6PL:H162	2.24	0.68
3:E:352:6PL:H32	3:E:352:6PL:O31	1.93	0.68
3:A:505:6PL:C35	3:A:506:6PL:H352	2.23	0.68
3:A:564:6PL:C11	3:A:564:6PL:O31	2.42	0.68
3:A:570:6PL:O4P	3:A:570:6PL:H72	1.93	0.68
3:E:307:6PL:H471	3:E:351:6PL:C18	2.23	0.68
3:E:332:6PL:H421	3:E:357:6PL:C24	2.16	0.68
3:A:510:6PL:O4P	3:A:510:6PL:C2	2.41	0.68
3:A:522:6PL:O4P	3:A:522:6PL:H63	1.93	0.68
3:A:526:6PL:H181	3:A:573:6PL:H451	1.73	0.68
3:A:529:6PL:H261	3:A:560:6PL:H342	1.74	0.68
3:A:530:6PL:H32	3:A:588:6PL:H71	1.75	0.68
3:A:538:6PL:H411	3:A:542:6PL:H362	1.76	0.68
3:A:562:6PL:H51	3:A:562:6PL:O2P	1.93	0.68
3:E:301:6PL:O4P	3:E:301:6PL:H63	1.93	0.68
3:E:332:6PL:H11	3:E:332:6PL:C8	2.15	0.68
3:E:352:6PL:O4P	3:E:352:6PL:H72	1.92	0.68
3:A:523:6PL:O4P	3:A:523:6PL:H83	1.93	0.68
3:E:310:6PL:H32	3:E:331:6PL:H131	1.73	0.68
3:E:321:6PL:C19	3:E:359:6PL:H121	2.24	0.68
3:A:518:6PL:O31	3:A:518:6PL:H31	1.93	0.68
3:A:543:6PL:H421	3:A:566:6PL:C48	2.23	0.68
3:A:562:6PL:H222	3:A:565:6PL:H31	1.75	0.68
3:E:317:6PL:H132	3:A:508:6PL:H212	1.76	0.68
3:E:368:6PL:O11	3:A:546:6PL:C23	2.42	0.68
3:A:524:6PL:C48	3:A:585:6PL:H212	2.24	0.68
3:A:527:6PL:C21	3:A:571:6PL:H431	2.23	0.68
3:E:310:6PL:H62	3:E:310:6PL:O4P	1.92	0.67
3:E:313:6PL:O4P	3:E:313:6PL:H72	1.93	0.67
3:A:570:6PL:H322	3:A:582:6PL:H73	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:318:6PL:H471	3:A:504:6PL:H232	1.76	0.67
3:E:323:6PL:H432	3:E:355:6PL:C26	2.24	0.67
3:E:340:6PL:C33	3:E:342:6PL:H181	2.23	0.67
3:E:307:6PL:H63	3:E:307:6PL:O4P	1.94	0.67
3:E:318:6PL:H242	3:A:518:6PL:C47	2.24	0.67
3:E:321:6PL:C26	3:E:326:6PL:H262	2.22	0.67
3:E:326:6PL:H392	3:E:364:6PL:H41	1.77	0.67
3:A:523:6PL:H431	3:A:572:6PL:H182	1.77	0.67
3:A:532:6PL:H263	3:A:588:6PL:H421	1.74	0.67
3:E:324:6PL:H151	3:E:361:6PL:H361	1.75	0.67
3:E:335:6PL:H131	3:E:356:6PL:H332	1.76	0.67
3:A:522:6PL:H12	3:A:522:6PL:O31	1.92	0.67
3:A:528:6PL:H232	3:A:528:6PL:C19	2.15	0.67
3:A:556:6PL:H83	3:A:556:6PL:O4P	1.94	0.67
3:A:578:6PL:O4P	3:A:578:6PL:H73	1.95	0.67
3:E:302:6PL:H142	3:E:302:6PL:O3	1.95	0.67
3:E:312:6PL:H32	3:E:312:6PL:O31	1.92	0.67
3:A:503:6PL:H62	3:A:503:6PL:O1P	1.95	0.67
3:E:310:6PL:H331	3:E:331:6PL:H152	1.76	0.67
3:E:321:6PL:H371	3:E:344:6PL:H341	1.76	0.67
3:E:324:6PL:C34	3:A:503:6PL:C3	2.65	0.67
3:E:330:6PL:H471	3:A:537:6PL:H231	1.76	0.67
3:E:346:6PL:H431	3:A:553:6PL:H241	1.76	0.67
3:E:350:6PL:H42	3:E:350:6PL:C1	2.25	0.67
3:A:557:6PL:O2P	3:A:565:6PL:H51	1.95	0.67
3:E:304:6PL:C36	3:E:308:6PL:H142	2.24	0.67
3:E:314:6PL:H2	3:E:314:6PL:O11	1.93	0.67
3:E:317:6PL:O31	3:E:317:6PL:H31	1.93	0.67
3:E:369:6PL:O4P	3:E:369:6PL:H63	1.93	0.67
3:E:357:6PL:H73	3:E:357:6PL:O2	1.95	0.67
3:A:503:6PL:H32	3:A:503:6PL:O31	1.94	0.67
3:A:520:6PL:C45	3:A:542:6PL:H422	2.20	0.67
3:A:521:6PL:H121	3:A:562:6PL:C15	2.25	0.67
3:A:528:6PL:H51	3:A:528:6PL:O2P	1.94	0.67
3:E:302:6PL:H82	3:E:302:6PL:O4P	1.95	0.67
3:E:359:6PL:C33	3:A:537:6PL:H462	2.23	0.67
3:A:548:6PL:H172	3:A:548:6PL:C40	2.19	0.67
3:A:566:6PL:O31	3:A:566:6PL:O3P	2.13	0.67
3:E:304:6PL:H341	3:E:355:6PL:C39	2.24	0.67
3:A:518:6PL:C45	3:A:560:6PL:H432	2.06	0.67
3:A:537:6PL:H431	3:A:586:6PL:H212	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:542:6PL:C43	3:A:542:6PL:H201	2.25	0.67
3:E:310:6PL:H361	3:E:310:6PL:H202	1.76	0.66
3:A:517:6PL:H221	3:A:522:6PL:H122	1.77	0.66
3:A:536:6PL:H2	3:A:536:6PL:O11	1.94	0.66
3:A:580:6PL:H362	3:A:588:6PL:C38	2.26	0.66
3:E:347:6PL:O2P	3:E:347:6PL:H51	1.95	0.66
3:A:546:6PL:O31	3:A:546:6PL:H12	1.93	0.66
3:E:313:6PL:H382	3:E:313:6PL:H182	1.77	0.66
3:A:513:6PL:H122	3:A:548:6PL:H321	1.78	0.66
3:A:513:6PL:O1P	3:A:513:6PL:H51	1.95	0.66
3:A:518:6PL:H452	3:A:558:6PL:H441	1.76	0.66
3:A:588:6PL:O2P	3:A:588:6PL:C3	2.43	0.66
3:E:308:6PL:H242	3:E:331:6PL:H442	1.77	0.66
3:E:323:6PL:H171	3:E:330:6PL:H421	1.76	0.66
3:E:326:6PL:C40	3:E:364:6PL:H11	2.26	0.66
3:E:326:6PL:H83	3:E:326:6PL:O4P	1.95	0.66
3:A:544:6PL:H372	3:A:572:6PL:H483	1.76	0.66
1:E:217:GLY:HA3	3:A:507:6PL:H332	1.77	0.66
3:E:305:6PL:H2	3:E:305:6PL:O11	1.94	0.66
3:E:316:6PL:H262	3:E:346:6PL:H211	1.77	0.66
3:A:506:6PL:H63	3:A:506:6PL:O3P	1.94	0.66
3:A:539:6PL:C26	3:A:563:6PL:H381	2.25	0.66
3:A:551:6PL:H12	3:A:551:6PL:O31	1.95	0.66
3:A:562:6PL:H392	3:A:579:6PL:H481	1.77	0.66
1:E:208:LYS:HB2	1:E:209:PRO:HD3	1.78	0.66
3:E:355:6PL:O31	3:E:355:6PL:C1	2.43	0.66
3:A:524:6PL:H482	3:A:585:6PL:H192	1.77	0.66
3:A:578:6PL:H421	3:A:578:6PL:C46	2.19	0.66
3:E:320:6PL:H32	3:E:320:6PL:O31	1.95	0.66
3:E:340:6PL:C45	3:E:350:6PL:H441	2.20	0.66
3:A:504:6PL:H242	3:A:561:6PL:H442	1.78	0.66
3:A:512:6PL:H141	3:A:582:6PL:H181	1.78	0.66
3:A:519:6PL:C25	3:A:549:6PL:H442	2.23	0.66
3:E:315:6PL:O2P	3:E:315:6PL:H2	1.94	0.66
3:E:316:6PL:H52	3:E:346:6PL:O1P	1.95	0.66
3:E:317:6PL:C41	3:E:353:6PL:H381	2.25	0.66
3:E:325:6PL:O31	3:E:325:6PL:H32	1.96	0.66
3:E:338:6PL:O2P	3:E:338:6PL:H52	1.94	0.66
3:A:512:6PL:O4P	3:A:512:6PL:H82	1.95	0.66
3:A:560:6PL:H41	3:A:560:6PL:H2	1.78	0.66
3:E:324:6PL:H321	3:A:503:6PL:C3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:366:6PL:C31	3:E:366:6PL:H352	2.25	0.66
3:A:525:6PL:H231	3:A:579:6PL:H251	1.77	0.66
3:A:563:6PL:H462	3:A:578:6PL:H341	1.77	0.66
3:A:580:6PL:H431	3:A:588:6PL:H242	1.77	0.66
3:E:322:6PL:H52	3:E:322:6PL:O3P	1.95	0.66
3:E:334:6PL:H452	3:A:534:6PL:H262	1.78	0.66
3:E:337:6PL:H142	3:E:337:6PL:H361	1.77	0.66
3:E:350:6PL:O31	3:E:350:6PL:H12	1.96	0.66
3:E:356:6PL:H452	3:E:362:6PL:H201	1.76	0.66
3:A:518:6PL:P	3:A:518:6PL:C8	2.84	0.66
3:E:353:6PL:O31	3:E:353:6PL:C3	2.30	0.65
3:E:369:6PL:O11	3:E:369:6PL:C31	2.44	0.65
3:A:518:6PL:C34	3:A:532:6PL:H391	2.21	0.65
3:A:532:6PL:O4P	3:A:532:6PL:H63	1.96	0.65
3:A:536:6PL:O4P	3:A:536:6PL:C8	2.44	0.65
3:A:587:6PL:C11	3:A:587:6PL:O31	2.45	0.65
3:E:345:6PL:H32	3:E:345:6PL:O31	1.94	0.65
3:E:365:6PL:O31	3:E:365:6PL:H11	1.95	0.65
3:E:366:6PL:H471	3:A:508:6PL:H262	1.78	0.65
3:A:520:6PL:C48	3:A:542:6PL:C44	2.71	0.65
3:A:527:6PL:H32	3:A:564:6PL:C17	2.26	0.65
3:A:547:6PL:H73	3:A:547:6PL:O4P	1.95	0.65
3:A:552:6PL:H63	3:A:552:6PL:P	2.36	0.65
3:A:565:6PL:H431	3:A:580:6PL:H432	1.77	0.65
3:A:588:6PL:O31	3:A:588:6PL:H11	1.95	0.65
3:E:302:6PL:O1P	3:E:302:6PL:H51	1.97	0.65
3:E:304:6PL:H372	3:E:312:6PL:H122	1.79	0.65
3:E:341:6PL:H211	3:E:341:6PL:C25	2.25	0.65
3:A:509:6PL:O4P	3:A:509:6PL:C6	2.42	0.65
3:A:539:6PL:H392	3:A:571:6PL:H391	1.78	0.65
3:A:564:6PL:H132	3:A:564:6PL:H331	1.78	0.65
3:A:565:6PL:H261	3:A:580:6PL:H211	1.77	0.65
3:E:346:6PL:C37	3:A:553:6PL:H471	2.26	0.65
3:A:515:6PL:H451	3:A:535:6PL:H231	1.77	0.65
3:A:520:6PL:H442	3:A:556:6PL:C25	2.26	0.65
3:A:546:6PL:H182	3:A:554:6PL:H121	1.78	0.65
3:A:556:6PL:H2	3:A:556:6PL:O11	1.96	0.65
3:E:302:6PL:H452	3:A:576:6PL:H241	1.78	0.65
3:E:332:6PL:C26	3:E:357:6PL:H231	2.22	0.65
3:A:524:6PL:C23	3:A:540:6PL:H362	2.23	0.65
3:A:539:6PL:H432	3:A:571:6PL:H401	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:552:6PL:O1P	3:A:552:6PL:H52	1.97	0.65
3:A:570:6PL:C48	3:A:582:6PL:H352	2.25	0.65
3:E:312:6PL:H461	3:E:323:6PL:H483	1.78	0.65
3:E:368:6PL:H73	3:E:368:6PL:O4P	1.96	0.65
3:A:511:6PL:P	3:A:511:6PL:H82	2.37	0.65
3:A:521:6PL:O31	3:A:521:6PL:H11	1.95	0.65
3:A:534:6PL:O4P	3:A:534:6PL:H83	1.97	0.65
3:A:572:6PL:O1P	3:A:572:6PL:C7	2.44	0.65
3:E:351:6PL:H442	1:A:365:LEU:HB3	1.78	0.65
1:A:402:LEU:HD23	3:A:503:6PL:H262	1.78	0.65
3:A:503:6PL:O4P	3:A:504:6PL:H31	1.97	0.65
3:A:520:6PL:C42	3:A:538:6PL:H263	2.25	0.65
3:A:578:6PL:H211	3:A:580:6PL:H251	1.79	0.65
3:E:334:6PL:H73	3:E:334:6PL:O4P	1.97	0.65
3:A:524:6PL:H82	3:A:524:6PL:P	2.36	0.65
3:A:540:6PL:O2P	3:A:540:6PL:H52	1.97	0.65
3:E:310:6PL:H131	3:E:318:6PL:C34	2.24	0.65
3:E:327:6PL:H191	3:E:340:6PL:H483	1.79	0.65
3:A:544:6PL:C40	3:A:551:6PL:H261	2.24	0.65
3:A:562:6PL:H392	3:A:579:6PL:C48	2.27	0.65
3:A:563:6PL:H202	3:A:567:6PL:H401	1.79	0.65
2:C:103:PHE:HA	2:C:143:PRO:HD2	1.79	0.65
3:E:301:6PL:H431	3:E:347:6PL:H372	1.78	0.65
3:E:302:6PL:H481	3:E:348:6PL:H483	1.77	0.65
3:A:543:6PL:H483	3:A:581:6PL:C24	2.27	0.65
3:A:587:6PL:O31	3:A:587:6PL:H341	1.96	0.65
3:E:332:6PL:C11	3:E:332:6PL:O31	2.45	0.64
3:E:335:6PL:H462	3:E:347:6PL:H251	1.79	0.64
3:E:350:6PL:H11	3:E:350:6PL:C4	2.27	0.64
3:E:350:6PL:O31	3:E:350:6PL:H32	1.97	0.64
1:A:435:TYR:CZ	3:A:537:6PL:H141	2.32	0.64
3:A:515:6PL:H482	3:A:519:6PL:H391	1.78	0.64
3:A:526:6PL:C24	3:A:575:6PL:H262	2.24	0.64
3:A:555:6PL:H12	3:A:555:6PL:O31	1.96	0.64
3:A:560:6PL:H62	3:A:560:6PL:P	2.36	0.64
3:E:321:6PL:H371	3:E:344:6PL:C34	2.28	0.64
3:E:368:6PL:H162	3:A:554:6PL:C23	2.27	0.64
3:A:560:6PL:H2	3:A:560:6PL:C4	2.27	0.64
3:E:321:6PL:H381	3:E:344:6PL:C3	2.27	0.64
3:E:368:6PL:H52	3:E:368:6PL:O2P	1.97	0.64
3:A:540:6PL:H12	3:A:540:6PL:O31	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:565:6PL:H442	3:A:580:6PL:H442	1.79	0.64
3:C:501:6PL:H352	3:C:501:6PL:C13	2.26	0.64
3:E:312:6PL:O11	3:E:312:6PL:H142	1.97	0.64
3:E:360:6PL:O31	3:E:360:6PL:C1	2.43	0.64
3:A:521:6PL:C23	3:A:557:6PL:H251	2.24	0.64
3:A:566:6PL:H452	3:A:587:6PL:H421	1.80	0.64
3:E:308:6PL:H422	3:E:353:6PL:H141	1.78	0.64
3:E:312:6PL:H263	3:E:315:6PL:H231	1.78	0.64
3:E:317:6PL:C33	3:A:508:6PL:H202	2.20	0.64
3:E:328:6PL:H122	3:E:330:6PL:H192	1.78	0.64
3:A:540:6PL:H132	3:A:540:6PL:C39	2.16	0.64
3:E:309:6PL:H342	3:E:309:6PL:O2	1.98	0.64
3:E:321:6PL:H341	3:E:339:6PL:H152	1.78	0.64
3:E:324:6PL:P	3:E:324:6PL:C6	2.85	0.64
3:E:341:6PL:H231	3:E:341:6PL:H402	1.78	0.64
3:E:342:6PL:H252	3:E:368:6PL:H241	1.79	0.64
3:E:363:6PL:H421	3:E:364:6PL:H212	1.80	0.64
3:A:505:6PL:H222	3:A:510:6PL:H201	1.76	0.64
3:A:524:6PL:P	3:A:524:6PL:C8	2.85	0.64
3:A:538:6PL:H191	3:A:552:6PL:H121	1.79	0.64
3:E:309:6PL:C12	3:E:326:6PL:H142	2.25	0.64
3:E:326:6PL:C48	3:E:364:6PL:H322	2.28	0.64
3:A:503:6PL:H72	3:A:504:6PL:H31	1.79	0.64
3:A:523:6PL:H461	3:A:544:6PL:H192	1.79	0.64
3:A:580:6PL:H372	3:A:588:6PL:C20	2.27	0.64
3:E:301:6PL:H382	3:E:343:6PL:H131	1.80	0.64
3:E:304:6PL:C32	3:E:355:6PL:H382	2.28	0.64
3:E:351:6PL:H442	1:A:365:LEU:CB	2.27	0.64
3:E:352:6PL:O31	3:E:352:6PL:H12	1.98	0.64
3:A:502:6PL:H461	3:A:510:6PL:H263	1.79	0.64
3:A:501:6PL:H2	3:A:501:6PL:O11	1.97	0.64
3:A:546:6PL:H191	3:A:554:6PL:H121	1.78	0.64
3:A:582:6PL:O4P	3:A:582:6PL:C6	2.45	0.64
3:E:304:6PL:H401	3:E:312:6PL:C12	2.27	0.64
3:E:333:6PL:C18	3:E:364:6PL:H362	2.28	0.64
3:E:357:6PL:H122	3:E:357:6PL:C34	2.28	0.64
3:E:358:6PL:H152	3:A:509:6PL:C2	2.28	0.64
3:A:501:6PL:O2P	3:A:502:6PL:H71	1.97	0.64
3:A:536:6PL:H121	3:A:546:6PL:H421	1.80	0.64
3:A:543:6PL:H172	3:A:566:6PL:C35	2.27	0.64
3:A:580:6PL:O4P	3:A:580:6PL:C2	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:581:6PL:H372	3:A:581:6PL:H431	1.78	0.64
3:E:304:6PL:H263	3:E:331:6PL:C22	2.28	0.63
3:E:309:6PL:H322	3:E:325:6PL:C12	2.27	0.63
3:E:318:6PL:C22	3:E:331:6PL:H252	2.24	0.63
3:E:320:6PL:H401	3:A:533:6PL:C25	2.27	0.63
3:E:351:6PL:H351	3:E:351:6PL:C15	2.28	0.63
3:E:358:6PL:H341	3:E:361:6PL:H32	1.78	0.63
3:E:364:6PL:H51	3:E:364:6PL:O2P	1.98	0.63
3:A:520:6PL:O31	3:A:520:6PL:C3	2.41	0.63
3:A:527:6PL:H352	3:A:530:6PL:H332	1.79	0.63
3:A:540:6PL:C37	3:A:550:6PL:H151	2.27	0.63
3:A:559:6PL:O2P	3:A:559:6PL:C5	2.46	0.63
2:B:103:PHE:HA	2:B:143:PRO:HD2	1.78	0.63
3:E:309:6PL:H362	3:E:325:6PL:C16	2.28	0.63
3:E:324:6PL:O3	3:E:324:6PL:O31	2.16	0.63
3:E:333:6PL:H372	3:E:363:6PL:C13	2.25	0.63
3:E:336:6PL:H392	3:E:336:6PL:C43	2.09	0.63
3:E:343:6PL:H73	3:E:343:6PL:O4P	1.97	0.63
2:C:68:LEU:HG	2:C:69:PRO:HD2	1.80	0.63
3:E:315:6PL:H122	3:E:326:6PL:H332	1.80	0.63
3:E:320:6PL:H422	3:A:533:6PL:H251	1.78	0.63
3:E:350:6PL:H262	3:E:360:6PL:H431	1.80	0.63
1:E:116:ARG:CZ	3:E:334:6PL:H42	2.28	0.63
3:E:344:6PL:O31	3:E:344:6PL:C3	2.42	0.63
3:A:529:6PL:H432	3:A:534:6PL:C38	2.28	0.63
3:A:539:6PL:H392	3:A:571:6PL:H382	1.78	0.63
3:E:309:6PL:C24	3:E:344:6PL:H171	2.28	0.63
3:E:318:6PL:H331	3:E:324:6PL:C45	2.26	0.63
3:E:321:6PL:H252	3:E:365:6PL:H222	1.81	0.63
3:E:332:6PL:O11	3:E:332:6PL:H2	1.98	0.63
3:E:348:6PL:H411	3:E:348:6PL:H262	1.79	0.63
3:E:356:6PL:O31	3:E:356:6PL:C11	2.46	0.63
3:A:533:6PL:H202	3:A:558:6PL:H201	1.80	0.63
1:E:108:TRP:CZ2	3:A:503:6PL:H381	2.34	0.63
1:A:351:TRP:CE3	3:A:536:6PL:H172	2.34	0.63
3:A:519:6PL:H62	3:A:519:6PL:O4P	1.98	0.63
3:A:529:6PL:C41	3:A:534:6PL:H361	2.28	0.63
3:A:532:6PL:H2	3:A:541:6PL:H83	1.81	0.63
3:A:549:6PL:H352	3:A:555:6PL:H191	1.80	0.63
3:E:343:6PL:O3P	3:E:343:6PL:C31	2.46	0.63
3:A:565:6PL:O31	3:A:565:6PL:H12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:574:6PL:H52	3:A:574:6PL:O3P	1.99	0.63
1:E:211:LEU:CD2	3:E:360:6PL:H472	2.28	0.62
3:E:305:6PL:H151	3:A:584:6PL:H252	1.81	0.62
3:E:345:6PL:O31	3:E:345:6PL:H12	1.99	0.62
3:E:347:6PL:H351	3:E:347:6PL:O2	1.98	0.62
3:E:355:6PL:O1P	3:E:355:6PL:H63	1.99	0.62
3:A:505:6PL:C22	3:A:510:6PL:C20	2.70	0.62
3:A:514:6PL:H51	3:A:514:6PL:O2P	1.99	0.62
3:A:515:6PL:H52	3:A:515:6PL:O3P	1.99	0.62
3:A:541:6PL:H31	3:A:557:6PL:C44	2.28	0.62
3:A:514:6PL:O2P	3:A:514:6PL:C7	2.46	0.62
3:A:565:6PL:H451	3:A:580:6PL:H231	1.80	0.62
3:A:578:6PL:C1	3:A:578:6PL:H42	2.29	0.62
3:A:580:6PL:H2	3:A:580:6PL:C4	2.29	0.62
3:E:308:6PL:O1P	3:E:308:6PL:H51	1.99	0.62
3:E:310:6PL:H391	3:E:331:6PL:H372	1.81	0.62
3:E:339:6PL:H83	3:E:339:6PL:O4P	1.96	0.62
3:A:501:6PL:C7	3:A:506:6PL:H121	2.29	0.62
3:A:525:6PL:C17	3:A:583:6PL:H251	2.19	0.62
3:A:540:6PL:H371	3:A:550:6PL:H162	1.78	0.62
3:A:580:6PL:C43	3:A:588:6PL:H242	2.29	0.62
3:C:501:6PL:H372	3:C:501:6PL:C14	2.17	0.62
3:E:304:6PL:C45	3:E:308:6PL:H241	2.29	0.62
3:E:321:6PL:H342	3:E:339:6PL:H152	1.81	0.62
3:E:333:6PL:H212	3:A:511:6PL:H442	1.80	0.62
3:A:533:6PL:H472	3:A:574:6PL:C14	2.25	0.62
3:E:335:6PL:H32	3:E:356:6PL:H32	1.82	0.62
3:E:328:6PL:C20	3:A:537:6PL:H261	2.26	0.62
3:A:524:6PL:H452	3:A:528:6PL:C26	2.27	0.62
3:A:560:6PL:P	3:A:560:6PL:C6	2.87	0.62
1:E:60:LEU:HD11	3:E:359:6PL:H481	1.81	0.62
3:E:306:6PL:H252	3:A:545:6PL:C42	2.29	0.62
3:E:310:6PL:C11	3:E:331:6PL:H141	2.29	0.62
3:E:354:6PL:O11	3:E:354:6PL:H2	1.98	0.62
3:A:532:6PL:C1	3:A:541:6PL:H83	2.30	0.62
3:A:546:6PL:H392	3:A:568:6PL:C13	2.23	0.62
3:A:570:6PL:H481	3:A:582:6PL:C12	2.29	0.62
3:E:306:6PL:C38	3:E:350:6PL:O11	2.47	0.62
3:E:328:6PL:O31	3:E:328:6PL:H32	1.99	0.62
3:E:335:6PL:H182	3:E:356:6PL:H172	1.82	0.62
3:A:533:6PL:H32	3:A:579:6PL:H361	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:LYS:HZ1	3:E:306:6PL:H2	1.64	0.62
3:E:315:6PL:O3	3:E:315:6PL:O31	2.18	0.62
3:A:544:6PL:C41	3:A:559:6PL:H212	2.30	0.62
3:A:548:6PL:H382	3:A:552:6PL:H451	1.80	0.62
3:E:308:6PL:H262	3:E:331:6PL:H462	1.82	0.62
1:A:250:PRO:HB2	3:A:575:6PL:H392	1.82	0.62
3:A:512:6PL:C31	3:A:587:6PL:H61	2.30	0.62
3:A:535:6PL:O1P	3:A:535:6PL:H51	1.99	0.62
3:A:566:6PL:H12	3:A:566:6PL:O31	1.98	0.62
3:A:576:6PL:P	3:A:576:6PL:H72	2.40	0.62
1:E:53:VAL:HB	3:A:586:6PL:H482	1.82	0.61
3:E:305:6PL:H261	3:A:528:6PL:H452	1.81	0.61
3:E:306:6PL:H382	3:E:350:6PL:O11	1.99	0.61
3:E:325:6PL:C18	3:E:325:6PL:C22	2.68	0.61
3:E:329:6PL:H351	3:E:340:6PL:H191	1.81	0.61
3:E:345:6PL:H11	3:C:501:6PL:H371	1.82	0.61
3:E:313:6PL:H263	3:A:553:6PL:H251	1.82	0.61
3:E:315:6PL:C18	3:E:323:6PL:H372	2.27	0.61
3:E:324:6PL:H341	3:E:358:6PL:C45	2.31	0.61
3:E:333:6PL:C7	3:E:333:6PL:O4P	2.48	0.61
1:A:276:PHE:HE1	3:A:507:6PL:H472	1.65	0.61
3:A:520:6PL:O2P	3:A:552:6PL:C8	2.48	0.61
3:A:540:6PL:H372	3:A:540:6PL:C13	2.26	0.61
3:A:570:6PL:C48	3:A:582:6PL:H132	2.25	0.61
3:E:310:6PL:H263	3:E:357:6PL:C21	2.05	0.61
3:E:369:6PL:H131	3:A:517:6PL:H432	1.82	0.61
3:A:540:6PL:H131	3:A:540:6PL:C38	2.30	0.61
3:A:549:6PL:O3P	3:A:549:6PL:C31	2.47	0.61
3:A:566:6PL:H83	3:A:566:6PL:P	2.40	0.61
1:E:43:ASN:HB3	3:E:322:6PL:H342	1.83	0.61
1:E:226:LYS:CG	3:E:327:6PL:H151	2.28	0.61
3:E:335:6PL:H132	3:E:356:6PL:H332	1.83	0.61
3:E:337:6PL:O4P	3:E:337:6PL:C7	2.48	0.61
3:A:505:6PL:H332	3:A:506:6PL:C34	2.29	0.61
3:A:572:6PL:H391	3:A:576:6PL:H172	1.82	0.61
3:A:578:6PL:H141	3:A:578:6PL:O11	2.00	0.61
3:E:304:6PL:H32	3:E:355:6PL:H372	1.82	0.61
3:E:326:6PL:H422	3:E:364:6PL:C1	2.29	0.61
3:A:511:6PL:H401	3:A:511:6PL:C36	2.17	0.61
3:A:518:6PL:H12	3:A:518:6PL:O11	2.01	0.61
3:A:558:6PL:C48	3:A:574:6PL:H222	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:565:6PL:H161	3:A:580:6PL:H411	1.82	0.61
3:A:566:6PL:O1P	3:A:566:6PL:H51	1.99	0.61
3:E:310:6PL:O31	3:E:310:6PL:H141	1.99	0.61
3:E:335:6PL:O2	3:E:335:6PL:O11	2.19	0.61
3:A:532:6PL:H171	3:A:541:6PL:H331	1.82	0.61
3:E:318:6PL:H211	3:E:331:6PL:H232	1.81	0.61
3:E:358:6PL:C25	3:A:509:6PL:H202	2.30	0.61
3:E:362:6PL:H83	3:E:362:6PL:P	2.40	0.61
3:A:504:6PL:C25	3:A:561:6PL:H241	2.30	0.61
3:A:505:6PL:H231	3:A:510:6PL:H212	1.83	0.61
3:A:522:6PL:C47	3:A:536:6PL:H351	2.30	0.61
3:A:541:6PL:O31	3:A:541:6PL:P	2.59	0.61
3:A:565:6PL:H181	3:A:565:6PL:H381	1.83	0.61
3:E:301:6PL:C46	3:E:347:6PL:H392	2.30	0.61
3:E:325:6PL:H252	3:E:344:6PL:H342	1.81	0.61
3:E:333:6PL:C40	3:E:363:6PL:H141	2.26	0.61
1:A:250:PRO:CB	3:A:575:6PL:H392	2.31	0.61
1:A:363:GLU:OE2	3:A:522:6PL:H52	2.00	0.61
3:A:558:6PL:C1	3:A:558:6PL:H41	2.30	0.61
3:A:578:6PL:O11	3:A:578:6PL:C31	2.48	0.61
3:E:303:6PL:O2P	3:E:303:6PL:H52	2.01	0.61
3:E:304:6PL:C47	3:E:308:6PL:H263	2.31	0.61
3:E:333:6PL:H161	3:E:364:6PL:C35	2.31	0.61
3:A:533:6PL:H441	3:A:574:6PL:C14	2.30	0.61
3:A:556:6PL:H12	3:A:556:6PL:O31	2.01	0.61
3:A:503:6PL:O4P	3:A:503:6PL:H63	2.00	0.61
3:A:512:6PL:C5	3:A:524:6PL:C12	2.65	0.61
3:A:525:6PL:H181	3:A:579:6PL:H212	1.81	0.61
3:A:538:6PL:H442	3:A:542:6PL:C22	2.26	0.61
3:A:538:6PL:H352	3:A:587:6PL:H342	1.82	0.61
3:A:539:6PL:O3	3:A:539:6PL:O31	2.19	0.61
1:E:149:ARG:HG3	3:C:501:6PL:H472	1.82	0.60
1:E:186:GLY:HA2	3:E:341:6PL:O3	2.01	0.60
3:E:347:6PL:H241	3:E:356:6PL:H212	1.83	0.60
3:E:358:6PL:H392	3:E:358:6PL:C43	2.26	0.60
3:E:368:6PL:O11	3:A:546:6PL:H231	2.01	0.60
3:A:502:6PL:H371	3:A:505:6PL:H441	1.83	0.60
3:A:531:6PL:H342	3:A:555:6PL:H351	1.82	0.60
3:A:551:6PL:C6	3:A:551:6PL:P	2.89	0.60
3:A:580:6PL:H441	3:A:588:6PL:H262	1.83	0.60
3:E:308:6PL:H262	3:E:331:6PL:C46	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:321:6PL:H61	3:E:365:6PL:H12	1.83	0.60
3:E:328:6PL:H162	3:A:537:6PL:H221	1.83	0.60
3:A:514:6PL:C46	3:A:567:6PL:H202	2.31	0.60
3:A:566:6PL:H452	3:A:587:6PL:C43	2.30	0.60
3:E:306:6PL:H372	3:E:350:6PL:O11	2.01	0.60
3:E:345:6PL:H32	3:C:501:6PL:H141	1.84	0.60
3:E:358:6PL:H232	3:A:509:6PL:C15	2.30	0.60
3:A:517:6PL:O31	3:A:517:6PL:C1	2.45	0.60
3:A:573:6PL:H451	3:A:575:6PL:H191	1.83	0.60
3:E:330:6PL:O1P	3:E:330:6PL:H51	2.00	0.60
3:E:368:6PL:O31	3:A:546:6PL:H201	2.02	0.60
3:A:516:6PL:O11	3:A:516:6PL:H2	2.00	0.60
3:A:535:6PL:H351	3:A:564:6PL:C39	2.25	0.60
3:E:301:6PL:H462	3:E:347:6PL:H392	1.82	0.60
3:E:347:6PL:C31	3:E:347:6PL:C35	2.80	0.60
1:A:485:THR:O	3:A:526:6PL:H71	2.01	0.60
3:A:546:6PL:H481	3:A:554:6PL:H201	1.83	0.60
3:A:548:6PL:H341	3:A:570:6PL:H171	1.83	0.60
3:A:578:6PL:C42	3:A:578:6PL:C46	2.77	0.60
3:C:501:6PL:O31	3:C:501:6PL:H12	1.99	0.60
3:E:326:6PL:H401	3:E:364:6PL:H11	1.83	0.60
3:A:538:6PL:P	3:A:542:6PL:H71	2.41	0.60
3:A:540:6PL:O31	3:A:540:6PL:H32	2.01	0.60
3:A:542:6PL:H421	3:A:542:6PL:C20	2.29	0.60
3:A:549:6PL:O3P	3:A:549:6PL:O31	2.20	0.60
1:E:211:LEU:HD23	3:E:360:6PL:H472	1.84	0.60
3:A:513:6PL:H212	3:A:548:6PL:H422	1.82	0.60
3:A:517:6PL:O11	3:A:517:6PL:H2	2.01	0.60
3:E:302:6PL:H202	3:E:308:6PL:H211	1.82	0.60
3:E:314:6PL:O31	3:E:314:6PL:H32	2.00	0.60
3:E:359:6PL:O3	3:E:359:6PL:O31	2.19	0.60
3:A:532:6PL:C2	3:A:541:6PL:H83	2.32	0.60
3:A:548:6PL:O4P	3:A:548:6PL:C8	2.47	0.60
3:E:333:6PL:H411	3:E:363:6PL:C35	2.32	0.60
3:E:369:6PL:H192	3:A:533:6PL:C40	2.30	0.60
3:A:559:6PL:H162	3:A:572:6PL:H441	1.84	0.60
3:A:576:6PL:O4P	3:A:576:6PL:C7	2.49	0.60
3:E:324:6PL:H342	3:A:503:6PL:O3	2.02	0.60
3:A:546:6PL:C18	3:A:554:6PL:H121	2.31	0.60
3:E:306:6PL:O2	3:E:306:6PL:O11	2.20	0.59
3:E:312:6PL:H241	3:E:315:6PL:H262	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:315:6PL:H451	3:E:355:6PL:H261	1.83	0.59
3:E:337:6PL:H192	3:E:362:6PL:H152	1.82	0.59
3:E:351:6PL:O4P	3:E:351:6PL:C6	2.50	0.59
3:E:351:6PL:O31	3:E:351:6PL:C3	2.48	0.59
3:A:526:6PL:H171	3:A:573:6PL:C47	2.31	0.59
3:A:541:6PL:H441	3:A:541:6PL:C40	2.14	0.59
3:E:304:6PL:H401	3:E:312:6PL:H121	1.84	0.59
3:E:324:6PL:C15	3:E:361:6PL:H361	2.32	0.59
3:E:335:6PL:H191	3:E:347:6PL:H201	1.83	0.59
1:A:435:TYR:CE2	3:A:537:6PL:H141	2.36	0.59
3:A:540:6PL:H41	3:A:550:6PL:C2	2.31	0.59
3:A:572:6PL:O31	3:A:572:6PL:H11	2.02	0.59
1:E:211:LEU:HD22	3:E:360:6PL:H412	1.83	0.59
3:E:325:6PL:H262	3:E:363:6PL:H212	1.84	0.59
3:E:359:6PL:H201	3:A:516:6PL:H242	1.84	0.59
3:E:368:6PL:H372	3:A:577:6PL:H481	1.84	0.59
3:A:503:6PL:O1P	3:A:503:6PL:H52	2.03	0.59
3:A:539:6PL:H263	3:A:563:6PL:H381	1.84	0.59
3:A:539:6PL:H52	3:A:539:6PL:O1P	2.02	0.59
3:A:542:6PL:O4P	3:A:542:6PL:H63	2.03	0.59
3:A:573:6PL:H342	3:A:575:6PL:C20	2.07	0.59
3:A:587:6PL:H362	3:A:587:6PL:H121	1.84	0.59
3:E:322:6PL:H263	3:E:339:6PL:H392	1.84	0.59
3:A:505:6PL:O4P	3:A:505:6PL:C6	2.45	0.59
3:A:506:6PL:C48	3:A:508:6PL:H482	2.24	0.59
3:E:350:6PL:O4P	3:E:350:6PL:H83	2.02	0.59
3:A:532:6PL:H12	3:A:541:6PL:H51	1.83	0.59
3:A:572:6PL:H401	3:A:576:6PL:C17	2.31	0.59
3:E:320:6PL:H372	3:E:338:6PL:H372	1.83	0.59
3:E:336:6PL:H382	3:E:362:6PL:C38	2.27	0.59
3:E:338:6PL:H152	3:E:352:6PL:H471	1.85	0.59
3:A:506:6PL:O31	3:A:506:6PL:H11	2.00	0.59
3:A:509:6PL:H32	3:A:509:6PL:O31	2.00	0.59
3:A:515:6PL:H261	3:A:531:6PL:H232	1.85	0.59
3:A:564:6PL:O4P	3:A:564:6PL:C8	2.50	0.59
3:A:573:6PL:H341	3:A:575:6PL:H222	1.83	0.59
3:E:318:6PL:H242	3:A:518:6PL:H462	1.83	0.59
3:E:319:6PL:H162	3:E:325:6PL:H392	1.83	0.59
3:E:325:6PL:H262	3:E:363:6PL:C21	2.32	0.59
3:E:327:6PL:C15	3:E:350:6PL:H381	2.32	0.59
3:E:333:6PL:H161	3:E:364:6PL:H352	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:345:6PL:O31	3:C:501:6PL:H141	2.03	0.59
3:E:363:6PL:H51	3:E:363:6PL:O2P	2.02	0.59
1:E:239:LYS:HD2	3:E:313:6PL:C33	2.31	0.59
3:E:301:6PL:H152	3:E:301:6PL:C11	2.32	0.59
3:E:321:6PL:H252	3:E:365:6PL:C23	2.33	0.59
3:E:345:6PL:H51	3:C:501:6PL:C36	2.32	0.59
3:E:352:6PL:O1P	3:E:352:6PL:H51	2.03	0.59
3:E:357:6PL:H2	3:E:357:6PL:O4P	2.03	0.59
3:A:511:6PL:O4P	3:A:511:6PL:C8	2.50	0.59
3:A:557:6PL:H371	3:A:557:6PL:H411	1.85	0.59
3:E:305:6PL:H222	3:A:550:6PL:H451	1.84	0.59
3:E:314:6PL:O1P	3:E:314:6PL:H52	2.01	0.59
3:A:506:6PL:H481	3:A:508:6PL:C48	2.27	0.59
3:A:508:6PL:H461	3:A:510:6PL:H411	1.85	0.59
3:A:517:6PL:H202	3:A:569:6PL:H382	1.85	0.59
3:A:529:6PL:H471	3:A:534:6PL:H401	1.85	0.59
3:A:574:6PL:O4P	3:A:574:6PL:C7	2.51	0.59
3:A:578:6PL:H42	3:A:578:6PL:H12	1.83	0.59
3:E:301:6PL:H451	3:E:347:6PL:H392	1.84	0.59
3:E:303:6PL:O4P	3:E:303:6PL:C6	2.46	0.59
3:E:310:6PL:O31	3:E:310:6PL:O3	2.21	0.59
3:E:317:6PL:H442	3:E:366:6PL:H483	1.83	0.59
3:E:323:6PL:H82	3:E:330:6PL:O31	2.03	0.59
3:E:331:6PL:H63	3:E:331:6PL:P	2.43	0.59
3:A:515:6PL:C26	3:A:531:6PL:H212	2.30	0.59
3:A:527:6PL:C15	3:A:571:6PL:O2	2.50	0.59
3:A:568:6PL:O2	3:A:568:6PL:H342	2.00	0.59
3:A:580:6PL:H362	3:A:588:6PL:H382	1.85	0.59
3:A:517:6PL:O4P	3:A:517:6PL:C6	2.47	0.58
3:A:535:6PL:O4P	3:A:535:6PL:C6	2.51	0.58
3:A:538:6PL:H483	3:A:542:6PL:H232	1.85	0.58
3:A:550:6PL:H483	3:A:584:6PL:H472	1.86	0.58
3:A:557:6PL:O3P	3:A:565:6PL:H52	2.03	0.58
3:E:308:6PL:O11	3:E:308:6PL:O2	2.21	0.58
3:E:313:6PL:H12	3:E:313:6PL:C4	2.33	0.58
3:A:525:6PL:H401	3:A:583:6PL:H483	1.85	0.58
3:A:542:6PL:H152	3:A:581:6PL:H182	1.80	0.58
3:A:588:6PL:O2P	3:A:588:6PL:H73	2.03	0.58
3:E:321:6PL:H381	3:E:344:6PL:H32	1.83	0.58
3:E:329:6PL:C42	3:A:548:6PL:H221	2.33	0.58
3:E:337:6PL:C44	3:E:347:6PL:H151	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:543:6PL:H483	3:A:581:6PL:H242	1.86	0.58
3:A:543:6PL:C41	3:A:566:6PL:H441	2.19	0.58
3:A:552:6PL:O31	3:A:552:6PL:H132	2.03	0.58
1:E:131:ARG:NH1	3:E:320:6PL:C2	2.66	0.58
3:E:301:6PL:C45	3:E:347:6PL:H392	2.34	0.58
3:E:324:6PL:O4P	3:E:324:6PL:C6	2.47	0.58
3:E:353:6PL:O2P	3:E:353:6PL:O2	2.21	0.58
3:E:355:6PL:O1P	3:E:355:6PL:H51	2.01	0.58
3:E:359:6PL:H63	3:E:359:6PL:P	2.43	0.58
3:A:541:6PL:H242	3:A:580:6PL:C39	2.28	0.58
3:A:586:6PL:H421	3:A:586:6PL:H371	1.85	0.58
3:A:506:6PL:O1P	3:A:506:6PL:H62	2.04	0.58
3:A:516:6PL:H261	3:A:563:6PL:C23	2.24	0.58
3:A:533:6PL:H352	3:A:533:6PL:H171	1.84	0.58
3:A:565:6PL:H422	3:A:565:6PL:H182	1.85	0.58
3:A:588:6PL:O11	3:A:588:6PL:H2	2.02	0.58
3:E:315:6PL:O1P	3:E:315:6PL:H51	2.02	0.58
3:E:345:6PL:C37	3:E:351:6PL:H121	2.33	0.58
3:E:368:6PL:C14	3:A:513:6PL:H442	2.33	0.58
3:A:520:6PL:C48	3:A:542:6PL:H422	2.17	0.58
3:A:531:6PL:H442	3:A:555:6PL:H241	1.84	0.58
3:A:572:6PL:C40	3:A:576:6PL:C17	2.69	0.58
3:A:579:6PL:H172	3:A:579:6PL:C37	2.34	0.58
2:B:133:TYR:HB3	2:B:139:VAL:CG2	2.33	0.58
3:E:319:6PL:H262	3:E:344:6PL:C47	2.34	0.58
3:E:321:6PL:H181	3:E:359:6PL:C11	2.33	0.58
1:A:343:TYR:HB3	3:A:554:6PL:H483	1.84	0.58
3:A:529:6PL:O3	3:A:529:6PL:O31	2.22	0.58
3:E:314:6PL:H161	3:E:353:6PL:H11	1.84	0.58
3:E:340:6PL:O31	3:E:340:6PL:C11	2.52	0.58
3:E:368:6PL:O11	3:A:546:6PL:H232	2.03	0.58
3:A:504:6PL:H261	3:A:561:6PL:H263	1.85	0.58
3:A:532:6PL:H132	3:A:560:6PL:C37	2.34	0.58
3:A:536:6PL:O31	3:A:536:6PL:H32	2.02	0.58
3:A:543:6PL:H421	3:A:566:6PL:C47	2.34	0.58
3:E:318:6PL:H362	3:E:331:6PL:H172	1.85	0.58
3:E:333:6PL:H392	3:E:363:6PL:C14	2.34	0.58
3:E:337:6PL:H442	3:E:347:6PL:H151	1.86	0.58
3:A:531:6PL:C36	3:A:531:6PL:H162	2.33	0.58
3:A:565:6PL:H351	3:A:580:6PL:H131	1.86	0.58
3:A:581:6PL:O31	3:A:581:6PL:H12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:306:6PL:C7	3:E:306:6PL:O4P	2.52	0.58
3:E:333:6PL:O4P	3:E:333:6PL:H73	2.04	0.58
3:E:345:6PL:H372	3:E:351:6PL:C12	2.34	0.58
3:E:359:6PL:O3	3:E:359:6PL:C31	2.52	0.58
1:A:363:GLU:CD	3:A:522:6PL:H52	2.24	0.58
3:A:518:6PL:O31	3:A:518:6PL:C3	2.50	0.58
3:A:543:6PL:H392	3:A:566:6PL:H411	1.86	0.58
3:E:315:6PL:C3	3:E:326:6PL:H321	2.34	0.57
3:E:324:6PL:C33	3:E:358:6PL:H442	2.33	0.57
3:A:531:6PL:O31	3:A:531:6PL:H12	2.03	0.57
3:A:534:6PL:H192	3:A:534:6PL:C15	2.18	0.57
3:A:541:6PL:O4P	3:A:541:6PL:H73	2.04	0.57
3:A:575:6PL:O31	3:A:575:6PL:H32	2.04	0.57
1:E:43:ASN:HB3	3:E:322:6PL:H362	1.86	0.57
3:E:346:6PL:H382	3:A:553:6PL:H472	1.78	0.57
3:E:321:6PL:H71	3:E:365:6PL:O1P	2.05	0.57
3:E:362:6PL:P	3:E:362:6PL:C8	2.92	0.57
3:A:513:6PL:H211	3:A:548:6PL:H161	1.85	0.57
3:A:515:6PL:H52	3:A:515:6PL:C1	2.34	0.57
3:A:545:6PL:O4P	3:A:545:6PL:C6	2.46	0.57
2:C:133:TYR:HB3	2:C:139:VAL:CG2	2.34	0.57
3:E:346:6PL:C11	3:E:346:6PL:O31	2.53	0.57
3:E:351:6PL:H351	3:E:351:6PL:H151	1.85	0.57
3:E:367:6PL:C7	3:E:367:6PL:O4P	2.52	0.57
3:E:369:6PL:H62	3:E:369:6PL:H11	1.85	0.57
3:A:507:6PL:H361	3:A:507:6PL:C32	2.15	0.57
3:A:507:6PL:O4P	3:A:507:6PL:C6	2.52	0.57
3:A:512:6PL:H63	3:A:524:6PL:O11	2.04	0.57
3:A:518:6PL:O11	3:A:518:6PL:C1	2.52	0.57
3:A:531:6PL:C33	3:A:555:6PL:O2	2.46	0.57
3:A:561:6PL:O31	3:A:561:6PL:H11	2.05	0.57
3:A:584:6PL:O4P	3:A:584:6PL:C6	2.47	0.57
3:A:584:6PL:H483	3:A:584:6PL:C16	2.33	0.57
1:E:182:LYS:NZ	3:E:306:6PL:H2	2.20	0.57
3:E:304:6PL:H322	3:E:355:6PL:H382	1.86	0.57
3:E:321:6PL:C2	3:E:344:6PL:H81	2.26	0.57
3:E:331:6PL:O2P	3:E:331:6PL:H52	2.04	0.57
3:E:354:6PL:H252	3:A:561:6PL:C25	2.33	0.57
1:A:363:GLU:OE1	3:A:522:6PL:H62	2.05	0.57
3:A:532:6PL:C21	3:A:541:6PL:H372	2.32	0.57
3:A:543:6PL:H332	3:A:587:6PL:H322	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:570:6PL:O3	3:A:570:6PL:C31	2.52	0.57
3:A:580:6PL:H392	3:A:588:6PL:C20	2.32	0.57
3:E:309:6PL:H481	3:E:364:6PL:H412	1.86	0.57
3:E:320:6PL:O31	3:E:320:6PL:H11	2.03	0.57
3:E:321:6PL:C25	3:E:365:6PL:H231	2.34	0.57
3:E:339:6PL:C14	3:E:339:6PL:H332	2.34	0.57
3:E:369:6PL:O3P	3:E:369:6PL:C6	2.53	0.57
3:A:515:6PL:H263	3:A:531:6PL:C21	2.33	0.57
3:A:552:6PL:O4P	3:A:552:6PL:C6	2.46	0.57
3:A:578:6PL:O31	3:A:578:6PL:H31	2.05	0.57
3:E:325:6PL:H231	3:E:344:6PL:H321	1.85	0.57
3:E:325:6PL:C25	3:E:344:6PL:H342	2.35	0.57
3:A:516:6PL:C26	3:A:563:6PL:H231	2.25	0.57
3:A:535:6PL:O31	3:A:535:6PL:C3	2.51	0.57
2:B:256:ARG:HA	2:B:259:TRP:O	2.05	0.57
2:C:256:ARG:HA	2:C:259:TRP:O	2.04	0.57
3:E:319:6PL:H212	3:E:319:6PL:H431	1.86	0.57
3:E:320:6PL:C20	3:E:369:6PL:H441	2.27	0.57
3:E:333:6PL:H161	3:E:364:6PL:H362	1.86	0.57
3:E:357:6PL:O31	3:E:357:6PL:O3	2.22	0.57
3:A:525:6PL:C7	3:A:525:6PL:O4P	2.52	0.57
3:A:574:6PL:H72	3:A:574:6PL:P	2.45	0.57
3:E:304:6PL:H372	3:E:312:6PL:C12	2.34	0.57
3:E:305:6PL:O4P	3:E:305:6PL:C6	2.47	0.57
3:E:318:6PL:H371	3:E:331:6PL:H192	1.86	0.57
3:E:308:6PL:H372	3:E:326:6PL:H441	1.85	0.56
3:E:308:6PL:H72	3:E:355:6PL:H11	1.86	0.56
3:E:369:6PL:H131	3:A:517:6PL:H442	1.87	0.56
3:A:530:6PL:H472	3:A:541:6PL:H221	1.87	0.56
3:A:533:6PL:H63	3:A:579:6PL:O1P	2.05	0.56
3:A:580:6PL:H61	3:A:588:6PL:O31	2.05	0.56
3:E:311:6PL:O31	3:E:313:6PL:H52	2.04	0.56
3:E:315:6PL:H162	3:E:323:6PL:C37	2.36	0.56
3:E:343:6PL:O4P	3:E:343:6PL:C7	2.52	0.56
3:A:503:6PL:H342	3:A:504:6PL:H141	1.87	0.56
3:A:515:6PL:H73	3:A:515:6PL:O4P	2.04	0.56
3:A:520:6PL:O4P	3:A:520:6PL:C6	2.49	0.56
3:A:538:6PL:H391	3:A:542:6PL:C34	2.35	0.56
3:A:542:6PL:O31	3:A:542:6PL:H32	2.04	0.56
3:A:577:6PL:H221	3:A:583:6PL:H482	1.87	0.56
1:E:94:LYS:HA	1:E:97:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:307:6PL:H481	3:E:345:6PL:H461	1.87	0.56
3:E:315:6PL:H162	3:E:323:6PL:C35	2.34	0.56
3:E:317:6PL:C14	3:E:366:6PL:H382	2.29	0.56
3:E:322:6PL:C17	3:E:339:6PL:H361	2.36	0.56
3:E:337:6PL:C1	3:E:337:6PL:O31	2.51	0.56
3:E:341:6PL:H461	3:E:350:6PL:H182	1.86	0.56
3:E:345:6PL:C42	3:E:351:6PL:H191	2.35	0.56
3:A:513:6PL:O31	3:A:513:6PL:H31	2.04	0.56
3:A:520:6PL:C44	3:A:556:6PL:H242	2.30	0.56
3:E:329:6PL:O4P	3:E:329:6PL:C6	2.53	0.56
3:E:361:6PL:H481	3:A:544:6PL:C34	2.35	0.56
3:E:366:6PL:H351	3:E:366:6PL:C3	2.35	0.56
3:A:521:6PL:H321	3:A:562:6PL:H331	1.88	0.56
3:A:582:6PL:H472	3:A:584:6PL:H452	1.88	0.56
3:E:302:6PL:H82	3:E:302:6PL:P	2.46	0.56
3:E:304:6PL:H452	3:E:308:6PL:C22	2.30	0.56
3:E:306:6PL:H252	3:A:545:6PL:H442	1.86	0.56
3:E:318:6PL:H242	3:A:518:6PL:H471	1.87	0.56
3:E:333:6PL:H161	3:E:364:6PL:C36	2.35	0.56
3:E:336:6PL:O31	3:E:336:6PL:H32	2.06	0.56
3:E:359:6PL:O2P	3:E:359:6PL:H52	2.05	0.56
3:A:519:6PL:O11	3:A:519:6PL:H2	2.05	0.56
3:A:531:6PL:O4P	3:A:531:6PL:C7	2.54	0.56
3:A:557:6PL:O4P	3:A:565:6PL:H42	2.05	0.56
2:C:256:ARG:HD3	2:C:261:GLU:HB3	1.87	0.56
3:E:306:6PL:H482	3:A:513:6PL:H202	1.87	0.56
3:E:315:6PL:H162	3:E:323:6PL:H371	1.88	0.56
3:E:317:6PL:H201	3:E:366:6PL:H421	1.87	0.56
3:E:324:6PL:C36	3:E:358:6PL:C43	2.83	0.56
3:E:329:6PL:O2P	3:E:329:6PL:H52	2.06	0.56
3:E:332:6PL:O4P	3:E:332:6PL:C6	2.51	0.56
3:E:369:6PL:H231	3:A:533:6PL:H452	1.86	0.56
3:A:507:6PL:H31	3:A:507:6PL:O31	2.06	0.56
3:A:563:6PL:H32	3:A:563:6PL:O31	2.04	0.56
3:E:317:6PL:H181	3:E:366:6PL:H421	1.88	0.56
3:E:344:6PL:O11	3:E:344:6PL:H2	2.04	0.56
3:E:369:6PL:C36	3:E:369:6PL:C40	2.73	0.56
3:A:546:6PL:C43	3:A:554:6PL:H381	2.23	0.56
3:A:565:6PL:H381	3:A:565:6PL:C18	2.36	0.56
2:B:256:ARG:HD3	2:B:261:GLU:HB3	1.87	0.56
2:C:120:TYR:CE2	2:C:121:LEU:HG	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:304:6PL:H462	3:E:312:6PL:H421	1.88	0.56
3:A:543:6PL:H251	3:A:566:6PL:H232	1.87	0.56
3:A:572:6PL:O1P	3:A:572:6PL:C5	2.50	0.56
3:E:308:6PL:H72	3:E:355:6PL:C1	2.36	0.56
3:E:316:6PL:O3	3:E:316:6PL:C31	2.53	0.56
3:E:358:6PL:H181	3:A:509:6PL:H151	1.88	0.56
3:A:515:6PL:O31	3:A:515:6PL:C1	2.40	0.56
3:A:528:6PL:H221	3:A:528:6PL:C42	2.26	0.56
3:E:306:6PL:H351	3:E:306:6PL:C17	2.35	0.56
3:E:335:6PL:O3	3:E:356:6PL:H331	2.05	0.56
3:A:532:6PL:O31	3:A:532:6PL:C1	2.49	0.56
3:A:546:6PL:H341	3:A:554:6PL:C3	2.36	0.56
3:E:310:6PL:H252	3:A:544:6PL:C48	2.35	0.55
3:E:319:6PL:O31	3:E:319:6PL:H11	2.06	0.55
3:E:329:6PL:C4	3:E:366:6PL:H131	2.35	0.55
3:A:538:6PL:H161	3:A:542:6PL:H321	1.87	0.55
3:A:542:6PL:H421	3:A:542:6PL:H211	1.79	0.55
3:A:563:6PL:H472	3:A:578:6PL:H392	1.87	0.55
3:A:576:6PL:O4P	3:A:576:6PL:H73	2.04	0.55
1:E:7:PRO:HD2	3:E:319:6PL:P	2.46	0.55
3:E:306:6PL:C48	3:A:513:6PL:H222	2.33	0.55
3:E:307:6PL:H52	3:E:307:6PL:O3P	2.06	0.55
3:E:321:6PL:H251	3:E:365:6PL:H231	1.88	0.55
3:E:340:6PL:H451	3:E:350:6PL:C44	2.26	0.55
3:A:535:6PL:H451	3:A:564:6PL:H262	1.87	0.55
3:E:304:6PL:H452	3:E:308:6PL:H241	1.89	0.55
3:E:321:6PL:H252	3:E:365:6PL:C22	2.36	0.55
3:E:360:6PL:O2	3:E:360:6PL:O11	2.24	0.55
3:A:510:6PL:H151	3:A:510:6PL:C36	2.36	0.55
3:A:512:6PL:H201	3:A:582:6PL:C22	2.35	0.55
3:A:525:6PL:O4P	3:A:525:6PL:H73	2.06	0.55
3:A:529:6PL:H462	3:A:534:6PL:C38	2.37	0.55
3:A:543:6PL:H381	3:A:581:6PL:H192	1.88	0.55
3:A:573:6PL:H341	3:A:575:6PL:H202	1.83	0.55
3:E:332:6PL:O31	3:E:332:6PL:O3	2.25	0.55
3:E:344:6PL:H191	3:E:363:6PL:H252	1.88	0.55
3:A:501:6PL:O1P	3:A:501:6PL:H51	2.05	0.55
3:A:529:6PL:O4P	3:A:529:6PL:C7	2.53	0.55
3:A:530:6PL:O4P	3:A:530:6PL:C6	2.48	0.55
3:A:562:6PL:H72	3:A:562:6PL:C1	2.36	0.55
3:A:578:6PL:H191	3:A:580:6PL:H242	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:306:6PL:H182	3:E:306:6PL:H362	1.89	0.55
3:E:328:6PL:H181	3:A:537:6PL:C25	2.37	0.55
3:A:518:6PL:H182	3:A:529:6PL:C17	2.36	0.55
3:A:573:6PL:C45	3:A:575:6PL:H191	2.37	0.55
3:A:580:6PL:H392	3:A:588:6PL:H222	1.88	0.55
3:E:312:6PL:H222	3:E:315:6PL:C41	2.35	0.55
3:E:324:6PL:C12	3:E:349:6PL:H211	2.33	0.55
3:E:349:6PL:H251	1:A:413:LEU:HD22	1.87	0.55
1:A:384:LEU:HB3	3:A:534:6PL:H422	1.88	0.55
3:A:514:6PL:O31	3:A:514:6PL:H342	2.06	0.55
3:A:519:6PL:H252	3:A:549:6PL:C43	2.34	0.55
3:A:552:6PL:O31	3:A:552:6PL:O3	2.24	0.55
2:B:360:GLN:HG2	2:B:367:VAL:HB	1.89	0.55
3:E:306:6PL:O4P	3:E:306:6PL:H73	2.07	0.55
3:E:313:6PL:H162	3:E:313:6PL:H361	1.89	0.55
3:E:324:6PL:H352	3:E:358:6PL:H431	1.87	0.55
3:E:326:6PL:H481	3:E:364:6PL:H342	1.87	0.55
3:E:340:6PL:H481	3:E:360:6PL:H202	1.88	0.55
1:A:351:TRP:NE1	3:A:536:6PL:H131	2.21	0.55
3:A:514:6PL:P	3:A:514:6PL:C7	2.93	0.55
3:A:540:6PL:H371	3:A:550:6PL:C17	2.37	0.55
3:A:588:6PL:C44	3:A:588:6PL:C48	2.78	0.55
3:E:317:6PL:H341	3:E:335:6PL:H342	1.88	0.55
3:E:369:6PL:C15	3:A:533:6PL:H321	2.26	0.55
3:A:502:6PL:C11	3:A:511:6PL:H122	2.37	0.55
3:A:513:6PL:O3	3:A:548:6PL:C32	2.55	0.55
3:E:305:6PL:C15	3:A:584:6PL:H252	2.36	0.55
1:A:426:GLU:OE2	3:A:519:6PL:H73	2.06	0.55
3:A:530:6PL:H391	3:A:564:6PL:H231	1.87	0.55
3:A:536:6PL:H162	3:A:554:6PL:H391	1.89	0.55
3:A:563:6PL:H362	3:A:567:6PL:H121	1.88	0.55
3:A:588:6PL:O4P	3:A:588:6PL:C7	2.55	0.55
1:A:370:GLN:NE2	3:A:517:6PL:H422	2.21	0.55
3:A:535:6PL:H402	3:A:564:6PL:H452	1.87	0.55
3:A:567:6PL:O1P	3:A:567:6PL:C6	2.55	0.55
2:B:120:TYR:CE2	2:B:121:LEU:HG	2.42	0.55
3:E:333:6PL:C16	3:E:364:6PL:H362	2.37	0.54
3:A:506:6PL:O1P	3:A:506:6PL:C6	2.55	0.54
3:A:533:6PL:O4P	3:A:533:6PL:C8	2.54	0.54
3:A:539:6PL:C40	3:A:571:6PL:H391	2.36	0.54
3:A:566:6PL:O3P	3:A:578:6PL:H63	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:568:6PL:O4P	3:A:568:6PL:C6	2.54	0.54
2:C:360:GLN:HG2	2:C:367:VAL:HB	1.89	0.54
3:A:518:6PL:C19	3:A:529:6PL:H181	2.37	0.54
3:A:572:6PL:H152	3:A:576:6PL:H162	1.88	0.54
3:A:577:6PL:H122	3:A:583:6PL:H322	1.89	0.54
3:A:580:6PL:O4P	3:A:580:6PL:C7	2.54	0.54
3:E:306:6PL:H351	3:E:306:6PL:H162	0.69	0.54
3:E:308:6PL:H362	3:E:326:6PL:H421	1.89	0.54
3:E:341:6PL:H481	3:A:513:6PL:H262	1.88	0.54
3:A:543:6PL:C16	3:A:566:6PL:H152	2.32	0.54
3:A:547:6PL:H391	3:A:555:6PL:C45	2.30	0.54
3:A:562:6PL:H72	3:A:562:6PL:O4P	2.07	0.54
3:A:565:6PL:O4P	3:A:565:6PL:C8	2.53	0.54
3:E:301:6PL:O2P	3:E:301:6PL:H52	2.08	0.54
3:E:309:6PL:C37	3:E:325:6PL:H172	2.38	0.54
3:E:350:6PL:C26	3:E:360:6PL:H431	2.37	0.54
3:E:362:6PL:C41	3:E:362:6PL:C45	2.86	0.54
3:E:369:6PL:H132	3:A:533:6PL:C31	2.37	0.54
3:A:502:6PL:O31	3:A:502:6PL:C3	2.41	0.54
3:A:505:6PL:C15	3:A:510:6PL:H122	2.37	0.54
3:A:515:6PL:H263	3:A:531:6PL:C23	2.36	0.54
3:A:520:6PL:H202	3:A:556:6PL:C47	2.37	0.54
3:A:538:6PL:H451	3:A:542:6PL:C22	2.38	0.54
3:A:553:6PL:H171	3:A:554:6PL:H182	1.88	0.54
3:A:575:6PL:O4P	3:A:575:6PL:C7	2.54	0.54
3:E:309:6PL:C13	3:E:344:6PL:H52	2.37	0.54
3:E:320:6PL:H381	3:E:338:6PL:C39	2.28	0.54
3:E:325:6PL:H262	3:E:363:6PL:H202	1.89	0.54
3:E:327:6PL:O4P	3:E:327:6PL:C6	2.54	0.54
3:E:360:6PL:H142	3:E:360:6PL:C33	2.36	0.54
3:E:366:6PL:C35	3:E:366:6PL:O3	2.56	0.54
3:A:534:6PL:C19	3:A:534:6PL:C15	2.82	0.54
3:A:570:6PL:H322	3:A:582:6PL:H71	1.89	0.54
3:E:304:6PL:H471	3:E:308:6PL:H263	1.88	0.54
3:E:313:6PL:H12	3:E:313:6PL:H41	1.90	0.54
3:E:338:6PL:O4P	3:E:338:6PL:C7	2.55	0.54
3:E:345:6PL:O4P	3:E:345:6PL:C8	2.53	0.54
3:E:354:6PL:O31	3:E:354:6PL:H12	2.06	0.54
3:A:503:6PL:O4P	3:A:504:6PL:C3	2.55	0.54
3:A:523:6PL:H471	3:A:544:6PL:H212	1.89	0.54
3:A:531:6PL:H161	3:A:531:6PL:H372	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:556:6PL:H351	3:A:557:6PL:C15	2.37	0.54
3:A:570:6PL:O31	3:A:570:6PL:H12	2.08	0.54
1:E:115:TYR:HB3	3:A:534:6PL:H472	1.89	0.54
3:E:314:6PL:H391	3:A:510:6PL:H322	1.89	0.54
3:E:332:6PL:C26	3:E:357:6PL:C23	2.83	0.54
3:E:346:6PL:H461	3:A:553:6PL:H432	1.90	0.54
3:E:359:6PL:H351	3:A:537:6PL:H451	1.90	0.54
3:E:363:6PL:O2P	3:E:363:6PL:H73	2.08	0.54
3:A:505:6PL:O1P	3:A:508:6PL:H2	2.08	0.54
3:A:513:6PL:H401	3:A:552:6PL:H471	1.89	0.54
3:A:517:6PL:H221	3:A:522:6PL:C12	2.38	0.54
3:E:309:6PL:O4P	3:E:309:6PL:C7	2.53	0.54
3:A:511:6PL:H83	3:A:511:6PL:P	2.47	0.54
3:A:548:6PL:O3P	3:A:548:6PL:H82	2.08	0.54
3:A:551:6PL:H62	3:A:551:6PL:P	2.48	0.54
3:A:582:6PL:H472	3:A:584:6PL:H431	1.90	0.54
2:C:66:MET:HA	3:C:501:6PL:H81	1.90	0.54
3:E:301:6PL:C7	3:E:307:6PL:O2P	2.49	0.54
3:E:317:6PL:H151	3:A:508:6PL:H231	1.88	0.54
3:E:319:6PL:H2	3:E:319:6PL:O11	2.06	0.54
3:E:340:6PL:C33	3:E:342:6PL:C18	2.85	0.54
1:A:387:LEU:CB	3:A:534:6PL:H432	2.38	0.54
1:A:407:ALA:HB3	1:A:408:PRO:HD3	1.89	0.54
3:A:528:6PL:H332	3:A:584:6PL:H32	1.88	0.54
3:A:546:6PL:H2	3:A:546:6PL:O11	2.06	0.54
3:A:568:6PL:H121	3:A:568:6PL:H361	1.90	0.54
3:E:320:6PL:O4P	3:E:320:6PL:H72	2.08	0.54
3:E:324:6PL:H372	3:E:358:6PL:H381	1.88	0.54
3:E:334:6PL:H482	3:A:534:6PL:H221	1.88	0.54
3:E:369:6PL:H131	3:A:517:6PL:C44	2.38	0.54
1:A:303:LEU:HD23	3:A:550:6PL:H431	1.91	0.54
1:A:399:VAL:CG2	3:A:503:6PL:H481	2.37	0.54
3:A:502:6PL:H12	3:A:511:6PL:H121	1.90	0.54
3:A:522:6PL:O31	3:A:522:6PL:C1	2.52	0.54
3:E:306:6PL:H162	3:E:306:6PL:C34	2.31	0.53
3:E:316:6PL:H82	3:E:346:6PL:O2P	2.08	0.53
3:E:321:6PL:H371	3:E:344:6PL:C33	2.39	0.53
3:E:327:6PL:H262	3:E:350:6PL:H452	1.89	0.53
3:E:329:6PL:H12	3:E:329:6PL:H42	1.90	0.53
3:E:358:6PL:H172	3:A:509:6PL:C2	2.39	0.53
3:A:513:6PL:H11	3:A:548:6PL:H322	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:515:6PL:H141	3:A:515:6PL:O11	2.08	0.53
3:A:529:6PL:H231	3:A:551:6PL:H442	1.90	0.53
3:A:530:6PL:H382	3:A:564:6PL:H222	1.90	0.53
3:E:309:6PL:H361	3:E:325:6PL:H152	1.90	0.53
3:E:323:6PL:C8	3:E:330:6PL:O31	2.56	0.53
3:E:323:6PL:H151	3:E:330:6PL:H412	1.91	0.53
3:E:369:6PL:C26	3:A:533:6PL:H451	2.36	0.53
3:A:517:6PL:H151	3:A:579:6PL:O11	2.09	0.53
3:A:528:6PL:H341	3:A:528:6PL:O31	2.09	0.53
3:A:541:6PL:H332	3:A:557:6PL:C36	2.38	0.53
3:A:553:6PL:H371	3:A:554:6PL:H452	1.90	0.53
3:A:556:6PL:O31	3:A:556:6PL:H31	2.09	0.53
3:A:563:6PL:O31	3:A:563:6PL:H11	2.06	0.53
3:A:566:6PL:C45	3:A:587:6PL:H432	2.38	0.53
3:E:302:6PL:H211	3:E:348:6PL:H251	1.90	0.53
3:E:303:6PL:P	3:E:303:6PL:C6	2.96	0.53
3:E:341:6PL:C47	3:E:360:6PL:H261	2.29	0.53
3:E:363:6PL:O4P	3:E:363:6PL:C7	2.56	0.53
1:A:351:TRP:CZ3	3:A:536:6PL:H172	2.43	0.53
3:A:516:6PL:H401	3:A:586:6PL:O2	2.08	0.53
3:A:563:6PL:H462	3:A:578:6PL:C34	2.38	0.53
3:E:331:6PL:H412	3:E:357:6PL:H391	1.89	0.53
3:A:543:6PL:H12	3:A:581:6PL:H362	1.90	0.53
3:A:547:6PL:C39	3:A:555:6PL:H452	2.31	0.53
3:A:566:6PL:H452	3:A:587:6PL:C42	2.38	0.53
3:E:328:6PL:H263	3:E:348:6PL:O3P	2.08	0.53
3:E:335:6PL:H162	3:E:356:6PL:C15	2.38	0.53
3:E:368:6PL:C16	3:A:513:6PL:H442	2.38	0.53
3:E:369:6PL:H402	3:E:369:6PL:H361	1.86	0.53
3:A:530:6PL:H331	3:A:588:6PL:H122	1.90	0.53
3:A:533:6PL:C4	3:A:579:6PL:O31	2.56	0.53
3:E:312:6PL:H461	3:E:323:6PL:C48	2.37	0.53
3:E:322:6PL:O4P	3:E:322:6PL:C8	2.56	0.53
3:E:330:6PL:H72	3:E:330:6PL:P	2.49	0.53
3:E:337:6PL:O31	3:E:337:6PL:H11	2.08	0.53
1:A:386:PRO:HA	2:B:239:LEU:H	1.73	0.53
3:A:522:6PL:H452	3:A:536:6PL:H372	1.91	0.53
3:A:532:6PL:C19	3:A:557:6PL:H392	2.39	0.53
3:A:552:6PL:P	3:A:552:6PL:C6	2.97	0.53
3:A:578:6PL:C1	3:A:578:6PL:C4	2.87	0.53
2:C:35:GLN:HG2	2:C:112:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:339:6PL:H263	3:A:567:6PL:H442	1.89	0.53
3:A:505:6PL:H51	3:A:508:6PL:O3P	2.08	0.53
3:A:558:6PL:H52	3:A:574:6PL:O2P	2.09	0.53
1:E:43:ASN:CB	3:E:322:6PL:H362	2.38	0.53
1:E:182:LYS:NZ	3:E:306:6PL:H31	2.23	0.53
3:E:359:6PL:H361	3:A:537:6PL:C43	2.37	0.53
3:A:506:6PL:C11	3:A:506:6PL:O2	2.57	0.53
3:A:514:6PL:O31	3:A:514:6PL:C11	2.57	0.53
3:A:515:6PL:H12	3:A:515:6PL:H52	1.91	0.53
3:A:561:6PL:O1P	3:A:561:6PL:H51	2.09	0.53
1:E:219:LEU:HB3	1:E:220:PRO:HD3	1.91	0.53
3:E:304:6PL:H161	3:E:331:6PL:C11	2.38	0.53
3:E:313:6PL:H41	3:E:313:6PL:C1	2.39	0.53
3:E:322:6PL:H263	3:E:339:6PL:C40	2.33	0.53
3:E:338:6PL:O31	3:E:338:6PL:O3	2.27	0.53
3:E:344:6PL:O31	3:E:344:6PL:H12	2.09	0.53
3:A:507:6PL:O1P	3:A:507:6PL:H52	2.09	0.53
3:A:513:6PL:H432	3:A:552:6PL:H382	1.90	0.53
3:A:519:6PL:H221	3:A:549:6PL:C42	2.38	0.53
3:A:539:6PL:H483	3:A:588:6PL:H232	1.91	0.53
3:A:548:6PL:H402	3:A:548:6PL:C17	2.24	0.53
3:A:550:6PL:C26	3:A:550:6PL:C22	2.76	0.53
3:C:501:6PL:H2	3:C:501:6PL:O2P	2.09	0.53
3:E:330:6PL:H452	3:A:537:6PL:C24	2.33	0.53
3:E:364:6PL:H141	3:E:364:6PL:H331	1.91	0.53
3:A:504:6PL:H472	3:A:534:6PL:H482	1.91	0.53
3:A:511:6PL:O1P	3:A:511:6PL:C5	2.48	0.53
3:A:528:6PL:C23	3:A:528:6PL:C19	2.78	0.53
3:A:533:6PL:C14	3:A:579:6PL:H202	2.30	0.53
3:A:557:6PL:P	3:A:565:6PL:H42	2.49	0.53
3:A:565:6PL:H152	3:A:580:6PL:H381	1.91	0.53
3:A:566:6PL:O1P	3:A:566:6PL:C5	2.56	0.53
1:E:229:PHE:CE2	3:E:316:6PL:H372	2.44	0.52
3:E:337:6PL:H142	3:E:337:6PL:C36	2.38	0.52
3:E:341:6PL:O11	3:E:341:6PL:O2	2.26	0.52
3:E:354:6PL:O31	3:E:354:6PL:C3	2.50	0.52
3:A:558:6PL:O11	3:A:574:6PL:H11	2.09	0.52
1:E:189:LEU:HD23	3:E:341:6PL:C2	2.38	0.52
3:E:304:6PL:H142	3:E:331:6PL:C2	2.39	0.52
3:E:306:6PL:H372	3:E:350:6PL:C11	2.39	0.52
3:E:313:6PL:H321	3:E:342:6PL:O2P	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:323:6PL:H171	3:E:330:6PL:C42	2.39	0.52
3:E:329:6PL:H52	3:E:366:6PL:H131	1.85	0.52
3:A:502:6PL:H371	3:A:505:6PL:C42	2.37	0.52
3:A:512:6PL:H31	3:A:524:6PL:C41	2.34	0.52
3:A:536:6PL:C8	3:A:536:6PL:P	2.97	0.52
3:A:541:6PL:O31	3:A:541:6PL:O3P	2.28	0.52
3:A:542:6PL:H201	3:A:542:6PL:H431	1.89	0.52
3:A:546:6PL:O4P	3:A:546:6PL:C6	2.55	0.52
3:E:354:6PL:O4P	3:E:354:6PL:C8	2.57	0.52
3:E:358:6PL:H242	3:A:509:6PL:C19	2.39	0.52
3:E:358:6PL:H342	3:E:361:6PL:O31	2.09	0.52
3:A:516:6PL:H201	3:A:547:6PL:H451	1.91	0.52
3:A:521:6PL:C11	3:A:562:6PL:H142	2.39	0.52
3:A:530:6PL:C17	3:A:535:6PL:H332	2.35	0.52
3:A:531:6PL:O4P	3:A:531:6PL:H73	2.10	0.52
3:A:551:6PL:O4P	3:A:551:6PL:C6	2.56	0.52
3:A:577:6PL:O11	3:A:577:6PL:H2	2.09	0.52
3:A:581:6PL:C8	3:A:581:6PL:O4P	2.57	0.52
3:E:302:6PL:C48	3:E:348:6PL:H483	2.39	0.52
3:E:314:6PL:H242	3:E:353:6PL:H162	1.91	0.52
3:E:317:6PL:O1P	3:E:317:6PL:H52	2.10	0.52
3:E:321:6PL:H182	3:E:365:6PL:H182	1.91	0.52
3:E:345:6PL:O11	3:C:501:6PL:H431	2.10	0.52
3:A:505:6PL:H32	3:A:505:6PL:O31	2.09	0.52
3:A:536:6PL:O2P	3:A:536:6PL:H52	2.10	0.52
3:E:338:6PL:C47	3:A:522:6PL:H231	2.32	0.52
3:E:344:6PL:H462	3:E:344:6PL:H231	1.90	0.52
3:E:346:6PL:O31	3:E:346:6PL:O3	2.27	0.52
3:A:515:6PL:H451	3:A:535:6PL:C24	2.39	0.52
3:A:519:6PL:H411	3:A:549:6PL:H431	1.92	0.52
3:A:520:6PL:H122	3:A:520:6PL:H362	1.91	0.52
3:A:522:6PL:H451	3:A:522:6PL:H142	1.91	0.52
3:A:570:6PL:H2	3:A:570:6PL:O1P	2.09	0.52
3:A:581:6PL:O1P	3:A:581:6PL:H51	2.10	0.52
2:B:67:PHE:O	2:B:240:LYS:HG3	2.09	0.52
3:E:304:6PL:C34	3:E:355:6PL:C38	2.81	0.52
3:E:315:6PL:C6	3:E:315:6PL:P	2.98	0.52
3:E:323:6PL:O31	3:E:323:6PL:O3	2.28	0.52
3:A:503:6PL:H41	3:A:504:6PL:C3	2.34	0.52
3:A:557:6PL:O4P	3:A:557:6PL:C7	2.56	0.52
3:E:309:6PL:C47	3:E:363:6PL:H251	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:523:6PL:H422	3:A:572:6PL:C47	2.38	0.52
3:A:531:6PL:O2P	3:A:571:6PL:H63	2.09	0.52
3:A:532:6PL:H191	3:A:541:6PL:C37	2.27	0.52
3:A:580:6PL:C36	3:A:588:6PL:H372	2.40	0.52
3:E:309:6PL:H131	3:E:344:6PL:H52	1.91	0.52
3:E:321:6PL:H192	3:E:365:6PL:H202	1.92	0.52
3:E:333:6PL:H412	3:E:363:6PL:C35	2.31	0.52
3:A:517:6PL:H182	3:A:569:6PL:H361	1.90	0.52
3:A:520:6PL:C42	3:A:538:6PL:H242	2.40	0.52
3:A:521:6PL:H222	3:A:557:6PL:H231	1.90	0.52
3:A:525:6PL:H321	3:A:557:6PL:H162	1.92	0.52
3:A:570:6PL:H51	3:A:570:6PL:O3P	2.10	0.52
3:A:572:6PL:H72	3:A:572:6PL:P	2.46	0.52
2:C:174:PRO:HB2	2:C:204:ASP:HB2	1.92	0.52
3:E:317:6PL:H161	3:E:366:6PL:H402	1.92	0.52
3:E:348:6PL:H62	3:E:348:6PL:O1P	2.10	0.52
1:A:250:PRO:HG2	3:A:575:6PL:H392	1.92	0.52
3:A:514:6PL:O2P	3:A:514:6PL:H73	2.10	0.52
3:A:519:6PL:C19	3:A:549:6PL:H422	2.39	0.52
3:A:540:6PL:C38	3:A:550:6PL:H171	2.40	0.52
3:A:543:6PL:H322	3:A:581:6PL:H132	1.92	0.52
3:A:549:6PL:O1P	3:A:549:6PL:H51	2.10	0.52
3:A:570:6PL:O4P	3:A:570:6PL:C7	2.58	0.52
3:A:577:6PL:O4P	3:A:577:6PL:C6	2.52	0.52
3:A:579:6PL:O4P	3:A:579:6PL:C7	2.58	0.52
2:B:293:MET:HA	2:B:293:MET:CE	2.39	0.52
3:E:302:6PL:H52	3:A:509:6PL:C13	2.40	0.52
3:E:315:6PL:O4P	3:E:315:6PL:C6	2.58	0.52
3:E:330:6PL:H262	3:A:537:6PL:C18	2.40	0.52
3:E:348:6PL:H63	3:E:348:6PL:P	2.49	0.52
3:E:366:6PL:H52	3:E:366:6PL:O1P	2.09	0.52
3:E:369:6PL:H211	3:A:574:6PL:H2	1.89	0.52
3:A:508:6PL:O31	3:A:508:6PL:H32	2.09	0.52
3:A:516:6PL:C7	3:A:516:6PL:O4P	2.57	0.52
3:A:531:6PL:H331	3:A:555:6PL:C2	2.40	0.52
3:A:535:6PL:H392	3:A:564:6PL:H432	1.91	0.52
3:A:541:6PL:C24	3:A:580:6PL:H391	2.33	0.52
3:A:566:6PL:H222	3:A:578:6PL:C41	2.39	0.52
2:C:293:MET:HA	2:C:293:MET:CE	2.40	0.52
3:E:326:6PL:C39	3:E:364:6PL:H41	2.40	0.51
3:E:335:6PL:H481	3:E:353:6PL:H431	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:365:6PL:O2P	3:E:365:6PL:C8	2.58	0.51
3:A:525:6PL:O31	3:A:525:6PL:H11	2.09	0.51
3:A:533:6PL:C8	3:A:533:6PL:P	2.98	0.51
3:A:539:6PL:C39	3:A:571:6PL:H391	2.40	0.51
3:A:577:6PL:H62	3:A:577:6PL:O1P	2.10	0.51
3:E:306:6PL:C47	3:A:582:6PL:H483	2.38	0.51
3:E:306:6PL:C37	3:E:350:6PL:O11	2.58	0.51
3:E:310:6PL:H472	3:A:544:6PL:C46	2.40	0.51
3:E:355:6PL:O4P	3:E:355:6PL:H2	2.11	0.51
3:E:368:6PL:C31	3:E:368:6PL:H351	2.40	0.51
3:A:518:6PL:H441	3:A:560:6PL:H412	1.92	0.51
3:A:541:6PL:C14	3:A:588:6PL:H332	2.40	0.51
3:E:302:6PL:H192	3:E:348:6PL:H231	1.92	0.51
3:E:305:6PL:H11	3:E:305:6PL:O31	2.10	0.51
3:E:310:6PL:C3	3:E:331:6PL:H131	2.40	0.51
3:E:311:6PL:C6	3:E:311:6PL:P	2.99	0.51
3:E:318:6PL:C24	3:A:518:6PL:H471	2.40	0.51
3:E:348:6PL:O31	3:E:348:6PL:C1	2.49	0.51
1:A:432:LEU:HD23	3:A:519:6PL:C3	2.38	0.51
3:A:508:6PL:O11	3:A:508:6PL:H142	2.09	0.51
3:A:525:6PL:H372	3:A:562:6PL:H483	1.92	0.51
3:A:525:6PL:H72	3:A:525:6PL:P	2.49	0.51
3:A:527:6PL:H151	3:A:571:6PL:H2	1.92	0.51
3:A:529:6PL:O31	3:A:529:6PL:C1	2.52	0.51
1:E:7:PRO:HD2	3:E:319:6PL:O2P	2.11	0.51
1:E:163:LEU:HD23	3:E:346:6PL:H372	1.92	0.51
3:E:321:6PL:H261	3:E:365:6PL:C24	2.29	0.51
3:E:322:6PL:H442	1:A:461:LEU:HD12	1.91	0.51
3:E:335:6PL:H352	3:E:353:6PL:C32	2.39	0.51
3:E:337:6PL:H172	3:E:362:6PL:H132	1.92	0.51
3:E:359:6PL:O2P	3:E:359:6PL:H62	2.11	0.51
3:A:524:6PL:O1P	3:A:524:6PL:C5	2.57	0.51
3:A:528:6PL:O4P	3:A:528:6PL:C8	2.55	0.51
3:A:568:6PL:H452	3:A:569:6PL:H481	1.92	0.51
3:A:580:6PL:C35	3:A:588:6PL:H182	2.40	0.51
3:A:582:6PL:H481	3:A:584:6PL:H442	1.91	0.51
3:E:308:6PL:H242	3:E:331:6PL:C44	2.40	0.51
3:E:311:6PL:O31	3:E:311:6PL:H342	2.11	0.51
3:E:324:6PL:C35	3:E:358:6PL:H431	2.41	0.51
3:E:325:6PL:H262	3:E:363:6PL:H201	1.87	0.51
3:A:515:6PL:H451	3:A:535:6PL:H242	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:532:6PL:O31	3:A:532:6PL:H32	2.11	0.51
3:A:540:6PL:H51	3:A:550:6PL:O3P	2.09	0.51
3:A:556:6PL:O2P	3:A:556:6PL:H82	2.11	0.51
3:A:558:6PL:O4P	3:A:558:6PL:C8	2.54	0.51
3:E:309:6PL:H131	3:E:344:6PL:H62	1.84	0.51
3:E:318:6PL:H481	3:A:504:6PL:H263	1.92	0.51
3:E:321:6PL:H181	3:E:359:6PL:H121	1.93	0.51
3:E:324:6PL:O2P	3:E:324:6PL:C6	2.57	0.51
3:E:340:6PL:H481	3:E:360:6PL:H201	1.92	0.51
3:A:504:6PL:H482	3:A:534:6PL:H241	1.92	0.51
3:A:522:6PL:H342	3:A:522:6PL:C14	2.38	0.51
3:A:549:6PL:O11	3:A:549:6PL:O2	2.29	0.51
3:A:553:6PL:O4P	3:A:553:6PL:C8	2.59	0.51
3:E:311:6PL:O4P	3:E:311:6PL:C6	2.58	0.51
3:E:321:6PL:O31	3:E:321:6PL:H12	2.10	0.51
3:E:324:6PL:H161	3:E:361:6PL:H361	1.93	0.51
3:E:326:6PL:O31	3:E:326:6PL:H11	2.09	0.51
3:E:327:6PL:C26	3:E:350:6PL:H452	2.41	0.51
3:E:333:6PL:H182	3:E:364:6PL:C38	2.38	0.51
3:E:357:6PL:O3	3:E:357:6PL:C31	2.57	0.51
3:E:358:6PL:H232	3:A:509:6PL:H131	1.93	0.51
3:A:506:6PL:O2	3:A:506:6PL:O11	2.29	0.51
3:A:528:6PL:H342	3:A:550:6PL:H351	1.92	0.51
3:A:532:6PL:H192	3:A:557:6PL:H392	1.93	0.51
3:E:312:6PL:O31	3:E:312:6PL:C3	2.56	0.51
3:E:337:6PL:H442	3:E:347:6PL:C15	2.40	0.51
3:A:567:6PL:O4P	3:A:567:6PL:C6	2.59	0.51
3:E:306:6PL:H182	3:E:306:6PL:C36	2.41	0.51
3:E:313:6PL:O4P	3:E:313:6PL:C7	2.58	0.51
3:E:329:6PL:H362	3:E:340:6PL:H221	1.91	0.51
3:E:337:6PL:H422	3:E:347:6PL:H152	1.93	0.51
3:E:356:6PL:C7	3:E:357:6PL:O1P	2.58	0.51
3:E:366:6PL:O31	3:E:366:6PL:C11	2.58	0.51
3:A:540:6PL:C13	3:A:540:6PL:C39	2.83	0.51
3:A:541:6PL:C37	3:A:557:6PL:H381	2.41	0.51
3:E:301:6PL:O4P	3:E:301:6PL:C6	2.58	0.51
3:E:306:6PL:H471	3:A:582:6PL:C48	2.36	0.51
3:E:326:6PL:H401	3:E:364:6PL:C1	2.41	0.51
3:E:351:6PL:H351	3:E:351:6PL:H152	1.93	0.51
3:A:512:6PL:H63	3:A:524:6PL:H341	1.93	0.51
3:A:517:6PL:H171	3:A:579:6PL:H122	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:518:6PL:H382	3:A:560:6PL:C40	2.41	0.51
3:A:523:6PL:H332	3:A:544:6PL:C5	2.39	0.51
3:E:304:6PL:H142	3:E:331:6PL:O3P	2.12	0.50
3:E:337:6PL:C1	3:E:337:6PL:C4	2.84	0.50
3:E:354:6PL:H131	3:E:354:6PL:H361	1.93	0.50
3:E:368:6PL:O31	3:E:368:6PL:C3	2.48	0.50
3:A:543:6PL:H262	3:A:566:6PL:H252	1.92	0.50
1:E:46:LEU:HB3	3:E:322:6PL:H402	1.94	0.50
3:E:321:6PL:C25	3:E:365:6PL:C23	2.89	0.50
3:E:329:6PL:H31	3:E:366:6PL:H142	1.93	0.50
3:E:358:6PL:H242	3:A:509:6PL:H191	1.92	0.50
1:A:387:LEU:HG	3:A:534:6PL:H432	1.93	0.50
3:A:520:6PL:H202	3:A:556:6PL:H472	1.92	0.50
3:A:532:6PL:H12	3:A:541:6PL:C5	2.40	0.50
3:A:573:6PL:O4P	3:A:573:6PL:C8	2.59	0.50
3:A:578:6PL:H151	3:A:580:6PL:H201	1.92	0.50
3:A:580:6PL:C37	3:A:588:6PL:H182	2.40	0.50
3:A:580:6PL:C38	3:A:588:6PL:H381	2.39	0.50
3:E:304:6PL:H361	3:E:308:6PL:H122	1.93	0.50
3:E:315:6PL:H332	3:E:326:6PL:C38	2.40	0.50
3:E:316:6PL:C32	3:E:327:6PL:H331	2.26	0.50
3:E:317:6PL:H181	3:E:366:6PL:H402	1.93	0.50
3:E:318:6PL:H52	3:E:318:6PL:O1P	2.11	0.50
3:E:328:6PL:C26	3:E:348:6PL:O3P	2.59	0.50
3:E:339:6PL:H442	3:A:575:6PL:H442	1.93	0.50
3:A:502:6PL:C12	3:A:511:6PL:O3	2.60	0.50
3:A:506:6PL:H332	3:A:506:6PL:C13	2.42	0.50
3:A:543:6PL:H483	3:A:581:6PL:H241	1.93	0.50
3:A:576:6PL:O1P	3:A:576:6PL:C5	2.54	0.50
3:A:580:6PL:H372	3:A:588:6PL:H182	1.93	0.50
3:E:304:6PL:O4P	3:E:304:6PL:C6	2.56	0.50
3:E:321:6PL:H371	3:E:344:6PL:H332	1.93	0.50
3:E:321:6PL:C25	3:E:365:6PL:H241	2.41	0.50
3:E:329:6PL:O2	3:E:329:6PL:O11	2.29	0.50
3:E:330:6PL:O4P	3:E:330:6PL:C7	2.59	0.50
3:A:513:6PL:O4P	3:A:513:6PL:C8	2.59	0.50
3:A:520:6PL:H2	3:A:520:6PL:O11	2.09	0.50
3:A:541:6PL:H141	3:A:588:6PL:H332	1.94	0.50
3:A:542:6PL:C42	3:A:542:6PL:H201	2.42	0.50
2:C:239:LEU:HG	2:C:239:LEU:O	2.11	0.50
