



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 09:17 pm BST

PDB ID : 5Z84
Title : The structure of azide-bound cytochrome c oxidase determined using the crystals exposed to 20 mM azide solution for 4 days
Authors : Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on : 2018-01-31
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

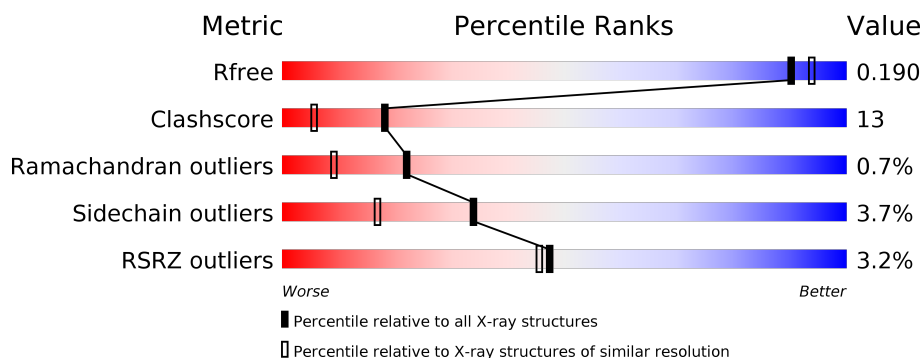
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	N	514	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	B	227	<div> <div>73%</div> <div>25%</div> <div>.</div> </div>
2	O	227	<div> <div>%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
3	C	261	<div> <div>84%</div> <div>14%</div> <div>..</div> </div>
3	P	261	<div> <div>%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
14	HEA	A	601	X	-	-	-
14	HEA	A	602[A]	X	-	-	-
14	HEA	A	602[B]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
14	HEA	N	603[A]	X	-	-	-
14	HEA	N	603[B]	X	-	-	-
18	AZI	A	606	-	-	X	-
18	AZI	A	607	-	-	X	-
18	AZI	N	608	-	-	X	-
19	TGL	D	201	-	-	X	-
21	EDO	A	615	-	X	X	-
21	EDO	A	621	-	-	X	-
21	EDO	C	319	-	-	-	X
21	EDO	D	202	-	-	X	-
21	EDO	D	203	-	-	X	X
21	EDO	F	105	-	-	X	-
21	EDO	N	618	-	-	X	-
21	EDO	N	621	-	-	X	-
21	EDO	N	622	-	-	X	-
22	CHD	J	101	-	-	-	X
24	PSC	B	303	-	-	X	-
28	CDL	C	306	-	-	X	-
28	CDL	P	304	-	-	X	-
9	SAC	V	1	-	X	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33735 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	22	0
			4193	2793	649	709	42			
1	N	514	Total	C	N	O	S	0	20	0
			4179	2786	647	704	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	10	0
			1904	1239	292	353	20			
2	O	227	Total	C	N	O	S	0	4	0
			1859	1206	287	346	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	4	0
			1231	800	205	222	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	4	0
			778	481	139	152	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	1
			686	440	130	114	1	1		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	1	0
			469	302	79	85	3			

- Molecule 11 is a protein called cytochrome c oxidase subunit 11, Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

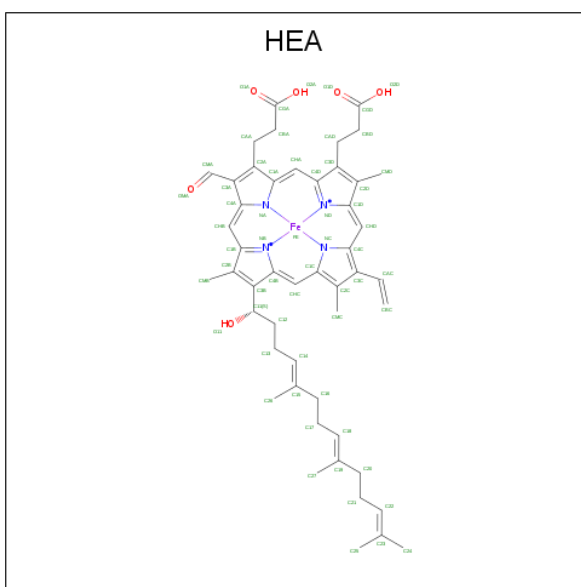
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			385	258	64	60	3			
12	Y	46	Total	C	N	O	S	0	1	0
			388	259	65	61	3			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 120	C 98	Fe 2	N 8	O 12	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 120	C 98	Fe 2	N 8	O 12	0	1

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	N	1	Total	Cu	0	0
			1	1		

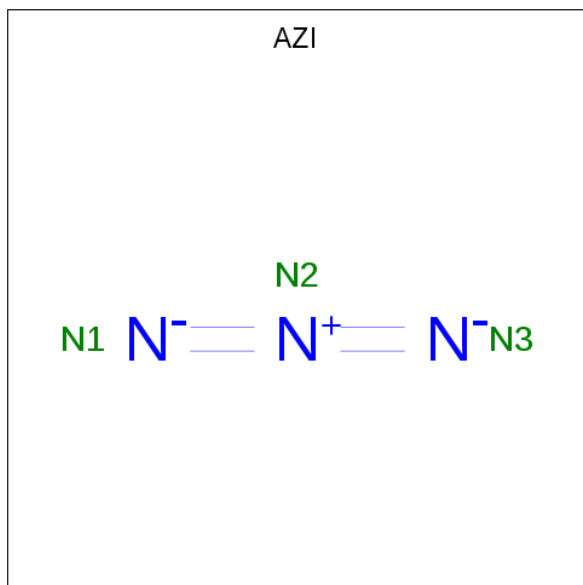
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

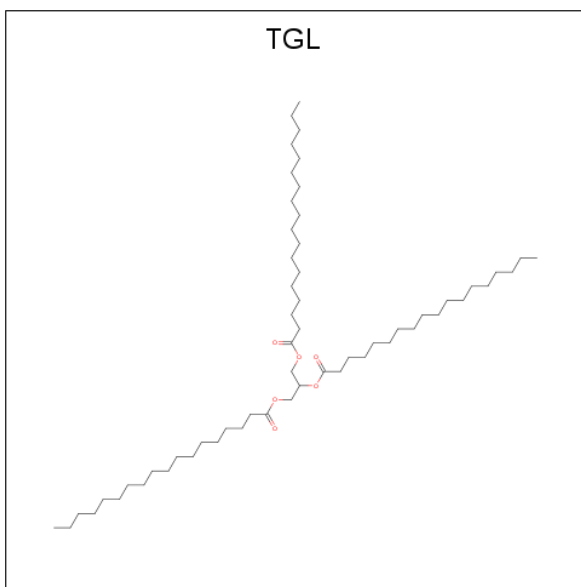
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is AZIDE ION (three-letter code: AZI) (formula: N₃).



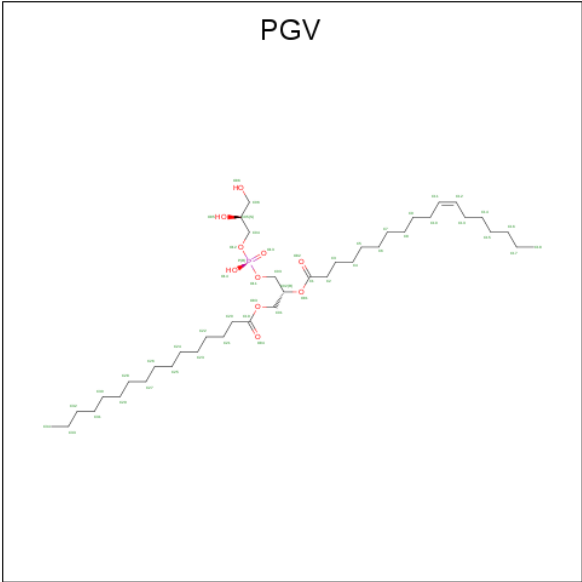
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	0
18	A	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	G	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	Z	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0

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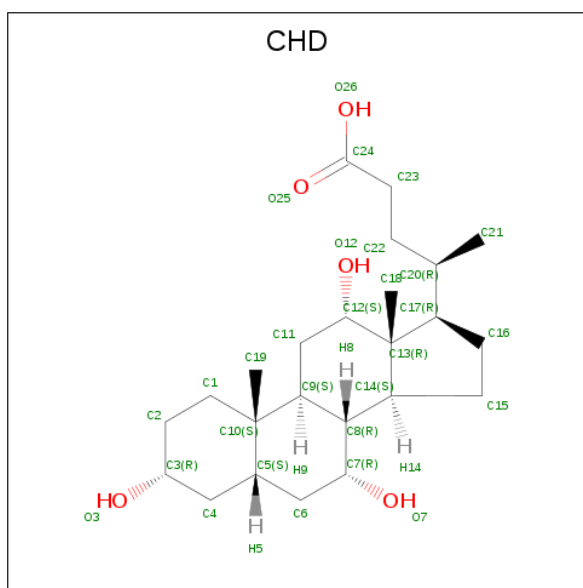
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	H	1	Total 4	C 2	O 2	0	0
21	H	1	Total 4	C 2	O 2	0	0
21	J	1	Total 4	C 2	O 2	0	0
21	L	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0

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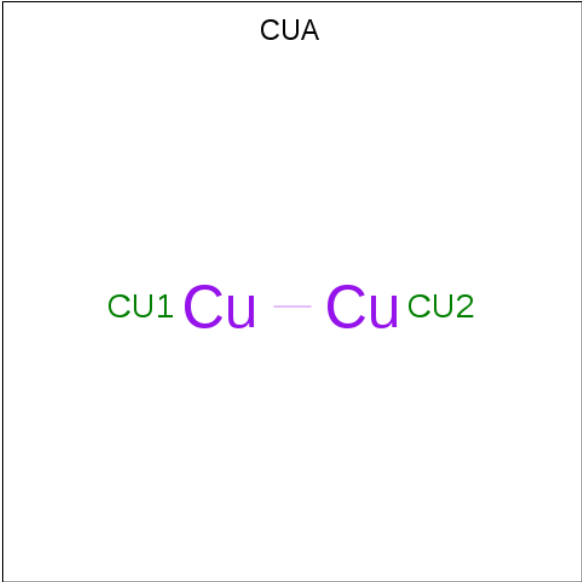
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	T	1	Total 4	C 2	O 2	0	0
21	U	1	Total 4	C 2	O 2	0	0
21	V	1	Total 4	C 2	O 2	0	0

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



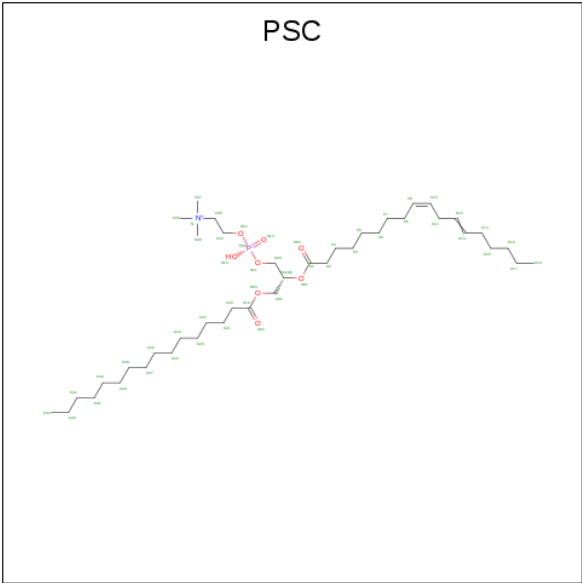
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Cu	0	0
			2	2		
23	O	1	Total	Cu	0	0
			2	2		

- Molecule 24 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



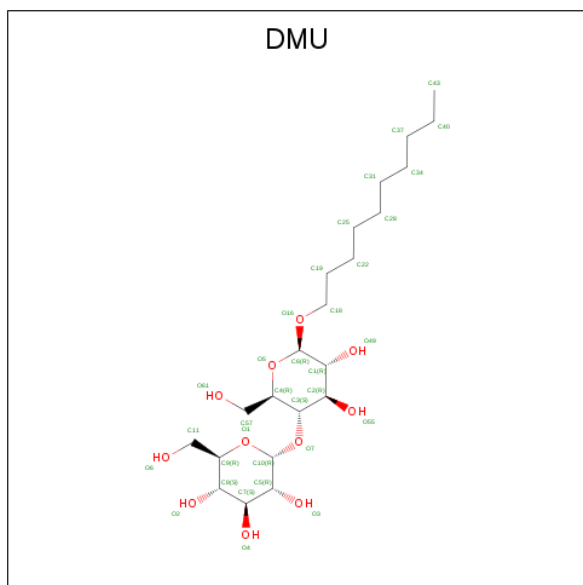
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

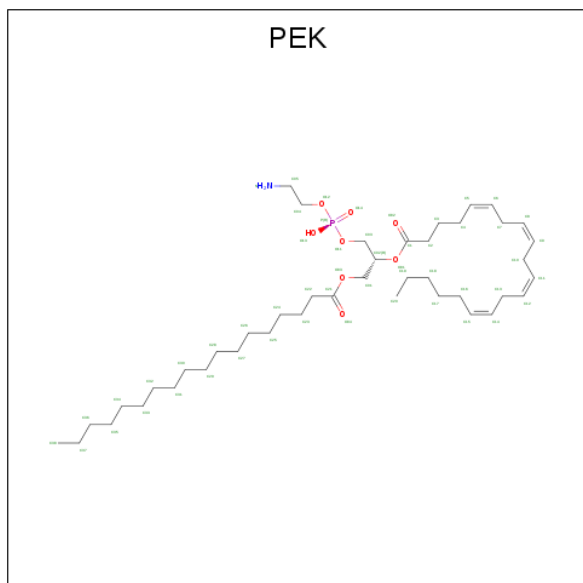


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			33	22	11		
25	L	1	Total	C	O	0	0
			33	22	11		
25	M	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 26 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

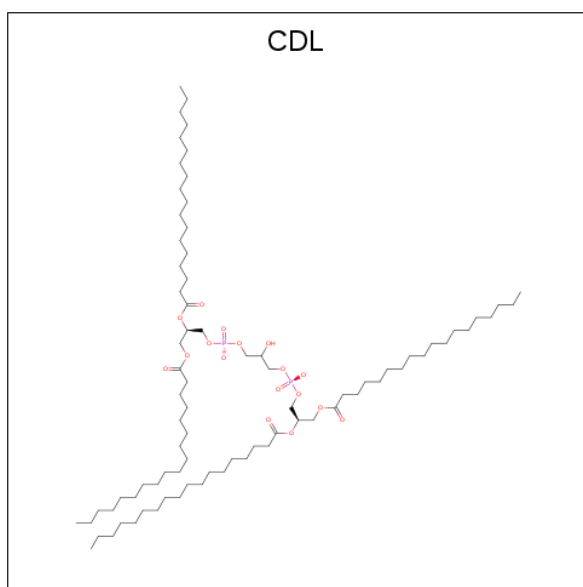
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	P	1	Total X 1 1	0	0
26	C	1	Total X 1 1	0	0

- Molecule 27 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 28 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	C	1	Total	C	O	P	0	0
			100	81	17	2		
28	N	1	Total	C	O	P	0	0
			100	81	17	2		
28	P	1	Total	C	O	P	0	0
			100	81	17	2		
28	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	S	1	Total	Zn	0	0
			1	1		
29	F	1	Total	Zn	0	0
			1	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	232	Total	O	0	1
			233	233		
30	B	139	Total	O	0	1
			140	140		
30	C	101	Total	O	0	0
			101	101		

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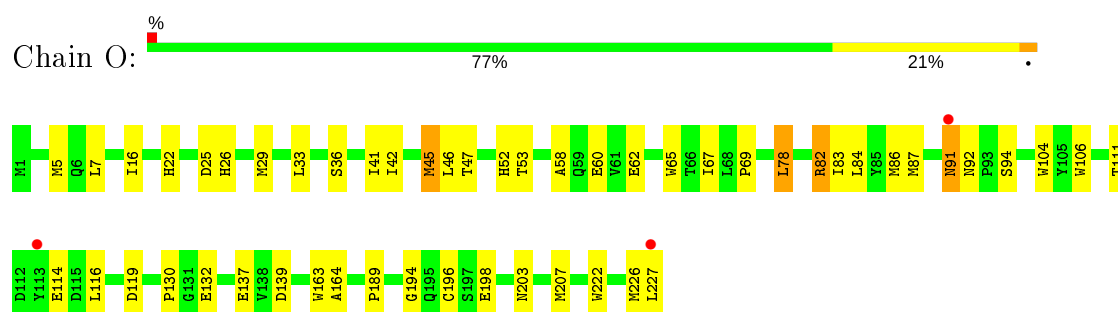
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	D	110	Total 110	O 110	0	0
30	E	85	Total 85	O 85	0	0
30	F	78	Total 78	O 78	0	0
30	G	51	Total 51	O 51	0	0
30	H	45	Total 45	O 45	0	0
30	I	25	Total 25	O 25	0	0
30	J	28	Total 28	O 28	0	0
30	K	21	Total 21	O 21	0	0
30	L	29	Total 29	O 29	0	0
30	M	27	Total 27	O 27	0	0
30	N	218	Total 219	O 219	0	1
30	O	114	Total 115	O 115	0	1
30	P	90	Total 90	O 90	0	0
30	Q	36	Total 36	O 36	0	0
30	R	39	Total 39	O 39	0	0
30	S	55	Total 55	O 55	0	0
30	T	39	Total 39	O 39	0	0
30	U	33	Total 33	O 33	0	0
30	V	14	Total 14	O 14	0	0
30	W	11	Total 11	O 11	0	0
30	X	11	Total 11	O 11	0	0

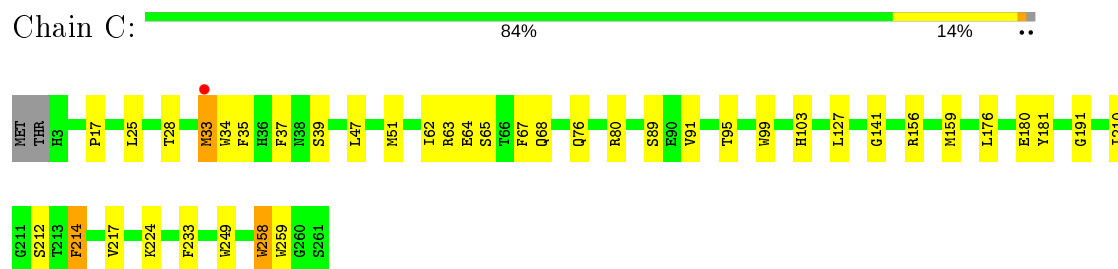
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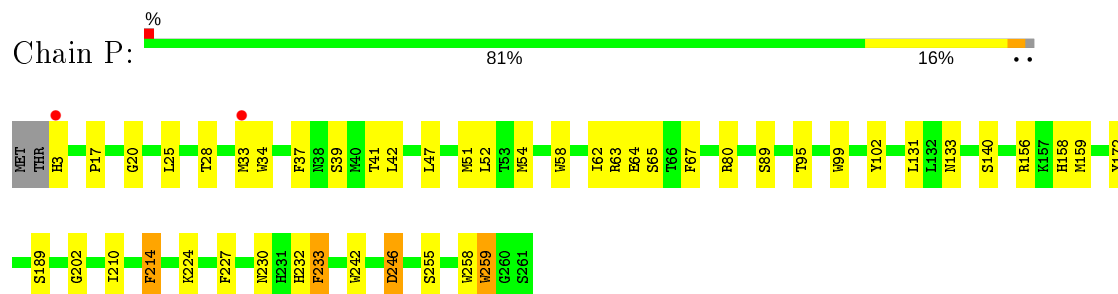
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	Y	14	Total 14	O 14	0	0
30	Z	16	Total 16	O 16	0	0



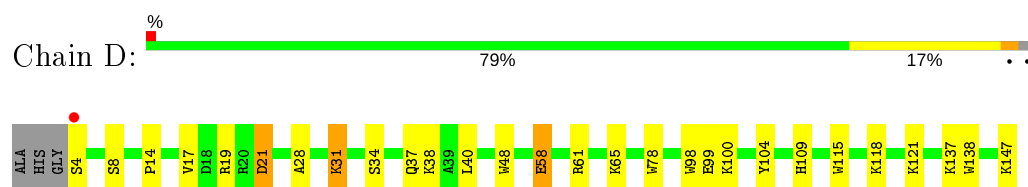
• Molecule 3: Cytochrome c oxidase subunit 3



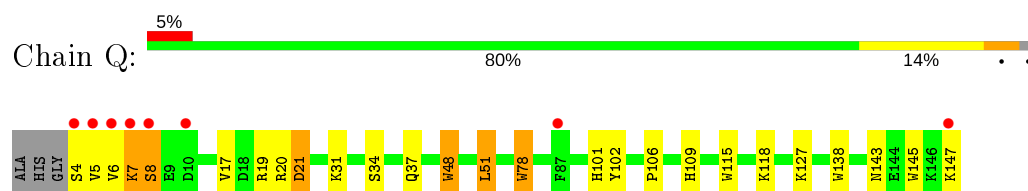
• Molecule 3: Cytochrome c oxidase subunit 3



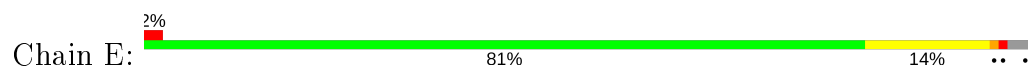
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

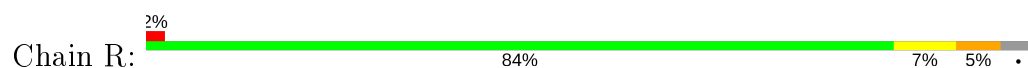


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

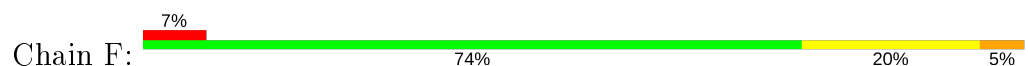




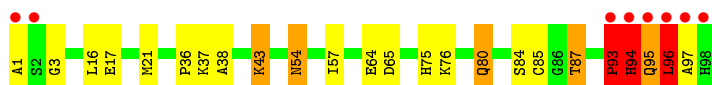
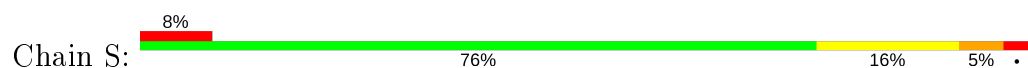
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



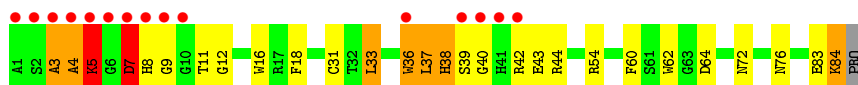
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



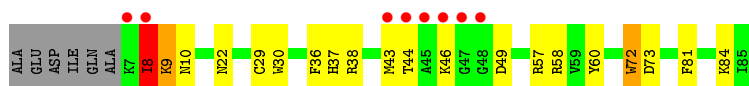
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



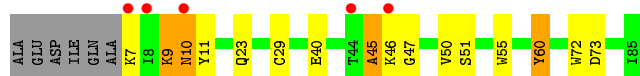
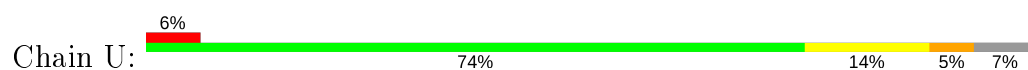
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1



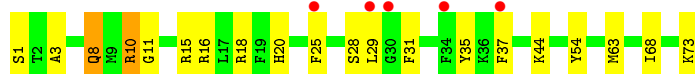
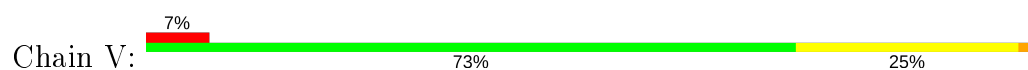
- Molecule 8: Cytochrome c oxidase subunit 6B1



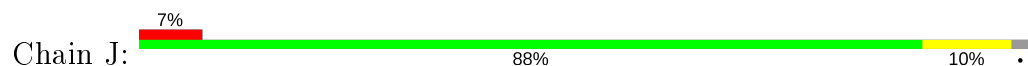
- Molecule 9: Cytochrome c oxidase subunit 6C



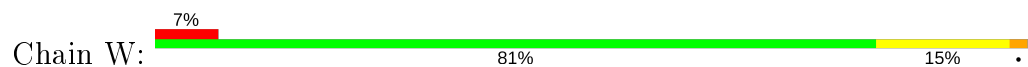
- Molecule 9: Cytochrome c oxidase subunit 6C



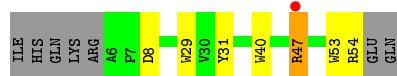
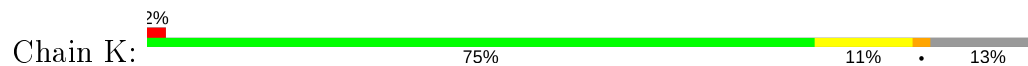
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 11: cytochrome c oxidase subunit 11, Cytochrome c oxidase subunit 7B, mitochondrial

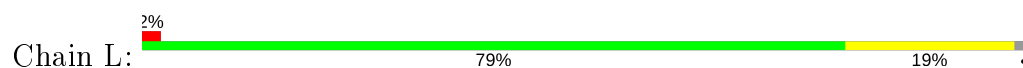


- Molecule 11: cytochrome c oxidase subunit 11, Cytochrome c oxidase subunit 7B, mitochondrial

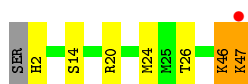
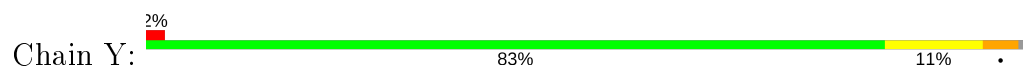




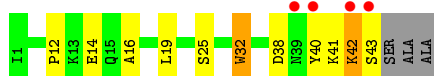
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



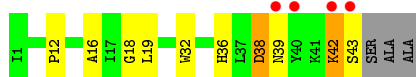
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.41Å 206.27Å 177.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 134.59 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-1.85) 99.4 (134.59-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.163 , 0.189 0.164 , 0.190	Depositor DCC
R_{free} test set	28371 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33735	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, ZN, CHD, HEA, SAC, TPO, PSC, PEK, MG, TGL, EDO, PGV, CDL, UNX, CUA, NA, FME, CU, DMU

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	1.60	21/4322 (0.5%)	1.28	28/5897 (0.5%)
1	N	1.51	22/4308 (0.5%)	1.19	15/5878 (0.3%)
2	B	1.46	6/1945 (0.3%)	1.25	7/2649 (0.3%)
2	O	1.22	6/1896 (0.3%)	1.08	7/2581 (0.3%)
3	C	1.53	12/2272 (0.5%)	1.09	1/3102 (0.0%)
3	P	1.55	16/2272 (0.7%)	1.14	3/3102 (0.1%)
4	D	1.49	4/1265 (0.3%)	1.22	5/1704 (0.3%)
4	Q	1.11	4/1259 (0.3%)	1.10	5/1698 (0.3%)
5	E	1.45	3/871 (0.3%)	1.27	5/1182 (0.4%)
5	R	1.25	3/871 (0.3%)	1.11	3/1182 (0.3%)
6	F	1.31	3/795 (0.4%)	1.18	3/1079 (0.3%)
6	S	1.25	0/780	1.19	3/1058 (0.3%)
7	G	1.50	3/690 (0.4%)	1.21	7/937 (0.7%)
7	T	1.51	6/702 (0.9%)	1.18	4/953 (0.4%)
8	H	1.29	4/682 (0.6%)	1.02	2/921 (0.2%)
8	U	1.11	2/682 (0.3%)	0.94	1/921 (0.1%)
9	I	1.20	1/605 (0.2%)	1.10	2/802 (0.2%)
9	V	1.04	0/605	1.07	2/802 (0.2%)
10	J	1.21	0/471	1.03	0/636
10	W	1.22	1/480 (0.2%)	1.01	0/648
11	K	1.41	4/398 (1.0%)	1.15	2/546 (0.4%)
11	X	1.15	2/405 (0.5%)	0.85	0/556
12	L	1.36	2/401 (0.5%)	1.12	1/536 (0.2%)
12	Y	1.21	0/401	1.01	0/536
13	M	1.41	2/345 (0.6%)	1.06	0/470
13	Z	1.23	2/345 (0.6%)	0.90	0/470
All	All	1.42	129/30068 (0.4%)	1.16	106/40846 (0.3%)

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	A	0	2
1	N	0	1
6	S	0	1
7	T	0	1
12	Y	0	1
All	All	0	6

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	CD-OE2	-9.33	1.15	1.25
11	K	29	TRP	CD2-CE2	8.56	1.51	1.41
4	D	58	GLU	CD-OE1	8.54	1.35	1.25
2	O	65	TRP	CD2-CE2	8.50	1.51	1.41
3	C	89	SER	CB-OG	8.48	1.53	1.42
1	A	281	GLY	N-CA	8.30	1.58	1.46
2	B	65	TRP	CD2-CE2	8.15	1.51	1.41
1	A	96	ARG	CZ-NH1	8.13	1.43	1.33
3	P	20	GLY	N-CA	8.04	1.58	1.46
2	O	198	GLU	CD-OE2	-7.56	1.17	1.25
1	N	49	GLY	C-O	7.55	1.35	1.23
1	N	409	TRP	CD2-CE2	7.30	1.50	1.41
3	C	181	TYR	CE1-CZ	7.23	1.48	1.38
1	A	409	TRP	CD2-CE2	7.22	1.50	1.41
1	N	288	TRP	CD2-CE2	7.10	1.49	1.41
3	P	172	TYR	CG-CD1	6.99	1.48	1.39
4	Q	78	TRP	CD2-CE2	6.95	1.49	1.41
13	M	14	GLU	CD-OE1	-6.94	1.18	1.25
3	P	89	SER	CB-OG	6.94	1.51	1.42
13	M	32	TRP	CD2-CE2	6.91	1.49	1.41
1	A	101	SER	CB-OG	6.91	1.51	1.42
1	N	179	TYR	CE1-CZ	6.67	1.47	1.38
7	T	16	TRP	CD2-CE2	6.66	1.49	1.41
7	G	36	TRP	CD2-CE2	6.66	1.49	1.41
1	N	25	TRP	CD2-CE2	6.56	1.49	1.41
7	G	16	TRP	CD2-CE2	6.54	1.49	1.41
1	A	279	SER	CA-CB	6.53	1.62	1.52
3	C	249	TRP	CD2-CE2	6.52	1.49	1.41
7	T	36	TRP	CD2-CE2	6.52	1.49	1.41
3	C	35	PHE	CG-CD2	6.51	1.48	1.38
1	A	49	GLY	C-O	6.51	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	225	SER	CA-CB	6.50	1.62	1.52
1	A	179	TYR	CG-CD1	6.49	1.47	1.39
2	O	36	SER	CB-OG	6.45	1.50	1.42
13	Z	32	TRP	CD2-CE2	6.45	1.49	1.41
4	D	115	TRP	CD2-CE2	6.39	1.49	1.41
4	Q	145	TRP	CD2-CE2	6.25	1.48	1.41
3	P	189	SER	CA-CB	6.24	1.62	1.52
1	N	279	SER	CA-CB	6.21	1.62	1.52
4	D	48	TRP	CD2-CE2	6.21	1.48	1.41
11	K	40	TRP	CD2-CE2	6.15	1.48	1.41
4	D	138	TRP	CD2-CE2	6.10	1.48	1.41
8	U	72	TRP	CD2-CE2	6.10	1.48	1.41
3	C	34	TRP	CD2-CE2	6.08	1.48	1.41
5	E	78	HIS	N-CA	6.08	1.58	1.46
1	A	74	MET	CB-CG	6.05	1.70	1.51
1	N	270	TYR	CB-CG	6.03	1.60	1.51
1	N	473	TRP	CD2-CE2	6.01	1.48	1.41
1	A	244	TYR	CG-CD1	6.01	1.47	1.39
3	C	181	TYR	CB-CG	5.99	1.60	1.51
5	R	69	GLU	CD-OE2	-5.98	1.19	1.25
3	C	141	GLY	N-CA	5.96	1.54	1.46
3	P	246	ASP	CB-CG	5.95	1.64	1.51
7	T	62	TRP	CD2-CE2	5.95	1.48	1.41
12	L	19	TRP	CD2-CE2	5.94	1.48	1.41
3	C	259	TRP	CD2-CE2	5.92	1.48	1.41
3	P	99	TRP	CD2-CE2	5.91	1.48	1.41
3	P	140	SER	CB-OG	5.91	1.50	1.42
3	C	258	TRP	CD2-CE2	5.87	1.48	1.41
1	N	25	TRP	CG-CD1	5.82	1.44	1.36
8	H	58	ARG	CZ-NH1	5.81	1.40	1.33
8	H	30	TRP	CD2-CE2	5.80	1.48	1.41
1	A	447	TYR	CG-CD1	5.80	1.46	1.39
1	A	261	TYR	CE2-CZ	5.79	1.46	1.38
1	N	414	PHE	CG-CD1	5.78	1.47	1.38
3	P	258	TRP	CD2-CE2	5.75	1.48	1.41
3	P	34	TRP	CD2-CE2	5.75	1.48	1.41
6	F	73	TRP	CE3-CZ3	5.74	1.48	1.38
2	O	106	TRP	CD2-CE2	5.74	1.48	1.41
6	F	18	ARG	CZ-NH1	5.74	1.40	1.33
1	N	323	TRP	CD2-CE2	5.73	1.48	1.41
3	C	65	SER	CA-CB	5.72	1.61	1.52
5	E	15	TRP	CD2-CE2	5.71	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	65	SER	CB-OG	5.71	1.49	1.42
1	A	74	MET	CG-SD	-5.69	1.66	1.81
7	T	60	PHE	CG-CD1	5.69	1.47	1.38
11	K	31	TYR	CG-CD1	5.68	1.46	1.39
11	X	29	TRP	CD2-CE2	5.67	1.48	1.41
11	K	53	TRP	CD2-CE2	5.66	1.48	1.41
1	A	379	TYR	CE2-CZ	5.66	1.46	1.38
3	P	64	GLU	CD-OE2	5.63	1.31	1.25
3	C	212	SER	CA-CB	5.56	1.61	1.52
8	H	72	TRP	CD2-CE2	5.56	1.48	1.41
1	N	335	SER	CB-OG	5.54	1.49	1.42
10	W	26	ALA	CA-CB	5.53	1.64	1.52
12	L	32	GLY	N-CA	5.49	1.54	1.46
1	N	334	TRP	CD2-CE2	5.49	1.48	1.41
3	P	255	SER	CA-CB	5.48	1.61	1.52
11	X	53	TRP	CD2-CE2	5.44	1.47	1.41
7	T	36	TRP	CG-CD2	5.42	1.52	1.43
4	Q	138	TRP	CD2-CE2	5.42	1.47	1.41
3	P	65	SER	CB-OG	5.39	1.49	1.42
1	A	376	HIS	CG-CD2	5.35	1.44	1.35
1	N	244	TYR	CE2-CZ	5.34	1.45	1.38
3	P	227	PHE	CG-CD1	5.34	1.46	1.38
1	N	6	TRP	CD2-CE2	5.32	1.47	1.41
1	N	244	TYR	CE1-CZ	5.31	1.45	1.38
1	A	226	GLY	N-CA	5.29	1.53	1.46
5	R	27	TRP	CG-CD1	5.27	1.44	1.36
2	O	163	TRP	CD2-CE2	5.27	1.47	1.41
5	E	38	GLY	N-CA	5.26	1.53	1.46
1	N	288	TRP	CE3-CZ3	5.26	1.47	1.38
3	P	259	TRP	CD2-CE2	5.26	1.47	1.41
1	N	457	GLY	N-CA	5.25	1.53	1.46
1	A	340	TRP	CD2-CE2	5.23	1.47	1.41
6	F	8	THR	CB-CG2	5.23	1.69	1.52
4	Q	48	TRP	CD2-CE2	5.23	1.47	1.41
5	R	27	TRP	CD2-CE2	5.21	1.47	1.41
3	P	232	HIS	CG-CD2	5.20	1.44	1.35
2	B	223	SER	CA-CB	5.19	1.60	1.52
9	I	69	PHE	CG-CD1	5.17	1.46	1.38
7	T	83	GLU	CD-OE1	5.17	1.31	1.25
2	O	222	TRP	CG-CD2	5.16	1.52	1.43
2	B	222	TRP	CD2-CE2	5.14	1.47	1.41
2	B	167	SER	CB-OG	-5.14	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	81	TRP	CG-CD1	5.12	1.44	1.36
13	Z	18	GLY	N-CA	5.12	1.53	1.46
1	N	379	TYR	CE1-CZ	5.11	1.45	1.38
1	A	275	TRP	CD2-CE3	5.10	1.48	1.40
1	A	450	TRP	CD2-CE2	5.08	1.47	1.41
1	N	396	TRP	CD2-CE2	5.08	1.47	1.41
1	A	244	TYR	CB-CG	-5.06	1.44	1.51
1	A	275	TRP	CG-CD1	5.06	1.43	1.36
8	H	81	PHE	CE2-CZ	5.04	1.47	1.37
1	N	148	PHE	CG-CD2	5.03	1.46	1.38
1	A	235	PHE	CG-CD2	5.02	1.46	1.38
7	G	36	TRP	CG-CD2	5.02	1.52	1.43
8	U	55	TRP	CD2-CE2	5.02	1.47	1.41
3	P	242	TRP	CD2-CE2	5.02	1.47	1.41