3:E:304:6PL:H401	3:E:312:6PL:H132	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:305:6PL:O11	3:E:305:6PL:C2	2.52	0.50
3:E:326:6PL:O4P	3:E:326:6PL:C8	2.60	0.50
3:A:522:6PL:H371	3:A:536:6PL:C38	2.33	0.50
3:A:585:6PL:O4P	3:A:585:6PL:C6	2.58	0.50
3:E:341:6PL:O1P	3:E:341:6PL:H51	2.10	0.50
3:E:347:6PL:H362	3:E:347:6PL:H121	1.94	0.50
3:A:510:6PL:H171	3:A:510:6PL:H391	1.94	0.50
2:C:260:PRO:HB2	2:C:262:ASP:OD1	2.12	0.50
3:E:321:6PL:C36	3:E:344:6PL:O31	2.60	0.50
3:E:342:6PL:O4P	3:E:342:6PL:C6	2.59	0.50
3:A:505:6PL:H162	3:A:510:6PL:H122	1.94	0.50
3:A:526:6PL:H52	3:A:526:6PL:O1P	2.12	0.50
3:A:556:6PL:H351	3:A:557:6PL:H151	1.92	0.50
3:A:571:6PL:O4P	3:A:571:6PL:C8	2.59	0.50
2:B:149:GLU:OE2	2:B:250:PRO:HD2	2.12	0.50
1:E:90:LEU:HB3	3:E:349:6PL:H162	1.93	0.50
3:E:309:6PL:O1P	3:E:326:6PL:H51	2.12	0.50
3:E:324:6PL:H372	3:E:358:6PL:C39	2.40	0.50
3:E:324:6PL:O31	3:E:324:6PL:H132	2.12	0.50
3:E:358:6PL:H232	3:A:509:6PL:C13	2.42	0.50
3:E:362:6PL:O31	3:E:362:6PL:H11	2.12	0.50
1:A:251:TRP:HB2	3:A:575:6PL:H341	1.93	0.50
3:A:501:6PL:O31	3:A:501:6PL:H32	2.12	0.50
3:A:524:6PL:O11	3:A:524:6PL:O2	2.30	0.50
3:A:532:6PL:O4P	3:A:532:6PL:C6	2.60	0.50
3:A:543:6PL:H421	3:A:566:6PL:H471	1.93	0.50
3:A:563:6PL:H452	3:A:567:6PL:H221	1.93	0.50
3:A:579:6PL:H122	3:A:583:6PL:H181	1.93	0.50
3:E:309:6PL:H252	3:E:309:6PL:H472	1.93	0.50
3:A:512:6PL:O31	3:A:587:6PL:C8	2.55	0.50
3:A:558:6PL:C1	3:A:558:6PL:C4	2.86	0.50
2:B:260:PRO:HB2	2:B:262:ASP:OD1	2.12	0.50
3:E:322:6PL:H171	3:E:339:6PL:H361	1.93	0.49
1:A:312:GLN:NE2	3:A:584:6PL:H61	2.27	0.49
3:A:527:6PL:C5	3:A:530:6PL:O2P	2.59	0.49
3:A:538:6PL:C45	3:A:542:6PL:H221	2.41	0.49
3:A:540:6PL:H371	3:A:550:6PL:H171	1.94	0.49
3:A:546:6PL:H483	3:A:554:6PL:H192	1.92	0.49
3:A:579:6PL:O4P	3:A:579:6PL:H73	2.11	0.49
2:B:190:PHE:O	2:B:194:GLN:HG2	2.12	0.49
1:E:22:LEU:HD21	3:E:339:6PL:H412	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:GLU:OE2	3:E:306:6PL:H31	2.12	0.49
3:E:319:6PL:H251	3:E:363:6PL:C23	2.41	0.49
3:E:332:6PL:H381	3:E:357:6PL:H192	1.93	0.49
3:E:350:6PL:O31	3:E:350:6PL:C3	2.54	0.49
3:E:358:6PL:H422	3:E:358:6PL:C46	2.38	0.49
3:A:512:6PL:H121	3:A:585:6PL:H191	1.93	0.49
3:A:515:6PL:H481	3:A:576:6PL:H342	1.94	0.49
3:A:531:6PL:H42	3:A:555:6PL:O1P	2.11	0.49
2:C:190:PHE:O	2:C:194:GLN:HG2	2.11	0.49
3:E:302:6PL:H321	3:A:509:6PL:H171	1.95	0.49
3:E:302:6PL:H141	3:E:355:6PL:H412	1.94	0.49
3:E:329:6PL:H351	3:E:340:6PL:H222	1.95	0.49
1:A:363:GLU:HB3	1:A:364:PRO:HD3	1.94	0.49
3:A:503:6PL:C33	3:A:504:6PL:H121	2.41	0.49
3:A:503:6PL:H421	3:A:560:6PL:H252	1.94	0.49
3:A:520:6PL:H321	3:A:552:6PL:H51	1.94	0.49
3:A:538:6PL:H391	3:A:542:6PL:H341	1.93	0.49
3:A:541:6PL:H382	3:A:557:6PL:C38	2.42	0.49
3:A:547:6PL:H263	3:A:563:6PL:H451	1.93	0.49
3:A:558:6PL:H41	3:A:558:6PL:C2	2.42	0.49
3:A:566:6PL:O1P	3:A:566:6PL:C8	2.59	0.49
3:A:569:6PL:O31	3:A:569:6PL:C3	2.47	0.49
3:E:310:6PL:H161	3:E:332:6PL:H31	1.93	0.49
3:E:345:6PL:H372	3:E:351:6PL:H121	1.94	0.49
3:E:353:6PL:H52	3:E:353:6PL:O3P	2.13	0.49
3:E:366:6PL:H351	3:E:366:6PL:O3	2.12	0.49
3:E:367:6PL:H451	3:E:367:6PL:H192	1.94	0.49
3:A:503:6PL:H322	3:A:504:6PL:C11	2.42	0.49
3:A:523:6PL:C4	3:A:572:6PL:H321	2.38	0.49
3:A:543:6PL:H251	3:A:578:6PL:H232	1.94	0.49
3:A:551:6PL:P	3:A:551:6PL:H63	2.53	0.49
3:A:563:6PL:C19	3:A:567:6PL:H381	2.42	0.49
3:A:570:6PL:O1P	3:A:570:6PL:H73	2.12	0.49
3:A:578:6PL:O11	3:A:578:6PL:O2	2.30	0.49
3:A:580:6PL:H362	3:A:588:6PL:H372	1.94	0.49
3:E:321:6PL:H2	3:E:344:6PL:C8	2.26	0.49
3:E:336:6PL:C39	3:E:362:6PL:H391	2.43	0.49
3:A:521:6PL:H322	3:A:562:6PL:H362	1.95	0.49
3:A:540:6PL:O1P	3:A:540:6PL:O2	2.30	0.49
3:A:541:6PL:O2P	3:A:541:6PL:H2	2.12	0.49
3:A:544:6PL:O31	3:A:544:6PL:H342	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:583:6PL:C8	3:A:583:6PL:O4P	2.61	0.49
1:E:174:LEU:HD13	3:E:346:6PL:H242	1.94	0.49
3:E:335:6PL:C35	3:E:353:6PL:H322	2.42	0.49
3:E:336:6PL:H421	3:E:352:6PL:H431	1.93	0.49
3:E:366:6PL:C31	3:E:366:6PL:H351	2.40	0.49
3:A:518:6PL:O2P	3:A:518:6PL:C5	2.59	0.49
3:A:543:6PL:C25	3:A:566:6PL:H232	2.43	0.49
3:A:546:6PL:H391	3:A:568:6PL:O11	2.12	0.49
3:A:548:6PL:C34	3:A:570:6PL:H171	2.42	0.49
3:A:562:6PL:H392	3:A:579:6PL:C47	2.43	0.49
2:C:37:GLU:HG3	2:C:101:PRO:HG3	1.94	0.49
1:E:141:LEU:HG	3:A:536:6PL:H483	1.93	0.49
1:E:163:LEU:HB3	3:E:346:6PL:H352	1.94	0.49
3:E:326:6PL:C48	3:E:364:6PL:C32	2.90	0.49
1:A:363:GLU:HB2	3:A:522:6PL:H62	1.94	0.49
3:A:519:6PL:H192	3:A:549:6PL:H422	1.95	0.49
3:A:524:6PL:O4P	3:A:524:6PL:C8	2.57	0.49
3:A:527:6PL:H202	3:A:571:6PL:C40	2.38	0.49
3:A:540:6PL:C13	3:A:540:6PL:C38	2.90	0.49
3:A:540:6PL:H382	3:A:550:6PL:H171	1.93	0.49
3:A:546:6PL:H462	3:A:546:6PL:H221	1.93	0.49
3:A:551:6PL:H162	3:A:561:6PL:H121	1.93	0.49
3:A:559:6PL:O3	3:A:559:6PL:C31	2.61	0.49
3:A:561:6PL:O4P	3:A:561:6PL:C8	2.58	0.49
3:A:562:6PL:H392	3:A:579:6PL:H472	1.95	0.49
3:A:587:6PL:O4P	3:A:587:6PL:C8	2.60	0.49
2:B:174:PRO:HB2	2:B:204:ASP:HB2	1.93	0.49
3:E:335:6PL:H352	3:E:353:6PL:H322	1.94	0.49
3:E:346:6PL:O4P	3:E:346:6PL:C6	2.58	0.49
1:A:451:LYS:HB3	1:A:452:PRO:HD3	1.94	0.49
3:A:504:6PL:H461	3:A:534:6PL:H263	1.95	0.49
3:A:510:6PL:H2	3:A:510:6PL:H42	1.91	0.49
3:A:521:6PL:H121	3:A:562:6PL:C14	2.42	0.49
3:A:531:6PL:H372	3:A:531:6PL:C16	2.43	0.49
3:A:543:6PL:H52	3:A:581:6PL:O31	2.12	0.49
3:A:561:6PL:H401	3:A:561:6PL:H161	1.95	0.49
3:A:563:6PL:H261	3:A:567:6PL:C47	2.37	0.49
3:A:584:6PL:H412	3:A:584:6PL:H361	1.92	0.49
1:E:33:PHE:HE2	3:E:322:6PL:H361	1.77	0.49
3:E:324:6PL:C36	3:E:358:6PL:H431	2.43	0.49
3:E:345:6PL:C44	3:E:351:6PL:H202	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:352:6PL:C16	3:E:352:6PL:C12	2.82	0.49
3:E:357:6PL:H352	3:E:357:6PL:H142	1.94	0.49
1:A:359:ARG:HD3	3:A:522:6PL:O1P	2.12	0.49
3:E:302:6PL:O31	3:A:509:6PL:H161	2.13	0.49
3:E:306:6PL:H391	3:E:350:6PL:C11	2.43	0.49
3:E:307:6PL:H452	3:E:351:6PL:H171	1.95	0.49
1:A:363:GLU:OE1	3:A:522:6PL:H52	2.12	0.49
3:A:529:6PL:H261	3:A:560:6PL:C34	2.43	0.49
3:A:537:6PL:O4P	3:A:537:6PL:C6	2.47	0.49
3:A:540:6PL:O31	3:A:540:6PL:C3	2.56	0.49
3:A:544:6PL:C31	3:A:559:6PL:H122	2.43	0.49
3:A:549:6PL:O4P	3:A:549:6PL:C8	2.58	0.49
3:A:562:6PL:C22	3:A:565:6PL:H31	2.42	0.49
3:E:320:6PL:H211	3:E:369:6PL:H421	1.94	0.48
3:E:332:6PL:C26	3:E:357:6PL:C24	2.91	0.48
3:E:345:6PL:H132	3:C:501:6PL:H182	1.95	0.48
3:E:369:6PL:H132	3:A:533:6PL:H321	1.95	0.48
3:A:502:6PL:H341	3:A:511:6PL:C15	2.42	0.48
3:A:508:6PL:H381	3:A:510:6PL:H332	1.95	0.48
3:A:512:6PL:H191	3:A:585:6PL:H483	1.95	0.48
3:A:535:6PL:H481	3:A:571:6PL:C23	2.43	0.48
3:A:540:6PL:H382	3:A:550:6PL:H202	1.95	0.48
3:A:543:6PL:C24	3:A:566:6PL:H232	2.42	0.48
3:A:543:6PL:C34	3:A:581:6PL:H152	2.28	0.48
3:A:587:6PL:O31	3:A:587:6PL:O3	2.31	0.48
3:E:315:6PL:H62	3:E:315:6PL:P	2.53	0.48
3:E:316:6PL:H431	3:E:327:6PL:H462	1.94	0.48
3:E:345:6PL:H372	3:E:351:6PL:H122	1.95	0.48
3:E:367:6PL:H161	3:A:526:6PL:H402	1.95	0.48
1:A:468:PHE:HE1	3:A:567:6PL:H382	1.78	0.48
3:A:510:6PL:H41	3:A:510:6PL:O31	2.13	0.48
3:A:528:6PL:H411	3:A:528:6PL:H201	1.95	0.48
3:A:530:6PL:H422	3:A:571:6PL:H191	1.95	0.48
3:A:541:6PL:H402	3:A:541:6PL:C45	2.42	0.48
3:E:318:6PL:C26	3:A:561:6PL:H262	2.43	0.48
3:E:361:6PL:H461	3:A:523:6PL:H441	1.95	0.48
3:E:367:6PL:O31	3:E:367:6PL:C3	2.57	0.48
3:A:504:6PL:O2P	3:A:504:6PL:H52	2.12	0.48
3:A:519:6PL:C25	3:A:549:6PL:C43	2.91	0.48
3:A:555:6PL:O31	3:A:555:6PL:H32	2.12	0.48
2:C:129:VAL:HA	2:C:133:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:TRP:CH2	3:A:503:6PL:H361	2.48	0.48
1:E:229:PHE:HE2	3:E:316:6PL:H372	1.77	0.48
3:E:301:6PL:H482	3:E:317:6PL:C22	2.18	0.48
3:E:308:6PL:H262	3:E:331:6PL:C44	2.44	0.48
3:E:333:6PL:H172	3:E:364:6PL:H362	1.95	0.48
3:E:338:6PL:O4P	3:E:338:6PL:H73	2.12	0.48
3:A:512:6PL:H51	3:A:524:6PL:H361	1.95	0.48
3:A:517:6PL:C17	3:A:579:6PL:C12	2.90	0.48
3:A:557:6PL:O3P	3:A:565:6PL:C5	2.61	0.48
1:E:193:HIS:NE2	3:E:341:6PL:O31	2.43	0.48
3:E:309:6PL:H402	3:E:363:6PL:H161	1.94	0.48
3:E:335:6PL:O4P	3:E:335:6PL:C7	2.61	0.48
3:E:350:6PL:H122	3:E:360:6PL:H182	1.90	0.48
3:E:364:6PL:H181	3:E:364:6PL:H361	1.94	0.48
3:A:544:6PL:H351	3:A:559:6PL:C13	2.41	0.48
2:B:177:LEU:HD13	2:B:187:LEU:HD22	1.94	0.48
3:C:501:6PL:H211	3:C:501:6PL:H471	1.95	0.48
1:E:212:GLU:OE2	1:E:215:ARG:HD3	2.14	0.48
3:E:321:6PL:H392	3:E:365:6PL:H172	1.96	0.48
3:E:336:6PL:C38	3:E:362:6PL:H391	2.43	0.48
3:A:501:6PL:O4P	3:A:501:6PL:C8	2.61	0.48
3:A:502:6PL:H371	3:A:505:6PL:C44	2.44	0.48
3:A:532:6PL:H232	3:A:541:6PL:H381	1.96	0.48
3:A:535:6PL:H482	3:A:571:6PL:H252	1.95	0.48
3:A:548:6PL:C19	3:A:582:6PL:H421	2.43	0.48
3:A:580:6PL:C39	3:A:588:6PL:H202	2.36	0.48
3:A:583:6PL:O3	3:A:583:6PL:O31	2.30	0.48
1:E:149:ARG:HB2	3:C:501:6PL:H192	1.95	0.48
3:E:318:6PL:C48	3:A:504:6PL:H263	2.44	0.48
3:E:320:6PL:H191	3:E:369:6PL:H421	1.94	0.48
3:E:331:6PL:C41	3:E:357:6PL:C39	2.91	0.48
3:E:340:6PL:H242	3:E:340:6PL:C43	2.37	0.48
3:E:345:6PL:C11	3:C:501:6PL:H431	2.43	0.48
3:E:357:6PL:O4P	3:E:357:6PL:C8	2.61	0.48
3:E:362:6PL:O1P	3:E:362:6PL:C5	2.60	0.48
3:A:512:6PL:C26	3:A:587:6PL:H251	2.40	0.48
3:A:524:6PL:H472	3:A:585:6PL:C21	2.33	0.48
3:A:563:6PL:C36	3:A:567:6PL:H121	2.44	0.48
3:A:570:6PL:H481	3:A:582:6PL:H121	1.94	0.48
2:B:364:PRO:HD2	2:B:365:GLN:OE1	2.13	0.48
2:C:364:PRO:HD2	2:C:365:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:302:6PL:C18	3:E:308:6PL:H191	2.40	0.48
3:E:348:6PL:O4P	3:E:348:6PL:C6	2.50	0.48
3:E:355:6PL:O4P	3:E:355:6PL:C6	2.59	0.48
3:E:364:6PL:C31	3:E:364:6PL:C11	2.91	0.48
3:E:369:6PL:H132	3:A:533:6PL:C32	2.43	0.48
3:A:502:6PL:H192	3:A:502:6PL:C42	2.31	0.48
3:A:518:6PL:H382	3:A:560:6PL:H401	1.95	0.48
3:A:523:6PL:H341	3:A:544:6PL:O4P	2.14	0.48
3:A:535:6PL:O31	3:A:535:6PL:H12	2.13	0.48
3:A:538:6PL:H382	3:A:542:6PL:O2	2.14	0.48
3:A:553:6PL:H411	3:A:553:6PL:H141	1.96	0.48
3:A:558:6PL:C48	3:A:574:6PL:H241	2.43	0.48
3:A:565:6PL:C43	3:A:580:6PL:H432	2.42	0.48
3:A:570:6PL:O1P	3:A:570:6PL:C2	2.61	0.48
3:A:580:6PL:C32	3:A:588:6PL:C16	2.92	0.48
3:C:501:6PL:O4P	3:C:501:6PL:C7	2.61	0.48
1:E:131:ARG:NH2	3:E:320:6PL:H12	2.29	0.48
1:E:171:ARG:HB2	3:E:346:6PL:H132	1.95	0.48
3:E:309:6PL:H322	3:E:325:6PL:C13	2.43	0.48
3:E:328:6PL:O4P	3:E:328:6PL:C7	2.59	0.48
3:E:358:6PL:H172	3:A:509:6PL:O3	2.14	0.48
3:E:369:6PL:C13	3:A:517:6PL:H432	2.44	0.48
3:A:525:6PL:H42	3:A:583:6PL:H351	1.94	0.48
3:A:543:6PL:H422	3:A:566:6PL:H483	1.95	0.48
1:E:118:LYS:HA	1:E:118:LYS:HE3	1.96	0.48
3:E:320:6PL:O11	3:E:320:6PL:C2	2.51	0.48
3:E:323:6PL:C39	3:E:326:6PL:H212	2.44	0.48
3:E:336:6PL:C41	3:E:352:6PL:H431	2.44	0.48
3:A:505:6PL:H192	3:A:506:6PL:H412	1.96	0.48
3:A:518:6PL:H171	3:A:529:6PL:H201	1.96	0.48
3:A:525:6PL:H372	3:A:562:6PL:C48	2.44	0.48
3:A:539:6PL:H412	3:A:571:6PL:C40	2.40	0.48
3:A:543:6PL:O4P	3:A:543:6PL:C6	2.59	0.48
2:B:60:ILE:O	2:B:61:TRP:HB2	2.13	0.48
1:E:61:ARG:CD	3:E:330:6PL:H181	2.39	0.47
3:E:307:6PL:O1P	3:E:307:6PL:C6	2.61	0.47
3:E:361:6PL:O4P	3:E:361:6PL:C8	2.62	0.47
3:E:368:6PL:H181	3:A:554:6PL:H241	1.95	0.47
3:A:502:6PL:H121	3:A:511:6PL:O3	2.14	0.47
3:A:502:6PL:H322	3:A:511:6PL:H141	1.95	0.47
3:A:514:6PL:O2	3:A:514:6PL:O1P	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:518:6PL:O4P	3:A:518:6PL:C8	2.61	0.47
3:E:322:6PL:H141	3:E:365:6PL:H431	1.95	0.47
3:E:367:6PL:O4P	3:E:367:6PL:H73	2.12	0.47
1:A:389:GLU:HG2	2:B:239:LEU:HD22	1.96	0.47
3:A:518:6PL:H382	3:A:560:6PL:C41	2.43	0.47
3:A:554:6PL:O31	3:A:554:6PL:C11	2.62	0.47
3:E:321:6PL:H422	3:E:339:6PL:H262	1.94	0.47
3:E:359:6PL:H422	3:A:586:6PL:C44	2.37	0.47
3:A:506:6PL:O1P	3:A:506:6PL:C5	2.61	0.47
3:A:520:6PL:O4P	3:A:520:6PL:H73	2.13	0.47
3:A:533:6PL:C44	3:A:574:6PL:H141	2.38	0.47
3:A:538:6PL:H411	3:A:542:6PL:H361	1.96	0.47
3:A:539:6PL:H392	3:A:571:6PL:C39	2.43	0.47
3:A:546:6PL:C48	3:A:554:6PL:H201	2.43	0.47
1:E:86:MET:SD	1:A:420:ARG:HG3	2.53	0.47
3:E:325:6PL:O4P	3:E:325:6PL:C7	2.61	0.47
3:E:327:6PL:C19	3:E:340:6PL:H483	2.44	0.47
3:E:330:6PL:P	3:E:330:6PL:C7	3.02	0.47
3:E:333:6PL:H411	3:E:363:6PL:H351	1.95	0.47
3:E:358:6PL:C17	3:A:509:6PL:O2	2.52	0.47
3:E:368:6PL:C16	3:A:554:6PL:H231	2.38	0.47
3:A:503:6PL:H342	3:A:504:6PL:H121	1.96	0.47
3:A:518:6PL:H331	3:A:560:6PL:H341	1.97	0.47
3:A:521:6PL:H482	3:A:558:6PL:H421	1.97	0.47
3:A:532:6PL:H431	3:A:558:6PL:H382	1.96	0.47
3:A:543:6PL:C25	3:A:578:6PL:H232	2.45	0.47
3:A:578:6PL:H191	3:A:580:6PL:C24	2.44	0.47
3:A:584:6PL:H362	3:A:584:6PL:C40	2.44	0.47
2:C:120:TYR:CD2	2:C:121:LEU:HG	2.49	0.47
2:C:129:VAL:HG21	2:C:135:ARG:HD2	1.95	0.47
3:E:308:6PL:H261	3:E:348:6PL:H451	1.96	0.47
1:A:359:ARG:NH2	3:A:536:6PL:H73	2.28	0.47
3:A:504:6PL:H252	3:A:561:6PL:H462	1.97	0.47
3:A:536:6PL:H162	3:A:554:6PL:H372	1.95	0.47
3:A:543:6PL:H332	3:A:587:6PL:C33	2.44	0.47
3:A:559:6PL:H52	3:A:559:6PL:H2	1.94	0.47
1:E:119:VAL:HG21	3:A:534:6PL:H451	1.96	0.47
3:E:306:6PL:H382	3:E:341:6PL:H142	1.96	0.47
3:E:318:6PL:O31	3:E:318:6PL:H11	2.13	0.47
3:E:352:6PL:O4P	3:E:352:6PL:C7	2.60	0.47
3:E:363:6PL:H51	3:E:363:6PL:H31	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:369:6PL:O11	3:A:517:6PL:H431	2.13	0.47
1:A:381:GLN:CG	3:A:534:6PL:H321	2.45	0.47
3:A:503:6PL:C3	3:A:503:6PL:O31	2.58	0.47
3:A:528:6PL:C33	3:A:584:6PL:H32	2.45	0.47
3:A:535:6PL:C4	3:A:564:6PL:O1P	2.50	0.47
3:A:542:6PL:H361	3:A:542:6PL:H122	1.95	0.47
3:A:549:6PL:H321	3:A:555:6PL:C15	2.43	0.47
1:E:61:ARG:HD2	3:E:328:6PL:C11	2.44	0.47
3:E:301:6PL:H63	3:E:307:6PL:O2P	2.15	0.47
3:E:309:6PL:H131	3:E:344:6PL:C5	2.44	0.47
3:E:315:6PL:O31	3:E:315:6PL:C1	2.50	0.47
3:E:321:6PL:H142	3:E:365:6PL:C13	2.44	0.47
3:E:331:6PL:C41	3:E:357:6PL:H391	2.44	0.47
3:E:331:6PL:H81	3:E:354:6PL:O1P	2.15	0.47
3:E:335:6PL:H131	3:E:356:6PL:C35	2.41	0.47
3:E:335:6PL:O31	3:E:335:6PL:H11	2.15	0.47
3:E:343:6PL:H132	3:E:343:6PL:H352	1.95	0.47
3:A:502:6PL:O4P	3:A:502:6PL:H2	2.15	0.47
3:A:505:6PL:H51	3:A:508:6PL:P	2.55	0.47
3:A:516:6PL:H471	3:A:547:6PL:H392	1.97	0.47
3:A:528:6PL:H391	3:A:528:6PL:H361	1.61	0.47
3:A:536:6PL:H83	3:A:536:6PL:P	2.55	0.47
3:A:538:6PL:O11	3:A:538:6PL:H2	2.14	0.47
3:A:542:6PL:H201	3:A:542:6PL:H402	1.95	0.47
3:A:543:6PL:H52	3:A:581:6PL:H12	1.97	0.47
3:A:558:6PL:O11	3:A:574:6PL:C1	2.62	0.47
3:A:563:6PL:H382	3:A:563:6PL:H411	1.68	0.47
3:A:580:6PL:C32	3:A:588:6PL:H161	2.44	0.47
2:B:31:TYR:CD2	2:B:32:LEU:HG	2.49	0.47
1:E:61:ARG:HE	1:E:61:ARG:HB3	1.47	0.47
1:E:155:HIS:HB2	3:A:536:6PL:H242	1.95	0.47
1:E:182:LYS:NZ	3:E:306:6PL:C2	2.78	0.47
3:E:322:6PL:H141	3:E:365:6PL:C43	2.45	0.47
3:E:348:6PL:H52	3:E:355:6PL:H132	1.96	0.47
3:E:368:6PL:H151	3:A:554:6PL:H211	1.97	0.47
3:A:503:6PL:O31	3:A:503:6PL:H12	2.13	0.47
3:A:519:6PL:H251	3:A:549:6PL:C44	2.34	0.47
3:A:521:6PL:C7	3:A:562:6PL:H321	2.45	0.47
3:A:560:6PL:O2P	3:A:560:6PL:C5	2.60	0.47
3:A:565:6PL:C32	3:A:580:6PL:H31	2.44	0.47
3:A:584:6PL:O3	3:A:584:6PL:O31	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:TYR:CD2	2:C:32:LEU:HG	2.50	0.47
1:E:239:LYS:CD	3:E:313:6PL:H331	2.41	0.47
3:E:302:6PL:C5	3:A:509:6PL:H132	2.42	0.47
3:E:306:6PL:H141	3:E:306:6PL:H331	1.95	0.47
3:E:318:6PL:H371	3:E:331:6PL:C17	2.38	0.47
3:E:351:6PL:H442	1:A:365:LEU:HB2	1.96	0.47
3:A:516:6PL:H62	3:A:516:6PL:H41	1.55	0.47
3:A:528:6PL:H422	3:A:528:6PL:C22	2.32	0.47
3:A:566:6PL:C8	3:A:566:6PL:O4P	2.63	0.47
3:E:307:6PL:O1P	3:E:307:6PL:H62	2.15	0.47
3:E:316:6PL:H483	3:E:327:6PL:H461	1.97	0.47
3:E:317:6PL:H161	3:E:366:6PL:C38	2.43	0.47
3:E:334:6PL:O31	3:E:334:6PL:H11	2.14	0.47
3:E:335:6PL:H151	3:E:356:6PL:H382	1.97	0.47
3:E:352:6PL:H2	3:E:352:6PL:O2P	2.15	0.47
3:A:522:6PL:O4P	3:A:522:6PL:C6	2.63	0.47
3:E:309:6PL:C36	3:E:325:6PL:H152	2.45	0.46
3:E:318:6PL:H471	3:A:504:6PL:H211	1.97	0.46
3:E:320:6PL:O2P	3:E:338:6PL:H11	2.14	0.46
3:E:333:6PL:C42	3:E:363:6PL:H352	2.44	0.46
3:E:359:6PL:H431	3:A:537:6PL:H402	1.96	0.46
3:E:367:6PL:H62	3:E:367:6PL:H41	1.59	0.46
1:A:387:LEU:CG	3:A:534:6PL:H432	2.45	0.46
3:A:537:6PL:H422	3:A:586:6PL:C20	2.45	0.46
3:A:573:6PL:C34	3:A:575:6PL:C20	2.74	0.46
3:E:317:6PL:O4P	3:E:317:6PL:C6	2.63	0.46
3:E:325:6PL:H242	3:E:363:6PL:H201	1.96	0.46
3:E:337:6PL:H442	3:E:347:6PL:C17	2.46	0.46
3:E:365:6PL:O2P	3:E:365:6PL:H82	2.15	0.46
3:A:501:6PL:H362	3:A:501:6PL:H392	1.85	0.46
3:A:513:6PL:H151	3:A:548:6PL:H351	1.98	0.46
3:A:515:6PL:H252	3:A:555:6PL:C47	2.25	0.46
3:A:538:6PL:C45	3:A:542:6PL:C22	2.93	0.46
3:A:551:6PL:H201	3:A:559:6PL:H362	1.98	0.46
3:A:552:6PL:C37	3:A:570:6PL:H241	2.22	0.46
3:A:560:6PL:O4P	3:A:560:6PL:C6	2.59	0.46
3:A:565:6PL:H351	3:A:580:6PL:C13	2.45	0.46
3:A:566:6PL:H452	3:A:587:6PL:H432	1.96	0.46
2:B:129:VAL:HG21	2:B:135:ARG:HD2	1.95	0.46
1:E:116:ARG:NH1	3:E:334:6PL:O1P	2.49	0.46
1:E:148:MET:HB3	3:C:501:6PL:H231	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:302:6PL:C21	3:E:308:6PL:H231	2.39	0.46
3:E:310:6PL:O4P	3:E:310:6PL:C6	2.61	0.46
3:E:313:6PL:C4	3:E:313:6PL:C1	2.93	0.46
3:E:316:6PL:H461	3:E:327:6PL:H462	1.96	0.46
3:E:320:6PL:H431	3:E:320:6PL:H402	1.81	0.46
3:E:323:6PL:H171	3:E:330:6PL:C41	2.46	0.46
3:E:323:6PL:H52	3:E:323:6PL:O3P	2.16	0.46
3:E:341:6PL:O11	3:E:341:6PL:H342	2.14	0.46
3:E:368:6PL:H142	3:A:554:6PL:H231	1.95	0.46
3:A:547:6PL:H141	3:A:547:6PL:O3	2.14	0.46
3:A:551:6PL:H201	3:A:559:6PL:C35	2.45	0.46
3:A:565:6PL:H162	3:A:580:6PL:C42	2.45	0.46
3:A:580:6PL:H322	3:A:588:6PL:C16	2.45	0.46
3:E:324:6PL:C35	3:E:358:6PL:C43	2.94	0.46
3:E:367:6PL:H401	3:E:367:6PL:H172	1.97	0.46
3:A:509:6PL:O31	3:A:509:6PL:C1	2.57	0.46
3:A:525:6PL:O11	3:A:525:6PL:O2	2.33	0.46
3:A:537:6PL:H181	3:A:549:6PL:C25	2.41	0.46
3:A:539:6PL:H392	3:A:571:6PL:C38	2.45	0.46
2:B:129:VAL:HA	2:B:133:TYR:O	2.16	0.46
3:E:312:6PL:H72	3:E:357:6PL:O3P	2.15	0.46
3:E:318:6PL:O2	3:E:336:6PL:H171	2.14	0.46
3:E:330:6PL:C25	3:A:537:6PL:H171	2.46	0.46
3:E:331:6PL:C37	3:E:355:6PL:H461	2.41	0.46
3:E:360:6PL:O4P	3:E:360:6PL:C7	2.59	0.46
3:E:369:6PL:O4P	3:E:369:6PL:C6	2.61	0.46
3:A:519:6PL:C25	3:A:549:6PL:C44	2.90	0.46
3:A:525:6PL:O1P	3:A:525:6PL:C5	2.58	0.46
3:A:528:6PL:H82	3:A:528:6PL:P	2.55	0.46
3:A:587:6PL:H141	3:A:587:6PL:H392	1.97	0.46
2:B:24:PRO:HB3	2:B:167:MET:CE	2.46	0.46
2:B:178:ILE:HG12	2:B:207:ILE:HB	1.97	0.46
3:E:335:6PL:H131	3:E:356:6PL:C33	2.44	0.46
1:A:289:LEU:HD21	3:A:573:6PL:H161	1.98	0.46
3:A:501:6PL:O11	3:A:501:6PL:C2	2.57	0.46
3:A:513:6PL:O31	3:A:513:6PL:C1	2.50	0.46
3:A:516:6PL:O11	3:A:516:6PL:C2	2.61	0.46
3:A:520:6PL:H442	3:A:556:6PL:H251	1.97	0.46
3:A:531:6PL:H221	3:A:547:6PL:C40	2.46	0.46
3:A:550:6PL:C8	3:A:550:6PL:O4P	2.64	0.46
3:A:565:6PL:H362	3:A:565:6PL:H391	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:572:6PL:H232	3:A:576:6PL:H182	1.97	0.46
2:C:63:ASP:O	2:C:66:MET:HG2	2.16	0.46
1:E:233:LEU:O	1:E:236:TYR:HB3	2.15	0.46
3:E:304:6PL:O31	3:E:304:6PL:O3	2.33	0.46
3:E:309:6PL:C32	3:E:325:6PL:H132	2.45	0.46
3:E:331:6PL:H432	3:E:331:6PL:H401	1.85	0.46
3:E:337:6PL:H52	3:E:337:6PL:C2	2.46	0.46
3:A:521:6PL:C11	3:A:579:6PL:H481	2.46	0.46
3:A:528:6PL:C8	3:A:528:6PL:P	3.04	0.46
3:A:543:6PL:H341	3:A:581:6PL:C15	2.26	0.46
2:C:251:TRP:CD1	2:C:297:SER:HB2	2.51	0.46
1:E:142:SER:HB2	1:E:143:PRO:HD3	1.98	0.46
3:E:321:6PL:H152	3:E:359:6PL:O11	2.15	0.46
3:E:329:6PL:H31	3:E:366:6PL:C16	2.39	0.46
3:E:331:6PL:H412	3:E:357:6PL:C39	2.45	0.46
3:E:333:6PL:H392	3:E:363:6PL:H141	1.98	0.46
3:E:339:6PL:H332	3:E:339:6PL:H142	1.98	0.46
3:E:340:6PL:C26	3:A:513:6PL:H252	2.35	0.46
3:E:368:6PL:O4P	3:E:368:6PL:C7	2.63	0.46
3:A:505:6PL:H251	3:A:505:6PL:H481	1.97	0.46
3:A:514:6PL:H222	3:A:567:6PL:C17	2.40	0.46
3:A:520:6PL:H421	3:A:538:6PL:C26	2.41	0.46
3:A:527:6PL:H231	3:A:535:6PL:H471	1.98	0.46
3:A:543:6PL:H401	3:A:581:6PL:H212	1.97	0.46
3:A:568:6PL:H381	3:A:568:6PL:H412	1.56	0.46
3:A:577:6PL:H151	3:A:577:6PL:C38	2.41	0.46
2:B:239:LEU:O	2:B:239:LEU:HG	2.16	0.46
1:E:94:LYS:NZ	3:E:361:6PL:O2P	2.49	0.46
3:E:317:6PL:H411	3:E:353:6PL:H381	1.96	0.46
3:E:317:6PL:C41	3:E:353:6PL:C40	2.92	0.46
3:A:512:6PL:C3	3:A:524:6PL:H412	2.38	0.46
3:A:513:6PL:H122	3:A:548:6PL:H351	1.97	0.46
3:A:517:6PL:O2P	3:A:517:6PL:H62	2.16	0.46
3:A:519:6PL:H221	3:A:549:6PL:H421	1.97	0.46
3:A:573:6PL:H451	3:A:575:6PL:C19	2.45	0.46
3:A:580:6PL:C35	3:A:588:6PL:H372	2.45	0.46
3:A:582:6PL:O31	3:A:582:6PL:H32	2.14	0.46
3:E:306:6PL:H482	3:A:513:6PL:C22	2.37	0.46
3:E:311:6PL:H63	3:E:311:6PL:P	2.56	0.46
3:E:329:6PL:C35	3:E:340:6PL:H191	2.46	0.46
3:E:351:6PL:C6	3:E:351:6PL:P	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:503:6PL:O1P	3:A:503:6PL:C6	2.63	0.46
3:A:512:6PL:H72	3:A:524:6PL:C11	2.44	0.46
3:A:512:6PL:C4	3:A:524:6PL:H121	2.46	0.46
3:A:513:6PL:H63	3:A:513:6PL:H42	1.63	0.46
3:A:518:6PL:C17	3:A:529:6PL:H202	2.42	0.46
3:A:520:6PL:H421	3:A:538:6PL:H242	1.98	0.46
3:A:523:6PL:H431	3:A:523:6PL:H402	1.84	0.46
3:A:528:6PL:H432	3:A:528:6PL:H402	1.85	0.46
3:A:535:6PL:H83	3:A:564:6PL:P	2.54	0.46
3:A:543:6PL:H361	3:A:581:6PL:H192	1.96	0.46
3:A:548:6PL:H2	3:A:548:6PL:O11	2.15	0.46
3:A:572:6PL:H391	3:A:576:6PL:C15	2.38	0.46
2:B:27:LEU:HD23	2:B:178:ILE:HB	1.96	0.46
2:B:144:TYR:HB3	2:B:156:TYR:CE1	2.51	0.46
3:E:302:6PL:H172	3:E:348:6PL:H211	1.98	0.45
3:E:348:6PL:O1P	3:E:348:6PL:C6	2.64	0.45
3:E:354:6PL:H462	3:E:354:6PL:H262	1.98	0.45
3:A:505:6PL:C47	3:A:506:6PL:H462	2.46	0.45
3:A:536:6PL:C46	3:C:501:6PL:H241	2.46	0.45
3:A:557:6PL:O11	3:A:565:6PL:H73	2.14	0.45
3:A:564:6PL:H381	3:A:564:6PL:H411	1.71	0.45
3:A:574:6PL:O4P	3:A:574:6PL:H73	2.16	0.45
3:E:304:6PL:C31	3:E:355:6PL:H382	2.46	0.45
3:E:345:6PL:H442	3:E:351:6PL:H202	1.98	0.45
3:A:502:6PL:H12	3:A:511:6PL:C12	2.46	0.45
3:A:552:6PL:O31	3:A:552:6PL:C13	2.64	0.45
3:A:562:6PL:H382	3:A:562:6PL:H411	1.68	0.45
3:C:501:6PL:O2	3:C:501:6PL:O11	2.33	0.45
1:E:214:LEU:HG	3:A:507:6PL:C35	2.46	0.45
3:E:310:6PL:H342	3:E:310:6PL:C18	2.47	0.45
3:E:312:6PL:H222	3:E:315:6PL:C40	2.46	0.45
3:E:314:6PL:H221	3:E:353:6PL:H141	1.97	0.45
3:E:321:6PL:H351	3:E:344:6PL:H332	1.97	0.45
3:E:355:6PL:H362	3:E:355:6PL:H392	1.78	0.45
3:A:517:6PL:C19	3:A:579:6PL:H121	2.46	0.45
3:A:527:6PL:H52	3:A:527:6PL:O1P	2.17	0.45
3:A:541:6PL:H332	3:A:557:6PL:H362	1.97	0.45
3:A:559:6PL:O2P	3:A:559:6PL:C2	2.59	0.45
3:A:581:6PL:H411	3:A:581:6PL:H381	1.77	0.45
2:B:120:TYR:CD2	2:B:121:LEU:HG	2.51	0.45
3:E:310:6PL:H171	3:E:332:6PL:C12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:314:6PL:H411	3:A:508:6PL:H421	1.99	0.45
3:E:333:6PL:H182	3:E:364:6PL:C36	2.46	0.45
3:E:333:6PL:H411	3:E:333:6PL:H381	1.67	0.45
3:E:347:6PL:O4P	3:E:347:6PL:C7	2.60	0.45
1:A:399:VAL:HG23	3:A:503:6PL:H481	1.98	0.45
3:A:519:6PL:H191	3:A:549:6PL:H392	1.94	0.45
3:A:522:6PL:H441	3:A:536:6PL:H351	1.98	0.45
3:A:540:6PL:H332	3:A:550:6PL:H142	1.98	0.45
3:A:544:6PL:C39	3:A:551:6PL:H261	2.47	0.45
3:A:552:6PL:O3	3:A:552:6PL:C31	2.65	0.45
3:A:564:6PL:C16	3:A:564:6PL:H391	2.46	0.45
3:A:577:6PL:C22	3:A:583:6PL:H482	2.46	0.45
3:E:345:6PL:C12	3:C:501:6PL:H431	2.47	0.45
3:A:530:6PL:H442	3:A:571:6PL:H191	1.98	0.45
3:A:540:6PL:O4P	3:A:540:6PL:C7	2.62	0.45
3:A:559:6PL:O31	3:A:559:6PL:C1	2.64	0.45
3:A:566:6PL:P	3:A:566:6PL:C8	3.04	0.45
2:C:26:ILE:HA	2:C:140:ARG:O	2.17	0.45
3:E:307:6PL:H63	3:E:307:6PL:P	2.56	0.45
3:A:520:6PL:H411	3:A:538:6PL:H242	1.99	0.45
3:A:563:6PL:O31	3:A:563:6PL:C3	2.62	0.45
3:A:576:6PL:P	3:A:576:6PL:C7	3.05	0.45
3:A:580:6PL:H362	3:A:588:6PL:C37	2.46	0.45
2:B:24:PRO:HB3	2:B:167:MET:HE1	1.99	0.45
2:B:160:LEU:O	2:B:164:VAL:HG23	2.17	0.45
3:E:303:6PL:C11	3:E:362:6PL:H73	2.47	0.45
3:A:514:6PL:O2P	3:A:514:6PL:C5	2.64	0.45
3:A:517:6PL:O2P	3:A:517:6PL:C5	2.62	0.45
3:A:526:6PL:H242	3:A:575:6PL:H232	1.99	0.45
3:E:322:6PL:H263	3:E:339:6PL:C39	2.47	0.45
3:E:344:6PL:H382	3:E:344:6PL:H411	1.61	0.45
3:E:358:6PL:H252	3:A:509:6PL:H202	1.98	0.45
3:E:363:6PL:H411	3:E:363:6PL:H382	1.57	0.45
3:A:547:6PL:H352	3:A:547:6PL:H152	1.99	0.45
3:A:588:6PL:O31	3:A:588:6PL:C1	2.58	0.45
2:C:149:GLU:OE1	2:C:251:TRP:HB2	2.16	0.45
3:E:323:6PL:H481	3:A:578:6PL:C43	2.47	0.45
3:E:328:6PL:H181	3:A:537:6PL:H252	1.97	0.45
3:E:331:6PL:O4P	3:E:331:6PL:C6	2.54	0.45
3:E:339:6PL:H332	3:E:339:6PL:H141	1.98	0.45
3:E:341:6PL:H481	3:A:513:6PL:H242	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:357:6PL:O31	3:E:357:6PL:C1	2.46	0.45
3:E:367:6PL:O2P	3:E:367:6PL:C5	2.64	0.45
3:E:368:6PL:H2	3:E:368:6PL:O1P	2.17	0.45
3:A:503:6PL:C4	3:A:504:6PL:C3	2.87	0.45
3:A:512:6PL:H82	3:A:512:6PL:P	2.56	0.45
3:A:516:6PL:H381	3:A:516:6PL:H411	1.49	0.45
3:A:538:6PL:O3P	3:A:542:6PL:H71	2.17	0.45
3:A:540:6PL:H41	3:A:550:6PL:C1	2.47	0.45
3:E:303:6PL:H362	3:E:303:6PL:H391	1.91	0.45
3:E:320:6PL:O31	3:E:320:6PL:C3	2.54	0.45
3:E:326:6PL:H481	3:E:364:6PL:C32	2.43	0.45
3:E:332:6PL:H361	3:E:357:6PL:H172	1.99	0.45
3:E:340:6PL:H432	3:E:340:6PL:C24	2.41	0.45
3:E:355:6PL:O4P	3:E:355:6PL:C2	2.65	0.45
3:E:362:6PL:O4P	3:E:362:6PL:C8	2.61	0.45
3:A:503:6PL:C41	3:A:560:6PL:C26	2.86	0.45
3:A:520:6PL:C41	3:A:538:6PL:H263	2.46	0.45
3:A:533:6PL:H202	3:A:558:6PL:C20	2.46	0.45
3:A:568:6PL:H452	3:A:569:6PL:C48	2.47	0.45
3:A:577:6PL:H381	3:A:577:6PL:C15	2.42	0.45
2:C:160:LEU:O	2:C:164:VAL:HG23	2.17	0.45
3:E:324:6PL:O2P	3:E:324:6PL:C5	2.62	0.44
3:E:328:6PL:H381	3:E:328:6PL:H411	1.65	0.44
3:E:360:6PL:O11	3:E:360:6PL:H331	2.16	0.44
1:A:355:MET:CE	3:A:536:6PL:H322	2.46	0.44
3:A:502:6PL:H431	3:A:502:6PL:H401	1.73	0.44
3:A:531:6PL:H201	3:A:531:6PL:H172	1.74	0.44
3:A:580:6PL:C40	3:A:588:6PL:H222	2.43	0.44
2:B:68:LEU:CG	2:B:69:PRO:HD2	2.42	0.44
2:C:177:LEU:HD13	2:C:187:LEU:HD22	1.98	0.44
3:E:304:6PL:H401	3:E:312:6PL:C13	2.47	0.44
3:E:344:6PL:C31	3:E:344:6PL:O2P	2.65	0.44
3:E:356:6PL:O31	3:E:356:6PL:O3	2.35	0.44
3:E:361:6PL:C24	3:A:509:6PL:H422	2.46	0.44
3:A:513:6PL:O1P	3:A:513:6PL:C5	2.65	0.44
3:A:517:6PL:H432	3:A:517:6PL:H401	1.85	0.44
3:A:521:6PL:H72	3:A:562:6PL:H321	1.99	0.44
3:A:523:6PL:H462	3:A:572:6PL:H182	1.99	0.44
3:A:542:6PL:O31	3:A:542:6PL:C3	2.61	0.44
3:A:543:6PL:H451	3:A:566:6PL:H483	2.00	0.44
3:A:547:6PL:O4P	3:A:547:6PL:C7	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:568:6PL:O11	3:A:568:6PL:H2	2.15	0.44
1:E:90:LEU:CD1	3:E:349:6PL:H151	2.42	0.44
3:E:309:6PL:H462	3:E:309:6PL:C24	2.37	0.44
3:E:333:6PL:C16	3:A:511:6PL:H392	2.47	0.44
3:E:339:6PL:H442	3:A:575:6PL:H422	1.99	0.44
3:A:513:6PL:C11	3:A:548:6PL:H321	2.47	0.44
3:A:519:6PL:O4P	3:A:519:6PL:C6	2.64	0.44
3:A:557:6PL:O11	3:A:565:6PL:C8	2.54	0.44
2:B:105:LYS:HA	2:B:136:ASP:OD1	2.17	0.44
1:E:239:LYS:NZ	3:E:342:6PL:O1P	2.51	0.44
3:E:317:6PL:H372	3:E:353:6PL:H361	1.99	0.44
3:E:320:6PL:H182	3:E:320:6PL:H432	1.99	0.44
3:E:337:6PL:H31	3:E:362:6PL:H41	1.99	0.44
3:E:343:6PL:C36	3:E:343:6PL:H152	2.48	0.44
3:E:359:6PL:O4P	3:E:359:6PL:C6	2.54	0.44
3:E:359:6PL:P	3:E:359:6PL:C6	3.06	0.44
1:A:369:LEU:HD11	3:A:522:6PL:H263	1.99	0.44
1:A:392:ARG:CZ	1:A:393:ASP:HB2	2.48	0.44
3:A:506:6PL:H332	3:A:506:6PL:H131	1.99	0.44
3:A:525:6PL:H41	3:A:525:6PL:H62	1.57	0.44
3:A:541:6PL:H251	3:A:571:6PL:H212	2.00	0.44
3:E:324:6PL:H401	3:E:324:6PL:H432	1.71	0.44
1:A:345:ASP:OD1	1:A:349:LYS:NZ	2.49	0.44
3:A:532:6PL:H221	3:A:557:6PL:H392	2.00	0.44
3:A:535:6PL:H481	3:A:571:6PL:H231	1.98	0.44
3:A:540:6PL:H73	3:A:540:6PL:H12	2.00	0.44
3:A:543:6PL:C40	3:A:581:6PL:H212	2.47	0.44
3:A:552:6PL:H192	3:A:552:6PL:H161	1.83	0.44
3:A:567:6PL:O11	3:A:567:6PL:H142	2.17	0.44
3:A:572:6PL:C7	3:A:572:6PL:O4P	2.60	0.44
3:A:584:6PL:O4P	3:A:584:6PL:H73	2.18	0.44
3:E:306:6PL:O2	3:E:306:6PL:C11	2.64	0.44
3:E:320:6PL:C37	3:E:338:6PL:H392	2.48	0.44
3:E:328:6PL:C12	3:E:330:6PL:H192	2.44	0.44
3:E:334:6PL:H211	3:E:362:6PL:H481	1.99	0.44
3:A:512:6PL:H442	3:A:512:6PL:H241	1.99	0.44
3:A:516:6PL:H261	3:A:563:6PL:H211	1.99	0.44
3:A:531:6PL:H162	3:A:531:6PL:H362	2.00	0.44
3:A:532:6PL:H12	3:A:541:6PL:H83	1.97	0.44
3:A:543:6PL:H171	3:A:566:6PL:H351	1.97	0.44
3:A:544:6PL:O2	3:A:559:6PL:H122	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:551:6PL:H221	3:A:559:6PL:H362	1.99	0.44
3:A:570:6PL:H481	3:A:582:6PL:H131	1.88	0.44
3:A:580:6PL:H351	3:A:588:6PL:H372	2.00	0.44
2:C:125:VAL:O	2:C:129:VAL:HG23	2.18	0.44
3:E:322:6PL:H171	3:E:339:6PL:C36	2.47	0.44
3:E:329:6PL:H51	3:E:366:6PL:C13	2.36	0.44
3:E:345:6PL:H131	3:C:501:6PL:H451	1.99	0.44
3:E:356:6PL:H452	3:E:362:6PL:C20	2.47	0.44
3:A:541:6PL:H141	3:A:588:6PL:O2	2.17	0.44
3:A:556:6PL:H32	3:A:556:6PL:H371	1.99	0.44
3:A:573:6PL:H411	3:A:573:6PL:H381	1.68	0.44
3:A:581:6PL:H381	3:A:581:6PL:C43	2.47	0.44
2:B:37:GLU:OE1	2:B:99:ARG:HD2	2.18	0.44
3:E:305:6PL:H371	1:A:303:LEU:HD22	1.99	0.44
3:E:306:6PL:H472	3:E:341:6PL:H482	2.00	0.44
3:E:318:6PL:H381	3:E:318:6PL:H412	1.73	0.44
1:A:351:TRP:CE2	3:A:536:6PL:H131	2.53	0.44
3:A:532:6PL:C20	3:A:541:6PL:H372	2.48	0.44
3:A:535:6PL:O1P	3:A:535:6PL:H63	2.17	0.44
3:A:542:6PL:H421	3:A:542:6PL:H201	1.96	0.44
3:A:583:6PL:H63	3:A:583:6PL:H42	1.61	0.44
2:B:383:SER:HB3	2:B:386:THR:OG1	2.18	0.44
3:E:317:6PL:C40	3:E:353:6PL:H381	2.47	0.44
3:E:317:6PL:C44	3:E:366:6PL:H483	2.48	0.44
3:E:329:6PL:H42	3:E:366:6PL:H131	1.99	0.44
3:E:335:6PL:O2	3:E:335:6PL:C11	2.65	0.44
3:E:341:6PL:H252	3:E:341:6PL:C21	2.36	0.44
3:E:346:6PL:H431	3:A:553:6PL:H212	1.99	0.44
3:E:364:6PL:O4P	3:E:364:6PL:C6	2.61	0.44
3:A:520:6PL:C3	3:A:556:6PL:H141	2.48	0.44
3:A:520:6PL:H412	3:A:538:6PL:H263	2.00	0.44
3:A:521:6PL:H171	3:A:562:6PL:H421	2.00	0.44
3:A:529:6PL:C26	3:A:560:6PL:H342	2.46	0.44
3:A:532:6PL:H162	3:A:541:6PL:H12	1.99	0.44
3:A:543:6PL:H242	3:A:566:6PL:H232	2.00	0.44
3:A:564:6PL:H391	3:A:564:6PL:H162	1.99	0.44
3:A:576:6PL:H62	3:A:576:6PL:H41	1.60	0.44
2:C:32:LEU:HD23	2:C:146:TRP:CH2	2.53	0.44
3:E:306:6PL:H141	3:E:306:6PL:C33	2.48	0.43
3:E:306:6PL:H62	3:E:306:6PL:H41	1.52	0.43
3:E:308:6PL:C7	3:E:355:6PL:H11	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:313:6PL:O11	3:E:313:6PL:H2	2.17	0.43
3:E:324:6PL:H362	3:A:503:6PL:O31	2.18	0.43
3:E:331:6PL:H371	3:E:355:6PL:C47	2.48	0.43
3:E:350:6PL:H62	3:E:350:6PL:H41	1.75	0.43
3:E:367:6PL:H361	3:E:367:6PL:H412	1.99	0.43
1:A:316:ASP:O	1:A:320:LYS:HD3	2.18	0.43
3:A:504:6PL:H362	3:A:504:6PL:H391	1.81	0.43
3:A:515:6PL:C25	3:A:555:6PL:H472	2.25	0.43
3:A:524:6PL:H161	3:A:585:6PL:H152	2.00	0.43
3:A:530:6PL:C3	3:A:588:6PL:H71	2.46	0.43
3:A:546:6PL:H451	3:A:554:6PL:C38	2.48	0.43
3:E:301:6PL:H392	3:E:311:6PL:H482	2.00	0.43
3:E:309:6PL:H402	3:E:363:6PL:C16	2.48	0.43
3:E:317:6PL:H2	3:E:335:6PL:H81	1.99	0.43
3:E:329:6PL:C4	3:E:329:6PL:H12	2.49	0.43
3:E:339:6PL:O2P	3:E:339:6PL:H52	2.18	0.43
1:A:250:PRO:CG	3:A:575:6PL:H392	2.47	0.43
3:A:505:6PL:C35	3:A:506:6PL:H382	2.32	0.43
3:A:517:6PL:C17	3:A:579:6PL:H121	2.48	0.43
3:A:518:6PL:H332	3:A:532:6PL:C37	2.33	0.43
3:A:535:6PL:C35	3:A:564:6PL:H392	2.30	0.43
3:A:537:6PL:H391	3:A:537:6PL:H362	1.68	0.43
3:A:542:6PL:C15	3:A:581:6PL:C18	2.75	0.43
3:A:563:6PL:H152	3:A:563:6PL:H181	1.85	0.43
3:E:330:6PL:H171	3:A:537:6PL:H251	2.00	0.43
1:A:304:ARG:CZ	3:A:550:6PL:H371	2.48	0.43
3:A:501:6PL:H412	3:A:501:6PL:H371	2.00	0.43
3:A:517:6PL:H171	3:A:579:6PL:C11	2.47	0.43
3:A:520:6PL:H482	3:A:542:6PL:H441	1.90	0.43
3:A:524:6PL:P	3:A:524:6PL:H83	2.57	0.43
3:A:535:6PL:O2	3:A:564:6PL:H332	2.18	0.43
3:A:540:6PL:H421	3:A:550:6PL:H262	2.00	0.43
3:A:556:6PL:O4P	3:A:556:6PL:C8	2.64	0.43
3:A:572:6PL:H392	3:A:576:6PL:H172	1.93	0.43
1:E:108:TRP:CZ2	3:A:503:6PL:H361	2.54	0.43
3:E:306:6PL:H321	3:E:350:6PL:O31	2.18	0.43
3:E:325:6PL:C26	3:E:363:6PL:H202	2.48	0.43
3:E:367:6PL:H382	3:E:367:6PL:H411	1.72	0.43
1:A:454:LEU:HD11	3:A:586:6PL:C36	2.40	0.43
3:A:505:6PL:O31	3:A:506:6PL:H83	2.18	0.43
3:A:512:6PL:C6	3:A:524:6PL:H341	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:525:6PL:H411	3:A:525:6PL:H381	1.77	0.43
3:A:563:6PL:H161	3:A:567:6PL:H362	1.99	0.43
3:A:571:6PL:H381	3:A:571:6PL:H411	1.61	0.43
3:A:580:6PL:H372	3:A:588:6PL:C19	2.48	0.43
1:E:243:GLN:NE2	1:E:243:GLN:HA	2.33	0.43
3:E:301:6PL:H362	3:E:343:6PL:C11	2.48	0.43
3:E:322:6PL:C33	3:E:365:6PL:H402	2.33	0.43
3:E:343:6PL:H411	3:E:343:6PL:H181	2.00	0.43
3:E:353:6PL:H63	3:E:353:6PL:P	2.56	0.43
1:A:251:TRP:HZ2	3:A:573:6PL:H322	1.83	0.43
1:A:399:VAL:HG22	3:A:503:6PL:H481	1.99	0.43
3:A:516:6PL:H412	3:A:555:6PL:H181	1.99	0.43
3:A:550:6PL:H63	3:A:550:6PL:H42	1.67	0.43
3:A:573:6PL:H451	3:A:575:6PL:C17	2.45	0.43
3:A:578:6PL:O4P	3:A:578:6PL:C7	2.65	0.43
3:A:580:6PL:H352	3:A:588:6PL:H182	1.99	0.43
2:C:128:LEU:O	2:C:133:TYR:HB2	2.18	0.43
3:E:307:6PL:O4P	3:E:307:6PL:C6	2.66	0.43
3:E:308:6PL:H262	3:E:331:6PL:H442	2.01	0.43
3:E:317:6PL:C16	3:E:366:6PL:H382	2.43	0.43
3:E:333:6PL:H151	3:A:511:6PL:H392	1.99	0.43
3:E:339:6PL:H422	3:A:575:6PL:H442	2.01	0.43
3:E:363:6PL:H421	3:E:364:6PL:C21	2.45	0.43
3:A:523:6PL:H392	3:A:572:6PL:H162	2.01	0.43
3:A:528:6PL:H332	3:A:584:6PL:C3	2.48	0.43
3:A:536:6PL:H11	3:A:568:6PL:O31	2.18	0.43
3:A:571:6PL:C8	3:A:571:6PL:P	3.07	0.43
1:E:160:ARG:HA	3:E:346:6PL:C34	2.49	0.43
3:E:304:6PL:H422	3:E:308:6PL:H221	1.99	0.43
3:E:329:6PL:H362	3:E:329:6PL:H391	1.77	0.43
3:E:332:6PL:C26	3:E:357:6PL:H242	2.39	0.43
3:E:341:6PL:O2	3:E:341:6PL:H342	2.18	0.43
3:E:345:6PL:H122	3:C:501:6PL:H431	2.00	0.43
3:E:348:6PL:H73	3:E:355:6PL:C14	2.49	0.43
3:A:518:6PL:H441	3:A:518:6PL:H401	1.97	0.43
3:A:519:6PL:H42	3:A:519:6PL:H83	1.80	0.43
3:A:521:6PL:H122	3:A:579:6PL:H481	2.00	0.43
3:A:522:6PL:O3	3:A:522:6PL:C31	2.67	0.43
3:A:524:6PL:H261	3:A:585:6PL:H241	1.99	0.43
3:A:535:6PL:C6	3:A:535:6PL:P	3.07	0.43
3:C:501:6PL:H72	3:C:501:6PL:P	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:LYS:HA	3:E:341:6PL:H141	2.00	0.43
3:E:308:6PL:O2	3:E:308:6PL:C11	2.67	0.43
3:E:333:6PL:H62	3:E:333:6PL:H41	1.54	0.43
3:E:340:6PL:H331	3:E:342:6PL:H201	2.00	0.43
3:E:355:6PL:C6	3:E:355:6PL:P	3.07	0.43
3:A:504:6PL:H382	3:A:504:6PL:H411	1.69	0.43
3:A:505:6PL:H41	3:A:508:6PL:C2	2.47	0.43
3:A:513:6PL:H421	3:A:552:6PL:H412	1.97	0.43
3:A:518:6PL:C19	3:A:529:6PL:H202	2.46	0.43
3:A:523:6PL:H411	3:A:523:6PL:C37	2.39	0.43
3:A:523:6PL:O4P	3:A:523:6PL:C8	2.64	0.43
3:A:536:6PL:C4	3:A:568:6PL:H321	2.49	0.43
3:A:553:6PL:H431	3:A:553:6PL:H401	1.81	0.43
3:A:562:6PL:H222	3:A:565:6PL:C3	2.44	0.43
2:B:125:VAL:O	2:B:129:VAL:HG23	2.19	0.43
3:C:501:6PL:O1P	3:C:501:6PL:H73	2.19	0.43
3:C:501:6PL:C7	3:C:501:6PL:P	3.06	0.43
3:E:326:6PL:H392	3:E:326:6PL:H361	1.83	0.43
3:E:337:6PL:C5	3:E:337:6PL:C1	2.72	0.43
3:E:345:6PL:C1	3:C:501:6PL:H371	2.49	0.43
3:E:369:6PL:H202	3:A:574:6PL:C11	2.49	0.43
3:A:512:6PL:C5	3:A:512:6PL:O1P	2.63	0.43
3:A:522:6PL:H322	3:A:522:6PL:H132	2.01	0.43
3:A:535:6PL:H411	3:A:535:6PL:H382	1.68	0.43
3:A:539:6PL:O3	3:A:539:6PL:C31	2.66	0.43
3:A:544:6PL:H381	3:A:551:6PL:H251	2.01	0.43
3:E:301:6PL:H161	3:E:343:6PL:H51	2.00	0.43
3:E:310:6PL:H161	3:E:332:6PL:C3	2.49	0.43
3:E:335:6PL:H462	3:E:347:6PL:C25	2.48	0.43
3:E:345:6PL:H131	3:C:501:6PL:C17	2.44	0.43
3:E:345:6PL:H141	3:C:501:6PL:H451	2.01	0.43
3:E:355:6PL:H42	3:E:355:6PL:H83	1.80	0.43
3:E:369:6PL:H442	1:A:376:LYS:HB3	2.01	0.43
1:A:248:GLN:HG2	3:A:575:6PL:H352	2.01	0.43
1:A:319:GLU:HG2	3:A:548:6PL:H71	2.01	0.43
3:A:503:6PL:H41	3:A:503:6PL:H72	1.81	0.43
3:A:519:6PL:H261	3:A:549:6PL:H451	2.00	0.43
3:A:538:6PL:O4P	3:A:538:6PL:C8	2.66	0.43
3:A:544:6PL:H432	3:A:559:6PL:C23	2.43	0.43
3:A:558:6PL:H321	3:A:562:6PL:H332	2.00	0.43
3:A:566:6PL:H222	3:A:578:6PL:C42	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:306:6PL:H411	3:E:360:6PL:H232	2.00	0.42
3:E:310:6PL:C45	3:A:509:6PL:H441	2.48	0.42
3:E:314:6PL:H392	3:E:364:6PL:H152	2.00	0.42
3:E:329:6PL:H63	3:E:340:6PL:H31	2.01	0.42
3:E:336:6PL:H391	3:E:362:6PL:H391	2.01	0.42
3:E:364:6PL:H141	3:E:364:6PL:C33	2.49	0.42
3:A:518:6PL:H202	3:A:529:6PL:H181	2.00	0.42
3:A:522:6PL:H362	3:A:522:6PL:H392	1.88	0.42
3:A:528:6PL:C33	3:A:584:6PL:C3	2.97	0.42
3:A:530:6PL:H352	3:A:588:6PL:H121	2.01	0.42
3:A:533:6PL:O11	3:A:579:6PL:H372	2.19	0.42
3:A:544:6PL:H432	3:A:559:6PL:H212	2.01	0.42
3:A:546:6PL:C36	3:A:554:6PL:O3	2.66	0.42
3:A:556:6PL:O2P	3:A:556:6PL:C5	2.64	0.42
2:B:251:TRP:CD1	2:B:297:SER:HB2	2.54	0.42
1:E:53:VAL:HB	3:A:586:6PL:C48	2.48	0.42
3:E:311:6PL:O2P	3:E:311:6PL:C5	2.60	0.42
3:E:318:6PL:H211	3:E:331:6PL:C23	2.48	0.42
3:E:361:6PL:H381	3:A:544:6PL:C22	2.49	0.42
3:A:515:6PL:C26	3:A:531:6PL:C23	2.91	0.42
3:A:527:6PL:O3	3:A:564:6PL:C18	2.57	0.42
3:A:569:6PL:O31	3:A:569:6PL:H12	2.19	0.42
3:A:569:6PL:H411	3:A:569:6PL:H381	1.67	0.42
1:E:77:LYS:NZ	1:E:80:GLU:OE2	2.52	0.42
1:E:163:LEU:CD2	3:E:346:6PL:H372	2.50	0.42
3:E:301:6PL:H381	3:E:311:6PL:H472	2.01	0.42
3:E:302:6PL:H202	3:E:308:6PL:C21	2.49	0.42
3:E:310:6PL:H472	3:A:544:6PL:H462	2.00	0.42
3:E:326:6PL:H392	3:E:364:6PL:C4	2.46	0.42
3:E:328:6PL:C26	3:E:348:6PL:C1	2.97	0.42
3:A:512:6PL:O4P	3:A:512:6PL:C8	2.67	0.42
3:A:525:6PL:H231	3:A:579:6PL:C25	2.48	0.42
3:A:556:6PL:H351	3:A:557:6PL:H152	2.01	0.42
3:A:576:6PL:H11	3:A:576:6PL:H42	2.01	0.42
2:B:358:LEU:O	2:B:362:ARG:HD2	2.18	0.42
1:E:34:GLU:OE2	1:E:40:LYS:HG3	2.19	0.42
1:E:82:LEU:HD11	3:E:349:6PL:H481	2.01	0.42
3:E:309:6PL:H371	3:E:325:6PL:H172	2.00	0.42
3:E:316:6PL:H432	3:E:316:6PL:H401	1.87	0.42
3:E:350:6PL:C14	3:E:360:6PL:H231	2.49	0.42
3:E:361:6PL:H241	3:A:509:6PL:H422	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:521:6PL:H83	3:A:521:6PL:O4P	2.20	0.42
3:A:555:6PL:H351	3:A:555:6PL:H322	1.87	0.42
3:A:556:6PL:C8	3:A:556:6PL:P	3.07	0.42
3:A:556:6PL:H232	3:A:577:6PL:H231	1.99	0.42
3:A:572:6PL:H412	3:A:572:6PL:H382	1.58	0.42
3:A:578:6PL:H131	3:A:580:6PL:H182	2.00	0.42
2:C:358:LEU:O	2:C:362:ARG:HD2	2.18	0.42
3:E:313:6PL:H12	3:E:313:6PL:O31	2.18	0.42
3:E:335:6PL:C48	3:E:353:6PL:H431	2.49	0.42
3:E:337:6PL:H441	3:E:347:6PL:H151	2.00	0.42
3:E:344:6PL:H483	3:E:344:6PL:C23	2.41	0.42
3:E:349:6PL:H162	3:E:349:6PL:H191	1.79	0.42
3:E:350:6PL:H142	3:E:360:6PL:H231	2.01	0.42
3:E:363:6PL:H421	3:E:364:6PL:C22	2.50	0.42
1:A:440:THR:HG23	3:A:537:6PL:H42	2.00	0.42
3:A:502:6PL:H382	3:A:505:6PL:H222	2.00	0.42
3:A:505:6PL:H63	3:A:508:6PL:O2P	2.19	0.42
3:A:522:6PL:H141	3:A:522:6PL:C34	2.48	0.42
3:A:534:6PL:O4P	3:A:534:6PL:C8	2.67	0.42
3:A:564:6PL:H431	3:A:564:6PL:C26	2.45	0.42
3:A:574:6PL:H41	3:A:574:6PL:H62	1.65	0.42
2:C:24:PRO:HB3	2:C:167:MET:CE	2.48	0.42
2:C:105:LYS:HA	2:C:136:ASP:OD1	2.19	0.42
2:C:135:ARG:H	2:C:135:ARG:HG2	1.62	0.42
1:E:236:TYR:HB2	3:E:313:6PL:H431	2.00	0.42
3:E:319:6PL:H242	3:E:325:6PL:C45	2.46	0.42
3:E:348:6PL:H202	3:E:348:6PL:H171	1.84	0.42
3:E:359:6PL:O31	3:E:359:6PL:C11	2.67	0.42
1:A:387:LEU:HB2	3:A:534:6PL:H432	2.02	0.42
3:A:512:6PL:H481	3:A:566:6PL:H451	2.02	0.42
3:A:513:6PL:H362	3:A:513:6PL:H391	1.83	0.42
3:A:517:6PL:P	3:A:517:6PL:H62	2.56	0.42
3:A:543:6PL:H392	3:A:566:6PL:H402	2.02	0.42
3:A:548:6PL:H412	3:A:548:6PL:H381	1.53	0.42
3:A:560:6PL:P	3:A:560:6PL:H63	2.60	0.42
3:A:562:6PL:H63	3:A:562:6PL:H42	1.80	0.42
3:A:565:6PL:H162	3:A:580:6PL:H421	2.01	0.42
3:A:581:6PL:H381	3:A:581:6PL:H432	2.01	0.42
2:B:365:GLN:HA	2:B:366:PRO:HD3	1.92	0.42
2:C:128:LEU:C	2:C:133:TYR:HB2	2.40	0.42
3:E:303:6PL:O2P	3:E:303:6PL:H62	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:321:6PL:O1P	3:E:344:6PL:H81	2.19	0.42
3:E:345:6PL:H142	3:C:501:6PL:H191	2.00	0.42
3:E:351:6PL:C44	1:A:365:LEU:HB3	2.47	0.42
1:A:381:GLN:NE2	3:A:534:6PL:H321	2.34	0.42
3:A:504:6PL:H432	3:A:504:6PL:H402	1.87	0.42
3:A:505:6PL:O31	3:A:505:6PL:C3	2.65	0.42
3:A:505:6PL:O31	3:A:506:6PL:C8	2.68	0.42
3:A:540:6PL:C37	3:A:550:6PL:H171	2.50	0.42
3:A:541:6PL:H31	3:A:557:6PL:H442	2.01	0.42
3:A:543:6PL:H392	3:A:566:6PL:C41	2.49	0.42
3:A:580:6PL:H81	3:A:588:6PL:H322	2.02	0.42
2:C:331:PHE:HA	2:C:332:PRO:HA	1.84	0.42
1:E:82:LEU:CD1	3:E:349:6PL:H481	2.50	0.42
3:E:321:6PL:H2	3:E:321:6PL:O1P	2.19	0.42
3:E:367:6PL:H132	3:A:575:6PL:H483	2.01	0.42
1:A:320:LYS:N	1:A:320:LYS:HD2	2.34	0.42
3:A:505:6PL:H252	3:A:506:6PL:H472	2.00	0.42
3:A:522:6PL:H141	3:A:522:6PL:C32	2.49	0.42
3:A:544:6PL:H141	3:A:544:6PL:O11	2.18	0.42
3:A:552:6PL:O1P	3:A:552:6PL:H62	2.19	0.42
2:B:188:LEU:O	2:B:192:LEU:HG	2.20	0.42
2:C:178:ILE:HG12	2:C:207:ILE:HB	2.00	0.42
3:E:308:6PL:O31	3:E:308:6PL:H12	2.18	0.42
3:E:310:6PL:H152	3:E:310:6PL:H181	1.89	0.42
3:E:310:6PL:H42	3:E:310:6PL:H83	1.84	0.42
3:E:328:6PL:C45	3:A:549:6PL:H262	2.35	0.42
3:E:335:6PL:C37	3:E:353:6PL:H332	2.50	0.42
3:E:347:6PL:O11	3:E:347:6PL:H2	2.19	0.42
3:E:353:6PL:C48	3:A:542:6PL:H452	2.36	0.42
3:E:364:6PL:H62	3:E:364:6PL:P	2.60	0.42
3:E:365:6PL:H412	3:E:365:6PL:H381	1.50	0.42
3:E:368:6PL:H362	3:E:368:6PL:H122	2.01	0.42
3:E:368:6PL:H371	3:A:568:6PL:C24	2.49	0.42
3:E:369:6PL:H432	3:E:369:6PL:H461	1.85	0.42
3:A:518:6PL:H51	3:A:521:6PL:H61	2.02	0.42
3:A:521:6PL:H352	3:A:562:6PL:H381	2.02	0.42
3:A:535:6PL:H362	3:A:535:6PL:H391	1.95	0.42
3:A:576:6PL:H381	3:A:576:6PL:H412	1.68	0.42
2:C:27:LEU:HD23	2:C:178:ILE:HB	2.01	0.42
3:E:302:6PL:P	3:E:302:6PL:C8	3.08	0.42
3:E:310:6PL:H472	3:A:544:6PL:H461	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:318:6PL:H152	3:E:332:6PL:H151	2.01	0.42
3:E:324:6PL:H12	3:E:361:6PL:O1P	2.20	0.42
3:E:346:6PL:C43	3:A:553:6PL:H241	2.46	0.42
1:A:376:LYS:HA	1:A:376:LYS:HD3	1.79	0.42
3:A:518:6PL:P	3:A:518:6PL:H83	2.59	0.42
3:A:518:6PL:H12	3:A:518:6PL:C11	2.49	0.42
3:A:519:6PL:H191	3:A:549:6PL:H422	2.01	0.42
3:A:522:6PL:H442	3:A:569:6PL:H431	2.01	0.42
3:A:557:6PL:H481	3:A:559:6PL:H342	2.01	0.42
2:B:26:ILE:HA	2:B:140:ARG:O	2.19	0.42
2:B:109:VAL:HG22	2:B:121:LEU:HD12	2.02	0.42
1:E:3:PRO:HA	1:E:4:PRO:C	2.40	0.41
3:E:314:6PL:C43	3:A:508:6PL:H421	2.37	0.41
3:E:330:6PL:O1P	3:E:330:6PL:H73	2.20	0.41
3:E:339:6PL:O4P	3:E:339:6PL:C8	2.65	0.41
3:E:340:6PL:H371	3:E:342:6PL:H251	2.02	0.41
3:A:513:6PL:O4P	3:A:513:6PL:H82	2.19	0.41
3:A:516:6PL:O4P	3:A:516:6PL:H73	2.20	0.41
3:A:542:6PL:H161	3:A:581:6PL:H202	2.01	0.41
3:A:561:6PL:H401	3:A:561:6PL:H181	2.01	0.41
3:A:570:6PL:H382	3:A:570:6PL:H411	1.68	0.41
1:E:33:PHE:CE2	3:E:322:6PL:H361	2.54	0.41
3:E:321:6PL:H362	3:E:344:6PL:O31	2.18	0.41
1:A:251:TRP:CZ2	3:A:573:6PL:H322	2.55	0.41
3:A:512:6PL:H181	3:A:582:6PL:H202	2.02	0.41
3:A:514:6PL:P	3:A:514:6PL:O2	2.78	0.41
3:A:528:6PL:H411	3:A:528:6PL:H382	1.75	0.41
3:A:533:6PL:H82	3:A:533:6PL:P	2.59	0.41
3:A:533:6PL:P	3:A:533:6PL:H83	2.60	0.41
3:A:535:6PL:H161	3:A:564:6PL:C44	2.39	0.41
3:A:539:6PL:H412	3:A:571:6PL:H401	2.02	0.41
3:A:542:6PL:C20	3:A:542:6PL:H402	2.50	0.41
3:E:301:6PL:H72	3:E:301:6PL:H41	1.86	0.41
3:E:318:6PL:H362	3:E:331:6PL:H161	2.01	0.41
3:E:324:6PL:H372	3:E:358:6PL:C38	2.51	0.41
3:E:331:6PL:H371	3:E:355:6PL:H471	2.02	0.41
3:E:338:6PL:H461	3:E:351:6PL:C22	2.44	0.41
3:E:344:6PL:H141	3:E:344:6PL:H172	1.87	0.41
3:A:505:6PL:C25	3:A:506:6PL:H472	2.51	0.41
3:A:527:6PL:C16	3:A:571:6PL:O2	2.68	0.41
3:A:531:6PL:H41	3:A:531:6PL:H62	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:545:6PL:H141	3:A:545:6PL:O11	2.20	0.41
3:A:556:6PL:O31	3:A:556:6PL:C1	2.61	0.41
1:E:8:TRP:HB2	3:E:319:6PL:H41	2.01	0.41
3:E:317:6PL:O31	3:A:508:6PL:H171	2.20	0.41
3:E:343:6PL:H41	3:E:343:6PL:H62	1.54	0.41
3:E:345:6PL:O11	3:C:501:6PL:H401	2.20	0.41
3:E:349:6PL:H62	3:A:509:6PL:O2P	2.20	0.41
3:E:360:6PL:H411	3:E:360:6PL:H381	1.69	0.41
3:A:505:6PL:H472	3:A:506:6PL:H462	2.02	0.41
3:A:514:6PL:H72	3:A:514:6PL:O4P	2.20	0.41
3:A:518:6PL:H62	3:A:521:6PL:H63	1.97	0.41
3:A:524:6PL:H483	3:A:528:6PL:H231	2.02	0.41
3:A:529:6PL:H471	3:A:534:6PL:C40	2.49	0.41
3:A:530:6PL:C38	3:A:564:6PL:H222	2.50	0.41
3:A:539:6PL:H261	3:A:563:6PL:H381	2.01	0.41
3:A:540:6PL:H131	3:A:540:6PL:H382	2.03	0.41
3:A:555:6PL:H83	3:A:555:6PL:O4P	2.20	0.41
3:A:579:6PL:H62	3:A:579:6PL:H41	1.46	0.41
3:E:304:6PL:H251	3:A:509:6PL:H432	2.02	0.41
3:E:322:6PL:H452	3:E:322:6PL:H421	1.73	0.41
3:E:328:6PL:H262	3:E:348:6PL:C1	2.51	0.41
3:E:329:6PL:H42	3:E:366:6PL:C13	2.51	0.41
3:E:329:6PL:H71	3:E:340:6PL:O2P	2.20	0.41
3:E:336:6PL:H421	3:E:352:6PL:C43	2.50	0.41
3:E:351:6PL:H151	3:E:351:6PL:H122	1.80	0.41
3:E:357:6PL:H412	3:E:357:6PL:H381	1.58	0.41
3:A:502:6PL:H162	3:A:502:6PL:H132	1.83	0.41
3:A:505:6PL:H352	3:A:506:6PL:C32	2.39	0.41
3:A:551:6PL:O2P	3:A:551:6PL:C5	2.61	0.41
3:A:555:6PL:H332	3:A:564:6PL:H172	2.01	0.41
3:A:572:6PL:O11	3:A:572:6PL:H2	2.20	0.41
1:E:119:VAL:HG13	1:A:384:LEU:HD21	2.02	0.41
3:E:306:6PL:H251	3:A:545:6PL:H422	2.00	0.41
3:E:356:6PL:H422	3:E:362:6PL:H201	2.03	0.41
3:E:365:6PL:O2P	3:E:365:6PL:H52	2.19	0.41
3:A:520:6PL:C11	3:A:556:6PL:H412	2.51	0.41
3:A:524:6PL:H441	3:A:528:6PL:C18	2.38	0.41
3:A:546:6PL:H251	3:A:554:6PL:H212	2.02	0.41
3:A:549:6PL:O31	3:A:549:6PL:H41	2.21	0.41
3:A:553:6PL:H52	3:A:553:6PL:O1P	2.21	0.41
3:A:562:6PL:O31	3:A:562:6PL:O3	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:581:6PL:O2	3:A:581:6PL:O2P	2.38	0.41
2:C:376:GLN:HB2	2:C:379:ASN:HB2	2.03	0.41
3:E:316:6PL:H362	3:E:316:6PL:H391	1.92	0.41
3:E:325:6PL:H82	3:E:325:6PL:H41	1.82	0.41
3:E:330:6PL:C26	3:A:537:6PL:C17	2.91	0.41
3:E:344:6PL:H52	3:E:344:6PL:O3P	2.20	0.41
3:A:506:6PL:C6	3:A:506:6PL:O3P	2.66	0.41
3:A:536:6PL:P	3:A:536:6PL:H82	2.61	0.41
3:A:538:6PL:H391	3:A:542:6PL:H342	2.02	0.41
3:A:563:6PL:H191	3:A:567:6PL:H381	2.01	0.41
2:C:24:PRO:HB3	2:C:167:MET:HE1	2.03	0.41
2:C:188:LEU:O	2:C:192:LEU:HG	2.20	0.41
3:E:302:6PL:H261	3:A:523:6PL:H261	2.02	0.41
3:E:307:6PL:H411	3:E:307:6PL:H382	1.65	0.41
3:E:308:6PL:H42	3:E:308:6PL:H73	1.83	0.41
3:E:321:6PL:H181	3:E:359:6PL:C12	2.50	0.41
3:E:321:6PL:C25	3:E:365:6PL:C24	2.99	0.41
3:E:330:6PL:H262	3:A:537:6PL:H182	2.01	0.41
3:E:345:6PL:O11	3:C:501:6PL:C43	2.68	0.41
3:A:513:6PL:C21	3:A:548:6PL:C42	2.97	0.41
3:A:516:6PL:H431	3:A:516:6PL:H402	1.72	0.41
3:A:521:6PL:H332	3:A:558:6PL:O31	2.21	0.41
3:A:528:6PL:H171	3:A:528:6PL:H202	1.86	0.41
3:A:538:6PL:O31	3:A:542:6PL:C7	2.64	0.41
3:A:545:6PL:O1P	3:A:545:6PL:H2	2.21	0.41
3:A:549:6PL:O11	3:A:549:6PL:H142	2.20	0.41
3:A:570:6PL:O2	3:A:570:6PL:P	2.78	0.41
3:A:581:6PL:H42	3:A:581:6PL:H63	1.64	0.41
2:B:149:GLU:OE1	2:B:251:TRP:HB2	2.21	0.41
3:E:302:6PL:H162	3:E:355:6PL:H431	1.98	0.41
3:E:309:6PL:H132	3:E:344:6PL:H52	2.01	0.41
3:E:315:6PL:O3	3:E:315:6PL:C31	2.68	0.41
3:E:326:6PL:H422	3:E:364:6PL:O2	2.20	0.41
3:E:342:6PL:H361	3:E:342:6PL:H392	1.90	0.41
3:E:349:6PL:O31	3:E:349:6PL:O3	2.38	0.41
3:E:352:6PL:H42	3:E:352:6PL:H63	1.85	0.41
3:E:355:6PL:H62	3:E:355:6PL:P	2.60	0.41
3:E:361:6PL:H461	3:A:523:6PL:C44	2.51	0.41
3:A:502:6PL:H442	3:A:510:6PL:H242	2.01	0.41
3:A:520:6PL:H142	3:A:542:6PL:C12	2.51	0.41
3:A:526:6PL:H12	3:A:526:6PL:C4	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:527:6PL:H362	3:A:527:6PL:H391	1.92	0.41
3:A:528:6PL:H151	3:A:528:6PL:H122	1.84	0.41
3:A:530:6PL:C41	3:A:571:6PL:H171	2.51	0.41
3:A:532:6PL:H191	3:A:557:6PL:H392	2.03	0.41
3:A:536:6PL:H452	3:C:501:6PL:H263	2.03	0.41
3:A:538:6PL:H451	3:A:542:6PL:H221	2.02	0.41
3:A:543:6PL:C42	3:A:566:6PL:H462	2.51	0.41
3:A:565:6PL:H231	3:A:565:6PL:H202	1.87	0.41
3:A:573:6PL:H461	3:A:575:6PL:C17	2.41	0.41
3:A:580:6PL:H41	3:A:580:6PL:O31	2.20	0.41
2:B:245:ILE:HG22	2:B:247:THR:H	1.86	0.41
2:C:249:SER:HA	2:C:250:PRO:HD3	1.94	0.41
3:C:501:6PL:H142	3:C:501:6PL:C36	2.51	0.41
1:E:61:ARG:HG3	3:E:330:6PL:H201	2.02	0.41
1:E:159:LEU:HD12	3:A:554:6PL:H471	2.02	0.41
3:E:333:6PL:H171	3:A:511:6PL:H411	2.03	0.41
1:A:381:GLN:HG2	3:A:534:6PL:H321	2.02	0.41
3:E:306:6PL:O1P	3:E:306:6PL:C2	2.59	0.40
3:E:312:6PL:H382	3:E:357:6PL:H451	2.01	0.40
3:E:319:6PL:O4P	3:E:319:6PL:H83	2.21	0.40
3:E:333:6PL:H192	3:A:511:6PL:C42	2.50	0.40
3:E:360:6PL:H362	3:E:360:6PL:H392	1.90	0.40
3:A:532:6PL:H263	3:A:588:6PL:C42	2.47	0.40
3:A:532:6PL:C26	3:A:588:6PL:H442	2.51	0.40
3:A:535:6PL:H172	3:A:564:6PL:C46	2.19	0.40
1:E:146:GLU:O	1:E:149:ARG:HB3	2.22	0.40
3:E:308:6PL:O4P	3:E:308:6PL:C8	2.63	0.40
3:E:318:6PL:H362	3:E:331:6PL:C16	2.52	0.40
3:E:318:6PL:H231	3:A:518:6PL:H471	2.04	0.40
3:E:322:6PL:H352	3:E:365:6PL:H402	2.03	0.40
3:E:325:6PL:H382	3:E:325:6PL:H411	1.86	0.40
3:E:338:6PL:H41	3:E:338:6PL:H62	1.54	0.40
3:A:503:6PL:O4P	3:A:503:6PL:C6	2.69	0.40
3:A:528:6PL:H322	3:A:584:6PL:C11	2.51	0.40
3:A:533:6PL:H42	3:A:579:6PL:O31	2.21	0.40
3:A:540:6PL:H41	3:A:540:6PL:H82	1.87	0.40
3:A:543:6PL:H422	3:A:566:6PL:H462	2.02	0.40
3:A:543:6PL:H332	3:A:587:6PL:C32	2.49	0.40
3:A:571:6PL:H82	3:A:571:6PL:P	2.60	0.40
3:A:586:6PL:O4P	3:A:586:6PL:H72	2.21	0.40
2:B:376:GLN:HB2	2:B:379:ASN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:109:VAL:HG22	2:C:121:LEU:HD12	2.03	0.40
3:C:501:6PL:O1P	3:C:501:6PL:C5	2.67	0.40
1:E:4:PRO:O	1:E:5:GLN:HB2	2.22	0.40
3:E:324:6PL:H161	3:E:361:6PL:H382	2.03	0.40
3:E:337:6PL:H441	3:E:347:6PL:H122	2.03	0.40
3:E:341:6PL:H471	3:E:350:6PL:H191	2.03	0.40
3:E:345:6PL:C14	3:C:501:6PL:H451	2.51	0.40
3:E:345:6PL:H371	3:E:351:6PL:H121	2.03	0.40
3:E:351:6PL:H263	3:A:536:6PL:H471	2.03	0.40
3:E:355:6PL:O1P	3:E:355:6PL:C6	2.67	0.40
3:E:366:6PL:H441	3:E:366:6PL:H472	1.91	0.40
3:E:367:6PL:P	3:E:367:6PL:H72	2.62	0.40
3:A:502:6PL:C37	3:A:505:6PL:H421	2.47	0.40
3:A:518:6PL:C45	3:A:558:6PL:H441	2.46	0.40
3:A:527:6PL:H63	3:A:530:6PL:O1P	2.21	0.40
3:A:553:6PL:H411	3:A:553:6PL:C14	2.49	0.40
3:A:582:6PL:H51	3:A:582:6PL:O3P	2.21	0.40
3:A:586:6PL:H172	3:A:586:6PL:H201	1.90	0.40
2:B:140:ARG:HD3	2:B:167:MET:SD	2.61	0.40
2:C:144:TYR:HB3	2:C:156:TYR:CE1	2.56	0.40
1:E:87:SER:HA	1:E:90:LEU:HD12	2.04	0.40
1:E:137:LEU:HB3	3:E:351:6PL:H401	2.03	0.40
3:E:306:6PL:H402	3:E:341:6PL:H162	2.03	0.40
3:E:308:6PL:H321	3:E:315:6PL:H342	2.04	0.40
3:E:326:6PL:H41	3:E:326:6PL:H62	1.83	0.40
3:E:342:6PL:H411	3:E:342:6PL:H381	1.66	0.40
3:E:350:6PL:H52	3:E:350:6PL:O1P	2.21	0.40
3:E:351:6PL:O31	3:E:351:6PL:H32	2.19	0.40
3:E:357:6PL:H82	3:E:357:6PL:C2	2.30	0.40
3:E:359:6PL:H192	3:E:359:6PL:H161	1.95	0.40
3:E:360:6PL:H141	3:E:360:6PL:H352	2.02	0.40
1:A:341:GLN:HB2	1:A:342:PRO:HD3	2.04	0.40
1:A:359:ARG:NH1	3:A:522:6PL:O2	2.53	0.40
1:A:381:GLN:HE21	3:A:534:6PL:H321	1.87	0.40
1:A:455:GLU:O	1:A:459:GLN:HG2	2.20	0.40
3:A:521:6PL:H431	3:A:558:6PL:H351	2.03	0.40
3:A:527:6PL:H262	3:A:571:6PL:H482	2.04	0.40
3:A:529:6PL:H411	3:A:534:6PL:H122	2.03	0.40
3:A:537:6PL:C19	3:A:549:6PL:H263	2.42	0.40
3:A:556:6PL:C23	3:A:577:6PL:H231	2.52	0.40
3:A:558:6PL:H482	3:A:574:6PL:C23	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:563:6PL:H61	3:A:567:6PL:O2P	2.22	0.40
3:A:566:6PL:H63	3:A:566:6PL:H42	1.61	0.40
2:B:321:THR:HA	2:B:322:PRO:HD3	1.95	0.40
1:E:173:ARG:HA	1:E:173:ARG:HD2	1.82	0.40
3:E:305:6PL:H222	3:A:550:6PL:C45	2.49	0.40
3:E:306:6PL:H481	3:A:548:6PL:C16	2.52	0.40
3:E:306:6PL:H122	3:E:327:6PL:H322	2.04	0.40
3:E:321:6PL:H371	3:E:344:6PL:O31	2.21	0.40
3:E:338:6PL:C47	3:A:522:6PL:H211	2.52	0.40
3:E:351:6PL:H431	3:E:351:6PL:H402	1.63	0.40
3:E:354:6PL:C25	3:A:561:6PL:H252	2.42	0.40
3:E:357:6PL:O31	3:E:357:6PL:H342	2.22	0.40
3:E:367:6PL:C13	3:A:526:6PL:H381	2.50	0.40
3:E:369:6PL:C22	3:A:574:6PL:H83	2.51	0.40
3:A:512:6PL:P	3:A:512:6PL:C8	3.09	0.40
3:A:527:6PL:O31	3:A:527:6PL:C11	2.70	0.40
3:A:543:6PL:H181	3:A:566:6PL:H361	2.03	0.40
3:A:549:6PL:H42	3:A:549:6PL:H73	1.84	0.40
3:A:552:6PL:H372	3:A:570:6PL:H242	1.96	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	A	241/243 (99%)	238 (99%)	3 (1%)	0	100	100
1	E	241/243 (99%)	237 (98%)	3 (1%)	1 (0%)	30	68
2	B	365/396 (92%)	341 (93%)	20 (6%)	4 (1%)	12	47
2	C	365/396 (92%)	341 (93%)	21 (6%)	3 (1%)	16	55
All	All	1212/1278 (95%)	1157 (96%)	47 (4%)	8 (1%)	21	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	38	LEU
2	B	62	LEU
2	C	62	LEU
2	B	41	ASP
2	C	243	GLN
2	C	346	ASP
2	B	243	GLN
2	B	346	ASP

5.3.2 Protein sidechains [i](#)

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	A	214/214 (100%)	195 (91%)	19 (9%)	8	25
1	E	214/214 (100%)	194 (91%)	20 (9%)	7	23
2	B	319/342 (93%)	299 (94%)	20 (6%)	15	36
2	C	319/342 (93%)	296 (93%)	23 (7%)	12	32
All	All	1066/1112 (96%)	984 (92%)	82 (8%)	13	30

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	20	ASP
1	E	24	ASP
1	E	31	SER
1	E	45	LYS
1	E	54	THR
1	E	55	SER
1	E	58	SER
1	E	61	ARG
1	E	77	LYS
1	E	92	GLU
1	E	118	LYS
1	E	138	GLN

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Mol	Chain	Res	Type
1	E	151	ARG
1	E	200	LEU
1	E	203	LEU
1	E	214	LEU
1	E	224	SER
1	E	228	SER
1	E	242	THR
1	E	243	GLN
1	A	244	ASP
1	A	268	SER
1	A	274	SER
1	A	275	GLN
1	A	301	SER
1	A	331	LYS
1	A	348	GLN
1	A	370	GLN
1	A	375	GLN
1	A	381	GLN
1	A	382	GLU
1	A	385	SER
1	A	392	ARG
1	A	396	ARG
1	A	444	SER
1	A	445	THR
1	A	474	SER
1	A	480	THR
1	A	485	THR
2	B	45	VAL
2	B	59	THR
2	B	62	LEU
2	B	85	ARG
2	B	96	VAL
2	B	99	ARG
2	B	109	VAL
2	B	115	SER
2	B	135	ARG
2	B	138	THR
2	B	176	PHE
2	B	201	ARG
2	B	240	LYS
2	B	244	ARG
2	B	246	THR

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Mol	Chain	Res	Type
2	B	263	HIS
2	B	270	SER
2	B	277	ASP
2	B	313	CYS
2	B	346	ASP
2	C	51	TYR
2	C	52	ARG
2	C	54	THR
2	C	59	THR
2	C	85	ARG
2	C	91	SER
2	C	96	VAL
2	C	99	ARG
2	C	109	VAL
2	C	115	SER
2	C	135	ARG
2	C	138	THR
2	C	176	PHE
2	C	181	SER
2	C	201	ARG
2	C	244	ARG
2	C	246	THR
2	C	263	HIS
2	C	270	SER
2	C	277	ASP
2	C	297	SER
2	C	313	CYS
2	C	346	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	49	ASN
1	A	370	GLN
1	A	381	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

158 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	6PL	E	362	-	51,51,51	0.84	3 (5%)	57,59,59	1.05	3 (5%)
3	6PL	E	326	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	4 (7%)
3	6PL	E	345	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	4 (7%)
3	6PL	E	324	-	51,51,51	0.84	3 (5%)	57,59,59	1.51	8 (14%)
3	6PL	A	516	-	51,51,51	0.84	3 (5%)	57,59,59	1.52	8 (14%)
3	6PL	A	585	-	51,51,51	0.84	3 (5%)	57,59,59	1.06	5 (8%)
3	6PL	A	519	-	51,51,51	0.84	3 (5%)	57,59,59	1.20	6 (10%)
3	6PL	A	573	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	4 (7%)
3	6PL	A	520	-	51,51,51	0.84	3 (5%)	57,59,59	1.51	8 (14%)
3	6PL	A	544	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	9 (15%)
3	6PL	E	359	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	E	315	-	51,51,51	0.84	3 (5%)	57,59,59	0.96	4 (7%)
3	6PL	E	337	-	51,51,51	0.84	3 (5%)	57,59,59	1.04	5 (8%)
3	6PL	E	309	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	3 (5%)
3	6PL	E	314	-	51,51,51	0.84	3 (5%)	57,59,59	1.53	8 (14%)
3	6PL	E	356	-	51,51,51	0.84	3 (5%)	57,59,59	1.56	10 (17%)
3	6PL	A	527	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	8 (14%)
3	6PL	E	308	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6PL	A	587	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	4 (7%)
3	6PL	E	330	-	51,51,51	0.84	3 (5%)	57,59,59	1.08	4 (7%)
3	6PL	E	361	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	5 (8%)
3	6PL	A	531	-	51,51,51	0.83	3 (5%)	57,59,59	1.63	9 (15%)
3	6PL	A	513	-	51,51,51	0.84	3 (5%)	57,59,59	1.52	8 (14%)
3	6PL	A	525	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	8 (14%)
3	6PL	E	338	-	51,51,51	0.84	3 (5%)	57,59,59	1.56	8 (14%)
3	6PL	E	346	-	51,51,51	0.84	3 (5%)	57,59,59	0.96	2 (3%)
3	6PL	E	368	-	51,51,51	0.84	3 (5%)	57,59,59	0.99	4 (7%)
3	6PL	A	509	-	51,51,51	0.84	3 (5%)	57,59,59	1.50	8 (14%)
3	6PL	A	541	-	51,51,51	0.84	3 (5%)	57,59,59	1.04	5 (8%)
3	6PL	A	584	-	51,51,51	0.84	3 (5%)	57,59,59	1.60	8 (14%)
3	6PL	A	502	-	51,51,51	0.83	3 (5%)	57,59,59	1.06	4 (7%)
3	6PL	E	367	-	51,51,51	0.84	3 (5%)	57,59,59	1.52	8 (14%)
3	6PL	A	510	-	51,51,51	0.83	3 (5%)	57,59,59	1.76	10 (17%)
3	6PL	E	328	-	51,51,51	0.84	3 (5%)	57,59,59	1.07	4 (7%)
3	6PL	A	571	-	51,51,51	0.84	3 (5%)	57,59,59	0.90	3 (5%)
3	6PL	E	333	-	51,51,51	0.84	3 (5%)	57,59,59	1.54	8 (14%)
3	6PL	A	563	-	51,51,51	0.84	3 (5%)	57,59,59	1.49	8 (14%)
3	6PL	A	523	-	51,51,51	0.83	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	E	339	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	3 (5%)
3	6PL	A	570	-	51,51,51	0.84	3 (5%)	57,59,59	1.05	4 (7%)
3	6PL	A	561	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	3 (5%)
3	6PL	A	536	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	3 (5%)
3	6PL	E	317	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	A	508	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	A	507	-	51,51,51	0.83	3 (5%)	57,59,59	1.07	4 (7%)
3	6PL	E	369	-	51,51,51	0.84	3 (5%)	57,59,59	1.06	3 (5%)
3	6PL	A	521	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	10 (17%)
3	6PL	A	526	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	A	574	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	8 (14%)
3	6PL	A	558	-	51,51,51	0.84	3 (5%)	57,59,59	1.13	6 (10%)
3	6PL	E	366	-	51,51,51	0.84	3 (5%)	57,59,59	1.53	9 (15%)
3	6PL	A	556	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	3 (5%)
3	6PL	A	576	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6PL	A	560	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	C	501	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	3 (5%)
3	6PL	E	331	-	51,51,51	0.84	3 (5%)	57,59,59	1.59	9 (15%)
3	6PL	A	511	-	51,51,51	0.83	3 (5%)	57,59,59	1.09	4 (7%)
3	6PL	A	546	-	51,51,51	0.84	3 (5%)	57,59,59	1.06	3 (5%)
3	6PL	A	514	-	51,51,51	0.84	3 (5%)	57,59,59	1.60	9 (15%)
3	6PL	E	354	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	E	343	-	51,51,51	0.84	3 (5%)	57,59,59	1.56	8 (14%)
3	6PL	E	349	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	10 (17%)
3	6PL	E	365	-	51,51,51	0.84	3 (5%)	57,59,59	1.63	8 (14%)
3	6PL	A	504	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	9 (15%)
3	6PL	E	363	-	51,51,51	0.84	3 (5%)	57,59,59	1.10	4 (7%)
3	6PL	E	307	-	51,51,51	0.84	3 (5%)	57,59,59	1.05	3 (5%)
3	6PL	A	505	-	51,51,51	0.83	3 (5%)	57,59,59	1.46	7 (12%)
3	6PL	E	335	-	51,51,51	0.84	3 (5%)	57,59,59	0.99	3 (5%)
3	6PL	E	319	-	51,51,51	0.84	3 (5%)	57,59,59	1.60	9 (15%)
3	6PL	A	503	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	2 (3%)
3	6PL	E	327	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	A	547	-	51,51,51	0.84	3 (5%)	57,59,59	1.28	8 (14%)
3	6PL	A	537	-	51,51,51	0.84	3 (5%)	57,59,59	1.61	8 (14%)
3	6PL	A	586	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	E	310	-	51,51,51	0.84	3 (5%)	57,59,59	1.08	4 (7%)
3	6PL	E	322	-	51,51,51	0.83	3 (5%)	57,59,59	1.16	3 (5%)
3	6PL	A	588	-	51,51,51	0.84	3 (5%)	57,59,59	1.04	4 (7%)
3	6PL	E	358	-	51,51,51	0.84	3 (5%)	57,59,59	1.61	10 (17%)
3	6PL	A	568	-	51,51,51	0.84	3 (5%)	57,59,59	1.04	4 (7%)
3	6PL	A	577	-	51,51,51	0.84	3 (5%)	57,59,59	1.51	9 (15%)
3	6PL	E	347	-	51,51,51	0.84	3 (5%)	57,59,59	1.05	3 (5%)
3	6PL	A	551	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	3 (5%)
3	6PL	E	316	-	51,51,51	0.84	3 (5%)	57,59,59	1.59	9 (15%)
3	6PL	E	336	-	51,51,51	0.84	3 (5%)	57,59,59	1.60	9 (15%)
3	6PL	E	332	-	51,51,51	0.84	3 (5%)	57,59,59	1.50	9 (15%)
3	6PL	A	524	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	4 (7%)
3	6PL	A	535	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	4 (7%)
3	6PL	A	538	-	51,51,51	0.84	3 (5%)	57,59,59	1.59	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6PL	A	543	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	3 (5%)
3	6PL	A	549	-	51,51,51	0.83	3 (5%)	57,59,59	1.10	3 (5%)
3	6PL	E	355	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	4 (7%)
3	6PL	A	533	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	3 (5%)
3	6PL	E	357	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	4 (7%)
3	6PL	E	325	-	51,51,51	0.84	3 (5%)	57,59,59	1.10	4 (7%)
3	6PL	E	340	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	8 (14%)
3	6PL	E	341	-	51,51,51	0.84	3 (5%)	57,59,59	1.59	8 (14%)
3	6PL	E	342	-	51,51,51	0.84	3 (5%)	57,59,59	0.99	2 (3%)
3	6PL	A	550	-	51,51,51	0.84	3 (5%)	57,59,59	1.51	8 (14%)
3	6PL	E	344	-	51,51,51	0.83	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	E	353	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	A	565	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	3 (5%)
3	6PL	A	548	-	51,51,51	0.84	3 (5%)	57,59,59	0.99	3 (5%)
3	6PL	E	334	-	51,51,51	0.84	3 (5%)	57,59,59	1.04	3 (5%)
3	6PL	A	559	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	3 (5%)
3	6PL	E	304	-	51,51,51	0.83	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	A	553	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	5 (8%)
3	6PL	A	506	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	A	518	-	51,51,51	0.84	3 (5%)	57,59,59	0.92	3 (5%)
3	6PL	A	534	-	51,51,51	0.84	3 (5%)	57,59,59	1.09	3 (5%)
3	6PL	A	555	-	51,51,51	0.84	3 (5%)	57,59,59	1.49	8 (14%)
3	6PL	A	562	-	51,51,51	0.84	3 (5%)	57,59,59	0.96	4 (7%)
3	6PL	E	301	-	51,51,51	0.84	3 (5%)	57,59,59	1.06	3 (5%)
3	6PL	E	364	-	51,51,51	0.83	3 (5%)	57,59,59	1.03	4 (7%)
3	6PL	A	542	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	3 (5%)
3	6PL	E	312	-	51,51,51	0.85	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	E	352	-	51,51,51	0.84	3 (5%)	57,59,59	1.09	5 (8%)
3	6PL	E	306	-	51,51,51	0.84	3 (5%)	57,59,59	1.63	9 (15%)
3	6PL	A	501	-	51,51,51	0.84	3 (5%)	57,59,59	0.97	3 (5%)
3	6PL	A	579	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	A	552	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	8 (14%)
3	6PL	A	582	-	51,51,51	0.84	3 (5%)	57,59,59	0.98	4 (7%)
3	6PL	A	529	-	51,51,51	0.84	3 (5%)	57,59,59	1.29	9 (15%)
3	6PL	A	512	-	51,51,51	0.84	3 (5%)	57,59,59	0.96	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6PL	A	530	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	A	572	-	51,51,51	0.84	3 (5%)	57,59,59	1.09	3 (5%)
3	6PL	E	302	-	51,51,51	0.84	3 (5%)	57,59,59	1.12	4 (7%)
3	6PL	E	360	-	51,51,51	0.84	3 (5%)	57,59,59	0.89	3 (5%)
3	6PL	A	532	-	51,51,51	0.84	3 (5%)	57,59,59	0.93	2 (3%)
3	6PL	E	348	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	E	311	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	A	515	-	51,51,51	0.83	3 (5%)	57,59,59	1.05	3 (5%)
3	6PL	A	557	-	51,51,51	0.84	3 (5%)	57,59,59	1.05	4 (7%)
3	6PL	A	567	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	5 (8%)
3	6PL	A	522	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	5 (8%)
3	6PL	E	318	-	51,51,51	0.84	3 (5%)	57,59,59	1.60	9 (15%)
3	6PL	E	321	-	51,51,51	0.84	3 (5%)	57,59,59	1.52	8 (14%)
3	6PL	A	566	-	51,51,51	0.83	3 (5%)	57,59,59	1.53	8 (14%)
3	6PL	A	528	-	51,51,51	0.83	3 (5%)	57,59,59	1.07	4 (7%)
3	6PL	A	564	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	3 (5%)
3	6PL	E	313	-	51,51,51	0.84	3 (5%)	57,59,59	1.25	8 (14%)
3	6PL	A	539	-	51,51,51	0.84	3 (5%)	57,59,59	1.54	9 (15%)
3	6PL	A	569	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	E	351	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	1 (1%)
3	6PL	E	303	-	51,51,51	0.84	3 (5%)	57,59,59	1.56	8 (14%)
3	6PL	A	554	-	51,51,51	0.84	3 (5%)	57,59,59	1.54	10 (17%)
3	6PL	E	320	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	3 (5%)
3	6PL	A	578	-	51,51,51	0.84	3 (5%)	57,59,59	1.21	8 (14%)
3	6PL	E	305	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	A	545	-	51,51,51	0.84	3 (5%)	57,59,59	1.59	8 (14%)
3	6PL	A	517	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	A	540	-	51,51,51	0.84	3 (5%)	57,59,59	0.93	3 (5%)
3	6PL	E	323	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	10 (17%)
3	6PL	A	575	-	51,51,51	0.84	3 (5%)	57,59,59	1.09	3 (5%)
3	6PL	E	329	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	3 (5%)
3	6PL	A	580	-	51,51,51	0.84	3 (5%)	57,59,59	1.08	4 (7%)
3	6PL	A	583	-	51,51,51	0.84	3 (5%)	57,59,59	1.54	9 (15%)
3	6PL	E	350	-	51,51,51	0.83	3 (5%)	57,59,59	1.14	5 (8%)
3	6PL	A	581	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	9 (15%)

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
3	6PL	E	362	-	-	6/55/55/55	-
3	6PL	E	326	-	-	14/55/55/55	-
3	6PL	E	345	-	-	8/55/55/55	-
3	6PL	E	324	-	-	7/55/55/55	-
3	6PL	A	516	-	-	10/55/55/55	-
3	6PL	A	585	-	-	3/55/55/55	-
3	6PL	A	519	-	-	6/55/55/55	-
3	6PL	A	573	-	-	4/55/55/55	-
3	6PL	A	520	-	-	11/55/55/55	-
3	6PL	A	544	-	-	1/55/55/55	-
3	6PL	E	359	-	-	6/55/55/55	-
3	6PL	E	315	-	-	11/55/55/55	-
3	6PL	E	337	-	-	6/55/55/55	-
3	6PL	E	309	-	-	4/55/55/55	-
3	6PL	E	314	-	-	10/55/55/55	-
3	6PL	E	356	-	-	4/55/55/55	-
3	6PL	A	527	-	-	3/55/55/55	-
3	6PL	E	308	-	-	5/55/55/55	-
3	6PL	A	587	-	-	6/55/55/55	-
3	6PL	E	330	-	-	5/55/55/55	-
3	6PL	E	361	-	-	8/55/55/55	-
3	6PL	A	531	-	-	9/55/55/55	-
3	6PL	A	513	-	-	8/55/55/55	-
3	6PL	A	525	-	-	6/55/55/55	-
3	6PL	E	338	-	-	2/55/55/55	-
3	6PL	E	346	-	-	2/55/55/55	-
3	6PL	E	368	-	-	9/55/55/55	-
3	6PL	A	509	-	-	12/55/55/55	-
3	6PL	A	541	-	-	6/55/55/55	-
3	6PL	A	584	-	-	11/55/55/55	-
3	6PL	A	502	-	-	5/55/55/55	-
3	6PL	E	367	-	-	14/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	A	510	-	-	8/55/55/55	-
3	6PL	E	328	-	-	6/55/55/55	-
3	6PL	A	571	-	-	10/55/55/55	-
3	6PL	E	333	-	-	12/55/55/55	-
3	6PL	A	563	-	-	14/55/55/55	-
3	6PL	A	523	-	-	8/55/55/55	-
3	6PL	E	339	-	-	6/55/55/55	-
3	6PL	A	570	-	-	9/55/55/55	-
3	6PL	A	561	-	-	7/55/55/55	-
3	6PL	A	536	-	-	7/55/55/55	-
3	6PL	E	317	-	-	6/55/55/55	-
3	6PL	A	508	-	-	7/55/55/55	-
3	6PL	A	507	-	-	6/55/55/55	-
3	6PL	E	369	-	-	11/55/55/55	-
3	6PL	A	521	-	-	5/55/55/55	-
3	6PL	A	526	-	-	10/55/55/55	-
3	6PL	A	574	-	-	7/55/55/55	-
3	6PL	A	558	-	-	8/55/55/55	-
3	6PL	E	366	-	-	6/55/55/55	-
3	6PL	A	556	-	-	8/55/55/55	-
3	6PL	A	576	-	-	10/55/55/55	-
3	6PL	A	560	-	-	8/55/55/55	-
3	6PL	C	501	-	-	5/55/55/55	-
3	6PL	E	331	-	-	7/55/55/55	-
3	6PL	A	511	-	-	12/55/55/55	-
3	6PL	A	546	-	-	10/55/55/55	-
3	6PL	A	514	-	-	9/55/55/55	-
3	6PL	E	354	-	-	4/55/55/55	-
3	6PL	E	343	-	-	8/55/55/55	-
3	6PL	E	349	-	-	9/55/55/55	-
3	6PL	E	365	-	-	10/55/55/55	-
3	6PL	A	504	-	-	6/55/55/55	-
3	6PL	E	363	-	-	7/55/55/55	-
3	6PL	E	307	-	-	12/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	A	505	-	-	6/55/55/55	-
3	6PL	E	335	-	-	11/55/55/55	-
3	6PL	E	319	-	-	7/55/55/55	-
3	6PL	A	503	-	-	8/55/55/55	-
3	6PL	E	327	-	-	5/55/55/55	-
3	6PL	A	547	-	-	9/55/55/55	-
3	6PL	A	537	-	-	11/55/55/55	-
3	6PL	A	586	-	-	10/55/55/55	-
3	6PL	E	310	-	-	7/55/55/55	-
3	6PL	E	322	-	-	10/55/55/55	-
3	6PL	A	588	-	-	8/55/55/55	-
3	6PL	E	358	-	-	7/55/55/55	-
3	6PL	A	568	-	-	6/55/55/55	-
3	6PL	A	577	-	-	10/55/55/55	-
3	6PL	E	347	-	-	4/55/55/55	-
3	6PL	A	551	-	-	13/55/55/55	-
3	6PL	E	316	-	-	10/55/55/55	-
3	6PL	E	336	-	-	5/55/55/55	-
3	6PL	E	332	-	-	5/55/55/55	-
3	6PL	A	524	-	-	7/55/55/55	-
3	6PL	A	535	-	-	10/55/55/55	-
3	6PL	A	538	-	-	4/55/55/55	-
3	6PL	A	543	-	-	5/55/55/55	-
3	6PL	A	549	-	-	7/55/55/55	-
3	6PL	E	355	-	-	6/55/55/55	-
3	6PL	A	533	-	-	9/55/55/55	-
3	6PL	E	357	-	-	5/55/55/55	-
3	6PL	E	325	-	-	12/55/55/55	-
3	6PL	E	340	-	-	7/55/55/55	-
3	6PL	E	341	-	-	5/55/55/55	-
3	6PL	E	342	-	-	12/55/55/55	-
3	6PL	A	550	-	-	7/55/55/55	-
3	6PL	E	344	-	-	9/55/55/55	-
3	6PL	E	353	-	-	14/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	A	565	-	-	10/55/55/55	-
3	6PL	A	548	-	-	11/55/55/55	-
3	6PL	E	334	-	-	5/55/55/55	-
3	6PL	A	559	-	-	15/55/55/55	-
3	6PL	E	304	-	-	6/55/55/55	-
3	6PL	A	553	-	-	6/55/55/55	-
3	6PL	A	506	-	-	12/55/55/55	-
3	6PL	A	518	-	-	11/55/55/55	-
3	6PL	A	534	-	-	9/55/55/55	-
3	6PL	A	555	-	-	9/55/55/55	-
3	6PL	A	562	-	-	6/55/55/55	-
3	6PL	E	301	-	-	7/55/55/55	-
3	6PL	E	364	-	-	8/55/55/55	-
3	6PL	A	542	-	-	10/55/55/55	-
3	6PL	E	312	-	-	14/55/55/55	-
3	6PL	E	352	-	-	10/55/55/55	-
3	6PL	E	306	-	-	6/55/55/55	-
3	6PL	A	501	-	-	7/55/55/55	-
3	6PL	A	579	-	-	8/55/55/55	-
3	6PL	A	552	-	-	5/55/55/55	-
3	6PL	A	582	-	-	9/55/55/55	-
3	6PL	A	529	-	-	7/55/55/55	-
3	6PL	A	512	-	-	7/55/55/55	-
3	6PL	A	530	-	-	3/55/55/55	-
3	6PL	A	572	-	-	5/55/55/55	-
3	6PL	E	302	-	-	8/55/55/55	-
3	6PL	E	360	-	-	11/55/55/55	-
3	6PL	A	532	-	-	6/55/55/55	-
3	6PL	E	348	-	-	12/55/55/55	-
3	6PL	E	311	-	-	3/55/55/55	-
3	6PL	A	515	-	-	7/55/55/55	-
3	6PL	A	557	-	-	5/55/55/55	-
3	6PL	A	567	-	-	4/55/55/55	-
3	6PL	A	522	-	-	15/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	E	318	-	-	6/55/55/55	-
3	6PL	E	321	-	-	11/55/55/55	-
3	6PL	A	566	-	-	6/55/55/55	-
3	6PL	A	528	-	-	10/55/55/55	-
3	6PL	A	564	-	-	9/55/55/55	-
3	6PL	E	313	-	-	9/55/55/55	-
3	6PL	A	539	-	-	3/55/55/55	-
3	6PL	A	569	-	-	7/55/55/55	-
3	6PL	E	351	-	-	13/55/55/55	-
3	6PL	E	303	-	-	7/55/55/55	-
3	6PL	A	554	-	-	4/55/55/55	-
3	6PL	E	320	-	-	7/55/55/55	-
3	6PL	A	578	-	-	8/55/55/55	-
3	6PL	E	305	-	-	10/55/55/55	-
3	6PL	A	545	-	-	6/55/55/55	-
3	6PL	A	517	-	-	9/55/55/55	-
3	6PL	A	540	-	-	9/55/55/55	-
3	6PL	E	323	-	-	5/55/55/55	-
3	6PL	A	575	-	-	11/55/55/55	-
3	6PL	E	329	-	-	6/55/55/55	-
3	6PL	A	580	-	-	8/55/55/55	-
3	6PL	A	583	-	-	3/55/55/55	-
3	6PL	E	350	-	-	6/55/55/55	-
3	6PL	A	581	-	-	11/55/55/55	-

All (474) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	306	6PL	C40-C39	-2.58	1.39	1.51
3	A	523	6PL	C40-C39	-2.56	1.39	1.51
3	E	369	6PL	C40-C39	-2.56	1.39	1.51
3	A	553	6PL	C41-C40	-2.55	1.39	1.51
3	A	507	6PL	C40-C39	-2.54	1.39	1.51
3	A	564	6PL	C40-C39	-2.53	1.39	1.51
3	E	321	6PL	C41-C40	-2.52	1.39	1.51
3	E	360	6PL	C41-C40	-2.51	1.39	1.51
3	E	305	6PL	C41-C40	-2.51	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	530	6PL	C41-C40	-2.51	1.39	1.51
3	A	521	6PL	C41-C40	-2.51	1.39	1.51
3	A	521	6PL	C39-C38	-2.51	1.39	1.51
3	A	566	6PL	C39-C38	-2.51	1.39	1.51
3	E	312	6PL	C40-C39	-2.51	1.39	1.51
3	E	367	6PL	C41-C40	-2.51	1.39	1.51
3	A	586	6PL	C41-C40	-2.51	1.39	1.51
3	A	566	6PL	C41-C40	-2.51	1.39	1.51
3	E	357	6PL	C39-C38	-2.51	1.39	1.51
3	E	320	6PL	C41-C40	-2.51	1.39	1.51
3	E	350	6PL	C39-C38	-2.51	1.39	1.51
3	A	526	6PL	C40-C39	-2.50	1.39	1.51
3	A	516	6PL	C40-C39	-2.50	1.39	1.51
3	A	536	6PL	C40-C39	-2.50	1.39	1.51
3	A	539	6PL	C39-C38	-2.50	1.39	1.51
3	A	559	6PL	C40-C39	-2.50	1.39	1.51
3	A	530	6PL	C40-C39	-2.50	1.39	1.51
3	A	587	6PL	C41-C40	-2.50	1.39	1.51
3	A	526	6PL	C41-C40	-2.50	1.39	1.51
3	A	543	6PL	C41-C40	-2.50	1.39	1.51
3	A	520	6PL	C39-C38	-2.50	1.39	1.51
3	A	586	6PL	C39-C38	-2.50	1.39	1.51
3	E	367	6PL	C39-C38	-2.50	1.39	1.51
3	E	350	6PL	C41-C40	-2.50	1.39	1.51
3	A	512	6PL	C39-C38	-2.50	1.39	1.51
3	A	556	6PL	C41-C40	-2.50	1.39	1.51
3	E	332	6PL	C41-C40	-2.50	1.39	1.51
3	E	366	6PL	C39-C38	-2.50	1.39	1.51
3	E	303	6PL	C39-C38	-2.50	1.39	1.51
3	E	343	6PL	C41-C40	-2.50	1.39	1.51
3	A	503	6PL	C41-C40	-2.50	1.39	1.51
3	A	537	6PL	C40-C39	-2.50	1.39	1.51
3	A	549	6PL	C40-C39	-2.50	1.39	1.51
3	A	558	6PL	C39-C38	-2.50	1.39	1.51
3	A	513	6PL	C39-C38	-2.50	1.39	1.51
3	A	530	6PL	C39-C38	-2.50	1.39	1.51
3	A	560	6PL	C41-C40	-2.50	1.39	1.51
3	E	328	6PL	C39-C38	-2.50	1.39	1.51
3	A	529	6PL	C41-C40	-2.50	1.39	1.51
3	E	325	6PL	C40-C39	-2.50	1.39	1.51
3	E	339	6PL	C39-C38	-2.50	1.39	1.51
3	A	554	6PL	C39-C38	-2.50	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	326	6PL	C39-C38	-2.50	1.39	1.51
3	A	506	6PL	C41-C40	-2.50	1.39	1.51
3	E	338	6PL	C41-C40	-2.50	1.39	1.51
3	A	565	6PL	C41-C40	-2.50	1.39	1.51
3	A	535	6PL	C40-C39	-2.50	1.39	1.51
3	A	550	6PL	C39-C38	-2.49	1.39	1.51
3	E	312	6PL	C39-C38	-2.49	1.39	1.51
3	E	337	6PL	C40-C39	-2.49	1.39	1.51
3	A	569	6PL	C40-C39	-2.49	1.39	1.51
3	A	558	6PL	C41-C40	-2.49	1.39	1.51
3	E	331	6PL	C39-C38	-2.49	1.39	1.51
3	A	584	6PL	C41-C40	-2.49	1.39	1.51
3	A	588	6PL	C40-C39	-2.49	1.39	1.51
3	E	324	6PL	C41-C40	-2.49	1.39	1.51
3	E	343	6PL	C39-C38	-2.49	1.39	1.51
3	A	513	6PL	C41-C40	-2.49	1.39	1.51
3	A	548	6PL	C40-C39	-2.49	1.39	1.51
3	A	576	6PL	C40-C39	-2.49	1.39	1.51
3	E	305	6PL	C39-C38	-2.49	1.39	1.51
3	A	547	6PL	C40-C39	-2.49	1.39	1.51
3	E	359	6PL	C40-C39	-2.49	1.39	1.51
3	A	587	6PL	C39-C38	-2.49	1.39	1.51
3	A	539	6PL	C40-C39	-2.49	1.39	1.51
3	A	551	6PL	C41-C40	-2.49	1.39	1.51
3	E	368	6PL	C41-C40	-2.49	1.39	1.51
3	E	321	6PL	C39-C38	-2.49	1.39	1.51
3	E	361	6PL	C41-C40	-2.49	1.39	1.51
3	E	368	6PL	C40-C39	-2.49	1.39	1.51
3	A	541	6PL	C40-C39	-2.49	1.39	1.51
3	E	328	6PL	C41-C40	-2.49	1.39	1.51
3	E	330	6PL	C39-C38	-2.49	1.39	1.51
3	A	540	6PL	C41-C40	-2.49	1.39	1.51
3	A	585	6PL	C40-C39	-2.49	1.39	1.51
3	E	310	6PL	C40-C39	-2.49	1.39	1.51
3	E	319	6PL	C40-C39	-2.49	1.39	1.51
3	A	567	6PL	C40-C39	-2.49	1.39	1.51
3	C	501	6PL	C40-C39	-2.49	1.39	1.51
3	E	323	6PL	C39-C38	-2.49	1.39	1.51
3	E	302	6PL	C41-C40	-2.49	1.39	1.51
3	E	325	6PL	C41-C40	-2.49	1.39	1.51
3	E	354	6PL	C39-C38	-2.49	1.39	1.51
3	A	522	6PL	C40-C39	-2.49	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	528	6PL	C40-C39	-2.49	1.39	1.51
3	A	535	6PL	C39-C38	-2.49	1.39	1.51
3	A	584	6PL	C39-C38	-2.49	1.39	1.51
3	E	342	6PL	C40-C39	-2.49	1.39	1.51
3	E	360	6PL	C39-C38	-2.49	1.39	1.51
3	E	309	6PL	C39-C38	-2.49	1.39	1.51
3	E	351	6PL	C39-C38	-2.49	1.39	1.51
3	A	543	6PL	C39-C38	-2.49	1.39	1.51
3	A	547	6PL	C39-C38	-2.49	1.39	1.51
3	A	559	6PL	C41-C40	-2.49	1.39	1.51
3	E	319	6PL	C39-C38	-2.49	1.39	1.51
3	E	337	6PL	C39-C38	-2.49	1.39	1.51
3	A	546	6PL	C39-C38	-2.49	1.39	1.51
3	A	518	6PL	C41-C40	-2.49	1.39	1.51
3	E	328	6PL	C40-C39	-2.49	1.39	1.51
3	A	518	6PL	C40-C39	-2.49	1.39	1.51
3	A	555	6PL	C41-C40	-2.49	1.39	1.51
3	A	556	6PL	C39-C38	-2.49	1.39	1.51
3	A	504	6PL	C39-C38	-2.49	1.39	1.51
3	E	308	6PL	C39-C38	-2.49	1.39	1.51
3	E	345	6PL	C39-C38	-2.49	1.39	1.51
3	E	361	6PL	C40-C39	-2.49	1.39	1.51
3	A	561	6PL	C39-C38	-2.49	1.39	1.51
3	A	544	6PL	C41-C40	-2.49	1.39	1.51
3	E	331	6PL	C41-C40	-2.49	1.39	1.51
3	E	365	6PL	C41-C40	-2.49	1.39	1.51
3	A	516	6PL	C39-C38	-2.49	1.39	1.51
3	A	568	6PL	C41-C40	-2.49	1.39	1.51
3	E	316	6PL	C41-C40	-2.49	1.39	1.51
3	E	346	6PL	C41-C40	-2.49	1.39	1.51
3	A	525	6PL	C40-C39	-2.49	1.39	1.51
3	E	307	6PL	C41-C40	-2.49	1.39	1.51
3	A	514	6PL	C39-C38	-2.49	1.39	1.51
3	A	520	6PL	C40-C39	-2.49	1.39	1.51
3	A	522	6PL	C39-C38	-2.49	1.39	1.51
3	A	534	6PL	C39-C38	-2.49	1.39	1.51
3	A	556	6PL	C40-C39	-2.49	1.39	1.51
3	E	305	6PL	C40-C39	-2.49	1.39	1.51
3	A	505	6PL	C39-C38	-2.49	1.39	1.51
3	A	534	6PL	C40-C39	-2.49	1.39	1.51
3	A	546	6PL	C41-C40	-2.49	1.39	1.51
3	E	324	6PL	C40-C39	-2.49	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	330	6PL	C41-C40	-2.49	1.39	1.51
3	A	504	6PL	C40-C39	-2.49	1.39	1.51
3	E	301	6PL	C40-C39	-2.49	1.39	1.51
3	E	314	6PL	C41-C40	-2.49	1.39	1.51
3	E	334	6PL	C39-C38	-2.49	1.39	1.51
3	E	347	6PL	C41-C40	-2.49	1.39	1.51
3	E	356	6PL	C39-C38	-2.49	1.39	1.51
3	A	572	6PL	C41-C40	-2.49	1.39	1.51
3	E	301	6PL	C39-C38	-2.49	1.39	1.51
3	A	517	6PL	C41-C40	-2.49	1.39	1.51
3	E	334	6PL	C41-C40	-2.48	1.39	1.51
3	A	565	6PL	C40-C39	-2.48	1.39	1.51
3	E	308	6PL	C40-C39	-2.48	1.39	1.51
3	E	342	6PL	C41-C40	-2.48	1.39	1.51
3	E	349	6PL	C40-C39	-2.48	1.39	1.51
3	A	540	6PL	C39-C38	-2.48	1.39	1.51
3	A	543	6PL	C40-C39	-2.48	1.39	1.51
3	E	339	6PL	C40-C39	-2.48	1.39	1.51
3	E	322	6PL	C39-C38	-2.48	1.39	1.51
3	E	335	6PL	C41-C40	-2.48	1.39	1.51
3	E	348	6PL	C41-C40	-2.48	1.39	1.51
3	A	519	6PL	C41-C40	-2.48	1.39	1.51
3	A	529	6PL	C39-C38	-2.48	1.39	1.51
3	A	538	6PL	C41-C40	-2.48	1.39	1.51
3	E	347	6PL	C40-C39	-2.48	1.39	1.51
3	A	504	6PL	C41-C40	-2.48	1.39	1.51
3	A	553	6PL	C39-C38	-2.48	1.39	1.51
3	E	352	6PL	C39-C38	-2.48	1.39	1.51
3	A	550	6PL	C40-C39	-2.48	1.39	1.51
3	A	563	6PL	C39-C38	-2.48	1.39	1.51
3	E	346	6PL	C40-C39	-2.48	1.39	1.51
3	E	363	6PL	C41-C40	-2.48	1.39	1.51
3	E	317	6PL	C41-C40	-2.48	1.39	1.51
3	A	509	6PL	C39-C38	-2.48	1.39	1.51
3	A	527	6PL	C40-C39	-2.48	1.39	1.51
3	A	532	6PL	C40-C39	-2.48	1.39	1.51
3	E	316	6PL	C39-C38	-2.48	1.39	1.51
3	E	326	6PL	C41-C40	-2.48	1.39	1.51
3	E	349	6PL	C39-C38	-2.48	1.39	1.51
3	E	337	6PL	C41-C40	-2.48	1.39	1.51
3	A	583	6PL	C41-C40	-2.48	1.39	1.51
3	E	327	6PL	C41-C40	-2.48	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	558	6PL	C40-C39	-2.48	1.39	1.51
3	E	335	6PL	C40-C39	-2.48	1.39	1.51
3	A	554	6PL	C41-C40	-2.48	1.39	1.51
3	A	563	6PL	C41-C40	-2.48	1.39	1.51
3	E	318	6PL	C39-C38	-2.48	1.39	1.51
3	A	509	6PL	C41-C40	-2.48	1.39	1.51
3	A	588	6PL	C41-C40	-2.48	1.39	1.51
3	E	308	6PL	C41-C40	-2.48	1.39	1.51
3	E	310	6PL	C41-C40	-2.48	1.39	1.51
3	E	357	6PL	C41-C40	-2.48	1.39	1.51
3	A	506	6PL	C39-C38	-2.48	1.39	1.51
3	A	512	6PL	C40-C39	-2.48	1.39	1.51
3	A	525	6PL	C39-C38	-2.48	1.39	1.51
3	A	531	6PL	C40-C39	-2.48	1.39	1.51
3	A	547	6PL	C41-C40	-2.48	1.39	1.51
3	A	559	6PL	C39-C38	-2.48	1.39	1.51
3	E	340	6PL	C41-C40	-2.48	1.39	1.51
3	E	356	6PL	C40-C39	-2.48	1.39	1.51
3	A	540	6PL	C40-C39	-2.48	1.39	1.51
3	E	301	6PL	C41-C40	-2.48	1.39	1.51
3	E	333	6PL	C40-C39	-2.48	1.39	1.51
3	A	512	6PL	C41-C40	-2.48	1.39	1.51
3	E	363	6PL	C40-C39	-2.48	1.39	1.51
3	A	537	6PL	C41-C40	-2.48	1.39	1.51
3	E	307	6PL	C40-C39	-2.48	1.39	1.51
3	E	323	6PL	C41-C40	-2.48	1.39	1.51
3	E	339	6PL	C41-C40	-2.48	1.39	1.51
3	A	529	6PL	C40-C39	-2.48	1.39	1.51
3	E	358	6PL	C40-C39	-2.48	1.39	1.51
3	E	366	6PL	C41-C40	-2.48	1.39	1.51
3	A	539	6PL	C41-C40	-2.48	1.39	1.51
3	A	509	6PL	C40-C39	-2.48	1.39	1.51
3	A	517	6PL	C40-C39	-2.48	1.39	1.51
3	E	311	6PL	C39-C38	-2.48	1.39	1.51
3	E	334	6PL	C40-C39	-2.48	1.39	1.51
3	E	342	6PL	C39-C38	-2.48	1.39	1.51
3	A	575	6PL	C41-C40	-2.48	1.39	1.51
3	E	303	6PL	C41-C40	-2.48	1.39	1.51
3	E	333	6PL	C41-C40	-2.48	1.39	1.51
3	E	355	6PL	C39-C38	-2.48	1.39	1.51
3	E	355	6PL	C41-C40	-2.48	1.39	1.51
3	E	368	6PL	C39-C38	-2.48	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	516	6PL	C41-C40	-2.48	1.39	1.51
3	A	573	6PL	C40-C39	-2.48	1.39	1.51
3	A	580	6PL	C40-C39	-2.48	1.39	1.51
3	E	324	6PL	C39-C38	-2.48	1.39	1.51
3	E	352	6PL	C40-C39	-2.48	1.39	1.51
3	A	528	6PL	C41-C40	-2.48	1.39	1.51
3	A	570	6PL	C40-C39	-2.48	1.39	1.51
3	E	341	6PL	C39-C38	-2.48	1.39	1.51
3	A	578	6PL	C40-C39	-2.48	1.39	1.51
3	E	329	6PL	C40-C39	-2.48	1.39	1.51
3	A	520	6PL	C41-C40	-2.48	1.39	1.51
3	A	531	6PL	C41-C40	-2.48	1.39	1.51
3	A	536	6PL	C41-C40	-2.48	1.39	1.51
3	A	548	6PL	C39-C38	-2.48	1.39	1.51
3	A	581	6PL	C41-C40	-2.48	1.39	1.51
3	A	531	6PL	C39-C38	-2.48	1.39	1.51
3	A	572	6PL	C39-C38	-2.48	1.39	1.51
3	A	503	6PL	C40-C39	-2.48	1.39	1.51
3	A	560	6PL	C40-C39	-2.48	1.39	1.51
3	A	582	6PL	C40-C39	-2.48	1.39	1.51
3	E	315	6PL	C40-C39	-2.48	1.39	1.51
3	A	573	6PL	C41-C40	-2.48	1.39	1.51
3	E	313	6PL	C40-C39	-2.48	1.39	1.51
3	E	325	6PL	C39-C38	-2.48	1.39	1.51
3	E	343	6PL	C40-C39	-2.48	1.39	1.51
3	A	532	6PL	C41-C40	-2.48	1.39	1.51
3	A	585	6PL	C41-C40	-2.48	1.39	1.51
3	A	545	6PL	C39-C38	-2.48	1.39	1.51
3	A	583	6PL	C40-C39	-2.48	1.39	1.51
3	E	320	6PL	C40-C39	-2.48	1.39	1.51
3	E	347	6PL	C39-C38	-2.48	1.39	1.51
3	E	365	6PL	C39-C38	-2.48	1.39	1.51
3	A	532	6PL	C39-C38	-2.48	1.39	1.51
3	A	560	6PL	C39-C38	-2.48	1.39	1.51
3	E	332	6PL	C39-C38	-2.48	1.39	1.51
3	A	571	6PL	C39-C38	-2.48	1.39	1.51
3	E	358	6PL	C41-C40	-2.48	1.39	1.51
3	A	514	6PL	C41-C40	-2.48	1.39	1.51
3	A	527	6PL	C39-C38	-2.48	1.39	1.51
3	A	570	6PL	C39-C38	-2.48	1.39	1.51
3	A	578	6PL	C39-C38	-2.48	1.39	1.51
3	E	321	6PL	C40-C39	-2.48	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	340	6PL	C40-C39	-2.48	1.39	1.51
3	A	501	6PL	C41-C40	-2.48	1.39	1.51
3	E	332	6PL	C40-C39	-2.48	1.39	1.51
3	A	515	6PL	C41-C40	-2.48	1.39	1.51
3	A	573	6PL	C39-C38	-2.48	1.39	1.51
3	E	312	6PL	C41-C40	-2.48	1.39	1.51
3	A	582	6PL	C41-C40	-2.48	1.39	1.51
3	A	524	6PL	C39-C38	-2.48	1.39	1.51
3	A	574	6PL	C39-C38	-2.48	1.39	1.51
3	A	579	6PL	C40-C39	-2.48	1.39	1.51
3	A	581	6PL	C40-C39	-2.48	1.39	1.51
3	E	355	6PL	C40-C39	-2.48	1.39	1.51
3	E	365	6PL	C40-C39	-2.48	1.39	1.51
3	A	533	6PL	C39-C38	-2.48	1.39	1.51
3	A	588	6PL	C39-C38	-2.48	1.39	1.51
3	A	510	6PL	C40-C39	-2.48	1.39	1.51
3	E	302	6PL	C39-C38	-2.48	1.39	1.51
3	E	318	6PL	C41-C40	-2.48	1.39	1.51
3	E	351	6PL	C40-C39	-2.48	1.39	1.51
3	E	356	6PL	C41-C40	-2.48	1.39	1.51
3	E	358	6PL	C39-C38	-2.48	1.39	1.51
3	A	502	6PL	C40-C39	-2.48	1.39	1.51
3	A	506	6PL	C40-C39	-2.48	1.39	1.51
3	E	338	6PL	C40-C39	-2.48	1.39	1.51
3	E	341	6PL	C41-C40	-2.48	1.39	1.51
3	E	315	6PL	C41-C40	-2.48	1.39	1.51
3	A	502	6PL	C41-C40	-2.48	1.39	1.51
3	A	533	6PL	C41-C40	-2.48	1.39	1.51
3	E	313	6PL	C41-C40	-2.48	1.39	1.51
3	C	501	6PL	C39-C38	-2.48	1.39	1.51
3	E	310	6PL	C39-C38	-2.48	1.39	1.51
3	E	335	6PL	C39-C38	-2.48	1.39	1.51
3	A	574	6PL	C40-C39	-2.48	1.39	1.51
3	A	582	6PL	C39-C38	-2.48	1.39	1.51
3	A	571	6PL	C40-C39	-2.48	1.39	1.51
3	E	304	6PL	C40-C39	-2.48	1.39	1.51
3	A	538	6PL	C39-C38	-2.48	1.39	1.51
3	A	538	6PL	C40-C39	-2.48	1.39	1.51
3	A	581	6PL	C39-C38	-2.48	1.39	1.51
3	E	345	6PL	C41-C40	-2.47	1.39	1.51
3	E	364	6PL	C41-C40	-2.47	1.39	1.51
3	A	542	6PL	C41-C40	-2.47	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	557	6PL	C40-C39	-2.47	1.39	1.51
3	E	354	6PL	C40-C39	-2.47	1.39	1.51
3	A	544	6PL	C40-C39	-2.47	1.39	1.51
3	A	551	6PL	C40-C39	-2.47	1.39	1.51
3	A	578	6PL	C41-C40	-2.47	1.39	1.51
3	E	302	6PL	C40-C39	-2.47	1.39	1.51
3	E	316	6PL	C40-C39	-2.47	1.39	1.51
3	A	505	6PL	C40-C39	-2.47	1.39	1.51
3	A	508	6PL	C41-C40	-2.47	1.39	1.51
3	E	307	6PL	C39-C38	-2.47	1.39	1.51
3	E	309	6PL	C41-C40	-2.47	1.39	1.51
3	E	331	6PL	C40-C39	-2.47	1.39	1.51
3	A	583	6PL	C39-C38	-2.47	1.39	1.51
3	A	515	6PL	C40-C39	-2.47	1.39	1.51
3	E	327	6PL	C40-C39	-2.47	1.39	1.51
3	A	572	6PL	C40-C39	-2.47	1.39	1.51
3	E	344	6PL	C39-C38	-2.47	1.39	1.51
3	A	519	6PL	C39-C38	-2.47	1.39	1.51
3	A	579	6PL	C41-C40	-2.47	1.39	1.51
3	A	508	6PL	C40-C39	-2.47	1.39	1.51
3	E	336	6PL	C41-C40	-2.47	1.39	1.51
3	A	508	6PL	C39-C38	-2.47	1.39	1.51
3	E	313	6PL	C39-C38	-2.47	1.39	1.51
3	A	580	6PL	C41-C40	-2.47	1.39	1.51
3	E	345	6PL	C40-C39	-2.47	1.39	1.51
3	A	519	6PL	C40-C39	-2.47	1.39	1.51
3	A	534	6PL	C41-C40	-2.47	1.39	1.51
3	A	568	6PL	C39-C38	-2.47	1.39	1.51
3	A	585	6PL	C39-C38	-2.47	1.39	1.51
3	E	349	6PL	C41-C40	-2.47	1.39	1.51
3	A	557	6PL	C39-C38	-2.47	1.39	1.51
3	E	330	6PL	C40-C39	-2.47	1.39	1.51
3	E	344	6PL	C41-C40	-2.47	1.39	1.51
3	E	354	6PL	C41-C40	-2.47	1.39	1.51
3	A	584	6PL	C40-C39	-2.47	1.39	1.51
3	E	364	6PL	C40-C39	-2.47	1.39	1.51
3	A	551	6PL	C39-C38	-2.47	1.39	1.51
3	E	363	6PL	C39-C38	-2.47	1.39	1.51
3	A	568	6PL	C40-C39	-2.47	1.39	1.51
3	A	571	6PL	C41-C40	-2.47	1.39	1.51
3	A	576	6PL	C41-C40	-2.47	1.39	1.51
3	A	513	6PL	C40-C39	-2.47	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	524	6PL	C41-C40	-2.47	1.39	1.51
3	A	545	6PL	C41-C40	-2.47	1.39	1.51
3	A	555	6PL	C40-C39	-2.47	1.39	1.51
3	E	306	6PL	C39-C38	-2.47	1.39	1.51
3	E	333	6PL	C39-C38	-2.47	1.39	1.51
3	E	353	6PL	C39-C38	-2.47	1.39	1.51
3	A	562	6PL	C40-C39	-2.47	1.39	1.51
3	A	562	6PL	C41-C40	-2.47	1.39	1.51
3	E	329	6PL	C39-C38	-2.47	1.39	1.51
3	A	518	6PL	C39-C38	-2.47	1.39	1.51
3	E	309	6PL	C40-C39	-2.47	1.39	1.51
3	A	510	6PL	C39-C38	-2.47	1.39	1.51
3	E	315	6PL	C39-C38	-2.47	1.39	1.51
3	A	501	6PL	C39-C38	-2.47	1.39	1.51
3	E	327	6PL	C39-C38	-2.47	1.39	1.51
3	E	329	6PL	C41-C40	-2.47	1.39	1.51
3	E	348	6PL	C40-C39	-2.47	1.39	1.51
3	A	522	6PL	C41-C40	-2.47	1.39	1.51
3	A	565	6PL	C39-C38	-2.47	1.39	1.51
3	E	304	6PL	C39-C38	-2.47	1.39	1.51
3	E	314	6PL	C39-C38	-2.47	1.39	1.51
3	E	336	6PL	C39-C38	-2.47	1.39	1.51
3	A	524	6PL	C40-C39	-2.47	1.39	1.51
3	A	544	6PL	C39-C38	-2.47	1.39	1.51
3	C	501	6PL	C41-C40	-2.47	1.39	1.51
3	E	336	6PL	C40-C39	-2.47	1.39	1.51
3	A	501	6PL	C40-C39	-2.47	1.39	1.51
3	A	525	6PL	C41-C40	-2.47	1.39	1.51
3	A	542	6PL	C40-C39	-2.47	1.39	1.51
3	A	502	6PL	C39-C38	-2.47	1.39	1.51
3	E	362	6PL	C41-C40	-2.47	1.39	1.51
3	A	527	6PL	C41-C40	-2.47	1.39	1.51
3	A	536	6PL	C39-C38	-2.47	1.39	1.51
3	A	545	6PL	C40-C39	-2.47	1.39	1.51
3	E	311	6PL	C41-C40	-2.47	1.39	1.51
3	A	563	6PL	C40-C39	-2.47	1.39	1.51
3	A	505	6PL	C41-C40	-2.47	1.39	1.51
3	A	555	6PL	C39-C38	-2.47	1.39	1.51
3	E	338	6PL	C39-C38	-2.47	1.39	1.51
3	A	552	6PL	C40-C39	-2.47	1.39	1.51
3	E	322	6PL	C41-C40	-2.47	1.39	1.51
3	E	344	6PL	C40-C39	-2.47	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	366	6PL	C40-C39	-2.47	1.39	1.51
3	A	511	6PL	C39-C38	-2.47	1.39	1.51
3	A	550	6PL	C41-C40	-2.47	1.39	1.51
3	A	535	6PL	C41-C40	-2.47	1.39	1.51
3	E	319	6PL	C41-C40	-2.47	1.39	1.51
3	A	569	6PL	C39-C38	-2.47	1.39	1.51
3	A	511	6PL	C40-C39	-2.47	1.39	1.51
3	A	562	6PL	C39-C38	-2.47	1.39	1.51
3	A	577	6PL	C40-C39	-2.47	1.39	1.51
3	A	576	6PL	C39-C38	-2.47	1.39	1.51
3	A	569	6PL	C41-C40	-2.47	1.39	1.51
3	A	570	6PL	C41-C40	-2.47	1.39	1.51
3	E	317	6PL	C39-C38	-2.47	1.39	1.51
3	E	364	6PL	C39-C38	-2.47	1.39	1.51
3	A	511	6PL	C41-C40	-2.47	1.39	1.51
3	A	575	6PL	C39-C38	-2.47	1.39	1.51
3	E	361	6PL	C39-C38	-2.47	1.39	1.51
3	E	304	6PL	C41-C40	-2.47	1.39	1.51
3	E	348	6PL	C39-C38	-2.47	1.39	1.51
3	A	574	6PL	C41-C40	-2.47	1.39	1.51
3	A	552	6PL	C41-C40	-2.47	1.39	1.51
3	E	341	6PL	C40-C39	-2.46	1.39	1.51
3	A	567	6PL	C39-C38	-2.46	1.39	1.51
3	A	546	6PL	C40-C39	-2.46	1.39	1.51
3	A	552	6PL	C39-C38	-2.46	1.39	1.51
3	A	579	6PL	C39-C38	-2.46	1.39	1.51
3	E	322	6PL	C40-C39	-2.46	1.39	1.51
3	E	352	6PL	C41-C40	-2.46	1.39	1.51
3	E	369	6PL	C41-C40	-2.46	1.39	1.51
3	E	359	6PL	C41-C40	-2.46	1.39	1.51
3	A	528	6PL	C39-C38	-2.46	1.39	1.51
3	A	541	6PL	C41-C40	-2.46	1.39	1.51
3	E	311	6PL	C40-C39	-2.46	1.39	1.51
3	A	541	6PL	C39-C38	-2.46	1.39	1.51
3	A	526	6PL	C39-C38	-2.46	1.39	1.51
3	A	548	6PL	C41-C40	-2.46	1.39	1.51
3	A	580	6PL	C39-C38	-2.46	1.39	1.51
3	A	533	6PL	C40-C39	-2.46	1.39	1.51
3	A	549	6PL	C41-C40	-2.46	1.39	1.51
3	A	561	6PL	C41-C40	-2.46	1.39	1.51
3	E	357	6PL	C40-C39	-2.46	1.39	1.51
3	A	577	6PL	C41-C40	-2.46	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	317	6PL	C40-C39	-2.46	1.39	1.51
3	A	510	6PL	C41-C40	-2.46	1.39	1.51
3	E	318	6PL	C40-C39	-2.46	1.39	1.51
3	A	517	6PL	C39-C38	-2.46	1.39	1.51
3	A	515	6PL	C39-C38	-2.46	1.39	1.51
3	E	326	6PL	C40-C39	-2.46	1.39	1.51
3	E	351	6PL	C41-C40	-2.46	1.39	1.51
3	A	537	6PL	C39-C38	-2.46	1.39	1.51
3	A	561	6PL	C40-C39	-2.46	1.39	1.51
3	A	567	6PL	C41-C40	-2.46	1.39	1.51
3	E	362	6PL	C40-C39	-2.46	1.39	1.51
3	E	360	6PL	C40-C39	-2.46	1.39	1.51
3	E	359	6PL	C39-C38	-2.46	1.39	1.51
3	A	549	6PL	C39-C38	-2.46	1.39	1.51
3	A	557	6PL	C41-C40	-2.46	1.39	1.51
3	A	586	6PL	C40-C39	-2.46	1.39	1.51
3	E	340	6PL	C39-C38	-2.46	1.39	1.51
3	E	353	6PL	C41-C40	-2.46	1.39	1.51
3	A	577	6PL	C39-C38	-2.46	1.39	1.51
3	E	320	6PL	C39-C38	-2.46	1.39	1.51
3	E	353	6PL	C40-C39	-2.46	1.39	1.51
3	A	503	6PL	C39-C38	-2.46	1.39	1.51
3	E	323	6PL	C40-C39	-2.46	1.39	1.51
3	A	514	6PL	C40-C39	-2.45	1.39	1.51
3	A	587	6PL	C40-C39	-2.45	1.39	1.51
3	A	554	6PL	C40-C39	-2.45	1.39	1.51
3	E	350	6PL	C40-C39	-2.45	1.39	1.51
3	E	362	6PL	C39-C38	-2.45	1.39	1.51
3	A	542	6PL	C39-C38	-2.45	1.39	1.51
3	E	314	6PL	C40-C39	-2.45	1.39	1.51
3	E	306	6PL	C41-C40	-2.45	1.39	1.51
3	E	303	6PL	C40-C39	-2.45	1.39	1.51
3	A	507	6PL	C41-C40	-2.45	1.39	1.51
3	A	564	6PL	C39-C38	-2.44	1.39	1.51
3	A	564	6PL	C41-C40	-2.44	1.39	1.51
3	A	507	6PL	C39-C38	-2.44	1.39	1.51
3	E	346	6PL	C39-C38	-2.44	1.39	1.51
3	E	369	6PL	C39-C38	-2.44	1.39	1.51
3	A	575	6PL	C40-C39	-2.44	1.39	1.51
3	A	553	6PL	C40-C39	-2.43	1.39	1.51
3	A	521	6PL	C40-C39	-2.43	1.39	1.51
3	A	523	6PL	C41-C40	-2.42	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	566	6PL	C40-C39	-2.41	1.39	1.51
3	E	367	6PL	C40-C39	-2.40	1.39	1.51
3	A	523	6PL	C39-C38	-2.39	1.39	1.51

All (909) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	510	6PL	C2-O2-C31	-5.12	105.54	117.80
3	A	569	6PL	C6-N-C8	-4.92	96.05	108.98
3	A	531	6PL	C6-N-C8	-4.92	96.07	108.98
3	A	508	6PL	C6-N-C8	-4.91	96.07	108.98
3	A	579	6PL	C6-N-C8	-4.90	96.10	108.98
3	E	365	6PL	C6-N-C8	-4.90	96.11	108.98
3	A	506	6PL	C6-N-C8	-4.88	96.16	108.98
3	E	306	6PL	C6-N-C8	-4.88	96.16	108.98
3	E	338	6PL	C6-N-C8	-4.87	96.17	108.98
3	E	343	6PL	C6-N-C8	-4.87	96.18	108.98
3	E	341	6PL	C6-N-C8	-4.86	96.21	108.98
3	A	516	6PL	C6-N-C8	-4.86	96.22	108.98
3	E	333	6PL	C6-N-C8	-4.86	96.22	108.98
3	A	525	6PL	C6-N-C8	-4.85	96.23	108.98
3	A	505	6PL	C6-N-C8	-4.84	96.26	108.98
3	E	366	6PL	C6-N-C8	-4.84	96.26	108.98
3	A	581	6PL	C6-N-C8	-4.83	96.29	108.98
3	E	318	6PL	C6-N-C8	-4.83	96.30	108.98
3	E	336	6PL	C6-N-C8	-4.82	96.32	108.98
3	A	550	6PL	C6-N-C8	-4.82	96.32	108.98
3	A	552	6PL	C6-N-C8	-4.82	96.32	108.98
3	A	538	6PL	C6-N-C8	-4.82	96.32	108.98
3	A	504	6PL	C6-N-C8	-4.81	96.33	108.98
3	E	353	6PL	C6-N-C7	-4.81	96.34	108.98
3	E	367	6PL	C6-N-C8	-4.81	96.34	108.98
3	A	563	6PL	C6-N-C8	-4.81	96.35	108.98
3	A	584	6PL	C6-N-C8	-4.80	96.38	108.98
3	A	566	6PL	C6-N-C8	-4.80	96.38	108.98
3	E	303	6PL	C6-N-C8	-4.79	96.39	108.98
3	E	340	6PL	C6-N-C8	-4.79	96.39	108.98
3	A	527	6PL	C6-N-C8	-4.79	96.40	108.98
3	E	305	6PL	C6-N-C8	-4.78	96.41	108.98
3	A	526	6PL	C6-N-C8	-4.78	96.42	108.98
3	A	576	6PL	C6-N-C8	-4.78	96.43	108.98
3	A	574	6PL	C6-N-C8	-4.78	96.43	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	316	6PL	C6-N-C8	-4.78	96.43	108.98
3	A	586	6PL	C6-N-C8	-4.77	96.44	108.98
3	A	509	6PL	C6-N-C8	-4.77	96.45	108.98
3	E	312	6PL	C6-N-C8	-4.76	96.46	108.98
3	A	555	6PL	C6-N-C8	-4.76	96.46	108.98
3	E	356	6PL	C6-N-C8	-4.76	96.48	108.98
3	A	513	6PL	C6-N-C8	-4.75	96.49	108.98
3	E	331	6PL	C6-N-C8	-4.75	96.49	108.98
3	A	517	6PL	C6-N-C8	-4.75	96.50	108.98
3	A	545	6PL	C6-N-C8	-4.75	96.50	108.98
3	E	344	6PL	C6-N-C8	-4.75	96.50	108.98
3	A	554	6PL	C6-N-C8	-4.75	96.50	108.98
3	E	314	6PL	C6-N-C8	-4.75	96.50	108.98
3	A	510	6PL	O2-C31-C32	4.75	121.75	111.48
3	E	324	6PL	C6-N-C8	-4.74	96.53	108.98
3	A	583	6PL	C6-N-C8	-4.73	96.54	108.98
3	A	530	6PL	C6-N-C8	-4.73	96.55	108.98
3	E	319	6PL	C6-N-C8	-4.73	96.56	108.98
3	E	353	6PL	C6-N-C8	-4.73	96.56	108.98
3	E	359	6PL	C6-N-C8	-4.73	96.56	108.98
3	E	349	6PL	C6-N-C8	-4.72	96.57	108.98
3	A	544	6PL	C6-N-C8	-4.72	96.58	108.98
3	E	348	6PL	C6-N-C8	-4.71	96.60	108.98
3	A	537	6PL	C6-N-C8	-4.71	96.61	108.98
3	A	510	6PL	C6-N-C7	-4.70	96.62	108.98
3	E	358	6PL	C6-N-C8	-4.70	96.62	108.98
3	A	510	6PL	C6-N-C8	-4.70	96.63	108.98
3	A	577	6PL	C6-N-C8	-4.69	96.66	108.98
3	A	569	6PL	C6-N-C7	-4.67	96.70	108.98
3	E	321	6PL	C6-N-C8	-4.66	96.73	108.98
3	A	539	6PL	C6-N-C8	-4.66	96.73	108.98
3	E	338	6PL	C6-N-C7	-4.66	96.74	108.98
3	A	521	6PL	C6-N-C8	-4.65	96.75	108.98
3	A	579	6PL	C6-N-C7	-4.63	96.80	108.98
3	A	574	6PL	C6-N-C7	-4.63	96.82	108.98
3	E	341	6PL	C6-N-C7	-4.63	96.82	108.98
3	E	316	6PL	C6-N-C7	-4.62	96.83	108.98
3	E	332	6PL	C6-N-C8	-4.62	96.85	108.98
3	A	531	6PL	C6-N-C7	-4.62	96.85	108.98
3	A	516	6PL	C6-N-C7	-4.61	96.87	108.98
3	E	365	6PL	C6-N-C7	-4.60	96.88	108.98
3	A	525	6PL	C6-N-C7	-4.60	96.88	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	323	6PL	C6-N-C8	-4.60	96.88	108.98
3	E	358	6PL	C6-N-C7	-4.59	96.92	108.98
3	A	514	6PL	C6-N-C7	-4.58	96.95	108.98
3	A	514	6PL	C6-N-C8	-4.58	96.95	108.98
3	A	526	6PL	C6-N-C7	-4.57	96.97	108.98
3	E	344	6PL	C6-N-C7	-4.57	96.98	108.98
3	A	527	6PL	C6-N-C7	-4.57	96.98	108.98
3	A	508	6PL	C6-N-C7	-4.57	96.98	108.98
3	A	552	6PL	C6-N-C7	-4.56	97.00	108.98
3	E	340	6PL	C6-N-C7	-4.55	97.01	108.98
3	E	367	6PL	C6-N-C7	-4.55	97.02	108.98
3	A	506	6PL	C6-N-C7	-4.54	97.04	108.98
3	E	303	6PL	C6-N-C7	-4.54	97.04	108.98
3	A	555	6PL	C6-N-C7	-4.54	97.06	108.98
3	A	576	6PL	C6-N-C7	-4.52	97.09	108.98
3	A	550	6PL	C6-N-C7	-4.52	97.11	108.98
3	A	584	6PL	C6-N-C7	-4.52	97.11	108.98
3	A	520	6PL	C6-N-C7	-4.51	97.12	108.98
3	A	517	6PL	C6-N-C7	-4.51	97.12	108.98
3	E	319	6PL	C6-N-C7	-4.51	97.12	108.98
3	A	544	6PL	C6-N-C7	-4.51	97.13	108.98
3	A	520	6PL	C6-N-C8	-4.51	97.14	108.98
3	E	349	6PL	C6-N-C7	-4.50	97.15	108.98
3	E	318	6PL	C6-N-C7	-4.50	97.15	108.98
3	A	538	6PL	C6-N-C7	-4.50	97.15	108.98
3	A	586	6PL	C6-N-C7	-4.49	97.19	108.98
3	E	324	6PL	C6-N-C7	-4.48	97.20	108.98
3	A	537	6PL	C6-N-C7	-4.48	97.20	108.98
3	E	306	6PL	C6-N-C7	-4.48	97.21	108.98
3	A	505	6PL	C6-N-C7	-4.48	97.22	108.98
3	E	331	6PL	C6-N-C7	-4.48	97.22	108.98
3	E	336	6PL	C6-N-C7	-4.46	97.26	108.98
3	E	366	6PL	C6-N-C7	-4.46	97.26	108.98
3	A	521	6PL	C6-N-C7	-4.46	97.26	108.98
3	E	314	6PL	C6-N-C7	-4.45	97.28	108.98
3	E	312	6PL	C6-N-C7	-4.45	97.28	108.98
3	E	305	6PL	C6-N-C7	-4.44	97.31	108.98
3	A	577	6PL	C6-N-C7	-4.42	97.35	108.98
3	E	359	6PL	C6-N-C7	-4.42	97.36	108.98
3	A	583	6PL	C6-N-C7	-4.42	97.36	108.98
3	E	343	6PL	C6-N-C7	-4.42	97.37	108.98
3	E	356	6PL	C6-N-C7	-4.42	97.38	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	530	6PL	C6-N-C7	-4.41	97.38	108.98
3	A	554	6PL	C6-N-C7	-4.40	97.41	108.98
3	A	563	6PL	C6-N-C7	-4.40	97.42	108.98
3	E	348	6PL	C6-N-C7	-4.40	97.42	108.98
3	A	513	6PL	C6-N-C7	-4.39	97.44	108.98
3	A	545	6PL	C6-N-C7	-4.39	97.44	108.98
3	E	333	6PL	C6-N-C7	-4.38	97.47	108.98
3	A	566	6PL	C6-N-C7	-4.37	97.49	108.98
3	E	323	6PL	C6-N-C7	-4.37	97.49	108.98
3	A	539	6PL	C8-N-C7	4.37	120.45	108.98
3	A	552	6PL	C8-N-C7	4.37	120.45	108.98
3	A	539	6PL	C6-N-C7	-4.36	97.52	108.98
3	A	581	6PL	C6-N-C7	-4.36	97.52	108.98
3	E	344	6PL	C8-N-C7	4.35	120.39	108.98
3	E	332	6PL	C6-N-C7	-4.34	97.58	108.98
3	E	349	6PL	C8-N-C7	4.33	120.35	108.98
3	E	306	6PL	C2-O2-C31	-4.33	107.44	117.80
3	A	510	6PL	C8-N-C7	4.31	120.31	108.98
3	A	577	6PL	C8-N-C7	4.31	120.30	108.98
3	E	358	6PL	C8-N-C7	4.31	120.30	108.98
3	E	321	6PL	C6-N-C7	-4.31	97.66	108.98
3	A	504	6PL	C6-N-C7	-4.30	97.67	108.98
3	A	509	6PL	C6-N-C7	-4.30	97.69	108.98
3	A	526	6PL	C8-N-C7	4.30	120.26	108.98
3	E	303	6PL	C8-N-C7	4.30	120.26	108.98
3	E	336	6PL	C8-N-C7	4.29	120.25	108.98
3	A	517	6PL	C8-N-C7	4.29	120.24	108.98
3	A	586	6PL	C8-N-C7	4.29	120.24	108.98
3	A	521	6PL	C8-N-C7	4.29	120.23	108.98
3	A	537	6PL	C8-N-C7	4.29	120.23	108.98
3	E	340	6PL	C8-N-C7	4.29	120.23	108.98
3	E	312	6PL	C8-N-C7	4.28	120.23	108.98
3	E	319	6PL	C8-N-C7	4.28	120.21	108.98
3	A	544	6PL	C8-N-C7	4.27	120.20	108.98
3	E	318	6PL	C8-N-C7	4.27	120.20	108.98
3	E	353	6PL	C8-N-C7	4.27	120.19	108.98
3	E	325	6PL	O2-C31-C32	4.27	120.71	111.48
3	A	504	6PL	C8-N-C7	4.27	120.18	108.98
3	A	554	6PL	C8-N-C7	4.26	120.18	108.98
3	E	331	6PL	C8-N-C7	4.26	120.18	108.98
3	A	545	6PL	C8-N-C7	4.26	120.17	108.98
3	A	506	6PL	C8-N-C7	4.26	120.16	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	341	6PL	C8-N-C7	4.26	120.16	108.98
3	A	579	6PL	C8-N-C7	4.26	120.16	108.98
3	E	322	6PL	O2-C31-C32	4.26	120.69	111.48
3	E	316	6PL	C8-N-C7	4.25	120.15	108.98
3	E	332	6PL	C8-N-C7	4.25	120.15	108.98
3	E	324	6PL	C8-N-C7	4.25	120.14	108.98
3	A	584	6PL	C8-N-C7	4.25	120.14	108.98
3	A	527	6PL	C8-N-C7	4.25	120.14	108.98
3	E	343	6PL	C8-N-C7	4.25	120.13	108.98
3	E	306	6PL	C8-N-C7	4.25	120.13	108.98
3	E	305	6PL	C8-N-C7	4.25	120.13	108.98
3	E	348	6PL	C8-N-C7	4.25	120.13	108.98
3	A	516	6PL	C8-N-C7	4.24	120.12	108.98
3	E	321	6PL	C8-N-C7	4.24	120.12	108.98
3	E	366	6PL	C8-N-C7	4.24	120.12	108.98
3	A	550	6PL	C8-N-C7	4.24	120.11	108.98
3	A	525	6PL	C8-N-C7	4.23	120.09	108.98
3	A	505	6PL	C8-N-C7	4.23	120.08	108.98
3	A	530	6PL	C8-N-C7	4.23	120.08	108.98
3	A	569	6PL	C8-N-C7	4.23	120.08	108.98
3	A	581	6PL	C8-N-C7	4.23	120.08	108.98
3	E	356	6PL	C8-N-C7	4.22	120.06	108.98
3	E	365	6PL	C8-N-C7	4.22	120.06	108.98
3	E	314	6PL	C8-N-C7	4.22	120.05	108.98
3	E	323	6PL	C8-N-C7	4.21	120.04	108.98
3	A	555	6PL	C8-N-C7	4.21	120.03	108.98
3	E	359	6PL	C8-N-C7	4.21	120.03	108.98
3	A	520	6PL	C8-N-C7	4.20	120.02	108.98
3	A	538	6PL	C8-N-C7	4.20	120.01	108.98
3	E	338	6PL	C8-N-C7	4.20	120.01	108.98
3	A	515	6PL	O2-C31-C32	4.20	120.57	111.48
3	A	513	6PL	C8-N-C7	4.20	120.01	108.98
3	E	363	6PL	O2-C31-C32	4.20	120.56	111.48
3	A	563	6PL	C8-N-C7	4.19	119.99	108.98
3	A	509	6PL	C8-N-C7	4.19	119.98	108.98
3	E	367	6PL	C8-N-C7	4.19	119.98	108.98
3	A	574	6PL	C8-N-C7	4.18	119.96	108.98
3	A	583	6PL	C8-N-C7	4.18	119.96	108.98
3	A	531	6PL	C8-N-C7	4.18	119.94	108.98
3	A	576	6PL	C8-N-C7	4.17	119.94	108.98
3	A	566	6PL	C8-N-C7	4.16	119.90	108.98
3	E	333	6PL	C8-N-C7	4.15	119.88	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	6PL	C8-N-C7	4.15	119.87	108.98
3	A	549	6PL	O2-C31-C32	4.08	120.30	111.48
3	A	575	6PL	O2-C31-C32	4.07	120.30	111.48
3	E	302	6PL	O2-C31-C32	4.07	120.29	111.48
3	A	537	6PL	O2-C31-C32	4.06	120.27	111.48
3	A	514	6PL	C8-N-C7	4.06	119.64	108.98
3	A	534	6PL	O2-C31-C32	4.05	120.25	111.48
3	A	572	6PL	O2-C31-C32	4.05	120.24	111.48
3	E	336	6PL	O2-C31-C32	4.03	120.19	111.48
3	E	322	6PL	C2-O2-C31	-4.01	108.19	117.80
3	A	545	6PL	O2-C31-C32	3.99	120.11	111.48
3	A	534	6PL	C2-O2-C31	-3.97	108.30	117.80
3	E	301	6PL	O2-C31-C32	3.95	120.04	111.48
3	A	574	6PL	O2-C31-C32	3.94	120.00	111.48
3	A	564	6PL	O2-C31-C32	3.91	119.95	111.48
3	E	334	6PL	O2-C31-C32	3.91	119.94	111.48
3	A	560	6PL	O2-C31-C32	3.91	119.93	111.48
3	E	348	6PL	O2-C31-C32	3.91	119.93	111.48
3	A	572	6PL	C2-O2-C31	-3.90	108.45	117.80
3	A	514	6PL	O2-C31-C32	3.90	119.92	111.48
3	A	507	6PL	O2-C31-C32	3.90	119.91	111.48
3	E	331	6PL	O2-C31-C32	3.88	119.88	111.48
3	A	508	6PL	O2-C31-C32	3.87	119.85	111.48
3	A	580	6PL	O2-C31-C32	3.87	119.85	111.48
3	E	347	6PL	O2-C31-C32	3.87	119.84	111.48
3	E	328	6PL	O2-C31-C32	3.86	119.83	111.48
3	E	319	6PL	O2-C31-C32	3.85	119.82	111.48
3	A	561	6PL	O2-C31-C32	3.85	119.80	111.48
3	A	503	6PL	O2-C31-C32	3.84	119.79	111.48
3	A	538	6PL	O2-C31-C32	3.82	119.75	111.48
3	E	317	6PL	O2-C31-C32	3.82	119.74	111.48
3	E	365	6PL	O2-C31-C32	3.81	119.73	111.48
3	E	341	6PL	O2-C31-C32	3.81	119.73	111.48
3	E	359	6PL	O2-C31-C32	3.81	119.73	111.48
3	A	537	6PL	C2-O2-C31	-3.80	108.70	117.80
3	A	546	6PL	O2-C31-C32	3.80	119.70	111.48
3	A	511	6PL	O2-C31-C32	3.79	119.69	111.48
3	A	545	6PL	C2-O2-C31	-3.79	108.72	117.80
3	E	307	6PL	O2-C31-C32	3.78	119.67	111.48
3	A	584	6PL	O2-C31-C32	3.78	119.66	111.48
3	A	582	6PL	O2-C31-C32	3.78	119.65	111.48
3	A	548	6PL	O2-C31-C32	3.77	119.64	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	576	6PL	O2-C31-C32	3.77	119.64	111.48
3	E	339	6PL	O2-C31-C32	3.77	119.63	111.48
3	A	527	6PL	O2-C31-C32	3.77	119.63	111.48
3	E	303	6PL	O2-C31-C32	3.77	119.63	111.48
3	E	321	6PL	O2-C31-C32	3.76	119.62	111.48
3	A	587	6PL	O2-C31-C32	3.76	119.62	111.48
3	A	526	6PL	O2-C31-C32	3.76	119.61	111.48
3	E	343	6PL	O2-C31-C32	3.75	119.59	111.48
3	E	302	6PL	C2-O2-C31	-3.75	108.83	117.80
3	E	330	6PL	O2-C31-C32	3.75	119.58	111.48
3	E	313	6PL	O2-C31-C32	3.74	119.57	111.48
3	C	501	6PL	O2-C31-C32	3.74	119.56	111.48
3	A	539	6PL	O2-C31-C32	3.73	119.55	111.48
3	E	356	6PL	O2-C31-C32	3.73	119.55	111.48
3	A	531	6PL	O2-C31-C32	3.73	119.55	111.48
3	E	342	6PL	O2-C31-C32	3.72	119.54	111.48
3	A	552	6PL	O2-C31-C32	3.72	119.54	111.48
3	E	353	6PL	O2-C31-C32	3.72	119.53	111.48
3	A	521	6PL	O2-C31-C32	3.72	119.53	111.48
3	E	318	6PL	O2-C31-C32	3.72	119.53	111.48
3	A	524	6PL	O2-C31-C32	3.72	119.53	111.48
3	A	533	6PL	O2-C31-C32	3.72	119.53	111.48
3	A	547	6PL	O2-C31-C32	3.72	119.53	111.48
3	E	362	6PL	O2-C31-C32	3.72	119.52	111.48
3	E	316	6PL	O2-C31-C32	3.71	119.51	111.48
3	E	350	6PL	O2-C31-C32	3.71	119.50	111.48
3	E	344	6PL	O2-C31-C32	3.70	119.49	111.48
3	E	354	6PL	O2-C31-C32	3.70	119.48	111.48
3	E	358	6PL	O2-C31-C32	3.70	119.47	111.48
3	A	543	6PL	O2-C31-C32	3.69	119.47	111.48
3	A	502	6PL	O2-C31-C32	3.69	119.47	111.48
3	A	569	6PL	O2-C31-C32	3.69	119.46	111.48
3	E	305	6PL	O2-C31-C32	3.69	119.46	111.48
3	A	530	6PL	O2-C31-C32	3.69	119.45	111.48
3	A	528	6PL	O2-C31-C32	3.67	119.42	111.48
3	E	323	6PL	O2-C31-C32	3.66	119.41	111.48
3	A	525	6PL	O2-C31-C32	3.66	119.41	111.48
3	A	506	6PL	O2-C31-C32	3.65	119.38	111.48
3	E	349	6PL	O2-C31-C32	3.65	119.38	111.48
3	E	369	6PL	C2-O2-C31	-3.65	109.07	117.80
3	A	549	6PL	C2-O2-C31	-3.64	109.09	117.80
3	A	551	6PL	O2-C31-C32	3.64	119.35	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	517	6PL	O2-C31-C32	3.64	119.35	111.48
3	A	511	6PL	C2-O2-C31	-3.64	109.09	117.80
3	E	363	6PL	C2-O2-C31	-3.63	109.11	117.80
3	A	577	6PL	O2-C31-C32	3.63	119.33	111.48
3	E	361	6PL	O2-C31-C32	3.61	119.29	111.48
3	A	581	6PL	O2-C31-C32	3.61	119.28	111.48
3	A	519	6PL	O2-C31-C32	3.61	119.28	111.48
3	A	504	6PL	O2-C31-C32	3.61	119.28	111.48
3	E	326	6PL	O2-C31-C32	3.60	119.28	111.48
3	A	574	6PL	C2-O2-C31	-3.60	109.18	117.80
3	A	536	6PL	O2-C31-C32	3.60	119.26	111.48
3	A	501	6PL	O2-C31-C32	3.59	119.25	111.48
3	A	541	6PL	O2-C31-C32	3.59	119.25	111.48
3	E	314	6PL	O2-C31-C32	3.59	119.25	111.48
3	E	329	6PL	O2-C31-C32	3.58	119.23	111.48
3	E	320	6PL	O2-C31-C32	3.58	119.23	111.48
3	E	365	6PL	C2-O2-C31	-3.58	109.22	117.80
3	E	311	6PL	O2-C31-C32	3.58	119.22	111.48
3	A	568	6PL	O2-C31-C32	3.57	119.20	111.48
3	E	357	6PL	O2-C31-C32	3.57	119.19	111.48
3	E	327	6PL	O2-C31-C32	3.56	119.18	111.48
3	E	369	6PL	O2-C31-C32	3.55	119.17	111.48
3	A	558	6PL	O2-C31-C32	3.55	119.15	111.48
3	E	310	6PL	O2-C31-C32	3.55	119.15	111.48
3	A	557	6PL	O2-C31-C32	3.54	119.13	111.48
3	A	578	6PL	O2-C31-C32	3.54	119.13	111.48
3	E	340	6PL	O2-C31-C32	3.53	119.12	111.48
3	A	554	6PL	O2-C31-C32	3.53	119.12	111.48
3	E	345	6PL	O2-C31-C32	3.53	119.12	111.48
3	A	583	6PL	O2-C31-C32	3.53	119.11	111.48
3	E	338	6PL	O2-C31-C32	3.53	119.11	111.48
3	E	327	6PL	C2-O2-C31	-3.52	109.36	117.80
3	E	311	6PL	C2-O2-C31	-3.51	109.39	117.80
3	E	319	6PL	C2-O2-C31	-3.51	109.40	117.80
3	A	507	6PL	C2-O2-C31	-3.50	109.42	117.80
3	A	516	6PL	O2-C31-C32	3.50	119.04	111.48
3	A	542	6PL	O2-C31-C32	3.50	119.04	111.48
3	E	308	6PL	O2-C31-C32	3.49	119.04	111.48
3	E	337	6PL	O2-C31-C32	3.49	119.04	111.48
3	A	513	6PL	O2-C31-C32	3.48	119.02	111.48
3	A	523	6PL	O2-C31-C32	3.48	119.01	111.48
3	E	332	6PL	O2-C31-C32	3.48	119.01	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	365	6PL	C6-N-C5	-3.47	96.11	109.91
3	E	307	6PL	C2-O2-C31	-3.47	109.49	117.80
3	A	518	6PL	O2-C31-C32	3.45	118.94	111.48
3	E	367	6PL	O2-C31-C32	3.45	118.94	111.48
3	A	562	6PL	O2-C31-C32	3.45	118.94	111.48
3	E	343	6PL	C2-O2-C31	-3.45	109.55	117.80
3	E	352	6PL	O2-C31-C32	3.45	118.94	111.48
3	A	544	6PL	O2-C31-C32	3.45	118.94	111.48
3	A	575	6PL	C2-O2-C31	-3.44	109.56	117.80
3	A	588	6PL	O2-C31-C32	3.44	118.92	111.48
3	A	529	6PL	O2-C31-C32	3.43	118.91	111.48
3	E	331	6PL	C2-O2-C31	-3.43	109.59	117.80
3	E	309	6PL	O2-C31-C32	3.42	118.89	111.48
3	A	508	6PL	C6-N-C5	-3.42	96.30	109.91
3	A	559	6PL	O2-C31-C32	3.42	118.87	111.48
3	A	573	6PL	O2-C31-C32	3.41	118.86	111.48
3	E	324	6PL	O2-C31-C32	3.40	118.84	111.48
3	E	329	6PL	C2-O2-C31	-3.39	109.67	117.80
3	A	520	6PL	O2-C31-C32	3.38	118.79	111.48
3	A	569	6PL	C6-N-C5	-3.38	96.48	109.91
3	A	565	6PL	O2-C31-C32	3.38	118.79	111.48
3	E	333	6PL	O2-C31-C32	3.38	118.78	111.48
3	E	301	6PL	C2-O2-C31	-3.37	109.72	117.80
3	A	535	6PL	O2-C31-C32	3.36	118.74	111.48
3	A	512	6PL	O2-C31-C32	3.35	118.73	111.48
3	A	586	6PL	O2-C31-C32	3.34	118.71	111.48
3	A	509	6PL	O2-C31-C32	3.34	118.70	111.48
3	E	342	6PL	C2-O2-C31	-3.34	109.81	117.80
3	A	588	6PL	C2-O2-C31	-3.33	109.82	117.80
3	A	538	6PL	C2-O2-C31	-3.33	109.83	117.80
3	A	516	6PL	C6-N-C5	-3.33	96.67	109.91
3	A	525	6PL	C2-O2-C31	-3.33	109.83	117.80
3	E	306	6PL	O2-C31-C32	3.33	118.68	111.48
3	E	364	6PL	O2-C31-C32	3.32	118.67	111.48
3	A	579	6PL	O2-C31-C32	3.32	118.67	111.48
3	A	556	6PL	O2-C31-C32	3.32	118.67	111.48
3	E	314	6PL	C6-N-C5	-3.32	96.71	109.91
3	E	312	6PL	O2-C31-C32	3.32	118.65	111.48
3	E	358	6PL	C2-O2-C31	-3.31	109.86	117.80
3	A	580	6PL	C2-O2-C31	-3.31	109.86	117.80
3	A	540	6PL	O2-C31-C32	3.31	118.63	111.48
3	E	368	6PL	O2-C31-C32	3.30	118.63	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	318	6PL	C2-O2-C31	-3.30	109.90	117.80
3	E	335	6PL	O2-C31-C32	3.30	118.61	111.48
3	A	528	6PL	C2-O2-C31	-3.29	109.91	117.80
3	A	571	6PL	O2-C31-C32	3.29	118.60	111.48
3	A	533	6PL	C2-O2-C31	-3.29	109.92	117.80
3	E	334	6PL	C2-O2-C31	-3.29	109.93	117.80
3	A	555	6PL	C6-N-C5	-3.28	96.87	109.91
3	A	526	6PL	C6-N-C5	-3.28	96.87	109.91
3	A	543	6PL	C2-O2-C31	-3.28	109.96	117.80
3	A	514	6PL	C6-N-C5	-3.26	96.94	109.91
3	E	305	6PL	C2-O2-C31	-3.26	109.99	117.80
3	E	316	6PL	C6-N-C5	-3.26	96.95	109.91
3	A	561	6PL	C2-O2-C31	-3.26	110.00	117.80
3	A	526	6PL	C2-O2-C31	-3.26	110.00	117.80
3	A	527	6PL	C6-N-C5	-3.26	96.97	109.91
3	A	584	6PL	C2-O2-C31	-3.25	110.01	117.80
3	E	362	6PL	C2-O2-C31	-3.25	110.01	117.80
3	A	527	6PL	C2-O2-C31	-3.25	110.01	117.80
3	A	504	6PL	C2-O2-C31	-3.25	110.02	117.80
3	E	340	6PL	C6-N-C5	-3.25	96.99	109.91
3	E	341	6PL	C6-N-C5	-3.25	97.00	109.91
3	A	555	6PL	O2-C31-C32	3.25	118.50	111.48
3	A	522	6PL	O2-C31-C32	3.24	118.50	111.48
3	E	366	6PL	C6-N-C5	-3.24	97.02	109.91
3	A	563	6PL	C6-N-C5	-3.24	97.02	109.91
3	E	347	6PL	C2-O2-C31	-3.24	110.05	117.80
3	A	519	6PL	O4P-P-O1P	-3.24	96.10	108.94
3	A	553	6PL	O2-C31-C32	3.24	118.49	111.48
3	E	367	6PL	C6-N-C5	-3.23	97.06	109.91
3	E	338	6PL	C6-N-C5	-3.23	97.07	109.91
3	A	520	6PL	C6-N-C5	-3.23	97.08	109.91
3	E	319	6PL	C6-N-C5	-3.23	97.09	109.91
3	E	333	6PL	C6-N-C5	-3.22	97.10	109.91
3	A	585	6PL	O2-C31-C32	3.22	118.45	111.48
3	E	349	6PL	C6-N-C5	-3.22	97.11	109.91
3	E	323	6PL	C6-N-C5	-3.22	97.12	109.91
3	A	566	6PL	O2-C31-C32	3.22	118.44	111.48
3	E	356	6PL	C6-N-C5	-3.22	97.12	109.91
3	A	538	6PL	C6-N-C5	-3.22	97.12	109.91
3	E	351	6PL	O2-C31-C32	3.21	118.44	111.48
3	A	579	6PL	C6-N-C5	-3.21	97.14	109.91
3	E	318	6PL	C6-N-C5	-3.21	97.15	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	570	6PL	O2-C31-C32	3.21	118.43	111.48
3	A	564	6PL	C2-O2-C31	-3.21	110.12	117.80
3	A	557	6PL	C2-O2-C31	-3.21	110.12	117.80
3	A	581	6PL	C6-N-C5	-3.20	97.17	109.91
3	A	554	6PL	C6-N-C5	-3.20	97.17	109.91
3	A	550	6PL	C6-N-C5	-3.20	97.19	109.91
3	E	346	6PL	O2-C31-C32	3.19	118.38	111.48
3	A	544	6PL	C6-N-C5	-3.18	97.26	109.91
3	A	583	6PL	C6-N-C5	-3.17	97.29	109.91
3	A	584	6PL	C6-N-C5	-3.17	97.30	109.91
3	A	574	6PL	C6-N-C5	-3.17	97.31	109.91
3	A	524	6PL	C2-O2-C31	-3.17	110.21	117.80
3	A	521	6PL	C6-N-C5	-3.17	97.32	109.91
3	A	563	6PL	O2-C31-C32	3.17	118.33	111.48
3	E	355	6PL	O2-C31-C32	3.17	118.33	111.48
3	A	576	6PL	C6-N-C5	-3.16	97.35	109.91
3	A	525	6PL	C6-N-C5	-3.16	97.35	109.91
3	E	306	6PL	C6-N-C5	-3.16	97.37	109.91
3	C	501	6PL	C2-O2-C31	-3.15	110.25	117.80
3	A	531	6PL	C6-N-C5	-3.15	97.39	109.91
3	E	344	6PL	C6-N-C5	-3.15	97.40	109.91
3	E	358	6PL	C6-N-C5	-3.15	97.41	109.91
3	A	586	6PL	C6-N-C5	-3.14	97.42	109.91
3	E	315	6PL	O2-C31-C32	3.14	118.27	111.48
3	A	510	6PL	C6-N-C5	-3.14	97.44	109.91
3	A	566	6PL	C6-N-C5	-3.13	97.47	109.91
3	A	546	6PL	C2-O2-C31	-3.13	110.31	117.80
3	A	547	6PL	C2-O2-C31	-3.13	110.32	117.80
3	E	313	6PL	O4P-P-O1P	-3.12	96.56	108.94
3	E	339	6PL	C2-O2-C31	-3.11	110.36	117.80
3	E	336	6PL	C6-N-C5	-3.10	97.59	109.91
3	A	517	6PL	C2-O2-C31	-3.10	110.39	117.80
3	E	343	6PL	C6-N-C5	-3.10	97.61	109.91
3	E	303	6PL	C2-O2-C31	-3.10	110.39	117.80
3	E	312	6PL	C6-N-C5	-3.09	97.61	109.91
3	A	532	6PL	O2-C31-C32	3.09	118.16	111.48
3	A	567	6PL	O2-C31-C32	3.08	118.15	111.48
3	A	530	6PL	C6-N-C5	-3.08	97.67	109.91
3	A	558	6PL	O3-C11-C12	3.08	121.22	111.83
3	E	321	6PL	C2-O2-C31	-3.08	110.44	117.80
3	A	505	6PL	C6-N-C5	-3.07	97.70	109.91
3	A	570	6PL	O3-C11-C12	3.07	121.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	537	6PL	C6-N-C5	-3.06	97.73	109.91
3	A	513	6PL	C6-N-C5	-3.06	97.74	109.91
3	E	353	6PL	C6-N-C5	-3.06	97.75	109.91
3	A	547	6PL	O4P-P-O1P	-3.05	96.84	108.94
3	E	359	6PL	C2-O2-C31	-3.05	110.51	117.80
3	A	506	6PL	C2-O2-C31	-3.04	110.51	117.80
3	A	585	6PL	C2-O2-C31	-3.04	110.52	117.80
3	A	504	6PL	C6-N-C5	-3.04	97.84	109.91
3	E	350	6PL	O3-C11-C12	3.03	121.08	111.83
3	A	545	6PL	C6-N-C5	-3.03	97.88	109.91
3	A	539	6PL	C6-N-C5	-3.02	97.90	109.91
3	E	316	6PL	C2-O2-C31	-3.02	110.57	117.80
3	E	348	6PL	C2-O2-C31	-3.02	110.58	117.80
3	A	509	6PL	C6-N-C5	-3.01	97.95	109.91
3	A	529	6PL	O3-C11-C12	3.00	121.00	111.83
3	E	331	6PL	C6-N-C5	-3.00	97.97	109.91
3	E	364	6PL	C2-O2-C31	-3.00	110.61	117.80
3	E	304	6PL	O2-C31-C32	3.00	117.96	111.48
3	E	341	6PL	C2-O2-C31	-2.99	110.64	117.80
3	A	515	6PL	C2-O2-C31	-2.99	110.65	117.80
3	A	531	6PL	O3-C11-C12	2.98	120.93	111.83
3	A	529	6PL	O4P-P-O1P	-2.98	97.14	108.94
3	E	310	6PL	O3-C11-C12	2.98	120.91	111.83
3	E	359	6PL	C6-N-C5	-2.98	98.08	109.91
3	E	330	6PL	C2-O2-C31	-2.97	110.69	117.80
3	E	303	6PL	C6-N-C5	-2.97	98.11	109.91
3	E	305	6PL	C6-N-C5	-2.96	98.14	109.91
3	A	552	6PL	C6-N-C5	-2.96	98.16	109.91
3	A	578	6PL	C2-O2-C31	-2.95	110.73	117.80
3	A	506	6PL	C6-N-C5	-2.94	98.21	109.91
3	E	313	6PL	C2-O2-C31	-2.94	110.75	117.80
3	A	530	6PL	C2-O2-C31	-2.93	110.79	117.80
3	E	348	6PL	C6-N-C5	-2.93	98.28	109.91
3	A	577	6PL	C6-N-C5	-2.92	98.29	109.91
3	A	578	6PL	O4P-P-O1P	-2.92	97.36	108.94
3	A	560	6PL	C2-O2-C31	-2.92	110.81	117.80
3	E	352	6PL	C3-O3-C11	-2.92	106.46	117.12
3	E	320	6PL	C2-O2-C31	-2.91	110.83	117.80
3	A	536	6PL	C2-O2-C31	-2.90	110.85	117.80
3	A	576	6PL	C2-O2-C31	-2.90	110.86	117.80
3	E	354	6PL	C2-O2-C31	-2.89	110.87	117.80
3	E	321	6PL	C6-N-C5	-2.89	98.44	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	344	6PL	C2-O2-C31	-2.88	110.89	117.80
3	A	513	6PL	C2-O2-C31	-2.88	110.91	117.80
3	A	517	6PL	C6-N-C5	-2.87	98.50	109.91
3	E	366	6PL	O2-C31-C32	2.87	117.68	111.48
3	A	505	6PL	O2-C31-C32	2.87	117.68	111.48
3	A	550	6PL	O2-C31-C32	2.86	117.66	111.48
3	A	514	6PL	C2-O2-C31	-2.85	110.97	117.80
3	E	352	6PL	O3-C11-C12	2.85	120.52	111.83
3	E	332	6PL	C6-N-C5	-2.84	98.62	109.91
3	E	328	6PL	C2-O2-C31	-2.84	111.00	117.80
3	A	579	6PL	C2-O2-C31	-2.84	111.00	117.80
3	E	309	6PL	C2-O2-C31	-2.83	111.02	117.80
3	E	324	6PL	C6-N-C5	-2.83	98.67	109.91
3	A	502	6PL	O3-C11-C12	2.83	120.45	111.83
3	A	565	6PL	C2-O2-C31	-2.83	111.03	117.80
3	A	502	6PL	C2-O2-C31	-2.82	111.06	117.80
3	A	550	6PL	C1-C2-C3	-2.81	105.24	111.78
3	A	558	6PL	C3-O3-C11	-2.80	106.87	117.12
3	A	568	6PL	C2-O2-C31	-2.80	111.09	117.80
3	E	349	6PL	C2-O2-C31	-2.80	111.10	117.80
3	A	529	6PL	C3-O3-C11	-2.79	106.91	117.12
3	E	336	6PL	O3-C11-C12	2.79	120.34	111.83
3	A	529	6PL	C2-O2-C31	-2.79	111.12	117.80
3	E	356	6PL	C2-O2-C31	-2.78	111.13	117.80
3	A	548	6PL	C2-O2-C31	-2.78	111.14	117.80
3	A	507	6PL	O3-C11-C12	2.78	120.31	111.83
3	A	552	6PL	C2-O2-C31	-2.77	111.16	117.80
3	E	304	6PL	O3-C11-C12	2.77	120.29	111.83
3	E	312	6PL	O3-C11-C12	2.77	120.29	111.83
3	E	308	6PL	O3-C11-C12	2.77	120.27	111.83
3	A	553	6PL	C1-C2-C3	-2.77	105.34	111.78
3	A	586	6PL	O3-C11-C12	2.76	120.26	111.83
3	A	531	6PL	C2-O2-C31	-2.76	111.18	117.80
3	A	563	6PL	C8-N-C5	2.76	120.89	109.91
3	E	335	6PL	O3-C11-C12	2.76	120.25	111.83
3	E	345	6PL	O3-C11-C12	2.76	120.25	111.83
3	A	587	6PL	C2-O2-C31	-2.76	111.20	117.80
3	E	368	6PL	O3-C11-C12	2.74	120.20	111.83
3	A	547	6PL	O2P-P-O1P	2.73	125.16	112.44
3	A	530	6PL	O3-C11-C12	2.73	120.16	111.83
3	A	566	6PL	C8-N-C5	2.73	120.75	109.91
3	E	313	6PL	O3-C11-C12	2.73	120.15	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	578	6PL	O2P-P-O1P	2.73	125.13	112.44
3	A	514	6PL	C8-N-C5	2.73	120.74	109.91
3	E	325	6PL	C2-O2-C31	-2.72	111.28	117.80
3	E	325	6PL	O3-C11-C12	2.71	120.11	111.83
3	A	514	6PL	O3-C11-C12	2.71	120.11	111.83
3	A	529	6PL	O2P-P-O1P	2.71	125.06	112.44
3	E	360	6PL	O2-C31-C32	2.71	117.33	111.48
3	A	583	6PL	C8-N-C5	2.70	120.66	109.91
3	A	508	6PL	C8-N-C5	2.70	120.65	109.91
3	A	566	6PL	O3-C11-C12	2.70	120.07	111.83
3	E	326	6PL	O3-C11-C12	2.70	120.06	111.83
3	E	345	6PL	C2-O2-C31	-2.70	111.34	117.80
3	A	551	6PL	C2-O2-C31	-2.70	111.34	117.80
3	A	568	6PL	O3-C11-C12	2.69	120.05	111.83
3	A	521	6PL	C2-O2-C31	-2.69	111.36	117.80
3	E	315	6PL	O3-C11-C12	2.69	120.03	111.83
3	A	539	6PL	C2-O2-C31	-2.69	111.37	117.80
3	E	357	6PL	O3-C11-C12	2.69	120.03	111.83
3	A	576	6PL	O3-C11-C12	2.69	120.02	111.83
3	E	314	6PL	C8-N-C5	2.68	120.58	109.91
3	E	313	6PL	O2P-P-O1P	2.68	124.93	112.44
3	A	538	6PL	C8-N-C5	2.68	120.56	109.91
3	E	338	6PL	C2-O2-C31	-2.68	111.38	117.80
3	E	356	6PL	C8-N-C5	2.68	120.56	109.91
3	E	357	6PL	C3-O3-C11	-2.68	107.33	117.12
3	A	513	6PL	C8-N-C5	2.67	120.54	109.91
3	E	350	6PL	C3-O3-C11	-2.67	107.34	117.12
3	A	505	6PL	C8-N-C5	2.67	120.53	109.91
3	E	369	6PL	O3-C11-C12	2.67	119.98	111.83
3	E	333	6PL	C8-N-C5	2.67	120.51	109.91
3	A	557	6PL	O3-C11-C12	2.66	119.96	111.83
3	E	355	6PL	O3-C11-C12	2.66	119.95	111.83
3	E	335	6PL	C2-O2-C31	-2.66	111.42	117.80
3	E	366	6PL	C8-N-C5	2.65	120.46	109.91
3	A	506	6PL	C8-N-C5	2.65	120.46	109.91
3	A	520	6PL	C8-N-C5	2.65	120.45	109.91
3	A	519	6PL	O2P-P-O1P	2.65	124.77	112.44
3	A	581	6PL	C2-O2-C31	-2.65	111.46	117.80
3	A	530	6PL	C8-N-C5	2.65	120.43	109.91
3	A	584	6PL	C8-N-C5	2.65	120.43	109.91
3	A	581	6PL	C8-N-C5	2.65	120.42	109.91
3	E	312	6PL	C8-N-C5	2.64	120.42	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	365	6PL	C8-N-C5	2.64	120.41	109.91
3	E	359	6PL	C8-N-C5	2.64	120.41	109.91
3	E	324	6PL	C8-N-C5	2.64	120.40	109.91
3	A	537	6PL	C8-N-C5	2.64	120.40	109.91
3	E	309	6PL	O3-C11-C12	2.64	119.88	111.83
3	A	550	6PL	C8-N-C5	2.64	120.39	109.91
3	E	332	6PL	C8-N-C5	2.64	120.39	109.91
3	A	559	6PL	O3-C11-C12	2.64	119.87	111.83
3	E	323	6PL	C8-N-C5	2.63	120.38	109.91
3	A	504	6PL	C8-N-C5	2.63	120.38	109.91
3	A	544	6PL	C8-N-C5	2.63	120.38	109.91
3	E	336	6PL	C8-N-C5	2.63	120.38	109.91
3	A	519	6PL	O2P-P-O4P	-2.63	95.63	107.57
3	E	326	6PL	C2-O2-C31	-2.63	111.50	117.80
3	A	516	6PL	O3-C11-C12	2.63	119.84	111.83
3	A	584	6PL	O3-C11-C12	2.63	119.84	111.83
3	A	546	6PL	O3-C11-C12	2.63	119.84	111.83
3	A	554	6PL	C2-O2-C31	-2.62	111.52	117.80
3	A	542	6PL	O3-C11-C12	2.62	119.83	111.83
3	A	573	6PL	O3-C11-C12	2.62	119.83	111.83
3	A	527	6PL	C8-N-C5	2.62	120.33	109.91
3	E	353	6PL	C8-N-C5	2.62	120.33	109.91
3	A	509	6PL	C8-N-C5	2.62	120.32	109.91
3	A	585	6PL	O3-C11-C12	2.62	119.82	111.83
3	E	312	6PL	C3-O3-C11	-2.62	107.55	117.12
3	A	526	6PL	C8-N-C5	2.62	120.32	109.91
3	A	573	6PL	C2-O2-C31	-2.61	111.54	117.80
3	E	318	6PL	C8-N-C5	2.61	120.29	109.91
3	E	344	6PL	C8-N-C5	2.61	120.29	109.91
3	A	509	6PL	C2-O2-C31	-2.61	111.56	117.80
3	E	310	6PL	C3-O3-C11	-2.61	107.59	117.12
3	A	531	6PL	C3-O3-C11	-2.61	107.59	117.12
3	E	314	6PL	C2-O2-C31	-2.60	111.57	117.80
3	E	332	6PL	O3-C11-C12	2.60	119.77	111.83
3	A	517	6PL	C8-N-C5	2.60	120.25	109.91
3	E	319	6PL	C8-N-C5	2.60	120.24	109.91
3	E	340	6PL	C8-N-C5	2.59	120.22	109.91
3	E	321	6PL	C8-N-C5	2.59	120.21	109.91
3	E	308	6PL	C2-O2-C31	-2.59	111.60	117.80
3	A	554	6PL	C8-N-C5	2.59	120.21	109.91
3	E	358	6PL	C8-N-C5	2.59	120.19	109.91
3	A	555	6PL	C8-N-C5	2.59	120.19	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	333	6PL	C2-O2-C31	-2.58	111.61	117.80
3	E	316	6PL	C8-N-C5	2.58	120.18	109.91
3	E	331	6PL	C8-N-C5	2.58	120.17	109.91
3	A	569	6PL	O3-C11-C12	2.58	119.70	111.83
3	A	580	6PL	O3-C11-C12	2.58	119.69	111.83
3	A	521	6PL	C8-N-C5	2.58	120.15	109.91
3	E	305	6PL	C8-N-C5	2.57	120.14	109.91
3	E	348	6PL	C8-N-C5	2.57	120.11	109.91
3	A	569	6PL	C8-N-C5	2.57	120.11	109.91
3	A	510	6PL	O3-C11-C12	2.57	119.66	111.83
3	E	304	6PL	C3-O3-C11	-2.57	107.74	117.12
3	A	545	6PL	C8-N-C5	2.56	120.10	109.91
3	A	586	6PL	C2-O2-C31	-2.56	111.66	117.80
3	E	337	6PL	O3-C11-C12	2.56	119.65	111.83
3	A	504	6PL	C1-C2-C3	-2.56	105.81	111.78
3	E	317	6PL	O3-C11-C12	2.56	119.64	111.83
3	A	567	6PL	O3-C11-C12	2.56	119.64	111.83
3	E	353	6PL	C2-O2-C31	-2.56	111.67	117.80
3	A	549	6PL	O3-C11-C12	2.56	119.63	111.83
3	A	588	6PL	O3-C11-C12	2.56	119.63	111.83
3	A	551	6PL	O3-C11-C12	2.55	119.62	111.83
3	A	531	6PL	C8-N-C5	2.55	120.06	109.91
3	E	302	6PL	O3-C11-C12	2.55	119.62	111.83
3	A	532	6PL	C2-O2-C31	-2.55	111.69	117.80
3	A	519	6PL	O3-C11-C12	2.55	119.61	111.83
3	E	330	6PL	O3-C11-C12	2.55	119.61	111.83
3	A	523	6PL	C1-C2-C3	-2.55	105.84	111.78
3	A	587	6PL	O3-C11-C12	2.55	119.60	111.83
3	A	576	6PL	C8-N-C5	2.55	120.03	109.91
3	A	541	6PL	O3-C11-C12	2.54	119.59	111.83
3	A	539	6PL	C8-N-C5	2.54	120.01	109.91
3	E	303	6PL	C8-N-C5	2.54	120.01	109.91
3	A	547	6PL	O3-C11-C12	2.54	119.58	111.83
3	A	574	6PL	C8-N-C5	2.54	120.00	109.91
3	E	349	6PL	C8-N-C5	2.54	120.00	109.91
3	A	586	6PL	C8-N-C5	2.54	120.00	109.91
3	E	367	6PL	C8-N-C5	2.54	119.99	109.91
3	A	536	6PL	O3-C11-C12	2.53	119.56	111.83
3	E	363	6PL	O3-C11-C12	2.53	119.56	111.83
3	A	577	6PL	O3-C11-C12	2.53	119.55	111.83
3	A	510	6PL	C8-N-C5	2.53	119.97	109.91
3	A	552	6PL	C8-N-C5	2.53	119.96	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	341	6PL	C8-N-C5	2.53	119.96	109.91
3	A	544	6PL	O3-C11-C12	2.53	119.53	111.83
3	A	533	6PL	O3-C11-C12	2.52	119.53	111.83
3	E	338	6PL	C8-N-C5	2.52	119.94	109.91
3	E	348	6PL	O3-C11-C12	2.52	119.51	111.83
3	E	307	6PL	O3-C11-C12	2.52	119.51	111.83
3	A	579	6PL	C8-N-C5	2.51	119.90	109.91
3	A	512	6PL	C2-O2-C31	-2.51	111.78	117.80
3	A	516	6PL	C8-N-C5	2.51	119.89	109.91
3	A	525	6PL	C8-N-C5	2.51	119.89	109.91
3	A	515	6PL	O3-C11-C12	2.51	119.48	111.83
3	E	365	6PL	C1-C2-C3	-2.51	105.94	111.78
3	E	306	6PL	C8-N-C5	2.50	119.86	109.91
3	A	512	6PL	O3-C11-C12	2.50	119.46	111.83
3	E	354	6PL	O3-C11-C12	2.50	119.46	111.83
3	A	556	6PL	O3-C11-C12	2.50	119.46	111.83
3	A	581	6PL	O3-C11-C12	2.50	119.45	111.83
3	C	501	6PL	O3-C11-C12	2.50	119.45	111.83
3	E	358	6PL	O3-C11-C12	2.50	119.45	111.83
3	A	570	6PL	C3-O3-C11	-2.50	107.99	117.12
3	A	583	6PL	C2-O2-C31	-2.50	111.82	117.80
3	A	522	6PL	O3-C3-C2	2.50	115.59	108.40
3	A	521	6PL	O3-C11-C12	2.50	119.45	111.83
3	A	518	6PL	C2-O2-C31	-2.49	111.83	117.80
3	A	553	6PL	C2-O2-C31	-2.49	111.83	117.80
3	E	353	6PL	O3-C11-C12	2.49	119.43	111.83
3	E	332	6PL	C3-O3-C11	-2.49	108.02	117.12
3	A	567	6PL	C3-O3-C11	-2.49	108.02	117.12
3	E	343	6PL	C8-N-C5	2.49	119.80	109.91
3	E	339	6PL	O3-C11-C12	2.49	119.42	111.83
3	E	330	6PL	C1-C2-C3	-2.49	105.99	111.78
3	E	331	6PL	O3-C11-C12	2.49	119.41	111.83
3	A	544	6PL	C2-O2-C31	-2.48	111.86	117.80
3	A	517	6PL	O3-C11-C12	2.48	119.40	111.83
3	A	577	6PL	C8-N-C5	2.48	119.75	109.91
3	E	316	6PL	O3-C11-C12	2.47	119.38	111.83
3	A	535	6PL	O3-C11-C12	2.47	119.38	111.83
3	A	525	6PL	O3-C11-C12	2.47	119.38	111.83
3	A	509	6PL	O3-C11-C12	2.47	119.37	111.83
3	E	318	6PL	O3-C11-C12	2.47	119.36	111.83
3	A	534	6PL	O3-C11-C12	2.47	119.36	111.83
3	A	569	6PL	C2-O2-C31	-2.47	111.89	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	538	6PL	O3-C11-C12	2.47	119.35	111.83
3	A	558	6PL	C2-O2-C31	-2.46	111.90	117.80
3	A	511	6PL	O3-C11-C12	2.46	119.34	111.83
3	E	367	6PL	C2-O2-C31	-2.46	111.91	117.80
3	E	334	6PL	O3-C11-C12	2.46	119.33	111.83
3	A	541	6PL	C3-O3-C11	-2.46	108.14	117.12
3	E	319	6PL	O3-C11-C12	2.45	119.31	111.83
3	E	350	6PL	C1-C2-C3	-2.45	106.07	111.78
3	E	328	6PL	O3-C11-C12	2.45	119.30	111.83
3	A	528	6PL	O3-C11-C12	2.45	119.30	111.83
3	E	352	6PL	C2-O2-C31	-2.44	111.95	117.80
3	E	336	6PL	C2-O2-C31	-2.44	111.95	117.80
3	A	579	6PL	O3-C11-C12	2.44	119.27	111.83
3	A	521	6PL	C1-C2-C3	-2.44	106.10	111.78
3	E	368	6PL	C2-O2-C31	-2.44	111.96	117.80
3	E	313	6PL	O2P-P-O3P	2.44	118.62	107.57
3	E	313	6PL	O2P-P-O4P	-2.44	96.52	107.57
3	E	340	6PL	C2-O2-C31	-2.44	111.97	117.80
3	A	542	6PL	C2-O2-C31	-2.44	111.97	117.80
3	A	523	6PL	O3-C11-C12	2.43	119.25	111.83
3	E	355	6PL	C3-O3-C11	-2.43	108.23	117.12
3	A	529	6PL	O2P-P-O4P	-2.43	96.55	107.57
3	E	323	6PL	C2-O2-C31	-2.43	111.99	117.80
3	A	513	6PL	O3-C11-C12	2.43	119.23	111.83
3	A	562	6PL	O3-C11-C12	2.42	119.23	111.83
3	A	562	6PL	C2-O2-C31	-2.42	112.00	117.80
3	A	554	6PL	O3-C11-C12	2.42	119.22	111.83
3	E	323	6PL	C1-C2-C3	-2.42	106.15	111.78
3	E	301	6PL	O3-C11-C12	2.41	119.20	111.83
3	E	337	6PL	C2-O2-C31	-2.41	112.02	117.80
3	A	506	6PL	O3-C11-C12	2.41	119.19	111.83
3	E	347	6PL	O3-C11-C12	2.41	119.18	111.83
3	E	356	6PL	O3-C11-C12	2.41	119.18	111.83
3	A	502	6PL	C3-O3-C11	-2.41	108.31	117.12
3	E	321	6PL	O3-C11-C12	2.41	119.17	111.83
3	E	322	6PL	O3-C11-C12	2.40	119.15	111.83
3	E	361	6PL	C1-C2-C3	-2.40	106.20	111.78
3	E	367	6PL	O3-C11-C12	2.39	119.12	111.83
3	E	305	6PL	O3-C11-C12	2.39	119.11	111.83
3	E	317	6PL	C2-O2-C31	-2.38	112.09	117.80
3	E	362	6PL	O3-C11-C12	2.38	119.10	111.83
3	A	578	6PL	O3-C11-C12	2.38	119.09	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	303	6PL	O3-C11-C12	2.38	119.08	111.83
3	E	324	6PL	O3-C11-C12	2.37	119.07	111.83
3	E	364	6PL	O3-C11-C12	2.37	119.07	111.83
3	A	547	6PL	O2P-P-O4P	-2.37	96.81	107.57
3	E	306	6PL	O3-C11-C12	2.37	119.06	111.83
3	A	527	6PL	O3-C11-C12	2.37	119.06	111.83
3	E	314	6PL	O3-C11-C12	2.37	119.05	111.83
3	E	361	6PL	C2-O2-C31	-2.37	112.14	117.80
3	A	508	6PL	O3-C11-C12	2.37	119.05	111.83
3	A	522	6PL	O3-C11-C12	2.37	119.05	111.83
3	E	349	6PL	O3-C11-C12	2.36	119.04	111.83
3	A	581	6PL	C3-O3-C11	-2.36	108.48	117.12
3	A	545	6PL	O3-C11-C12	2.36	119.04	111.83
3	A	529	6PL	O2P-P-O3P	2.36	118.25	107.57
3	A	520	6PL	C2-O2-C31	-2.36	112.16	117.80
3	A	541	6PL	C2-O2-C31	-2.36	112.16	117.80
3	E	311	6PL	O3-C11-C12	2.35	119.01	111.83
3	A	583	6PL	O3-C11-C12	2.35	119.01	111.83
3	E	338	6PL	O3-C11-C12	2.35	119.00	111.83
3	A	510	6PL	C3-O3-C11	-2.35	108.53	117.12
3	A	503	6PL	C2-O2-C31	-2.34	112.20	117.80
3	A	553	6PL	O3-C11-C12	2.34	118.96	111.83
3	E	350	6PL	C2-O2-C31	-2.34	112.20	117.80
3	A	586	6PL	C3-O3-C11	-2.34	108.58	117.12
3	E	337	6PL	C3-O3-C11	-2.33	108.59	117.12
3	E	340	6PL	O3-C11-C12	2.33	118.95	111.83
3	E	345	6PL	C3-O3-C11	-2.33	108.61	117.12
3	E	358	6PL	C3-O3-C11	-2.31	108.66	117.12
3	E	368	6PL	C3-O3-C11	-2.31	108.66	117.12
3	A	520	6PL	O3-C11-C12	2.31	118.89	111.83
3	A	548	6PL	O3-C11-C12	2.31	118.88	111.83
3	E	366	6PL	O3-C11-C12	2.31	118.88	111.83
3	A	567	6PL	C1-C2-C3	-2.31	106.40	111.78
3	A	530	6PL	C3-O3-C11	-2.31	108.69	117.12
3	A	571	6PL	O3-C11-C12	2.31	118.86	111.83
3	A	563	6PL	O3-C11-C12	2.30	118.86	111.83
3	A	578	6PL	C1-C2-C3	-2.30	106.43	111.78
3	A	558	6PL	O3-C3-C2	2.30	115.01	108.40
3	E	360	6PL	C2-O2-C31	-2.29	112.31	117.80
3	E	336	6PL	C3-O3-C11	-2.29	108.76	117.12
3	A	552	6PL	O3-C11-C12	2.28	118.80	111.83
3	A	547	6PL	O2P-P-O3P	2.28	117.92	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	333	6PL	O3-C11-C12	2.28	118.79	111.83
3	A	537	6PL	O3-C11-C12	2.28	118.78	111.83
3	E	325	6PL	C3-O3-C11	-2.28	108.80	117.12
3	A	561	6PL	O3-C11-C12	2.28	118.77	111.83
3	A	577	6PL	C2-O2-C31	-2.27	112.35	117.80
3	A	578	6PL	O2P-P-O4P	-2.27	97.27	107.57
3	A	501	6PL	O3-C11-C12	2.27	118.76	111.83
3	A	574	6PL	O3-C11-C12	2.27	118.76	111.83
3	A	562	6PL	C3-O3-C11	-2.27	108.82	117.12
3	A	535	6PL	C2-O2-C31	-2.27	112.36	117.80
3	A	547	6PL	C3-O3-C11	-2.27	108.83	117.12
3	A	582	6PL	O3-C11-C12	2.27	118.74	111.83
3	E	323	6PL	O3-C11-C12	2.26	118.73	111.83
3	A	553	6PL	O3-C3-C2	2.26	114.92	108.40
3	E	344	6PL	O3-C11-C12	2.26	118.73	111.83
3	A	543	6PL	O3-C11-C12	2.26	118.73	111.83
3	E	356	6PL	C3-O3-C11	-2.26	108.87	117.12
3	A	582	6PL	C2-O2-C31	-2.26	112.40	117.80
3	A	539	6PL	C4-C5-N	-2.26	108.58	115.82
3	A	575	6PL	O3-C11-C12	2.25	118.70	111.83
3	A	559	6PL	C2-O2-C31	-2.25	112.41	117.80
3	A	560	6PL	O3-C11-C12	2.25	118.69	111.83
3	A	566	6PL	C3-O3-C11	-2.25	108.90	117.12
3	A	555	6PL	O3-C11-C12	2.24	118.68	111.83
3	E	360	6PL	O3-C11-C12	2.24	118.66	111.83
3	A	522	6PL	C2-O2-C31	-2.24	112.44	117.80
3	E	343	6PL	O3-C11-C12	2.23	118.64	111.83
3	A	578	6PL	O2P-P-O3P	2.23	117.67	107.57
3	A	572	6PL	O3-C11-C12	2.22	118.62	111.83
3	E	329	6PL	O3-C11-C12	2.22	118.62	111.83
3	A	510	6PL	O2-C31-O31	-2.22	118.52	123.70
3	E	346	6PL	O3-C11-C12	2.22	118.59	111.83
3	A	521	6PL	C4-C5-N	-2.21	108.72	115.82
3	A	516	6PL	C2-O2-C31	-2.21	112.50	117.80
3	A	541	6PL	C1-C2-C3	-2.21	106.63	111.78
3	A	514	6PL	C3-O3-C11	-2.21	109.05	117.12
3	E	315	6PL	C3-O3-C11	-2.21	109.05	117.12
3	E	349	6PL	C3-O3-C11	-2.20	109.06	117.12
3	E	357	6PL	C2-O2-C31	-2.20	112.52	117.80
3	E	318	6PL	C3-O3-C11	-2.20	109.07	117.12
3	E	341	6PL	O3-C11-C12	2.20	118.55	111.83
3	A	540	6PL	C2-O2-C31	-2.20	112.53	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	524	6PL	O3-C11-C12	2.20	118.54	111.83
3	E	316	6PL	C1-C2-C3	-2.19	106.67	111.78
3	A	557	6PL	C3-O3-C11	-2.19	109.11	117.12
3	A	504	6PL	O3-C11-C12	2.19	118.51	111.83
3	A	508	6PL	C1-C2-C3	-2.19	106.68	111.78
3	E	352	6PL	C1-C2-C3	-2.19	106.69	111.78
3	E	313	6PL	C3-O3-C11	-2.18	109.15	117.12
3	E	364	6PL	O3-C3-C2	2.18	114.68	108.40
3	A	563	6PL	C2-O2-C31	-2.18	112.59	117.80
3	A	558	6PL	C4-C5-N	-2.18	108.84	115.82
3	A	540	6PL	O3-C11-C12	2.17	118.45	111.83
3	E	366	6PL	C1-C2-C3	-2.17	106.73	111.78
3	A	585	6PL	C3-O3-C11	-2.17	109.20	117.12
3	A	565	6PL	O3-C11-C12	2.16	118.44	111.83
3	E	331	6PL	C3-O3-C11	-2.16	109.21	117.12
3	A	568	6PL	C3-O3-C11	-2.16	109.21	117.12
3	E	328	6PL	C4-C5-N	-2.16	108.88	115.82
3	E	302	6PL	C3-O3-C11	-2.15	109.26	117.12
3	A	569	6PL	C3-O3-C11	-2.14	109.28	117.12
3	A	526	6PL	O3-C11-C12	2.14	118.36	111.83
3	A	519	6PL	O3P-P-O1P	2.14	117.41	108.94
3	E	359	6PL	O3-C11-C12	2.13	118.34	111.83
3	E	315	6PL	C2-O2-C31	-2.13	112.69	117.80
3	A	550	6PL	O3-C11-C12	2.13	118.32	111.83
3	A	507	6PL	C3-O3-C11	-2.12	109.37	117.12
3	A	587	6PL	C3-O3-C11	-2.12	109.37	117.12
3	E	323	6PL	C4-C5-N	-2.11	109.04	115.82
3	E	332	6PL	C2-O2-C31	-2.11	112.74	117.80
3	A	583	6PL	C1-C2-C3	-2.11	106.86	111.78
3	A	518	6PL	O3-C11-C12	2.11	118.27	111.83
3	A	582	6PL	C4-C5-N	-2.11	109.06	115.82
3	A	508	6PL	C3-O3-C11	-2.11	109.42	117.12
3	A	567	6PL	C2-O2-C31	-2.11	112.75	117.80
3	A	564	6PL	O3-C11-C12	2.11	118.26	111.83
3	A	511	6PL	C3-O3-C11	-2.10	109.45	117.12
3	E	310	6PL	C2-O2-C31	-2.10	112.78	117.80
3	A	555	6PL	C2-O2-C31	-2.10	112.78	117.80
3	E	324	6PL	C2-O2-C31	-2.10	112.78	117.80
3	E	353	6PL	C3-O3-C11	-2.10	109.45	117.12
3	A	544	6PL	C4-C5-N	-2.10	109.09	115.82
3	A	539	6PL	O3-C11-C12	2.09	118.21	111.83
3	E	306	6PL	C3-O3-C11	-2.09	109.48	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	358	6PL	C4-C5-N	-2.09	109.12	115.82
3	A	585	6PL	C1-C2-C3	-2.09	106.92	111.78
3	A	535	6PL	C3-O3-C11	-2.08	109.50	117.12
3	A	529	6PL	O3-C3-C2	2.08	114.40	108.40
3	A	570	6PL	C2-O2-C31	-2.08	112.82	117.80
3	A	571	6PL	C3-O3-C11	-2.08	109.53	117.12
3	A	528	6PL	C3-O3-C11	-2.08	109.53	117.12
3	A	556	6PL	C2-O2-C31	-2.07	112.83	117.80
3	A	526	6PL	C4-C5-N	-2.07	109.17	115.82
3	A	576	6PL	C3-O3-C11	-2.07	109.54	117.12
3	E	361	6PL	O3-C11-C12	2.06	118.13	111.83
3	E	355	6PL	C4-C5-N	-2.06	109.21	115.82
3	A	524	6PL	C1-C2-C3	-2.06	106.98	111.78
3	A	522	6PL	C3-O3-C11	-2.06	109.60	117.12
3	E	319	6PL	C4-C5-N	-2.06	109.22	115.82
3	E	327	6PL	O3-C11-C12	2.06	118.10	111.83
3	E	366	6PL	C4-C5-N	-2.05	109.23	115.82
3	A	577	6PL	C3-O3-C11	-2.05	109.61	117.12
3	A	501	6PL	C2-O2-C31	-2.05	112.88	117.80
3	E	348	6PL	C3-O3-C11	-2.05	109.62	117.12
3	A	588	6PL	O3-C3-C2	2.05	114.31	108.40
3	E	320	6PL	O3-C11-C12	2.05	118.08	111.83
3	E	337	6PL	O2-C2-C3	2.04	115.65	108.34
3	A	538	6PL	C3-O3-C11	-2.03	109.69	117.12
3	A	573	6PL	C3-O3-C11	-2.02	109.73	117.12
3	E	349	6PL	C4-C5-N	-2.02	109.34	115.82
3	E	363	6PL	C3-O3-C11	-2.02	109.73	117.12
3	E	326	6PL	C3-O3-C11	-2.02	109.75	117.12
3	A	580	6PL	C3-O3-C11	-2.02	109.75	117.12
3	A	554	6PL	C3-O3-C11	-2.01	109.77	117.12
3	A	505	6PL	O3-C11-C12	2.01	117.96	111.83
3	A	554	6PL	C4-C5-N	-2.01	109.38	115.82
3	E	361	6PL	O3-C3-C2	2.01	114.18	108.40
3	E	356	6PL	C4-C5-N	-2.00	109.39	115.82