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-15.54	75.34	100.20
4	Q	20	ARG	NE-CZ-NH2	-15.10	112.75	120.30
1	A	71	MET	CG-SD-CE	-15.09	76.06	100.20
5	E	90	ARG	NE-CZ-NH1	15.04	127.82	120.30
1	A	96	ARG	NE-CZ-NH2	-11.40	114.60	120.30
5	E	90	ARG	NE-CZ-NH2	-10.16	115.22	120.30
5	R	90	ARG	NE-CZ-NH2	-9.95	115.32	120.30
11	K	47	ARG	NE-CZ-NH1	9.89	125.25	120.30
4	Q	20	ARG	NE-CZ-NH1	9.86	125.23	120.30
6	F	18	ARG	NE-CZ-NH2	-9.01	115.79	120.30
2	O	82	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	A	189	MET	CG-SD-CE	-8.93	85.92	100.20
4	D	21	ASP	CB-CG-OD2	8.80	126.22	118.30
2	B	82	ARG	NE-CZ-NH2	-8.16	116.22	120.30
7	T	7	ASP	N-CA-C	8.05	132.73	111.00
2	B	45	MET	CG-SD-CE	7.74	112.58	100.20
5	E	49	ASP	CB-CG-OD1	7.53	125.07	118.30
1	A	112	LEU	CD1-CG-CD2	-7.50	88.00	110.50
6	F	18	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	310	MET	CA-CB-CG	-7.25	100.97	113.30
5	E	14	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	213	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	213	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	310	MET	CG-SD-CE	-6.92	89.13	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	42	ILE	CG1-CB-CG2	-6.87	96.28	111.40
1	A	35	LEU	CB-CG-CD2	6.86	122.66	111.00
1	A	439	ARG	NE-CZ-NH2	-6.85	116.88	120.30
7	T	33	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	347	LEU	CA-CB-CG	-6.74	99.80	115.30
4	D	61	ARG	NE-CZ-NH2	-6.71	116.94	120.30
4	Q	20	ARG	CG-CD-NE	-6.70	97.74	111.80
1	N	302[A]	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	N	302[B]	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	B	152	MET	CG-SD-CE	6.54	110.67	100.20
1	N	302[A]	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	N	302[B]	ARG	NE-CZ-NH2	-6.51	117.05	120.30
7	G	12	GLY	N-CA-C	6.46	129.25	113.10
6	S	94	HIS	N-CA-C	6.42	128.34	111.00
2	B	158	ASP	CB-CG-OD1	6.35	124.01	118.30
1	A	96	ARG	NE-CZ-NH1	6.33	123.47	120.30
8	U	73	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	297[A]	MET	CB-CG-SD	6.27	131.21	112.40
1	A	297[B]	MET	CB-CG-SD	6.27	131.21	112.40
1	N	369	ASP	CB-CG-OD1	6.22	123.89	118.30
6	S	17	GLU	OE1-CD-OE2	6.18	130.72	123.30
5	R	90	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	N	51	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	347	LEU	CB-CG-CD2	6.08	121.33	111.00
12	L	20	ARG	CG-CD-NE	-6.06	99.07	111.80
1	A	38	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	49	GLY	N-CA-C	-6.02	98.06	113.10
7	T	64	ASP	CB-CG-OD1	6.00	123.70	118.30
7	G	6	GLY	N-CA-C	5.98	128.06	113.10
7	G	7	ASP	N-CA-C	5.95	127.06	111.00
5	R	90	ARG	CG-CD-NE	-5.93	99.34	111.80
4	Q	21	ASP	CB-CG-OD2	5.90	123.61	118.30
2	B	133	LEU	CA-CB-CG	-5.88	101.78	115.30
3	C	214	PHE	CB-CG-CD1	5.83	124.88	120.80
3	P	214	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	A	513	LEU	CA-CB-CG	-5.78	102.01	115.30
9	V	10	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	O	198	GLU	OE1-CD-OE2	-5.71	116.45	123.30
9	I	58	LYS	CD-CE-NZ	-5.68	98.63	111.70
2	O	119	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	74	MET	CB-CG-SD	-5.61	95.56	112.40
1	A	242	GLU	OE1-CD-OE2	-5.60	116.58	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	ASP	CB-CG-OD1	5.59	123.33	118.30
3	P	102	TYR	CB-CG-CD1	-5.57	117.66	121.00
4	Q	127	LYS	CD-CE-NZ	5.57	124.51	111.70
1	A	38	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	N	310	MET	CA-CB-CG	-5.55	103.86	113.30
9	V	10	ARG	NE-CZ-NH1	5.55	123.07	120.30
2	B	139	ASP	CB-CG-OD1	5.54	123.29	118.30
8	H	73	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	N	7	LEU	CB-CG-CD1	5.50	120.34	111.00
4	D	118	LYS	CD-CE-NZ	-5.49	99.08	111.70
1	N	310	MET	CG-SD-CE	-5.45	91.48	100.20
2	O	65	TRP	CB-CA-C	-5.41	99.58	110.40
8	H	58	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	O	45	MET	CG-SD-CE	5.39	108.83	100.20
5	E	57	ARG	NE-CZ-NH1	5.37	122.98	120.30
3	P	233	PHE	CB-CG-CD1	-5.36	117.05	120.80
11	K	54	ARG	NE-CZ-NH1	-5.34	117.63	120.30
4	D	137	LYS	CD-CE-NZ	-5.31	99.48	111.70
2	O	139	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	64	VAL	CG1-CB-CG2	-5.29	102.44	110.90
7	G	54	ARG	NE-CZ-NH2	-5.29	117.66	120.30
6	S	3	GLY	N-CA-C	-5.28	99.89	113.10
1	N	38	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	O	82	ARG	NE-CZ-NH1	5.27	122.94	120.30
7	T	5	LYS	CB-CA-C	5.25	120.91	110.40
1	A	366	VAL	CA-CB-CG2	-5.25	103.03	110.90
1	A	129	TYR	CB-CG-CD2	-5.24	117.86	121.00
7	G	8	HIS	N-CA-C	5.22	125.09	111.00
4	D	38	LYS	CB-CG-CD	-5.21	98.06	111.60
9	I	16	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	363	LEU	CA-CB-CG	5.14	127.12	115.30
6	F	96	LEU	CA-CB-CG	5.13	127.09	115.30
1	N	179	TYR	CD1-CE1-CZ	-5.11	115.20	119.80
7	G	5	LYS	CB-CA-C	5.09	120.59	110.40
1	N	113[A]	LEU	CB-CA-C	5.05	119.79	110.20
1	N	113[B]	LEU	CB-CA-C	5.05	119.79	110.20
1	A	240	HIS	CA-CB-CG	-5.03	105.06	113.60
1	N	164	PHE	CB-CG-CD1	-5.03	117.28	120.80
1	A	353	LEU	CB-CG-CD1	-5.02	102.47	111.00
7	G	56	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
7	T	40	GLY	Peptide
12	Y	46	LYS	Peptide

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	4193	0	4162	95	0
1	N	4179	0	4154	86	0
2	B	1904	0	1909	57	0
2	O	1859	0	1860	38	1
3	C	2185	0	2097	54	0
3	P	2185	0	2097	47	0
4	D	1231	0	1227	47	0
4	Q	1224	0	1211	24	1
5	E	852	0	845	8	0
5	R	852	0	845	7	0
6	F	778	0	754	36	0
6	S	763	0	742	32	0
7	G	675	0	643	37	0
7	T	686	0	651	30	0
8	H	662	0	623	21	0
8	U	662	0	623	8	0
9	I	601	0	613	26	0
9	V	601	0	613	16	0
10	J	460	0	459	5	0
10	W	469	0	464	13	0
11	K	384	0	366	4	0
11	X	391	0	374	5	0
12	L	385	0	389	5	0
12	Y	388	0	388	14	0
13	M	335	0	352	10	0
13	Z	335	0	352	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	180	0	162	27	0
14	N	180	0	162	27	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	6	0	0	7	0
18	N	6	0	0	6	0
19	A	63	0	110	3	0
19	D	63	0	110	21	0
19	L	63	0	110	4	0
19	N	63	0	110	8	0
19	Q	63	0	110	10	0
19	Y	63	0	110	13	0
20	A	102	0	152	13	0
20	C	102	0	152	11	0
20	G	51	0	76	4	0
20	N	51	0	76	2	0
20	P	51	0	76	3	0
20	Z	51	0	76	12	0
21	A	52	0	78	20	0
21	B	8	0	12	0	0
21	C	36	0	54	4	0
21	D	24	0	36	15	0
21	E	20	0	30	0	0
21	F	16	0	24	5	0
21	G	8	0	12	1	0
21	H	8	0	12	4	0
21	J	4	0	6	0	0
21	L	4	0	6	0	0
21	N	48	0	72	23	0
21	O	12	0	18	2	0
21	P	16	0	24	1	0
21	Q	8	0	12	0	0
21	R	24	0	36	2	0
21	S	8	0	12	0	0
21	T	4	0	6	0	0
21	U	4	0	6	0	0
21	V	4	0	6	0	0
22	B	29	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	58	0	78	8	0
22	G	29	0	39	1	0
22	J	29	0	38	2	0
22	P	58	0	78	7	0
22	W	29	0	39	9	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	23	0
24	O	52	0	80	12	0
25	C	99	0	126	18	0
25	L	33	0	42	5	0
25	M	33	0	42	1	0
25	P	99	0	126	18	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0
26	P	1	0	0	0	0
27	C	106	0	154	19	0
27	G	53	0	77	10	0
27	P	53	0	77	10	0
27	T	106	0	154	8	0
28	C	100	0	156	30	0
28	N	100	0	156	15	0
28	P	100	0	156	25	0
28	T	100	0	156	20	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	233	0	0	15	0
30	B	140	0	0	13	1
30	C	101	0	0	4	0
30	D	110	0	0	19	1
30	E	85	0	0	3	0
30	F	78	0	0	7	0
30	G	51	0	0	4	0
30	H	45	0	0	3	0
30	I	25	0	0	5	0
30	J	28	0	0	2	0
30	K	21	0	0	4	0
30	L	29	0	0	3	0
30	M	27	0	0	3	0
30	N	219	0	0	17	0
30	O	115	0	0	3	0
30	P	90	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Q	36	0	0	3	0
30	R	39	0	0	0	0
30	S	55	0	0	6	0
30	T	39	0	0	3	0
30	U	33	0	0	0	0
30	V	14	0	0	3	0
30	W	11	0	0	2	0
30	X	11	0	0	0	0
30	Y	14	0	0	1	0
30	Z	16	0	0	1	0
All	All	33735	0	32802	872	2

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 13.

All (872) 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)
21:A:615:EDO:C2	21:A:615:EDO:C1	1.78	1.57
20:Z:101:PGV:C2	20:Z:101:PGV:H011	1.50	1.39
21:A:615:EDO:C1	21:A:615:EDO:O2	1.71	1.36
21:C:316:EDO:H11	30:C:486:HOH:O	1.23	1.29
30:A:705:HOH:O	19:D:201:TGL:HG11	1.32	1.26
19:D:201:TGL:HG31	30:D:364:HOH:O	1.24	1.26
19:N:610:TGL:H112	30:O:424:HOH:O	1.30	1.25
4:D:31[B]:LYS:HG3	30:D:401:HOH:O	1.33	1.24
5:E:100:THR:HG21	30:E:357:HOH:O	1.09	1.23
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD2	1.44	1.17
1:A:112:LEU:HG	30:A:911:HOH:O	1.43	1.15
4:D:100[B]:LYS:HE3	30:D:310:HOH:O	1.48	1.14
1:N:302[B]:ARG:HH12	1:N:365:ILE:HD11	1.12	1.13
1:N:417[A]:MET:CE	30:N:839:HOH:O	1.94	1.13
20:Z:101:PGV:H011	20:Z:101:PGV:H22	1.26	1.12
6:S:43:LYS:H	6:S:43:LYS:HE2	1.00	1.12
21:N:621:EDO:H11	6:S:36:PRO:HD3	1.24	1.11
3:P:67:PHE:HE2	28:P:304:CDL:H1	1.01	1.10
2:B:32[A]:PHE:O	2:B:35[A]:SER:OG	1.69	1.10
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	1.92	1.09
24:B:303:PSC:H241	24:B:303:PSC:H202	1.35	1.08
3:P:67:PHE:CE2	28:P:304:CDL:H1	1.89	1.08
7:G:84:LYS:HD2	7:G:84:LYS:H	1.18	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:309:PGV:H061	8:H:22:ASN:HD22	1.09	1.07
1:A:417[B]:MET:CE	30:A:867:HOH:O	2.03	1.06
20:Z:101:PGV:H21	20:Z:101:PGV:H011	1.33	1.06
28:P:304:CDL:H381	28:P:304:CDL:H271	1.32	1.06
1:A:39:ALA:HA	21:D:202:EDO:O1	1.52	1.06
8:H:9:LYS:HG3	8:H:10:ASN:H	1.15	1.06
21:N:618:EDO:H12	30:S:246:HOH:O	1.54	1.06
1:N:486:ASP:OD2	4:Q:19[B]:ARG:HD2	1.52	1.06
21:N:621:EDO:C1	6:S:36:PRO:HD3	1.86	1.05
21:A:615:EDO:H12	21:A:615:EDO:O2	1.53	1.04
1:N:297[B]:MET:CB	30:N:766:HOH:O	2.03	1.03
1:A:282:PHE:HA	7:T:4:ALA:CB	1.88	1.03
1:A:297[A]:MET:SD	1:A:302[A]:ARG:HG2	1.98	1.02
21:N:618:EDO:O2	30:N:701:HOH:O	1.76	1.02
1:A:513:LEU:O	1:A:514:LYS:HB2	1.59	1.01
1:N:297[B]:MET:HB2	30:N:766:HOH:O	1.59	1.01
3:C:33[A]:MET:HB2	25:C:302:DMU:C22	1.90	1.01
6:F:94:HIS:HD2	30:F:216:HOH:O	1.44	1.00
4:D:19[A]:ARG:CG	4:D:21:ASP:OD1	2.10	1.00
19:D:201:TGL:H361	30:I:125:HOH:O	1.62	0.99
20:Z:101:PGV:C2	20:Z:101:PGV:C01	2.42	0.98
1:N:178[B]:GLN:HG2	1:N:186:TRP:CZ2	1.99	0.98
6:F:1:ALA:HB3	21:F:105:EDO:O1	1.64	0.97
7:G:84:LYS:HD2	7:G:84:LYS:N	1.79	0.97
7:G:8:HIS:CD2	7:G:9:GLY:H	1.81	0.97
3:C:63:ARG:HE	28:C:306:CDL:HA22	1.27	0.97
1:N:302[B]:ARG:NH1	1:N:365:ILE:HD11	1.77	0.97
27:P:307:PEK:C04	6:S:1:ALA:N	2.26	0.97
27:C:308:PEK:H041	6:F:1:ALA:N	1.78	0.97
4:Q:19[A]:ARG:CD	4:Q:21:ASP:OD1	2.13	0.96
11:K:47:ARG:HD3	30:K:109:HOH:O	1.62	0.96
28:N:601:CDL:H371	2:O:78:LEU:HD12	1.48	0.96
28:P:304:CDL:H351	28:P:304:CDL:H391	1.45	0.96
6:F:1:ALA:CB	21:F:105:EDO:O1	2.14	0.95
27:P:307:PEK:H041	6:S:1:ALA:N	1.81	0.94
30:B:533:HOH:O	19:D:201:TGL:H281	1.67	0.94
28:T:103:CDL:H641	28:T:103:CDL:H602	1.49	0.94
7:T:11:TPO:O3P	7:T:11:TPO:HA	1.66	0.94
3:P:33[A]:MET:HE1	3:P:42:LEU:H	1.33	0.93
6:S:43:LYS:N	6:S:43:LYS:HE2	1.82	0.93
1:A:189:MET:HE2	30:A:907:HOH:O	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:12:GLY:HA3	30:G:237:HOH:O	1.67	0.92
1:N:513:LEU:O	1:N:514:LYS:HB2	1.68	0.92
1:A:221:ASP:OD1	21:A:621:EDO:H12	1.70	0.91
2:B:29[A]:MET:HE2	9:I:35:TYR:HD1	1.33	0.91
4:D:19[A]:ARG:HG2	4:D:21:ASP:OD1	1.71	0.91
4:Q:19[A]:ARG:HD3	4:Q:21:ASP:OD1	1.68	0.91
25:L:102:DMU:H26	30:L:229:HOH:O	1.71	0.91
12:Y:24[B]:MET:SD	19:Y:101:TGL:HC21	2.11	0.90
7:T:12:GLY:HA3	30:T:233:HOH:O	1.69	0.90
19:Y:101:TGL:OC1	19:Y:101:TGL:HC41	1.68	0.90
5:E:90:ARG:HD2	30:E:366:HOH:O	1.72	0.90
9:V:11:GLY:O	9:V:15:ARG:HG3	1.72	0.89
3:C:33[A]:MET:HB2	25:C:302:DMU:H11	1.52	0.89
21:D:203:EDO:H11	30:D:340:HOH:O	1.72	0.89
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.52	0.89
20:G:103:PGV:H71	20:G:103:PGV:H22	1.55	0.88
6:S:43:LYS:H	6:S:43:LYS:CE	1.87	0.88
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:CD	2.21	0.88
9:I:15:ARG:NH2	30:I:101:HOH:O	2.04	0.88
7:G:9:GLY:HA3	30:N:885:HOH:O	1.72	0.88
24:B:303:PSC:C24	24:B:303:PSC:H202	2.01	0.87
1:A:282:PHE:HA	7:T:4:ALA:HB1	1.55	0.87
7:G:42:ARG:NH1	7:G:42:ARG:HA	1.90	0.87
30:B:533:HOH:O	19:D:201:TGL:C28	2.19	0.86
27:P:307:PEK:C04	6:S:1:ALA:H1	1.83	0.86
2:O:16:ILE:HD12	2:O:87[A]:MET:HG2	1.57	0.86
3:C:67:PHE:HE2	28:C:306:CDL:C1	1.89	0.86
24:B:303:PSC:H51	30:I:110:HOH:O	1.75	0.85
27:P:307:PEK:H041	6:S:1:ALA:H1	1.36	0.85
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.16	0.85
27:C:308:PEK:H041	6:F:1:ALA:H2	1.36	0.85
24:O:302:PSC:C07	9:V:10:ARG:HH21	1.90	0.85
8:H:9:LYS:HG3	8:H:10:ASN:N	1.91	0.85
3:C:67:PHE:HE2	28:C:306:CDL:H1	1.40	0.85
3:P:33[B]:MET:SD	25:P:306:DMU:H8	2.16	0.85
10:W:33:ARG:HG2	22:W:101:CHD:H8	1.59	0.85
7:G:72:ASN:H	7:G:76:ASN:HD22	1.24	0.84
6:S:75:HIS:H	6:S:80:GLN:HE22	1.24	0.84
7:T:72:ASN:H	7:T:76:ASN:HD22	1.24	0.84
1:N:359:ALA:HA	14:N:603[B]:HEA:OMA	1.77	0.84
4:D:100[B]:LYS:HD2	4:D:100[B]:LYS:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:103:CDL:OA7	28:T:103:CDL:H331	1.78	0.84
1:N:417[A]:MET:HE2	30:N:839:HOH:O	1.63	0.83
27:C:304:PEK:HN2	7:G:76:ASN:HD21	1.26	0.83
3:P:63:ARG:HE	28:P:304:CDL:HA21	1.43	0.83
27:C:308:PEK:C04	6:F:1:ALA:N	2.42	0.83
1:N:178[B]:GLN:O	1:N:178[B]:GLN:HG3	1.78	0.83
7:G:42:ARG:HA	7:G:42:ARG:HH11	1.44	0.82
28:P:304:CDL:H392	28:P:304:CDL:H251	1.60	0.82
24:B:303:PSC:H081	5:E:8:ASP:OD1	1.79	0.82
24:B:303:PSC:C20	24:B:303:PSC:H241	2.05	0.82
7:G:46:ALA:HB3	30:G:247:HOH:O	1.78	0.81
3:C:51[B]:MET:CE	28:C:306:CDL:H392	2.10	0.81
27:P:307:PEK:H383	28:T:103:CDL:H273	1.63	0.81
3:C:67:PHE:CE2	28:C:306:CDL:H1	2.16	0.81
3:C:224:LYS:HE3	28:C:306:CDL:HB32	1.61	0.81
20:A:609:PGV:H343	27:C:304:PEK:H382	1.61	0.81
4:D:99:GLU:OE2	21:D:202:EDO:H22	1.81	0.81
1:A:297[A]:MET:SD	1:A:302[A]:ARG:CG	2.69	0.81
4:D:34:SER:H	4:D:37:GLN:HE21	1.26	0.80
13:M:38:ASP:OD2	13:M:42:LYS:HD3	1.81	0.80
27:P:307:PEK:H042	6:S:1:ALA:N	1.94	0.80
4:D:31[B]:LYS:CE	30:D:401:HOH:O	2.29	0.80
22:P:305:CHD:H231	22:P:305:CHD:H162	1.63	0.80
24:O:302:PSC:H142	24:O:302:PSC:H343	1.62	0.80
22:C:307:CHD:H162	22:C:307:CHD:H231	1.62	0.80
20:C:309:PGV:H061	8:H:22:ASN:ND2	1.93	0.80
6:F:75:HIS:H	6:F:80:GLN:HE22	1.24	0.80
4:D:65:LYS:HE3	30:D:389:HOH:O	1.82	0.79
3:C:224:LYS:CD	28:C:306:CDL:HB32	2.13	0.79
21:A:615:EDO:H22	30:M:217:HOH:O	1.82	0.79
20:C:309:PGV:H21	20:C:309:PGV:H72	1.63	0.78
25:P:306:DMU:H29	25:P:306:DMU:H35	1.65	0.78
3:C:51[B]:MET:HE3	28:C:306:CDL:H392	1.65	0.78
2:B:16[B]:ILE:HG23	30:B:502:HOH:O	1.83	0.78
2:B:41[A]:ILE:HD13	24:B:303:PSC:H342	1.66	0.78
18:A:606:AZI:N1	18:A:607:AZI:N1	2.32	0.77
1:A:359:ALA:HA	14:A:602[B]:HEA:OMA	1.83	0.77
24:B:303:PSC:C06	9:I:10:ARG:HH21	1.97	0.77
21:N:618:EDO:O1	30:N:702:HOH:O	2.01	0.77
27:P:307:PEK:C04	6:S:1:ALA:H2	1.98	0.77
21:A:618:EDO:H12	30:M:219:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31[B]:LYS:CD	30:D:401:HOH:O	2.31	0.77
11:K:47:ARG:CD	30:K:109:HOH:O	2.28	0.77
1:N:302[B]:ARG:HH12	1:N:365:ILE:CD1	1.93	0.77
3:C:180[B]:GLU:HG2	30:C:414:HOH:O	1.83	0.77
7:T:37:LEU:HD23	28:T:103:CDL:H381	1.67	0.76
3:P:63:ARG:HE	28:P:304:CDL:CA2	1.98	0.76
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.76
1:A:459:PHE:CE1	21:D:202:EDO:H11	2.20	0.76
21:N:622:EDO:H11	6:S:84:SER:OG	1.86	0.76
20:Z:101:PGV:C01	20:Z:101:PGV:H22	2.13	0.76
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.69	0.75
8:U:10:ASN:HD22	8:U:10:ASN:N	1.83	0.75
12:Y:20:ARG:HH12	19:Y:101:TGL:HC32	1.51	0.75
1:A:39:ALA:CA	21:D:202:EDO:O1	2.32	0.75
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.69	0.75
3:C:33[A]:MET:HB2	25:C:302:DMU:C25	2.18	0.74
14:N:603[B]:HEA:HMC1	14:N:603[B]:HEA:HBC1	1.69	0.74
8:H:38:ARG:HH22	21:H:101:EDO:H12	1.53	0.74
3:C:224:LYS:CE	28:C:306:CDL:HB32	2.18	0.74
3:C:33[A]:MET:HB2	25:C:302:DMU:H13	1.70	0.73
8:H:9:LYS:NZ	8:H:9:LYS:HA	2.03	0.73
1:N:178[B]:GLN:O	1:N:178[B]:GLN:CG	2.36	0.73
7:T:76:ASN:HD21	27:T:102:PEK:HN2	1.34	0.73
7:G:84:LYS:CD	7:G:84:LYS:H	1.99	0.73
13:M:42:LYS:HG2	13:M:42:LYS:O	1.89	0.73
4:Q:78:TRP:CA	19:Q:201:TGL:HB22	2.19	0.73
28:T:103:CDL:H311	28:T:103:CDL:OA7	1.89	0.73
8:U:10:ASN:HD22	8:U:10:ASN:H	1.33	0.73
1:A:112:LEU:C	1:A:112:LEU:HD23	2.10	0.73
14:N:603[A]:HEA:HBC1	14:N:603[A]:HEA:HMC1	1.69	0.73
1:N:105:LEU:HD11	21:N:612:EDO:H12	1.71	0.72
20:Z:101:PGV:H21	20:Z:101:PGV:C01	2.15	0.72
7:T:44:ARG:HH22	7:T:84:LYS:NZ	1.86	0.72
28:T:103:CDL:H311	28:T:103:CDL:HA4	1.72	0.72
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.72	0.72
3:C:33[A]:MET:CB	25:C:302:DMU:H11	2.19	0.72
20:A:610:PGV:H311	13:M:19:LEU:HD23	1.71	0.71
19:D:201:TGL:HA91	19:D:201:TGL:H242	1.70	0.71
6:F:95:GLN:C	6:F:97:ALA:H	1.93	0.71
1:N:362[B]:SER:OG	30:N:703:HOH:O	2.08	0.71
3:C:63:ARG:HE	28:C:306:CDL:CA2	2.01	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:602[A]:HEA:HMC1	14:A:602[A]:HEA:HBC1	1.72	0.71
4:D:100[B]:LYS:O	4:D:100[B]:LYS:CD	2.39	0.71
21:A:613:EDO:H21	30:A:906:HOH:O	1.91	0.71
1:N:28:MET:CE	14:N:602:HEA:H271	2.21	0.71
4:D:31[B]:LYS:CG	30:D:401:HOH:O	2.06	0.70
1:N:54:TYR:HB2	30:N:866:HOH:O	1.91	0.70
9:V:18:ARG:HD3	30:V:213:HOH:O	1.90	0.70
21:A:615:EDO:C1	21:A:615:EDO:HO2	2.03	0.70
28:T:103:CDL:H222	28:T:103:CDL:H522	1.74	0.70
3:P:67:PHE:HE2	28:P:304:CDL:C1	1.93	0.70
7:G:46:ALA:CB	30:G:247:HOH:O	2.37	0.70
8:H:9:LYS:HA	8:H:9:LYS:HZ1	1.56	0.70
1:A:221:ASP:OD1	21:A:621:EDO:C1	2.40	0.69
2:B:29[A]:MET:CE	9:I:35:TYR:HD1	2.04	0.69
1:N:297[B]:MET:HB3	30:N:766:HOH:O	1.75	0.69
12:L:24[B]:MET:HG2	19:L:101:TGL:HA22	1.74	0.69
2:O:29[B]:MET:HG3	9:V:35:TYR:CD1	2.27	0.69
2:O:47:THR:HB	19:Q:201:TGL:H181	1.73	0.69
2:B:29[A]:MET:HE2	9:I:35:TYR:CD1	2.23	0.69
27:C:308:PEK:H041	6:F:1:ALA:H1	1.56	0.68
3:P:51[B]:MET:CE	28:P:304:CDL:H273	2.22	0.68
12:Y:24[B]:MET:SD	19:Y:101:TGL:CC2	2.82	0.68
3:C:224:LYS:HE3	28:C:306:CDL:CB3	2.23	0.68
21:D:203:EDO:H21	30:F:201:HOH:O	1.94	0.68
7:T:36:TRP:CE3	7:T:39:SER:HB3	2.29	0.68
1:A:22:PHE:HA	19:L:101:TGL:HB71	1.74	0.68
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.91	0.68
14:N:603[B]:HEA:HMD1	14:N:603[B]:HEA:CBD	2.24	0.68
7:T:31:CYS:SG	28:T:103:CDL:H532	2.33	0.68
1:N:364:ASP:OD1	14:N:603[B]:HEA:O1A	2.12	0.68
9:V:18:ARG:HG3	30:V:211:HOH:O	1.94	0.68
1:A:417[B]:MET:HE1	30:A:867:HOH:O	1.83	0.67
3:P:33[B]:MET:SD	25:P:306:DMU:C19	2.82	0.67
20:A:609:PGV:H183	27:C:304:PEK:H322	1.76	0.67
7:G:8:HIS:HE1	27:G:102:PEK:H042	1.60	0.67
24:B:303:PSC:H31	9:I:17:LEU:HD23	1.76	0.67
14:N:603[B]:HEA:HBD1	14:N:603[B]:HEA:HMD1	1.77	0.67
3:P:51[B]:MET:HE3	28:P:304:CDL:H273	1.75	0.67
12:Y:26:THR:OG1	30:Y:201:HOH:O	2.13	0.67
28:T:103:CDL:H762	28:T:103:CDL:H252	1.76	0.67
3:P:133:ASN:ND2	30:P:401:HOH:O	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:90:LYS:HD2	30:F:276:HOH:O	1.94	0.67
18:N:607:AZI:N1	18:N:608:AZI:N1	2.42	0.67
4:Q:19[A]:ARG:CG	4:Q:21:ASP:OD1	2.43	0.66
4:D:4:SER:CB	30:D:302:HOH:O	2.44	0.66
9:I:73:LYS:O	30:I:102:HOH:O	2.13	0.66
4:D:28:ALA:H	4:D:31[B]:LYS:NZ	1.93	0.66
1:A:28:MET:CE	14:A:601:HEA:H271	2.26	0.66
13:M:41:LYS:O	13:M:43:SER:N	2.25	0.66
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.31	0.66
3:C:91:VAL:O	3:C:95:THR:HG23	1.95	0.66
1:N:309:THR:HG22	14:N:603[B]:HEA:HMB2	1.78	0.66
6:F:64:GLU:O	6:F:65:ASP:HB2	1.96	0.66
20:G:103:PGV:H292	3:P:95:THR:HG21	1.77	0.66
4:Q:19[A]:ARG:HG2	4:Q:21:ASP:OD1	1.95	0.66
1:N:265:LYS:HE3	21:N:622:EDO:O1	1.96	0.65
25:P:306:DMU:H29	25:P:306:DMU:C9	2.25	0.65
19:N:610:TGL:HB92	19:N:610:TGL:C28	2.26	0.65
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.24	0.65
5:E:72:LYS:HE2	30:E:349:HOH:O	1.95	0.65
4:Q:78:TRP:HA	19:Q:201:TGL:HB22	1.77	0.65
1:A:378:HIS:HA	1:A:382[B]:SER:HB2	1.79	0.65
6:S:64:GLU:O	6:S:65:ASP:HB2	1.96	0.65
4:D:100[A]:LYS:NZ	30:D:301:HOH:O	1.93	0.65
7:G:2:SER:OG	27:G:102:PEK:H301	1.97	0.65
1:A:177:SER:H	1:A:180:GLN:HE21	1.45	0.65
1:A:297[A]:MET:CG	1:A:302[A]:ARG:HG3	2.27	0.65
4:D:19[A]:ARG:HH21	4:D:21:ASP:CG	2.00	0.65
20:C:309:PGV:C06	8:H:22:ASN:HD22	1.98	0.65
19:A:608:TGL:HC22	30:A:918:HOH:O	1.96	0.65
6:F:87[B]:THR:HG21	30:F:258:HOH:O	1.97	0.65
2:O:114:GLU:HG3	2:O:227:LEU:HD21	1.79	0.65
4:Q:17[A]:VAL:O	4:Q:17[A]:VAL:HG23	1.97	0.64
28:P:304:CDL:H381	28:P:304:CDL:C27	2.19	0.64
1:N:28:MET:HE1	14:N:602:HEA:C27	2.27	0.64
1:A:282:PHE:CA	7:T:4:ALA:HB1	2.26	0.64
3:C:180[A]:GLU:OE2	30:C:401:HOH:O	2.15	0.64
4:D:4:SER:OG	30:D:302:HOH:O	2.14	0.64
3:P:33[A]:MET:HB2	25:P:306:DMU:C19	2.27	0.64
10:W:27:THR:HB	30:W:211:HOH:O	1.97	0.64
14:A:601:HEA:HBC1	14:A:601:HEA:HMC1	1.78	0.64
27:C:308:PEK:H382	28:N:601:CDL:H271	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:307:CHD:H162	22:C:307:CHD:C23	2.27	0.64
27:C:308:PEK:C04	6:F:1:ALA:H1	2.08	0.64
4:D:31[B]:LYS:HE3	30:D:401:HOH:O	1.92	0.64
24:B:303:PSC:O01	9:I:14:ALA:HB2	1.97	0.64
3:C:37:PHE:CG	25:C:302:DMU:H8	2.33	0.63
3:C:224:LYS:HD3	28:C:306:CDL:HB32	1.79	0.63
3:P:224:LYS:HE3	28:P:304:CDL:HB32	1.80	0.63
13:Z:19:LEU:HD23	20:Z:101:PGV:H312	1.80	0.63
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.13	0.63
4:D:58:GLU:OE2	21:D:204:EDO:H22	1.98	0.63
4:D:34:SER:H	4:D:37:GLN:NE2	1.95	0.63
1:N:356:ILE:HA	14:N:603[B]:HEA:HMB3	1.81	0.63
27:P:307:PEK:C38	28:T:103:CDL:H273	2.28	0.63
3:P:33[A]:MET:HB2	25:P:306:DMU:H9	1.81	0.63
8:U:10:ASN:ND2	8:U:10:ASN:N	2.47	0.63
3:C:33[A]:MET:HE3	25:C:302:DMU:H10	1.81	0.63
4:D:4:SER:HB3	30:D:302:HOH:O	1.98	0.63
7:G:59:PRO:O	21:G:104:EDO:H22	1.98	0.63
1:N:265:LYS:HD2	21:N:622:EDO:H12	1.80	0.63
6:S:85:CYS:SG	6:S:87[A]:THR:CG2	2.81	0.63
1:A:382[B]:SER:HB3	1:A:383[B]:MET:HE2	1.81	0.62
28:N:601:CDL:H161	28:N:601:CDL:OB3	1.98	0.62
19:Y:101:TGL:HC22	19:Y:101:TGL:HC81	1.81	0.62
7:T:5:LYS:HG3	27:T:101:PEK:H351	1.80	0.62
1:A:513:LEU:O	1:A:514:LYS:CB	2.38	0.62