There are no chirality outliers.

All (1232) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	302	6PL	C1-O3P-P-O1P
3	E	302	6PL	C1-O3P-P-O2P
3	E	302	6PL	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
3	E	302	6PL	C5-C4-O4P-P
3	E	303	6PL	C1-O3P-P-O1P
3	E	304	6PL	C2-C1-O3P-P
3	E	304	6PL	C1-O3P-P-O1P
3	E	304	6PL	C1-O3P-P-O4P
3	E	305	6PL	C4-O4P-P-O3P
3	E	305	6PL	C4-O4P-P-O1P
3	E	305	6PL	C4-O4P-P-O2P
3	E	306	6PL	C2-C1-O3P-P
3	E	307	6PL	C1-O3P-P-O4P
3	E	307	6PL	C4-O4P-P-O3P
3	E	307	6PL	C4-O4P-P-O1P
3	E	307	6PL	C4-O4P-P-O2P
3	E	307	6PL	C5-C4-O4P-P
3	E	310	6PL	C1-O3P-P-O1P
3	E	310	6PL	C4-O4P-P-O3P
3	E	310	6PL	C4-O4P-P-O1P
3	E	311	6PL	C5-C4-O4P-P
3	E	312	6PL	C4-O4P-P-O3P
3	E	312	6PL	C4-O4P-P-O2P
3	E	312	6PL	C5-C4-O4P-P
3	E	313	6PL	C1-O3P-P-O2P
3	E	314	6PL	C1-O3P-P-O2P
3	E	314	6PL	C5-C4-O4P-P
3	E	315	6PL	C2-C1-O3P-P
3	E	315	6PL	C4-O4P-P-O3P
3	E	315	6PL	C4-O4P-P-O1P
3	E	315	6PL	C5-C4-O4P-P
3	E	316	6PL	C1-O3P-P-O1P
3	E	316	6PL	C1-O3P-P-O2P
3	E	316	6PL	C4-O4P-P-O3P
3	E	316	6PL	C4-O4P-P-O1P
3	E	319	6PL	C4-O4P-P-O3P
3	E	319	6PL	C4-O4P-P-O1P
3	E	319	6PL	C4-O4P-P-O2P
3	E	320	6PL	C4-O4P-P-O3P
3	E	320	6PL	C4-O4P-P-O1P
3	E	321	6PL	C2-C1-O3P-P
3	E	321	6PL	C4-O4P-P-O3P
3	E	321	6PL	C4-O4P-P-O1P
3	E	321	6PL	C4-O4P-P-O2P
3	E	322	6PL	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	E	322	6PL	C1-O3P-P-O4P
3	E	323	6PL	C1-O3P-P-O2P
3	E	323	6PL	C1-O3P-P-O4P
3	E	324	6PL	C5-C4-O4P-P
3	E	325	6PL	C4-O4P-P-O3P
3	E	325	6PL	C4-O4P-P-O1P
3	E	325	6PL	C4-O4P-P-O2P
3	E	326	6PL	C1-O3P-P-O1P
3	E	326	6PL	C1-O3P-P-O2P
3	E	326	6PL	C1-O3P-P-O4P
3	E	326	6PL	C4-O4P-P-O3P
3	E	326	6PL	C4-O4P-P-O2P
3	E	327	6PL	C1-O3P-P-O1P
3	E	327	6PL	C1-O3P-P-O4P
3	E	329	6PL	C1-O3P-P-O1P
3	E	329	6PL	C1-O3P-P-O2P
3	E	329	6PL	C1-O3P-P-O4P
3	E	330	6PL	C5-C4-O4P-P
3	E	332	6PL	C4-O4P-P-O2P
3	E	333	6PL	C1-O3P-P-O1P
3	E	333	6PL	C1-O3P-P-O2P
3	E	333	6PL	C1-O3P-P-O4P
3	E	333	6PL	C4-O4P-P-O3P
3	E	333	6PL	C4-O4P-P-O2P
3	E	334	6PL	C1-O3P-P-O2P
3	E	335	6PL	C4-O4P-P-O3P
3	E	335	6PL	C4-O4P-P-O2P
3	E	338	6PL	C5-C4-O4P-P
3	E	340	6PL	C1-O3P-P-O4P
3	E	342	6PL	C1-O3P-P-O4P
3	E	342	6PL	C4-O4P-P-O3P
3	E	342	6PL	C4-O4P-P-O2P
3	E	343	6PL	C4-O4P-P-O1P
3	E	344	6PL	C2-C1-O3P-P
3	E	344	6PL	C1-O3P-P-O4P
3	E	345	6PL	C1-O3P-P-O2P
3	E	345	6PL	C1-O3P-P-O4P
3	E	345	6PL	C4-O4P-P-O1P
3	E	347	6PL	C5-C4-O4P-P
3	E	348	6PL	C2-C1-O3P-P
3	E	348	6PL	C1-O3P-P-O1P
3	E	348	6PL	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
3	E	349	6PL	C1-O3P-P-O4P
3	E	349	6PL	C4-O4P-P-O3P
3	E	349	6PL	C4-O4P-P-O2P
3	E	351	6PL	C1-O3P-P-O1P
3	E	351	6PL	C5-C4-O4P-P
3	E	352	6PL	C2-C1-O3P-P
3	E	352	6PL	C1-O3P-P-O4P
3	E	353	6PL	C2-C1-O3P-P
3	E	353	6PL	C1-O3P-P-O1P
3	E	353	6PL	C1-O3P-P-O4P
3	E	353	6PL	C4-O4P-P-O2P
3	E	355	6PL	C2-C1-O3P-P
3	E	355	6PL	C5-C4-O4P-P
3	E	357	6PL	C2-C1-O3P-P
3	E	360	6PL	C1-O3P-P-O1P
3	E	360	6PL	C4-O4P-P-O3P
3	E	360	6PL	C4-O4P-P-O2P
3	E	361	6PL	C5-C4-O4P-P
3	E	362	6PL	C5-C4-O4P-P
3	E	363	6PL	C2-C1-O3P-P
3	E	363	6PL	C1-O3P-P-O1P
3	E	363	6PL	C5-C4-O4P-P
3	E	364	6PL	C5-C4-O4P-P
3	E	365	6PL	C1-O3P-P-O1P
3	E	365	6PL	C1-O3P-P-O2P
3	E	365	6PL	C1-O3P-P-O4P
3	E	365	6PL	C5-C4-O4P-P
3	E	366	6PL	C1-O3P-P-O4P
3	E	367	6PL	C5-C4-O4P-P
3	E	368	6PL	C2-C1-O3P-P
3	E	368	6PL	C1-O3P-P-O1P
3	E	368	6PL	C1-O3P-P-O4P
3	E	368	6PL	C5-C4-O4P-P
3	E	369	6PL	C2-C1-O3P-P
3	E	369	6PL	C1-O3P-P-O1P
3	E	369	6PL	C1-O3P-P-O4P
3	E	369	6PL	C4-O4P-P-O3P
3	E	369	6PL	C4-O4P-P-O1P
3	E	369	6PL	C5-C4-O4P-P
3	A	502	6PL	C2-C1-O3P-P
3	A	503	6PL	C5-C4-O4P-P
3	A	505	6PL	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	A	505	6PL	C1-O3P-P-O2P
3	A	505	6PL	C1-O3P-P-O4P
3	A	506	6PL	C4-O4P-P-O3P
3	A	506	6PL	C4-O4P-P-O2P
3	A	506	6PL	C5-C4-O4P-P
3	A	507	6PL	C1-O3P-P-O1P
3	A	507	6PL	C1-O3P-P-O4P
3	A	507	6PL	C4-O4P-P-O1P
3	A	510	6PL	C2-C1-O3P-P
3	A	511	6PL	C1-O3P-P-O2P
3	A	511	6PL	C4-O4P-P-O1P
3	A	511	6PL	C5-C4-O4P-P
3	A	512	6PL	C1-O3P-P-O2P
3	A	512	6PL	C5-C4-O4P-P
3	A	513	6PL	C5-C4-O4P-P
3	A	514	6PL	C2-C1-O3P-P
3	A	514	6PL	C1-O3P-P-O1P
3	A	514	6PL	C5-C4-O4P-P
3	A	515	6PL	C1-O3P-P-O1P
3	A	515	6PL	C1-O3P-P-O2P
3	A	515	6PL	C1-O3P-P-O4P
3	A	516	6PL	C5-C4-O4P-P
3	A	517	6PL	C5-C4-O4P-P
3	A	518	6PL	C1-O3P-P-O1P
3	A	518	6PL	C4-O4P-P-O2P
3	A	518	6PL	C5-C4-O4P-P
3	A	519	6PL	C1-O3P-P-O2P
3	A	520	6PL	C1-O3P-P-O1P
3	A	520	6PL	C1-O3P-P-O4P
3	A	520	6PL	C4-O4P-P-O3P
3	A	520	6PL	C4-O4P-P-O2P
3	A	521	6PL	C4-O4P-P-O2P
3	A	522	6PL	C2-C1-O3P-P
3	A	522	6PL	C1-O3P-P-O1P
3	A	522	6PL	C1-O3P-P-O4P
3	A	522	6PL	C4-O4P-P-O2P
3	A	524	6PL	C4-O4P-P-O1P
3	A	524	6PL	C5-C4-O4P-P
3	A	525	6PL	C5-C4-O4P-P
3	A	526	6PL	C1-O3P-P-O1P
3	A	526	6PL	C1-O3P-P-O2P
3	A	526	6PL	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
3	A	527	6PL	C5-C4-O4P-P
3	A	528	6PL	C5-C4-O4P-P
3	A	529	6PL	C1-O3P-P-O2P
3	A	529	6PL	C1-O3P-P-O4P
3	A	531	6PL	C4-O4P-P-O3P
3	A	531	6PL	C4-O4P-P-O1P
3	A	532	6PL	C1-O3P-P-O1P
3	A	532	6PL	C1-O3P-P-O4P
3	A	533	6PL	C4-O4P-P-O2P
3	A	533	6PL	C5-C4-O4P-P
3	A	534	6PL	C2-C1-O3P-P
3	A	535	6PL	C1-O3P-P-O4P
3	A	535	6PL	C5-C4-O4P-P
3	A	536	6PL	C4-O4P-P-O3P
3	A	536	6PL	C4-O4P-P-O2P
3	A	537	6PL	C4-O4P-P-O1P
3	A	539	6PL	C2-C1-O3P-P
3	A	540	6PL	C2-C1-O3P-P
3	A	540	6PL	C4-O4P-P-O3P
3	A	540	6PL	C4-O4P-P-O2P
3	A	540	6PL	C5-C4-O4P-P
3	A	541	6PL	C2-C1-O3P-P
3	A	543	6PL	C2-C1-O3P-P
3	A	543	6PL	C1-O3P-P-O4P
3	A	545	6PL	C2-C1-O3P-P
3	A	546	6PL	C4-O4P-P-O3P
3	A	546	6PL	C5-C4-O4P-P
3	A	547	6PL	C1-O3P-P-O4P
3	A	547	6PL	C4-O4P-P-O3P
3	A	547	6PL	C4-O4P-P-O1P
3	A	548	6PL	C1-O3P-P-O1P
3	A	549	6PL	C1-O3P-P-O1P
3	A	549	6PL	C1-O3P-P-O2P
3	A	549	6PL	C1-O3P-P-O4P
3	A	550	6PL	C4-O4P-P-O3P
3	A	550	6PL	C4-O4P-P-O1P
3	A	550	6PL	C4-O4P-P-O2P
3	A	551	6PL	C4-O4P-P-O3P
3	A	551	6PL	C4-O4P-P-O2P
3	A	551	6PL	C5-C4-O4P-P
3	A	553	6PL	C4-O4P-P-O3P
3	A	553	6PL	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	A	555	6PL	C4-O4P-P-O3P
3	A	555	6PL	C4-O4P-P-O2P
3	A	556	6PL	C5-C4-O4P-P
3	A	557	6PL	C1-O3P-P-O1P
3	A	557	6PL	C1-O3P-P-O2P
3	A	557	6PL	C1-O3P-P-O4P
3	A	558	6PL	C1-O3P-P-O1P
3	A	559	6PL	C2-C1-O3P-P
3	A	559	6PL	C1-O3P-P-O1P
3	A	559	6PL	C1-O3P-P-O2P
3	A	559	6PL	C1-O3P-P-O4P
3	A	559	6PL	C5-C4-O4P-P
3	A	560	6PL	O2-C2-C3-O3
3	A	560	6PL	C1-O3P-P-O1P
3	A	560	6PL	C1-O3P-P-O4P
3	A	560	6PL	C5-C4-O4P-P
3	A	561	6PL	C1-O3P-P-O2P
3	A	562	6PL	C4-O4P-P-O3P
3	A	562	6PL	C4-O4P-P-O1P
3	A	562	6PL	C5-C4-O4P-P
3	A	563	6PL	C4-O4P-P-O3P
3	A	563	6PL	C4-O4P-P-O1P
3	A	564	6PL	C1-O3P-P-O4P
3	A	565	6PL	C4-O4P-P-O3P
3	A	565	6PL	C4-O4P-P-O2P
3	A	566	6PL	C5-C4-O4P-P
3	A	567	6PL	C1-O3P-P-O1P
3	A	567	6PL	C5-C4-O4P-P
3	A	569	6PL	C4-O4P-P-O3P
3	A	570	6PL	C2-C1-O3P-P
3	A	570	6PL	C4-O4P-P-O3P
3	A	570	6PL	C4-O4P-P-O2P
3	A	570	6PL	C5-C4-O4P-P
3	A	571	6PL	C1-O3P-P-O2P
3	A	571	6PL	C5-C4-O4P-P
3	A	572	6PL	C5-C4-O4P-P
3	A	574	6PL	C5-C4-O4P-P
3	A	575	6PL	C1-O3P-P-O4P
3	A	575	6PL	C4-O4P-P-O3P
3	A	575	6PL	C4-O4P-P-O1P
3	A	575	6PL	C4-O4P-P-O2P
3	A	576	6PL	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	A	576	6PL	C5-C4-O4P-P
3	A	577	6PL	C4-O4P-P-O3P
3	A	577	6PL	C4-O4P-P-O1P
3	A	578	6PL	C1-O3P-P-O2P
3	A	578	6PL	C4-O4P-P-O1P
3	A	578	6PL	C4-O4P-P-O2P
3	A	580	6PL	C2-C1-O3P-P
3	A	580	6PL	C4-O4P-P-O3P
3	A	580	6PL	C4-O4P-P-O1P
3	A	580	6PL	C4-O4P-P-O2P
3	A	581	6PL	C1-O3P-P-O2P
3	A	582	6PL	C1-O3P-P-O1P
3	A	582	6PL	C1-O3P-P-O2P
3	A	582	6PL	C1-O3P-P-O4P
3	A	582	6PL	C4-O4P-P-O1P
3	A	584	6PL	C2-C1-O3P-P
3	A	584	6PL	C1-O3P-P-O1P
3	A	584	6PL	C4-O4P-P-O3P
3	A	584	6PL	C4-O4P-P-O1P
3	A	584	6PL	C4-O4P-P-O2P
3	A	586	6PL	C2-C1-O3P-P
3	A	586	6PL	C1-O3P-P-O1P
3	A	586	6PL	C1-O3P-P-O2P
3	A	586	6PL	C1-O3P-P-O4P
3	A	586	6PL	C4-O4P-P-O1P
3	A	587	6PL	C4-O4P-P-O3P
3	A	587	6PL	C4-O4P-P-O2P
3	A	588	6PL	C4-O4P-P-O3P
3	A	588	6PL	C4-O4P-P-O1P
3	A	588	6PL	C4-O4P-P-O2P
3	A	588	6PL	C5-C4-O4P-P
3	C	501	6PL	C2-C1-O3P-P
3	C	501	6PL	C5-C4-O4P-P
3	A	532	6PL	C2-C3-O3-C11
3	E	320	6PL	C2-C3-O3-C11
3	E	307	6PL	C38-C39-C40-C41
3	E	333	6PL	C38-C39-C40-C41
3	E	334	6PL	C38-C39-C40-C41
3	E	344	6PL	C38-C39-C40-C41
3	E	346	6PL	C38-C39-C40-C41
3	E	348	6PL	C38-C39-C40-C41
3	E	352	6PL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
3	E	357	6PL	C38-C39-C40-C41
3	E	362	6PL	C38-C39-C40-C41
3	E	363	6PL	C38-C39-C40-C41
3	E	365	6PL	C38-C39-C40-C41
3	A	504	6PL	C38-C39-C40-C41
3	A	525	6PL	C38-C39-C40-C41
3	A	528	6PL	C38-C39-C40-C41
3	A	533	6PL	C38-C39-C40-C41
3	A	537	6PL	C38-C39-C40-C41
3	A	547	6PL	C38-C39-C40-C41
3	A	552	6PL	C38-C39-C40-C41
3	A	554	6PL	C38-C39-C40-C41
3	A	559	6PL	C38-C39-C40-C41
3	A	564	6PL	C38-C39-C40-C41
3	A	568	6PL	C38-C39-C40-C41
3	A	571	6PL	C38-C39-C40-C41
3	A	572	6PL	C38-C39-C40-C41
3	A	573	6PL	C38-C39-C40-C41
3	A	578	6PL	C38-C39-C40-C41
3	A	581	6PL	C38-C39-C40-C41
3	A	584	6PL	C38-C39-C40-C41
3	A	587	6PL	C38-C39-C40-C41
3	A	555	6PL	C38-C39-C40-C41
3	A	561	6PL	C38-C39-C40-C41
3	A	563	6PL	C38-C39-C40-C41
3	A	576	6PL	C38-C39-C40-C41
3	E	325	6PL	C38-C39-C40-C41
3	E	326	6PL	C38-C39-C40-C41
3	E	331	6PL	C38-C39-C40-C41
3	E	339	6PL	C38-C39-C40-C41
3	E	345	6PL	C38-C39-C40-C41
3	E	367	6PL	C38-C39-C40-C41
3	A	501	6PL	C38-C39-C40-C41
3	A	516	6PL	C38-C39-C40-C41
3	A	519	6PL	C38-C39-C40-C41
3	A	523	6PL	C38-C39-C40-C41
3	A	524	6PL	C38-C39-C40-C41
3	A	557	6PL	C38-C39-C40-C41
3	E	310	6PL	C38-C39-C40-C41
3	E	318	6PL	C38-C39-C40-C41
3	E	319	6PL	C38-C39-C40-C41
3	E	330	6PL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
3	E	342	6PL	C38-C39-C40-C41
3	A	506	6PL	C38-C39-C40-C41
3	A	510	6PL	C38-C39-C40-C41
3	A	562	6PL	C38-C39-C40-C41
3	A	570	6PL	C38-C39-C40-C41
3	E	323	6PL	C38-C39-C40-C41
3	E	328	6PL	C38-C39-C40-C41
3	E	351	6PL	C38-C39-C40-C41
3	E	359	6PL	C38-C39-C40-C41
3	E	360	6PL	C38-C39-C40-C41
3	A	513	6PL	C38-C39-C40-C41
3	A	530	6PL	C38-C39-C40-C41
3	A	535	6PL	C38-C39-C40-C41
3	A	548	6PL	C38-C39-C40-C41
3	A	565	6PL	C38-C39-C40-C41
3	A	566	6PL	C38-C39-C40-C41
3	A	569	6PL	C38-C39-C40-C41
3	A	580	6PL	C38-C39-C40-C41
3	A	586	6PL	C38-C39-C40-C41
3	A	546	6PL	C38-C39-C40-C41
3	A	503	6PL	C2-C3-O3-C11
3	A	513	6PL	C2-C3-O3-C11
3	E	305	6PL	C2-C3-O3-C11
3	E	310	6PL	C2-C1-O3P-P
3	E	316	6PL	C2-C1-O3P-P
3	E	317	6PL	C2-C1-O3P-P
3	A	529	6PL	C2-C1-O3P-P
3	A	581	6PL	C2-C1-O3P-P
3	A	545	6PL	C37-C38-C39-C40
3	A	511	6PL	C37-C38-C39-C40
3	A	506	6PL	C4-C5-N-C8
3	A	510	6PL	C4-C5-N-C7
3	E	336	6PL	C37-C38-C39-C40
3	A	501	6PL	C2-C3-O3-C11
3	E	336	6PL	C39-C40-C41-C42
3	E	314	6PL	C2-C3-O3-C11
3	A	520	6PL	C4-C5-N-C7
3	E	364	6PL	C2-C1-O3P-P
3	A	576	6PL	C2-C1-O3P-P
3	E	330	6PL	C2-C3-O3-C11
3	A	536	6PL	C2-C3-O3-C11
3	A	549	6PL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
3	A	584	6PL	C4-C5-N-C7
3	E	328	6PL	C31-C32-C33-C34
3	A	566	6PL	C2-C1-O3P-P
3	A	566	6PL	C1-C2-O2-C31
3	A	519	6PL	C2-C3-O3-C11
3	E	337	6PL	O2-C2-C3-O3
3	A	516	6PL	C2-C3-O3-C11
3	A	572	6PL	C37-C38-C39-C40
3	E	308	6PL	C37-C38-C39-C40
3	E	327	6PL	C37-C38-C39-C40
3	E	361	6PL	C37-C38-C39-C40
3	A	516	6PL	C37-C38-C39-C40
3	A	518	6PL	C37-C38-C39-C40
3	A	571	6PL	C39-C40-C41-C42
3	A	579	6PL	C37-C38-C39-C40
3	E	318	6PL	C39-C40-C41-C42
3	E	322	6PL	C37-C38-C39-C40
3	E	328	6PL	C37-C38-C39-C40
3	E	352	6PL	C37-C38-C39-C40
3	A	534	6PL	C37-C38-C39-C40
3	A	564	6PL	C39-C40-C41-C42
3	E	357	6PL	C37-C38-C39-C40
3	E	365	6PL	C37-C38-C39-C40
3	A	510	6PL	C37-C38-C39-C40
3	A	559	6PL	C39-C40-C41-C42
3	A	568	6PL	C37-C38-C39-C40
3	E	311	6PL	C39-C40-C41-C42
3	E	339	6PL	C37-C38-C39-C40
3	A	566	6PL	C37-C38-C39-C40
3	A	548	6PL	C37-C38-C39-C40
3	E	333	6PL	C39-C40-C41-C42
3	E	363	6PL	C39-C40-C41-C42
3	A	568	6PL	C39-C40-C41-C42
3	E	342	6PL	C39-C40-C41-C42
3	A	545	6PL	C39-C40-C41-C42
3	E	367	6PL	C37-C38-C39-C40
3	A	587	6PL	C39-C40-C41-C42
3	E	307	6PL	C37-C38-C39-C40
3	E	307	6PL	C39-C40-C41-C42
3	E	350	6PL	C37-C38-C39-C40
3	E	359	6PL	C37-C38-C39-C40
3	A	528	6PL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
3	A	553	6PL	C39-C40-C41-C42
3	A	582	6PL	C37-C38-C39-C40
3	A	583	6PL	C39-C40-C41-C42
3	E	344	6PL	C39-C40-C41-C42
3	A	526	6PL	C37-C38-C39-C40
3	E	317	6PL	C37-C38-C39-C40
3	A	542	6PL	C39-C40-C41-C42
3	A	558	6PL	C39-C40-C41-C42
3	E	367	6PL	C1-C2-C3-O3
3	A	555	6PL	C39-C40-C41-C42
3	A	582	6PL	C39-C40-C41-C42
3	E	352	6PL	C31-C32-C33-C34
3	A	531	6PL	C11-C12-C13-C14
3	E	325	6PL	C39-C40-C41-C42
3	E	341	6PL	C37-C38-C39-C40
3	E	360	6PL	C37-C38-C39-C40
3	A	509	6PL	C39-C40-C41-C42
3	A	513	6PL	C37-C38-C39-C40
3	A	523	6PL	C39-C40-C41-C42
3	A	560	6PL	C39-C40-C41-C42
3	E	328	6PL	C39-C40-C41-C42
3	E	316	6PL	C39-C40-C41-C42
3	E	321	6PL	C37-C38-C39-C40
3	A	540	6PL	C39-C40-C41-C42
3	A	544	6PL	C37-C38-C39-C40
3	A	573	6PL	C39-C40-C41-C42
3	A	576	6PL	C37-C38-C39-C40
3	A	551	6PL	C39-C40-C41-C42
3	A	553	6PL	C2-C1-O3P-P
3	E	318	6PL	C37-C38-C39-C40
3	E	366	6PL	C32-C33-C34-C35
3	A	574	6PL	C37-C38-C39-C40
3	E	312	6PL	C37-C38-C39-C40
3	E	317	6PL	C39-C40-C41-C42
3	A	519	6PL	C39-C40-C41-C42
3	A	539	6PL	C37-C38-C39-C40
3	A	508	6PL	C37-C38-C39-C40
3	E	354	6PL	C37-C38-C39-C40
3	E	369	6PL	C39-C40-C41-C42
3	A	529	6PL	C39-C40-C41-C42
3	A	542	6PL	C37-C38-C39-C40
3	A	572	6PL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
3	E	308	6PL	C39-C40-C41-C42
3	A	518	6PL	C39-C40-C41-C42
3	E	334	6PL	C37-C38-C39-C40
3	E	351	6PL	C37-C38-C39-C40
3	E	365	6PL	C39-C40-C41-C42
3	A	541	6PL	C37-C38-C39-C40
3	E	310	6PL	C37-C38-C39-C40
3	A	579	6PL	C39-C40-C41-C42
3	A	558	6PL	C37-C38-C39-C40
3	E	312	6PL	C39-C40-C41-C42
3	E	319	6PL	C39-C40-C41-C42
3	A	573	6PL	C37-C38-C39-C40
3	A	581	6PL	C37-C38-C39-C40
3	A	554	6PL	C39-C40-C41-C42
3	A	504	6PL	C39-C40-C41-C42
3	E	344	6PL	C2-C3-O3-C11
3	C	501	6PL	C37-C38-C39-C40
3	E	305	6PL	C37-C38-C39-C40
3	A	585	6PL	C39-C40-C41-C42
3	E	337	6PL	C37-C38-C39-C40
3	A	552	6PL	C39-C40-C41-C42
3	E	303	6PL	C39-C40-C41-C42
3	A	538	6PL	C37-C38-C39-C40
3	E	315	6PL	C39-C40-C41-C42
3	A	501	6PL	C39-C40-C41-C42
3	A	570	6PL	C37-C38-C39-C40
3	E	356	6PL	C39-C40-C41-C42
3	A	508	6PL	C39-C40-C41-C42
3	A	511	6PL	C39-C40-C41-C42
3	A	520	6PL	C37-C38-C39-C40
3	A	522	6PL	O2-C2-C3-O3
3	A	543	6PL	C37-C38-C39-C40
3	E	306	6PL	C39-C40-C41-C42
3	E	367	6PL	C35-C36-C37-C38
3	A	575	6PL	C39-C40-C41-C42
3	E	302	6PL	C37-C38-C39-C40
3	E	312	6PL	C2-C1-O3P-P
3	A	560	6PL	C2-C1-O3P-P
3	E	356	6PL	C37-C38-C39-C40
3	A	502	6PL	C37-C38-C39-C40
3	A	535	6PL	C39-C40-C41-C42
3	E	319	6PL	C2-C3-O3-C11

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Mol	Chain	Res	Type	Atoms
3	E	332	6PL	C2-C3-O3-C11
3	E	354	6PL	C2-C3-O3-C11
3	A	517	6PL	C2-C3-O3-C11
3	A	546	6PL	C2-C3-O3-C11
3	A	556	6PL	C2-C3-O3-C11
3	A	588	6PL	C2-C3-O3-C11
3	E	330	6PL	C39-C40-C41-C42
3	E	364	6PL	C39-C40-C41-C42
3	E	314	6PL	C37-C38-C39-C40
3	A	525	6PL	C39-C40-C41-C42
3	A	533	6PL	C37-C38-C39-C40
3	A	551	6PL	C42-C43-C44-C45
3	A	510	6PL	O3P-C1-C2-C3
3	A	529	6PL	O3P-C1-C2-C3
3	E	343	6PL	C37-C38-C39-C40
3	A	565	6PL	C39-C40-C41-C42
3	E	343	6PL	C35-C36-C37-C38
3	A	556	6PL	C37-C38-C39-C40
3	E	313	6PL	C39-C40-C41-C42
3	E	337	6PL	C1-C2-C3-O3
3	A	560	6PL	C1-C2-C3-O3
3	E	326	6PL	C37-C38-C39-C40
3	E	333	6PL	C37-C38-C39-C40
3	A	586	6PL	C37-C38-C39-C40
3	A	520	6PL	C2-C3-O3-C11
3	E	331	6PL	C4-C5-N-C8
3	A	526	6PL	C39-C40-C41-C42
3	E	313	6PL	C37-C38-C39-C40
3	A	587	6PL	C37-C38-C39-C40
3	E	308	6PL	C40-C41-C42-C43
3	A	563	6PL	C37-C38-C39-C40
3	E	323	6PL	C39-C40-C41-C42
3	A	521	6PL	C39-C40-C41-C42
3	A	571	6PL	C3-C2-O2-C31
3	A	586	6PL	C39-C40-C41-C42
3	E	309	6PL	C39-C40-C41-C42
3	A	505	6PL	C39-C40-C41-C42
3	E	301	6PL	C37-C38-C39-C40
3	A	531	6PL	C39-C40-C41-C42
3	E	358	6PL	C37-C38-C39-C40
3	A	559	6PL	O3P-C1-C2-O2
3	A	515	6PL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
3	A	543	6PL	C39-C40-C41-C42
3	A	581	6PL	C39-C40-C41-C42
3	A	572	6PL	C2-C3-O3-C11
3	E	309	6PL	C37-C38-C39-C40
3	A	569	6PL	C39-C40-C41-C42
3	E	363	6PL	C37-C38-C39-C40
3	A	570	6PL	C39-C40-C41-C42
3	A	575	6PL	C37-C38-C39-C40
3	A	576	6PL	C39-C40-C41-C42
3	E	351	6PL	O2-C2-C3-O3
3	E	367	6PL	O2-C2-C3-O3
3	E	321	6PL	C41-C42-C43-C44
3	E	353	6PL	C39-C40-C41-C42
3	A	568	6PL	C13-C14-C15-C16
3	A	506	6PL	O2-C31-C32-C33
3	E	353	6PL	C11-C12-C13-C14
3	A	528	6PL	C33-C34-C35-C36
3	E	367	6PL	C2-C3-O3-C11
3	A	524	6PL	C39-C40-C41-C42
3	E	324	6PL	C39-C40-C41-C42
3	E	345	6PL	C39-C40-C41-C42
3	E	335	6PL	C37-C38-C39-C40
3	E	313	6PL	C2-C1-O3P-P
3	E	322	6PL	C2-C1-O3P-P
3	E	333	6PL	C2-C1-O3P-P
3	E	339	6PL	C2-C1-O3P-P
3	A	509	6PL	C2-C1-O3P-P
3	A	577	6PL	C2-C1-O3P-P
3	A	578	6PL	C2-C1-O3P-P
3	A	588	6PL	C2-C1-O3P-P
3	E	353	6PL	C37-C38-C39-C40
3	E	305	6PL	O2-C31-C32-C33
3	A	522	6PL	O3P-C1-C2-C3
3	A	534	6PL	O3P-C1-C2-C3
3	A	522	6PL	O2-C31-C32-C33
3	E	366	6PL	C34-C35-C36-C37
3	A	538	6PL	C39-C40-C41-C42
3	A	571	6PL	C37-C38-C39-C40
3	E	330	6PL	C37-C38-C39-C40
3	A	534	6PL	C39-C40-C41-C42
3	A	535	6PL	C37-C38-C39-C40
3	A	537	6PL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
3	E	361	6PL	C39-C40-C41-C42
3	E	362	6PL	C37-C38-C39-C40
3	E	306	6PL	C31-C32-C33-C34
3	E	343	6PL	C39-C40-C41-C42
3	E	351	6PL	C1-C2-C3-O3
3	A	522	6PL	C1-C2-C3-O3
3	A	548	6PL	C39-C40-C41-C42
3	E	344	6PL	C37-C38-C39-C40
3	A	506	6PL	C39-C40-C41-C42
3	A	516	6PL	C39-C40-C41-C42
3	A	529	6PL	O3P-C1-C2-O2
3	A	534	6PL	O3P-C1-C2-O2
3	E	360	6PL	C39-C40-C41-C42
3	E	359	6PL	C2-C1-O3P-P
3	E	331	6PL	C37-C38-C39-C40
3	A	555	6PL	C37-C38-C39-C40
3	E	357	6PL	C39-C40-C41-C42
3	A	509	6PL	C33-C34-C35-C36
3	E	335	6PL	O2-C31-C32-C33
3	E	314	6PL	C39-C40-C41-C42
3	A	564	6PL	C37-C38-C39-C40
3	A	563	6PL	C4-C5-N-C8
3	A	510	6PL	C13-C14-C15-C16
3	A	561	6PL	O3-C11-C12-C13
3	A	586	6PL	O3-C11-C12-C13
3	E	349	6PL	C36-C37-C38-C39
3	E	301	6PL	C14-C15-C16-C17
3	A	527	6PL	C39-C40-C41-C42
3	A	509	6PL	O3P-C1-C2-C3
3	E	340	6PL	C2-C1-O3P-P
3	A	504	6PL	C2-C3-O3-C11
3	A	502	6PL	C39-C40-C41-C42
3	E	352	6PL	C39-C40-C41-C42
3	A	557	6PL	C39-C40-C41-C42
3	E	351	6PL	C3-C2-O2-C31
3	E	360	6PL	C1-C2-O2-C31
3	E	361	6PL	C3-C2-O2-C31
3	A	516	6PL	C1-C2-O2-C31
3	A	520	6PL	C3-C2-O2-C31
3	A	548	6PL	C3-C2-O2-C31
3	E	316	6PL	C37-C38-C39-C40
3	A	548	6PL	O3-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	E	329	6PL	C39-C40-C41-C42
3	E	342	6PL	C37-C38-C39-C40
3	A	562	6PL	C37-C38-C39-C40
3	E	301	6PL	C12-C13-C14-C15
3	E	301	6PL	C5-C4-O4P-P
3	E	303	6PL	C5-C4-O4P-P
3	E	305	6PL	C5-C4-O4P-P
3	E	308	6PL	C5-C4-O4P-P
3	E	316	6PL	C5-C4-O4P-P
3	E	317	6PL	C5-C4-O4P-P
3	E	318	6PL	C5-C4-O4P-P
3	E	321	6PL	C5-C4-O4P-P
3	E	322	6PL	C5-C4-O4P-P
3	E	323	6PL	C5-C4-O4P-P
3	E	325	6PL	C5-C4-O4P-P
3	E	329	6PL	C5-C4-O4P-P
3	E	331	6PL	C5-C4-O4P-P
3	E	335	6PL	C5-C4-O4P-P
3	E	339	6PL	C5-C4-O4P-P
3	E	341	6PL	C5-C4-O4P-P
3	E	344	6PL	C5-C4-O4P-P
3	E	348	6PL	C5-C4-O4P-P
3	E	350	6PL	C5-C4-O4P-P
3	E	352	6PL	C5-C4-O4P-P
3	E	353	6PL	C5-C4-O4P-P
3	E	359	6PL	C5-C4-O4P-P
3	E	366	6PL	C5-C4-O4P-P
3	A	501	6PL	C5-C4-O4P-P
3	A	502	6PL	C5-C4-O4P-P
3	A	504	6PL	C5-C4-O4P-P
3	A	507	6PL	C5-C4-O4P-P
3	A	515	6PL	C5-C4-O4P-P
3	A	523	6PL	C5-C4-O4P-P
3	A	526	6PL	C5-C4-O4P-P
3	A	531	6PL	C5-C4-O4P-P
3	A	536	6PL	C5-C4-O4P-P
3	A	539	6PL	C5-C4-O4P-P
3	A	548	6PL	C5-C4-O4P-P
3	A	549	6PL	C5-C4-O4P-P
3	A	550	6PL	C5-C4-O4P-P
3	A	552	6PL	C5-C4-O4P-P
3	A	553	6PL	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
3	A	558	6PL	C5-C4-O4P-P
3	A	561	6PL	C5-C4-O4P-P
3	A	577	6PL	C5-C4-O4P-P
3	A	579	6PL	C5-C4-O4P-P
3	A	580	6PL	C5-C4-O4P-P
3	A	581	6PL	C5-C4-O4P-P
3	A	577	6PL	C2-C3-O3-C11
3	A	565	6PL	C37-C38-C39-C40
3	A	567	6PL	C37-C38-C39-C40
3	A	503	6PL	C37-C38-C39-C40
3	A	562	6PL	C39-C40-C41-C42
3	E	367	6PL	C2-C1-O3P-P
3	E	312	6PL	O4P-C4-C5-N
3	E	349	6PL	O4P-C4-C5-N
3	E	358	6PL	O4P-C4-C5-N
3	A	504	6PL	O4P-C4-C5-N
3	A	559	6PL	O4P-C4-C5-N
3	E	355	6PL	C39-C40-C41-C42
3	A	554	6PL	C37-C38-C39-C40
3	A	584	6PL	C37-C38-C39-C40
3	E	361	6PL	C2-C3-O3-C11
3	A	548	6PL	C2-C3-O3-C11
3	E	303	6PL	C4-C5-N-C8
3	E	321	6PL	C4-C5-N-C8
3	E	348	6PL	C4-C5-N-C8
3	E	359	6PL	C4-C5-N-C8
3	A	537	6PL	C4-C5-N-C7
3	A	549	6PL	C37-C38-C39-C40
3	A	515	6PL	O2-C31-C32-C33
3	A	564	6PL	O3-C11-C12-C13
3	A	512	6PL	C39-C40-C41-C42
3	A	537	6PL	C31-C32-C33-C34
3	A	579	6PL	C35-C36-C37-C38
3	A	541	6PL	O2-C31-C32-C33
3	E	336	6PL	C40-C41-C42-C43
3	E	319	6PL	C37-C38-C39-C40
3	A	504	6PL	C37-C38-C39-C40
3	A	511	6PL	C40-C41-C42-C43
3	E	365	6PL	C31-C32-C33-C34
3	E	324	6PL	C2-C1-O3P-P
3	E	336	6PL	C2-C1-O3P-P
3	E	366	6PL	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
3	A	537	6PL	C2-C1-O3P-P
3	E	337	6PL	O3P-C1-C2-O2
3	A	509	6PL	O3P-C1-C2-O2
3	A	510	6PL	O3P-C1-C2-O2
3	A	522	6PL	O3P-C1-C2-O2
3	A	523	6PL	O3P-C1-C2-O2
3	A	538	6PL	C2-C3-O3-C11
3	E	340	6PL	C39-C40-C41-C42
3	A	505	6PL	C4-C5-N-C7
3	A	517	6PL	C4-C5-N-C8
3	A	530	6PL	C4-C5-N-C7
3	A	545	6PL	C4-C5-N-C7
3	A	550	6PL	C4-C5-N-C8
3	A	552	6PL	C4-C5-N-C8
3	A	577	6PL	C4-C5-N-C8
3	A	522	6PL	C39-C40-C41-C42
3	A	577	6PL	C39-C40-C41-C42
3	A	528	6PL	C34-C35-C36-C37
3	E	364	6PL	C16-C17-C18-C19
3	E	312	6PL	C36-C37-C38-C39
3	A	530	6PL	C37-C38-C39-C40
3	A	547	6PL	C13-C14-C15-C16
3	E	304	6PL	C39-C40-C41-C42
3	E	303	6PL	C1-O3P-P-O4P
3	E	304	6PL	C1-O3P-P-O2P
3	E	305	6PL	C1-O3P-P-O1P
3	E	305	6PL	C4-C5-N-C7
3	E	307	6PL	C1-O3P-P-O1P
3	E	312	6PL	C1-O3P-P-O1P
3	E	312	6PL	C1-O3P-P-O2P
3	E	312	6PL	C1-O3P-P-O4P
3	E	314	6PL	C1-O3P-P-O1P
3	E	314	6PL	C1-O3P-P-O4P
3	E	315	6PL	C4-O4P-P-O2P
3	E	316	6PL	C1-O3P-P-O4P
3	E	320	6PL	C4-O4P-P-O2P
3	E	322	6PL	C1-O3P-P-O2P
3	E	322	6PL	C4-O4P-P-O1P
3	E	324	6PL	C1-O3P-P-O2P
3	E	324	6PL	C1-O3P-P-O4P
3	E	326	6PL	C4-O4P-P-O1P
3	E	333	6PL	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	E	334	6PL	C1-O3P-P-O1P
3	E	334	6PL	C1-O3P-P-O4P
3	E	335	6PL	C1-O3P-P-O1P
3	E	335	6PL	C1-O3P-P-O2P
3	E	335	6PL	C1-O3P-P-O4P
3	E	335	6PL	C4-O4P-P-O1P
3	E	339	6PL	C1-O3P-P-O1P
3	E	340	6PL	C1-O3P-P-O1P
3	E	340	6PL	C1-O3P-P-O2P
3	E	342	6PL	C1-O3P-P-O1P
3	E	342	6PL	C1-O3P-P-O2P
3	E	343	6PL	C4-O4P-P-O3P
3	E	343	6PL	C4-O4P-P-O2P
3	E	344	6PL	C1-O3P-P-O1P
3	E	345	6PL	C1-O3P-P-O1P
3	E	348	6PL	C1-O3P-P-O4P
3	E	348	6PL	C4-O4P-P-O1P
3	E	349	6PL	C1-O3P-P-O1P
3	E	349	6PL	C4-O4P-P-O1P
3	E	350	6PL	C1-O3P-P-O1P
3	E	351	6PL	C1-O3P-P-O4P
3	E	352	6PL	C1-O3P-P-O1P
3	E	353	6PL	C4-O4P-P-O3P
3	E	353	6PL	C4-O4P-P-O1P
3	E	360	6PL	C1-O3P-P-O2P
3	E	360	6PL	C1-O3P-P-O4P
3	E	360	6PL	C4-O4P-P-O1P
3	E	361	6PL	C1-O3P-P-O1P
3	E	364	6PL	C1-O3P-P-O1P
3	E	368	6PL	C1-O3P-P-O2P
3	E	369	6PL	C1-O3P-P-O2P
3	E	369	6PL	C4-O4P-P-O2P
3	A	507	6PL	C4-O4P-P-O3P
3	A	507	6PL	C4-O4P-P-O2P
3	A	508	6PL	C1-O3P-P-O1P
3	A	509	6PL	C1-O3P-P-O1P
3	A	511	6PL	C1-O3P-P-O1P
3	A	511	6PL	C1-O3P-P-O4P
3	A	512	6PL	C1-O3P-P-O1P
3	A	512	6PL	C1-O3P-P-O4P
3	A	514	6PL	C1-O3P-P-O4P
3	A	517	6PL	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	A	517	6PL	C1-O3P-P-O2P
3	A	517	6PL	C1-O3P-P-O4P
3	A	518	6PL	C1-O3P-P-O2P
3	A	518	6PL	C1-O3P-P-O4P
3	A	518	6PL	C4-O4P-P-O3P
3	A	518	6PL	C4-O4P-P-O1P
3	A	520	6PL	C1-O3P-P-O2P
3	A	520	6PL	C4-O4P-P-O1P
3	A	521	6PL	C4-O4P-P-O3P
3	A	521	6PL	C4-O4P-P-O1P
3	A	522	6PL	C4-O4P-P-O3P
3	A	522	6PL	C4-O4P-P-O1P
3	A	528	6PL	C1-O3P-P-O1P
3	A	528	6PL	C1-O3P-P-O2P
3	A	528	6PL	C1-O3P-P-O4P
3	A	531	6PL	C4-O4P-P-O2P
3	A	532	6PL	C1-O3P-P-O2P
3	A	533	6PL	C4-O4P-P-O3P
3	A	533	6PL	C4-O4P-P-O1P
3	A	534	6PL	C1-O3P-P-O1P
3	A	535	6PL	C1-O3P-P-O1P
3	A	536	6PL	C4-O4P-P-O1P
3	A	537	6PL	C4-O4P-P-O3P
3	A	537	6PL	C4-O4P-P-O2P
3	A	540	6PL	C1-O3P-P-O1P
3	A	540	6PL	C4-O4P-P-O1P
3	A	543	6PL	C1-O3P-P-O1P
3	A	545	6PL	C1-O3P-P-O1P
3	A	546	6PL	C4-O4P-P-O1P
3	A	547	6PL	C1-O3P-P-O2P
3	A	547	6PL	C4-O4P-P-O2P
3	A	548	6PL	C1-O3P-P-O2P
3	A	548	6PL	C1-O3P-P-O4P
3	A	551	6PL	C1-O3P-P-O1P
3	A	551	6PL	C4-O4P-P-O1P
3	A	553	6PL	C4-O4P-P-O2P
3	A	554	6PL	C4-O4P-P-O1P
3	A	555	6PL	C4-O4P-P-O1P
3	A	558	6PL	C1-O3P-P-O2P
3	A	558	6PL	C1-O3P-P-O4P
3	A	560	6PL	C1-O3P-P-O2P
3	A	561	6PL	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	A	561	6PL	C1-O3P-P-O4P
3	A	563	6PL	C4-O4P-P-O2P
3	A	564	6PL	C1-O3P-P-O1P
3	A	564	6PL	C1-O3P-P-O2P
3	A	565	6PL	C1-O3P-P-O4P
3	A	567	6PL	C4-O4P-P-O1P
3	A	569	6PL	C4-O4P-P-O1P
3	A	570	6PL	C4-O4P-P-O1P
3	A	571	6PL	C1-O3P-P-O4P
3	A	573	6PL	C4-O4P-P-O3P
3	A	574	6PL	C4-O4P-P-O3P
3	A	574	6PL	C4-O4P-P-O1P
3	A	574	6PL	C4-O4P-P-O2P
3	A	575	6PL	C1-O3P-P-O1P
3	A	575	6PL	C1-O3P-P-O2P
3	A	576	6PL	C1-O3P-P-O1P
3	A	576	6PL	C1-O3P-P-O2P
3	A	576	6PL	C1-O3P-P-O4P
3	A	577	6PL	C4-O4P-P-O2P
3	A	578	6PL	C4-O4P-P-O3P
3	A	579	6PL	C1-O3P-P-O1P
3	A	579	6PL	C1-O3P-P-O2P
3	A	579	6PL	C1-O3P-P-O4P
3	A	580	6PL	C1-O3P-P-O1P
3	A	581	6PL	C1-O3P-P-O1P
3	A	581	6PL	C1-O3P-P-O4P
3	A	581	6PL	C4-C5-N-C8
3	A	585	6PL	C1-O3P-P-O2P
3	A	587	6PL	C4-O4P-P-O1P
3	A	566	6PL	C39-C40-C41-C42
3	E	314	6PL	C2-C1-O3P-P
3	E	335	6PL	C2-C1-O3P-P
3	A	519	6PL	C2-C1-O3P-P
3	A	558	6PL	C2-C1-O3P-P
3	A	583	6PL	C2-C1-O3P-P
3	A	583	6PL	C37-C38-C39-C40
3	E	312	6PL	C34-C35-C36-C37
3	A	520	6PL	C39-C40-C41-C42
3	A	542	6PL	C40-C41-C42-C43
3	E	312	6PL	C3-C2-O2-C31
3	E	315	6PL	C1-C2-O2-C31
3	E	337	6PL	C1-C2-O2-C31

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Mol	Chain	Res	Type	Atoms
3	E	344	6PL	C3-C2-O2-C31
3	E	347	6PL	C1-C2-O2-C31
3	E	348	6PL	C1-C2-O2-C31
3	E	353	6PL	C3-C2-O2-C31
3	E	355	6PL	C1-C2-O2-C31
3	E	357	6PL	C1-C2-O2-C31
3	E	367	6PL	C3-C2-O2-C31
3	E	368	6PL	C3-C2-O2-C31
3	A	501	6PL	C1-C2-O2-C31
3	A	502	6PL	C3-C2-O2-C31
3	A	513	6PL	C1-C2-O2-C31
3	A	515	6PL	C1-C2-O2-C31
3	A	519	6PL	C3-C2-O2-C31
3	A	522	6PL	C1-C2-O2-C31
3	A	529	6PL	C1-C2-O2-C31
3	A	532	6PL	C1-C2-O2-C31
3	A	536	6PL	C1-C2-O2-C31
3	A	558	6PL	C1-C2-O2-C31
3	A	569	6PL	C3-C2-O2-C31
3	A	575	6PL	C1-C2-O2-C31
3	A	581	6PL	C3-C2-O2-C31
3	E	368	6PL	C37-C38-C39-C40
3	A	512	6PL	O3-C11-C12-C13
3	A	571	6PL	O2-C31-C32-C33
3	E	349	6PL	C34-C35-C36-C37
3	E	358	6PL	C4-C5-N-C7
3	A	531	6PL	C37-C38-C39-C40
3	E	349	6PL	C35-C36-C37-C38
3	A	568	6PL	C2-C3-O3-C11
3	E	325	6PL	C2-C1-O3P-P
3	E	358	6PL	C2-C1-O3P-P
3	A	563	6PL	C39-C40-C41-C42
3	E	324	6PL	C4-C5-N-C8
3	A	549	6PL	O2-C31-C32-C33
3	E	304	6PL	C40-C41-C42-C43
3	E	360	6PL	O2-C31-C32-C33
3	A	508	6PL	O2-C31-C32-C33
3	A	563	6PL	C31-C32-C33-C34
3	A	532	6PL	C39-C40-C41-C42
3	A	516	6PL	C40-C41-C42-C43
3	E	358	6PL	C42-C43-C44-C45
3	A	574	6PL	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
3	E	361	6PL	O2-C2-C3-O3
3	A	550	6PL	C2-C3-O3-C11
3	A	506	6PL	O31-C31-C32-C33
3	A	546	6PL	C18-C19-C20-C21
3	E	341	6PL	C39-C40-C41-C42
3	A	555	6PL	C2-C1-O3P-P
3	A	575	6PL	C2-C1-O3P-P
3	E	369	6PL	C36-C37-C38-C39
3	E	341	6PL	C21-C22-C23-C24
3	A	559	6PL	C34-C35-C36-C37
3	A	508	6PL	C13-C14-C15-C16
3	E	310	6PL	C39-C40-C41-C42
3	E	362	6PL	C2-C3-O3-C11
3	E	303	6PL	C37-C38-C39-C40
3	E	362	6PL	C39-C40-C41-C42
3	E	359	6PL	C39-C40-C41-C42
3	A	569	6PL	C37-C38-C39-C40
3	E	368	6PL	C34-C35-C36-C37
3	E	314	6PL	C3-C2-O2-C31
3	E	314	6PL	C1-C2-O2-C31
3	E	317	6PL	C3-C2-O2-C31
3	E	320	6PL	C3-C2-O2-C31
3	E	325	6PL	C1-C2-O2-C31
3	E	326	6PL	C3-C2-O2-C31
3	E	328	6PL	C3-C2-O2-C31
3	E	328	6PL	C1-C2-O2-C31
3	E	336	6PL	C1-C2-O2-C31
3	E	341	6PL	C1-C2-O2-C31
3	E	345	6PL	C3-C2-O2-C31
3	E	345	6PL	C1-C2-O2-C31
3	E	350	6PL	C3-C2-O2-C31
3	E	350	6PL	C1-C2-O2-C31
3	E	352	6PL	C3-C2-O2-C31
3	E	352	6PL	C1-C2-O2-C31
3	E	354	6PL	C3-C2-O2-C31
3	E	365	6PL	C1-C2-O2-C31
3	E	367	6PL	C1-C2-O2-C31
3	A	505	6PL	C3-C2-O2-C31
3	A	508	6PL	C1-C2-O2-C31
3	A	509	6PL	C3-C2-O2-C31
3	A	509	6PL	C1-C2-O2-C31
3	A	517	6PL	C1-C2-O2-C31

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Mol	Chain	Res	Type	Atoms
3	A	518	6PL	C3-C2-O2-C31
3	A	518	6PL	C1-C2-O2-C31
3	A	521	6PL	C1-C2-O2-C31
3	A	526	6PL	C1-C2-O2-C31
3	A	531	6PL	C3-C2-O2-C31
3	A	531	6PL	C1-C2-O2-C31
3	A	535	6PL	C3-C2-O2-C31
3	A	540	6PL	C3-C2-O2-C31
3	A	546	6PL	C3-C2-O2-C31
3	A	551	6PL	C1-C2-O2-C31
3	A	555	6PL	C1-C2-O2-C31
3	A	556	6PL	C1-C2-O2-C31
3	A	563	6PL	C3-C2-O2-C31
3	A	565	6PL	C3-C2-O2-C31
3	A	565	6PL	C1-C2-O2-C31
3	A	577	6PL	C3-C2-O2-C31
3	A	578	6PL	C1-C2-O2-C31
3	A	582	6PL	C1-C2-O2-C31
3	A	584	6PL	C33-C34-C35-C36
3	A	565	6PL	O3-C11-C12-C13
3	A	563	6PL	C2-C3-O3-C11
3	E	308	6PL	C17-C18-C19-C20
3	A	511	6PL	C42-C43-C44-C45
3	E	312	6PL	C42-C43-C44-C45
3	A	506	6PL	C37-C38-C39-C40
3	E	351	6PL	C2-C1-O3P-P
3	E	327	6PL	C12-C13-C14-C15
3	A	523	6PL	O3P-C1-C2-C3
3	A	509	6PL	C37-C38-C39-C40
3	A	516	6PL	C36-C37-C38-C39
3	A	514	6PL	C39-C40-C41-C42
3	A	501	6PL	C37-C38-C39-C40
3	A	551	6PL	C37-C38-C39-C40
3	E	313	6PL	C2-C3-O3-C11
3	E	347	6PL	C2-C3-O3-C11
3	A	564	6PL	C2-C1-O3P-P
3	E	332	6PL	C4-C5-N-C8
3	E	351	6PL	C40-C41-C42-C43
3	E	354	6PL	O3-C11-C12-C13
3	A	579	6PL	C40-C41-C42-C43
3	E	303	6PL	O3-C11-C12-C13
3	E	350	6PL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
3	A	514	6PL	C33-C34-C35-C36
3	E	321	6PL	C40-C41-C42-C43
3	E	305	6PL	O31-C31-C32-C33
3	E	353	6PL	O3-C11-C12-C13
3	E	346	6PL	C39-C40-C41-C42
3	A	525	6PL	O2-C31-C32-C33
3	A	538	6PL	C4-C5-N-C8
3	A	522	6PL	O31-C31-C32-C33
3	A	559	6PL	O3P-C1-C2-C3
3	A	577	6PL	O3-C11-C12-C13
3	A	523	6PL	C2-C1-O3P-P
3	E	315	6PL	C37-C38-C39-C40
3	E	320	6PL	C37-C38-C39-C40
3	A	511	6PL	C32-C33-C34-C35
3	A	559	6PL	C37-C38-C39-C40
3	E	364	6PL	C11-C12-C13-C14
3	A	586	6PL	O11-C11-C12-C13
3	A	503	6PL	O3-C11-C12-C13
3	A	565	6PL	O2-C31-C32-C33
3	E	317	6PL	C1-C2-O2-C31
3	E	325	6PL	C3-C2-O2-C31
3	A	501	6PL	C3-C2-O2-C31
3	A	503	6PL	C3-C2-O2-C31
3	A	503	6PL	C1-C2-O2-C31
3	A	526	6PL	C3-C2-O2-C31
3	A	540	6PL	C1-C2-O2-C31
3	A	542	6PL	C3-C2-O2-C31
3	A	542	6PL	C1-C2-O2-C31
3	A	547	6PL	C3-C2-O2-C31
3	A	547	6PL	C1-C2-O2-C31
3	A	555	6PL	C3-C2-O2-C31
3	A	556	6PL	C3-C2-O2-C31
3	A	559	6PL	C1-C2-O2-C31
3	A	588	6PL	C1-C2-O2-C31
3	E	324	6PL	O3-C11-C12-C13
3	E	325	6PL	C18-C19-C20-C21
3	E	306	6PL	C37-C38-C39-C40
3	A	576	6PL	C16-C17-C18-C19
3	E	358	6PL	C18-C19-C20-C21
3	A	509	6PL	C31-C32-C33-C34
3	E	326	6PL	O3-C11-C12-C13
3	A	503	6PL	O2-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	A	528	6PL	C37-C38-C39-C40
3	A	546	6PL	C20-C21-C22-C23
3	E	335	6PL	O31-C31-C32-C33
3	E	301	6PL	C34-C35-C36-C37
3	E	318	6PL	O2-C31-C32-C33
3	E	325	6PL	O2-C31-C32-C33
3	E	348	6PL	O3-C11-C12-C13
3	A	517	6PL	O2-C31-C32-C33
3	E	356	6PL	C2-C3-O3-C11
3	E	332	6PL	C39-C40-C41-C42
3	E	367	6PL	C39-C40-C41-C42
3	A	509	6PL	C4-C5-N-C7
3	A	561	6PL	O11-C11-C12-C13
3	E	307	6PL	O3-C11-C12-C13
3	E	313	6PL	O3-C11-C12-C13
3	E	369	6PL	C18-C19-C20-C21
3	A	524	6PL	O2-C31-C32-C33
3	E	326	6PL	O2-C31-C32-C33
3	E	331	6PL	O3-C11-C12-C13
3	E	343	6PL	O2-C31-C32-C33
3	A	513	6PL	O2-C31-C32-C33
3	A	535	6PL	O3-C11-C12-C13
3	E	302	6PL	O3-C11-C12-C13
3	A	526	6PL	O2-C31-C32-C33
3	C	501	6PL	O2-C31-C32-C33
3	A	527	6PL	C37-C38-C39-C40
3	E	337	6PL	C2-C3-O3-C11
3	A	551	6PL	C2-C3-O3-C11
3	E	333	6PL	O2-C31-C32-C33
3	A	541	6PL	C39-C40-C41-C42
3	A	574	6PL	C39-C40-C41-C42
3	E	342	6PL	O2-C31-C32-C33
3	E	355	6PL	O2-C31-C32-C33
3	A	542	6PL	O3-C11-C12-C13
3	E	322	6PL	C42-C43-C44-C45
3	E	364	6PL	C12-C13-C14-C15
3	A	534	6PL	O2-C31-C32-C33
3	A	541	6PL	O3-C11-C12-C13
3	E	321	6PL	C39-C40-C41-C42
3	A	564	6PL	O11-C11-C12-C13
3	E	340	6PL	O3-C11-C12-C13
3	A	511	6PL	O3-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	A	559	6PL	O3-C11-C12-C13
3	A	534	6PL	C13-C14-C15-C16
3	E	327	6PL	C21-C22-C23-C24
3	E	351	6PL	C34-C35-C36-C37
3	E	343	6PL	C4-C5-N-C8
3	A	522	6PL	C13-C14-C15-C16
3	E	367	6PL	O2-C31-C32-C33
3	A	537	6PL	O3-C11-C12-C13
3	A	584	6PL	O2-C31-C32-C33
3	E	301	6PL	O3-C11-C12-C13
3	E	302	6PL	O2-C31-C32-C33
3	E	313	6PL	O2-C31-C32-C33
3	A	509	6PL	O2-C31-C32-C33
3	A	542	6PL	O2-C31-C32-C33
3	A	556	6PL	O3-C11-C12-C13
3	A	563	6PL	O3-C11-C12-C13
3	E	342	6PL	C14-C15-C16-C17
3	E	315	6PL	O3-C11-C12-C13
3	E	362	6PL	O2-C31-C32-C33
3	A	551	6PL	O3-C11-C12-C13
3	A	563	6PL	O2-C31-C32-C33
3	A	582	6PL	O2-C31-C32-C33
3	E	320	6PL	C1-C2-O2-C31
3	E	348	6PL	C3-C2-O2-C31
3	E	365	6PL	C3-C2-O2-C31
3	A	506	6PL	C3-C2-O2-C31
3	A	506	6PL	C1-C2-O2-C31
3	A	508	6PL	C3-C2-O2-C31
3	A	513	6PL	C3-C2-O2-C31
3	A	536	6PL	C3-C2-O2-C31
3	A	546	6PL	C1-C2-O2-C31
3	A	550	6PL	C3-C2-O2-C31
3	A	551	6PL	C3-C2-O2-C31
3	A	563	6PL	C1-C2-O2-C31
3	A	570	6PL	C3-C2-O2-C31
3	A	578	6PL	C3-C2-O2-C31
3	A	581	6PL	C1-C2-O2-C31
3	A	582	6PL	C3-C2-O2-C31
3	A	588	6PL	C3-C2-O2-C31
3	C	501	6PL	C1-C2-O2-C31
3	A	525	6PL	C37-C38-C39-C40
3	A	568	6PL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
3	E	367	6PL	C4-C5-N-C7
3	A	516	6PL	C4-C5-N-C7
3	E	353	6PL	C2-C3-O3-C11
3	A	533	6PL	O2-C31-C32-C33
3	A	575	6PL	C36-C37-C38-C39
3	E	364	6PL	C37-C38-C39-C40
3	A	537	6PL	C37-C38-C39-C40
3	A	514	6PL	O3-C11-C12-C13
3	A	503	6PL	O31-C31-C32-C33
3	A	534	6PL	O31-C31-C32-C33
3	E	351	6PL	O2-C31-C32-C33
3	E	353	6PL	O2-C31-C32-C33
3	E	307	6PL	O11-C11-C12-C13
3	E	318	6PL	O31-C31-C32-C33
3	E	326	6PL	O11-C11-C12-C13
3	E	340	6PL	O11-C11-C12-C13
3	E	342	6PL	O31-C31-C32-C33
3	A	528	6PL	C17-C18-C19-C20
3	A	506	6PL	C21-C22-C23-C24
3	E	315	6PL	C44-C45-C46-C47
3	E	326	6PL	O31-C31-C32-C33
3	E	333	6PL	O31-C31-C32-C33
3	A	517	6PL	O31-C31-C32-C33
3	E	368	6PL	C42-C43-C44-C45
3	E	342	6PL	C11-C12-C13-C14
3	E	316	6PL	C4-C5-N-C7
3	E	366	6PL	C4-C5-N-C8
3	E	322	6PL	O3-C11-C12-C13
3	A	523	6PL	O2-C31-C32-C33
3	E	355	6PL	O31-C31-C32-C33
3	A	526	6PL	O31-C31-C32-C33
3	E	306	6PL	C34-C35-C36-C37
3	A	580	6PL	C31-C32-C33-C34
3	E	331	6PL	C39-C40-C41-C42
3	E	348	6PL	O11-C11-C12-C13
3	A	542	6PL	O11-C11-C12-C13
3	A	548	6PL	O11-C11-C12-C13
3	E	309	6PL	C40-C41-C42-C43
3	A	585	6PL	O3-C11-C12-C13
3	A	524	6PL	O31-C31-C32-C33
3	A	535	6PL	O11-C11-C12-C13
3	E	309	6PL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
3	E	356	6PL	O2-C31-C32-C33
3	A	535	6PL	O2-C31-C32-C33
3	A	571	6PL	O3-C11-C12-C13
3	E	361	6PL	C40-C41-C42-C43
3	E	313	6PL	O11-C11-C12-C13
3	E	325	6PL	O31-C31-C32-C33
3	E	331	6PL	O11-C11-C12-C13
3	E	367	6PL	O31-C31-C32-C33
3	A	513	6PL	O31-C31-C32-C33
3	A	541	6PL	O11-C11-C12-C13
3	A	556	6PL	O11-C11-C12-C13
3	A	563	6PL	O11-C11-C12-C13
3	A	516	6PL	C44-C45-C46-C47
3	A	533	6PL	C21-C22-C23-C24
3	A	511	6PL	O11-C11-C12-C13
3	A	542	6PL	O31-C31-C32-C33
3	A	559	6PL	O11-C11-C12-C13
3	A	524	6PL	O3-C11-C12-C13
3	E	332	6PL	C45-C46-C47-C48
3	A	556	6PL	C34-C35-C36-C37
3	A	514	6PL	O11-C11-C12-C13
3	A	537	6PL	O11-C11-C12-C13
3	A	551	6PL	O11-C11-C12-C13
3	E	306	6PL	O2-C31-C32-C33
3	E	321	6PL	O2-C31-C32-C33
3	A	523	6PL	O3-C11-C12-C13
3	A	546	6PL	O3-C11-C12-C13
3	E	302	6PL	O31-C31-C32-C33
3	A	512	6PL	C37-C38-C39-C40
3	E	301	6PL	O11-C11-C12-C13
3	A	571	6PL	O11-C11-C12-C13
3	A	510	6PL	C36-C37-C38-C39
3	E	363	6PL	C23-C24-C25-C26
3	E	326	6PL	C39-C40-C41-C42
3	A	584	6PL	O31-C31-C32-C33
3	E	307	6PL	O2-C31-C32-C33
3	A	552	6PL	O3-C11-C12-C13
3	A	542	6PL	C14-C15-C16-C17
3	A	525	6PL	C40-C41-C42-C43
3	E	358	6PL	C39-C40-C41-C42
3	A	514	6PL	C37-C38-C39-C40
3	E	313	6PL	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	E	351	6PL	O31-C31-C32-C33
3	E	311	6PL	O3-C11-C12-C13
3	E	329	6PL	O3-C11-C12-C13
3	E	338	6PL	O3-C11-C12-C13
3	E	339	6PL	O3-C11-C12-C13
3	A	545	6PL	O3-C11-C12-C13
3	A	569	6PL	O3-C11-C12-C13
3	E	315	6PL	O11-C11-C12-C13
3	E	322	6PL	O11-C11-C12-C13
3	E	347	6PL	O2-C31-C32-C33
3	A	533	6PL	O31-C31-C32-C33

There are no ring outliers.

158 monomers are involved in 3163 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	362	6PL	28	0
3	E	326	6PL	42	0
3	E	345	6PL	35	0
3	E	324	6PL	47	0
3	A	516	6PL	22	0
3	A	585	6PL	14	0
3	A	519	6PL	30	0
3	A	573	6PL	28	0
3	A	520	6PL	52	0
3	A	544	6PL	31	0
3	E	359	6PL	32	0
3	E	315	6PL	31	0
3	E	337	6PL	26	0
3	E	309	6PL	40	0
3	E	314	6PL	14	0
3	E	356	6PL	24	0
3	A	527	6PL	31	0
3	E	308	6PL	44	0
3	A	587	6PL	28	0
3	E	330	6PL	32	0
3	E	361	6PL	23	0
3	A	531	6PL	32	0
3	A	513	6PL	43	0
3	A	525	6PL	26	0
3	E	338	6PL	17	0
3	E	346	6PL	28	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	368	6PL	31	0
3	A	509	6PL	35	0
3	A	541	6PL	51	0
3	A	584	6PL	24	0
3	A	502	6PL	33	0
3	E	367	6PL	21	0
3	A	510	6PL	31	0
3	E	328	6PL	24	0
3	A	571	6PL	40	0
3	E	333	6PL	45	0
3	A	563	6PL	32	0
3	A	523	6PL	25	0
3	E	339	6PL	22	0
3	A	570	6PL	29	0
3	A	561	6PL	16	0
3	A	536	6PL	35	0
3	E	317	6PL	41	0
3	A	508	6PL	34	0
3	A	507	6PL	10	0
3	E	369	6PL	42	0
3	A	521	6PL	26	0
3	A	526	6PL	30	0
3	A	574	6PL	24	0
3	A	558	6PL	27	0
3	E	366	6PL	34	0
3	A	556	6PL	36	0
3	A	576	6PL	23	0
3	A	560	6PL	33	0
3	C	501	6PL	45	0
3	E	331	6PL	54	0
3	A	511	6PL	28	0
3	A	546	6PL	34	0
3	A	514	6PL	20	0
3	E	354	6PL	12	0
3	E	343	6PL	13	0
3	E	349	6PL	14	0
3	E	365	6PL	36	0
3	A	504	6PL	30	0
3	E	363	6PL	50	0
3	E	307	6PL	16	0
3	A	505	6PL	51	0
3	E	335	6PL	34	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	319	6PL	17	0
3	A	503	6PL	43	0
3	E	327	6PL	17	0
3	A	547	6PL	14	0
3	A	537	6PL	41	0
3	A	586	6PL	17	0
3	E	310	6PL	34	0
3	E	322	6PL	27	0
3	A	588	6PL	58	0
3	E	358	6PL	41	0
3	A	568	6PL	14	0
3	A	577	6PL	16	0
3	E	347	6PL	28	0
3	A	551	6PL	18	0
3	E	316	6PL	15	0
3	E	336	6PL	13	0
3	E	332	6PL	26	0
3	A	524	6PL	38	0
3	A	535	6PL	43	0
3	A	538	6PL	34	0
3	A	543	6PL	53	0
3	A	549	6PL	48	0
3	E	355	6PL	50	0
3	A	533	6PL	38	0
3	E	357	6PL	42	0
3	E	325	6PL	37	0
3	E	340	6PL	32	0
3	E	341	6PL	23	0
3	E	342	6PL	15	0
3	A	550	6PL	39	0
3	E	344	6PL	48	0
3	E	353	6PL	34	0
3	A	565	6PL	42	0
3	A	548	6PL	34	0
3	E	334	6PL	8	0
3	A	559	6PL	23	0
3	E	304	6PL	46	0
3	A	553	6PL	20	0
3	A	506	6PL	41	0
3	A	518	6PL	58	0
3	A	534	6PL	34	0
3	A	555	6PL	33	0

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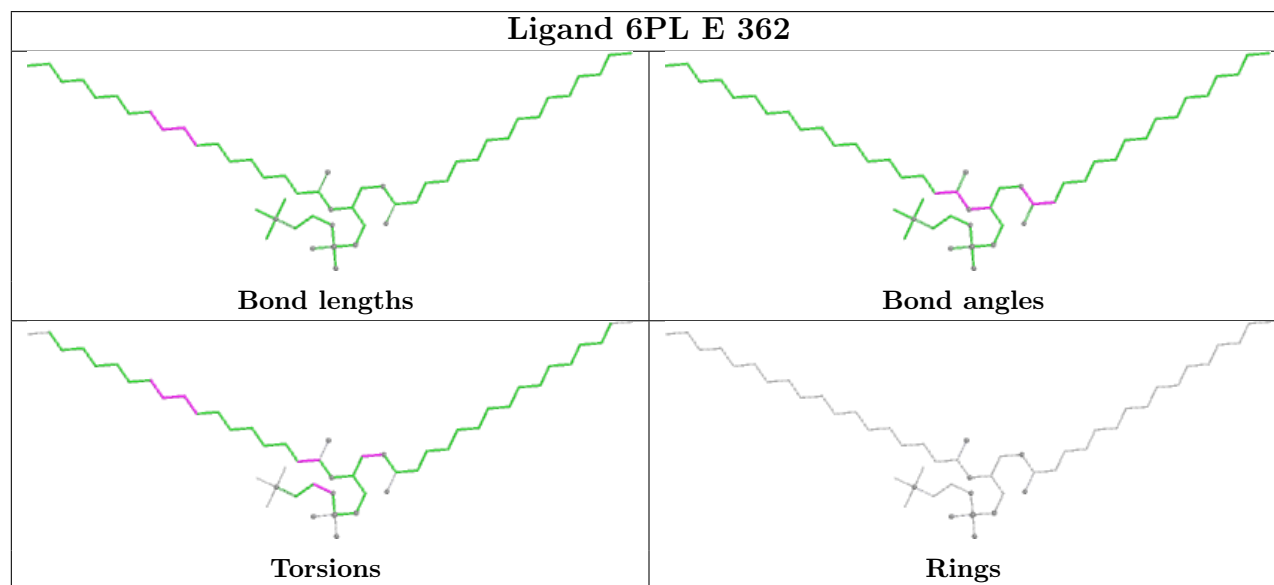
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	562	6PL	40	0
3	E	301	6PL	24	0
3	E	364	6PL	45	0
3	A	542	6PL	69	0
3	E	312	6PL	22	0
3	E	352	6PL	15	0
3	E	306	6PL	49	0
3	A	501	6PL	12	0
3	A	579	6PL	34	0
3	A	552	6PL	28	0
3	A	582	6PL	29	0
3	A	529	6PL	34	0
3	A	512	6PL	41	0
3	A	530	6PL	25	0
3	A	572	6PL	35	0
3	E	302	6PL	30	0
3	E	360	6PL	28	0
3	A	532	6PL	46	0
3	E	348	6PL	26	0
3	E	311	6PL	15	0
3	A	515	6PL	28	0
3	A	557	6PL	46	0
3	A	567	6PL	29	0
3	A	522	6PL	37	0
3	E	318	6PL	34	0
3	E	321	6PL	53	0
3	A	566	6PL	58	0
3	A	528	6PL	36	0
3	A	564	6PL	38	0
3	E	313	6PL	19	0
3	A	539	6PL	21	0
3	A	569	6PL	9	0
3	E	351	6PL	34	0
3	E	303	6PL	9	0
3	A	554	6PL	32	0
3	E	320	6PL	25	0
3	A	578	6PL	33	0
3	E	305	6PL	11	0
3	A	545	6PL	10	0
3	A	517	6PL	31	0
3	A	540	6PL	43	0
3	E	323	6PL	24	0

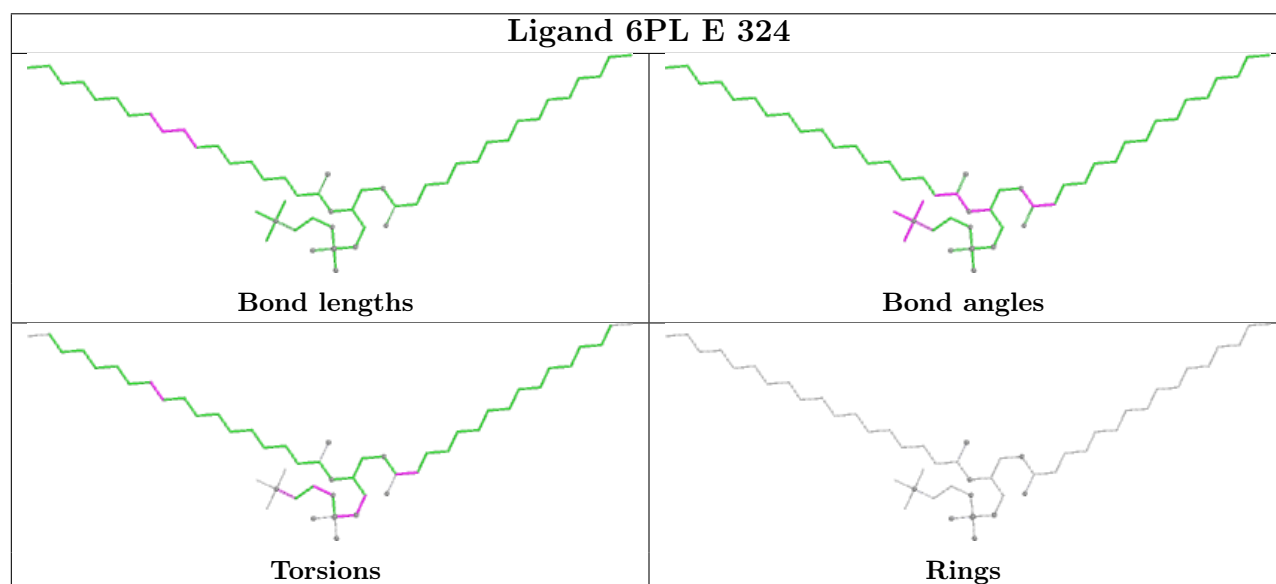
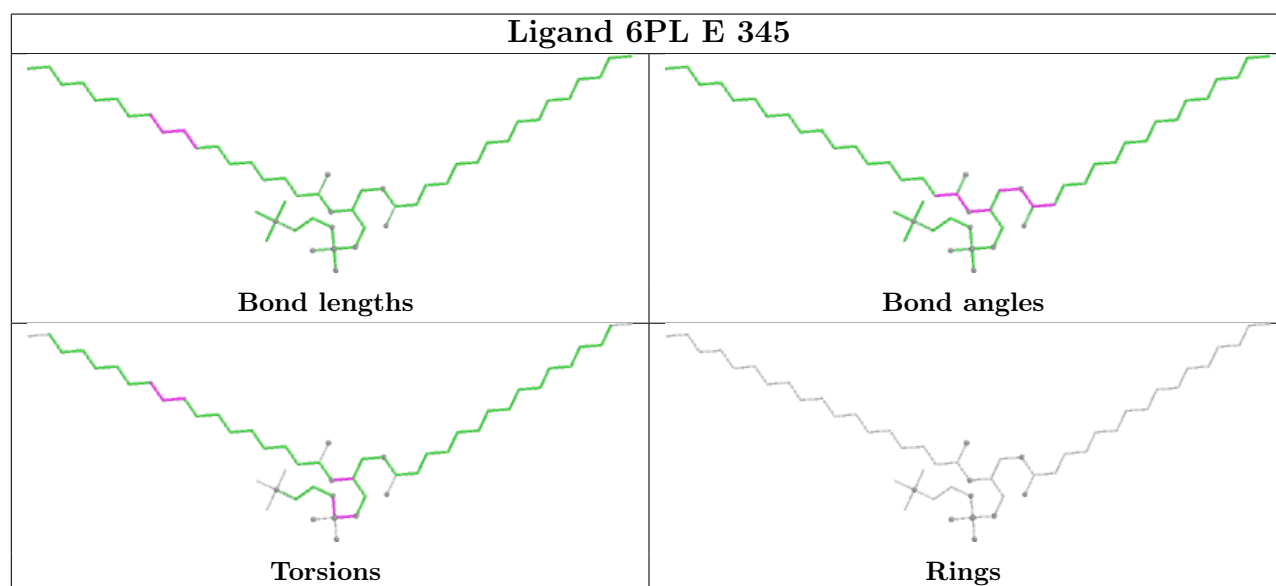
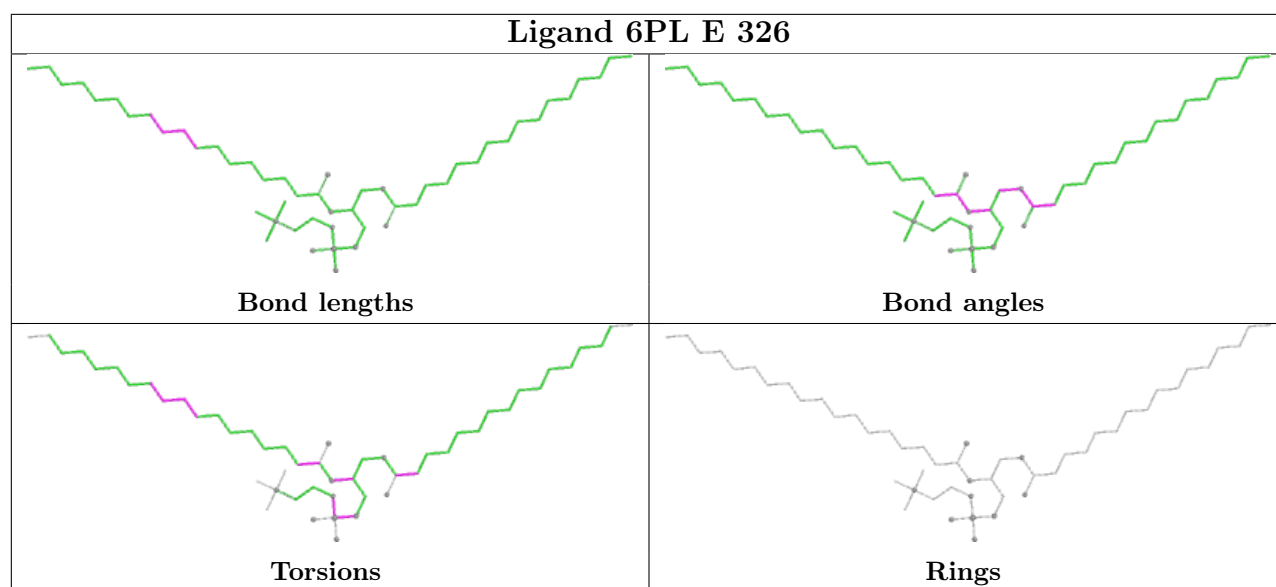
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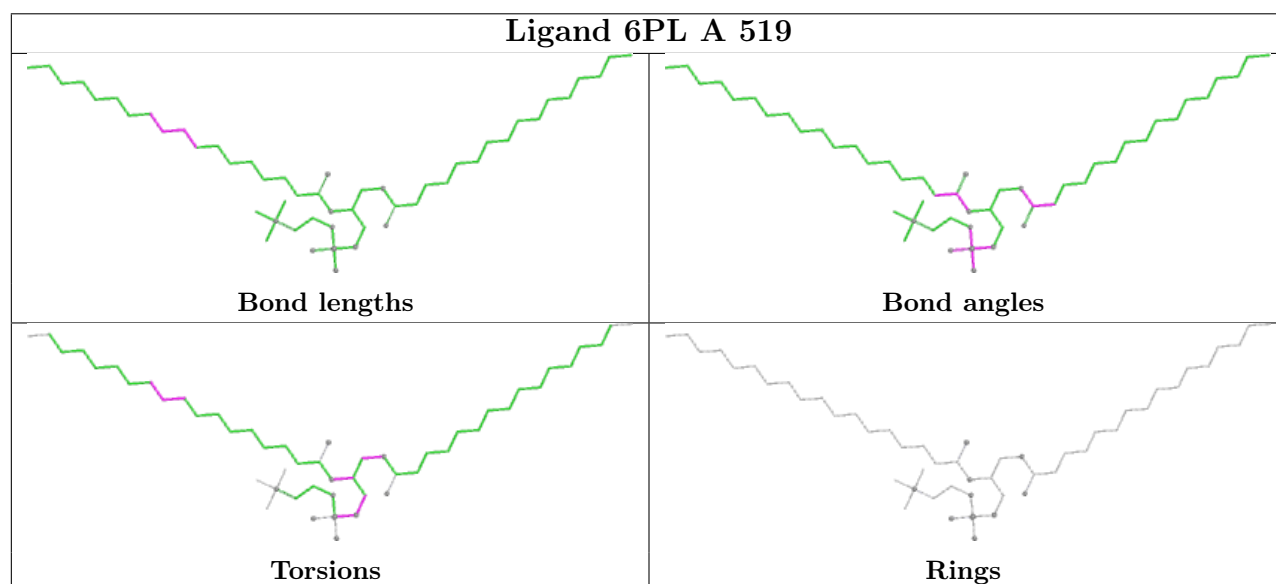
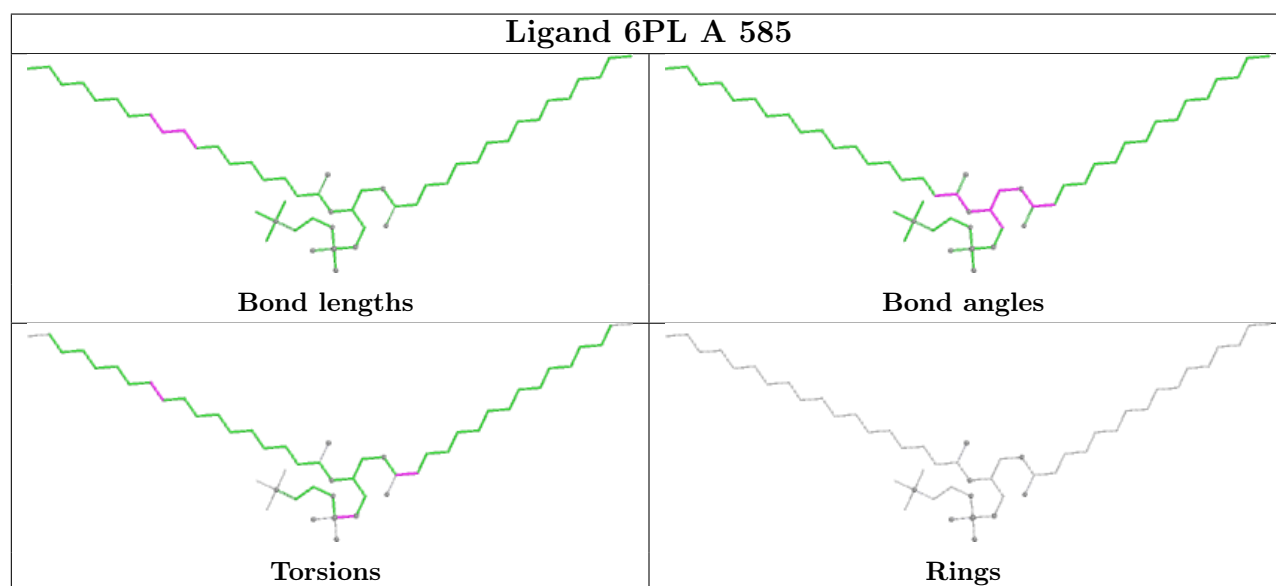
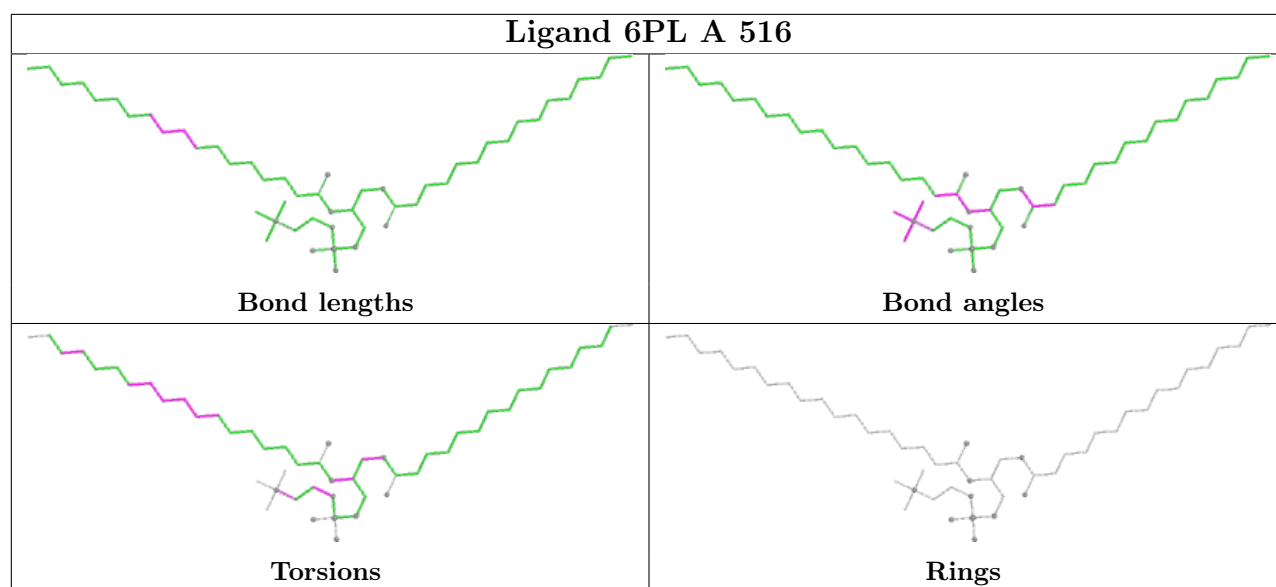
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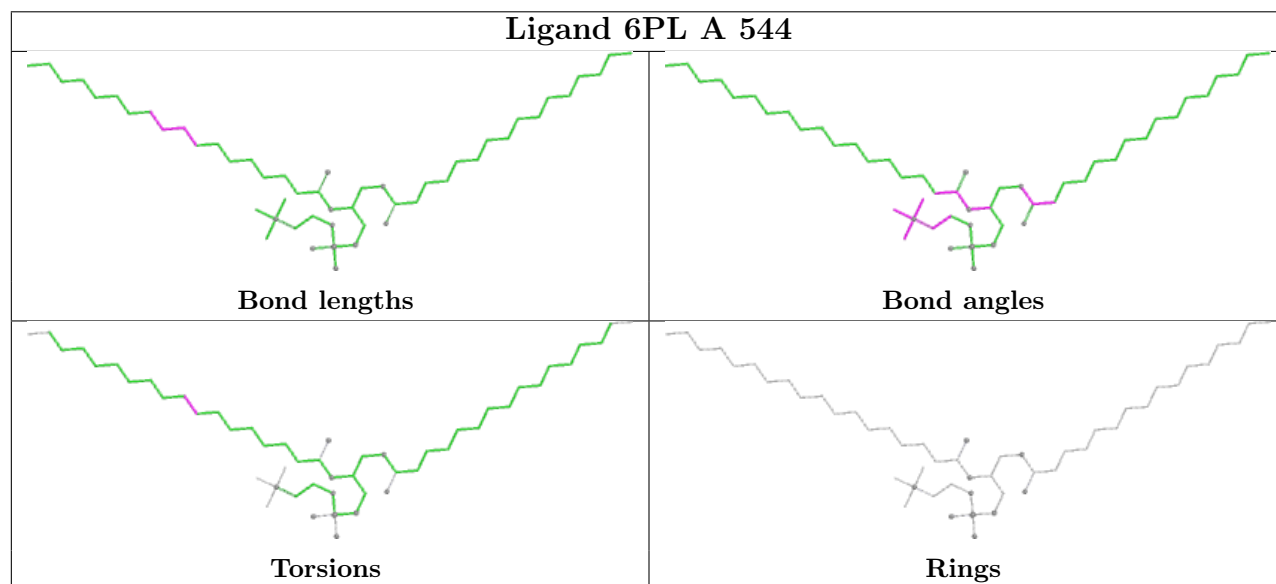
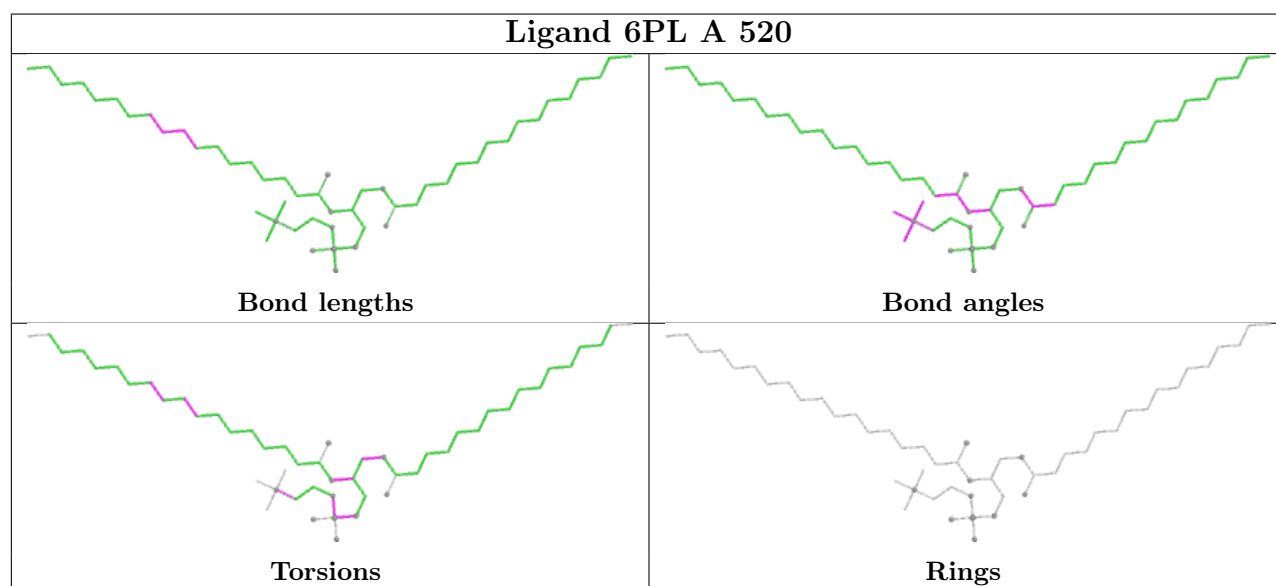
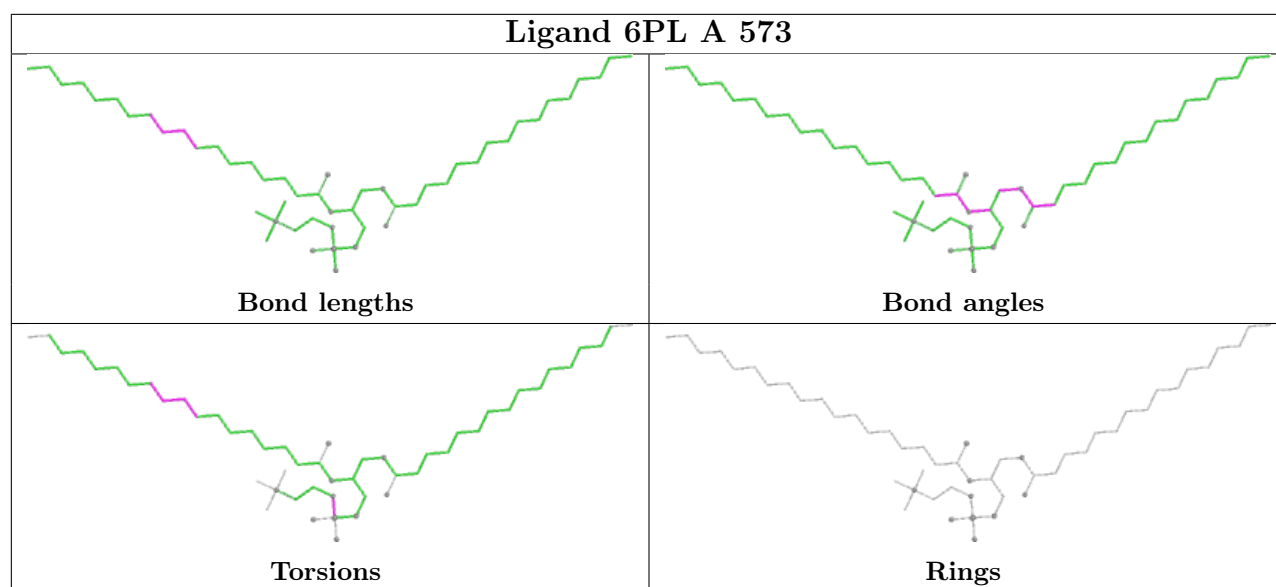
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	575	6PL	39	0
3	E	329	6PL	31	0
3	A	580	6PL	72	0
3	A	583	6PL	17	0
3	E	350	6PL	38	0
3	A	581	6PL	34	0

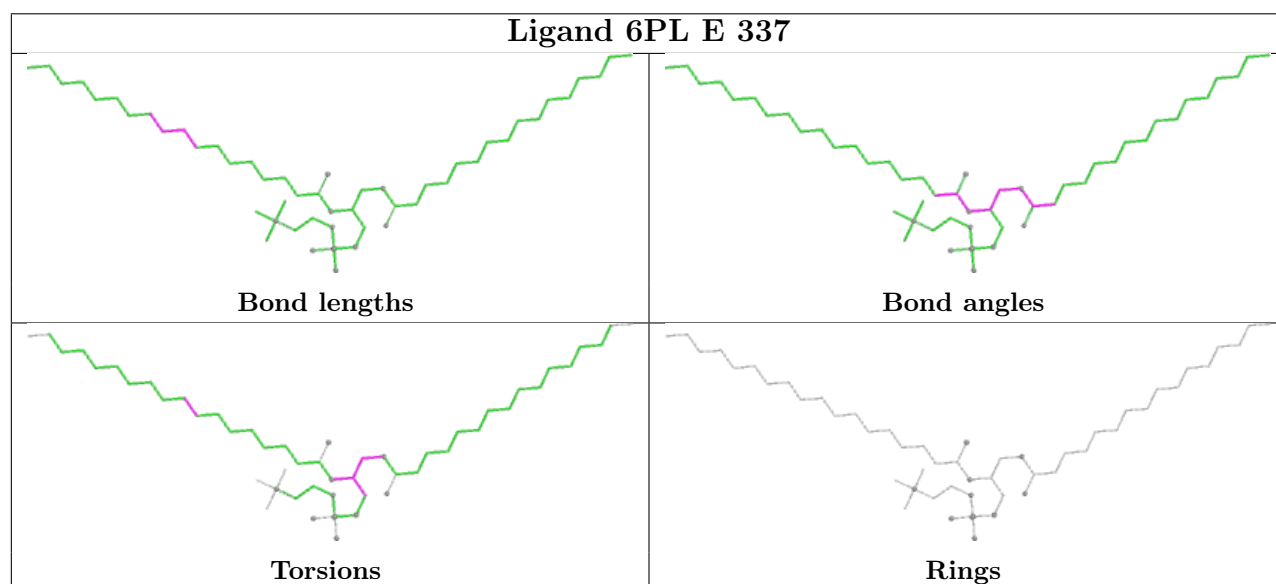
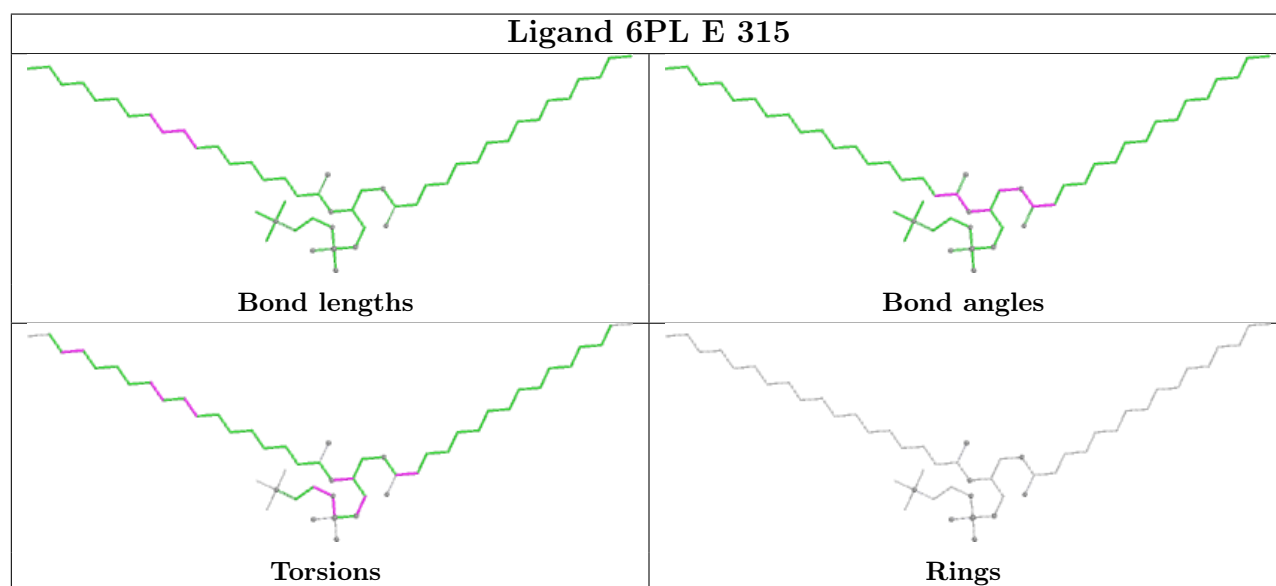
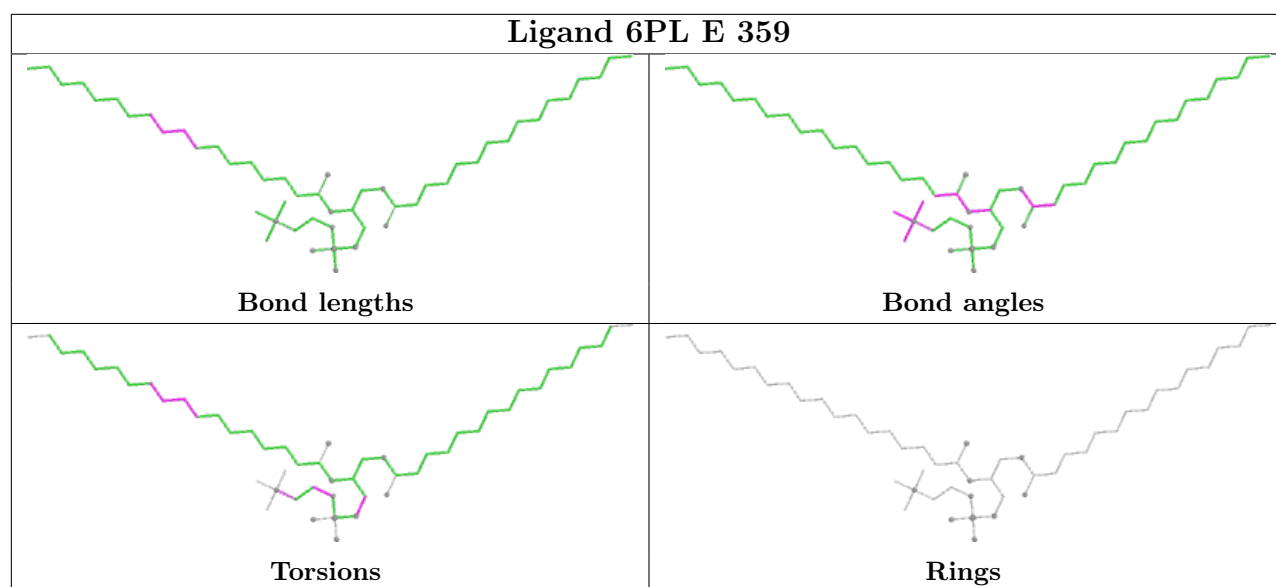
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

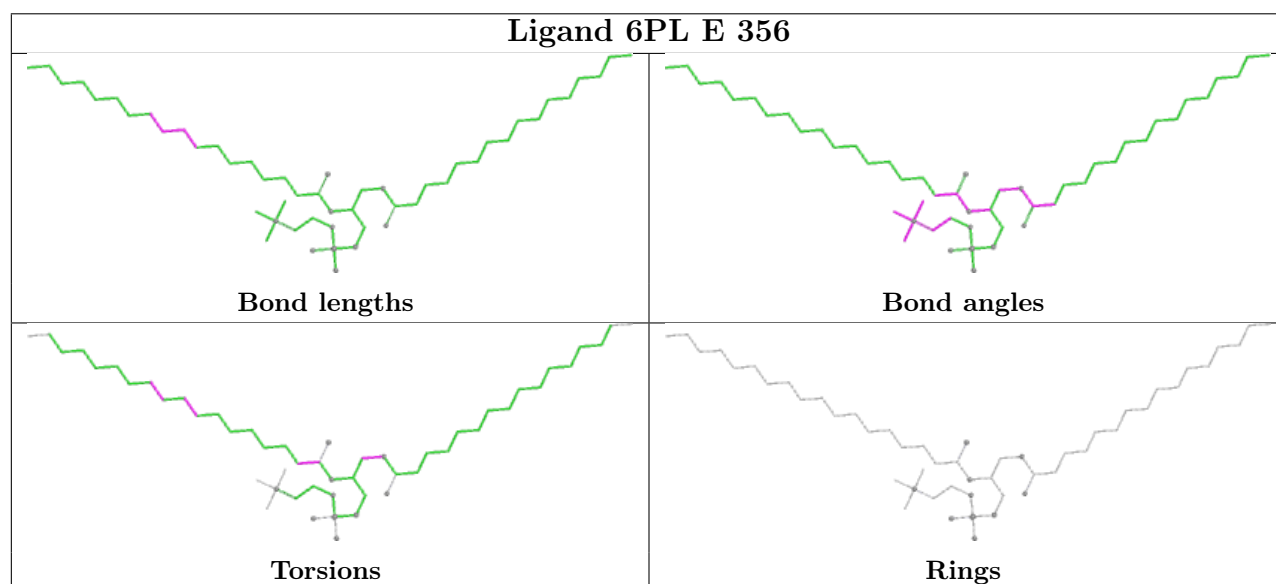
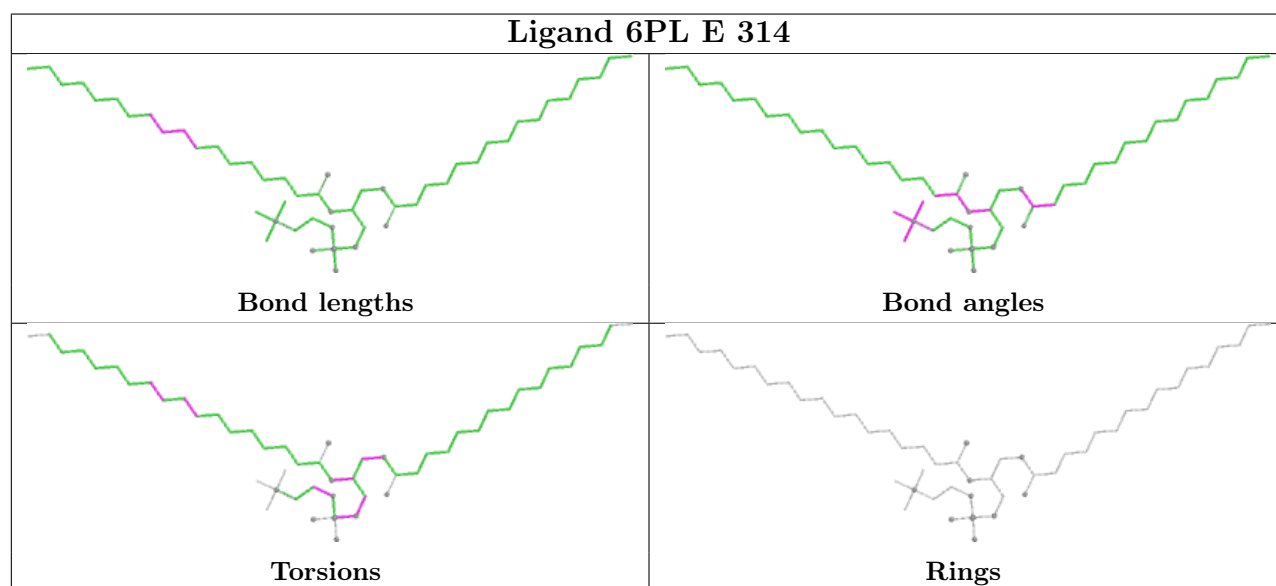
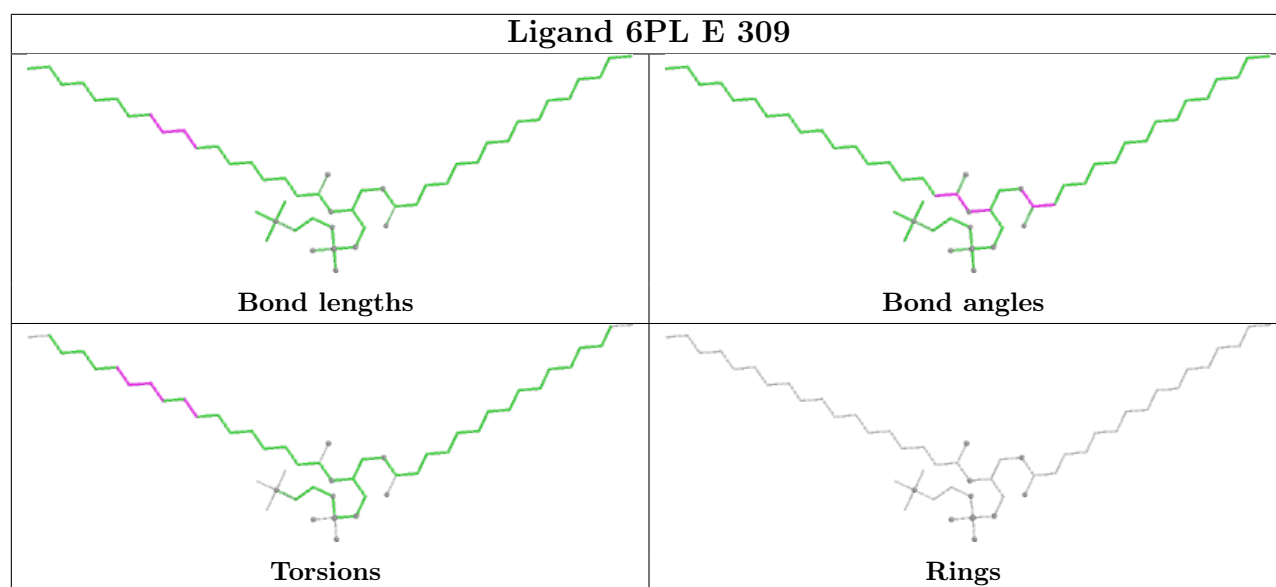


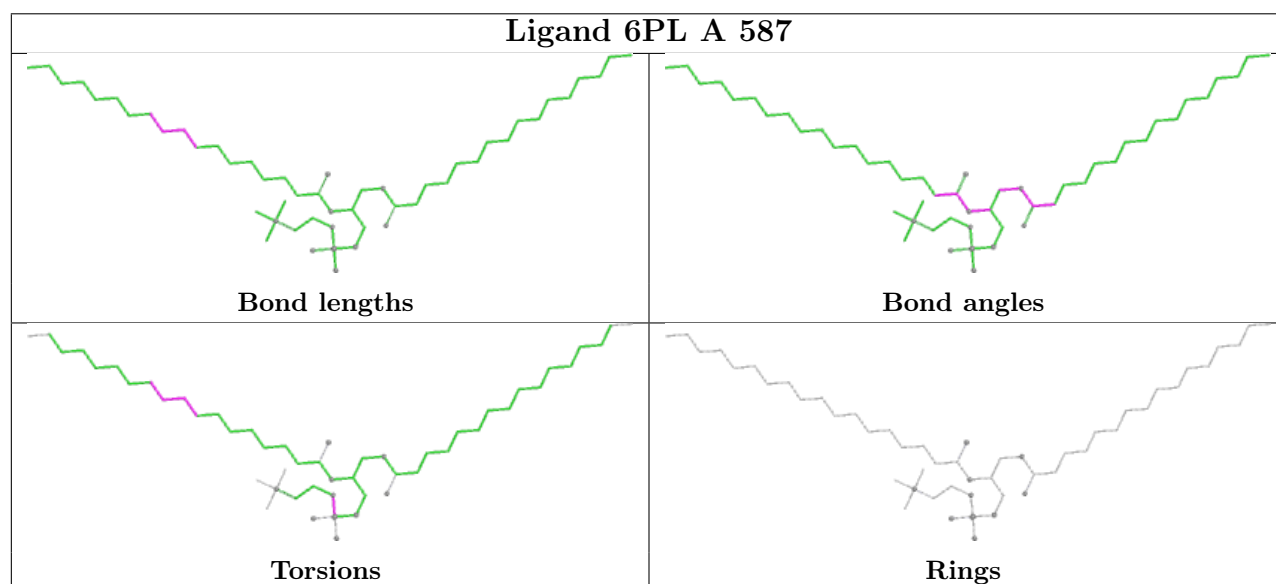
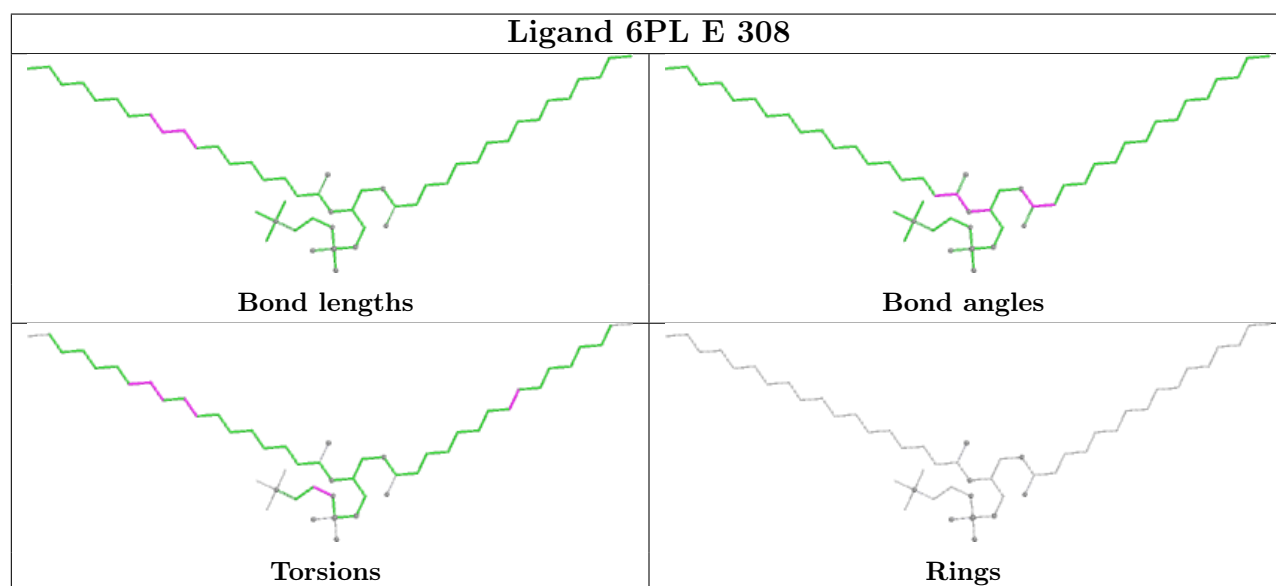
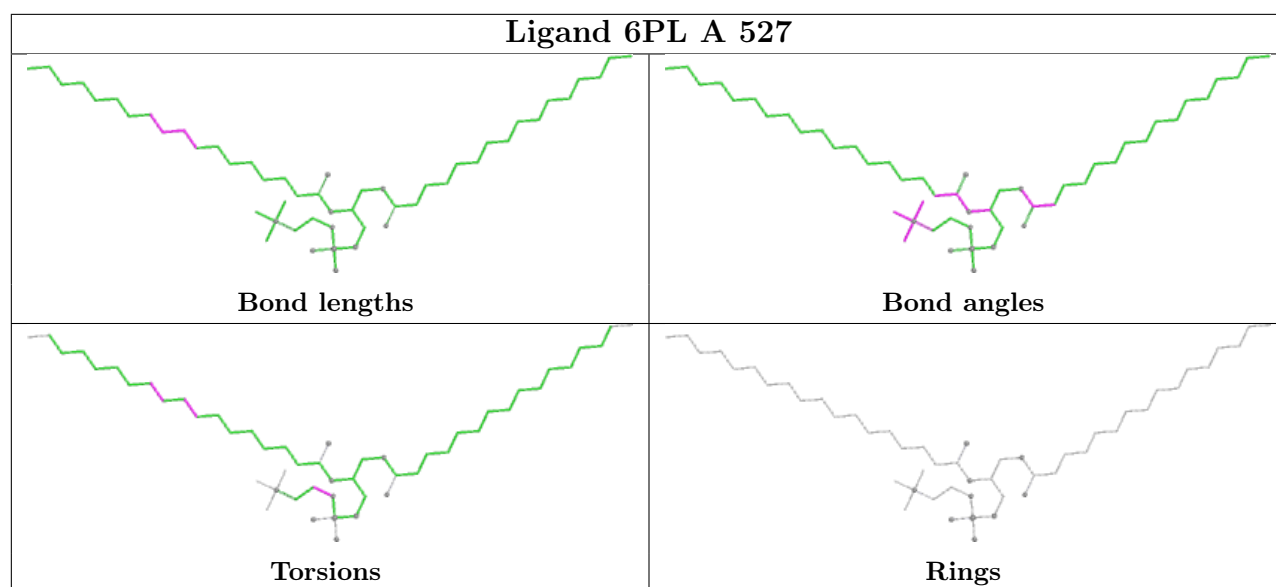


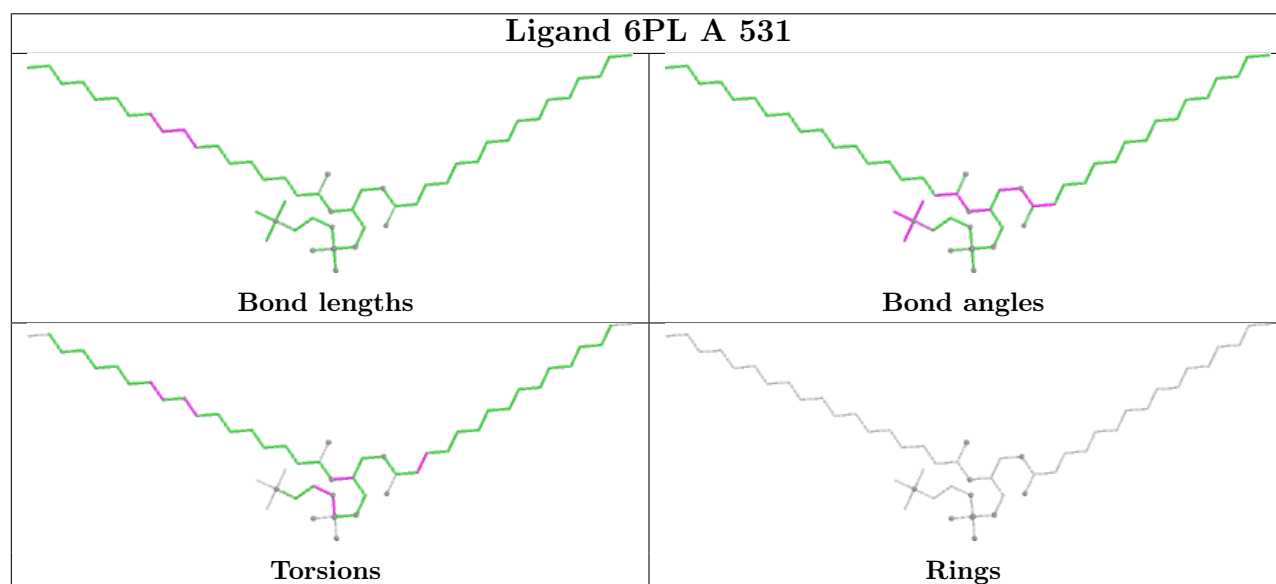
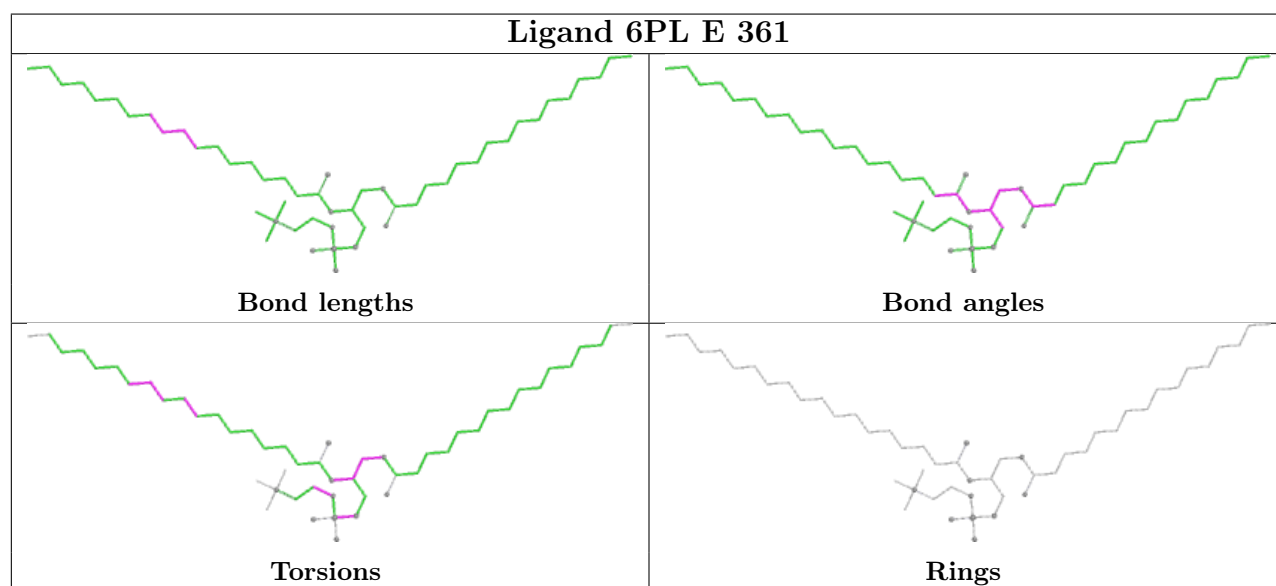
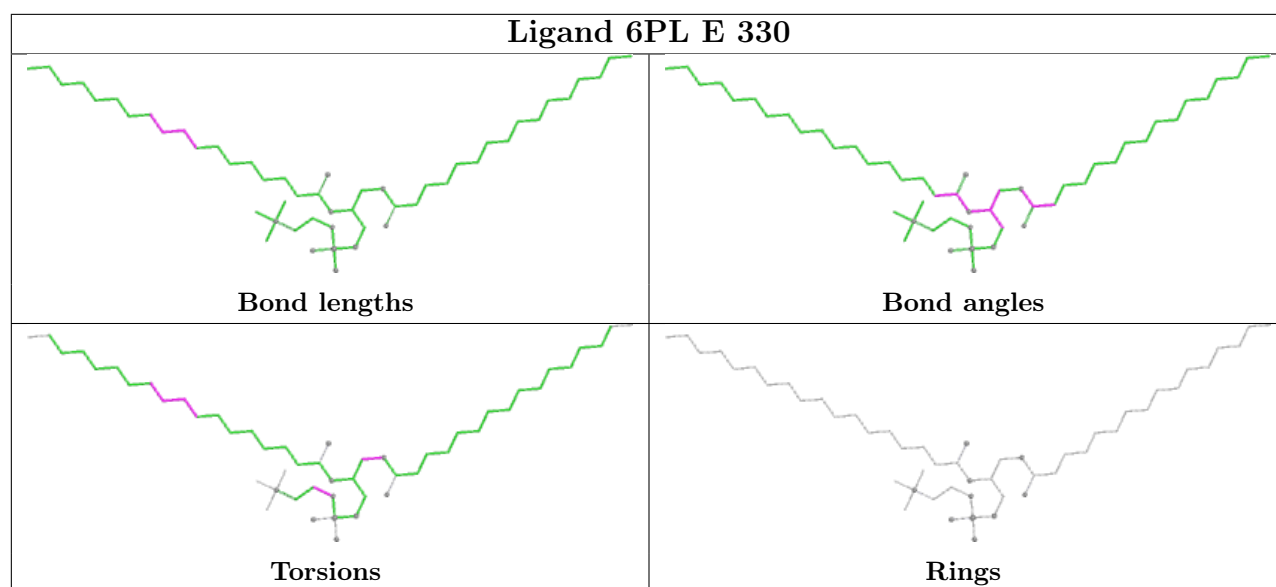


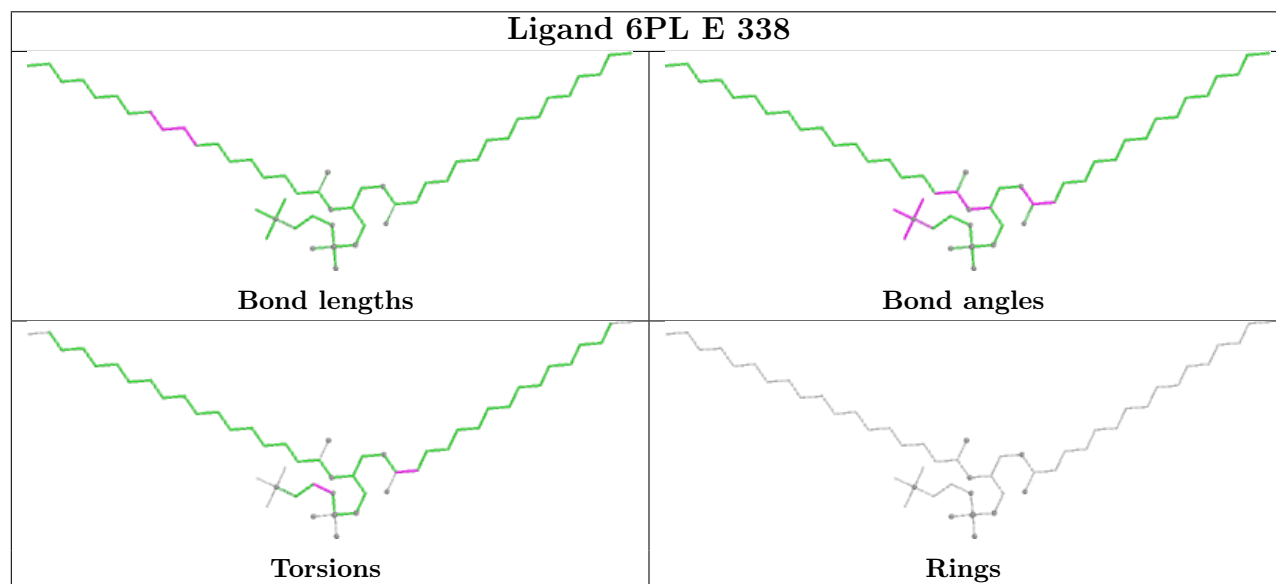
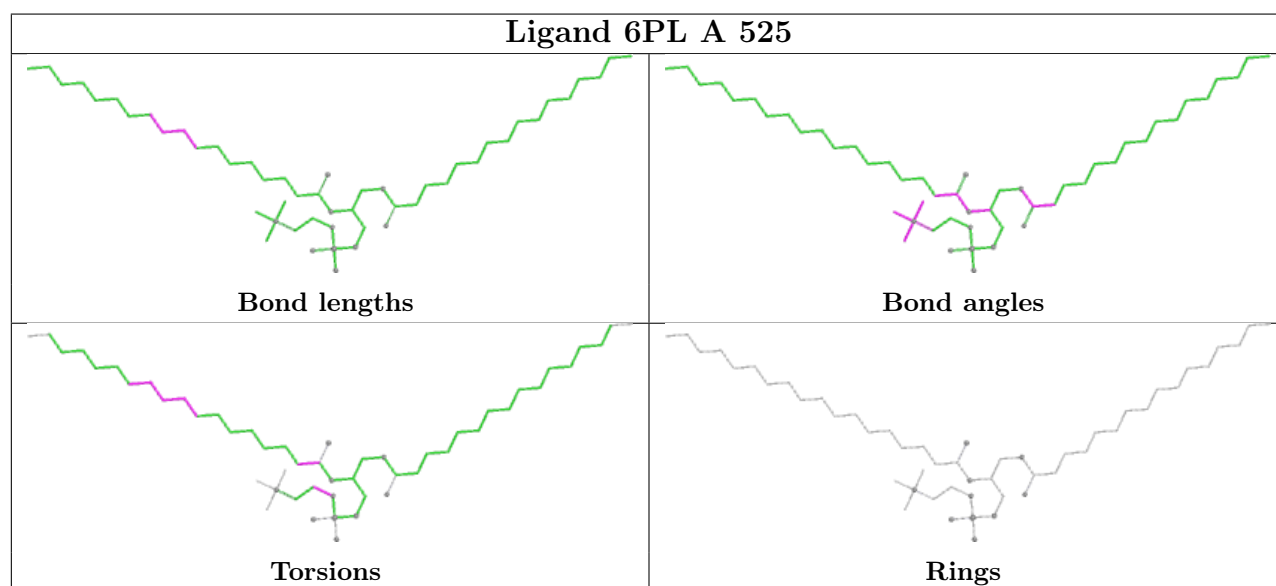
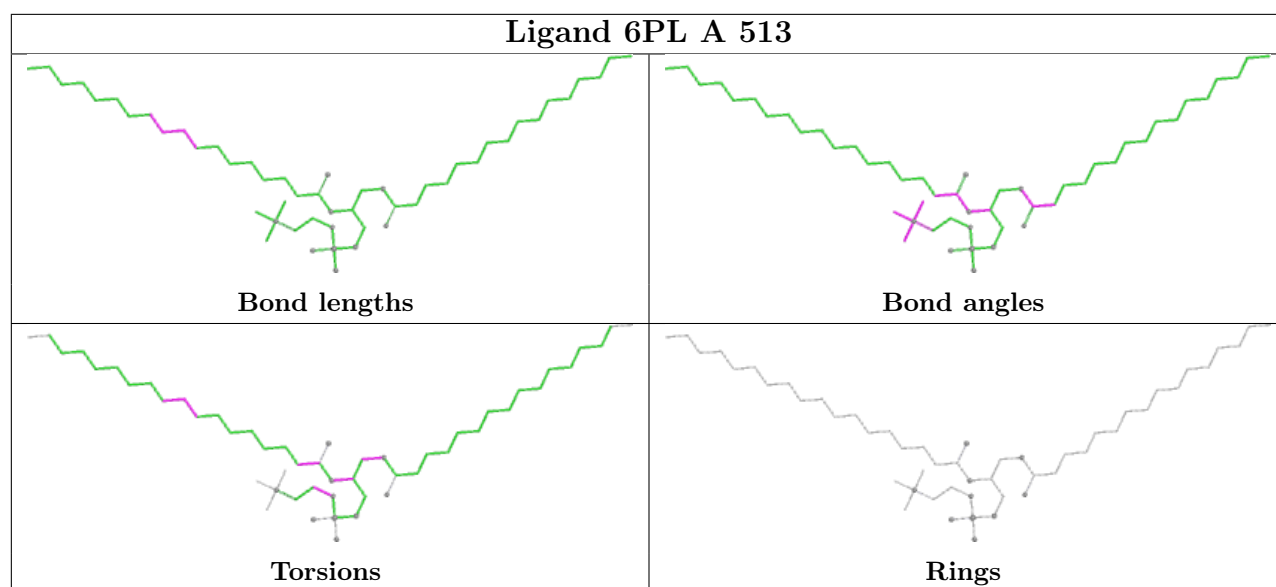


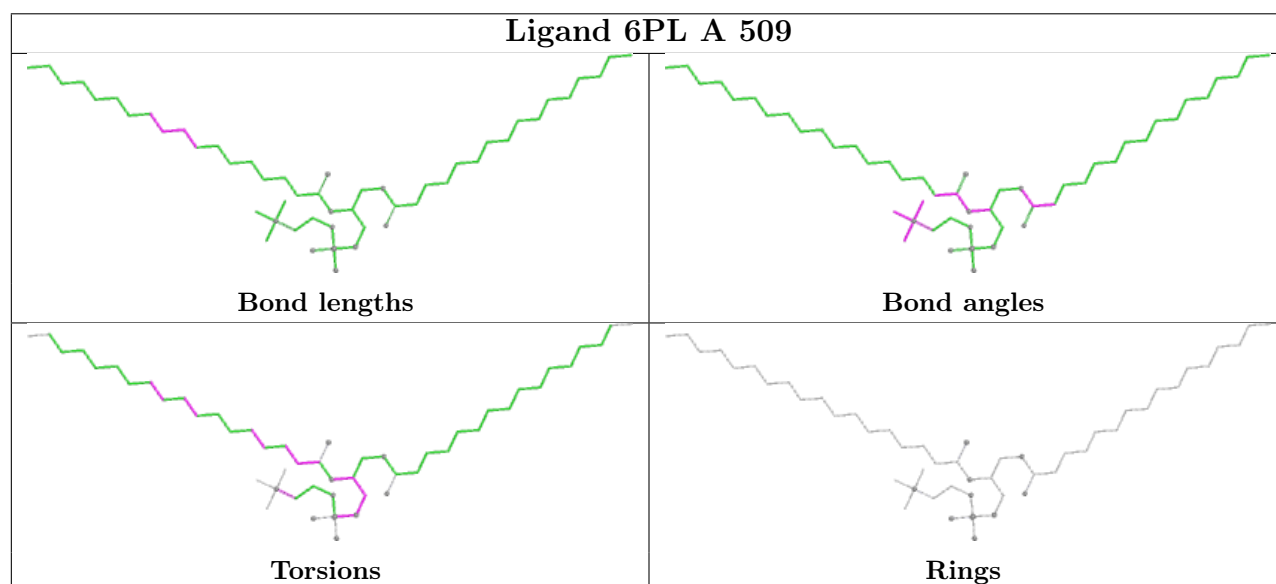
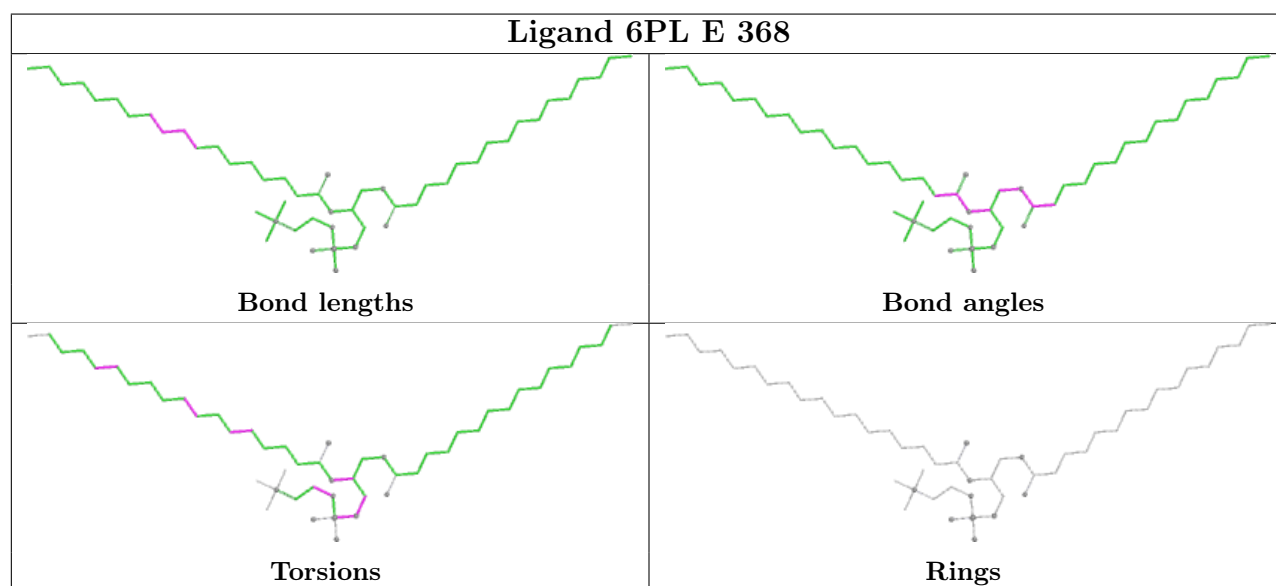
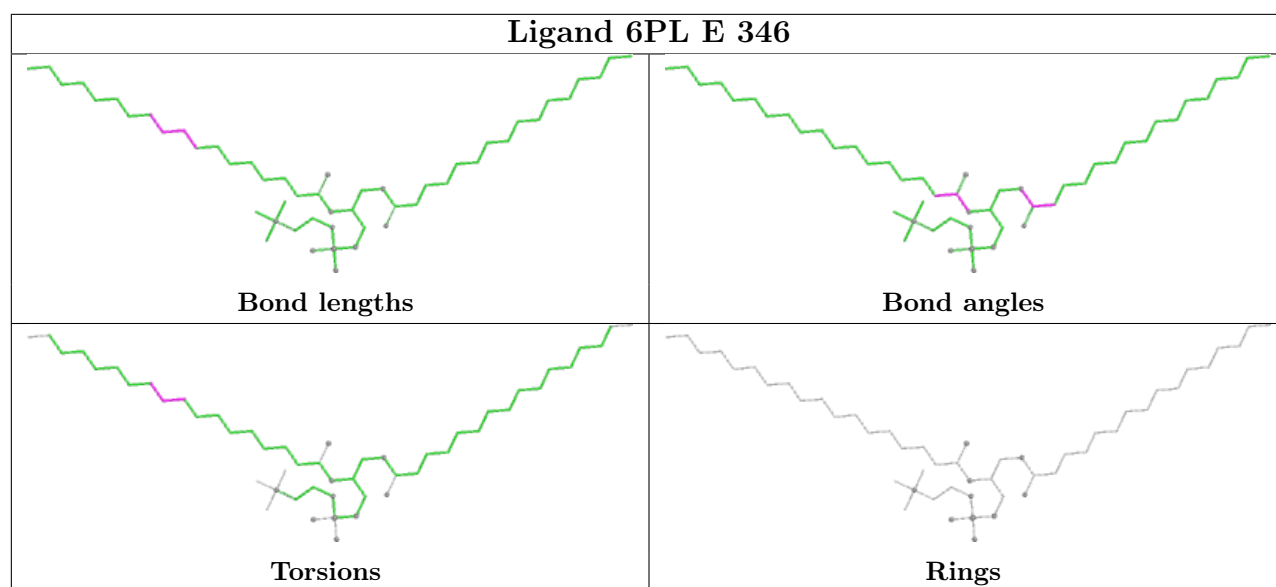


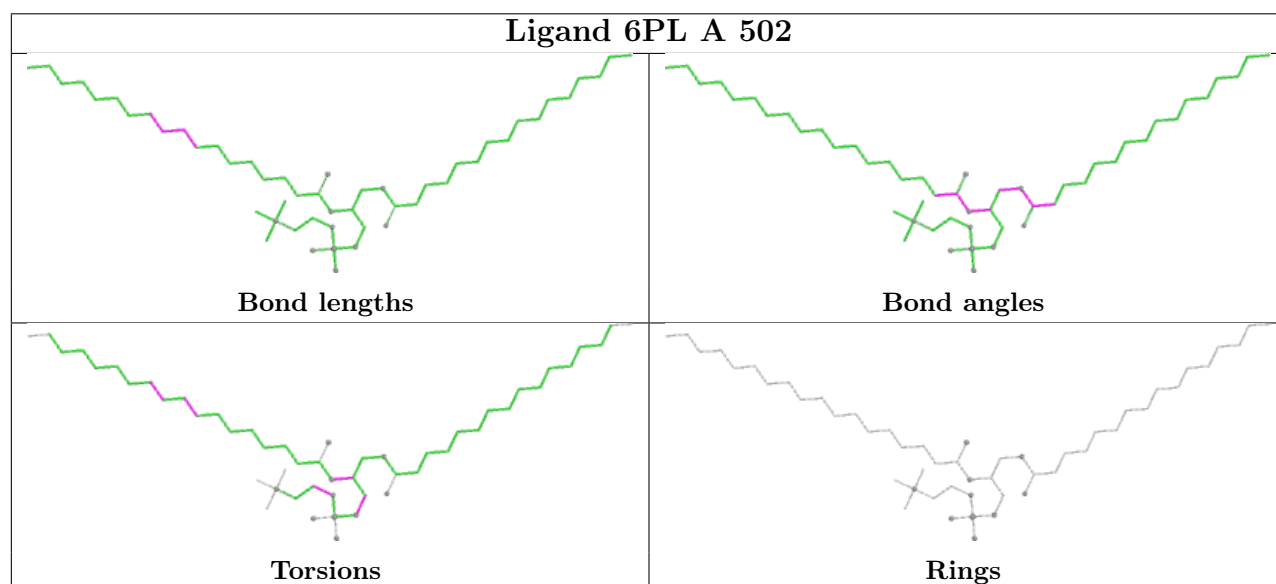
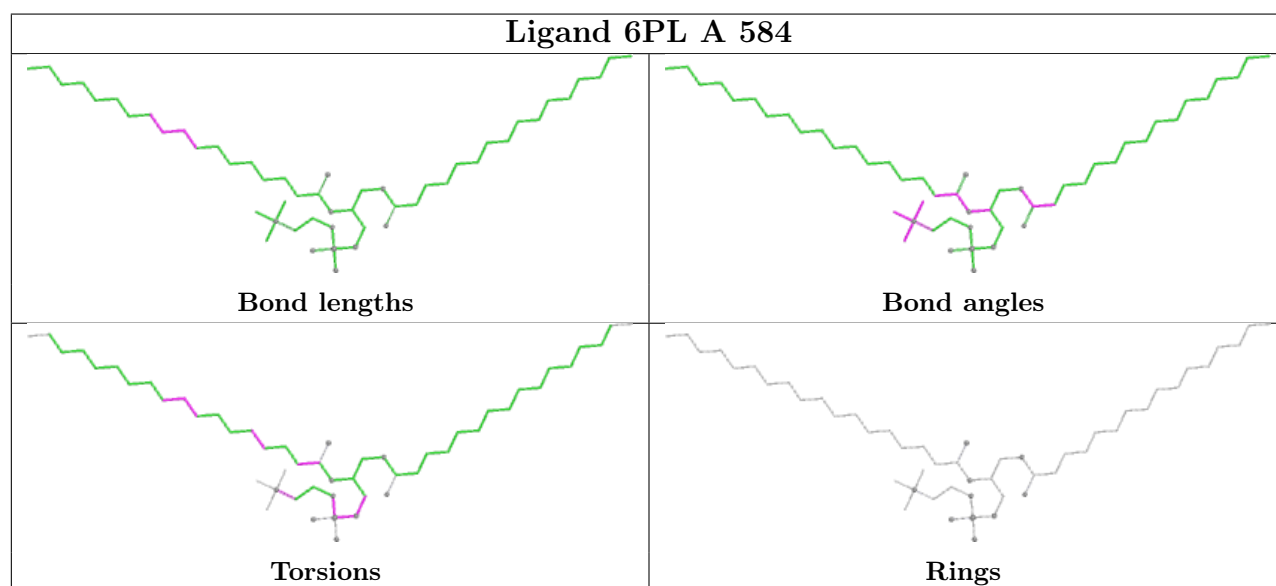
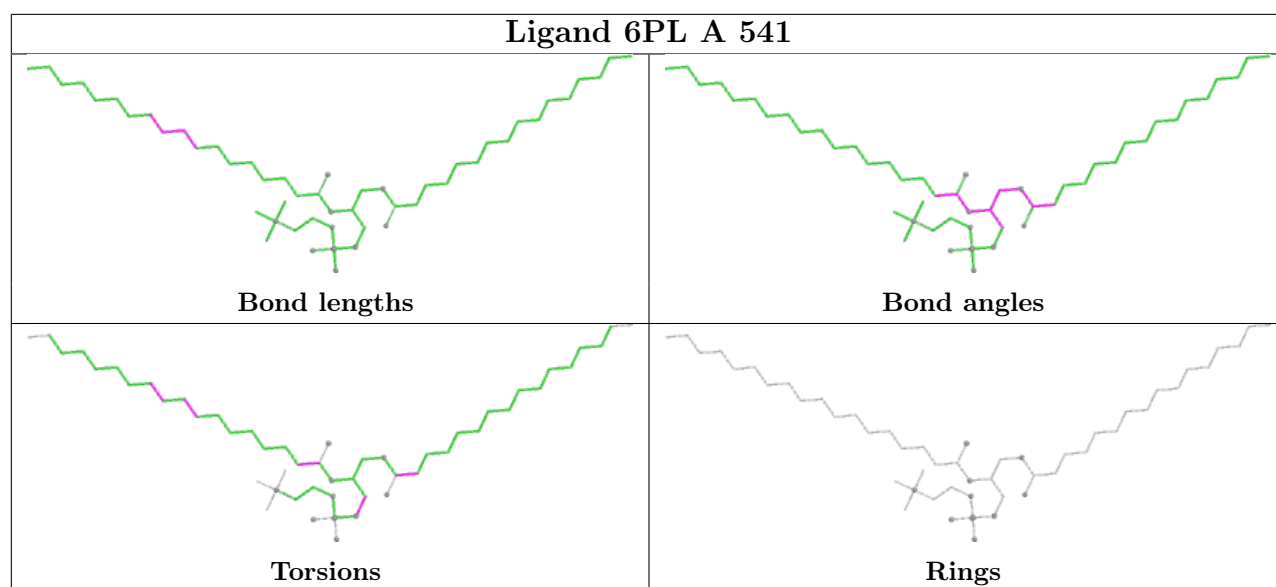


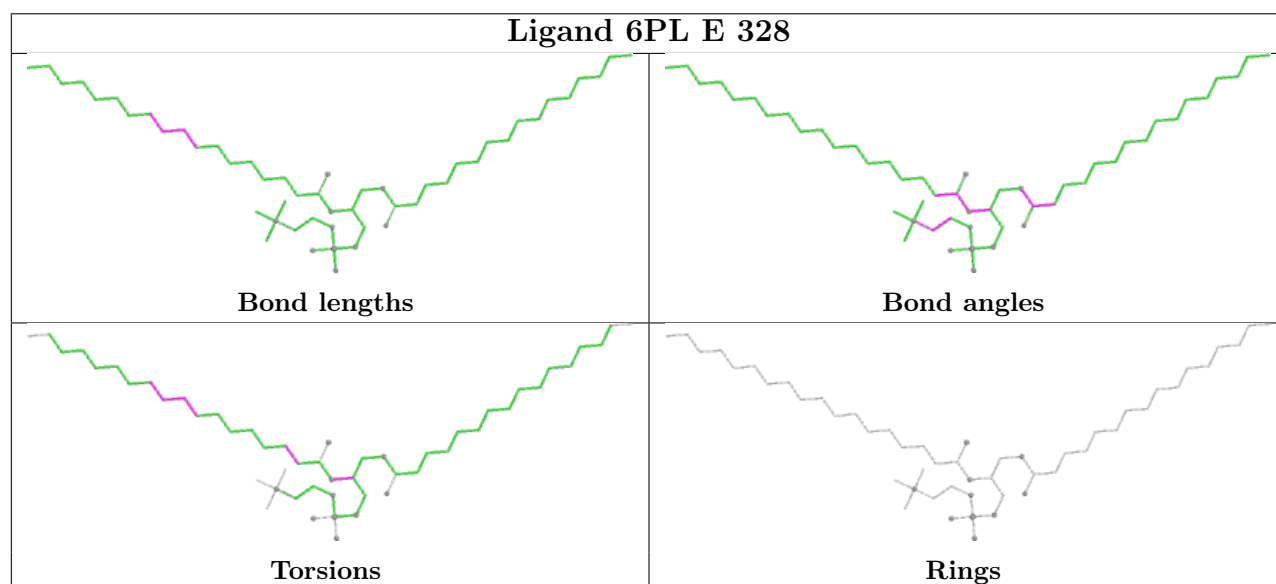
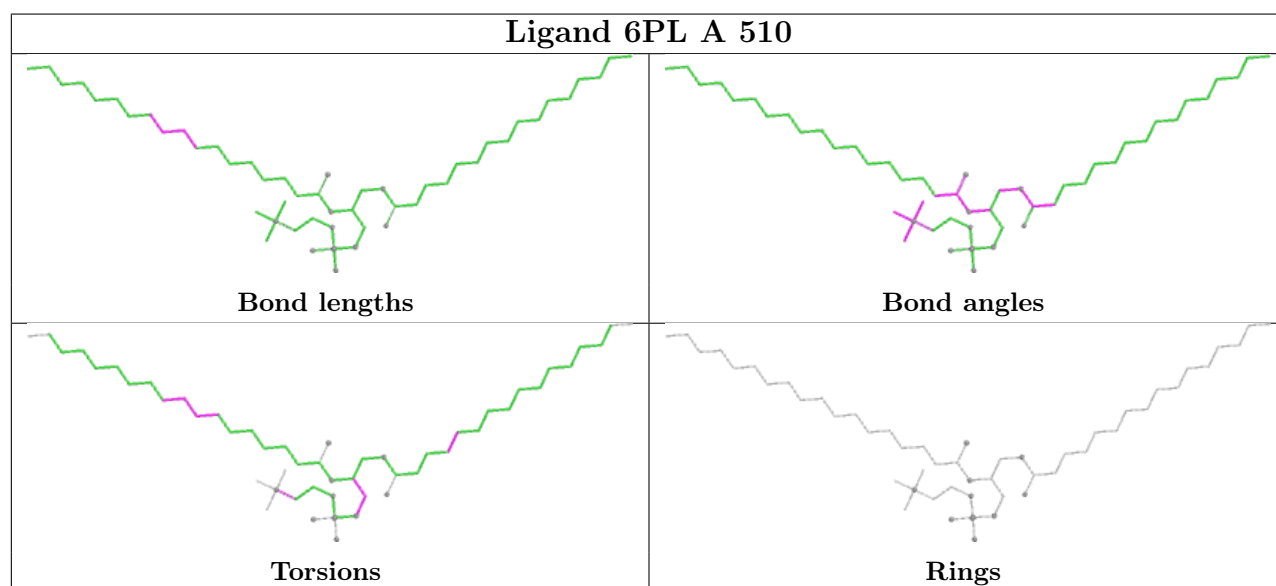
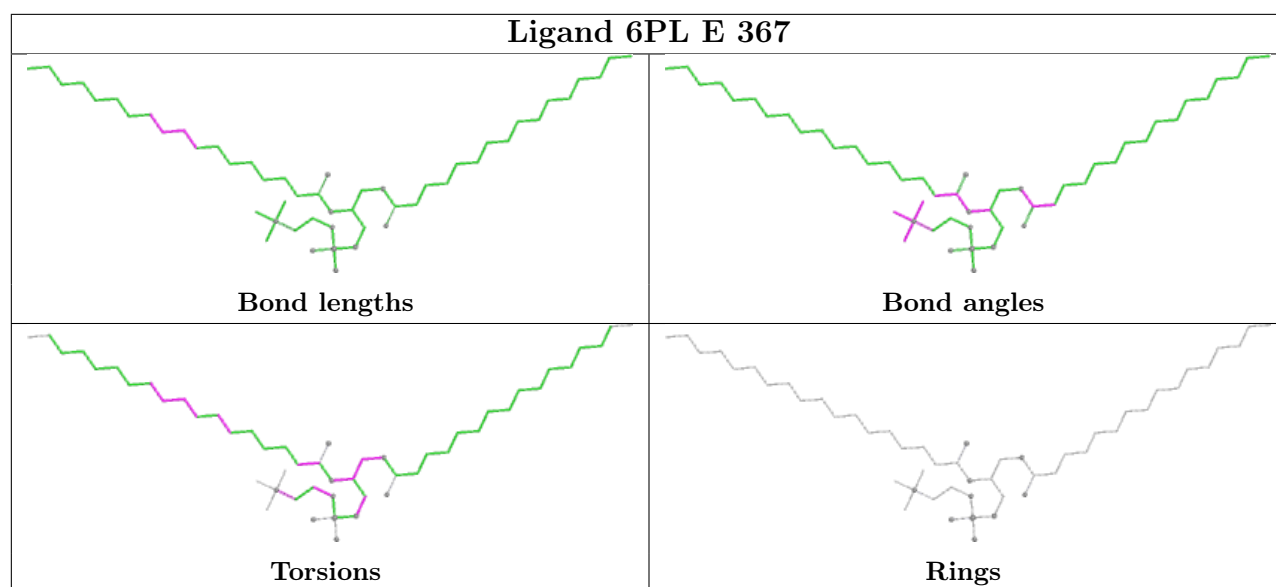


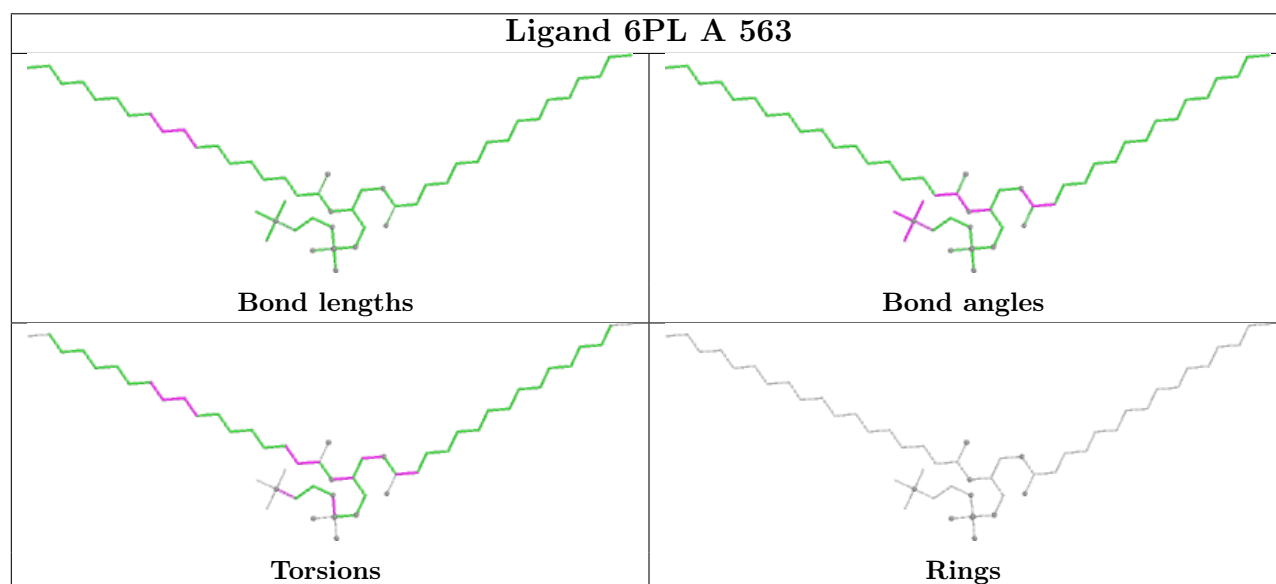
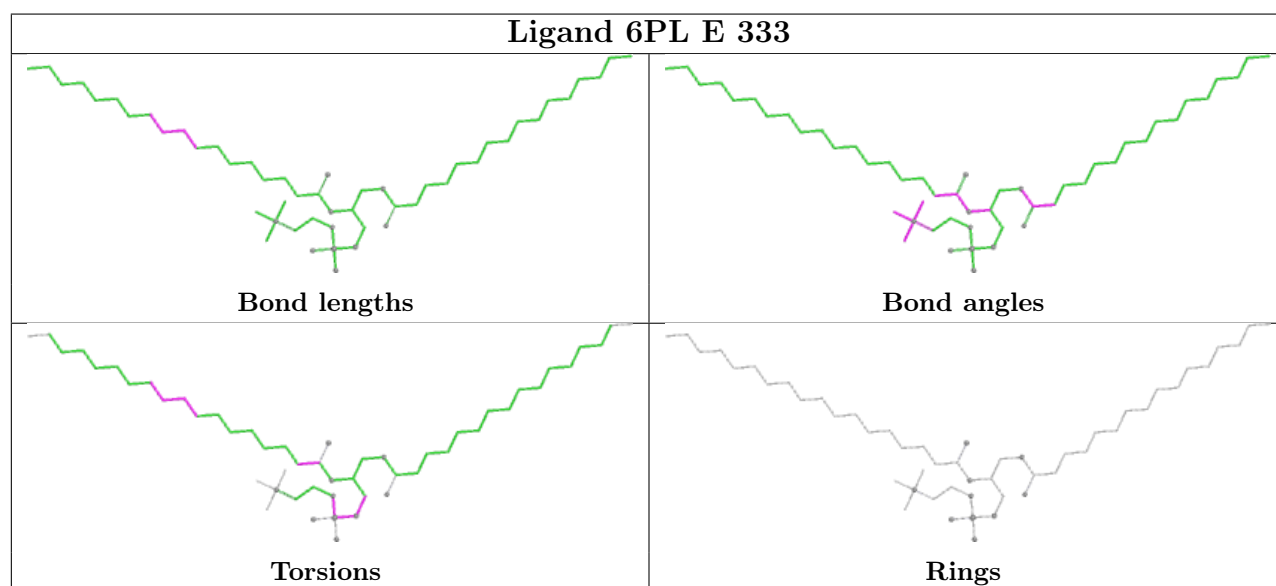
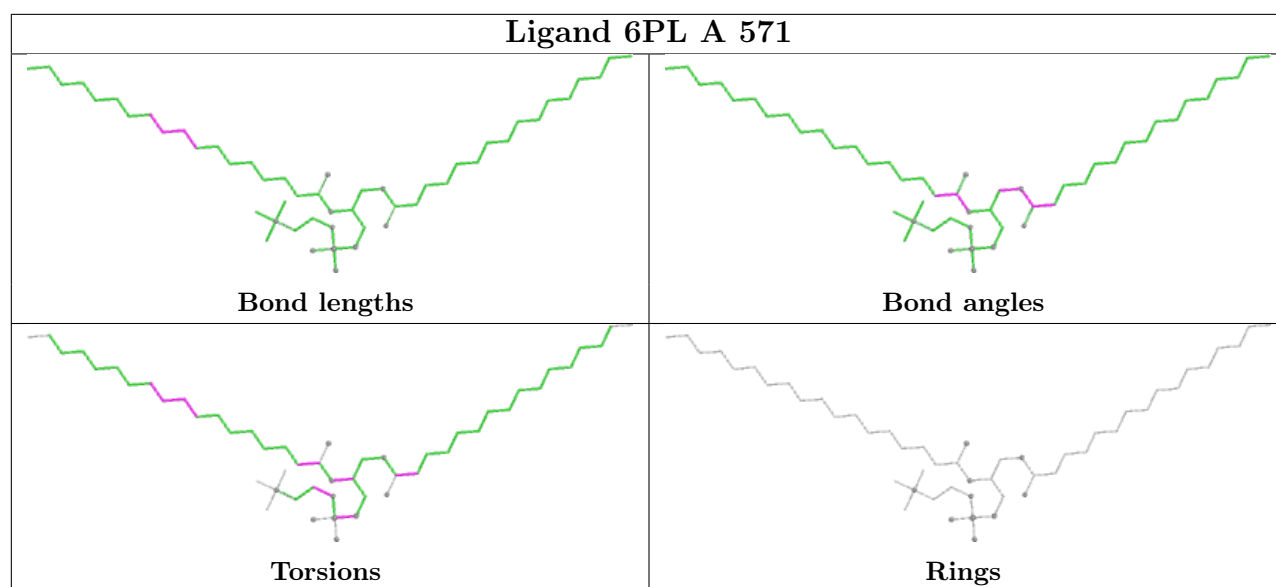