13:Z:12:PRO:HB3	20:Z:101:PGV:H251	1.79	0.62
24:B:303:PSC:C1	9:I:14:ALA:HB2	2.29	0.62
9:I:73:LYS:OXT	9:I:73:LYS:HD3	1.99	0.62
1:A:261:TYR:OH	21:A:615:EDO:H21	1.99	0.62
7:T:7:ASP:O	7:T:9:GLY:N	2.24	0.62
7:T:44:ARG:HH22	7:T:84:LYS:HZ1	1.46	0.62
28:C:306:CDL:OA5	28:C:306:CDL:HB21	1.99	0.62
1:A:177:SER:H	1:A:180:GLN:NE2	1.98	0.61
1:A:189:MET:CE	30:A:907:HOH:O	2.36	0.61
1:A:28:MET:HE1	14:A:601:HEA:C27	2.30	0.61
1:N:406:ASN:HD21	20:Z:101:PGV:H21	1.65	0.61
7:T:36:TRP:HE3	7:T:39:SER:HB3	1.66	0.61
28:P:304:CDL:H271	28:P:304:CDL:C38	2.21	0.61
4:D:58:GLU:OE2	21:D:204:EDO:C2	2.49	0.61
25:C:310:DMU:H32	25:C:310:DMU:H29	1.82	0.60
2:B:148:MET:HE2	30:B:527:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:28:MET:CE	14:N:602:HEA:C27	2.78	0.60
2:B:68[B]:LEU:HB3	2:B:69:PRO:HD3	1.82	0.60
3:C:80[B]:ARG:HG2	3:C:233:PHE:CE1	2.37	0.60
7:G:8:HIS:CE1	27:G:102:PEK:H051	2.37	0.60
7:T:5:LYS:HG3	27:T:101:PEK:C35	2.31	0.60
1:A:223:ALA:HB2	21:A:621:EDO:H11	1.82	0.60
27:C:304:PEK:H11	27:C:304:PEK:H172	1.84	0.60
4:D:78:TRP:N	19:D:201:TGL:HB21	2.17	0.60
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.30	0.60
13:M:40:TYR:O	13:M:43:SER:HB2	2.02	0.60
1:N:177:SER:H	1:N:180:GLN:HE21	1.48	0.60
28:N:601:CDL:H761	28:N:601:CDL:H561	1.83	0.60
21:N:612:EDO:H21	30:N:798:HOH:O	2.02	0.59
1:A:328:HIS:NE2	24:B:303:PSC:H22	2.16	0.59
14:A:602[B]:HEA:HMC1	14:A:602[B]:HEA:HBC1	1.85	0.59
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.84	0.59
1:N:177:SER:H	1:N:180:GLN:NE2	1.99	0.59
4:Q:109:HIS:HD2	30:Q:322:HOH:O	1.85	0.59
2:B:49:LYS:HD3	19:D:201:TGL:HC71	1.84	0.59
7:G:8:HIS:HE1	27:G:102:PEK:H051	1.67	0.59
28:C:306:CDL:H212	28:C:306:CDL:H772	1.84	0.59
9:I:73:LYS:HA	9:I:73:LYS:HE2	1.84	0.59
1:A:28:MET:CE	14:A:601:HEA:C27	2.80	0.59
12:L:42:HIS:ND1	25:L:102:DMU:O49	2.32	0.59
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.83	0.59
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.84	0.59
7:G:8:HIS:CD2	7:G:9:GLY:N	2.63	0.58
8:H:84:LYS:HG2	21:H:102:EDO:H11	1.83	0.58
21:A:621:EDO:C2	30:A:748:HOH:O	2.51	0.58
2:B:49:LYS:CE	30:D:394:HOH:O	2.51	0.58
2:B:60:GLU:CD	2:B:60:GLU:H	2.06	0.58
4:D:19[A]:ARG:HG3	4:D:21:ASP:OD1	1.97	0.58
19:N:610:TGL:HA71	19:N:610:TGL:H121	1.84	0.58
3:C:156:ARG:HE	22:C:307:CHD:C24	2.15	0.58
28:C:306:CDL:H221	28:C:306:CDL:H632	1.85	0.58
2:O:25:ASP:O	2:O:29[B]:MET:HB2	2.03	0.58
2:B:49:LYS:HE3	30:D:394:HOH:O	2.03	0.58
6:F:94:HIS:CD2	30:F:216:HOH:O	2.31	0.58
7:G:8:HIS:CG	7:G:9:GLY:H	2.20	0.58
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.84	0.58
20:A:610:PGV:H212	13:M:12:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:116:LEU:HD13	2:O:226:MET:CG	2.34	0.58
3:C:33[B]:MET:HA	25:C:302:DMU:H11	1.86	0.57
19:N:610:TGL:H121	19:N:610:TGL:CA7	2.34	0.57
24:O:302:PSC:H071	9:V:10:ARG:HH21	1.66	0.57
19:D:201:TGL:C36	30:I:125:HOH:O	2.32	0.57
8:H:37:HIS:HE1	30:H:208:HOH:O	1.86	0.57
1:N:243:VAL:HB	14:N:603[B]:HEA:HAC	1.86	0.57
20:C:309:PGV:H72	20:C:309:PGV:C2	2.31	0.57
2:B:26:HIS:O	2:B:29[B]:MET:HB3	2.03	0.57
1:N:178[B]:GLN:HG2	1:N:186:TRP:CE2	2.40	0.57
1:A:486[B]:ASP:OD1	30:A:701:HOH:O	2.17	0.57
6:F:87[B]:THR:HG21	30:F:263:HOH:O	2.05	0.57
1:A:178[B]:GLN:CD	1:A:178[B]:GLN:H	2.08	0.57
1:A:243:VAL:HB	14:A:602[B]:HEA:HAC	1.87	0.57
21:A:621:EDO:H22	30:A:748:HOH:O	2.04	0.57
2:B:68[B]:LEU:HD23	24:B:303:PSC:H172	1.86	0.57
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.87	0.57
12:Y:14:SER:H	19:Y:101:TGL:HC31	1.70	0.57
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.87	0.57
3:C:39:SER:OG	25:C:311:DMU:H2	2.04	0.57
3:P:33[B]:MET:SD	25:P:306:DMU:H6	2.44	0.57
19:Q:201:TGL:H362	9:V:20:HIS:CE1	2.39	0.57
4:D:19[A]:ARG:CD	4:D:21:ASP:OD1	2.52	0.57
3:C:62:ILE:CD1	28:C:306:CDL:H522	2.35	0.57
21:N:621:EDO:C1	6:S:36:PRO:CD	2.73	0.57
10:J:52:TRP:O	10:J:57:HIS:HE1	1.88	0.56
3:P:33[A]:MET:HE1	3:P:42:LEU:N	2.12	0.56
3:C:63:ARG:NE	28:C:306:CDL:HA22	2.09	0.56
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.03	0.56
1:N:112:LEU:HG	30:N:904:HOH:O	2.04	0.56
3:P:62:ILE:HD12	28:P:304:CDL:H522	1.86	0.56
4:Q:19[A]:ARG:HD3	4:Q:21:ASP:CG	2.25	0.56
1:A:382[B]:SER:HB3	1:A:383[B]:MET:CE	2.34	0.56
6:F:1:ALA:HB3	21:F:105:EDO:HO1	1.70	0.56
7:T:72:ASN:H	7:T:76:ASN:ND2	2.01	0.56
12:Y:47:LYS:HA	12:Y:47:LYS:HE3	1.88	0.56
21:N:621:EDO:H12	6:S:36:PRO:HD3	1.84	0.56
4:D:121:LYS:NZ	21:D:206:EDO:H22	2.21	0.56
22:W:101:CHD:O12	22:W:101:CHD:H222	2.06	0.56
3:C:51[B]:MET:HB3	28:C:306:CDL:H381	1.87	0.56
30:N:828:HOH:O	2:O:53:THR:HG21	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:GLN:OE1	6:F:98:HIS:HB3	2.05	0.56
10:W:14[B]:GLU:HG2	30:W:209:HOH:O	2.06	0.56
7:T:5:LYS:HB2	27:T:101:PEK:H331	1.87	0.56
27:T:102:PEK:H71	27:T:102:PEK:H32	1.87	0.56
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.88	0.56
24:B:303:PSC:H32	9:I:14:ALA:HA	1.88	0.55
25:L:102:DMU:C43	30:L:229:HOH:O	2.39	0.55
14:N:603[B]:HEA:CBC	14:N:603[B]:HEA:HMC1	2.36	0.55
3:P:156:ARG:HE	22:P:305:CHD:C24	2.19	0.55
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.07	0.55
8:U:45:ALA:O	8:U:47:GLY:N	2.39	0.55
8:H:37:HIS:CE1	30:H:208:HOH:O	2.59	0.55
1:N:311[B]:ILE:CD1	28:N:601:CDL:H232	2.37	0.55
2:O:83:ILE:O	2:O:87[A]:MET:HG3	2.06	0.55
3:P:224:LYS:CE	28:P:304:CDL:HB32	2.36	0.55
3:C:67:PHE:CE2	28:C:306:CDL:C1	2.79	0.55
4:D:14:PRO:CG	21:D:203:EDO:H22	2.36	0.55
7:G:8:HIS:CE1	27:G:102:PEK:H042	2.40	0.55
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.05	0.55
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.89	0.55
3:P:80[B]:ARG:HG2	3:P:233:PHE:CE1	2.41	0.55
3:P:33[B]:MET:CE	25:P:306:DMU:H6	2.36	0.55
20:G:103:PGV:H71	20:G:103:PGV:C2	2.33	0.55
10:W:32:TYR:OH	22:W:101:CHD:H213	2.07	0.55
1:A:136[B]:LEU:HD11	30:A:921:HOH:O	2.06	0.55
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.72	0.55
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.41	0.55
7:T:3:ALA:O	7:T:4:ALA:CB	2.55	0.55
11:X:47:ARG:CZ	11:X:47:ARG:HB3	2.37	0.55
1:A:172:LYS:HZ2	1:A:178[A]:GLN:HE22	1.53	0.55
21:N:618:EDO:C1	30:S:246:HOH:O	2.30	0.55
3:P:62:ILE:CD1	28:P:304:CDL:H522	2.36	0.55
20:A:610:PGV:C19	20:A:610:PGV:H231	2.36	0.54
6:F:87[A]:THR:HG21	30:F:263:HOH:O	2.05	0.54
22:P:305:CHD:H12	22:P:305:CHD:H212	1.89	0.54
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.07	0.54
2:B:49:LYS:HE3	30:B:526:HOH:O	2.06	0.54
3:C:67:PHE:HE2	28:C:306:CDL:H1O1	1.56	0.54
24:O:302:PSC:C34	24:O:302:PSC:H142	2.34	0.54
2:O:22[B]:HIS:CE1	9:V:44:LYS:NZ	2.76	0.54
4:D:78:TRP:CA	19:D:201:TGL:HB21	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:243:VAL:HG11	14:N:603[B]:HEA:HMD2	1.90	0.54
2:B:1:FME:HE3	2:B:133:LEU:HD22	1.89	0.54
2:B:217:LYS:HG2	30:B:468:HOH:O	2.06	0.54
6:F:1:ALA:CB	21:F:105:EDO:HO1	2.17	0.54
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.90	0.54
27:C:308:PEK:C04	6:F:1:ALA:H2	2.07	0.54
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.07	0.54
2:B:92:ASN:N	30:B:401:HOH:O	1.91	0.54
1:N:265:LYS:CE	21:N:622:EDO:O1	2.55	0.54
4:Q:19[B]:ARG:NH1	30:Q:301:HOH:O	2.18	0.54
1:A:281:GLY:C	7:T:4:ALA:HB1	2.29	0.54
14:A:602[A]:HEA:NB	18:A:607:AZI:N2	2.54	0.54
1:A:309:THR:HG22	14:A:602[B]:HEA:HMB2	1.89	0.53
27:P:307:PEK:H042	6:S:1:ALA:H1	1.62	0.53
27:C:308:PEK:H292	30:O:402:HOH:O	2.07	0.53
3:C:33[B]:MET:HG2	3:C:39:SER:O	2.08	0.53
9:I:31:PHE:C	9:I:31:PHE:CD1	2.82	0.53
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.27	0.53
21:A:618:EDO:H22	30:M:217:HOH:O	2.08	0.53
7:T:36:TRP:HE3	7:T:39:SER:CB	2.22	0.53
10:W:32:TYR:HE2	22:W:101:CHD:H181	1.73	0.53
6:F:75:HIS:H	6:F:80:GLN:NE2	2.02	0.53
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.43	0.53
19:Q:201:TGL:H231	19:Q:201:TGL:HA91	1.91	0.53
2:B:14:SER:HB3	2:B:168:LEU:CD2	2.39	0.53
2:B:83:ILE:O	2:B:87[B]:MET:HB2	2.09	0.53
3:P:210:ILE:HD13	20:P:303:PGV:H301	1.90	0.53
1:N:240:HIS:CE1	18:N:608:AZI:N2	2.77	0.53
1:A:243:VAL:HG11	14:A:602[B]:HEA:HMD2	1.91	0.52
1:N:240:HIS:HE1	18:N:608:AZI:N2	2.07	0.52
24:O:302:PSC:H342	24:O:302:PSC:H12	1.91	0.52
1:A:380[A]:VAL:HG21	14:A:602[A]:HEA:C3C	2.39	0.52
21:C:316:EDO:H22	8:H:72:TRP:HZ2	1.74	0.52
9:V:25:PHE:O	9:V:28:SER:HB2	2.10	0.52
2:B:29[A]:MET:CE	9:I:35:TYR:CD1	2.87	0.52
5:R:14:ARG:NH1	21:R:202:EDO:O2	2.41	0.52
10:J:7:GLU:HG3	30:J:219:HOH:O	2.10	0.52
21:N:618:EDO:H21	6:S:57:ILE:HD12	1.91	0.52
28:P:304:CDL:H651	28:P:304:CDL:H222	1.91	0.52
4:D:28:ALA:H	4:D:31[B]:LYS:HZ3	1.58	0.52
1:A:307:SER:HB2	28:T:103:CDL:H192	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17[A]:VAL:O	4:D:17[A]:VAL:HG23	2.09	0.52
1:N:380[A]:VAL:HG21	14:N:603[A]:HEA:C3C	2.39	0.52
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.54	0.52
13:Z:36:HIS:HD2	13:Z:39:ASN:ND2	2.06	0.52
7:G:41:HIS:HB3	7:G:74:ARG:CZ	2.40	0.52
12:Y:20:ARG:NH1	19:Y:101:TGL:HC32	2.20	0.52
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.52
20:N:609:PGV:H182	3:P:28:THR:HG22	1.92	0.52
6:S:94:HIS:CD2	6:S:95:GLN:N	2.78	0.52
9:V:8:GLN:HB3	9:V:15:ARG:NH2	2.24	0.52
10:W:32:TYR:CE2	22:W:101:CHD:H181	2.45	0.52
28:C:306:CDL:H811	28:C:306:CDL:H672	1.92	0.52
5:E:86:ILE:O	5:E:90:ARG:HG2	2.10	0.51
6:F:54[A]:ASN:C	6:F:54[A]:ASN:HD22	2.13	0.51
28:T:103:CDL:H311	28:T:103:CDL:CA4	2.39	0.51
24:B:303:PSC:H061	9:I:10:ARG:HH21	1.75	0.51
1:N:514:LYS:HE2	30:S:227:HOH:O	2.11	0.51
9:I:27:VAL:HG12	9:I:28:SER:N	2.24	0.51
7:G:8:HIS:HE1	27:G:102:PEK:C04	2.23	0.51
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	1.93	0.51
11:K:47:ARG:CG	30:K:109:HOH:O	2.58	0.51
3:P:33[A]:MET:CB	25:P:306:DMU:H9	2.40	0.51
6:S:54:ASN:HD22	6:S:54:ASN:C	2.12	0.51
12:Y:20:ARG:NH2	19:Y:101:TGL:HC52	2.26	0.51
24:B:303:PSC:H32	9:I:14:ALA:CB	2.41	0.51
6:S:76:LYS:HD2	6:S:93:PRO:HG2	1.92	0.51
1:A:484:THR:HA	21:A:619:EDO:H12	1.92	0.51
1:N:311[B]:ILE:HD11	28:N:601:CDL:H232	1.93	0.51
5:R:25:ASP:HB3	21:R:205:EDO:H11	1.91	0.51
12:Y:24[B]:MET:HG2	19:Y:101:TGL:HA21	1.92	0.51
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.93	0.51
19:Q:201:TGL:H352	9:V:16:ARG:HE	1.75	0.51
21:A:613:EDO:C2	30:A:906:HOH:O	2.54	0.50
19:L:101:TGL:HC92	19:L:101:TGL:CC5	2.41	0.50
21:N:612:EDO:O2	30:N:704:HOH:O	2.19	0.50
5:R:109:VAL:O	5:R:109:VAL:HG22	2.11	0.50
8:H:37:HIS:HD2	30:H:201:HOH:O	1.93	0.50
3:P:33[A]:MET:HE1	3:P:41:THR:HB	1.92	0.50
2:B:68[B]:LEU:CD2	24:B:303:PSC:H172	2.41	0.50
3:P:33[A]:MET:HB2	25:P:306:DMU:H8	1.93	0.50
27:C:308:PEK:O02	27:C:308:PEK:H42	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:ARG:HH12	21:H:101:EDO:C2	2.23	0.50
6:F:95:GLN:C	6:F:97:ALA:N	2.63	0.50
1:N:62:ALA:HB2	14:N:602:HEA:HBD1	1.94	0.50
3:P:246:ASP:HB2	30:P:481:HOH:O	2.11	0.50
7:G:72:ASN:H	7:G:76:ASN:ND2	2.00	0.50
14:A:601:HEA:H122	14:A:601:HEA:HHC	1.93	0.50
7:T:36:TRP:CE3	7:T:39:SER:CB	2.94	0.50
1:A:282:PHE:CA	7:T:4:ALA:CB	2.77	0.50
2:B:105:TYR:CD1	30:B:404:HOH:O	2.55	0.50
7:T:44:ARG:HH22	7:T:84:LYS:HZ3	1.60	0.50
2:B:58:ALA:O	2:B:62:GLU:HG3	2.11	0.49
3:C:62:ILE:HD12	28:C:306:CDL:H522	1.93	0.49
22:P:305:CHD:H231	22:P:305:CHD:C16	2.36	0.49
2:O:52:HIS:HE1	24:O:302:PSC:H212	1.77	0.49
3:P:33[A]:MET:CE	3:P:41:THR:HB	2.41	0.49
1:A:297[A]:MET:CG	1:A:302[A]:ARG:CG	2.90	0.49
1:A:356:ILE:HD13	14:A:602[B]:HEA:HMB1	1.92	0.49
2:B:41[B]:ILE:HG21	24:B:303:PSC:H342	1.94	0.49
3:C:51[B]:MET:HG2	28:C:306:CDL:H611	1.93	0.49
1:A:514:LYS:OXT	6:F:37:LYS:HE2	2.12	0.49
6:F:95:GLN:HG2	6:F:98:HIS:H	1.77	0.49
21:O:304:EDO:H21	30:O:475:HOH:O	2.11	0.49
12:Y:47:LYS:HA	12:Y:47:LYS:CE	2.40	0.49
1:A:39:ALA:HA	21:D:202:EDO:HO1	1.68	0.49
1:A:514:LYS:HA	6:F:38:ALA:CB	2.41	0.49
2:B:91:ASN:OD1	2:B:183[B]:THR:HG21	2.13	0.49
7:G:11:TPO:O2P	7:G:12:GLY:N	2.45	0.49
4:Q:17[A]:VAL:O	4:Q:17[A]:VAL:CG2	2.60	0.49
19:Y:101:TGL:OC1	19:Y:101:TGL:CC4	2.50	0.49
9:I:57:MET:O	9:I:61:GLU:HG2	2.13	0.49
28:T:103:CDL:H782	28:T:103:CDL:H571	1.94	0.49
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.94	0.49
14:A:602[B]:HEA:HBD2	14:A:602[B]:HEA:HMD1	1.94	0.49
22:P:305:CHD:C23	22:P:305:CHD:H162	2.37	0.49
22:C:307:CHD:C16	22:C:307:CHD:C23	2.91	0.49
4:D:78:TRP:CA	19:D:201:TGL:CB2	2.91	0.49
3:C:258:TRP:CZ3	25:C:310:DMU:H12	2.48	0.49
7:G:8:HIS:HE1	27:G:102:PEK:C05	2.26	0.49
1:A:240:HIS:HE1	18:A:607:AZI:N2	2.11	0.49
2:B:87[B]:MET:HB3	30:B:457:HOH:O	2.12	0.49
4:D:100[B]:LYS:CE	4:D:100[B]:LYS:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:608:TGL:HB21	19:A:608:TGL:HA21	1.95	0.48
28:P:304:CDL:H351	28:P:304:CDL:C39	2.28	0.48
13:Z:36:HIS:CD2	13:Z:39:ASN:ND2	2.80	0.48
2:B:60:GLU:N	2:B:60:GLU:CD	2.66	0.48
20:C:309:PGV:H21	20:C:309:PGV:C7	2.38	0.48
3:P:33[B]:MET:CB	25:P:306:DMU:H9	2.42	0.48
4:D:78:TRP:HA	19:D:201:TGL:HB21	1.95	0.48
2:O:26:HIS:O	2:O:29[B]:MET:HB3	2.12	0.48
5:R:5:HIS:O	5:R:6:GLU:HB3	2.13	0.48
11:X:7:PRO:HB2	11:X:12:LYS:NZ	2.27	0.48
30:L:221:HOH:O	13:M:32:TRP:HH2	1.96	0.48
6:S:85:CYS:SG	6:S:87[B]:THR:HG22	2.53	0.48
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.49	0.48
14:N:602:HEA:H122	14:N:602:HEA:H262	1.96	0.48
1:A:334:TRP:CZ3	19:D:201:TGL:HA52	2.49	0.48
6:F:95:GLN:HG2	6:F:98:HIS:N	2.28	0.48
22:P:301:CHD:H12	22:P:301:CHD:H212	1.96	0.48
4:D:78:TRP:HB3	19:D:201:TGL:CB2	2.34	0.47
14:N:603[A]:HEA:NB	18:N:608:AZI:N2	2.58	0.47
1:A:265:LYS:NZ	21:A:617:EDO:H22	2.29	0.47
2:B:41[B]:ILE:CD1	9:I:21:ILE:CD1	2.91	0.47
21:N:618:EDO:C2	30:S:246:HOH:O	2.61	0.47
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.94	0.47
3:P:259:TRP:CD1	25:P:308:DMU:H30	2.49	0.47
3:P:63:ARG:HE	28:P:304:CDL:HA22	1.78	0.47
9:I:35:TYR:CD1	9:I:35:TYR:C	2.88	0.47
3:C:258:TRP:CH2	25:C:310:DMU:H12	2.49	0.47
22:J:101:CHD:H222	22:J:101:CHD:H162	1.61	0.47
1:N:468:MET:HG3	30:N:910[A]:HOH:O	2.13	0.47
3:C:51[A]:MET:HE1	20:C:305:PGV:H161	1.95	0.47