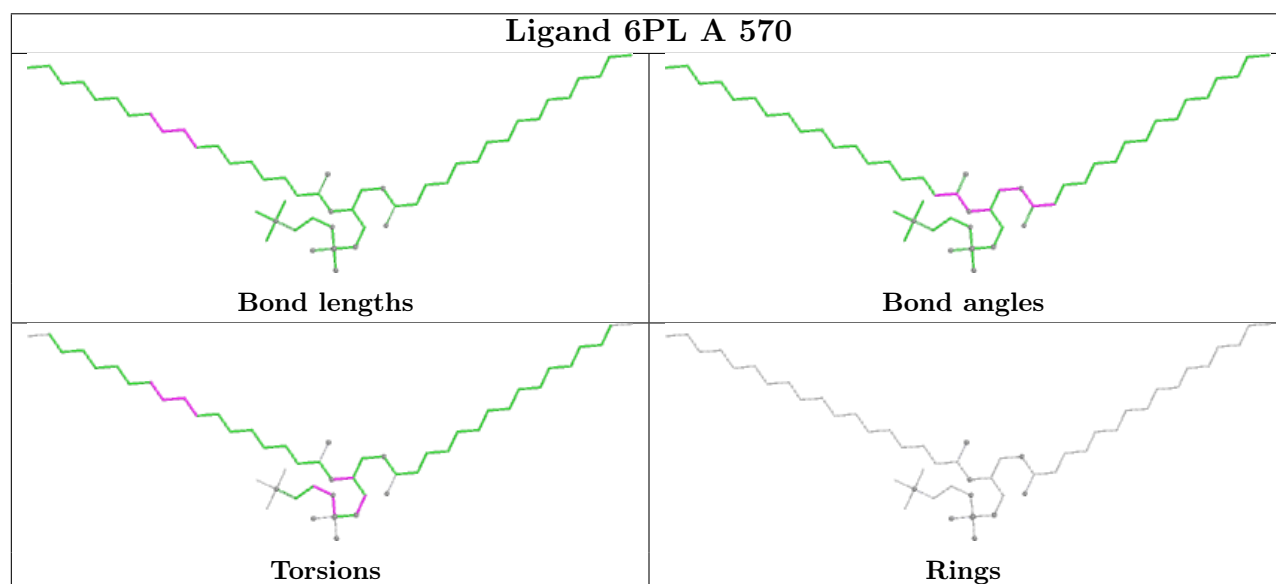
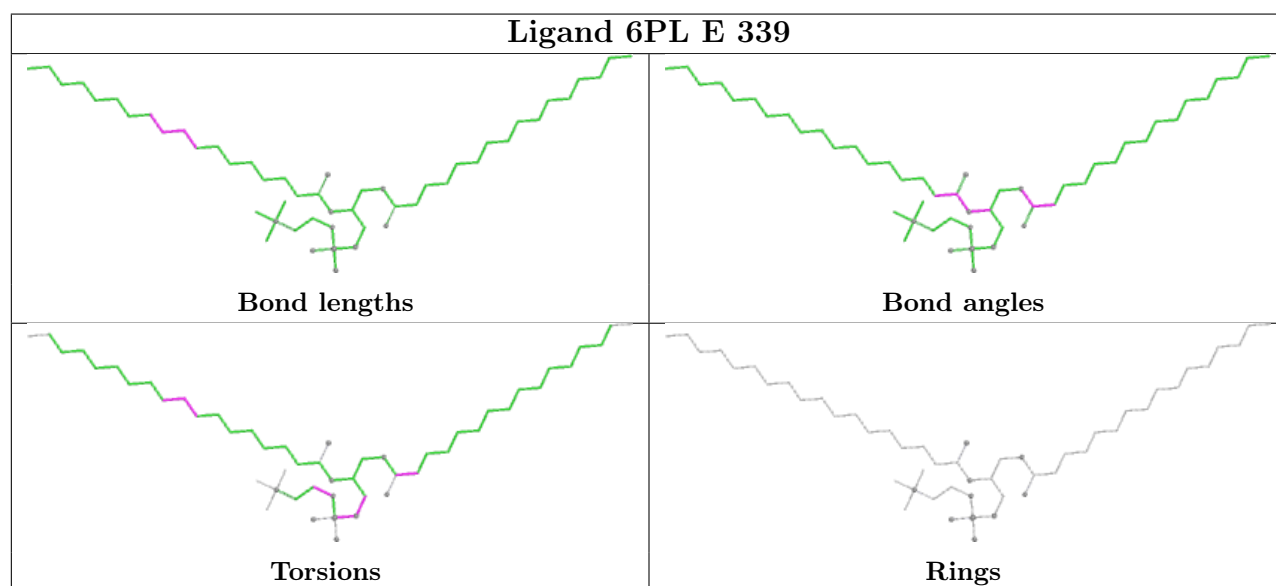
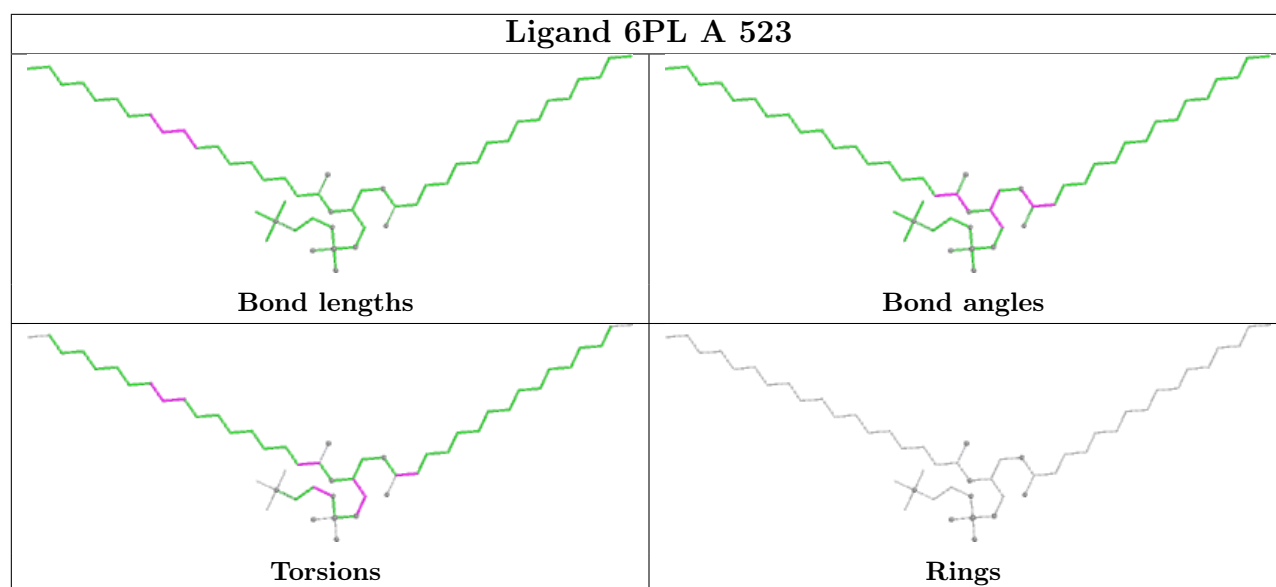


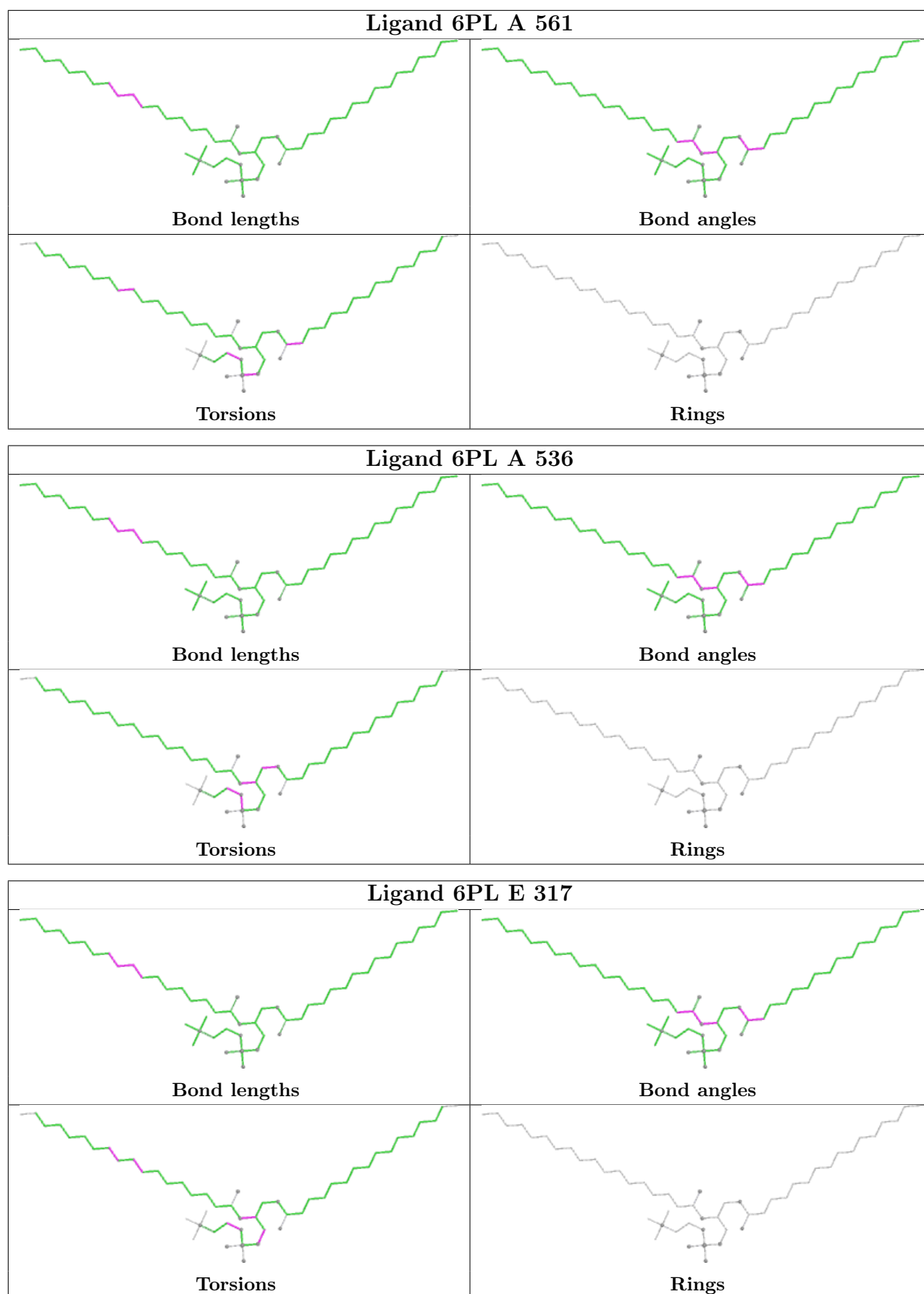


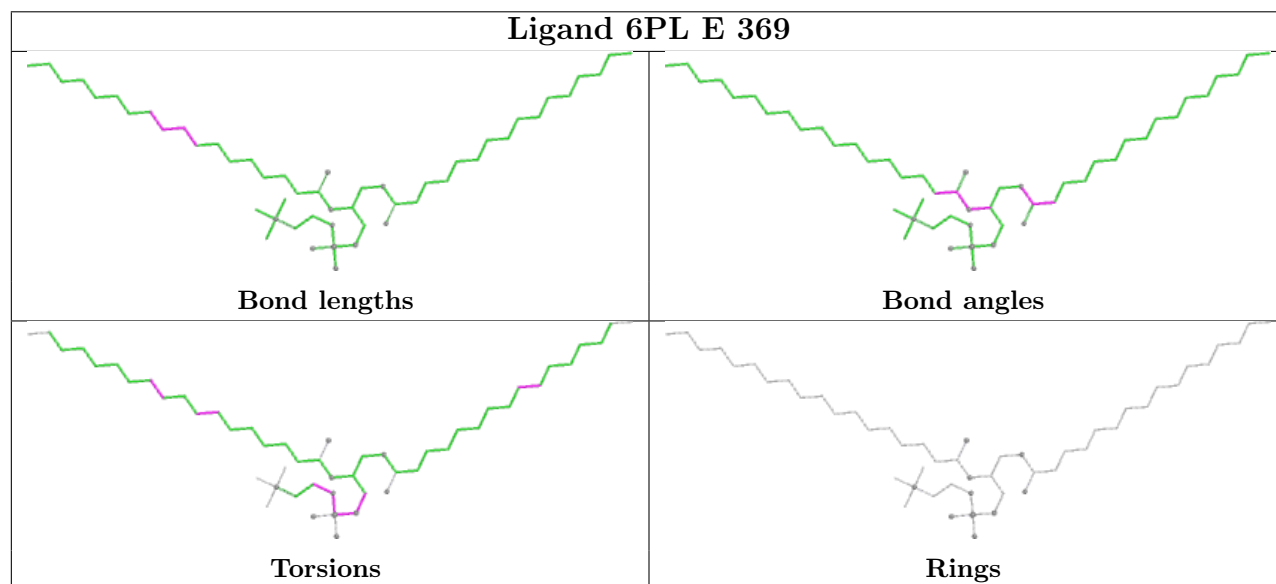
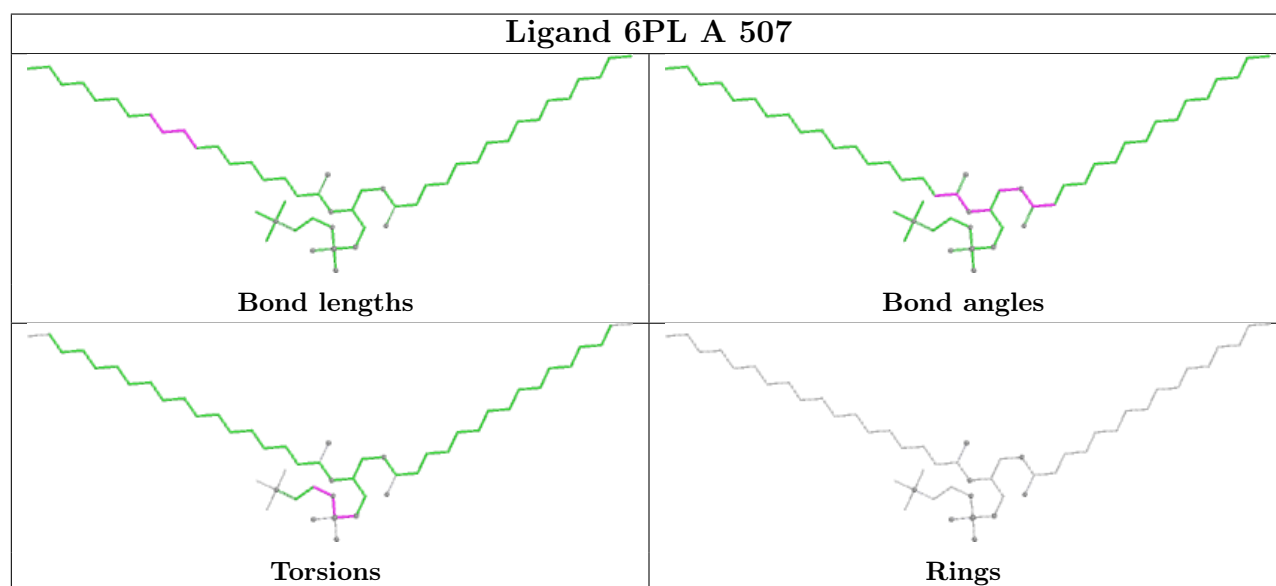
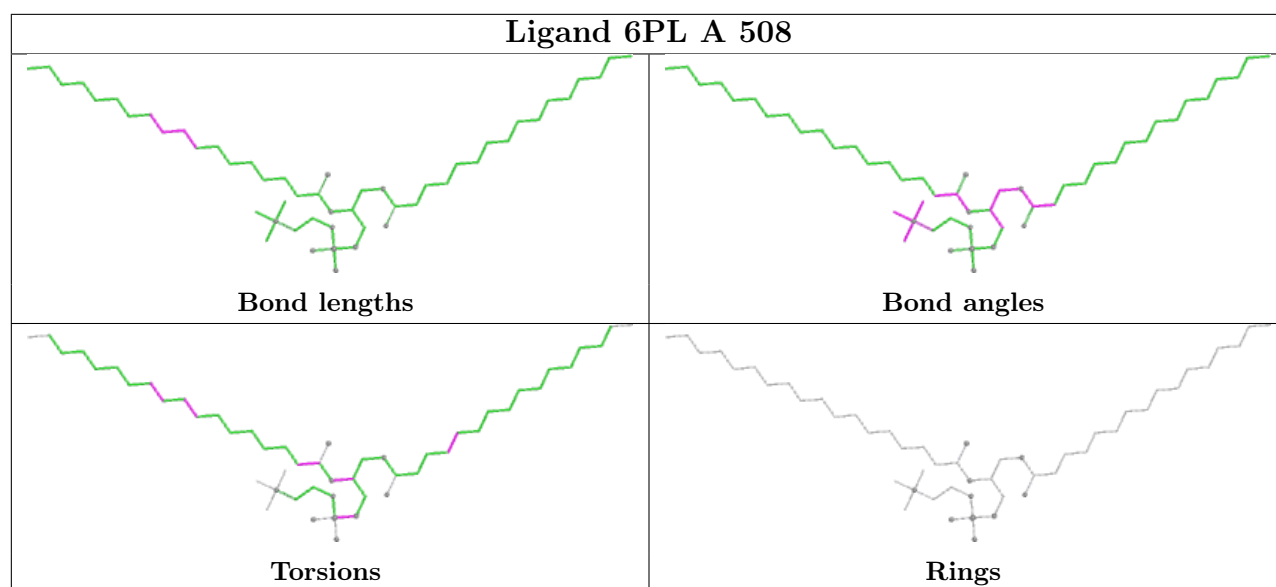


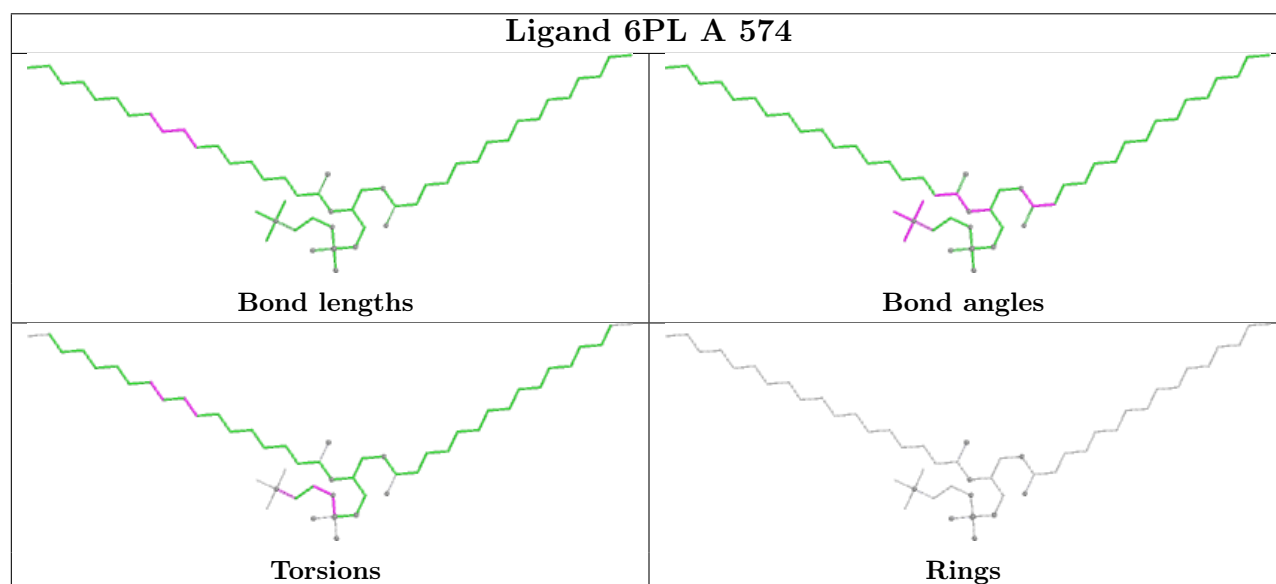
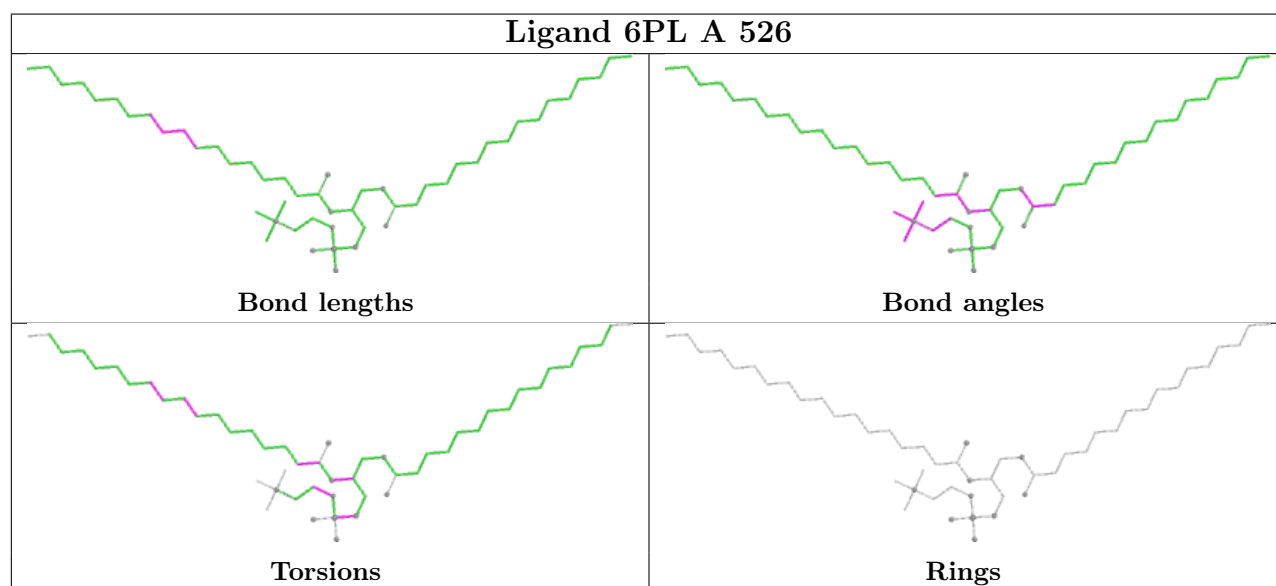
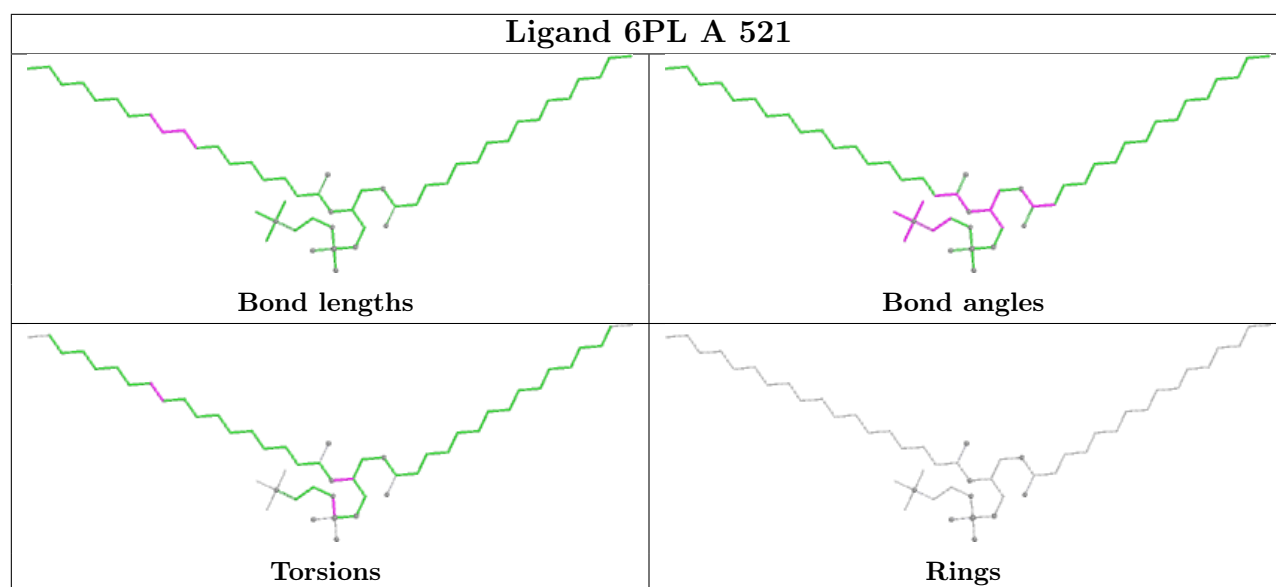


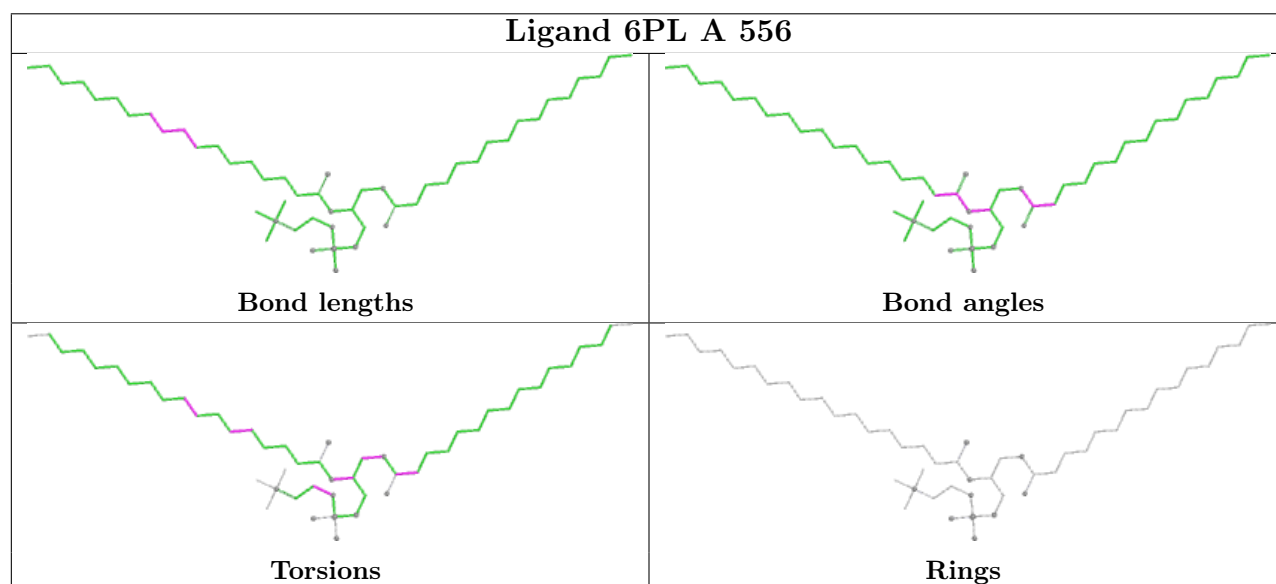
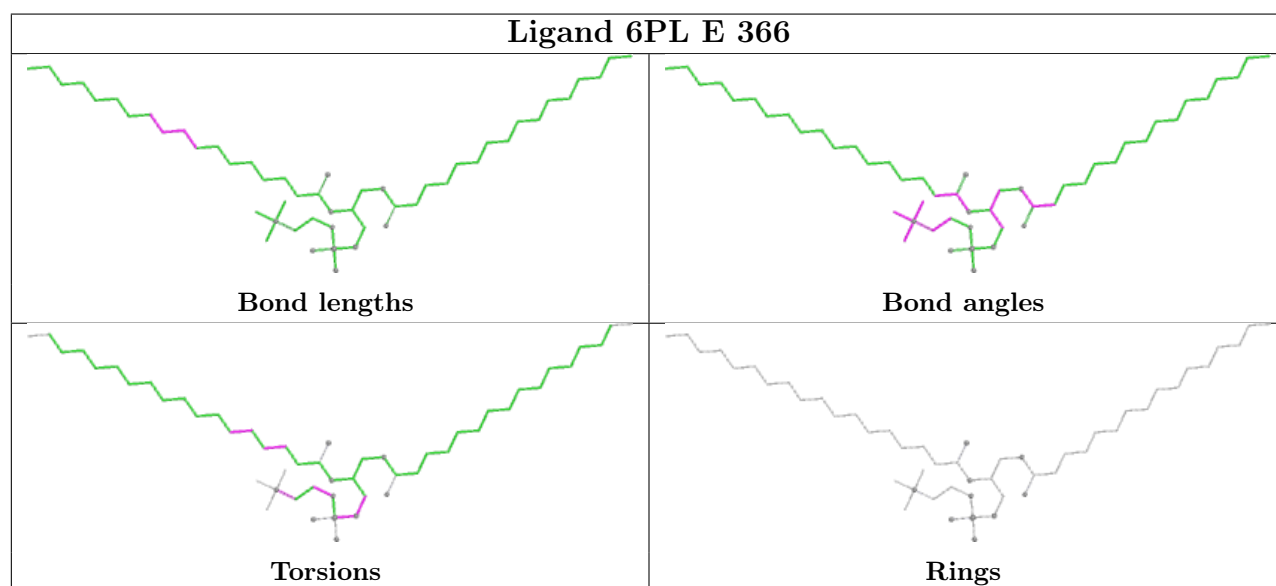
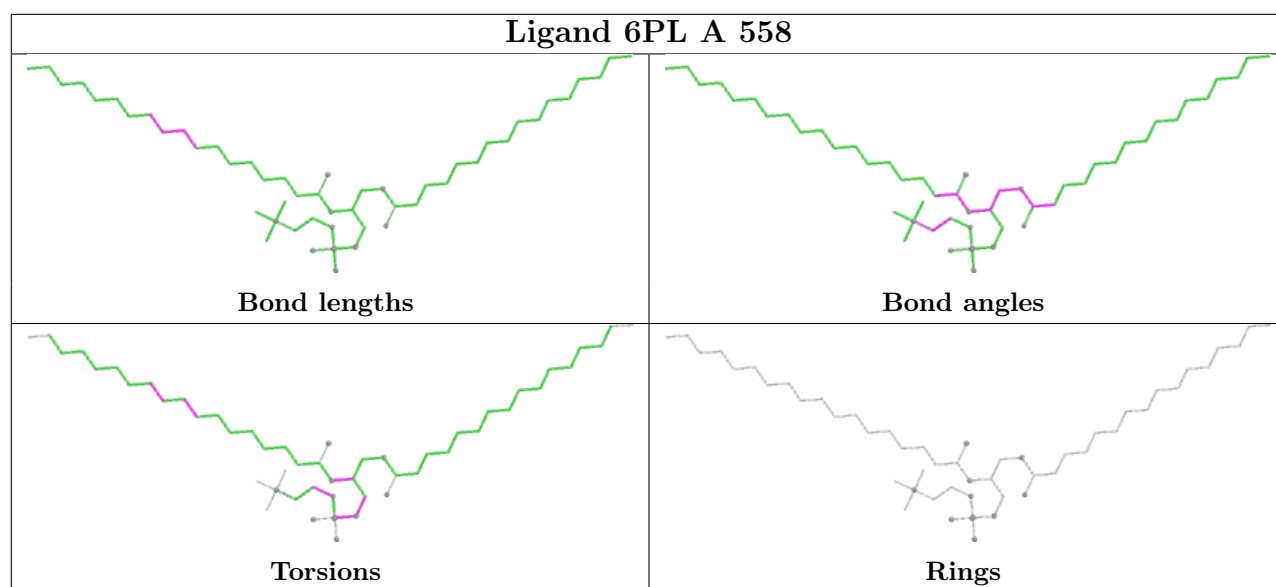


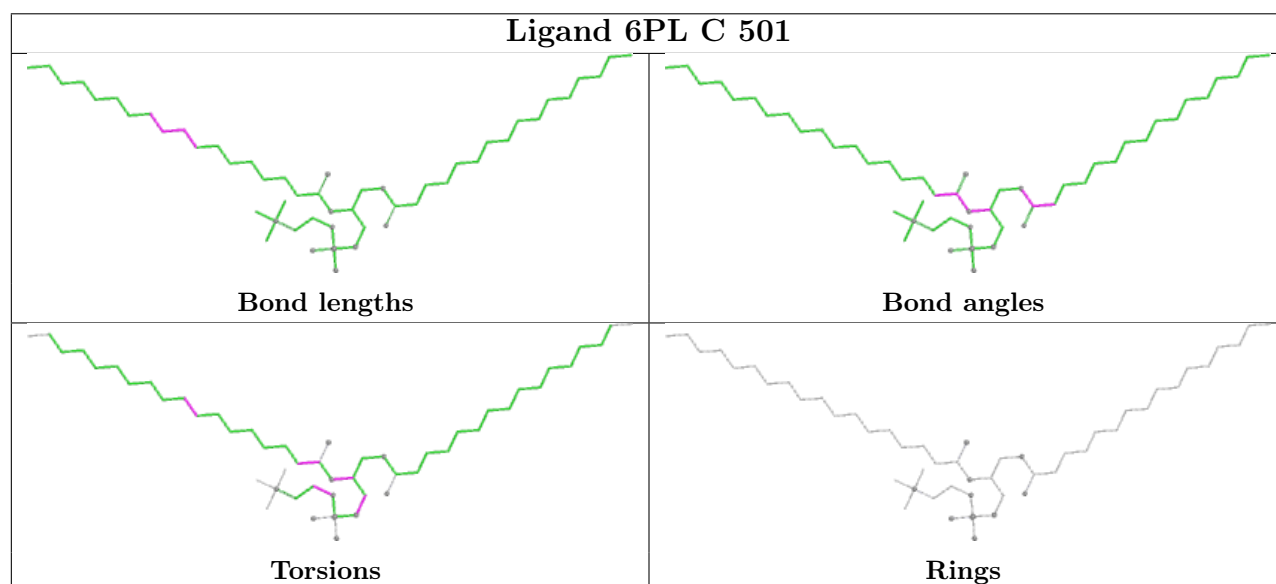
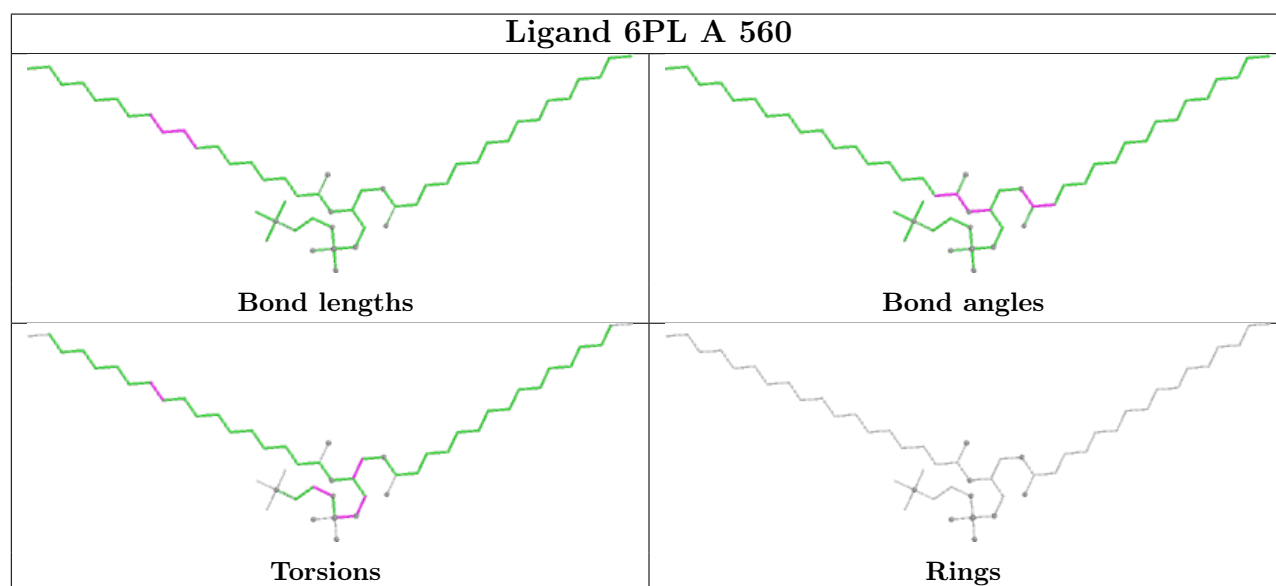
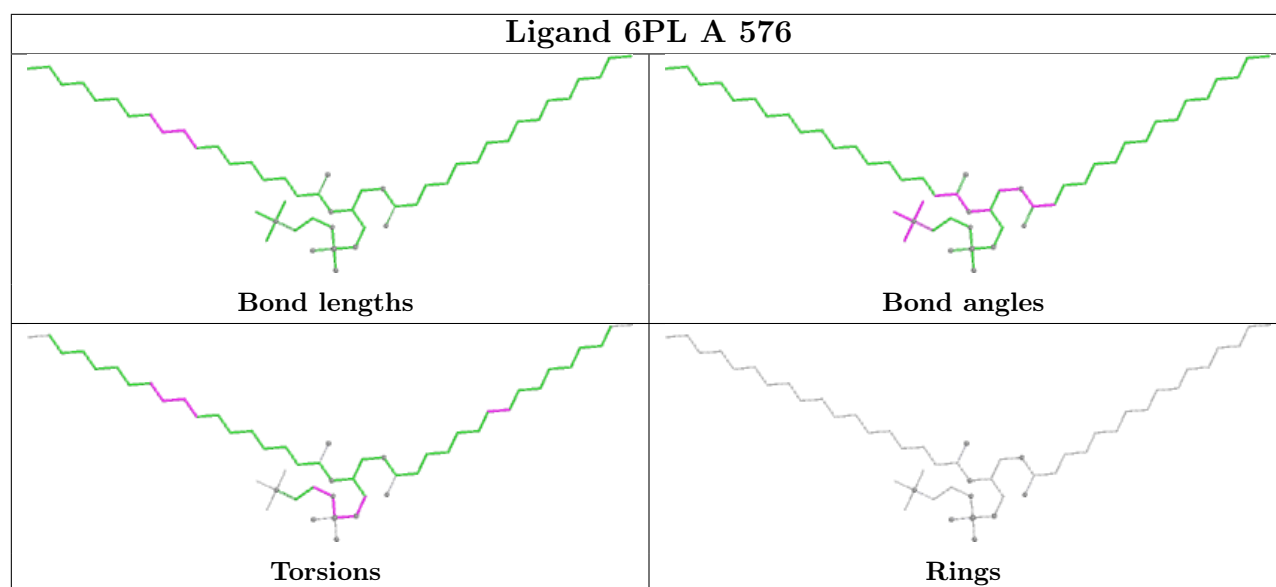


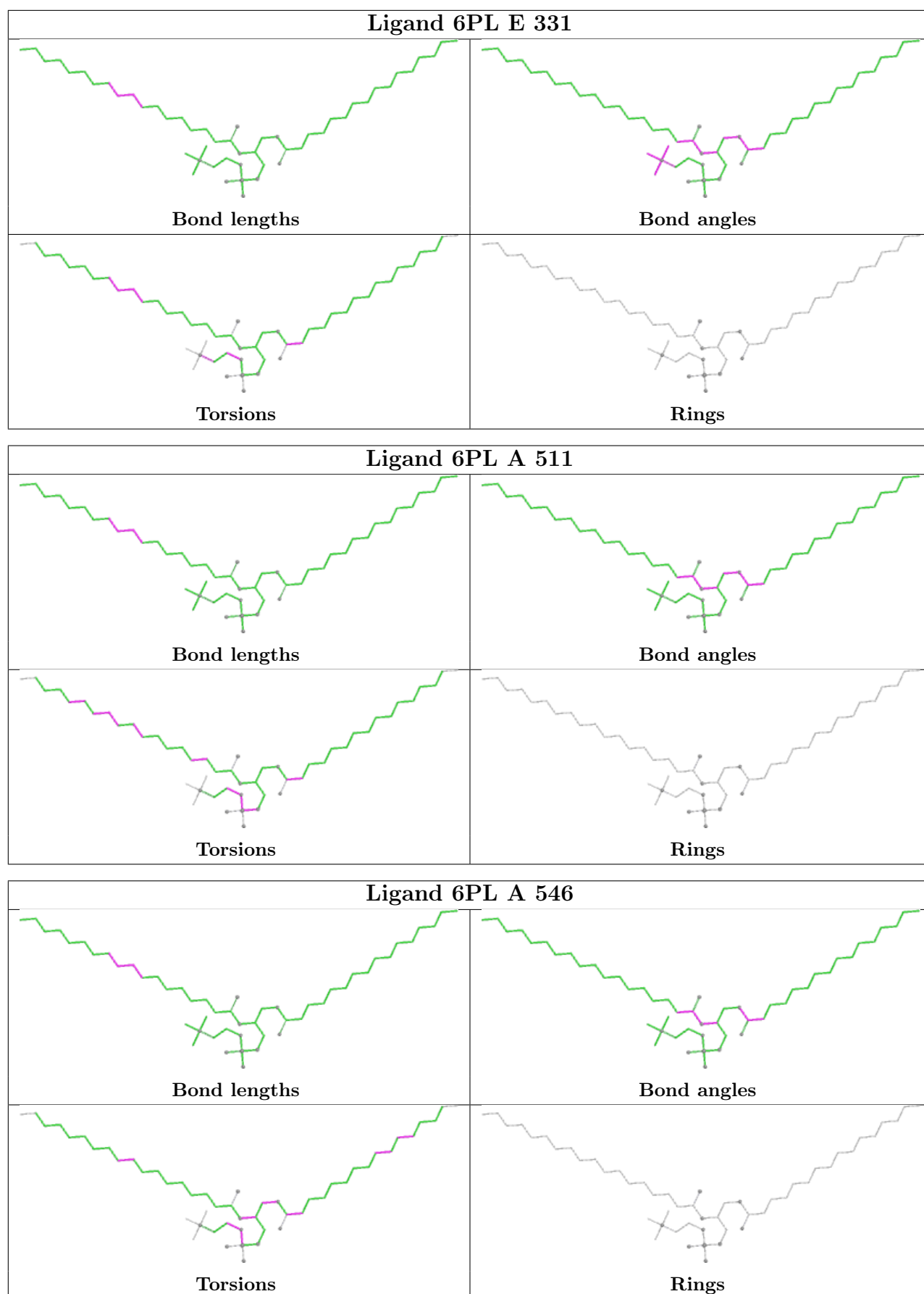


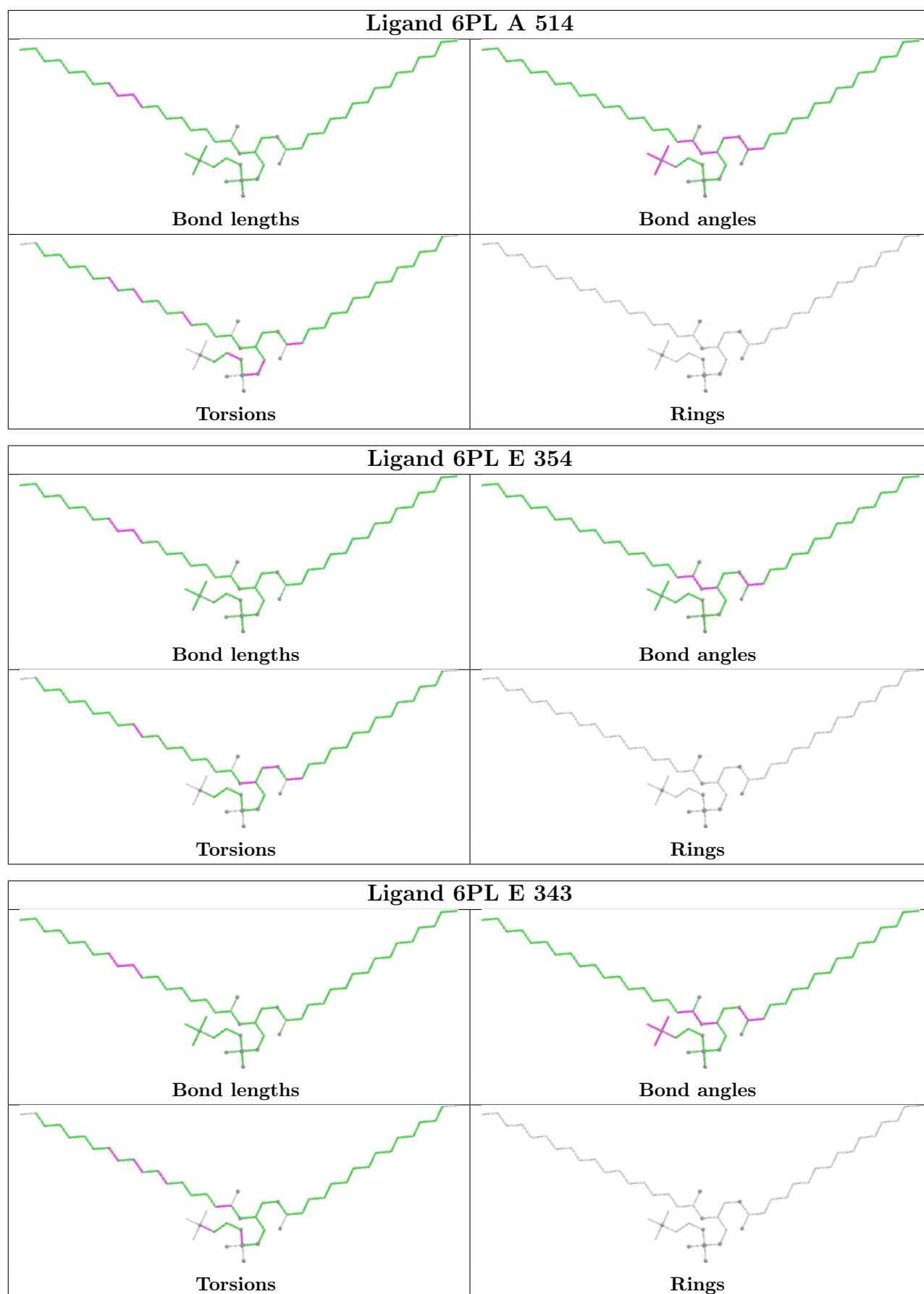


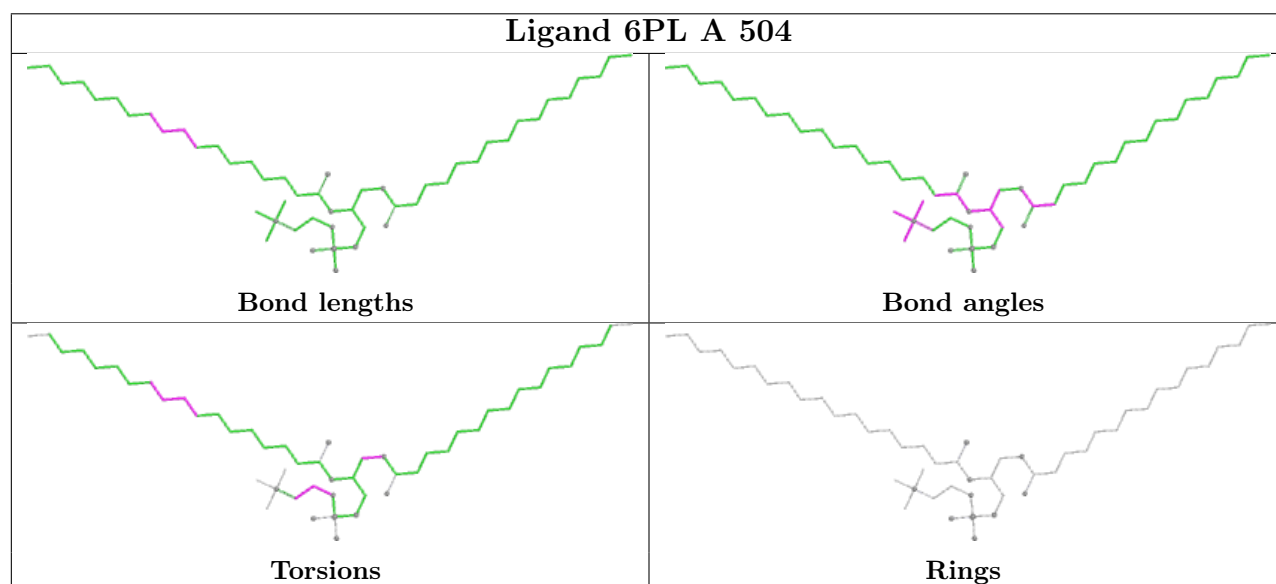
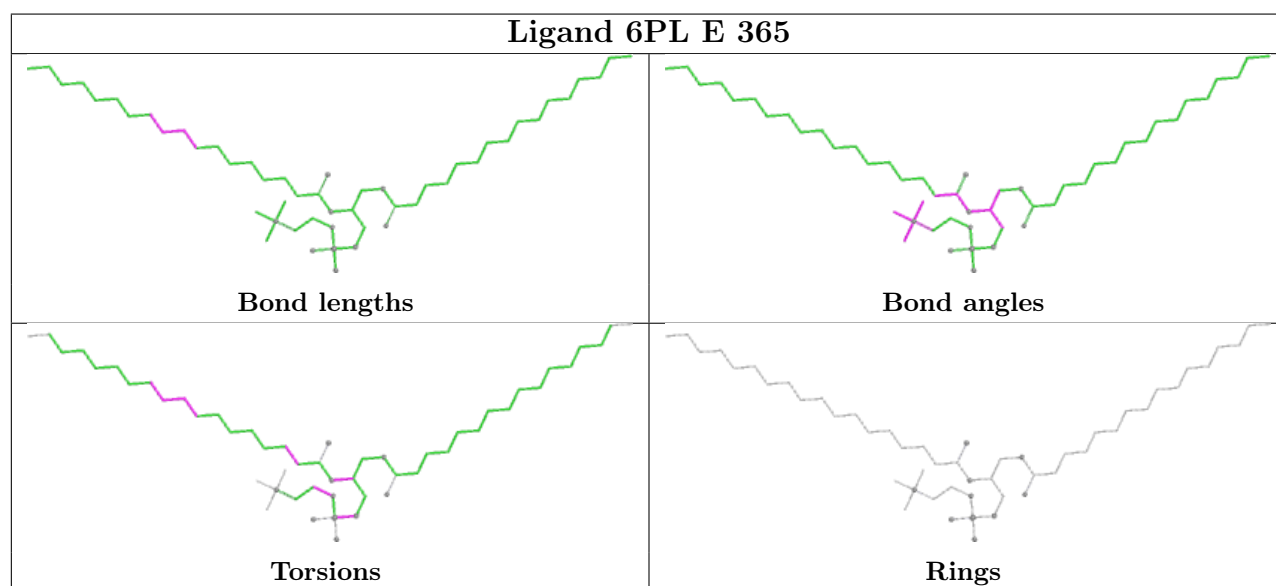
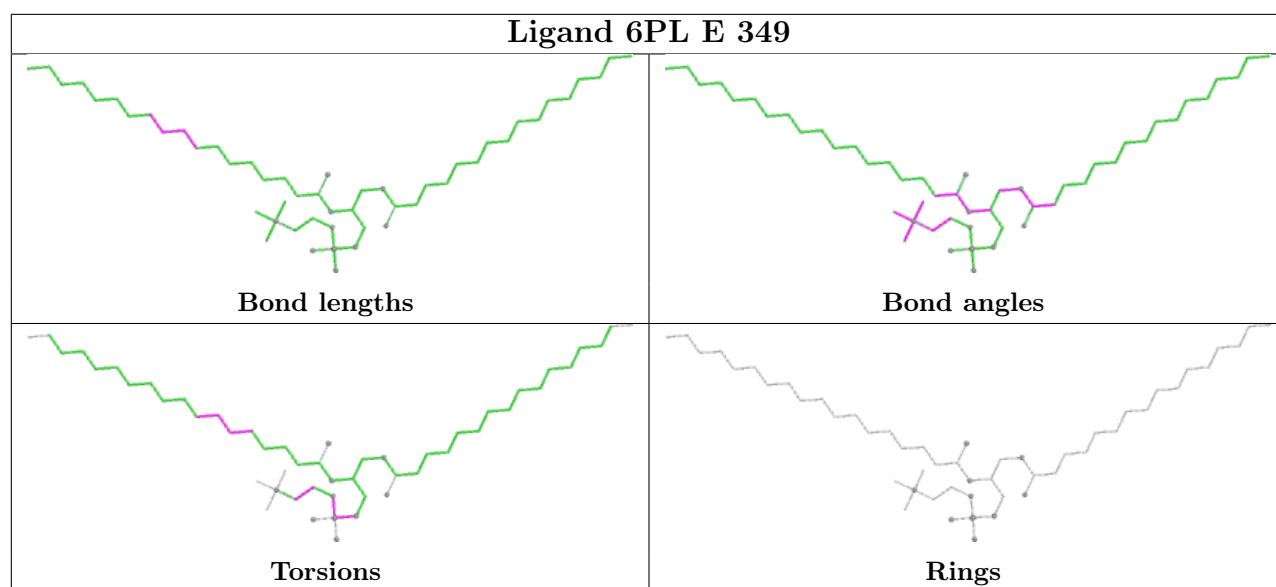


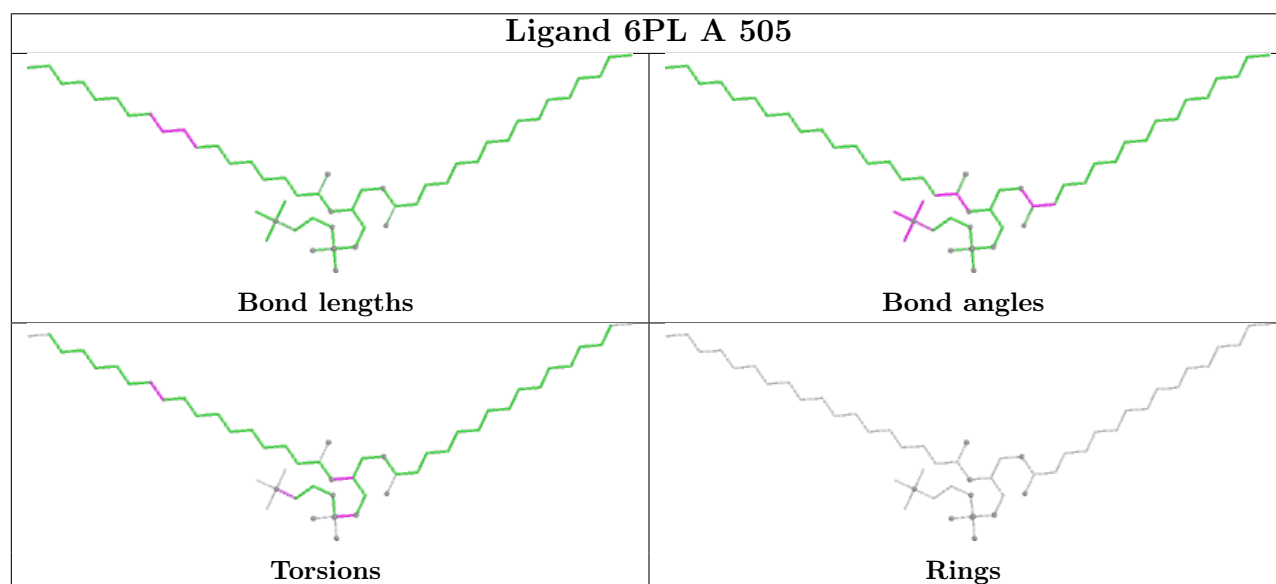
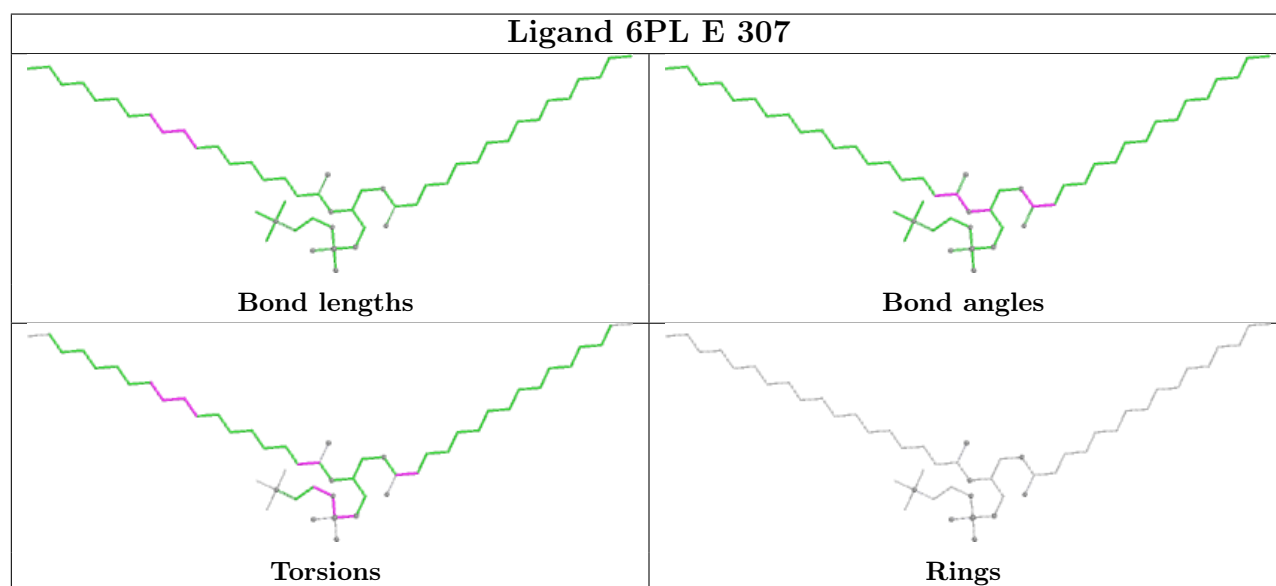
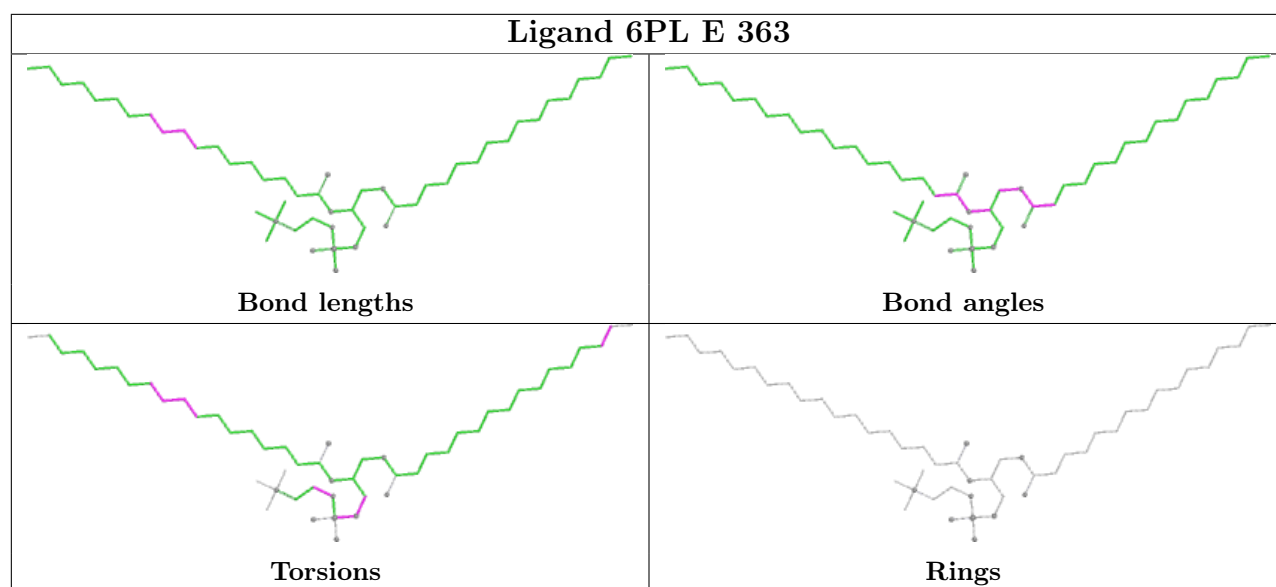


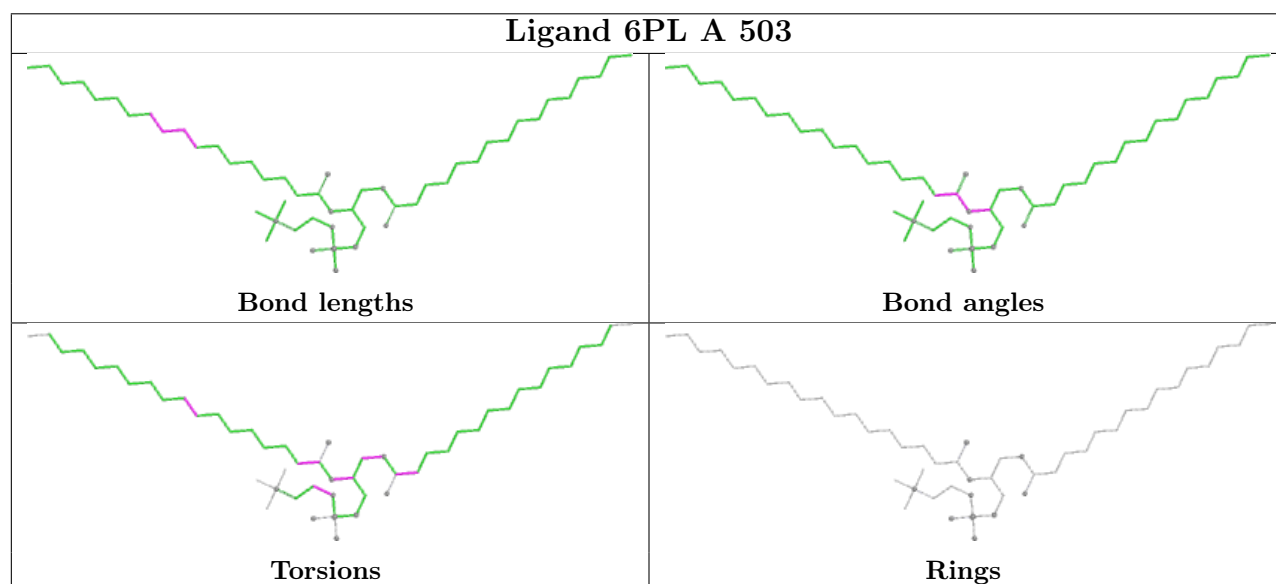
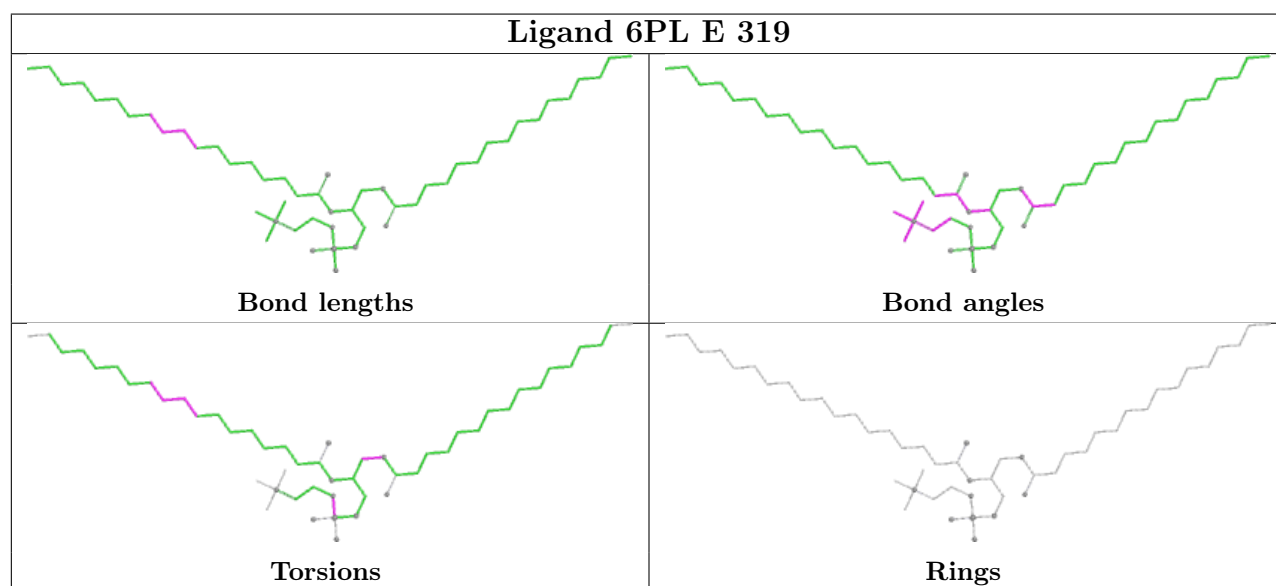
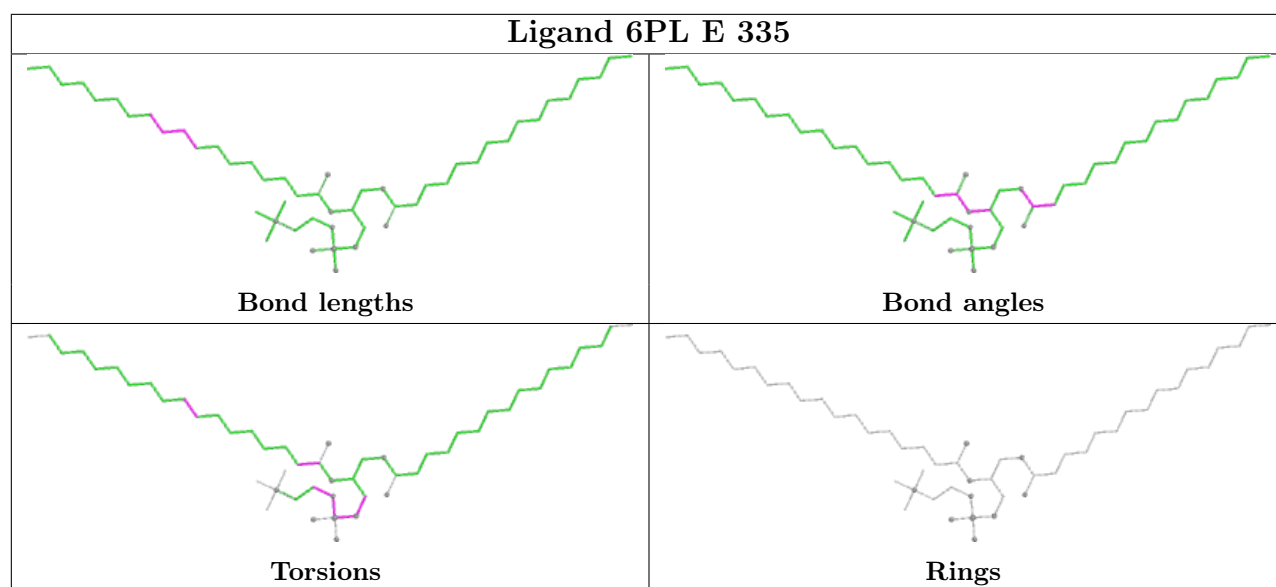


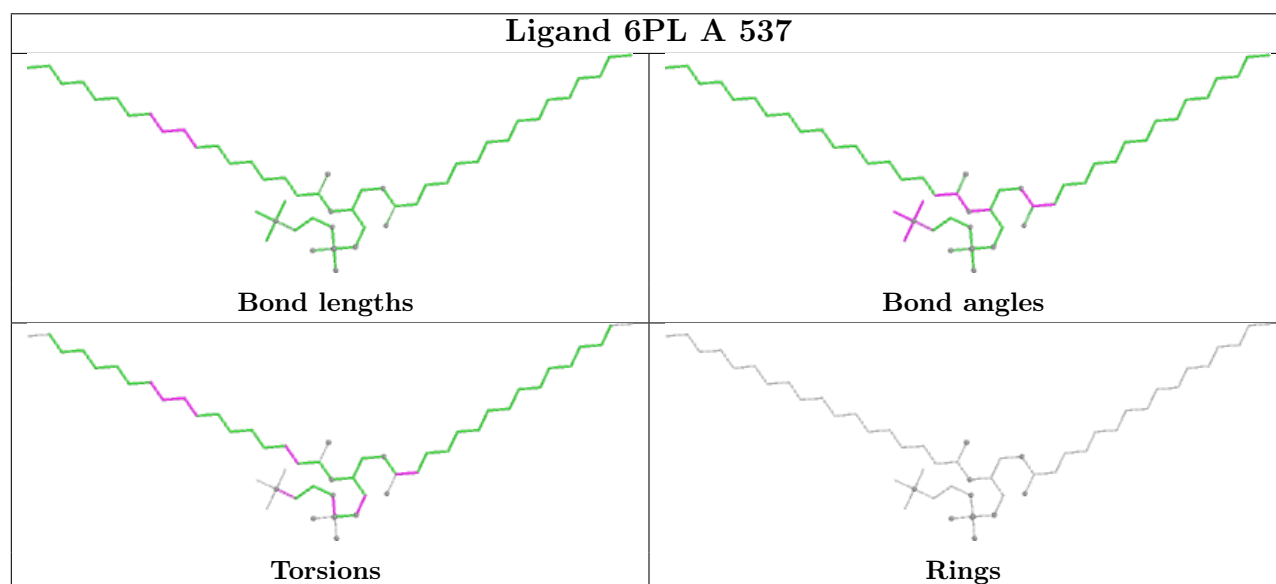
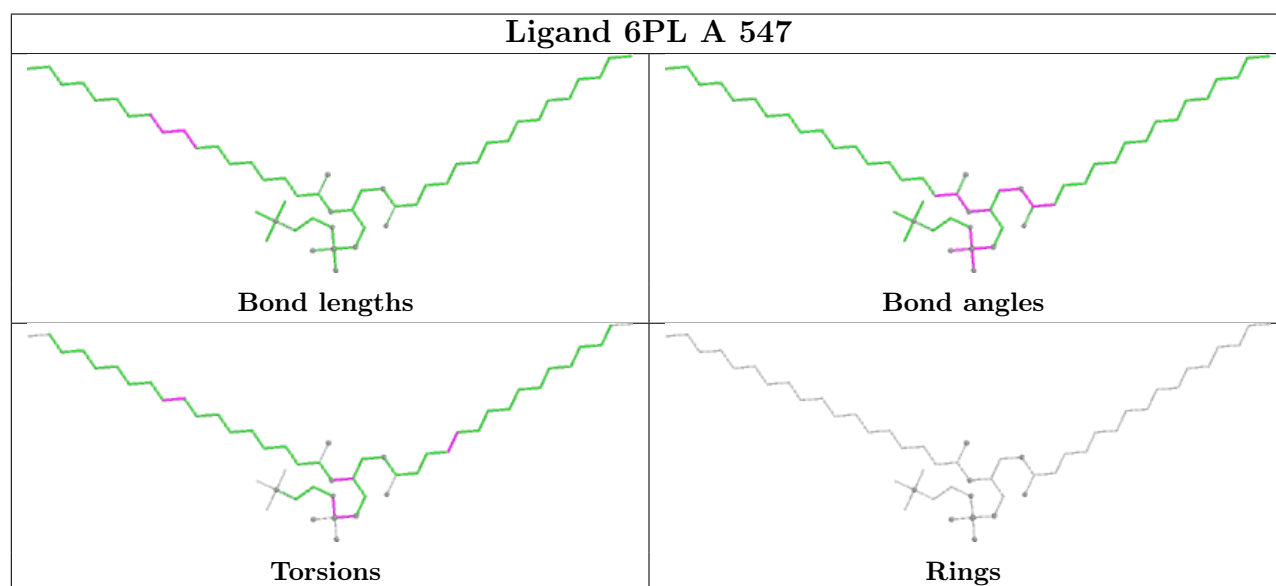
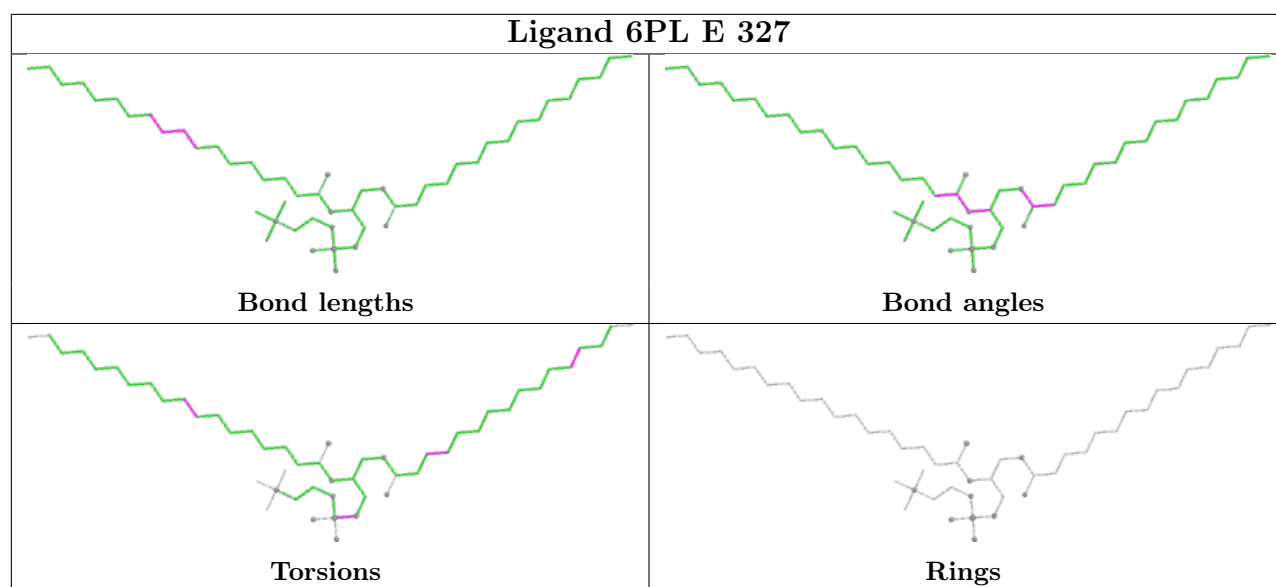


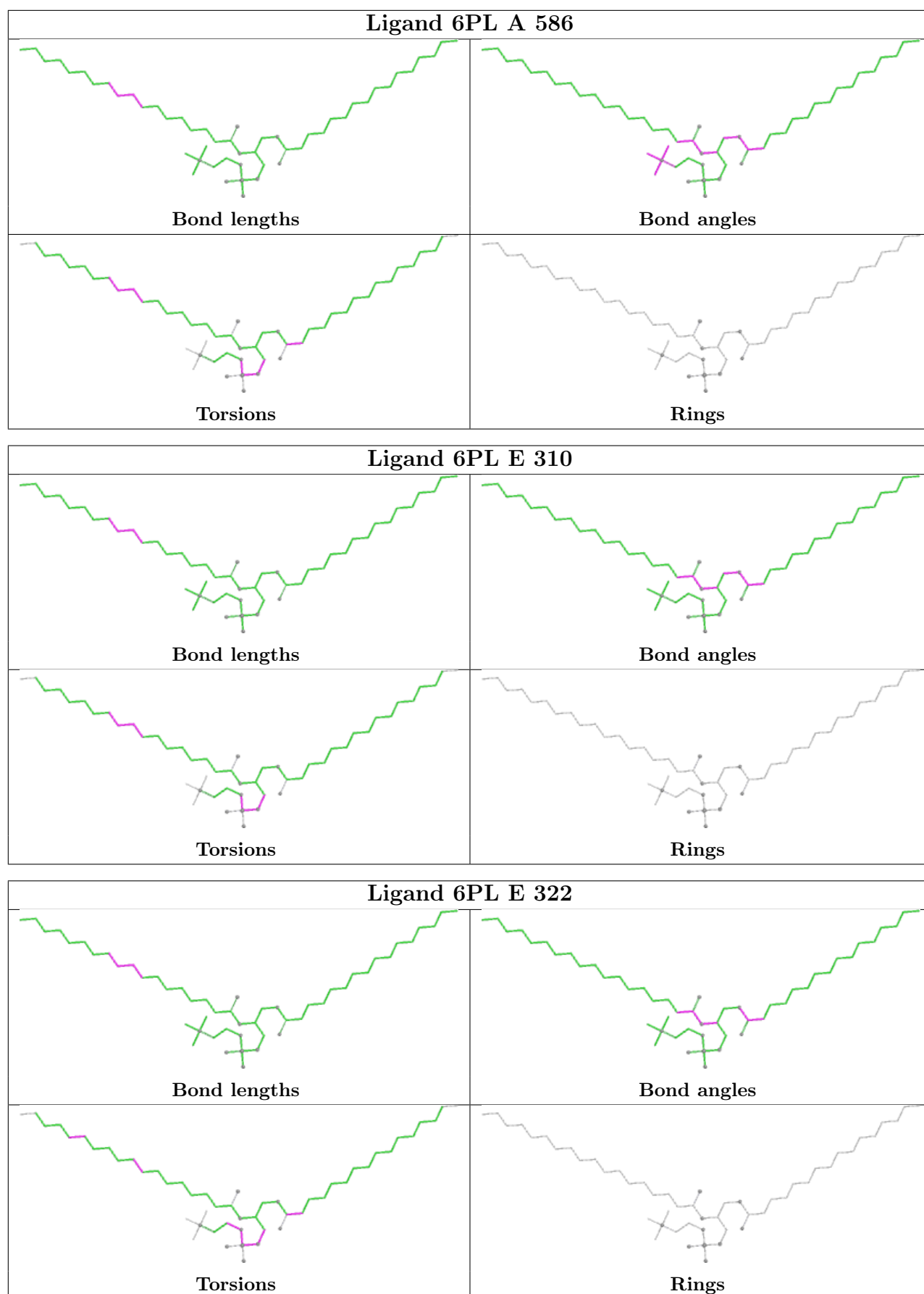


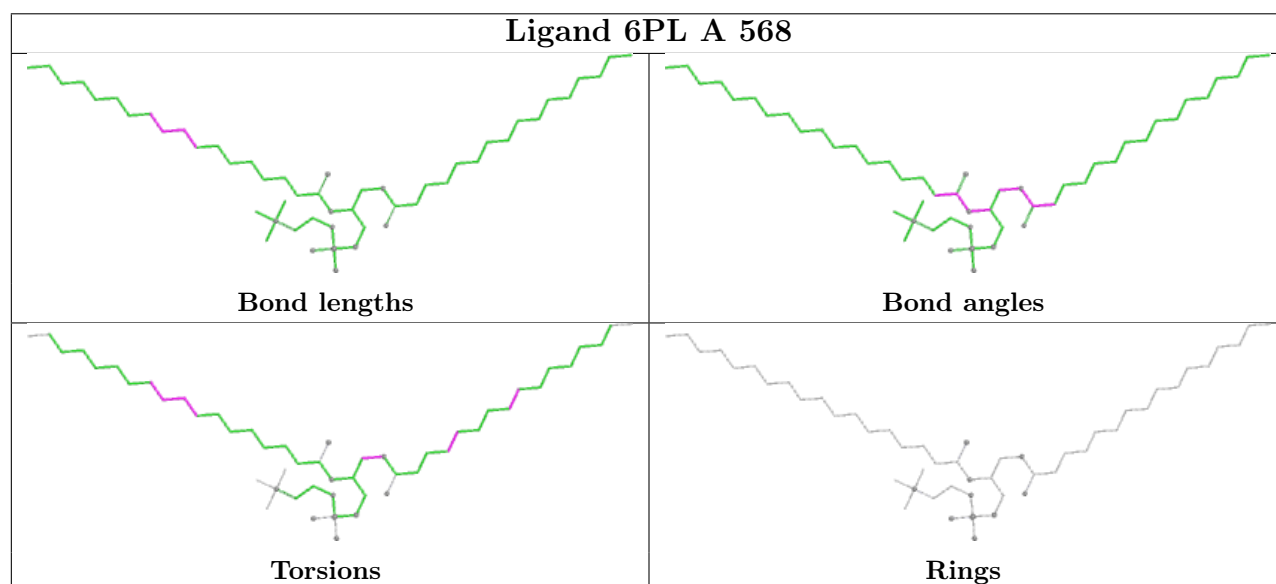
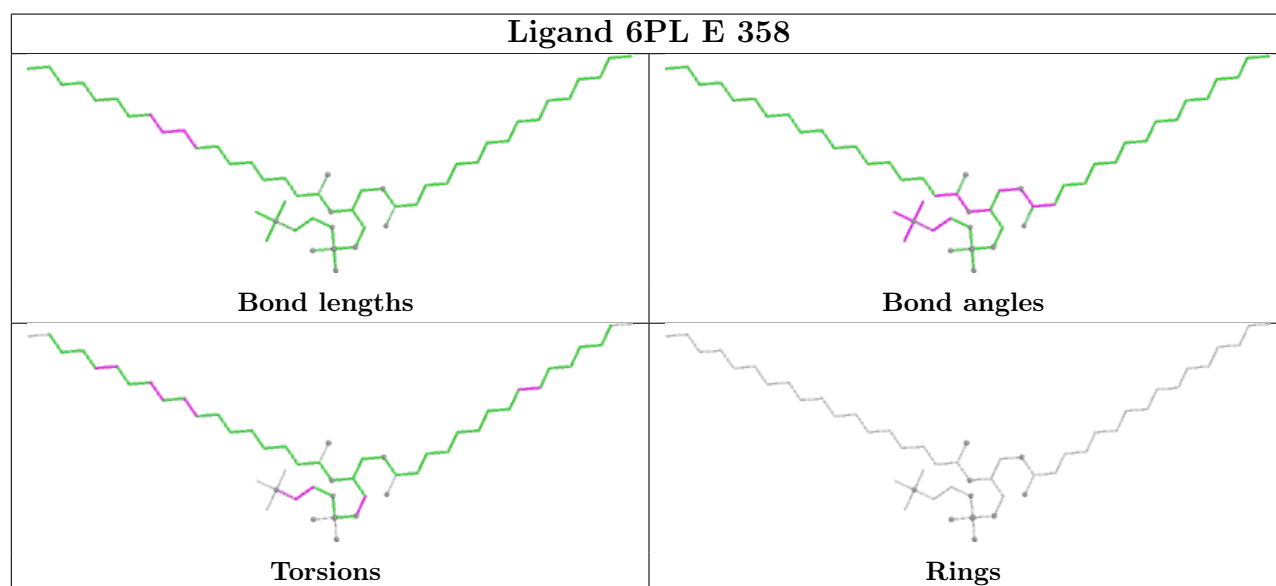
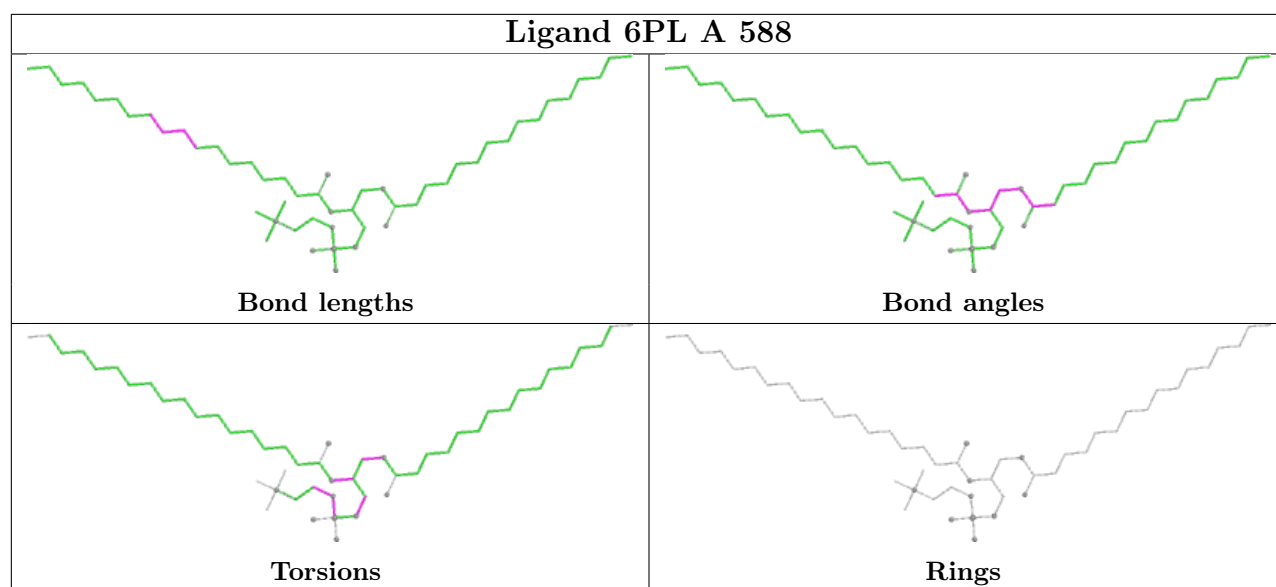


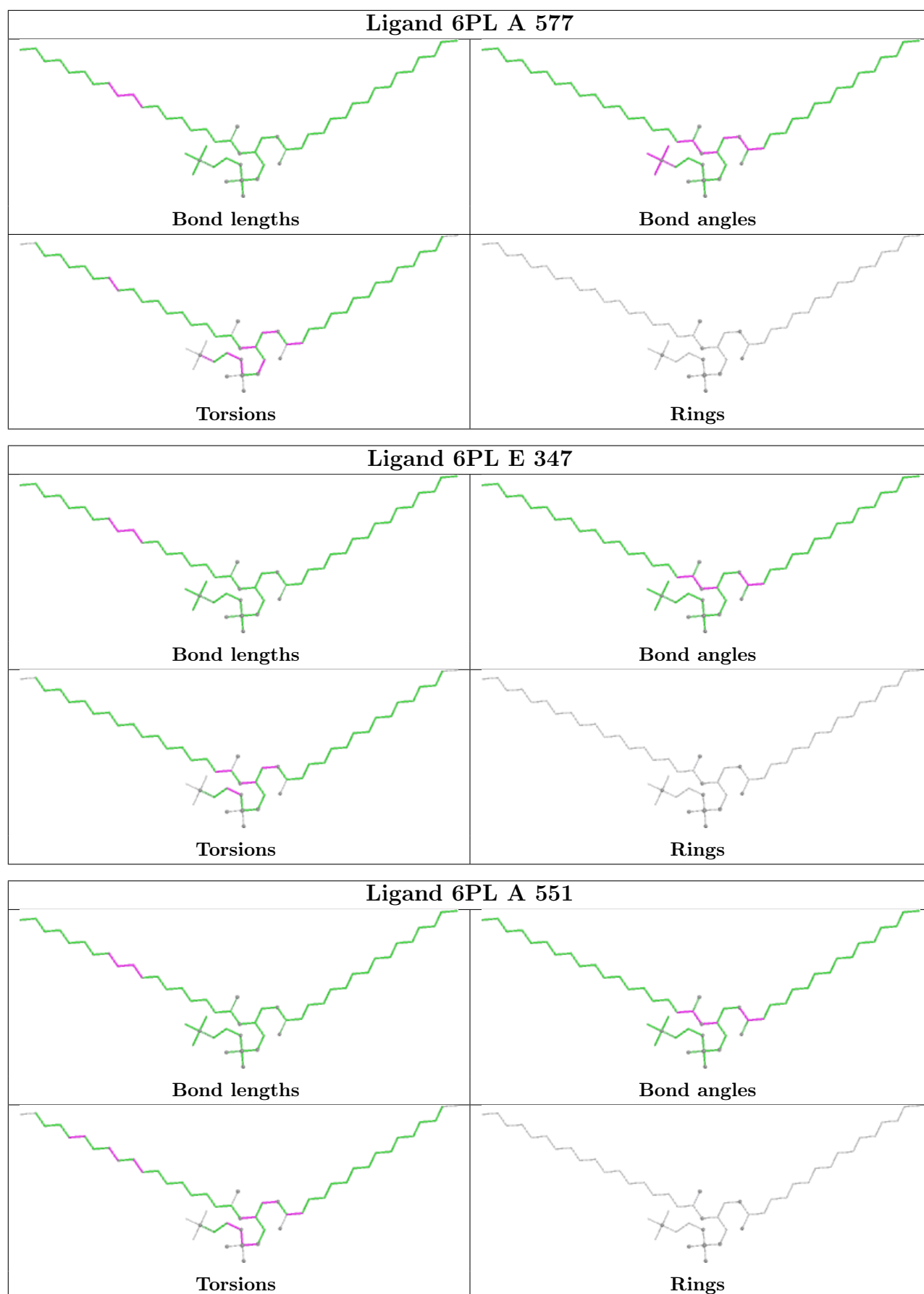


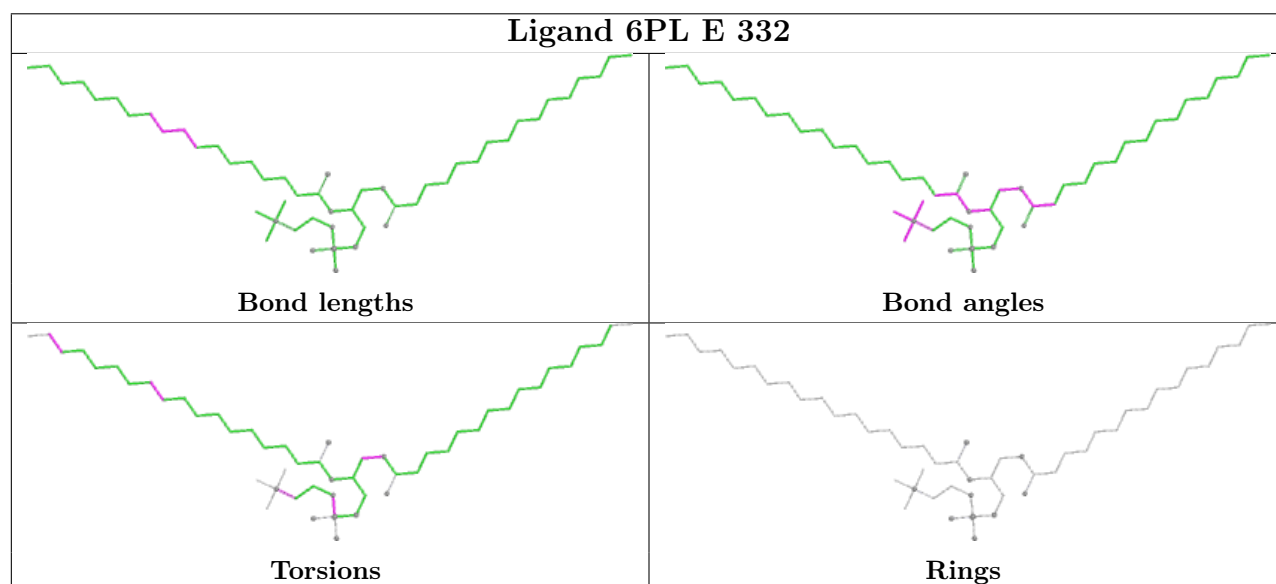
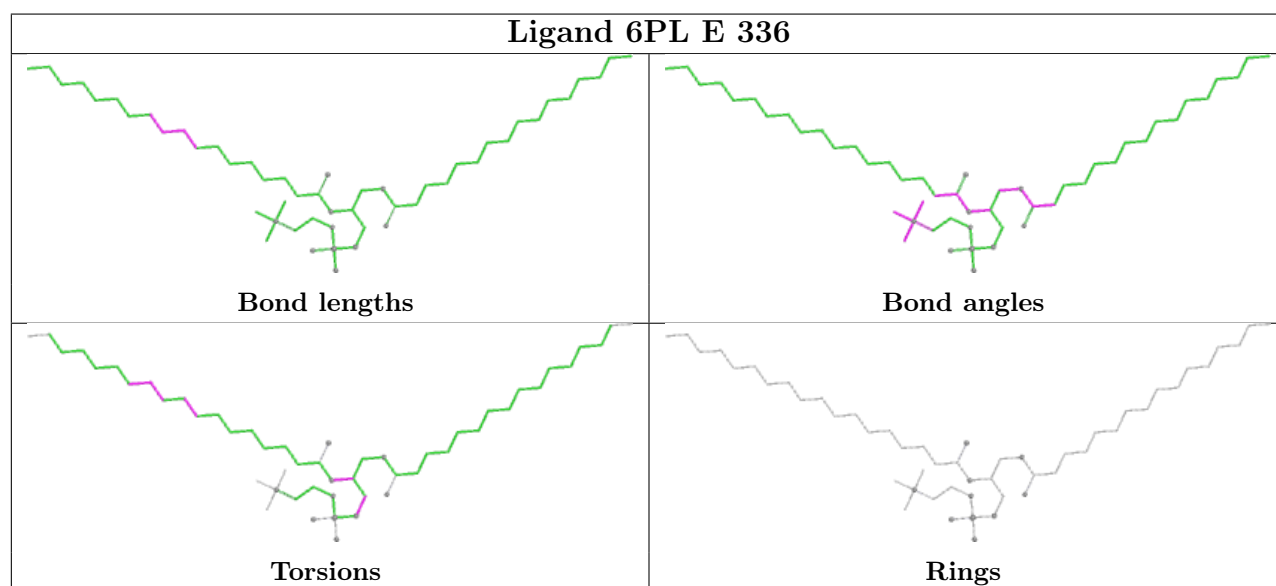
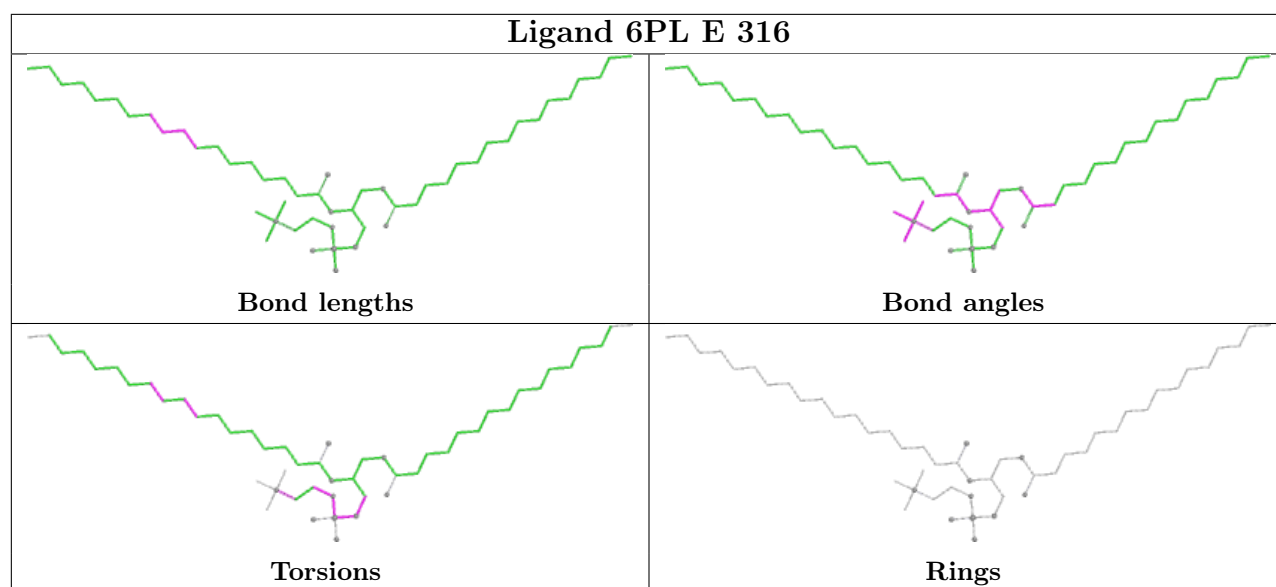