9:I:31:PHE:CZ	9:I:35:TYR:HB2	2.49	0.47
8:H:38:ARG:HH12	21:H:101:EDO:H21	1.80	0.47
1:A:243:VAL:HG11	18:A:606:AZI:N3	2.30	0.47
2:B:49:LYS:HE2	30:D:394:HOH:O	2.14	0.47
3:C:37:PHE:CD2	25:C:302:DMU:H8	2.49	0.47
7:G:4:ALA:CB	1:N:282:PHE:HA	2.44	0.47
20:P:303:PGV:H142	20:P:303:PGV:H11	1.70	0.47
28:T:103:CDL:C76	28:T:103:CDL:H252	2.44	0.47
9:V:31:PHE:C	9:V:31:PHE:CD1	2.87	0.47
10:W:33:ARG:HE	22:W:101:CHD:H7	1.79	0.47
11:X:26:VAL:O	11:X:30:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.95	0.47
20:C:309:PGV:C2	20:C:309:PGV:C7	2.93	0.47
13:Z:19:LEU:HD23	20:Z:101:PGV:C31	2.45	0.47
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.97	0.47
3:C:210:ILE:HG12	20:C:305:PGV:H132	1.96	0.47
1:N:173:PRO:HB3	30:N:864:HOH:O	2.14	0.47
1:N:359:ALA:CA	14:N:603[B]:HEA:OMA	2.58	0.47
13:Z:16:ALA:HA	20:Z:101:PGV:H291	1.97	0.47
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.97	0.47
2:B:40:TYR:CE2	9:I:24:ALA:HB2	2.50	0.47
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.97	0.47
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.15	0.47
1:A:240:HIS:CE1	18:A:607:AZI:N2	2.83	0.46
3:C:176:LEU:HD23	21:C:317:EDO:H12	1.96	0.46
9:V:1:SAC:OAC	9:V:3:ALA:HB3	2.14	0.46
19:Q:201:TGL:H362	9:V:20:HIS:HE1	1.80	0.46
1:A:378:HIS:HA	1:A:382[B]:SER:CB	2.43	0.46
20:A:609:PGV:H343	27:C:304:PEK:C38	2.41	0.46
20:A:610:PGV:H132	20:A:610:PGV:H302	1.98	0.46
6:S:64:GLU:O	6:S:65:ASP:CB	2.63	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.46
14:N:603[A]:HEA:CBC	14:N:603[A]:HEA:HMC1	2.43	0.46
3:P:33[B]:MET:HE3	25:P:306:DMU:H6	1.97	0.46
4:Q:78:TRP:CB	19:Q:201:TGL:HB22	2.45	0.46
7:T:44:ARG:NH2	7:T:84:LYS:NZ	2.59	0.46
4:Q:118:LYS:HE3	11:X:51:LYS:HE3	1.98	0.46
3:P:33[A]:MET:HG2	3:P:39:SER:O	2.14	0.46
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.50	0.46
6:S:96:LEU:HB3	6:S:97:ALA:H	1.56	0.46
4:D:121:LYS:HZ3	21:D:206:EDO:H22	1.80	0.46
10:W:32:TYR:CE2	22:W:101:CHD:C18	2.98	0.46
14:A:602[A]:HEA:C1B	18:A:607:AZI:N2	2.79	0.46
3:C:156:ARG:HH21	22:C:307:CHD:C24	2.28	0.46
3:C:51[B]:MET:HE2	28:C:306:CDL:H392	1.95	0.46
3:P:202:GLY:HA3	27:T:102:PEK:H21	1.98	0.46
3:P:224:LYS:HZ1	28:P:304:CDL:H112	1.80	0.46
19:Y:101:TGL:H202	19:Y:101:TGL:H231	1.78	0.46
22:J:101:CHD:H212	22:J:101:CHD:O12	2.15	0.46
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.04	0.46
7:T:12:GLY:HA3	30:T:226:HOH:O	2.15	0.46
11:X:47:ARG:CZ	11:X:47:ARG:CB	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:304:PEK:C11	27:C:304:PEK:H172	2.46	0.46
1:N:302[B]:ARG:HE	2:O:84:LEU:HD11	1.81	0.46
28:N:601:CDL:H371	2:O:78:LEU:CD1	2.34	0.46
24:B:303:PSC:H063	9:I:10:ARG:HH21	1.76	0.45
2:O:67:ILE:HD11	21:O:305:EDO:O2	2.16	0.45
10:W:33:ARG:HG2	22:W:101:CHD:H182	1.98	0.45
1:N:265:LYS:CD	21:N:622:EDO:H12	2.46	0.45
28:T:103:CDL:C33	28:T:103:CDL:OA7	2.58	0.45
28:T:103:CDL:OB4	28:T:103:CDL:H131	2.16	0.45
1:A:449:MET:SD	2:B:5:MET:HG2	2.57	0.45
3:P:52:LEU:HG	28:P:304:CDL:H382	1.98	0.45
1:A:363:LEU:HD22	2:B:23:PHE:CE2	2.51	0.45
4:D:109:HIS:HD2	30:D:359:HOH:O	1.98	0.45
27:G:102:PEK:H382	28:N:601:CDL:H861	1.99	0.45
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.51	0.45
1:N:112:LEU:C	1:N:112:LEU:HD23	2.37	0.45
1:N:513:LEU:O	1:N:514:LYS:CB	2.44	0.45
6:S:87[A]:THR:HG21	30:S:227:HOH:O	2.17	0.45
14:A:602[B]:HEA:H11	14:A:602[B]:HEA:HMB1	1.85	0.45
2:B:28:LEU:O	2:B:29[A]:MET:C	2.52	0.45
25:C:310:DMU:H32	25:C:310:DMU:C57	2.45	0.45
8:H:43:MET:HE3	8:H:49:ASP:N	2.32	0.45
19:N:610:TGL:HB92	19:N:610:TGL:H281	1.94	0.45
28:T:103:CDL:C31	28:T:103:CDL:HA4	2.43	0.45
20:Z:101:PGV:H202	20:Z:101:PGV:H22	1.99	0.45
25:C:310:DMU:H34	25:C:310:DMU:H36	1.30	0.45
28:N:601:CDL:H531	28:N:601:CDL:H261	1.97	0.45
2:O:69:PRO:HG3	24:O:302:PSC:H182	1.99	0.45
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.99	0.45
2:B:49:LYS:HD3	19:D:201:TGL:CC7	2.46	0.45
1:N:313:ALA:HB2	1:N:356:ILE:HD11	1.98	0.45
3:P:33[B]:MET:SD	25:P:306:DMU:C18	3.05	0.45
27:T:101:PEK:H361	28:T:103:CDL:C87	2.46	0.45
3:C:217:VAL:HG22	28:C:306:CDL:H732	1.98	0.45
21:D:203:EDO:C1	30:D:340:HOH:O	2.45	0.45
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.45	0.45
7:T:38:HIS:ND1	7:T:38:HIS:N	2.65	0.45
1:A:282:PHE:N	7:T:4:ALA:HB1	2.31	0.45
30:B:513:HOH:O	19:D:201:TGL:HC22	2.17	0.44
6:F:92:VAL:HG23	6:F:92:VAL:O	2.17	0.44
12:L:41:ARG:HH22	25:L:102:DMU:H30	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:610:PGV:H312	13:M:16:ALA:HA	1.99	0.44
14:N:603[A]:HEA:C1B	18:N:608:AZI:N3	2.80	0.44
2:O:114:GLU:CG	2:O:227:LEU:HD21	2.47	0.44
1:N:449:MET:SD	2:O:5:MET:HG2	2.57	0.44
1:A:172:LYS:HD2	1:A:181:THR:CG2	2.47	0.44
1:A:407:ASP:OD2	21:A:618:EDO:H11	2.18	0.44
4:D:99:GLU:OE2	21:D:202:EDO:C2	2.57	0.44
7:G:38:HIS:CE1	28:N:601:CDL:H141	2.51	0.44
21:C:315:EDO:H12	30:C:469:HOH:O	2.17	0.44
14:A:602[B]:HEA:CBD	14:A:602[B]:HEA:HMD1	2.47	0.44
28:C:306:CDL:H191	28:C:306:CDL:H752	2.00	0.44
2:O:111:THR:HA	2:O:114:GLU:O	2.18	0.44
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.99	0.44
12:Y:24[B]:MET:SD	19:Y:101:TGL:CC3	3.06	0.44
1:A:297[A]:MET:HG2	1:A:302[A]:ARG:HG3	1.99	0.44
4:D:19[A]:ARG:HD2	4:D:21:ASP:OD1	2.18	0.44
19:N:610:TGL:HA71	19:N:610:TGL:H102	2.00	0.44
19:A:608:TGL:H242	19:A:608:TGL:H272	1.72	0.44
24:O:302:PSC:C34	24:O:302:PSC:H12	2.48	0.44
21:N:622:EDO:C1	6:S:84:SER:OG	2.64	0.44
14:A:602[A]:HEA:C1B	18:A:607:AZI:N3	2.81	0.44
20:A:609:PGV:H312	20:C:305:PGV:H321	2.00	0.44
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.99	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.17	0.44
5:R:7:THR:HB	5:R:9:GLU:OE2	2.17	0.44
12:Y:20:ARG:NH1	12:Y:24[B]:MET:SD	2.90	0.44
25:L:102:DMU:H36	25:L:102:DMU:H2	1.55	0.44
25:P:309:DMU:H22	10:W:38:LEU:HD23	1.98	0.44
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.44	0.44
28:N:601:CDL:H362	28:N:601:CDL:H121	2.00	0.44
2:B:28:LEU:HG	2:B:32[A]:PHE:CE2	2.52	0.43
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.48	0.43
1:N:311[B]:ILE:HD11	28:N:601:CDL:C23	2.48	0.43
30:N:828:HOH:O	2:O:53:THR:CG2	2.66	0.43
19:Q:201:TGL:HG32	19:Q:201:TGL:OB1	2.17	0.43
3:C:103:HIS:ND1	22:C:301:CHD:O26	2.51	0.43
20:A:609:PGV:C18	27:C:304:PEK:H322	2.45	0.43
1:N:172:LYS:HZ2	1:N:178[A]:GLN:HE22	1.67	0.43
3:P:33[A]:MET:HA	25:P:306:DMU:H9	2.00	0.43
1:A:297[A]:MET:SD	1:A:302[A]:ARG:HG3	2.56	0.43
3:C:33[B]:MET:CG	3:C:39:SER:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:303:PSC:H072	5:E:11:PHE:HB2	2.00	0.43
7:G:72:ASN:N	7:G:76:ASN:HD22	2.05	0.43
2:O:82:ARG:HH11	2:O:86:MET:HE3	1.84	0.43
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.47	0.43
12:L:26:THR:HG23	13:M:25:SER:CB	2.48	0.43
4:Q:78:TRP:HB3	19:Q:201:TGL:HB22	1.99	0.43
1:A:316:THR:HG21	14:A:602[A]:HEA:H14	2.00	0.43
6:F:13:ALA:CB	6:F:21[B]:MET:HE1	2.48	0.43
3:P:37:PHE:CB	25:P:306:DMU:H7	2.49	0.43
27:C:308:PEK:H382	28:N:601:CDL:C27	2.46	0.43
1:N:328:HIS:HB2	2:O:45:MET:SD	2.58	0.43
19:N:610:TGL:HC31	2:O:7:LEU:HD12	2.00	0.43
1:A:328:HIS:NE2	24:B:303:PSC:C2	2.82	0.43
1:A:483:LEU:O	21:A:619:EDO:H12	2.19	0.43
4:D:17[A]:VAL:O	4:D:17[A]:VAL:CG2	2.66	0.43
22:G:101:CHD:H212	22:G:101:CHD:H12	2.01	0.43
1:N:307:SER:HB3	28:N:601:CDL:H191	1.99	0.43
8:U:50:VAL:O	8:U:51:SER:C	2.57	0.43
2:B:41[A]:ILE:O	2:B:42:ILE:C	2.51	0.43
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.54	0.43
2:O:91:ASN:HD22	2:O:92:ASN:N	2.17	0.43
1:A:406:ASN:HD21	20:A:610:PGV:H22	1.82	0.43
1:N:115[A]:SER:O	1:N:121:GLY:HA2	2.18	0.43
3:P:158:HIS:NE2	27:P:307:PEK:N	2.67	0.43
1:N:467:LEU:O	1:N:471:ILE:HG13	2.19	0.42
2:O:41:ILE:O	2:O:42:ILE:C	2.55	0.42
1:A:361[B]:SER:HB3	30:A:708:HOH:O	2.18	0.42
20:A:609:PGV:C34	27:C:304:PEK:H382	2.40	0.42
28:C:306:CDL:H521	28:C:306:CDL:OB9	2.19	0.42
1:N:311[A]:ILE:CG1	28:N:601:CDL:H442	2.49	0.42
2:B:16[A]:ILE:HD13	2:B:16[A]:ILE:HA	1.87	0.42
1:N:378:HIS:HA	1:N:382[B]:SER:HB2	2.00	0.42
13:Z:38:ASP:HB2	30:Z:202:HOH:O	2.18	0.42
1:A:131:PRO:HB3	21:A:622:EDO:H22	2.01	0.42
2:B:69:PRO:HG2	30:B:437:HOH:O	2.19	0.42
25:C:302:DMU:H12	10:J:49:CYS:HB3	2.00	0.42
4:D:98:TRP:CE2	25:M:101:DMU:H11	2.54	0.42
1:N:240:HIS:O	1:N:241:PRO:C	2.56	0.42
1:N:297[B]:MET:SD	1:N:302[B]:ARG:CG	3.07	0.42
24:O:302:PSC:H251	24:O:302:PSC:H221	1.63	0.42
28:T:103:CDL:H232	28:T:103:CDL:H262	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297[A]:MET:HG2	1:A:302[A]:ARG:CG	2.50	0.42
1:N:309:THR:HG22	14:N:603[A]:HEA:HMB2	2.01	0.42
14:N:602:HEA:H122	14:N:602:HEA:HHC	2.00	0.42
24:O:302:PSC:C12	24:O:302:PSC:H343	2.50	0.42
1:A:355:GLY:C	14:A:602[B]:HEA:HMB3	2.40	0.42
10:J:27:THR:HG22	30:J:214:HOH:O	2.18	0.42
11:K:8:ASP:HB2	30:K:110:HOH:O	2.19	0.42
21:N:622:EDO:H11	6:S:84:SER:CB	2.49	0.42
7:G:3:ALA:O	7:G:4:ALA:CB	2.66	0.42
1:N:131:PRO:HB3	21:N:613:EDO:H12	2.00	0.42
12:Y:20:ARG:HH22	19:Y:101:TGL:HC52	1.84	0.42
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.00	0.42
2:B:57:ASP:H	24:B:303:PSC:H212	1.83	0.42
3:C:51[B]:MET:HE1	28:C:306:CDL:H242	2.02	0.42
19:D:201:TGL:HC42	19:D:201:TGL:OA1	2.20	0.42
1:N:488:THR:HB	1:N:495:LEU:HD13	2.02	0.42
5:R:41:LEU:HA	30:V:209:HOH:O	2.20	0.42
3:P:131:LEU:HD11	28:T:103:CDL:H561	2.01	0.42
1:A:397:PHE:HB3	1:A:398:PRO:HD3	2.01	0.42
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.01	0.42
7:G:33:LEU:O	7:G:37:LEU:HB2	2.20	0.42
28:P:304:CDL:OA7	28:P:304:CDL:H162	2.20	0.42
5:R:77:PRO:O	5:R:79:LYS:HD2	2.20	0.42
22:C:307:CHD:H12A	22:C:307:CHD:H112	1.86	0.42
7:G:19:LEU:HD21	27:G:102:PEK:H372	2.02	0.41
20:G:103:PGV:H231	20:G:103:PGV:H202	1.82	0.41
8:H:8:ILE:O	8:H:8:ILE:CG2	2.68	0.41
28:P:304:CDL:OB9	28:P:304:CDL:HB4	2.20	0.41
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.20	0.41
1:A:54:TYR:HB2	30:A:744:HOH:O	2.20	0.41
1:N:377:PHE:CD2	14:N:603[A]:HEA:HAD1	2.55	0.41
4:Q:19[A]:ARG:HD2	4:Q:21:ASP:OD1	2.13	0.41
1:A:377:PHE:HB3	14:A:602[A]:HEA:C2D	2.50	0.41
25:C:302:DMU:H15	25:C:302:DMU:H9	1.74	0.41
25:C:302:DMU:H7	10:J:49:CYS:HB3	2.02	0.41
8:H:8:ILE:HG23	8:H:8:ILE:O	2.20	0.41
1:N:302[B]:ARG:HH21	2:O:84:LEU:CD1	2.33	0.41
14:N:603[A]:HEA:C1B	18:N:608:AZI:N2	2.84	0.41
1:N:511:VAL:H	21:N:621:EDO:H22	1.84	0.41
24:O:302:PSC:H231	24:O:302:PSC:H202	1.51	0.41
8:U:60:TYR:C	8:U:60:TYR:CD1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:26:MET:O	9:I:27:VAL:C	2.59	0.41
1:N:136[B]:LEU:HD21	30:T:237:HOH:O	2.19	0.41
7:G:2:SER:HB2	1:N:197:LEU:HD21	2.03	0.41
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG3	2.60	0.41
24:O:302:PSC:H292	24:O:302:PSC:H322	1.86	0.41
3:P:54[A]:MET:HB3	3:P:58:TRP:CZ3	2.55	0.41
7:T:3:ALA:O	7:T:4:ALA:HB2	2.20	0.41
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.02	0.41
2:B:32[B]:PHE:HE1	30:B:536:HOH:O	2.03	0.41
1:A:514:LYS:HG3	6:F:38:ALA:HB2	2.03	0.41
28:P:304:CDL:H842	28:P:304:CDL:H812	1.68	0.41
22:W:101:CHD:H7	22:W:101:CHD:H191	2.02	0.41
10:W:3:ASN:C	10:W:3:ASN:OD1	2.58	0.41
1:A:240:HIS:CD2	1:A:240:HIS:C	2.94	0.41
14:A:602[A]:HEA:H243	2:B:69:PRO:HB3	2.03	0.41
20:N:609:PGV:H262	20:P:303:PGV:H292	2.02	0.41
8:U:9:LYS:C	8:U:9:LYS:HD2	2.41	0.41
8:H:43:MET:HB3	8:H:43:MET:HE3	1.88	0.41
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.21	0.41
21:P:312:EDO:H11	6:S:16:LEU:HD13	2.02	0.41
6:S:87[A]:THR:HG22	30:S:254:HOH:O	2.21	0.41
1:A:302[B]:ARG:NE	1:A:361[B]:SER:OG	2.53	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.64	0.41
7:G:6:GLY:HA2	27:G:102:PEK:H322	2.03	0.41
19:N:610:TGL:HC32	19:N:610:TGL:HG12	2.02	0.41
14:A:602[A]:HEA:H11	14:A:602[A]:HEA:HMB1	1.90	0.41
2:B:108:TYR:O	2:B:117:SER:HA	2.20	0.41
2:B:65:TRP:CD1	24:B:303:PSC:H142	2.56	0.41
3:C:67:PHE:HE2	28:C:306:CDL:O1	2.02	0.41
19:D:201:TGL:CG3	30:D:364:HOH:O	2.11	0.41
6:F:1:ALA:HB3	21:F:105:EDO:C1	2.47	0.41
1:N:510:TYR:HA	21:N:621:EDO:C2	2.50	0.41
22:P:305:CHD:C16	22:P:305:CHD:C23	2.95	0.41
4:Q:109:HIS:CD2	30:Q:322:HOH:O	2.66	0.41
27:T:102:PEK:H221	27:T:102:PEK:H251	1.73	0.41
14:A:602[B]:HEA:HHC	14:A:602[B]:HEA:H122	2.03	0.41
24:B:303:PSC:H062	24:B:303:PSC:H042	1.79	0.41
19:L:101:TGL:HC92	19:L:101:TGL:HC52	2.02	0.41
28:P:304:CDL:HB21	28:P:304:CDL:OB6	2.21	0.41
2:B:37:LEU:O	2:B:41[B]:ILE:HG12	2.22	0.40
22:C:301:CHD:H212	22:C:301:CHD:H12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:TYR:OH	21:D:202:EDO:H21	2.21	0.40
27:C:308:PEK:H202	7:G:36:TRP:HE1	1.85	0.40
8:H:43:MET:CE	8:H:49:ASP:H	2.34	0.40
1:A:148:PHE:HB3	3:C:28:THR:HB	2.03	0.40
4:D:100[B]:LYS:HD2	4:D:100[B]:LYS:HA	1.87	0.40
1:N:399:LEU:O	1:N:499:PRO:HA	2.21	0.40
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.83	0.40
28:C:306:CDL:H761	28:C:306:CDL:H791	1.70	0.40
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.86	0.40
30:B:517:HOH:O	19:D:201:TGL:H332	2.21	0.40
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.57	0.40
20:A:610:PGV:H241	13:M:12:PRO:HG3	2.03	0.40
1:N:115[B]:SER:O	1:N:121:GLY:HA2	2.21	0.40
14:N:603[B]:HEA:HBD2	14:N:603[B]:HEA:HMD1	2.01	0.40
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.56	0.40
2:O:58:ALA:O	2:O:62:GLU:HG3	2.22	0.40
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.19	0.40
1:A:311[B]:ILE:HG13	1:A:314:ILE:HD12	2.04	0.40
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.04	0.40
2:B:42:ILE:HD13	2:B:42:ILE:HG21	1.88	0.40
3:C:76:GLN:O	3:C:80[A]:ARG:HG3	2.22	0.40
1:A:309:THR:HG22	14:A:602[A]:HEA:HMB2	2.04	0.40
3:C:191:GLY:HA3	30:G:218:HOH:O	2.20	0.40
3:C:99:TRP:CE2	20:C:309:PGV:H232	2.57	0.40
3:P:33[B]:MET:CG	25:P:306:DMU:C19	2.99	0.40
10:W:29:ASN:H	10:W:29:ASN:HD22	1.70	0.40
10:W:58:LYS:HE2	10:W:58:LYS:HB3	1.88	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:226:MET:O	4:Q:5:VAL:O[2_684]	2.13	0.07
30:B:466:HOH:O	30:D:302:HOH:O[2_584]	2.18	0.02