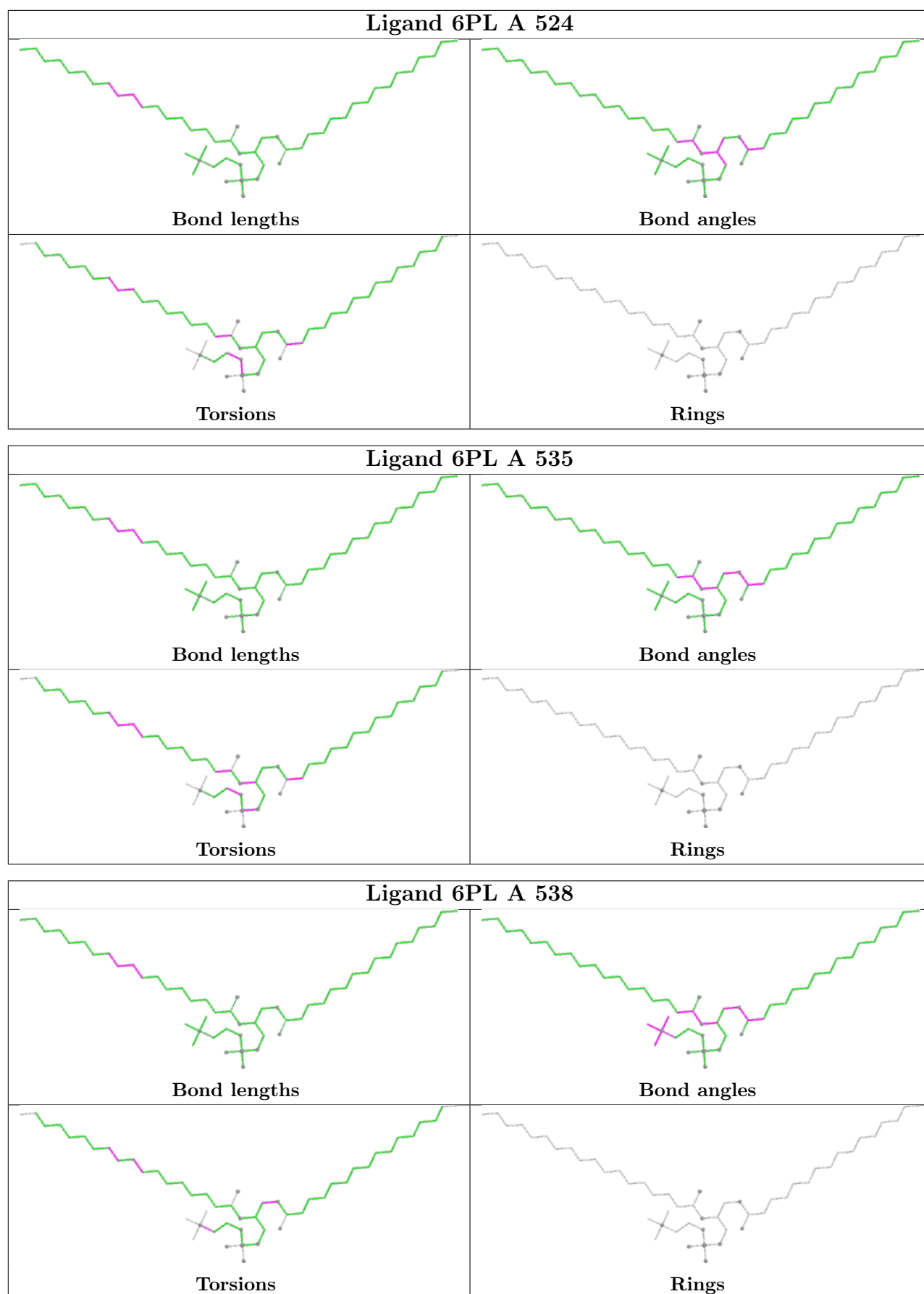


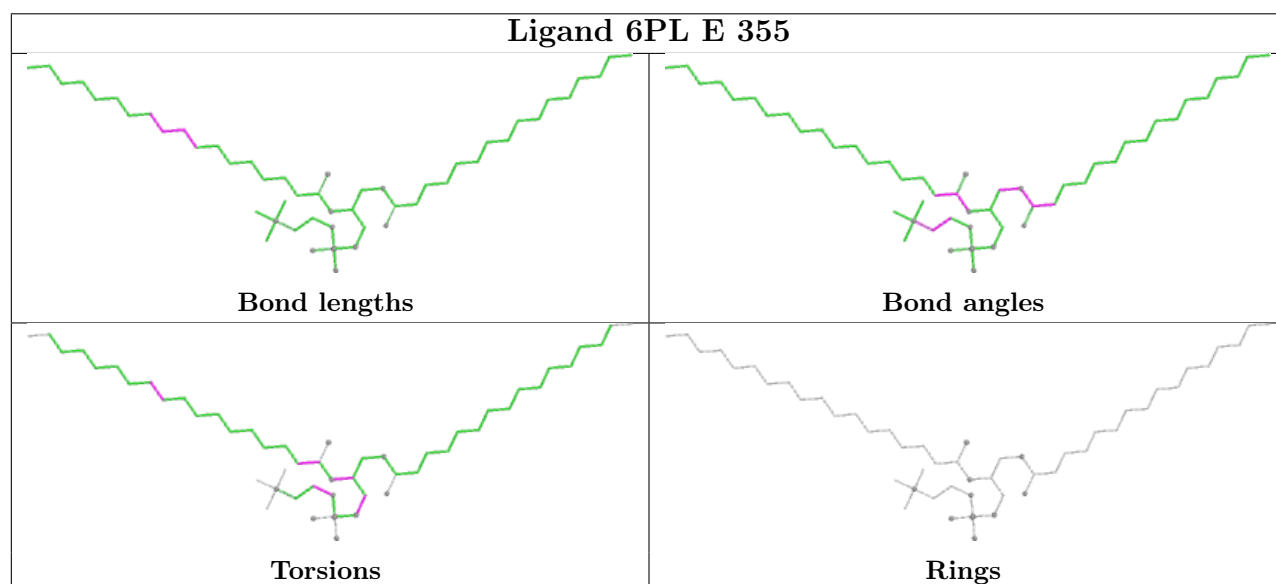
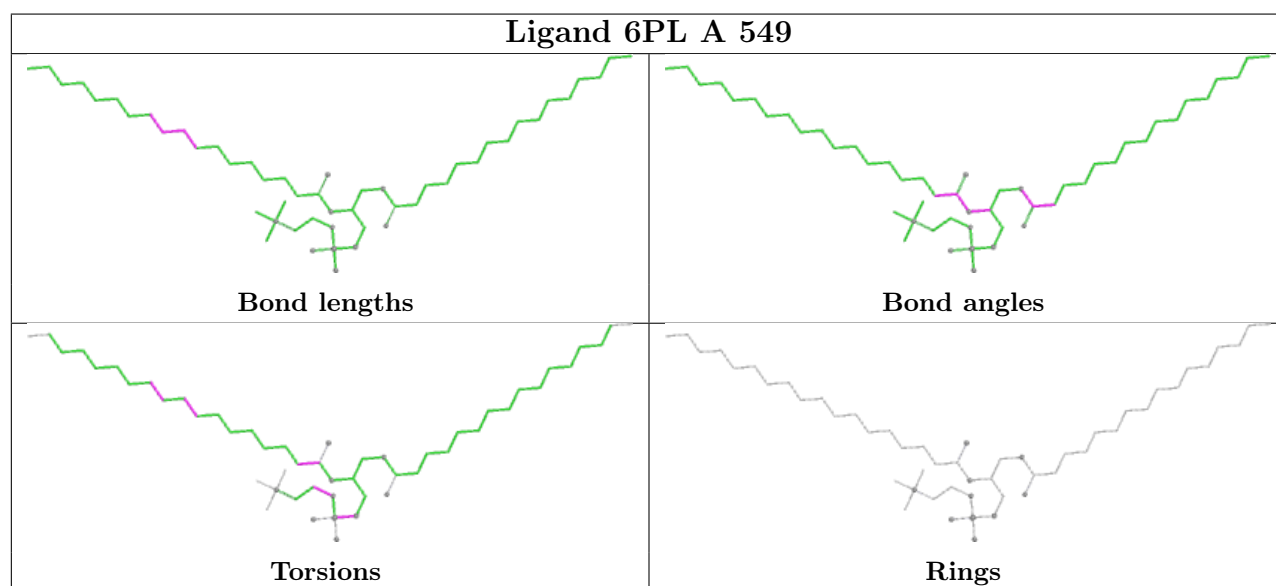
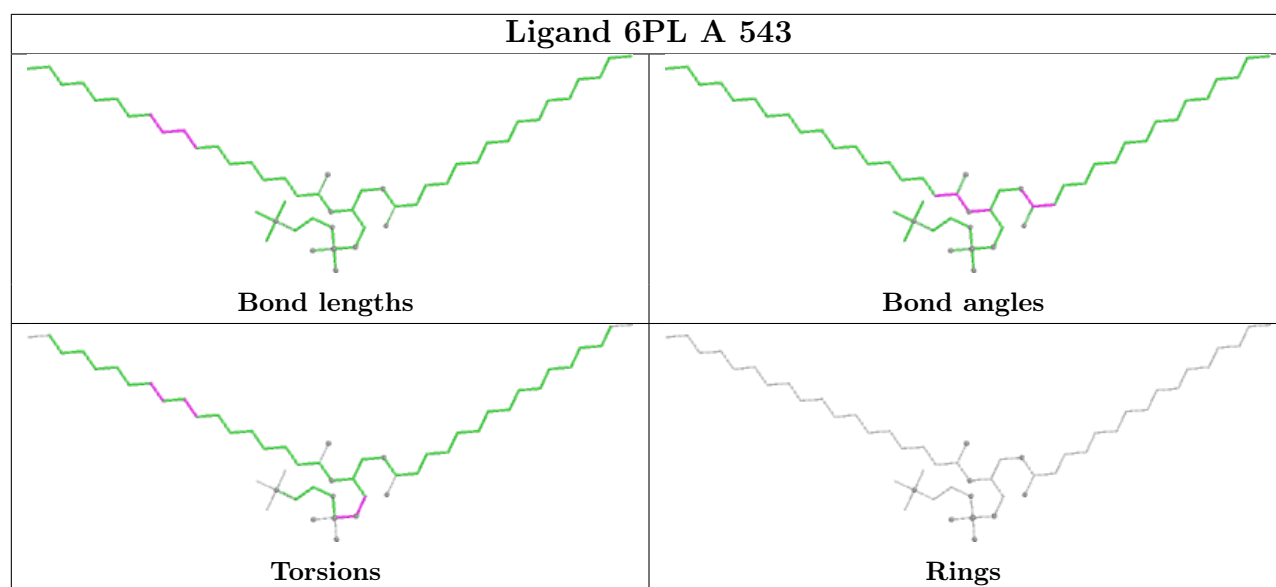


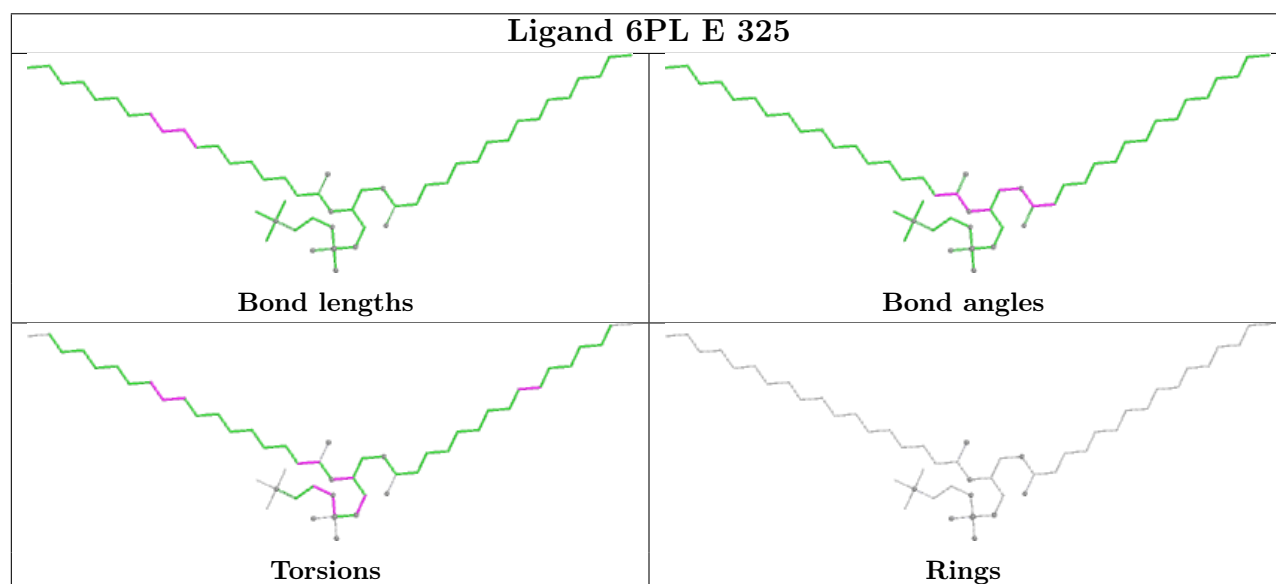
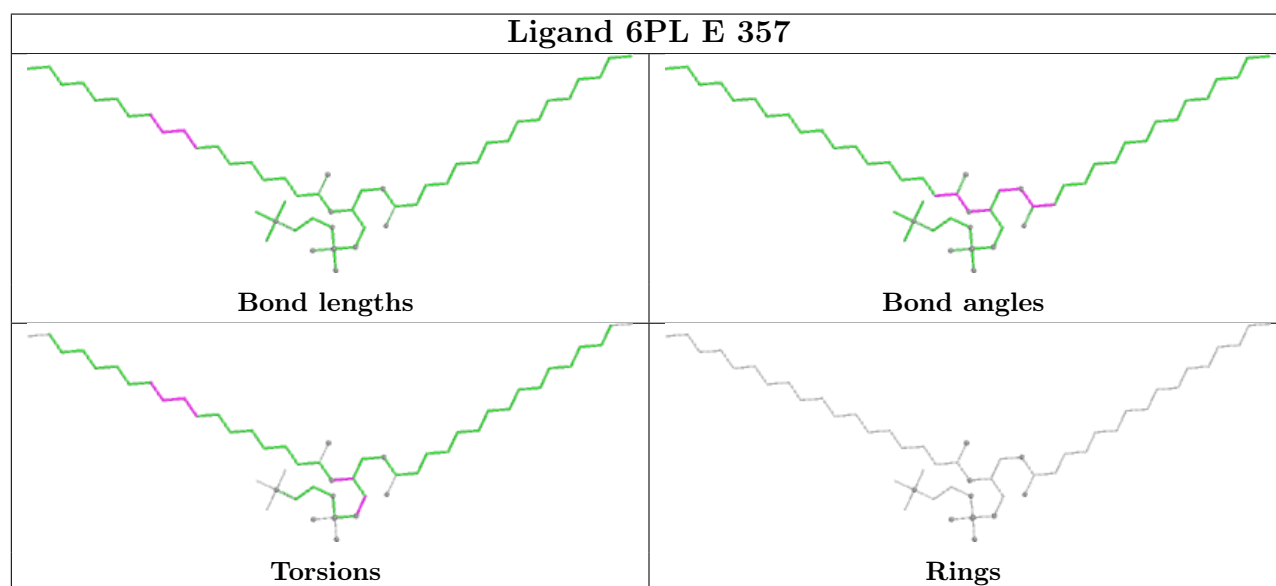
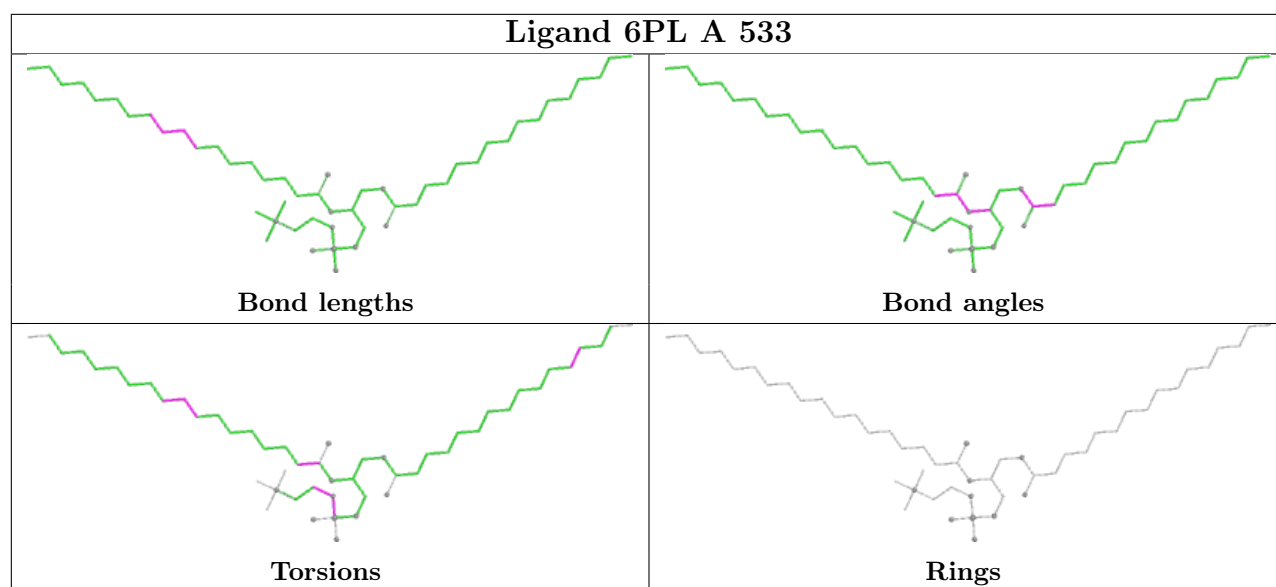


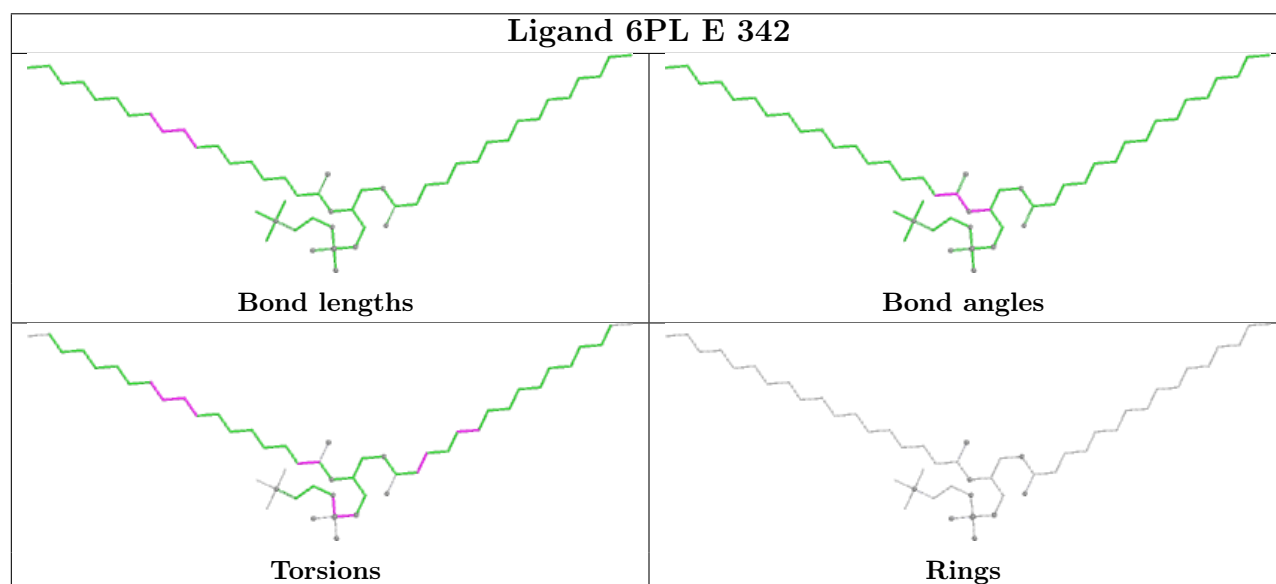
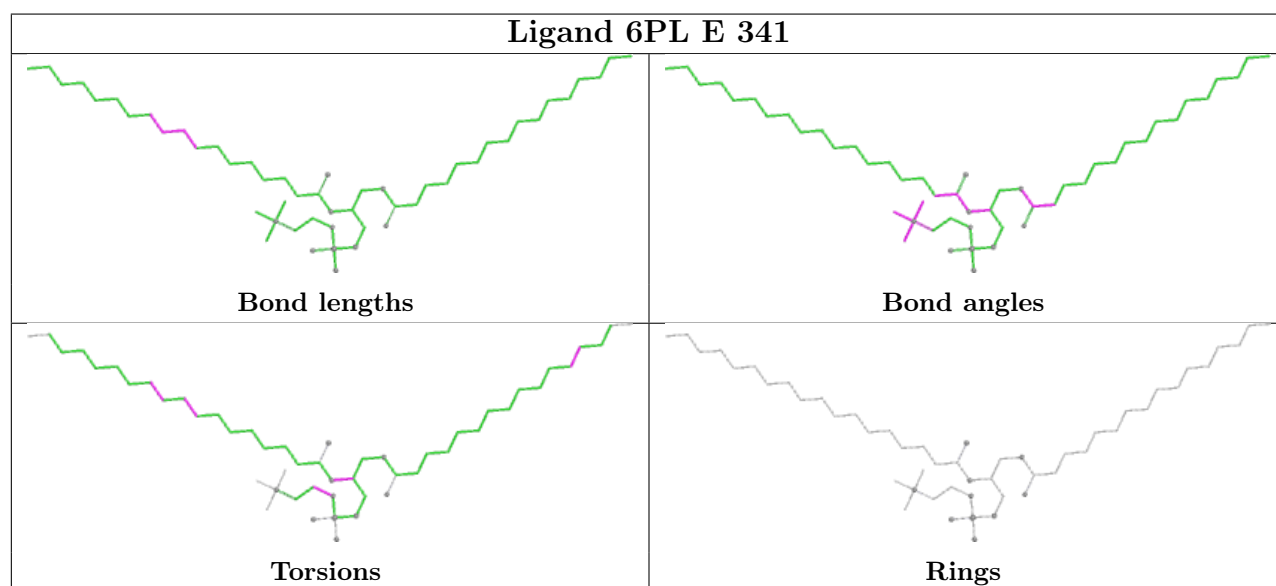
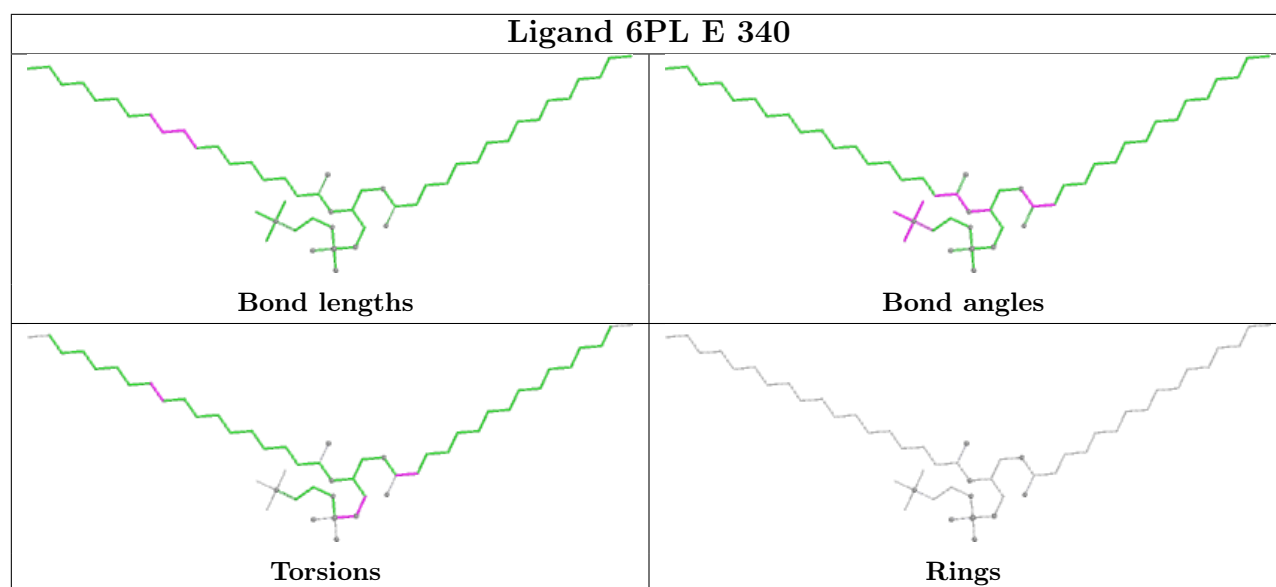


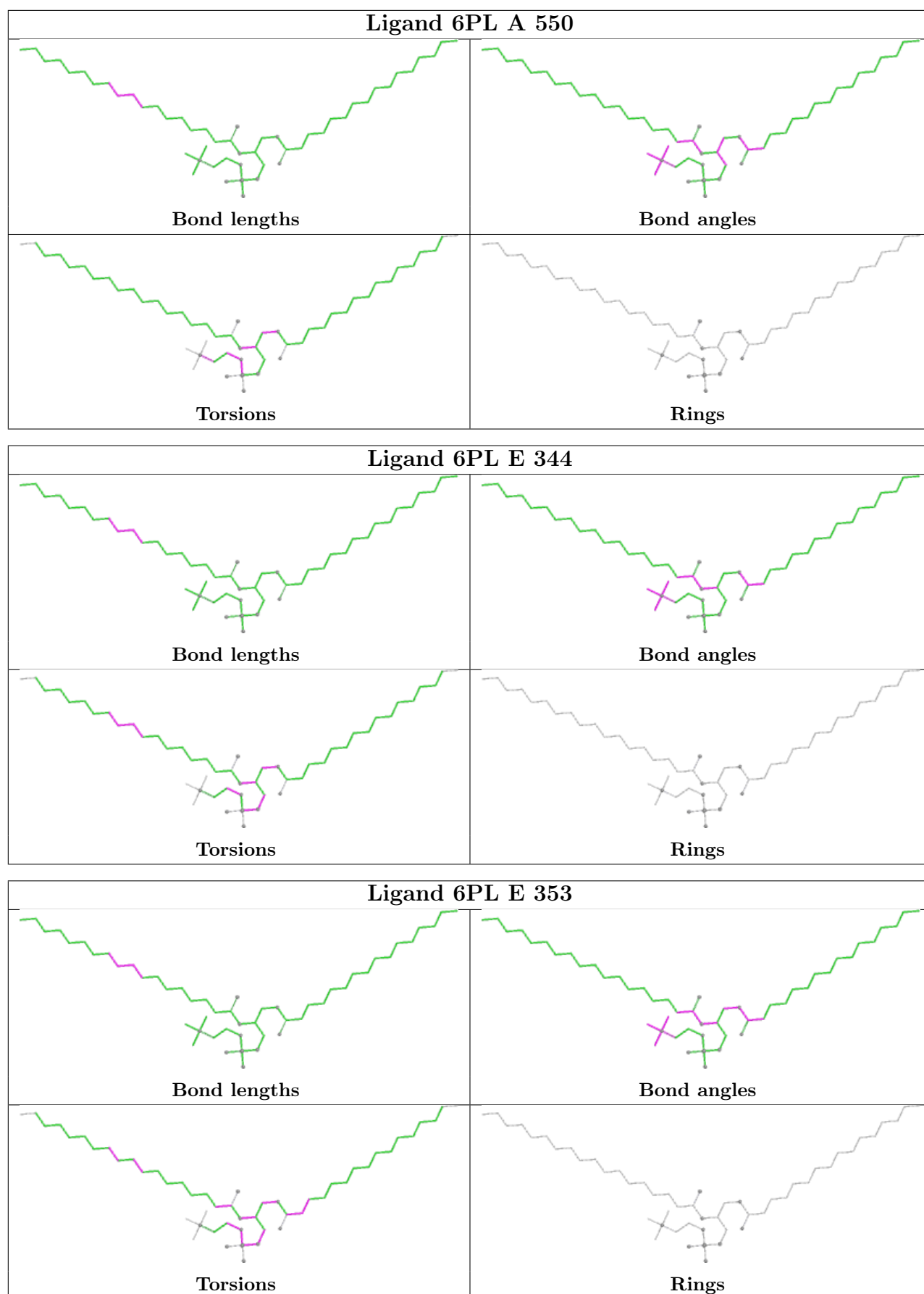


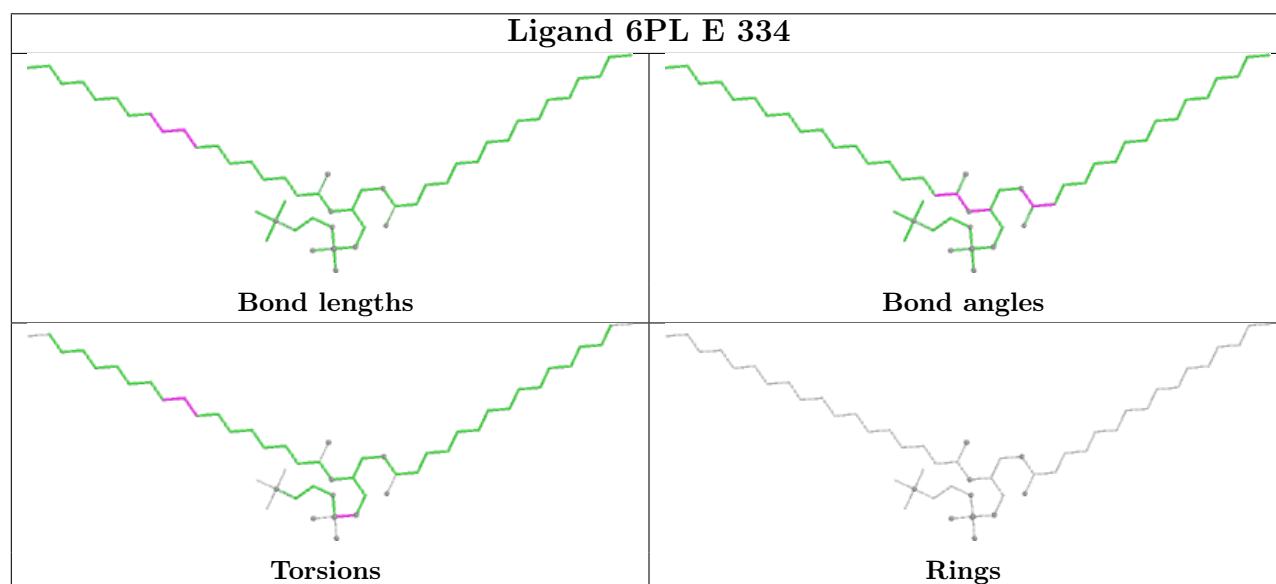
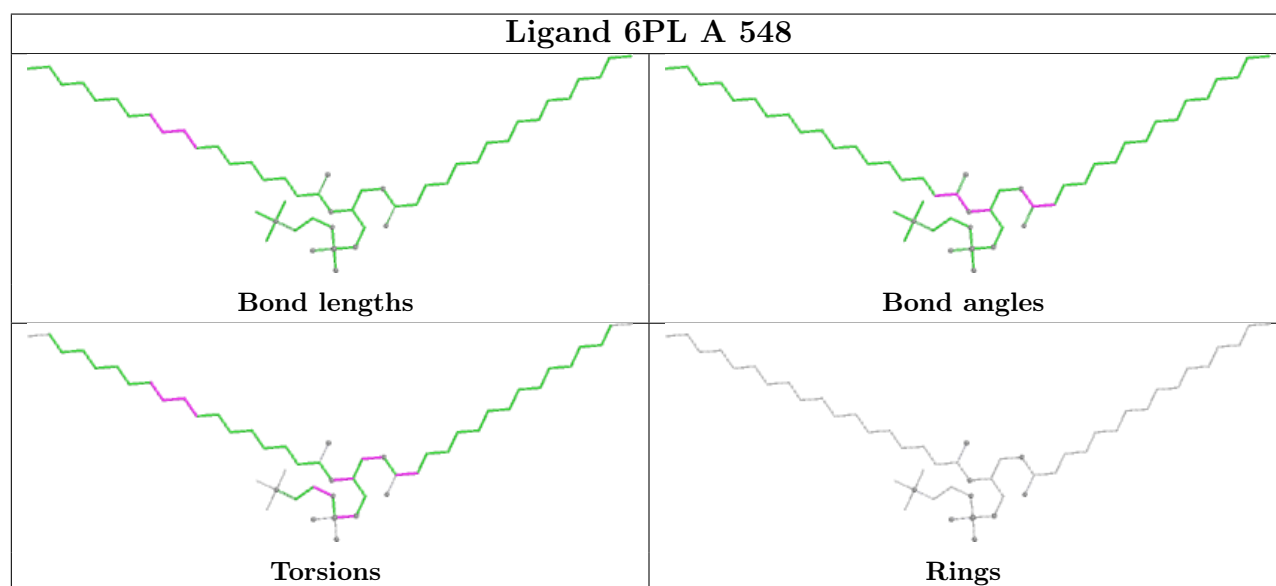
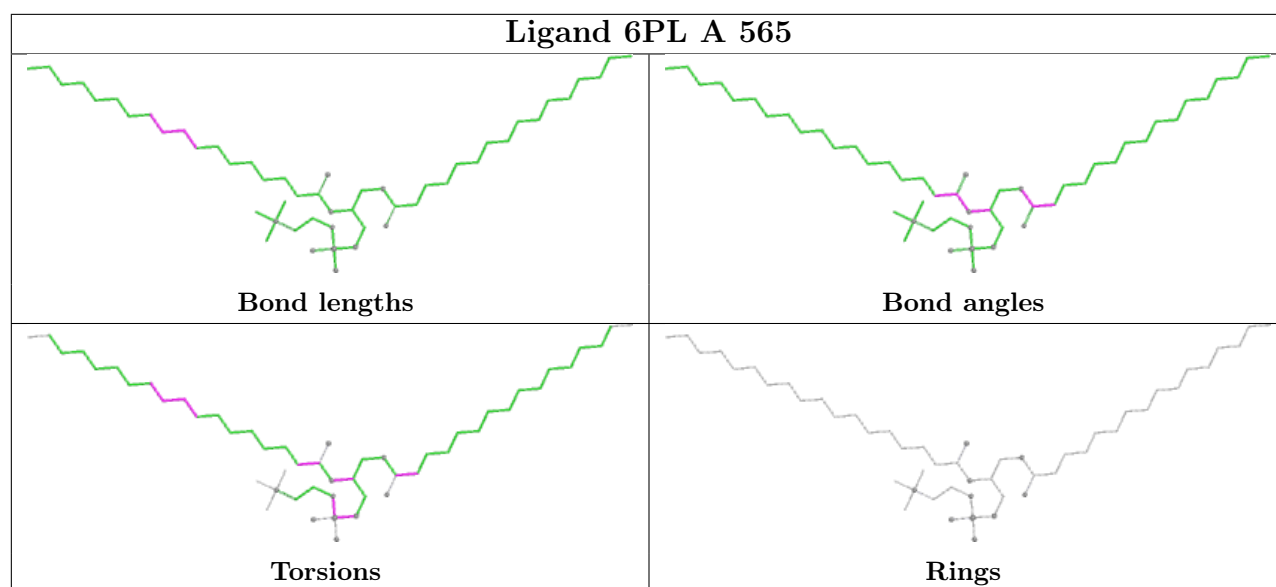


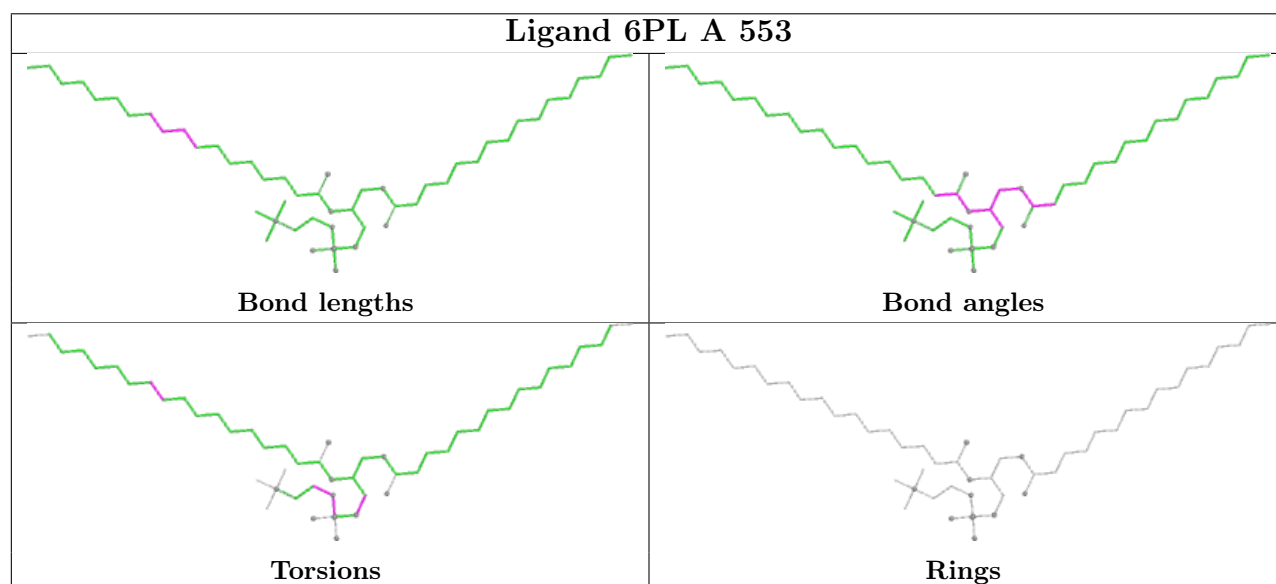
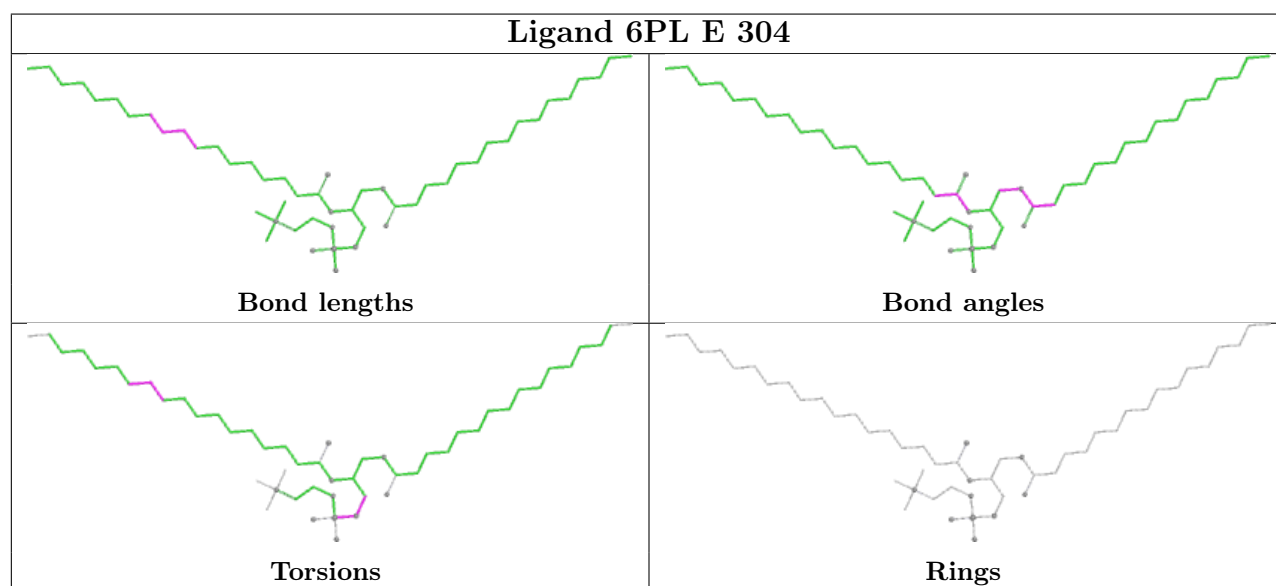
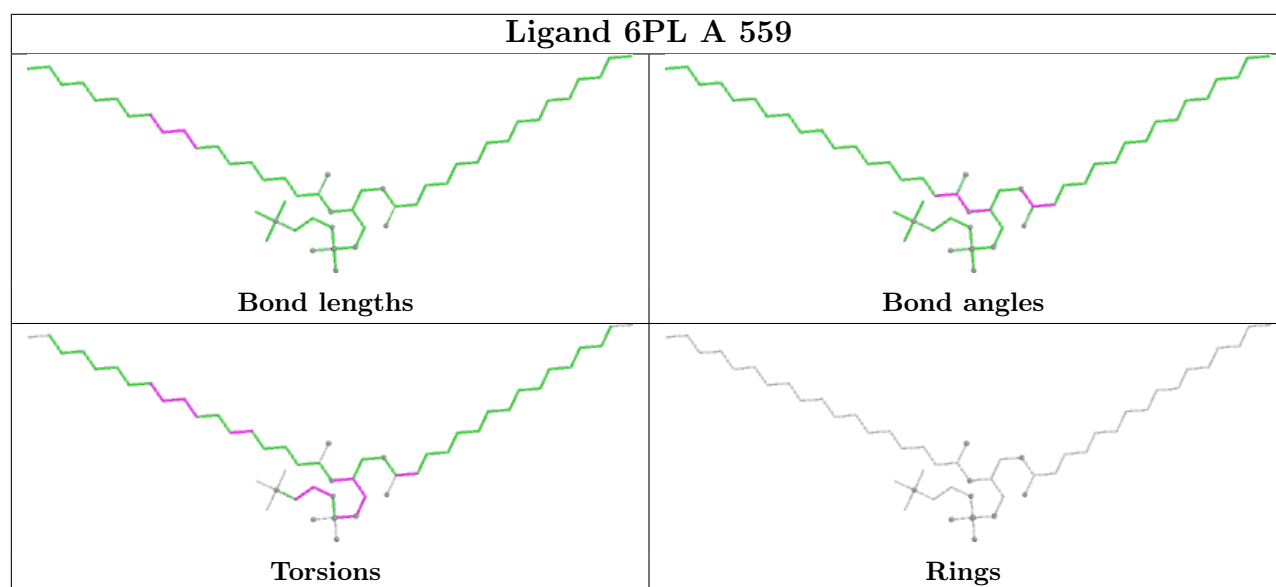


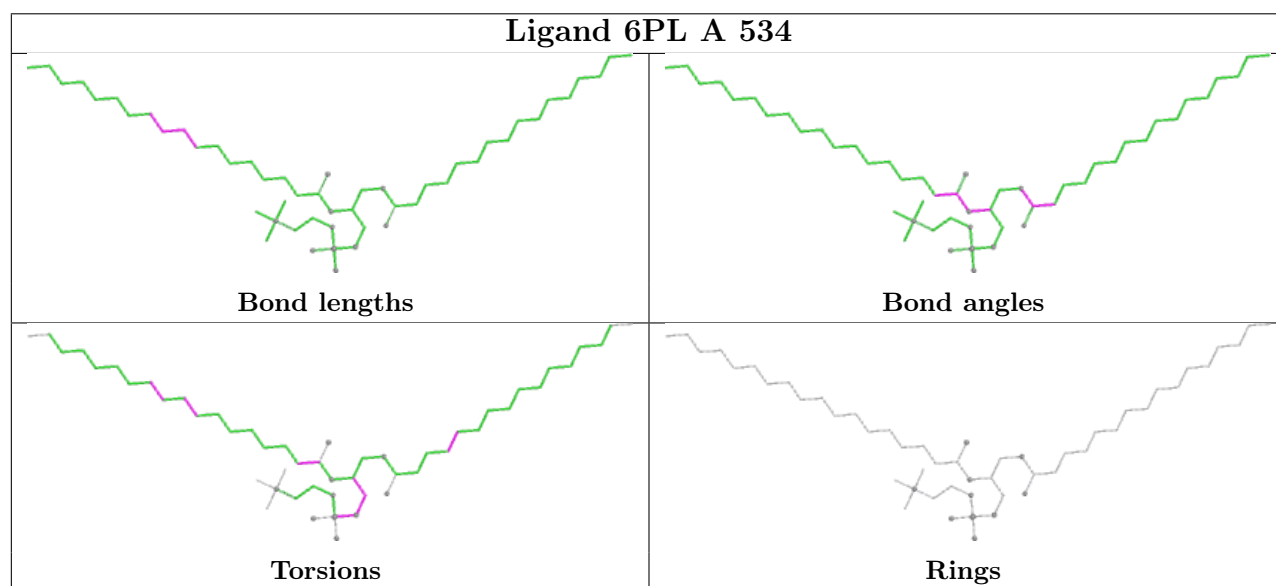
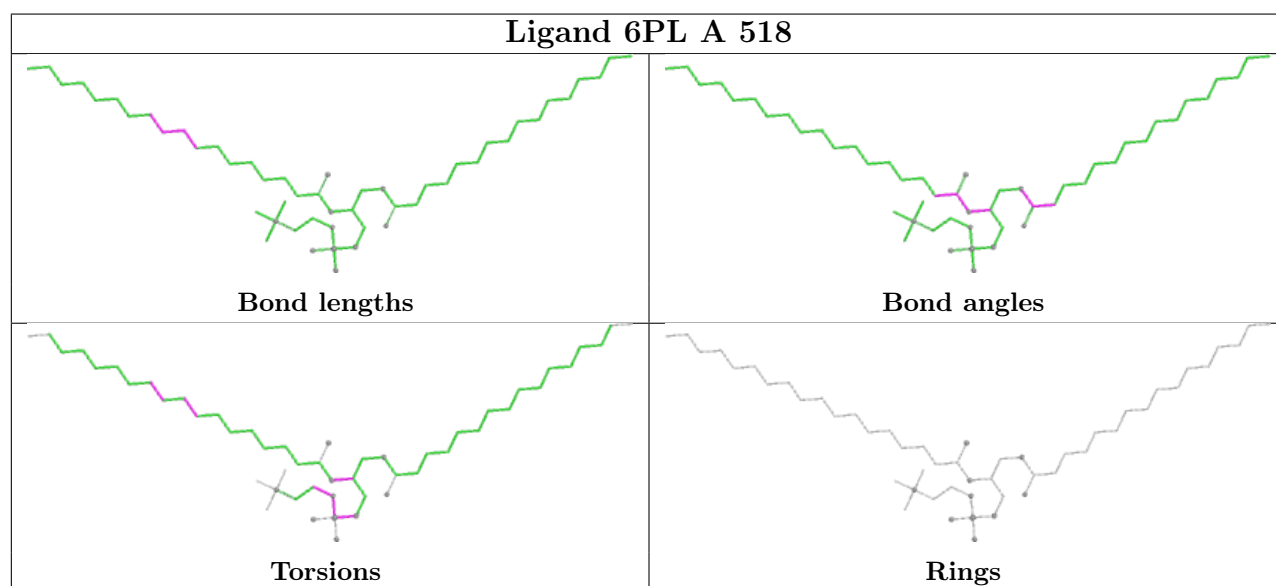
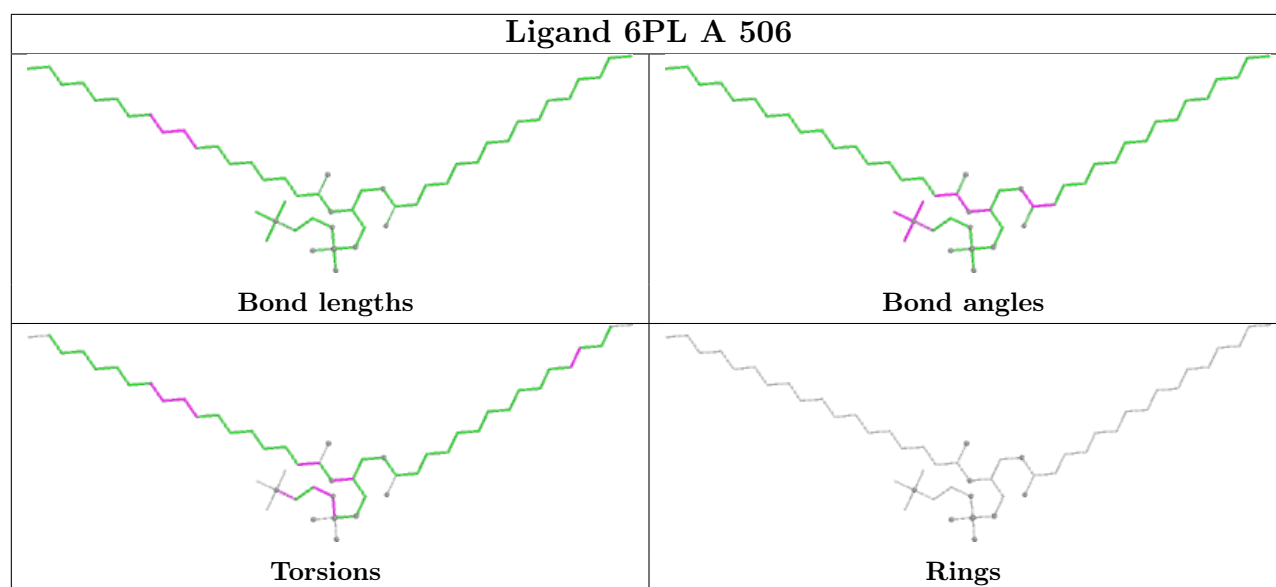


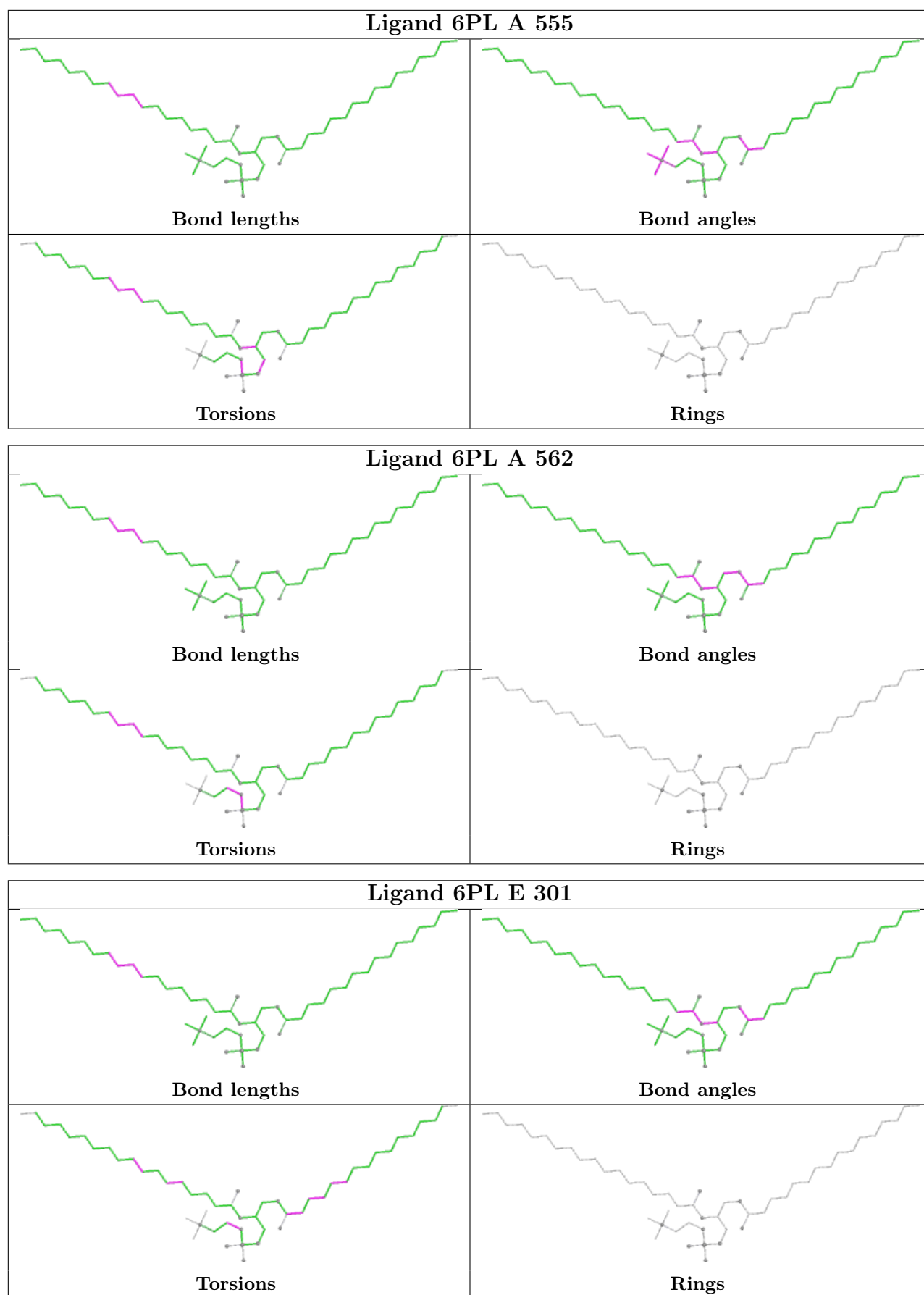


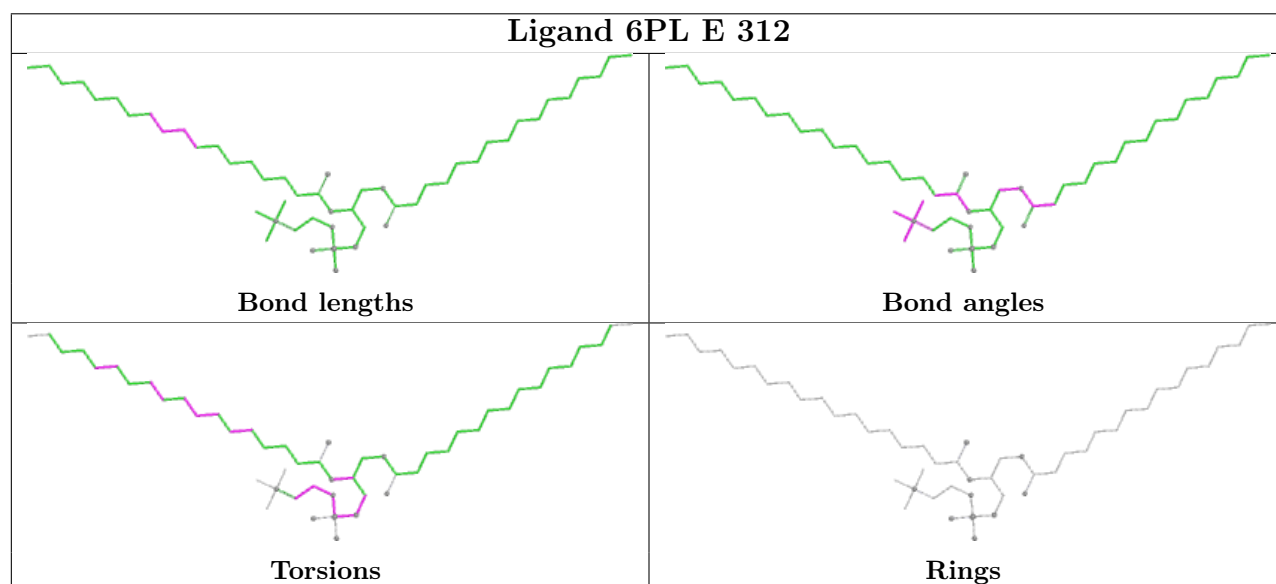
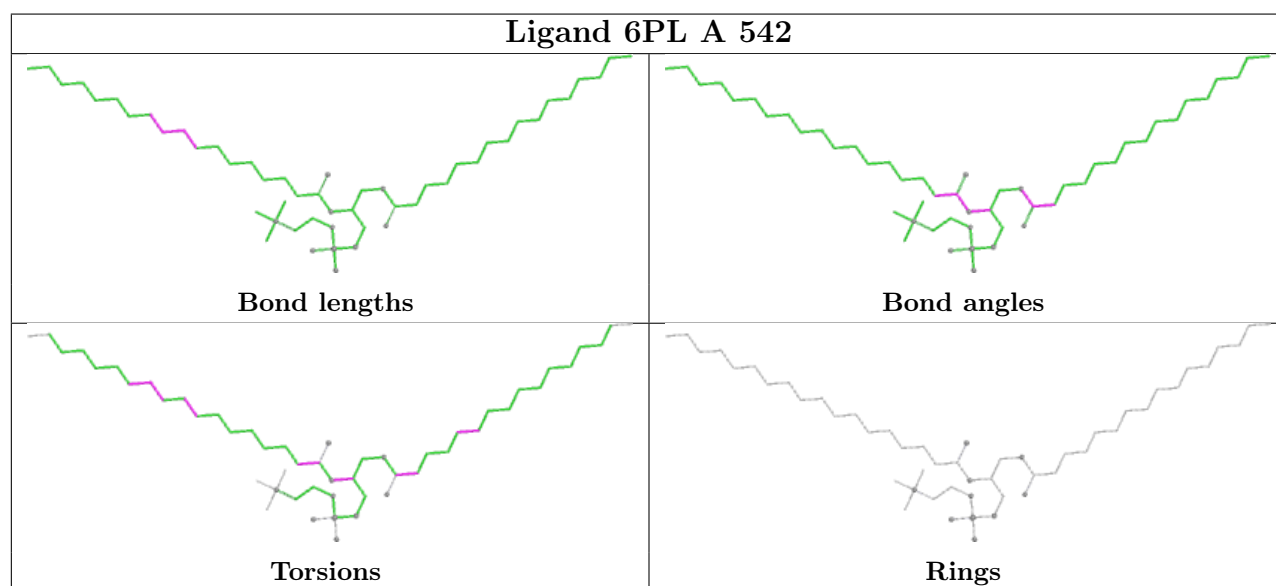
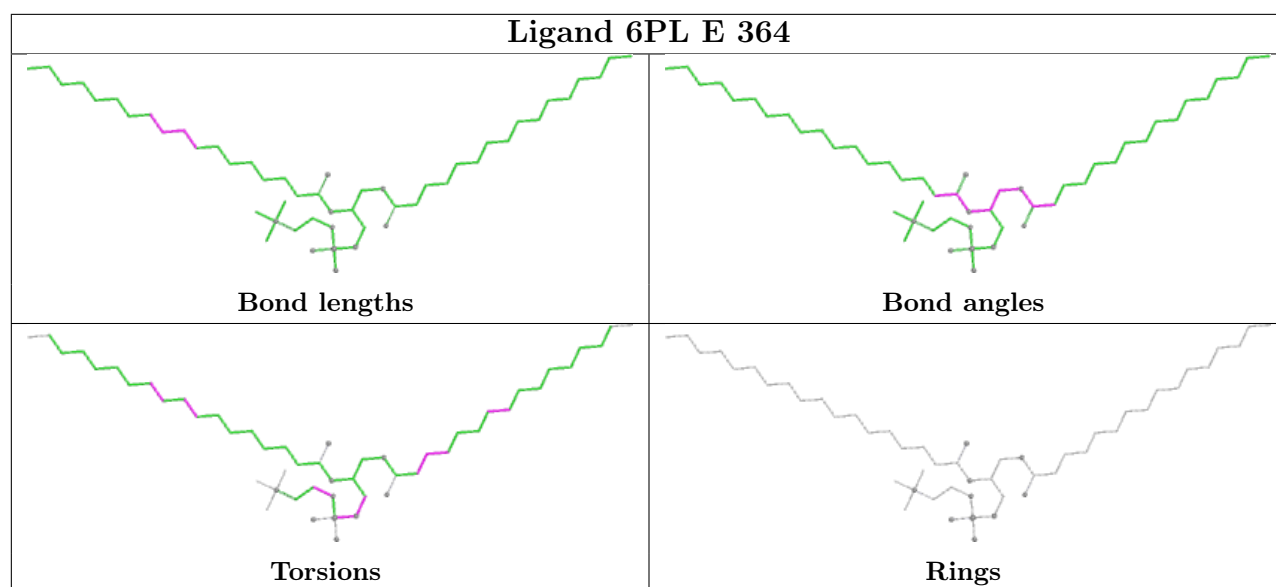


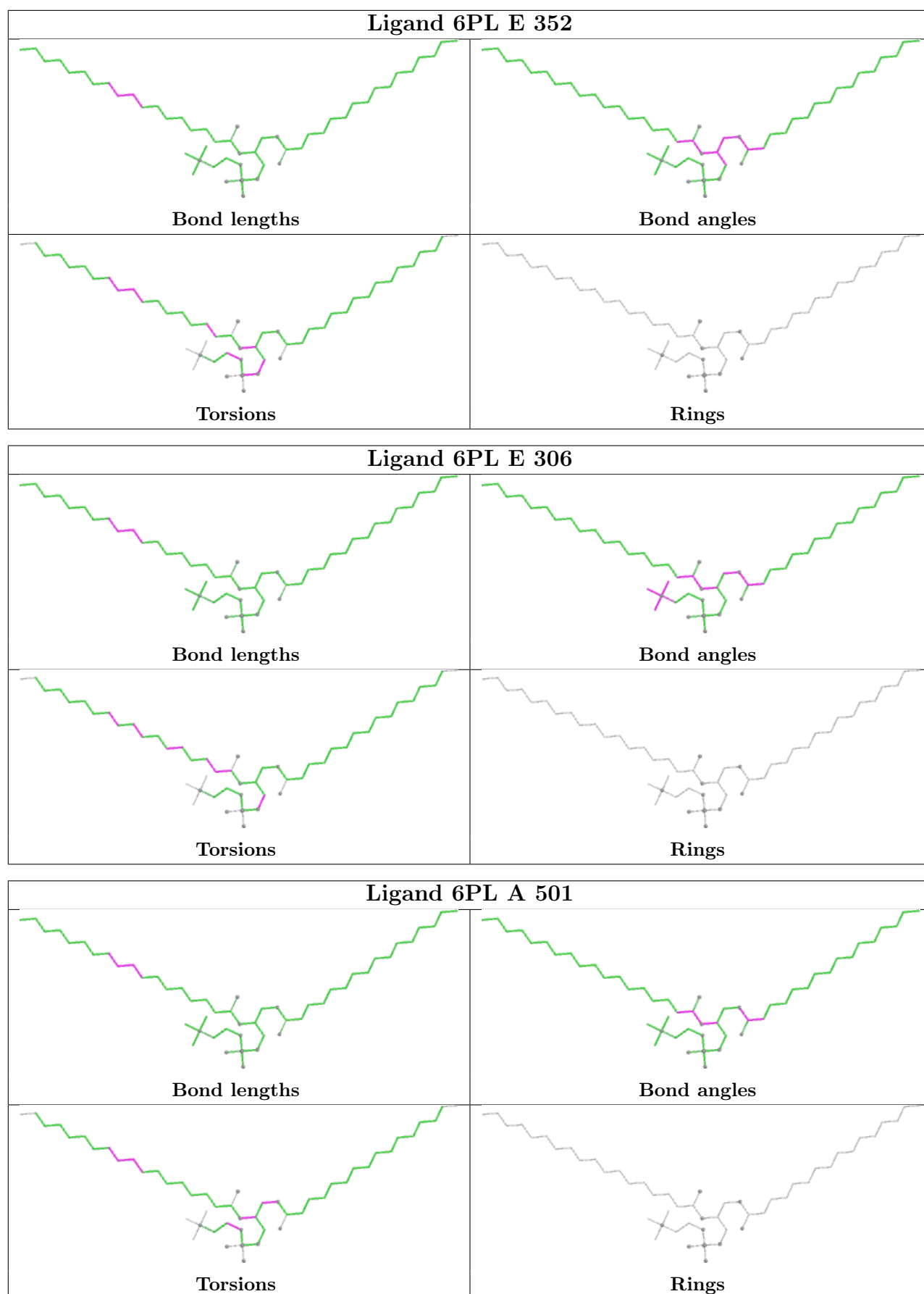


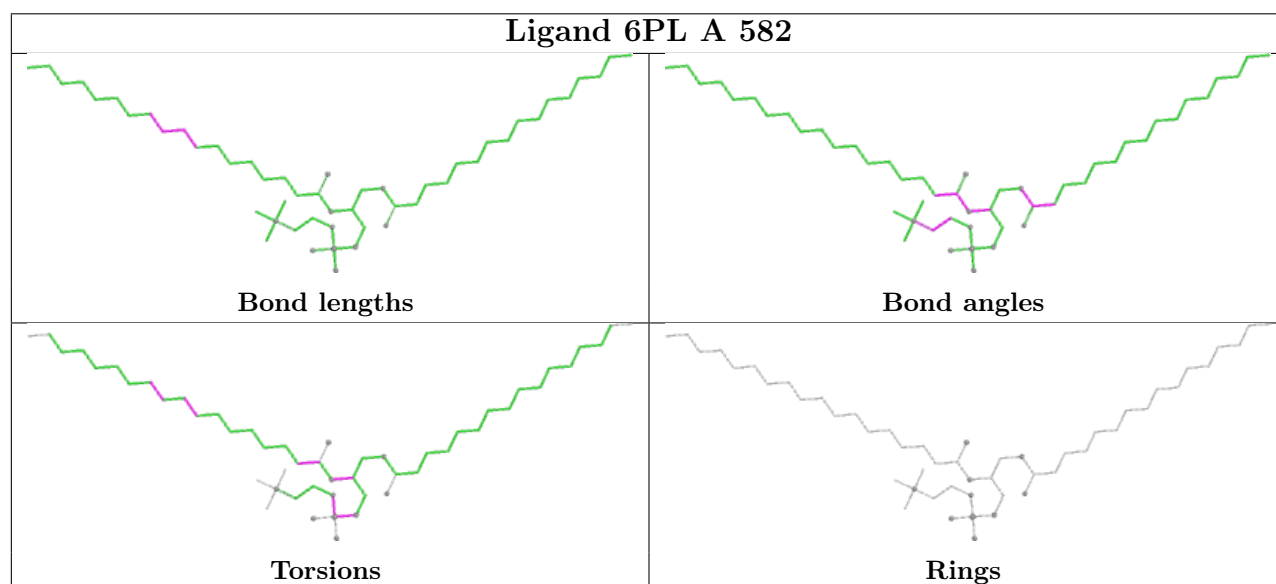
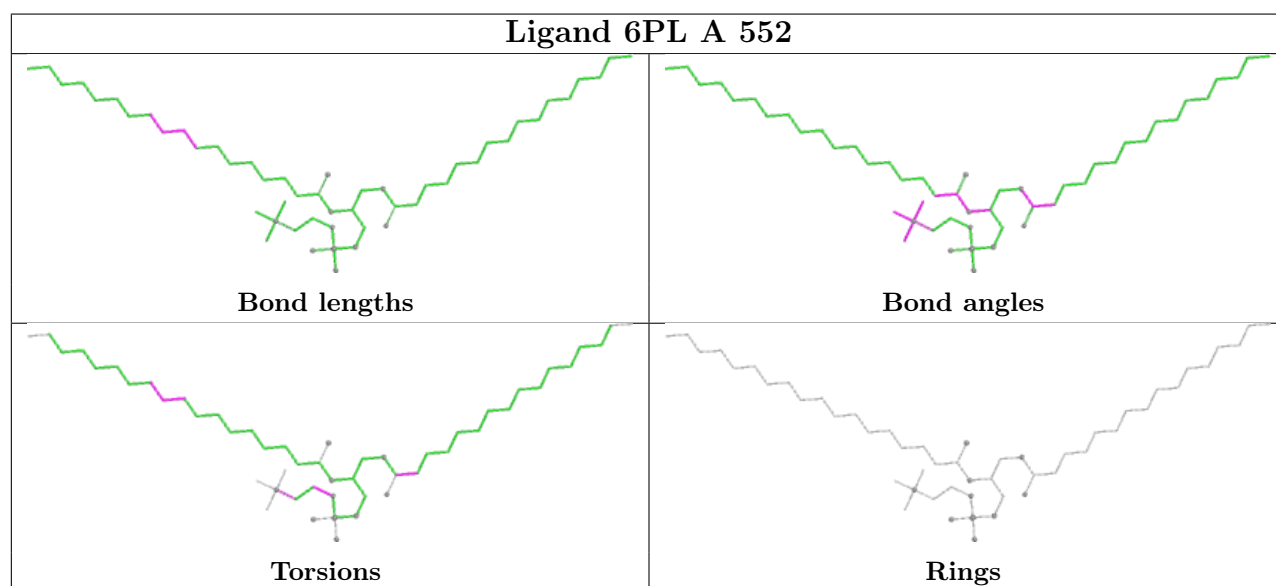
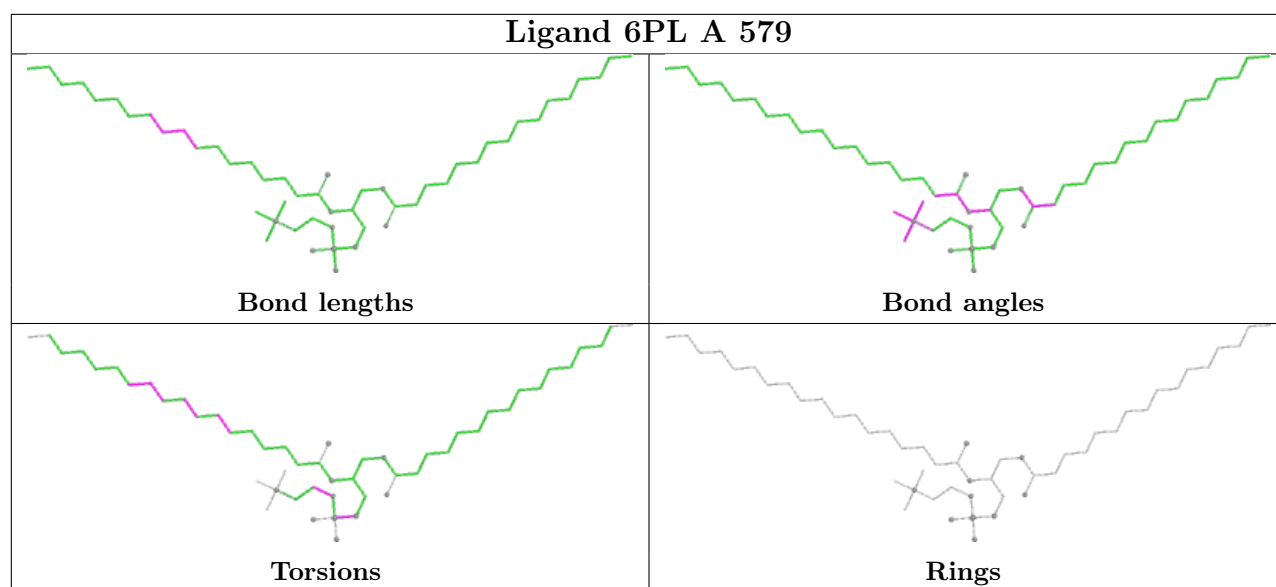


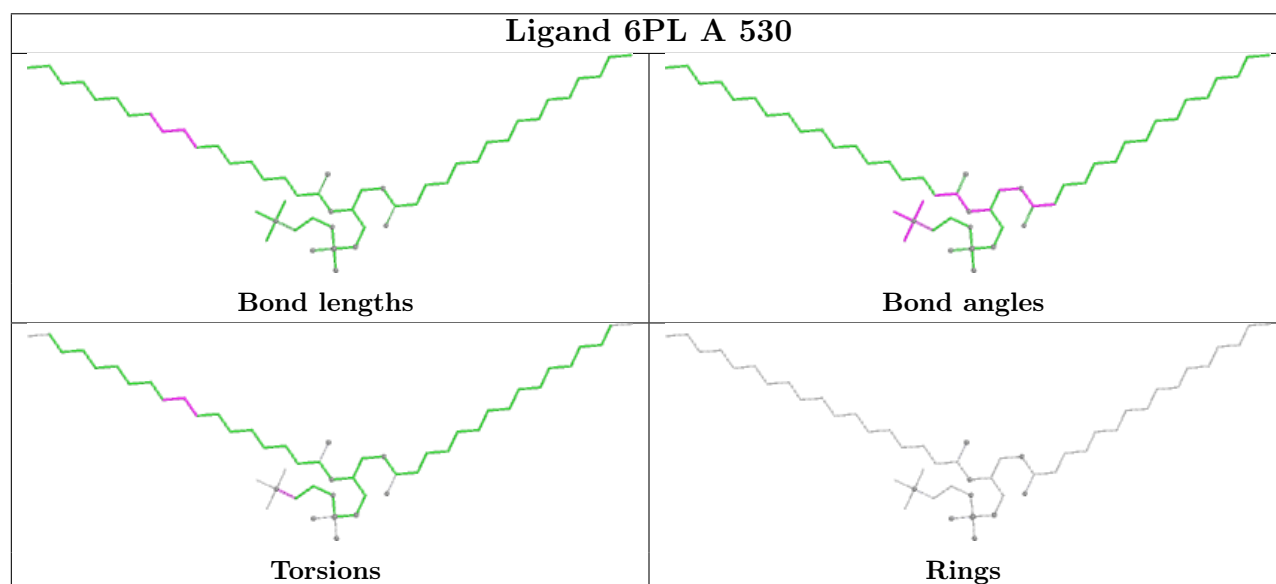
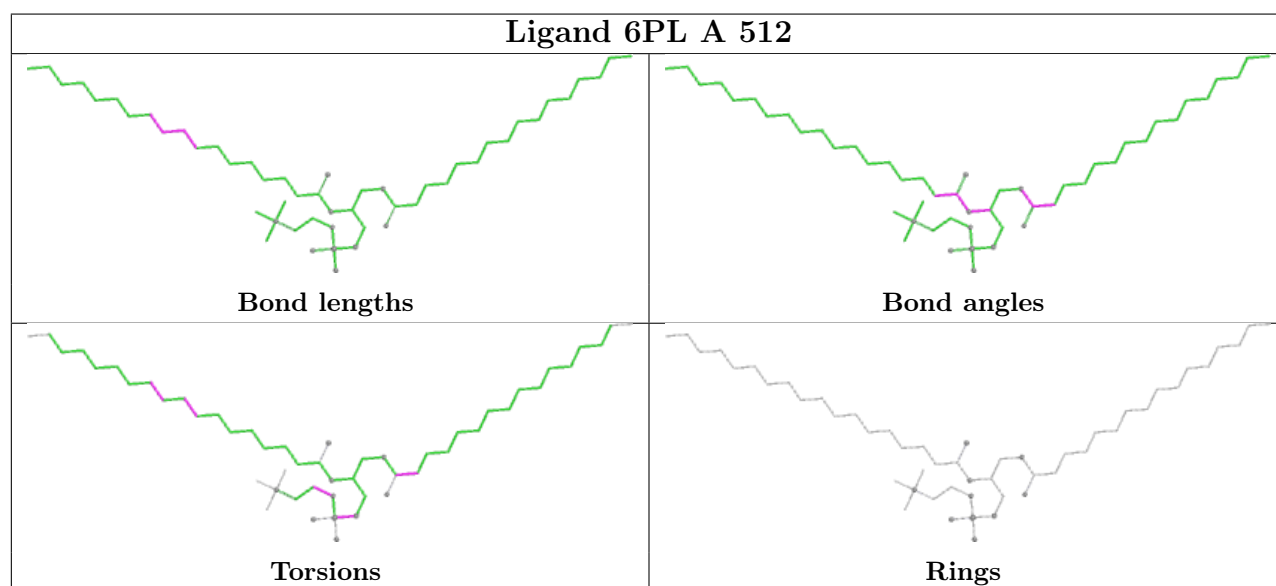
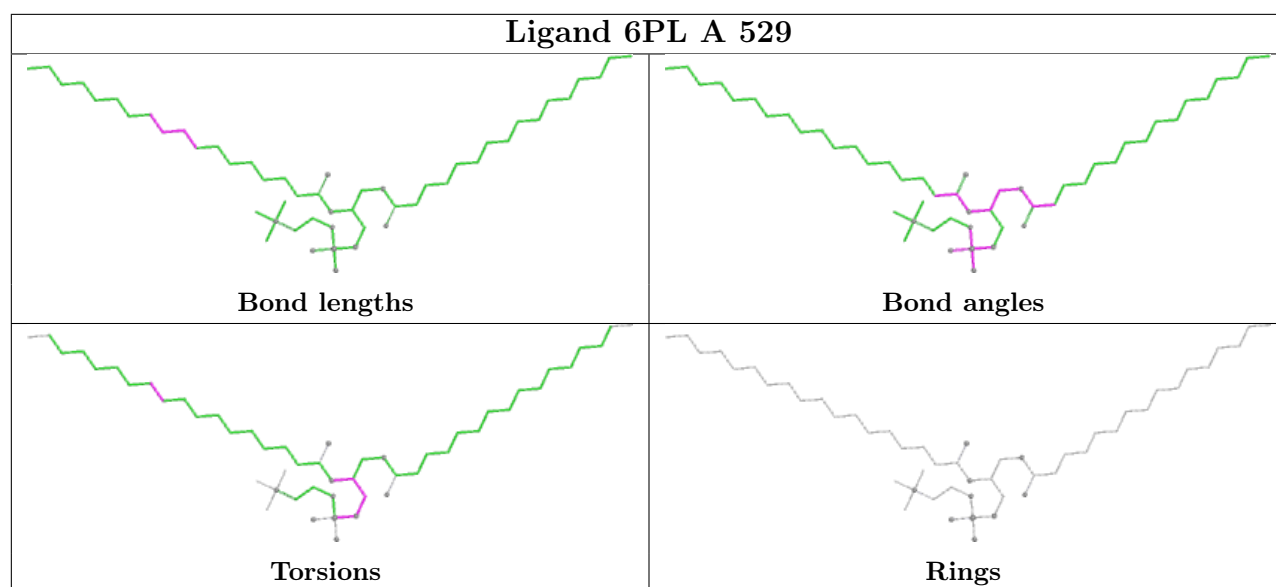


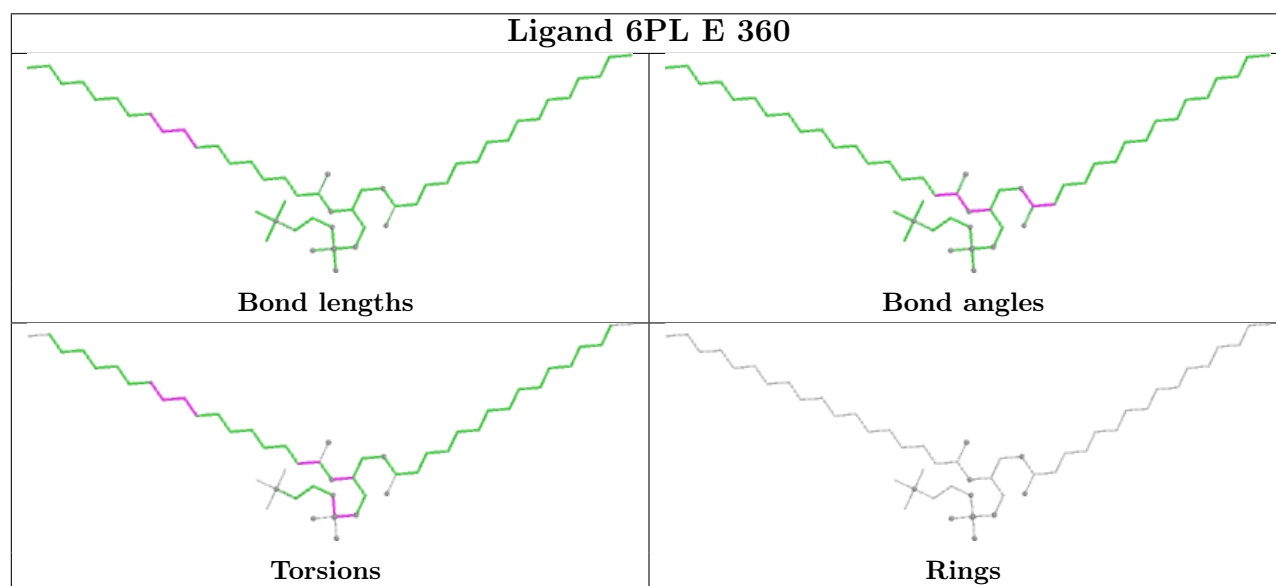
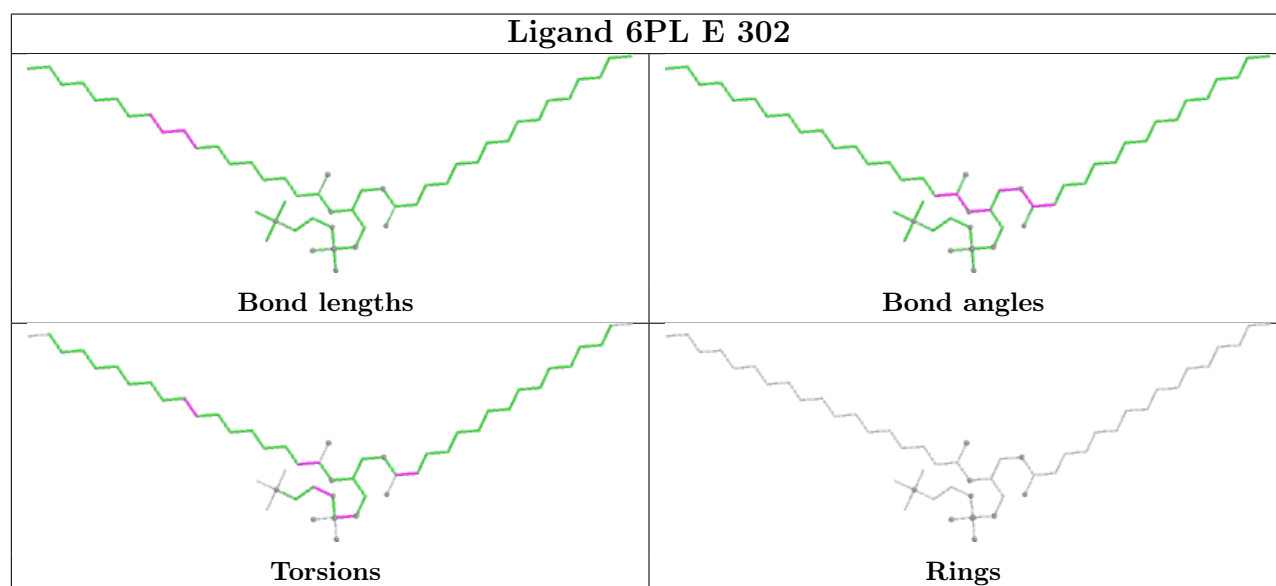
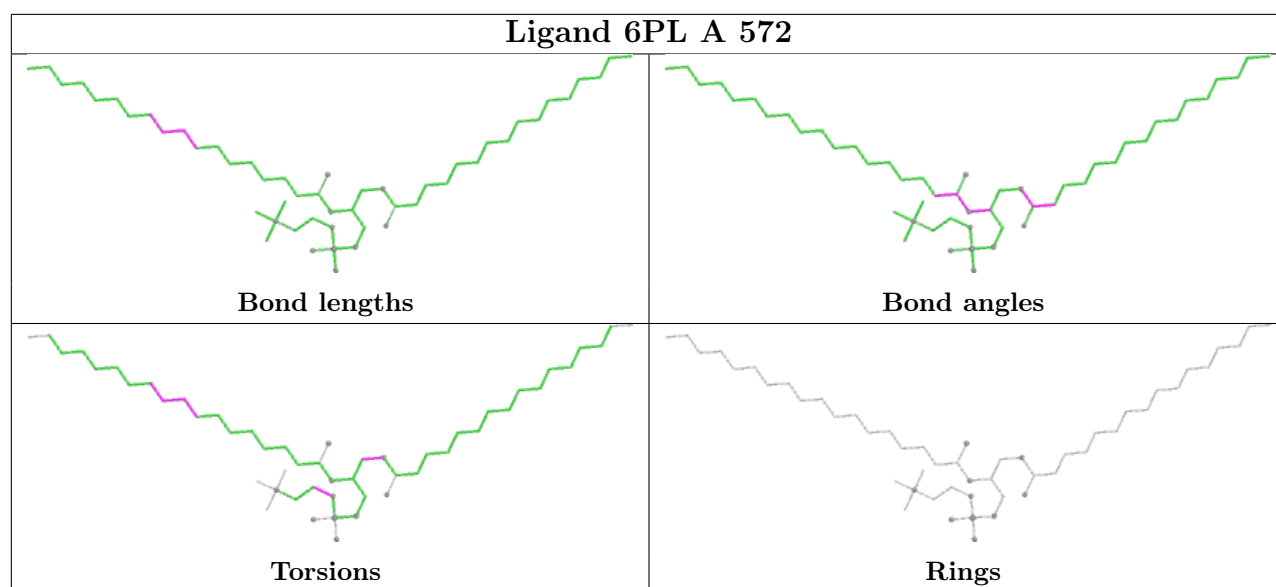