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 X-ray entries followed by that with respect to entries of similar resolution.

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	534/514 (104%)	519 (97%)	15 (3%)	0	100	100
1	N	532/514 (104%)	516 (97%)	16 (3%)	0	100	100
2	B	235/227 (104%)	224 (95%)	11 (5%)	0	100	100
2	O	229/227 (101%)	222 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	146/147 (99%)	141 (97%)	5 (3%)	0	100	100
4	Q	145/147 (99%)	139 (96%)	4 (3%)	2 (1%)	11	3
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	15	5
6	F	100/98 (102%)	96 (96%)	2 (2%)	2 (2%)	7	1
6	S	98/98 (100%)	89 (91%)	7 (7%)	2 (2%)	7	1
7	G	81/85 (95%)	70 (86%)	5 (6%)	6 (7%)	1	0
7	T	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	2	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	12	3
8	U	77/85 (91%)	67 (87%)	7 (9%)	3 (4%)	3	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	6	1
All	All	3596/3614 (100%)	3454 (96%)	119 (3%)	23 (1%)	22	12

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
7	G	4	ALA
7	G	5	LYS
7	G	8	HIS
13	M	42	LYS
4	Q	7	LYS
4	Q	8	SER
5	R	6	GLU
6	S	94	HIS
7	T	5	LYS
7	T	8	HIS
8	U	46	LYS
7	G	37	LEU
6	S	96	LEU
7	T	3	ALA
7	T	4	ALA
7	G	6	GLY
8	U	45	ALA
13	Z	42	LYS
6	F	96	LEU
7	G	3	ALA
8	U	11	TYR
8	H	8	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	447/426 (105%)	441 (99%)	6 (1%)	69	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	445/426 (104%)	437 (98%)	8 (2%)	59	45
2	B	220/210 (105%)	211 (96%)	9 (4%)	30	13
2	O	214/210 (102%)	209 (98%)	5 (2%)	50	34
3	C	233/226 (103%)	227 (97%)	6 (3%)	46	30
3	P	233/226 (103%)	228 (98%)	5 (2%)	53	38
4	D	132/129 (102%)	128 (97%)	4 (3%)	41	24
4	Q	131/129 (102%)	122 (93%)	9 (7%)	15	4
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	21
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	12
6	F	85/81 (105%)	80 (94%)	5 (6%)	19	6
6	S	83/81 (102%)	71 (86%)	12 (14%)	3	0
7	G	67/68 (98%)	62 (92%)	5 (8%)	13	3
7	T	68/68 (100%)	59 (87%)	9 (13%)	4	0
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	2
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	2
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	8
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	3
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	40
10	W	50/50 (100%)	48 (96%)	2 (4%)	31	14
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	39 (98%)	1 (2%)	47	31
12	L	40/40 (100%)	39 (98%)	1 (2%)	47	31
12	Y	40/40 (100%)	38 (95%)	2 (5%)	24	9
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	2
All	All	3130/3082 (102%)	3011 (96%)	119 (4%)	34	16

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	297[A]	MET
1	A	297[B]	MET
1	A	369	ASP
2	B	42	ILE
2	B	59	GLN
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	91	ASN
2	B	116	LEU
2	B	171	LYS
3	C	17	PRO
3	C	33[A]	MET
3	C	33[B]	MET
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
4	D	8	SER
4	D	31[A]	LYS
4	D	31[B]	LYS
4	D	147	LYS
5	E	5	HIS
5	E	70	VAL
5	E	90	ARG
6	F	37	LYS
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	80	GLN
6	F	95	GLN
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	54	ARG
7	G	84	LYS
8	H	8	ILE
8	H	9	LYS
8	H	29	CYS
8	H	44	THR
8	H	46	LYS
8	H	60	TYR
9	I	2	THR

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Mol	Chain	Res	Type
9	I	37	PHE
9	I	73	LYS
10	J	58	LYS
12	L	47	LYS
1	N	38	ARG
1	N	109	PHE
1	N	138	HIS
1	N	180	GLN
1	N	265	LYS
1	N	369	ASP
1	N	382[A]	SER
1	N	382[B]	SER
2	O	33	LEU
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
3	P	3	HIS
3	P	17	PRO
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	4	SER
4	Q	6	VAL
4	Q	7	LYS
4	Q	8	SER
4	Q	31	LYS
4	Q	51	LEU
4	Q	106	PRO
4	Q	143	ASN
4	Q	147	LYS
5	R	5	HIS
5	R	79	LYS
5	R	90	ARG
5	R	109	VAL
6	S	21[A]	MET
6	S	21[B]	MET
6	S	37	LYS
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
6	S	87[A]	THR

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Mol	Chain	Res	Type
6	S	87[B]	THR
6	S	93	PRO
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	7	ASP
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	38	HIS
7	T	42	ARG
7	T	43	GLU
7	T	54	ARG
7	T	84	LYS
8	U	7	LYS
8	U	9	LYS
8	U	10	ASN
8	U	29	CYS
8	U	40	GLU
8	U	60	TYR
9	V	8	GLN
9	V	29	LEU
9	V	37	PHE
9	V	73	LYS
10	W	50	LEU
10	W	58	LYS
11	X	54	ARG
12	Y	2	HIS
12	Y	47	LYS
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	10	GLN
2	B	59	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN

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Mol	Chain	Res	Type
3	C	149	HIS
4	D	29	HIS
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
5	E	94	ASN
6	F	80	GLN
7	G	8	HIS
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
8	H	22	ASN
10	J	29	ASN
10	J	57	HIS
1	N	180	GLN
2	O	10	GLN
2	O	52	HIS
2	O	181	GLN
2	O	195	GLN
3	P	38	ASN
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	76	ASN
8	U	10	ASN
8	U	22	ASN
8	U	37	HIS
10	W	29	ASN
13	Z	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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$
1	FME	A	1	1	8,9,10	0.87	0	7,9,11	2.27	3 (42%)
1	FME	N	1	1	8,9,10	1.52	1 (12%)	7,9,11	1.61	2 (28%)
7	TPO	T	11	7	8,10,11	1.82	2 (25%)	10,14,16	1.67	2 (20%)
9	SAC	V	1	9	7,8,9	1.64	1 (14%)	8,9,11	1.54	3 (37%)
2	FME	B	1	2	8,9,10	1.97	2 (25%)	7,9,11	2.29	2 (28%)
2	FME	O	1	2	8,9,10	1.21	1 (12%)	7,9,11	1.88	2 (28%)
7	TPO	G	11	7	8,10,11	2.02	2 (25%)	10,14,16	1.39	2 (20%)
9	SAC	I	1	9	7,8,9	1.12	1 (14%)	8,9,11	1.97	2 (25%)

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
1	FME	A	1	1	-	3/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
9	SAC	V	1	9	-	7/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.17	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CA-N	3.89	1.51	1.46
1	N	1	FME	CA-N	3.78	1.51	1.46
7	G	11	TPO	P-OG1	3.43	1.65	1.59
7	T	11	TPO	P-O1P	3.08	1.60	1.50
7	G	11	TPO	P-O1P	3.06	1.60	1.50
9	I	1	SAC	CA-N	2.63	1.50	1.46
2	B	1	FME	CB-CG	2.38	1.60	1.51
7	T	11	TPO	P-OG1	2.34	1.63	1.59
2	O	1	FME	CA-N	2.11	1.49	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	C-CA-N	-4.23	102.11	109.73
9	I	1	SAC	OG-CB-CA	-4.10	100.50	110.97
7	T	11	TPO	CG2-CB-CA	3.72	120.51	113.16
2	B	1	FME	CG-CB-CA	-3.71	102.63	112.95
2	O	1	FME	CG-CB-CA	-3.32	103.72	112.95
1	A	1	FME	CE-SD-CG	3.13	111.16	100.40
1	N	1	FME	CG-CB-CA	2.92	121.07	112.95
1	A	1	FME	C-CA-N	2.90	114.97	109.73
1	A	1	FME	CA-N-CN	2.81	127.14	122.82
9	I	1	SAC	C-CA-N	2.70	114.61	109.73
7	G	11	TPO	CG2-CB-CA	2.63	118.36	113.16
2	O	1	FME	CA-N-CN	2.53	126.71	122.82
9	V	1	SAC	CA-N-C1A	2.46	127.68	123.15
9	V	1	SAC	O-C-CA	-2.23	118.94	124.78
9	V	1	SAC	OG-CB-CA	-2.23	105.28	110.97
7	T	11	TPO	O3P-P-O1P	-2.09	102.50	110.68
7	G	11	TPO	O3P-P-OG1	2.07	115.26	105.99
1	N	1	FME	O-C-CA	-2.05	119.39	124.78

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
7	T	11	TPO	CA-CB-OG1-P
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	O-C-CA-CB
9	V	1	SAC	C-CA-CB-OG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
9	I	1	SAC	N-CA-CB-OG
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	CA-CB-CG-SD
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
1	N	1	FME	N-CA-CB-CG
9	V	1	SAC	N-CA-CB-OG
2	B	1	FME	CB-CG-SD-CE
1	N	1	FME	CB-CG-SD-CE
9	V	1	SAC	CB-CA-N-C1A
1	A	1	FME	CB-CG-SD-CE
9	V	1	SAC	C-CA-N-C1A

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
9	V	1	SAC	1	0
2	B	1	FME	1	0
7	G	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 142 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 132 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	N	603[B]	1,18	44,67,67	1.03	1 (2%)	37,103,103	1.92	10 (27%)
21	EDO	D	205	-	3,3,3	0.50	0	2,2,2	0.71	0
21	EDO	T	104	-	3,3,3	1.06	0	2,2,2	0.46	0
21	EDO	N	618	-	3,3,3	0.45	0	2,2,2	1.46	0
19	TGL	Q	201	-	62,62,62	1.49	4 (6%)	65,65,65	1.64	8 (12%)
22	CHD	C	301	-	29,32,32	1.64	5 (17%)	48,51,51	2.65	21 (43%)
27	PEK	C	304	-	52,52,52	1.06	5 (9%)	55,57,57	1.28	8 (14%)
27	PEK	C	308	-	52,52,52	1.27	3 (5%)	55,57,57	1.59	9 (16%)
21	EDO	E	204	-	3,3,3	0.79	0	2,2,2	0.39	0
21	EDO	O	305	-	3,3,3	0.39	0	2,2,2	0.52	0
21	EDO	D	202	-	3,3,3	0.55	0	2,2,2	0.74	0
21	EDO	U	101	-	3,3,3	0.36	0	2,2,2	0.82	0
21	EDO	D	206	-	3,3,3	0.26	0	2,2,2	1.32	0
21	EDO	A	623	-	3,3,3	0.53	0	2,2,2	0.80	0
21	EDO	A	616	-	3,3,3	1.02	0	2,2,2	0.33	0
14	HEA	A	601	1	44,67,67	1.62	7 (15%)	37,103,103	2.63	20 (54%)
21	EDO	A	614	-	3,3,3	0.39	0	2,2,2	1.18	0
21	EDO	P	312	-	3,3,3	0.59	0	2,2,2	0.63	0
21	EDO	A	611	-	3,3,3	0.37	0	2,2,2	1.14	0
21	EDO	C	320	-	3,3,3	0.79	0	2,2,2	1.30	0
21	EDO	N	620	-	3,3,3	0.43	0	2,2,2	0.73	0
22	CHD	W	101	-	29,32,32	0.97	0	48,51,51	3.35	20 (41%)
21	EDO	C	319	-	3,3,3	0.68	0	2,2,2	0.26	0
21	EDO	A	621	-	3,3,3	0.80	0	2,2,2	0.23	0
21	EDO	C	315	-	3,3,3	0.68	0	2,2,2	0.51	0
25	DMU	P	309	-	34,34,34	0.89	1 (2%)	45,45,45	1.26	3 (6%)
21	EDO	B	304	-	3,3,3	0.50	0	2,2,2	0.23	0
27	PEK	G	102	-	52,52,52	1.12	2 (3%)	55,57,57	1.49	5 (9%)
21	EDO	C	312	-	3,3,3	1.23	0	2,2,2	0.14	0
27	PEK	P	307	-	52,52,52	1.21	2 (3%)	55,57,57	1.32	6 (10%)
21	EDO	N	615	-	3,3,3	1.57	1 (33%)	2,2,2	0.65	0
20	PGV	A	609	-	50,50,50	1.11	5 (10%)	53,56,56	1.19	5 (9%)
21	EDO	Q	203	-	3,3,3	0.58	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	Z	101	-	50,50,50	1.15	2 (4%)	53,56,56	1.36	7 (13%)
21	EDO	D	204	-	3,3,3	0.61	0	2,2,2	0.98	0
21	EDO	R	202	-	3,3,3	0.18	0	2,2,2	1.29	0
22	CHD	C	307	-	29,32,32	1.12	3 (10%)	48,51,51	3.50	20 (41%)
21	EDO	A	618	-	3,3,3	0.23	0	2,2,2	1.43	0
27	PEK	T	101	-	52,52,52	1.30	2 (3%)	55,57,57	1.43	7 (12%)
18	AZI	A	607	14	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	R	205	-	3,3,3	0.32	0	2,2,2	1.05	0
22	CHD	P	301	-	29,32,32	1.55	7 (24%)	48,51,51	2.16	17 (35%)
19	TGL	A	608	-	62,62,62	1.37	5 (8%)	65,65,65	2.18	11 (16%)
21	EDO	C	316	-	3,3,3	0.52	0	2,2,2	1.52	0
21	EDO	V	101	-	3,3,3	0.39	0	2,2,2	0.90	0
14	HEA	A	602[B]	1,18	44,67,67	1.16	3 (6%)	37,103,103	2.54	15 (40%)
25	DMU	C	311	-	34,34,34	1.43	3 (8%)	45,45,45	2.32	11 (24%)
18	AZI	N	607	15	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	N	616	-	3,3,3	0.56	0	2,2,2	1.11	0
18	AZI	N	608	14	0,2,2	0.00	-	0,1,1	0.00	-
20	PGV	N	609	-	50,50,50	1.13	5 (10%)	53,56,56	1.32	5 (9%)
19	TGL	N	610	-	62,62,62	1.16	4 (6%)	65,65,65	1.77	12 (18%)
23	CUA	B	302	2	0,1,1	0.00	-	-	-	-
21	EDO	C	318	-	3,3,3	0.66	0	2,2,2	0.39	0
24	PSC	O	302	-	51,51,51	1.29	3 (5%)	57,59,59	1.34	4 (7%)
18	AZI	A	606	15	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	N	614	-	3,3,3	0.40	0	2,2,2	1.22	0
22	CHD	J	101	-	29,32,32	0.68	0	48,51,51	3.32	29 (60%)
21	EDO	A	622	-	3,3,3	0.30	0	2,2,2	0.48	0
21	EDO	A	617	-	3,3,3	1.21	0	2,2,2	1.28	0
14	HEA	N	603[A]	1,18	44,67,67	1.25	3 (6%)	37,103,103	2.88	14 (37%)
21	EDO	F	104	-	3,3,3	0.33	0	2,2,2	0.47	0
21	EDO	J	102	-	3,3,3	0.39	0	2,2,2	1.78	0
25	DMU	C	302	-	34,34,34	0.94	0	45,45,45	1.73	14 (31%)
21	EDO	H	102	-	3,3,3	0.59	0	2,2,2	1.26	0
21	EDO	R	206	-	3,3,3	1.02	0	2,2,2	0.48	0
21	EDO	P	311	-	3,3,3	0.84	0	2,2,2	0.14	0
21	EDO	R	203	-	3,3,3	0.54	0	2,2,2	0.82	0
21	EDO	E	202	-	3,3,3	0.53	0	2,2,2	0.84	0
21	EDO	O	304	-	3,3,3	0.35	0	2,2,2	0.92	0
21	EDO	D	203	-	3,3,3	0.45	0	2,2,2	0.71	0
21	EDO	R	201	-	3,3,3	1.14	0	2,2,2	1.17	0
21	EDO	O	303	-	3,3,3	0.68	0	2,2,2	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	N	602	1	44,67,67	1.24	3 (6%)	37,103,103	2.74	15 (40%)
28	CDL	T	103	-	99,99,99	1.51	14 (14%)	105,111,111	1.72	25 (23%)
21	EDO	H	101	-	3,3,3	0.24	0	2,2,2	2.63	2 (100%)
25	DMU	C	310	-	34,34,34	0.87	1 (2%)	45,45,45	2.11	9 (20%)
21	EDO	A	613	-	3,3,3	1.64	1 (33%)	2,2,2	0.92	0
21	EDO	E	203	-	3,3,3	0.31	0	2,2,2	1.26	0
21	EDO	N	611	-	3,3,3	0.36	0	2,2,2	1.12	0
25	DMU	Z	102	-	34,34,34	0.75	1 (2%)	45,45,45	1.33	5 (11%)
19	TGL	Y	101	-	62,62,62	1.45	5 (8%)	65,65,65	1.88	11 (16%)
20	PGV	P	303	-	50,50,50	0.80	1 (2%)	53,56,56	1.25	8 (15%)
21	EDO	E	205	-	3,3,3	0.38	0	2,2,2	0.80	0
21	EDO	P	310	-	3,3,3	0.67	0	2,2,2	2.16	1 (50%)
19	TGL	D	201	-	62,62,62	1.66	5 (8%)	65,65,65	2.26	11 (16%)
21	EDO	Q	202	-	3,3,3	0.36	0	2,2,2	1.09	0
25	DMU	P	306	-	34,34,34	1.02	1 (2%)	45,45,45	1.38	3 (6%)
21	EDO	S	102	-	3,3,3	1.13	0	2,2,2	0.39	0
21	EDO	A	620	-	3,3,3	0.68	0	2,2,2	0.65	0
22	CHD	P	305	-	29,32,32	1.30	4 (13%)	48,51,51	3.64	22 (45%)
21	EDO	C	317	-	3,3,3	0.47	0	2,2,2	0.37	0
21	EDO	G	104	-	3,3,3	0.58	0	2,2,2	0.47	0
25	DMU	P	308	-	34,34,34	0.75	0	45,45,45	2.19	13 (28%)
24	PSC	B	303	-	51,51,51	1.46	4 (7%)	57,59,59	1.46	7 (12%)
21	EDO	G	105	-	3,3,3	0.91	0	2,2,2	0.20	0
20	PGV	C	305	-	50,50,50	1.06	1 (2%)	53,56,56	1.36	7 (13%)
21	EDO	P	313	-	3,3,3	0.60	0	2,2,2	0.70	0
21	EDO	B	305	-	3,3,3	1.73	1 (33%)	2,2,2	0.11	0
20	PGV	G	103	-	50,50,50	1.25	2 (4%)	53,56,56	1.69	6 (11%)
21	EDO	N	612	-	3,3,3	1.36	0	2,2,2	1.62	0
21	EDO	N	617	-	3,3,3	1.05	0	2,2,2	0.14	0
21	EDO	N	619	-	3,3,3	0.55	0	2,2,2	0.04	0
21	EDO	S	103	-	3,3,3	0.68	0	2,2,2	1.76	1 (50%)
21	EDO	F	102	-	3,3,3	1.06	0	2,2,2	0.29	0
21	EDO	L	103	-	3,3,3	0.26	0	2,2,2	1.08	0
21	EDO	A	619	-	3,3,3	1.55	0	2,2,2	1.69	0
21	EDO	R	204	-	3,3,3	0.88	0	2,2,2	0.42	0
21	EDO	E	201	-	3,3,3	0.84	0	2,2,2	0.44	0
21	EDO	D	207	-	3,3,3	0.62	0	2,2,2	0.56	0
20	PGV	A	610	-	50,50,50	1.42	4 (8%)	53,56,56	1.63	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	A	612	-	3,3,3	0.51	0	2,2,2	1.15	0
21	EDO	C	313	-	3,3,3	0.36	0	2,2,2	0.80	0
14	HEA	A	602[A]	1,18	44,67,67	1.12	2 (4%)	37,103,103	2.15	11 (29%)
19	TGL	L	101	-	62,62,62	2.03	8 (12%)	65,65,65	2.34	17 (26%)
21	EDO	F	103	-	3,3,3	0.64	0	2,2,2	0.54	0
28	CDL	P	304	-	99,99,99	1.61	18 (18%)	105,111,111	1.60	19 (18%)
22	CHD	B	301	-	29,32,32	2.12	10 (34%)	48,51,51	2.00	15 (31%)
21	EDO	N	621	-	3,3,3	0.33	0	2,2,2	0.89	0
20	PGV	C	309	-	50,50,50	1.41	3 (6%)	53,56,56	1.48	8 (15%)
21	EDO	A	615	-	3,3,3	2.67	1 (33%)	2,2,2	4.78	1 (50%)
22	CHD	G	101	-	29,32,32	1.69	7 (24%)	48,51,51	1.81	10 (20%)
21	EDO	F	105	-	3,3,3	0.66	0	2,2,2	0.42	0
28	CDL	C	306	-	99,99,99	1.58	17 (17%)	105,111,111	1.66	20 (19%)
21	EDO	N	613	-	3,3,3	0.54	0	2,2,2	0.44	0
25	DMU	L	102	-	34,34,34	0.96	1 (2%)	45,45,45	1.73	11 (24%)
27	PEK	T	102	-	52,52,52	1.18	6 (11%)	55,57,57	2.57	7 (12%)
23	CUA	O	301	2	0,1,1	0.00	-	-	-	-
25	DMU	M	101	-	34,34,34	0.71	0	45,45,45	1.41	6 (13%)
21	EDO	N	622	-	3,3,3	0.51	0	2,2,2	0.70	0
21	EDO	C	314	-	3,3,3	0.54	0	2,2,2	0.77	0
28	CDL	N	601	-	99,99,99	1.54	14 (14%)	105,111,111	1.60	20 (19%)