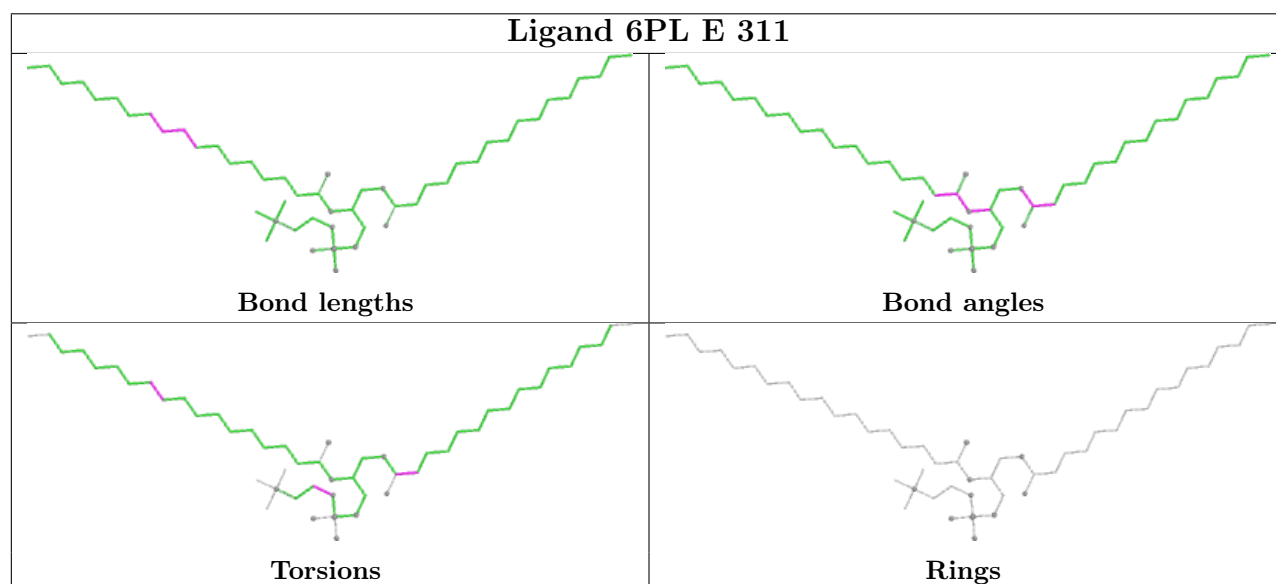
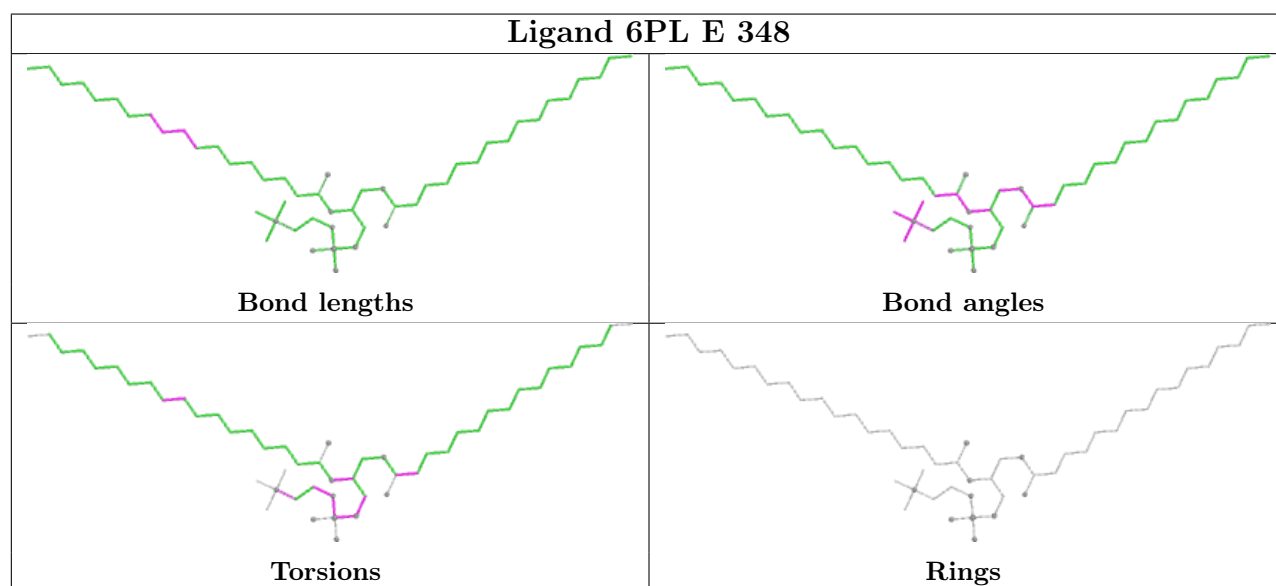
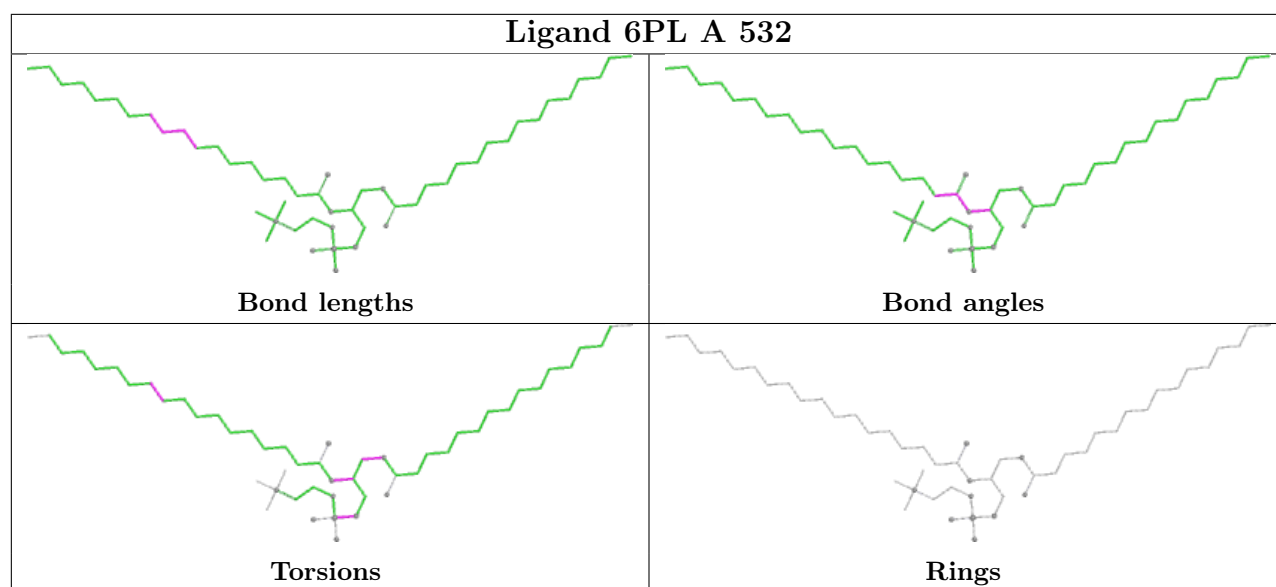


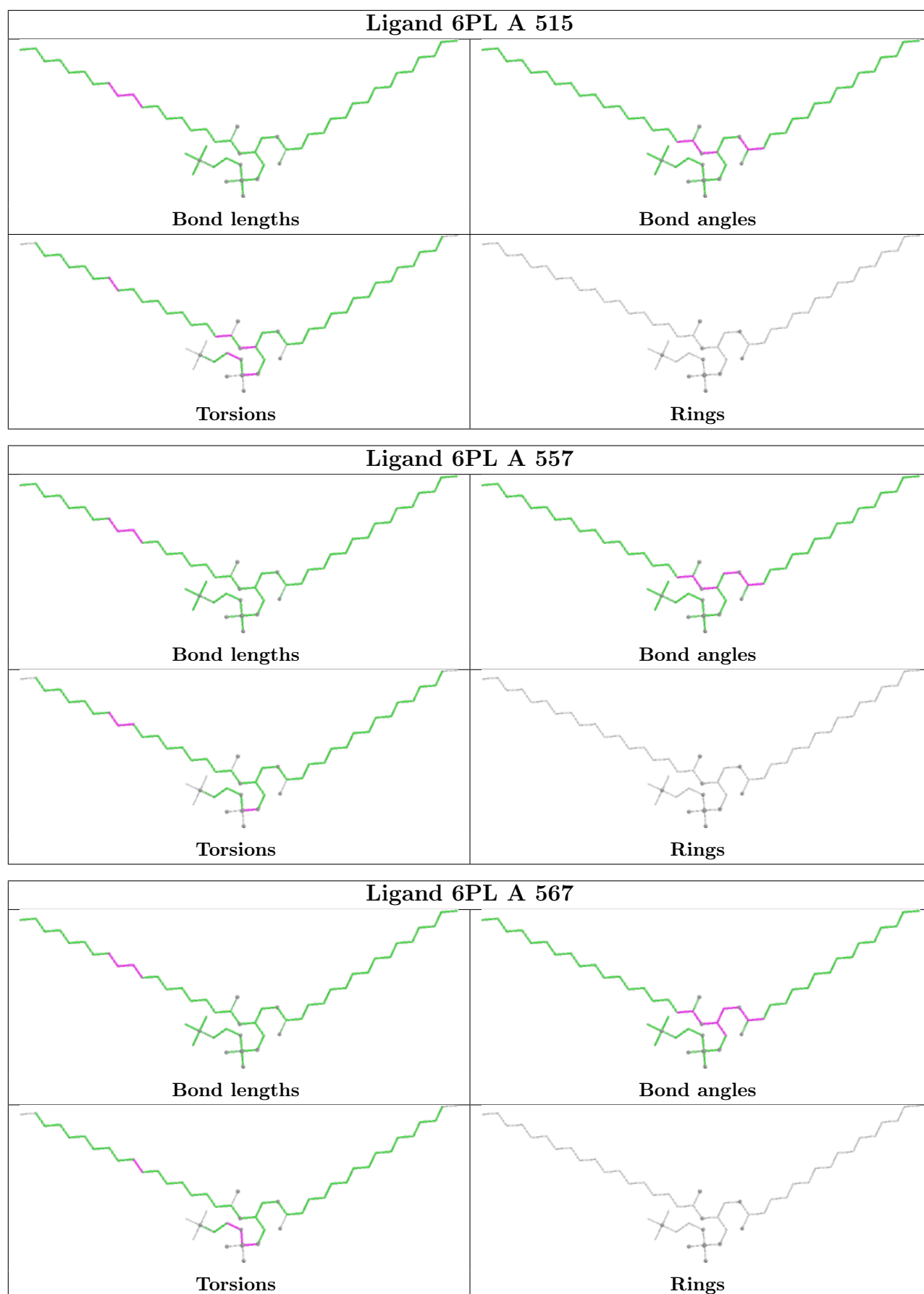


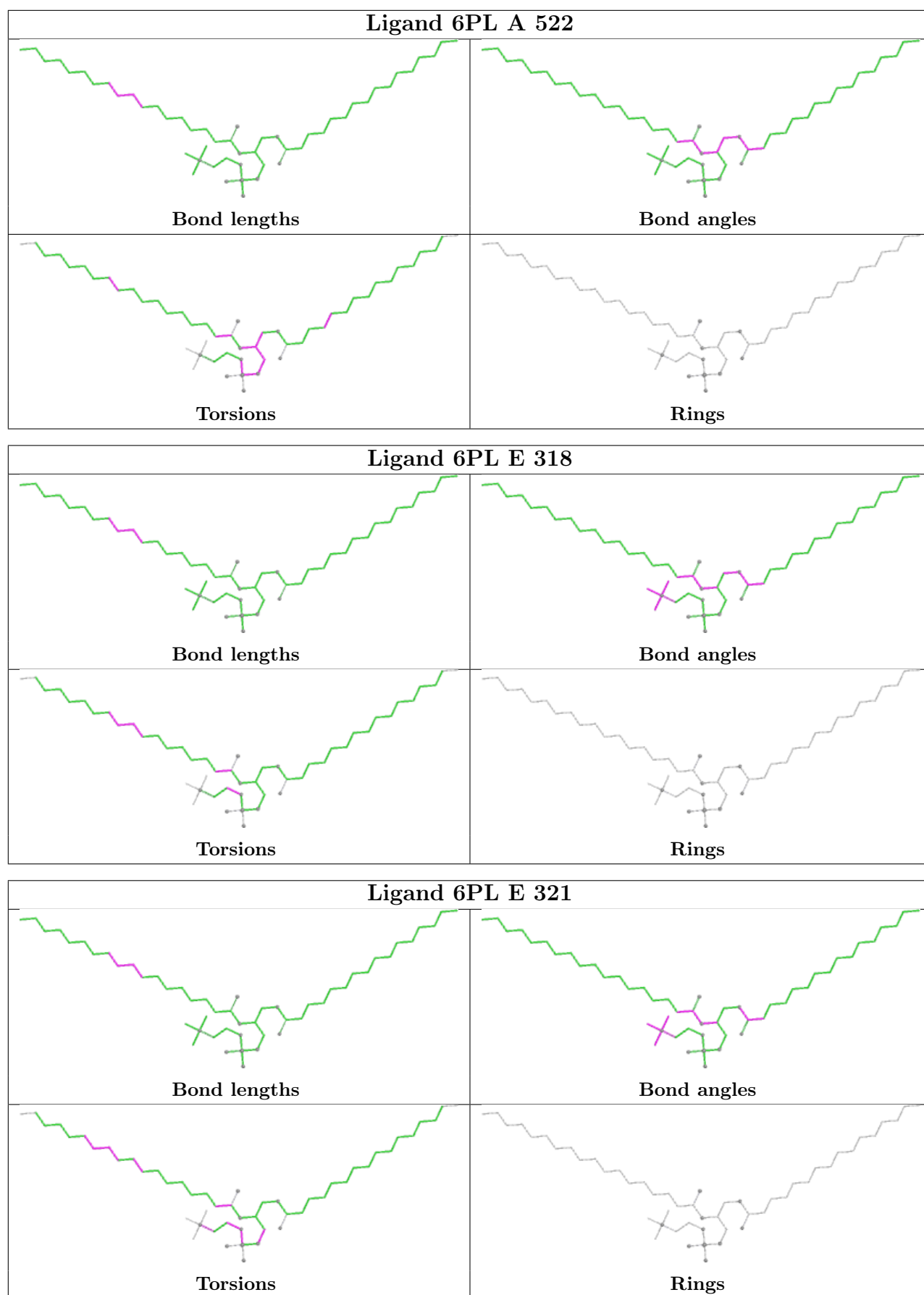


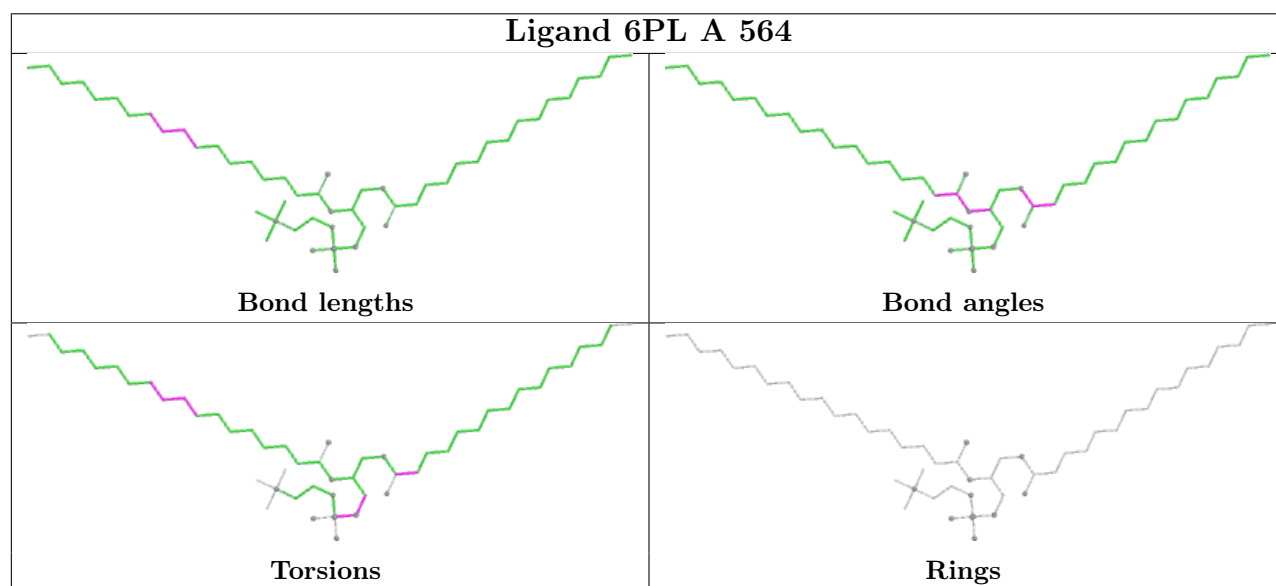
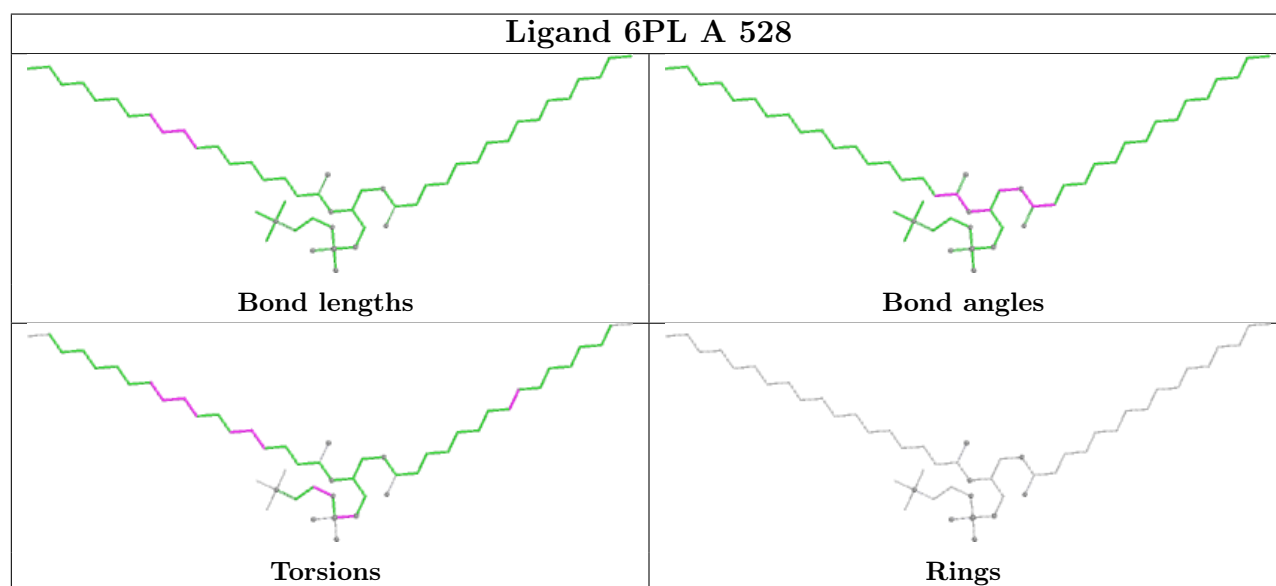
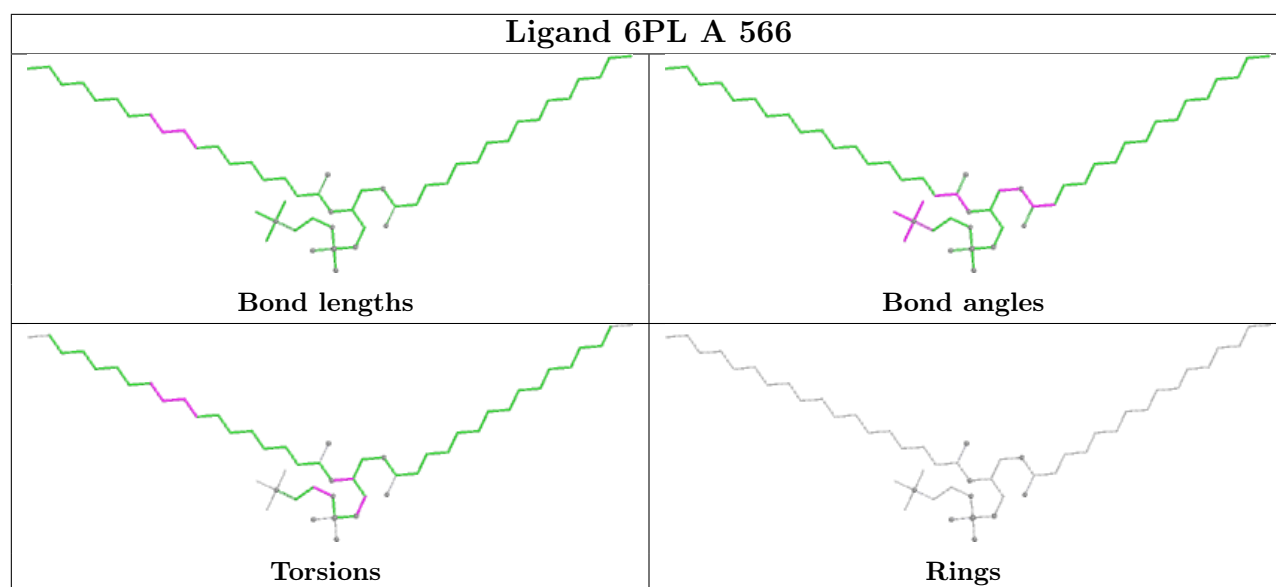


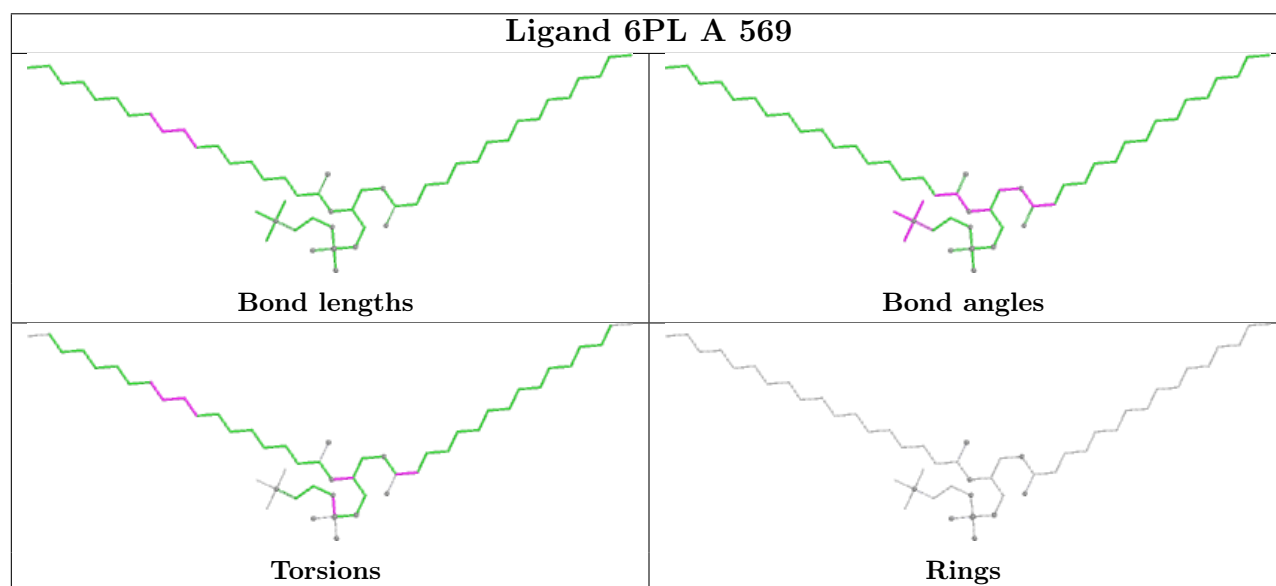
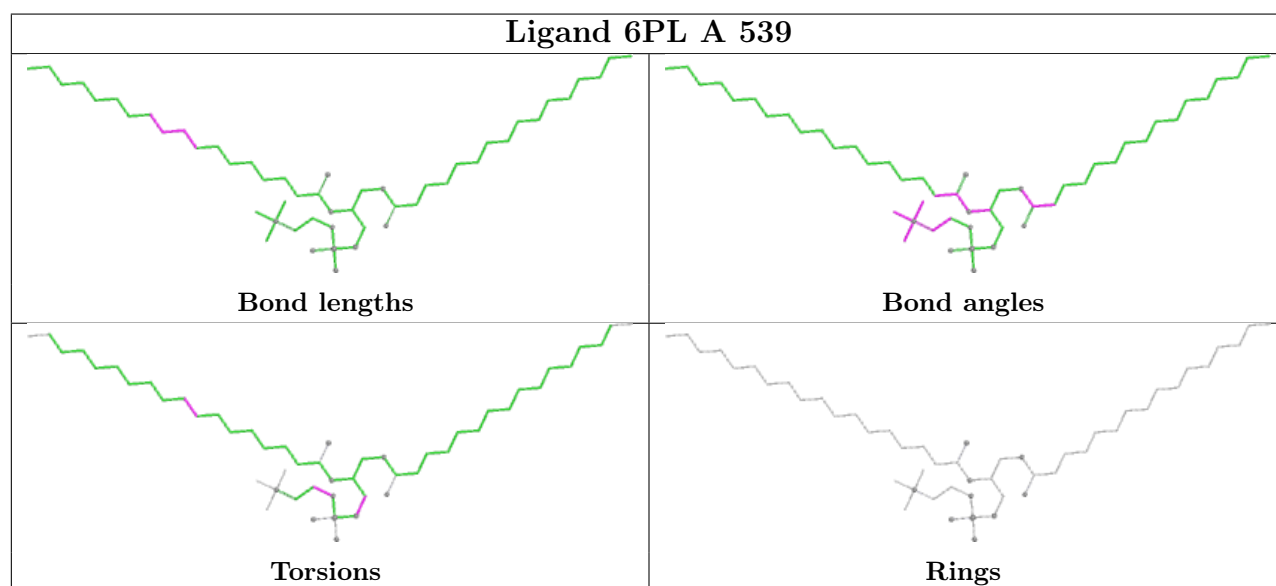
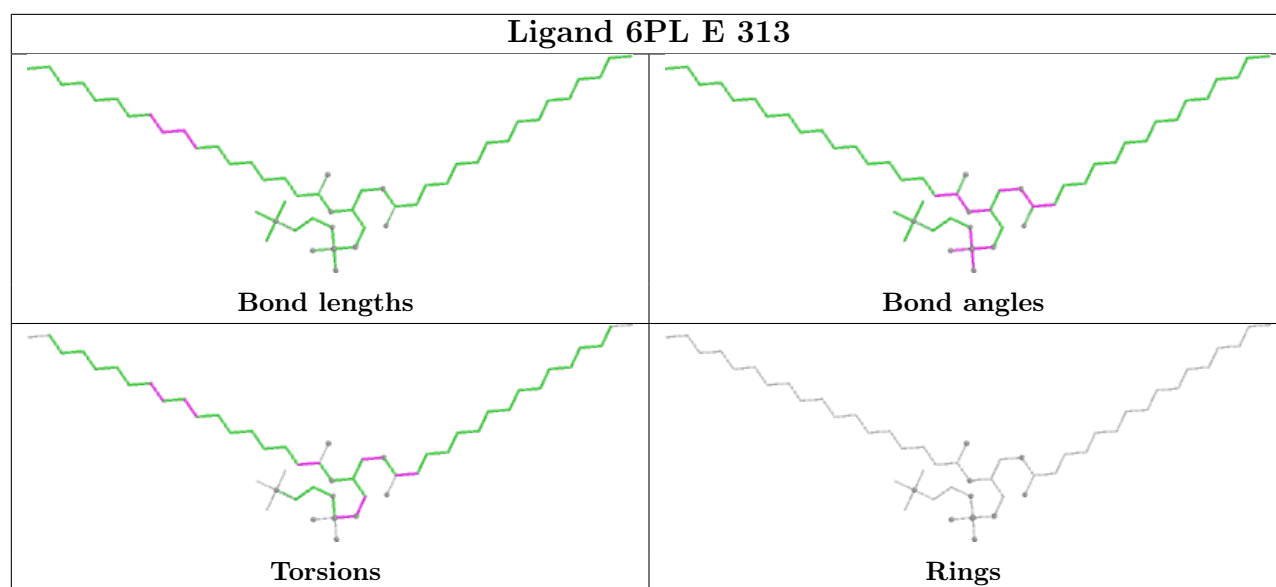


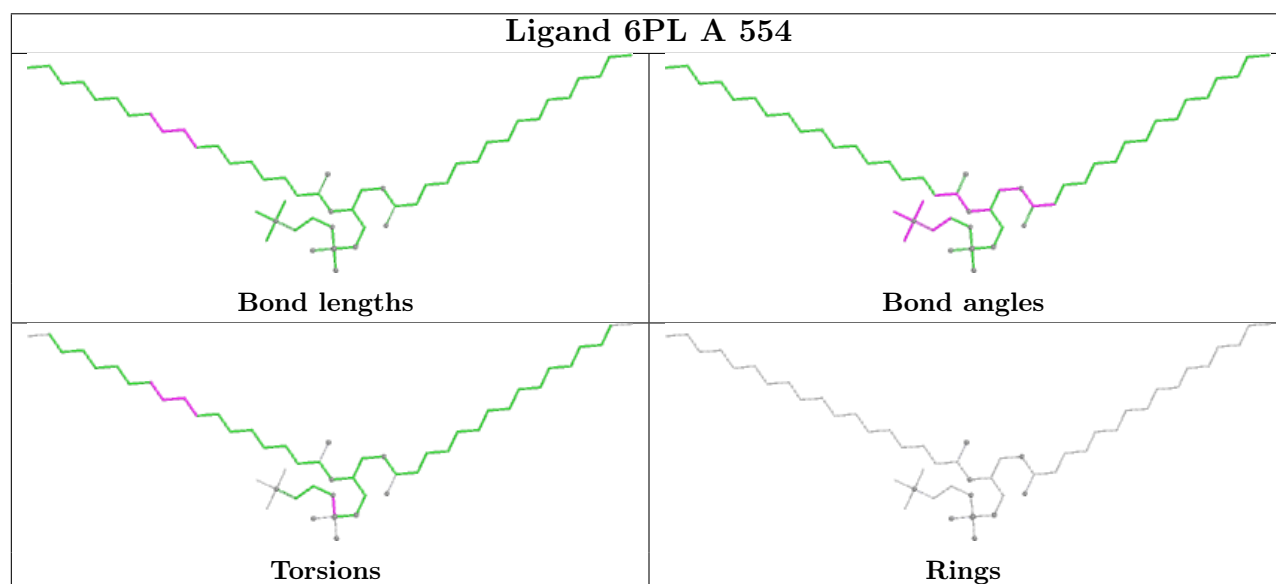
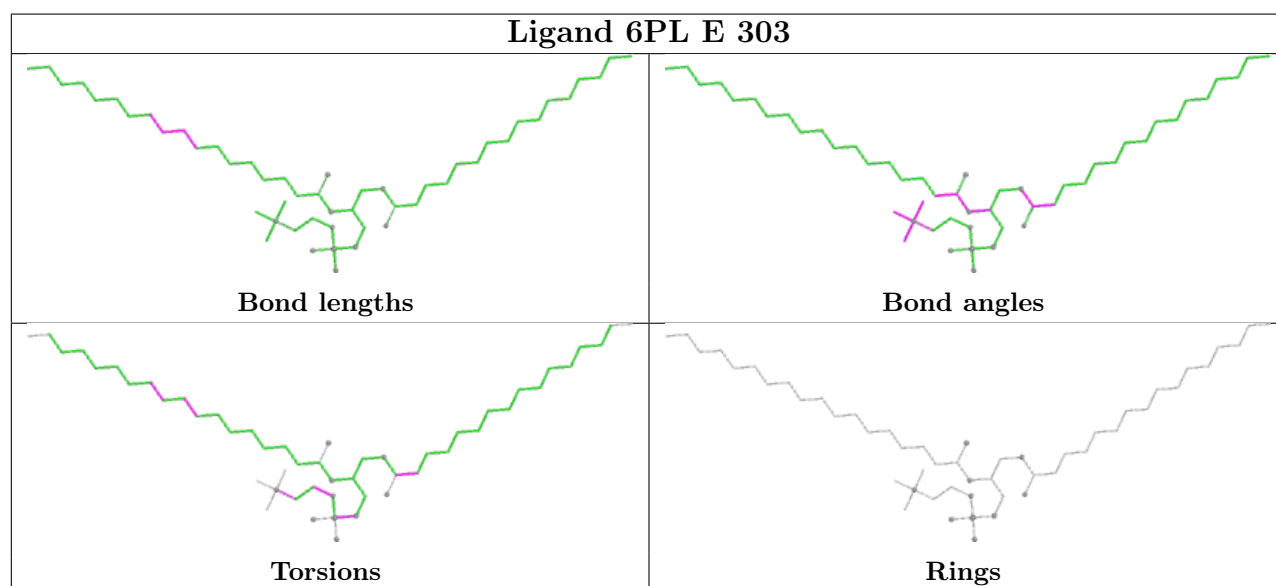
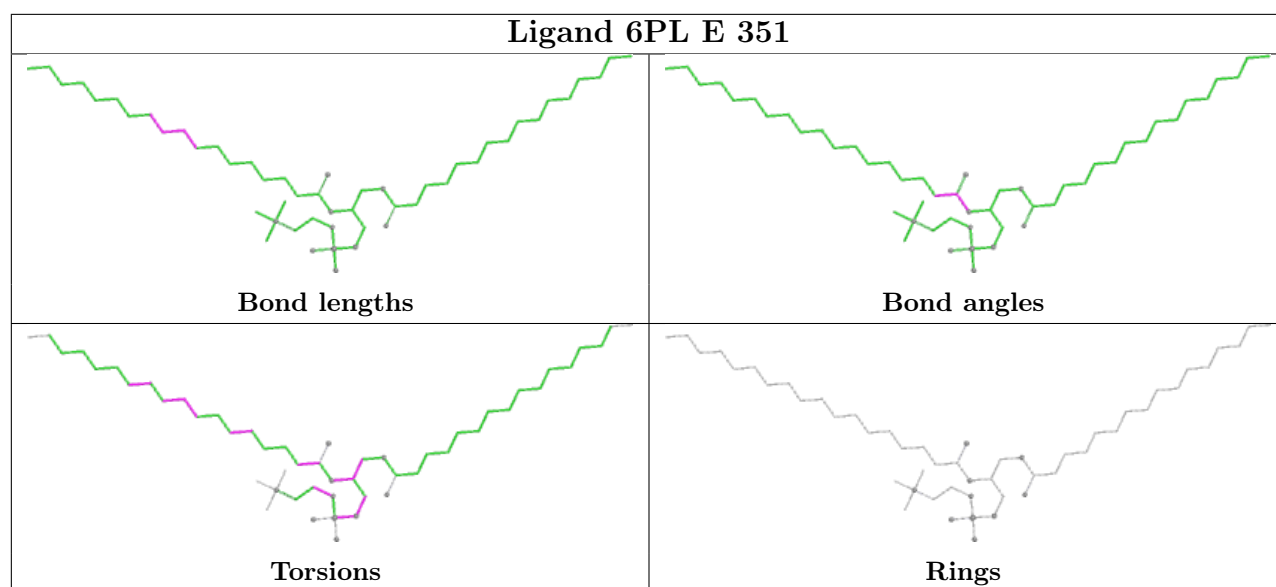


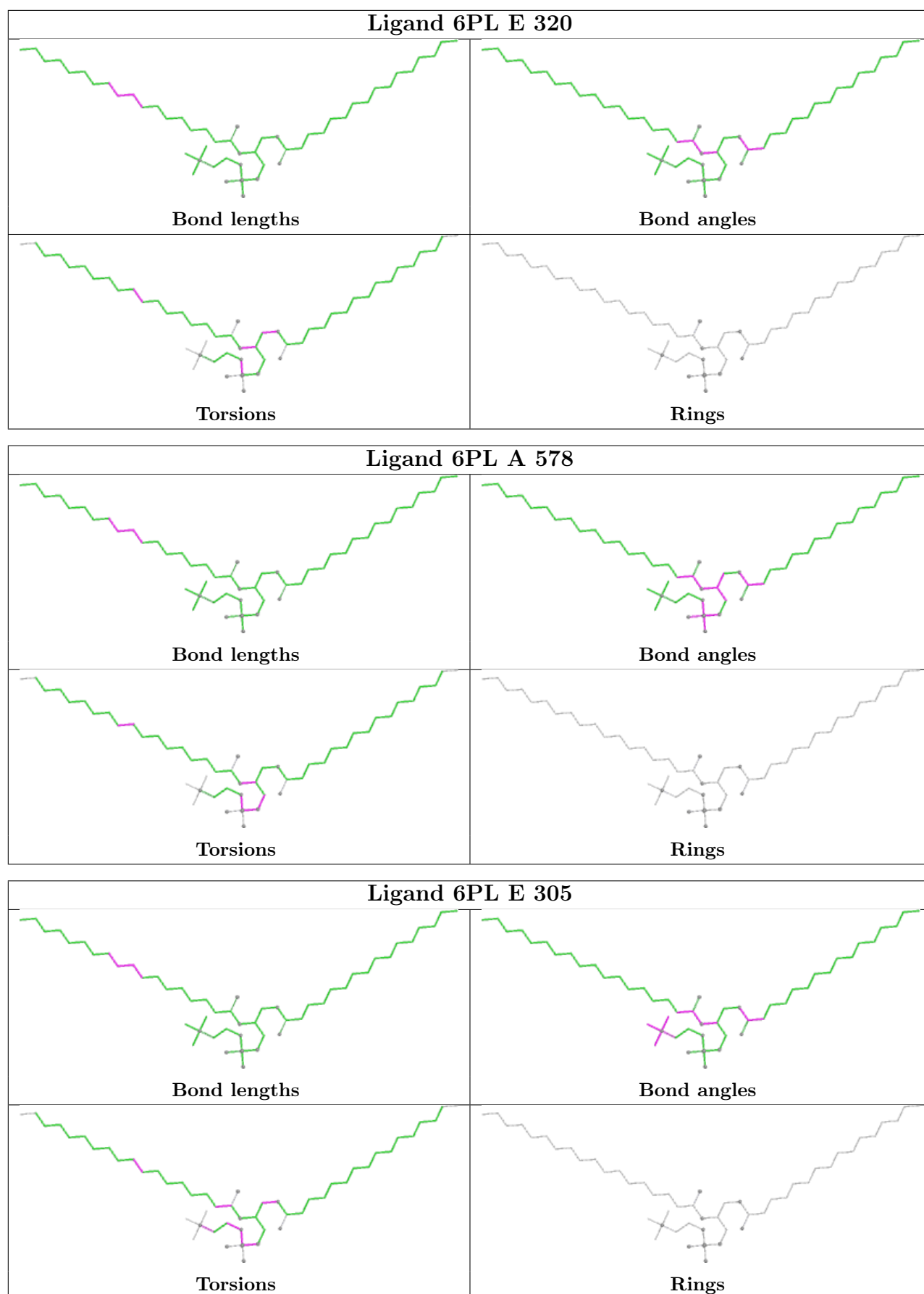


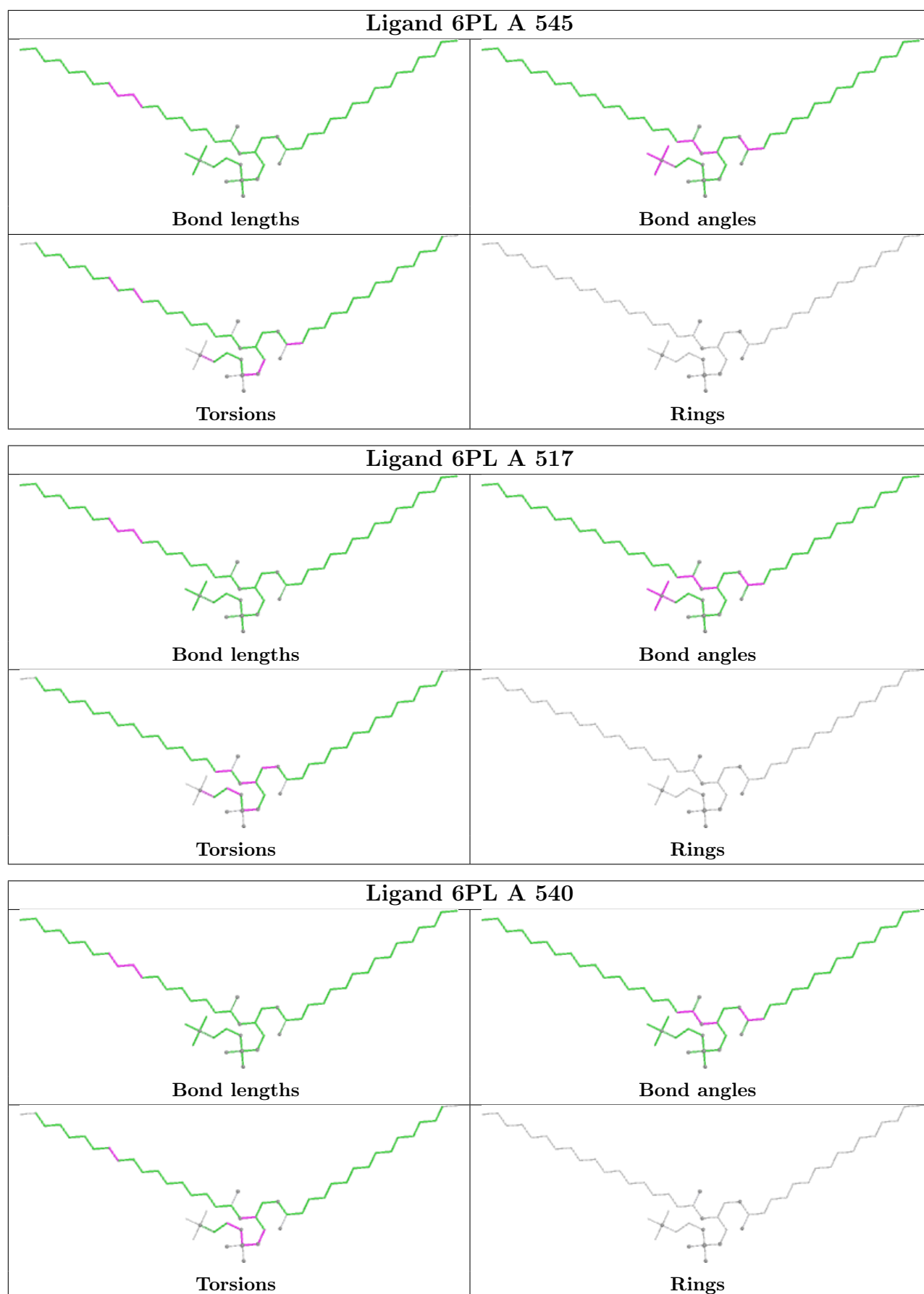


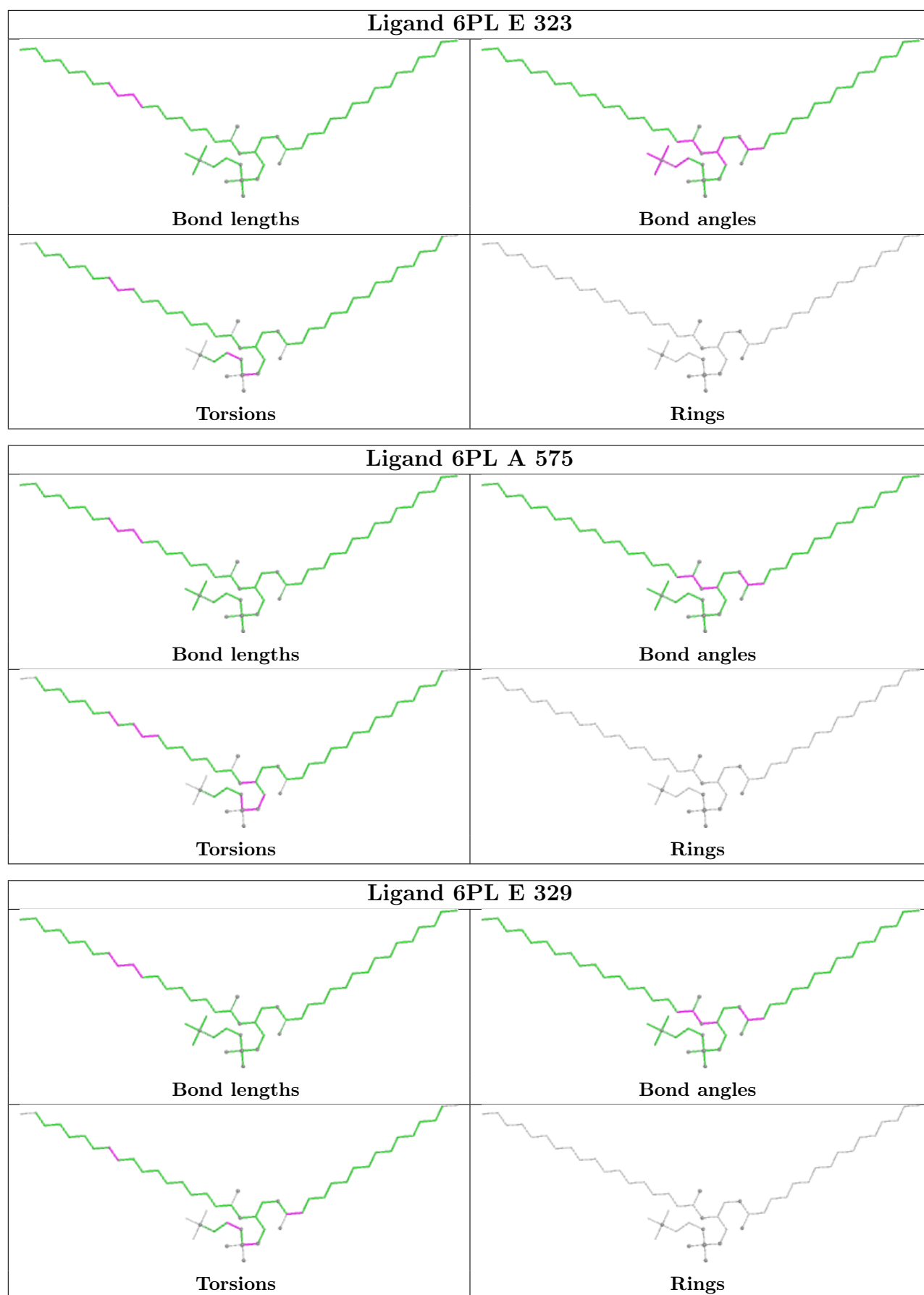


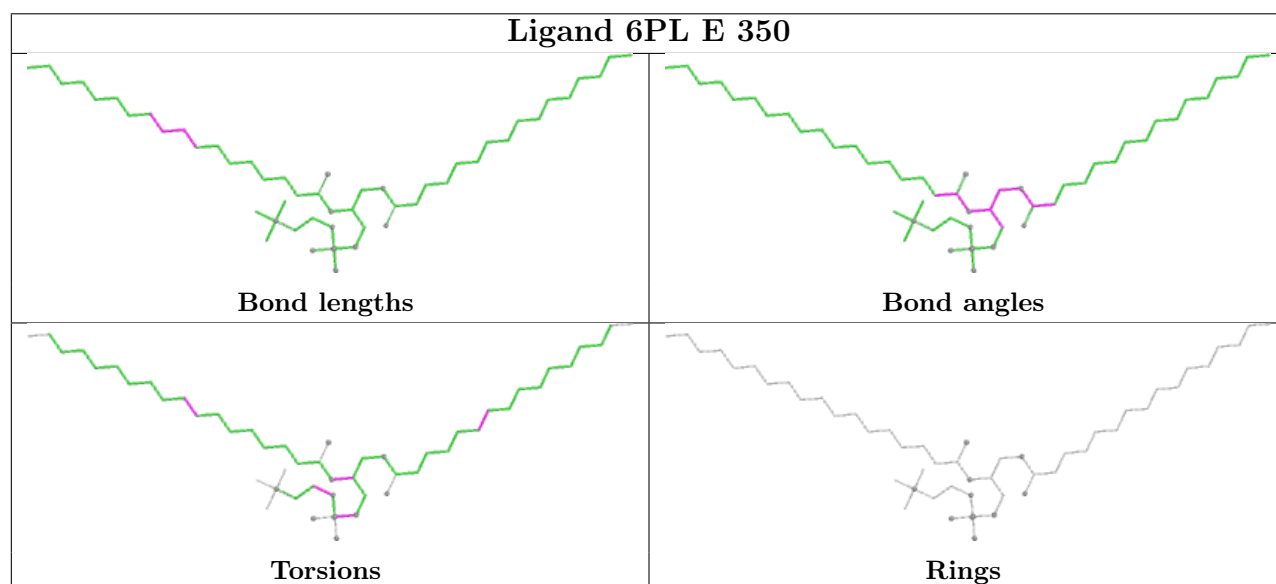
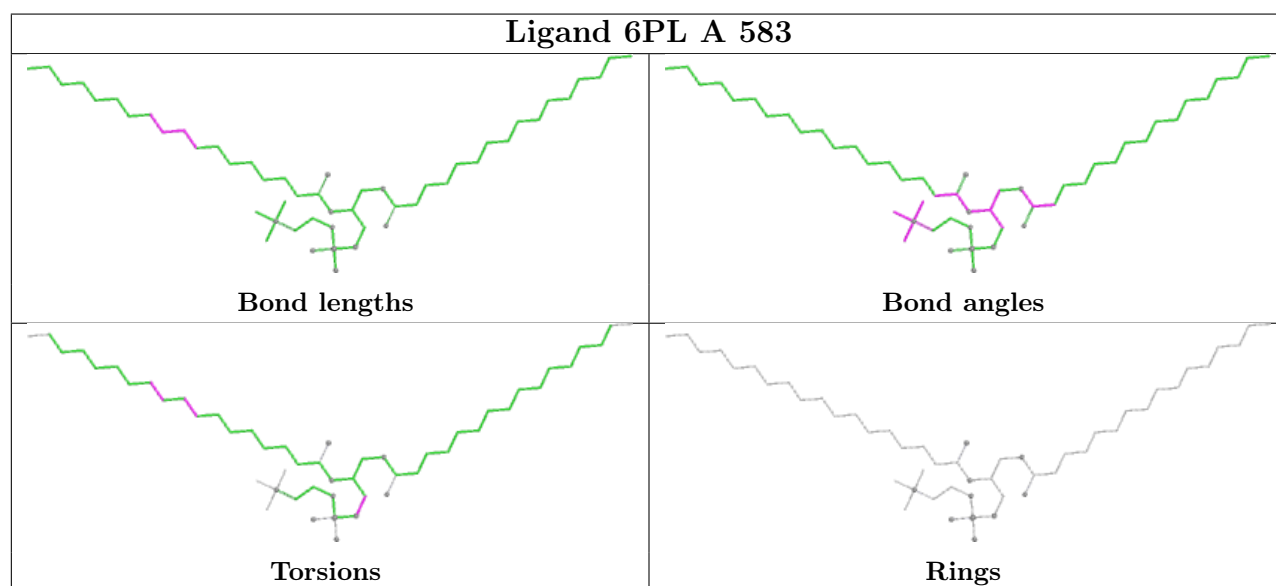
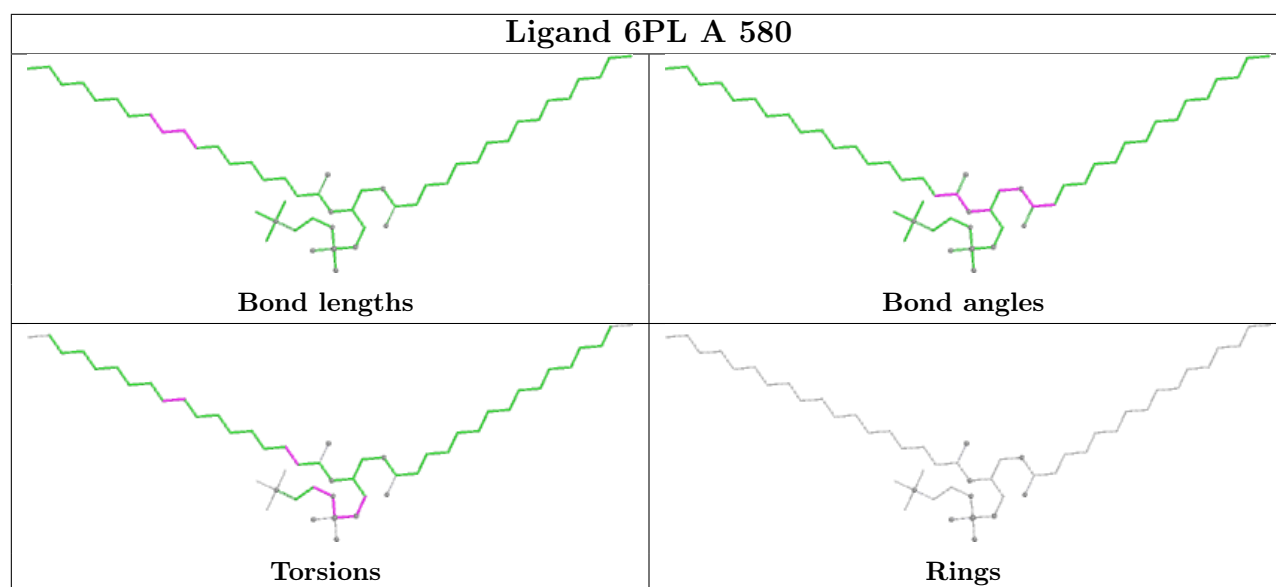


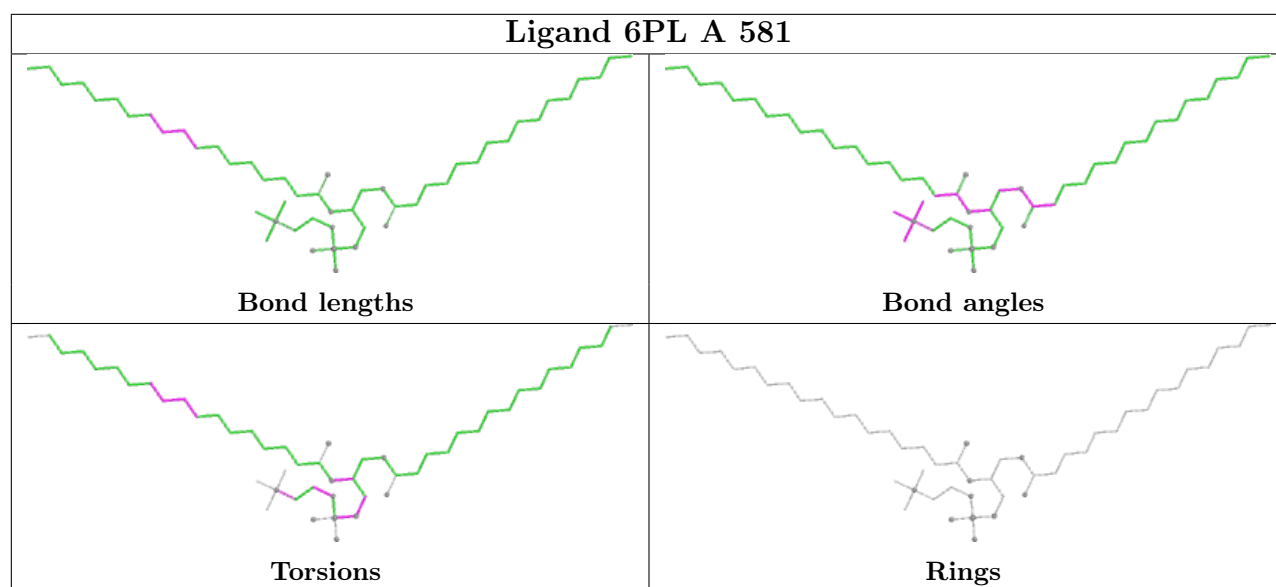












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

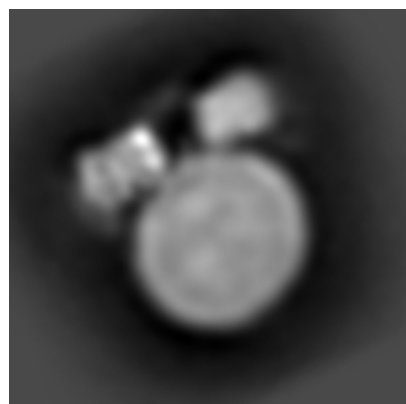
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48724. These allow visual inspection of the internal detail of the map and identification of artifacts.

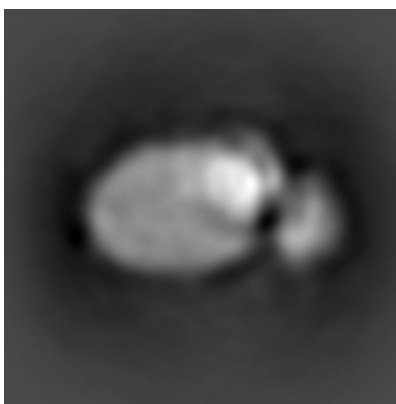
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

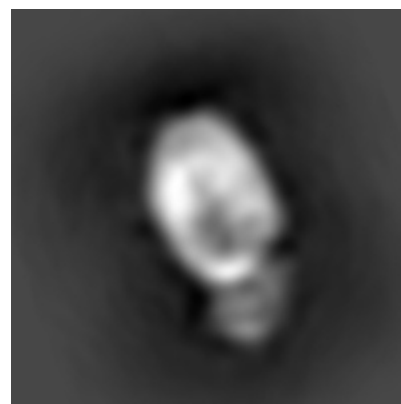
6.1.1 Primary map



X

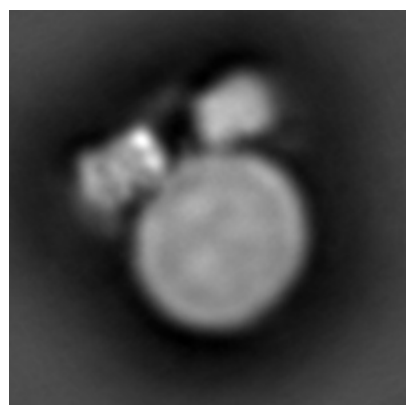


Y

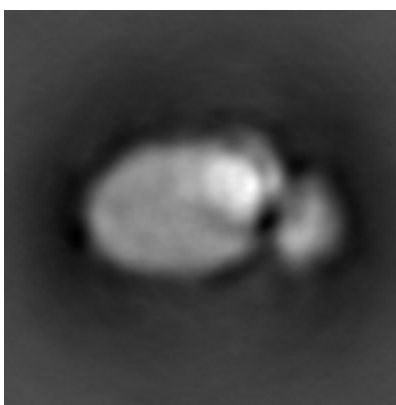


Z

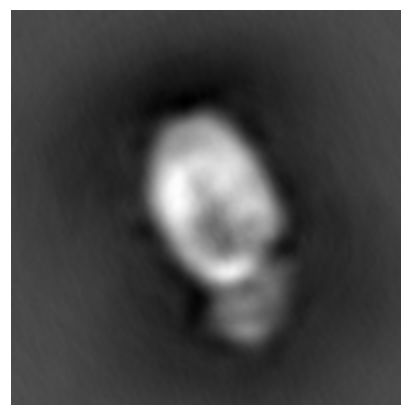
6.1.2 Raw map



X



Y

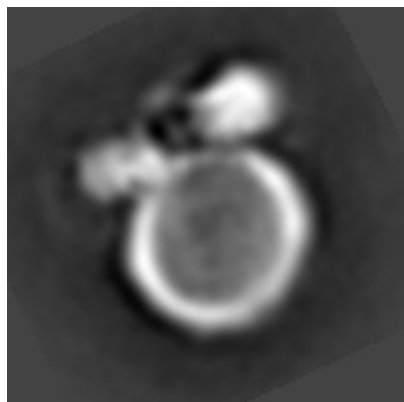


Z

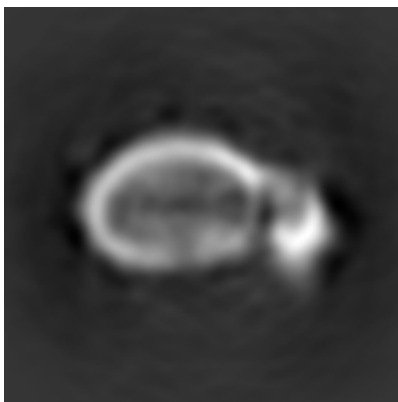
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

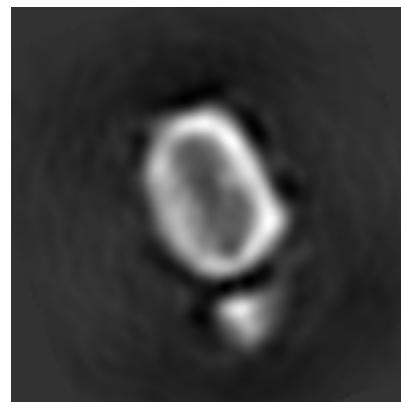
6.2.1 Primary map



X Index: 63

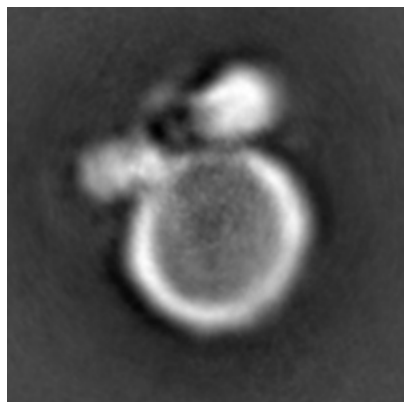


Y Index: 63

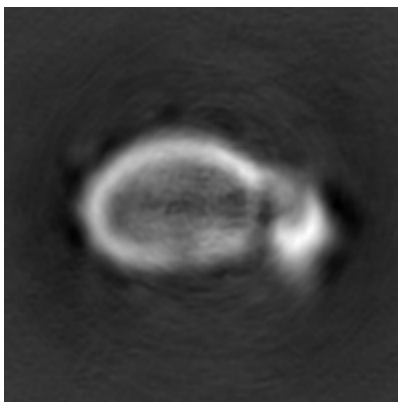


Z Index: 63

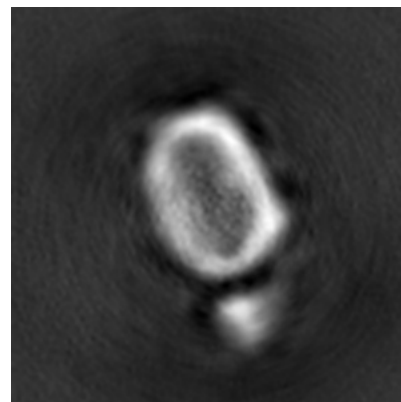
6.2.2 Raw map



X Index: 63



Y Index: 63

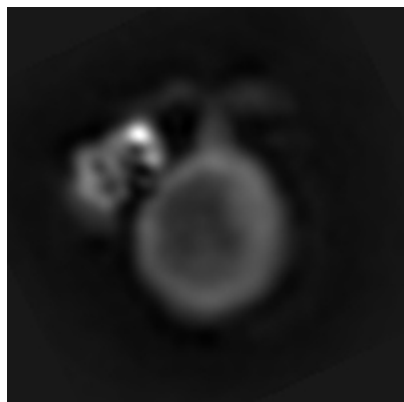


Z Index: 63

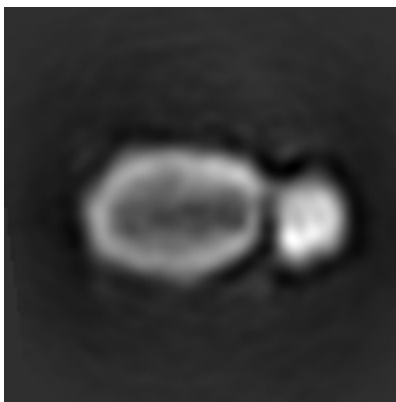
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

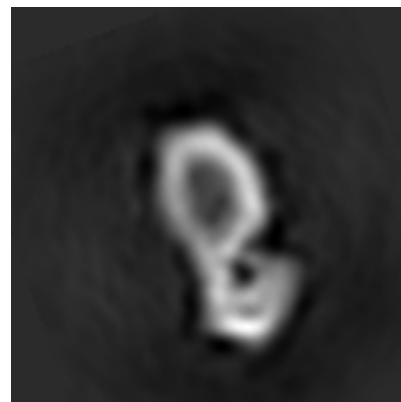
6.3.1 Primary map



X Index: 72

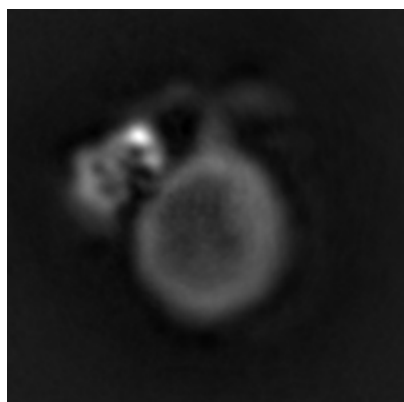


Y Index: 73

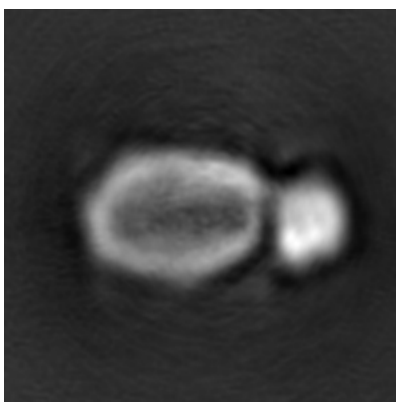


Z Index: 73

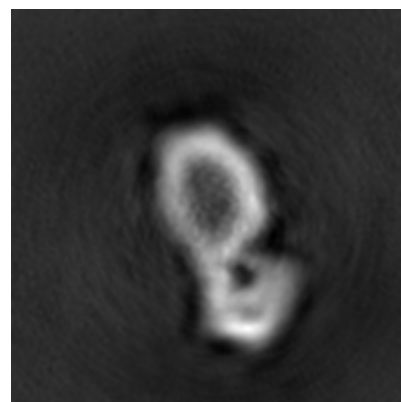
6.3.2 Raw map



X Index: 72



Y Index: 73

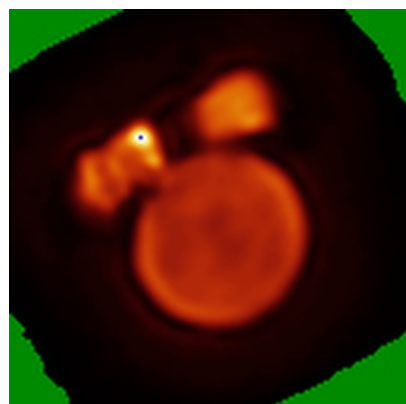


Z Index: 73

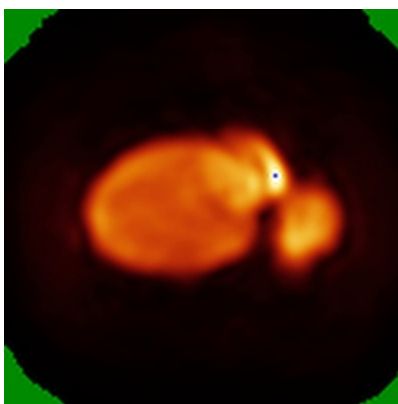
The images above show the largest variance slices of the map in three orthogonal directions.

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

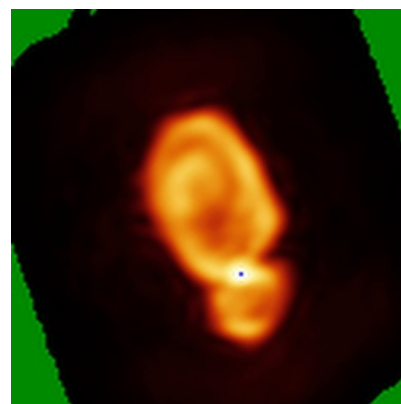
6.4.1 Primary map



X

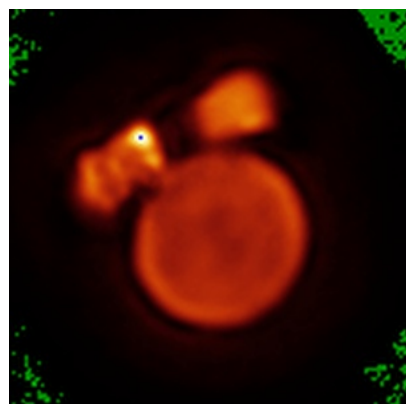


Y

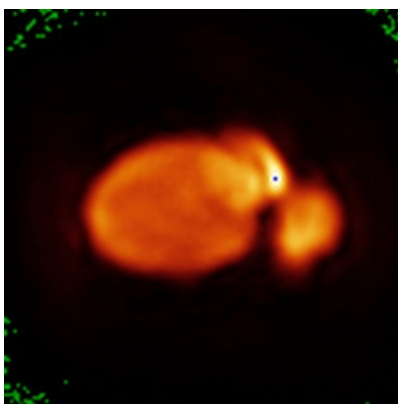


Z

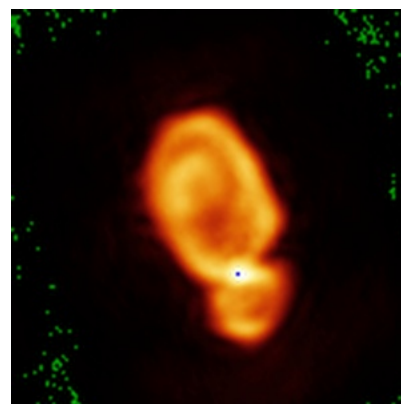
6.4.2 Raw map



X



Y

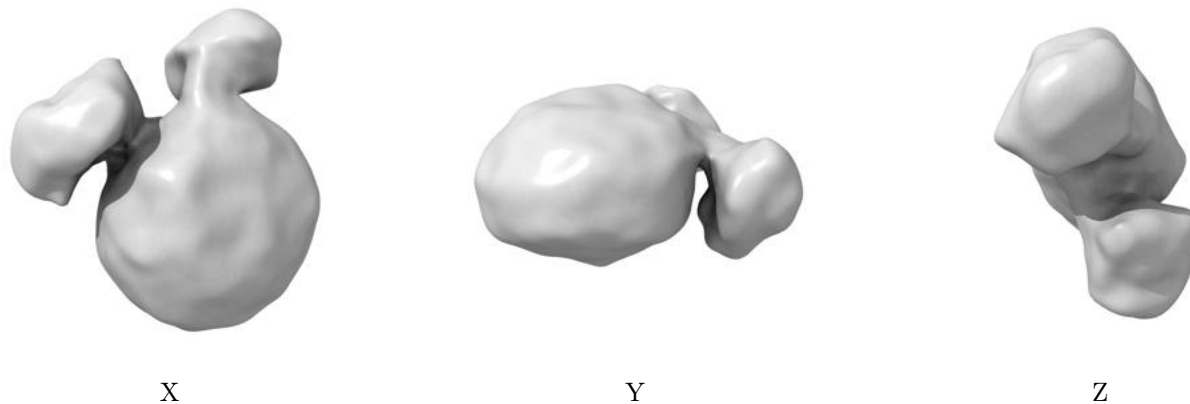


Z

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.

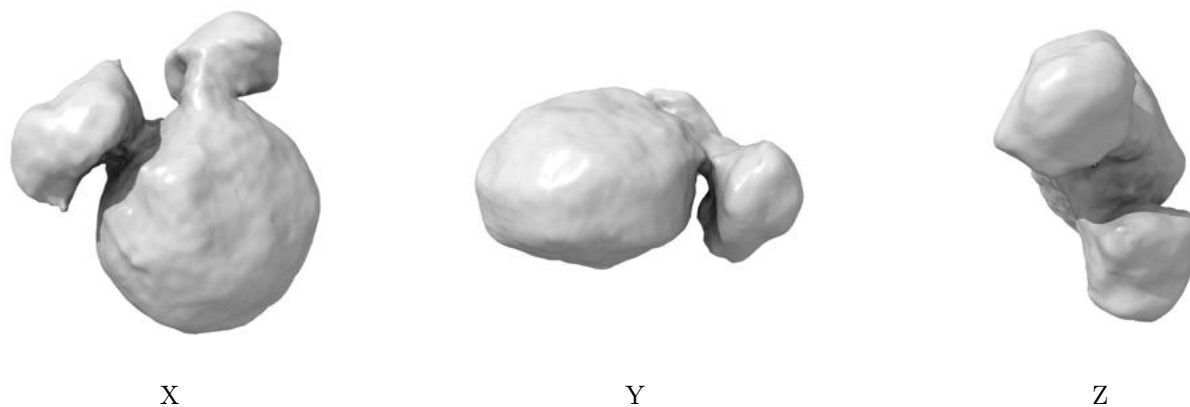
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

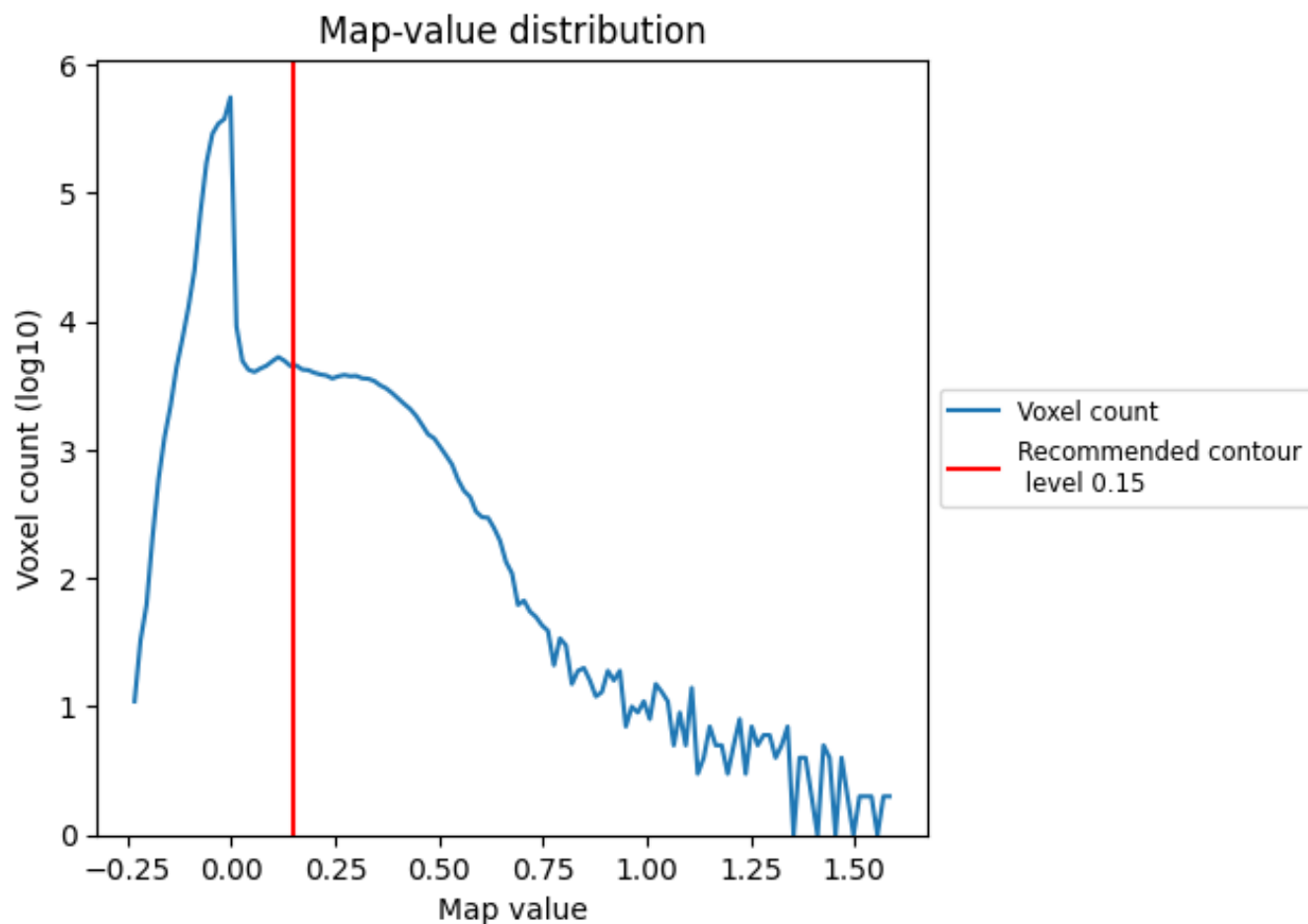
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

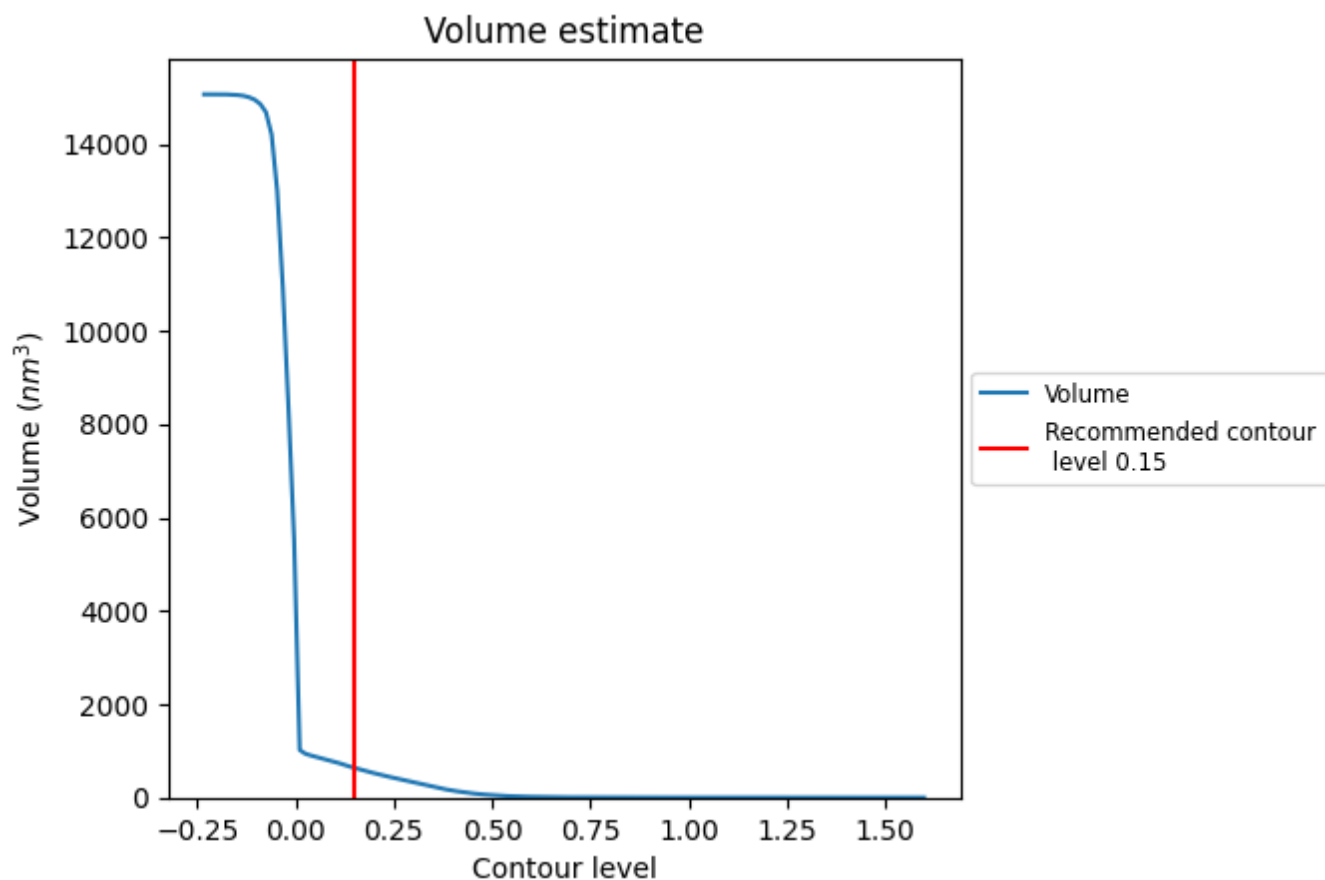
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

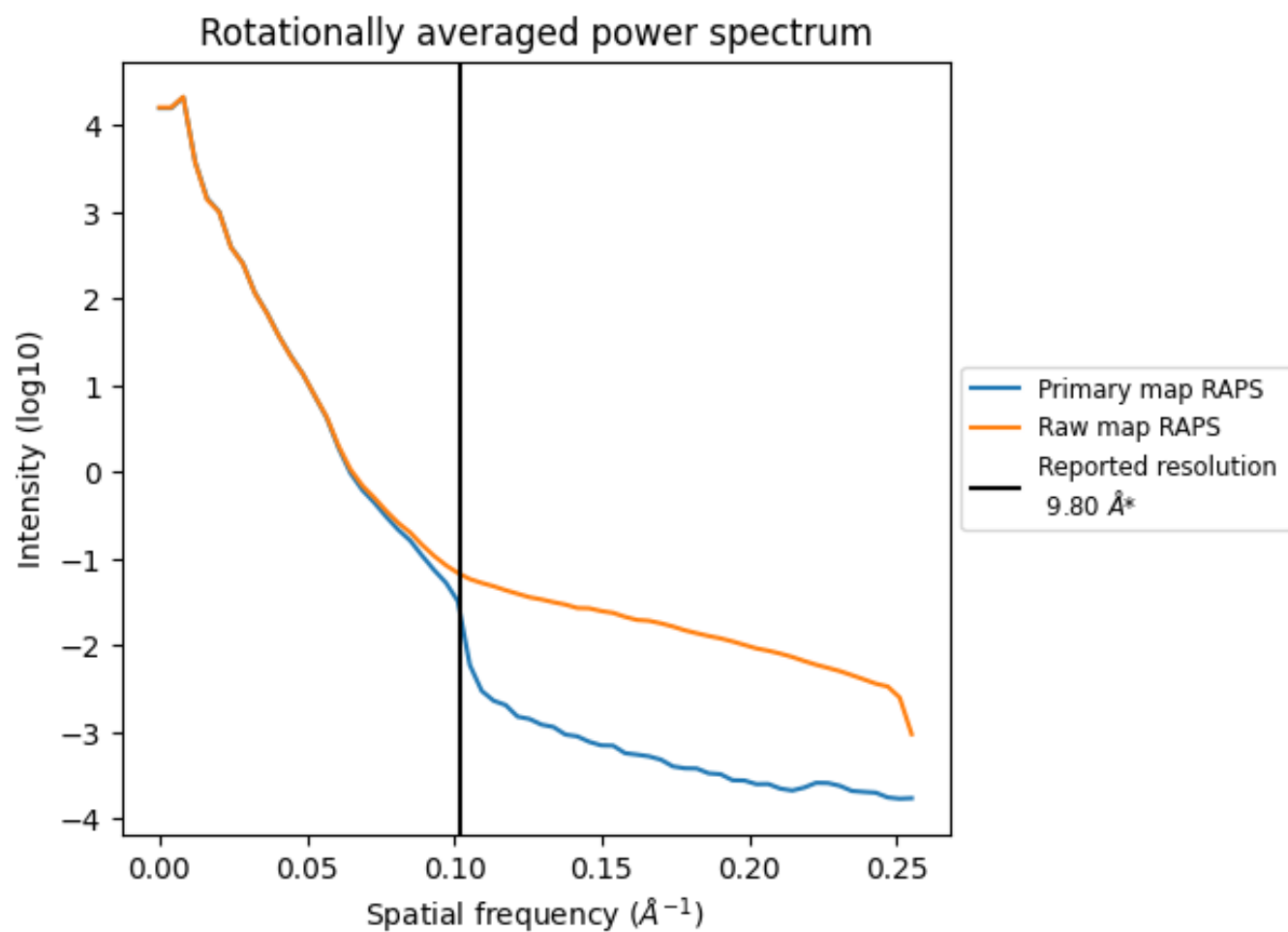
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 634 nm³; this corresponds to an approximate mass of 573 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 [i](#)

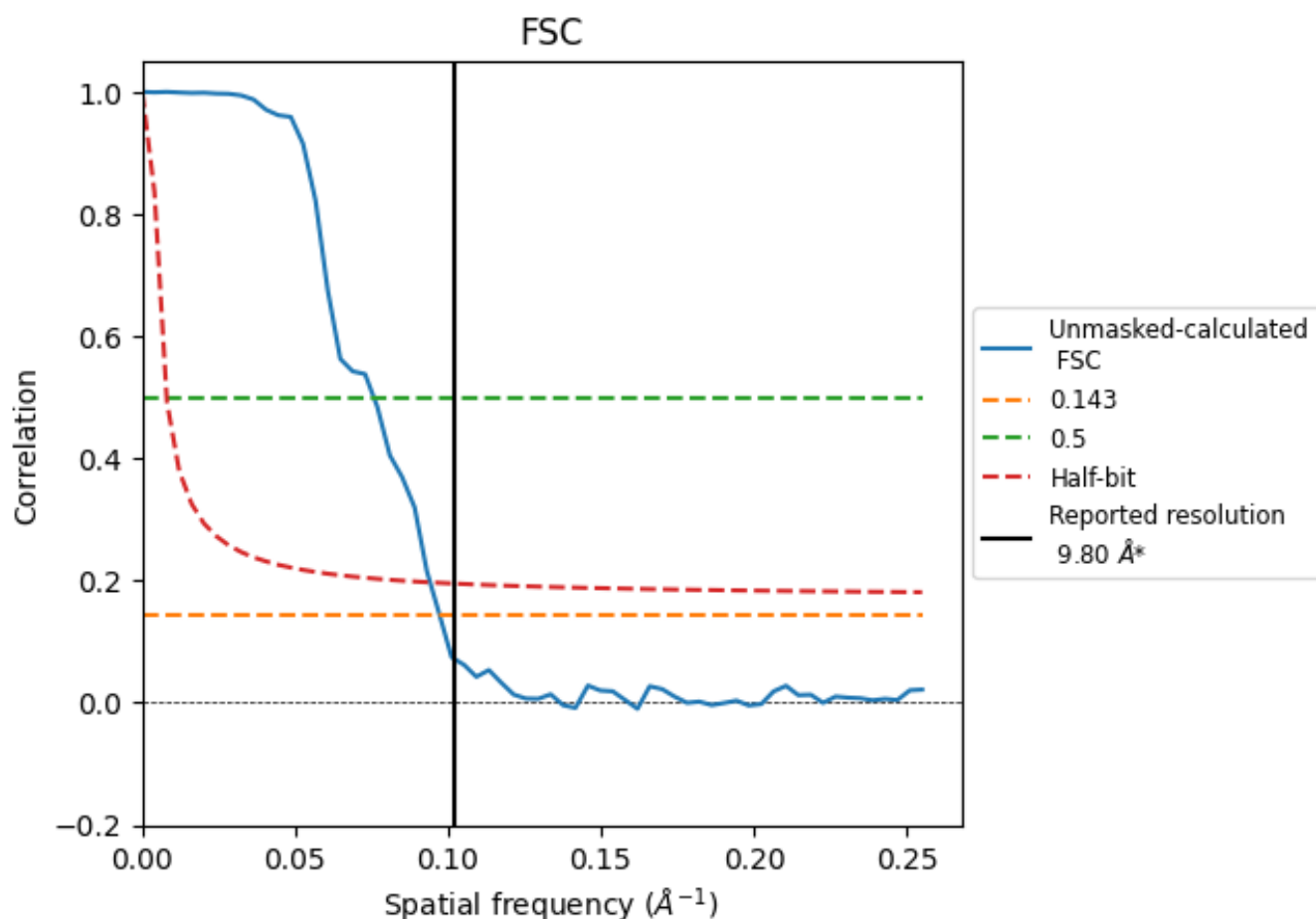


*Reported resolution corresponds to spatial frequency of 0.102 Å⁻¹

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 0.102 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.28	13.21	10.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

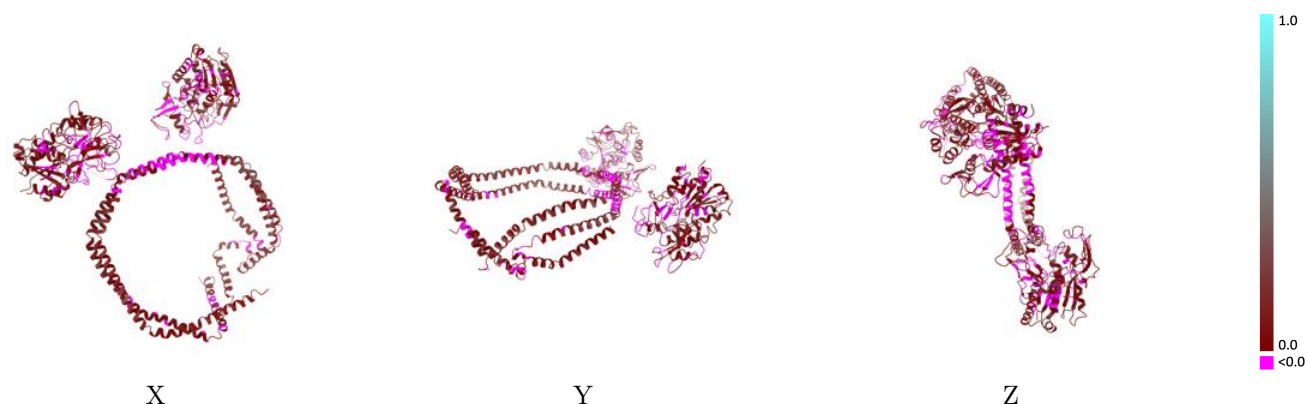
This section contains information regarding the fit between EMDB map EMD-48724 and PDB model 9MXZ. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



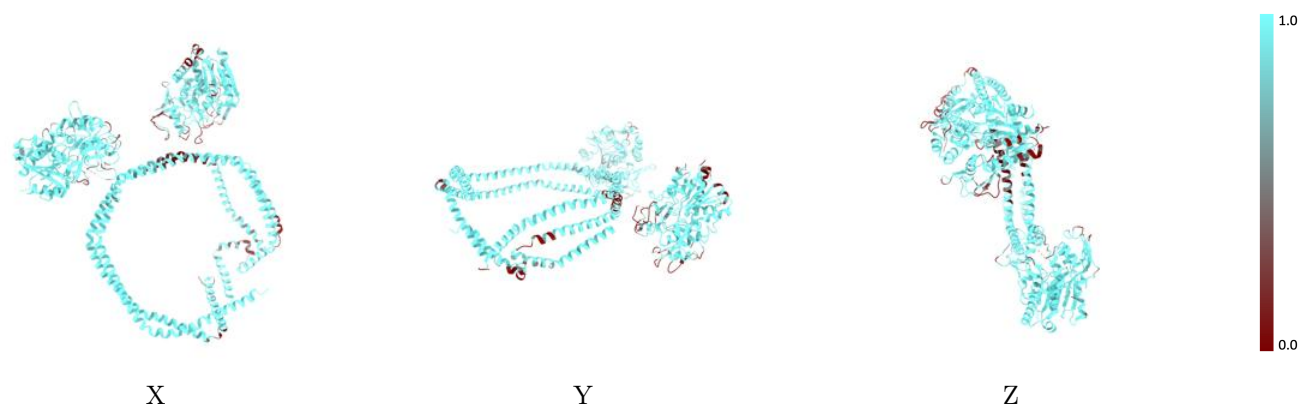
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



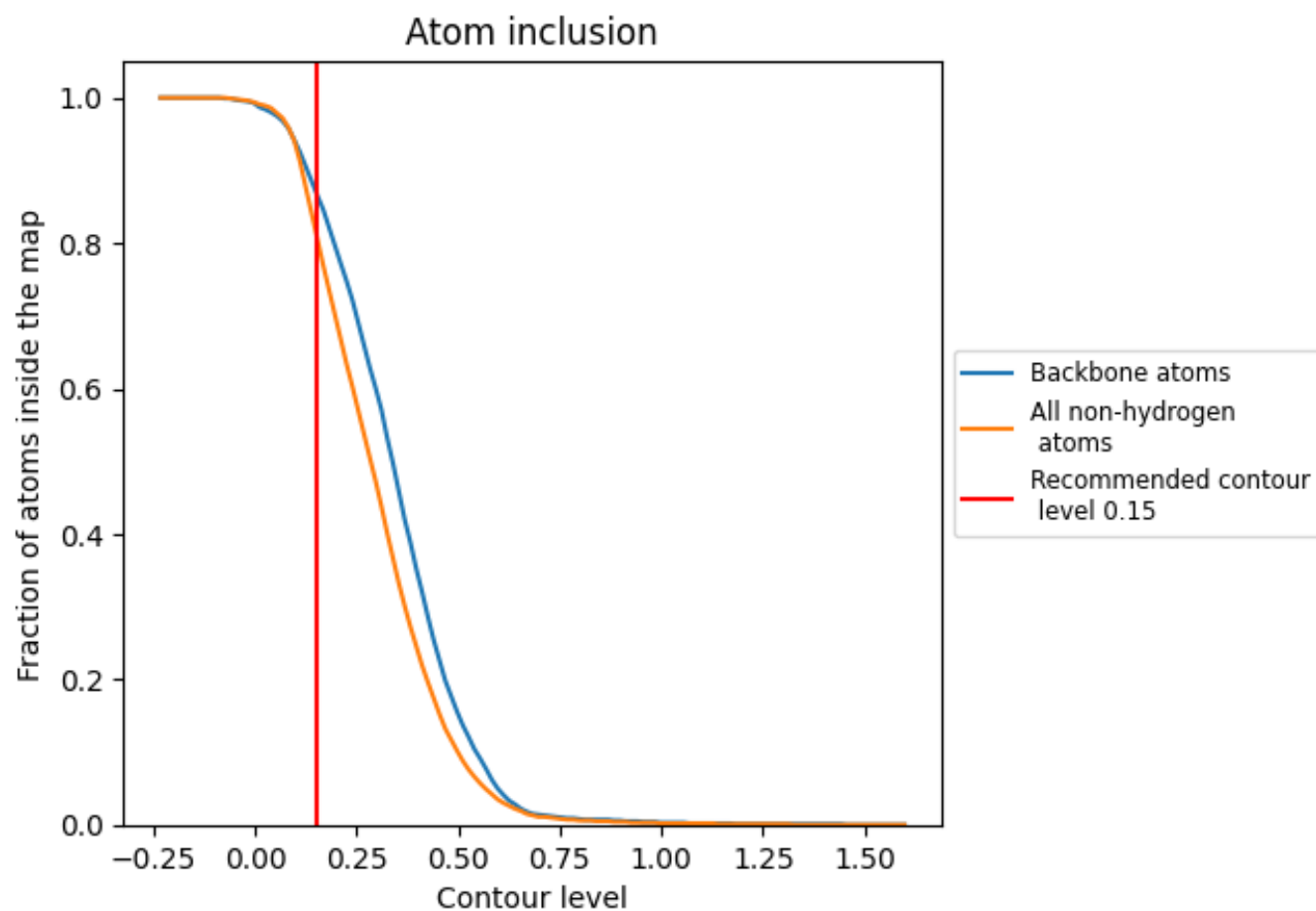
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 81% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8140	<div></div> 0.0340
A	<div></div> 0.8240	<div></div> 0.0370
B	<div></div> 0.9360	<div></div> 0.0490
C	<div></div> 0.8290	<div></div> 0.0470
E	<div></div> 0.7540	<div></div> 0.0150