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
14	HEA	N	603[B]	1,18	2/2/7/16	3/24/76/76	-
21	EDO	D	205	-	-	1/1/1/1	-
21	EDO	T	104	-	-	0/1/1/1	-
21	EDO	N	618	-	-	0/1/1/1	-
19	TGL	Q	201	-	-	37/65/65/65	-
22	CHD	C	301	-	-	1/7/74/74	0/4/4/4
27	PEK	C	304	-	-	12/56/56/56	-
27	PEK	C	308	-	-	28/56/56/56	-
21	EDO	E	204	-	-	1/1/1/1	-
21	EDO	O	305	-	-	0/1/1/1	-
21	EDO	D	202	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	U	101	-	-	1/1/1/1	-
21	EDO	D	206	-	-	1/1/1/1	-
21	EDO	A	623	-	-	0/1/1/1	-
21	EDO	A	616	-	-	0/1/1/1	-
14	HEA	A	601	1	3/3/7/16	2/24/76/76	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	P	312	-	-	0/1/1/1	-
21	EDO	A	611	-	-	1/1/1/1	-
21	EDO	C	320	-	-	1/1/1/1	-
21	EDO	N	620	-	-	0/1/1/1	-
22	CHD	W	101	-	-	5/7/74/74	0/4/4/4
21	EDO	C	319	-	-	1/1/1/1	-
21	EDO	A	621	-	-	1/1/1/1	-
21	EDO	C	315	-	-	1/1/1/1	-
25	DMU	P	309	-	-	7/19/59/59	0/2/2/2
21	EDO	B	304	-	-	0/1/1/1	-
27	PEK	G	102	-	-	34/56/56/56	-
21	EDO	C	312	-	-	0/1/1/1	-
27	PEK	P	307	-	-	27/56/56/56	-
21	EDO	N	615	-	-	0/1/1/1	-
20	PGV	A	609	-	-	8/55/55/55	-
21	EDO	Q	203	-	-	1/1/1/1	-
20	PGV	Z	101	-	-	31/55/55/55	-
21	EDO	D	204	-	-	1/1/1/1	-
21	EDO	R	202	-	-	1/1/1/1	-
22	CHD	C	307	-	-	6/7/74/74	0/4/4/4
21	EDO	A	618	-	-	1/1/1/1	-
27	PEK	T	101	-	-	29/56/56/56	-
21	EDO	R	205	-	-	1/1/1/1	-
22	CHD	P	301	-	-	0/7/74/74	0/4/4/4
19	TGL	A	608	-	-	36/65/65/65	-
21	EDO	C	316	-	-	0/1/1/1	-
21	EDO	V	101	-	-	0/1/1/1	-
14	HEA	A	602[B]	1,18	3/3/7/16	2/24/76/76	-
25	DMU	C	311	-	-	8/19/59/59	0/2/2/2
21	EDO	N	616	-	-	1/1/1/1	-
20	PGV	N	609	-	-	13/55/55/55	-
19	TGL	N	610	-	-	39/65/65/65	-
21	EDO	C	318	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSC	O	302	-	-	33/55/55/55	-
21	EDO	N	614	-	-	1/1/1/1	-
22	CHD	J	101	-	-	6/7/74/74	0/4/4/4
21	EDO	A	622	-	-	1/1/1/1	-
21	EDO	A	617	-	-	1/1/1/1	-
14	HEA	N	603[A]	1,18	3/3/7/16	0/24/76/76	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	J	102	-	-	1/1/1/1	-
25	DMU	C	302	-	-	7/19/59/59	0/2/2/2
21	EDO	H	102	-	-	1/1/1/1	-
21	EDO	R	206	-	-	1/1/1/1	-
21	EDO	P	311	-	-	0/1/1/1	-
21	EDO	R	203	-	-	1/1/1/1	-
21	EDO	E	202	-	-	0/1/1/1	-
21	EDO	O	304	-	-	1/1/1/1	-
21	EDO	D	203	-	-	1/1/1/1	-
21	EDO	R	201	-	-	0/1/1/1	-
21	EDO	O	303	-	-	0/1/1/1	-
14	HEA	N	602	1	2/2/7/16	3/24/76/76	-
28	CDL	T	103	-	-	63/110/110/110	-
21	EDO	H	101	-	-	0/1/1/1	-
25	DMU	C	310	-	-	6/19/59/59	0/2/2/2
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	E	203	-	-	1/1/1/1	-
21	EDO	N	611	-	-	1/1/1/1	-
25	DMU	Z	102	-	-	5/19/59/59	0/2/2/2
19	TGL	Y	101	-	-	34/65/65/65	-
20	PGV	P	303	-	-	11/55/55/55	-
21	EDO	E	205	-	-	0/1/1/1	-
21	EDO	P	310	-	-	1/1/1/1	-
19	TGL	D	201	-	-	40/65/65/65	-
21	EDO	Q	202	-	-	0/1/1/1	-
25	DMU	P	306	-	-	6/19/59/59	0/2/2/2
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	A	620	-	-	0/1/1/1	-
22	CHD	P	305	-	-	4/7/74/74	0/4/4/4
21	EDO	C	317	-	-	1/1/1/1	-
21	EDO	G	104	-	-	1/1/1/1	-
25	DMU	P	308	-	-	7/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSC	B	303	-	-	28/55/55/55	-
21	EDO	G	105	-	-	1/1/1/1	-
20	PGV	C	305	-	-	14/55/55/55	-
21	EDO	P	313	-	-	1/1/1/1	-
21	EDO	B	305	-	-	1/1/1/1	-
20	PGV	G	103	-	-	33/55/55/55	-
21	EDO	N	612	-	-	1/1/1/1	-
21	EDO	N	617	-	-	0/1/1/1	-
21	EDO	N	619	-	-	0/1/1/1	-
21	EDO	S	103	-	-	1/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	L	103	-	-	1/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
21	EDO	R	204	-	-	0/1/1/1	-
21	EDO	E	201	-	-	1/1/1/1	-
21	EDO	D	207	-	-	0/1/1/1	-
20	PGV	A	610	-	-	26/55/55/55	-
21	EDO	A	612	-	-	1/1/1/1	-
21	EDO	C	313	-	-	1/1/1/1	-
14	HEA	A	602[A]	1,18	3/3/7/16	2/24/76/76	-
19	TGL	L	101	-	-	38/65/65/65	-
21	EDO	F	103	-	-	0/1/1/1	-
28	CDL	P	304	-	-	56/110/110/110	-
22	CHD	B	301	-	-	0/7/74/74	0/4/4/4
21	EDO	N	621	-	-	0/1/1/1	-
20	PGV	C	309	-	-	27/55/55/55	-
21	EDO	A	615	-	-	1/1/1/1	-
22	CHD	G	101	-	-	0/7/74/74	0/4/4/4
21	EDO	F	105	-	-	0/1/1/1	-
28	CDL	C	306	-	-	70/110/110/110	-
21	EDO	N	613	-	-	1/1/1/1	-
25	DMU	L	102	-	-	12/19/59/59	0/2/2/2
27	PEK	T	102	-	-	23/56/56/56	-
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
21	EDO	N	622	-	-	1/1/1/1	-
21	EDO	C	314	-	-	0/1/1/1	-
28	CDL	N	601	-	-	53/110/110/110	-

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG3-CC1	9.15	1.60	1.33
19	L	101	TGL	OG2-CB1	9.01	1.59	1.34
19	D	201	TGL	OB1-CB1	7.45	1.44	1.22
19	Y	101	TGL	OG2-CB1	6.77	1.53	1.34
20	C	309	PGV	O01-C1	6.53	1.52	1.34
19	Q	201	TGL	OB1-CB1	6.41	1.41	1.22
19	D	201	TGL	OG1-CA1	6.22	1.51	1.33
28	N	601	CDL	OB6-CB5	6.20	1.51	1.34
24	B	303	PSC	O01-C1	6.11	1.51	1.34
28	T	103	CDL	OB6-CB5	6.08	1.51	1.34
19	Y	101	TGL	OG3-CC1	5.82	1.50	1.33
19	Q	201	TGL	OG2-CB1	5.80	1.50	1.34
28	P	304	CDL	OA8-CA7	5.77	1.50	1.33
28	P	304	CDL	OB8-CB7	5.75	1.50	1.33
20	G	103	PGV	O01-C1	5.71	1.50	1.34
19	A	608	TGL	OG1-CA1	5.68	1.49	1.33
28	C	306	CDL	OA8-CA7	5.63	1.49	1.33
20	A	610	PGV	O03-C19	5.62	1.49	1.33
27	T	101	PEK	O01-C1	5.58	1.50	1.34
28	N	601	CDL	OB8-CB7	5.52	1.49	1.33
28	C	306	CDL	OB8-CB7	5.52	1.49	1.33
27	T	101	PEK	O03-C21	5.41	1.49	1.33
27	C	308	PEK	O03-C21	5.40	1.49	1.33
20	Z	101	PGV	O03-C19	5.37	1.49	1.33
19	D	201	TGL	OG2-CB1	5.35	1.49	1.34
20	A	610	PGV	O01-C1	5.34	1.49	1.34
19	A	608	TGL	OG2-CB1	5.27	1.49	1.34
28	T	103	CDL	OB8-CB7	5.23	1.48	1.33
24	O	302	PSC	O01-C1	5.21	1.49	1.34
27	C	308	PEK	O01-C1	5.20	1.49	1.34
20	C	309	PGV	O03-C19	5.19	1.48	1.33
27	P	307	PEK	O01-C1	5.17	1.48	1.34
28	P	304	CDL	OA6-CA5	5.11	1.48	1.34
28	T	103	CDL	OA6-CA5	5.05	1.48	1.34
27	G	102	PEK	O01-C1	4.98	1.48	1.34
28	N	601	CDL	OA6-CA5	4.94	1.48	1.34
24	O	302	PSC	O03-C19	4.87	1.47	1.33
27	T	102	PEK	C2-C1	4.84	1.64	1.50
19	N	610	TGL	OG1-CA1	4.82	1.47	1.33
28	T	103	CDL	OA8-CA7	4.79	1.47	1.33
28	C	306	CDL	PB2-OB3	4.76	1.67	1.50
19	Q	201	TGL	OG1-CA1	4.75	1.47	1.33
20	G	103	PGV	O03-C19	4.75	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	P	307	PEK	O03-C21	4.74	1.47	1.33
25	C	311	DMU	O16-C6	4.72	1.48	1.40
27	G	102	PEK	O03-C21	4.68	1.47	1.33
20	Z	101	PGV	O01-C1	4.68	1.47	1.34
19	L	101	TGL	OG1-CA1	4.56	1.46	1.33
19	N	610	TGL	OG2-CB1	4.56	1.47	1.34
19	Y	101	TGL	OG1-CA1	4.54	1.46	1.33
14	A	601	HEA	C3A-C2A	-4.53	1.34	1.40
28	N	601	CDL	OA8-CA7	4.45	1.46	1.33
28	C	306	CDL	OA6-CA5	4.41	1.46	1.34
22	C	301	CHD	C11-C12	4.37	1.60	1.53
21	A	615	EDO	C2-C1	4.36	1.78	1.48
24	B	303	PSC	O03-C19	4.36	1.46	1.33
25	P	306	DMU	O16-C6	4.31	1.47	1.40
19	N	610	TGL	OG3-CC1	4.24	1.45	1.33
24	O	302	PSC	C13-C12	4.16	1.55	1.31
19	L	101	TGL	OG3-CG3	4.13	1.54	1.45
22	G	101	CHD	C4-C5	4.12	1.60	1.53
24	B	303	PSC	C13-C12	4.06	1.55	1.31
19	Q	201	TGL	OG3-CC1	4.04	1.45	1.33
22	B	301	CHD	C19-C10	4.04	1.61	1.54
19	L	101	TGL	CG3-CG2	4.03	1.63	1.50
28	P	304	CDL	PB2-OB3	4.02	1.65	1.50
20	C	305	PGV	O01-C02	-4.00	1.36	1.46
14	N	603[A]	HEA	O11-C11	3.92	1.51	1.42
28	C	306	CDL	OB6-CB5	3.80	1.45	1.34
14	A	601	HEA	CAD-C3D	3.79	1.57	1.52
22	B	301	CHD	C8-C7	3.77	1.59	1.53
28	P	304	CDL	OB6-CB5	3.75	1.44	1.34
24	B	303	PSC	C2-C1	3.70	1.61	1.50
19	D	201	TGL	OG3-CC1	3.66	1.44	1.33
19	A	608	TGL	OG3-CC1	3.63	1.43	1.33
19	A	608	TGL	OC1-CC1	-3.62	1.11	1.22
14	N	603[B]	HEA	C3B-C11	-3.43	1.50	1.52
22	B	301	CHD	C20-C17	3.42	1.60	1.54
20	A	610	PGV	O02-C1	3.38	1.32	1.22
25	C	310	DMU	O16-C6	3.35	1.45	1.40
22	B	301	CHD	C1-C2	3.33	1.60	1.53
25	P	309	DMU	O16-C6	3.33	1.45	1.40
28	C	306	CDL	PB2-OB2	3.33	1.72	1.59
28	C	306	CDL	C79-C78	-3.30	1.33	1.51
22	G	101	CHD	C1-C2	3.30	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	O11-C11	3.29	1.50	1.42
25	C	311	DMU	C10-C5	3.28	1.61	1.52
14	A	601	HEA	CMB-C2B	3.23	1.58	1.51
28	C	306	CDL	C59-C58	-3.22	1.33	1.51
27	C	304	PEK	P-O14	3.20	1.62	1.50
27	T	102	PEK	P-O14	3.14	1.62	1.50
19	L	101	TGL	OG2-CG2	3.12	1.54	1.46
28	N	601	CDL	C22-C21	-3.03	1.34	1.51
28	T	103	CDL	C59-C58	-3.03	1.34	1.51
28	C	306	CDL	C19-C18	-3.01	1.34	1.51
28	C	306	CDL	C82-C81	-3.00	1.34	1.51
20	N	609	PGV	O03-C19	2.98	1.42	1.33
14	N	602	HEA	CMC-C2C	2.98	1.57	1.51
20	A	609	PGV	O03-C19	2.97	1.42	1.33
20	N	609	PGV	O03-C01	2.97	1.51	1.45
28	T	103	CDL	C79-C78	-2.96	1.35	1.51
28	P	304	CDL	C42-C41	-2.96	1.35	1.51
22	P	301	CHD	C16-C15	2.95	1.62	1.54
22	B	301	CHD	C4-C3	2.95	1.57	1.51
22	P	305	CHD	C16-C17	2.95	1.60	1.54
28	C	306	CDL	C22-C21	-2.95	1.35	1.51
28	C	306	CDL	C62-C61	-2.95	1.35	1.51
28	P	304	CDL	PA1-OA5	2.93	1.71	1.59
27	C	304	PEK	O01-C1	2.93	1.42	1.34
22	G	101	CHD	C20-C17	2.93	1.59	1.54
14	A	601	HEA	C12-C13	2.90	1.62	1.53
28	P	304	CDL	C79-C78	-2.89	1.35	1.51
22	B	301	CHD	O7-C7	2.88	1.49	1.43
20	N	609	PGV	C01-C02	2.87	1.59	1.50
28	P	304	CDL	C22-C21	-2.86	1.35	1.51
28	N	601	CDL	C19-C18	-2.86	1.35	1.51
22	B	301	CHD	C10-C5	2.85	1.60	1.55
28	N	601	CDL	C62-C61	-2.85	1.35	1.51
28	P	304	CDL	C19-C18	-2.84	1.35	1.51
28	P	304	CDL	C82-C81	-2.84	1.35	1.51
27	C	304	PEK	O03-C21	2.83	1.41	1.33
28	T	103	CDL	C19-C18	-2.81	1.35	1.51
28	N	601	CDL	C59-C58	-2.80	1.35	1.51
28	N	601	CDL	C79-C78	-2.80	1.35	1.51
28	P	304	CDL	C62-C61	-2.78	1.35	1.51
28	N	601	CDL	C82-C81	-2.78	1.36	1.51
22	P	301	CHD	C11-C12	2.77	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	N	601	CDL	C42-C41	-2.75	1.36	1.51
28	T	103	CDL	C22-C21	-2.75	1.36	1.51
20	C	309	PGV	C01-C02	2.75	1.59	1.50
22	B	301	CHD	C13-C17	-2.74	1.50	1.55
22	G	101	CHD	C8-C7	2.71	1.58	1.53
27	C	304	PEK	O01-C02	2.71	1.53	1.46
28	T	103	CDL	C39-C38	-2.70	1.36	1.51
22	P	301	CHD	C8-C14	2.70	1.59	1.53
14	A	601	HEA	C3B-C2B	-2.70	1.32	1.41
28	T	103	CDL	C82-C81	-2.70	1.36	1.51
28	C	306	CDL	CB2-C1	2.69	1.60	1.51
22	B	301	CHD	C2-C3	2.67	1.58	1.51
25	C	311	DMU	O3-C5	2.66	1.49	1.43
14	A	602[B]	HEA	C4D-ND	-2.66	1.30	1.36
28	T	103	CDL	C62-C61	-2.63	1.36	1.51
28	P	304	CDL	C59-C58	-2.63	1.36	1.51
14	A	601	HEA	C3C-C2C	-2.63	1.36	1.40
19	A	608	TGL	OG2-CG2	2.62	1.53	1.46
28	C	306	CDL	C42-C41	-2.61	1.36	1.51
28	P	304	CDL	CB2-C1	2.61	1.60	1.51
22	G	101	CHD	O7-C7	2.60	1.48	1.43
22	P	305	CHD	C8-C9	2.60	1.58	1.53
28	T	103	CDL	C42-C41	-2.59	1.37	1.51
28	C	306	CDL	C39-C38	-2.59	1.37	1.51
28	N	601	CDL	CB3-CB4	2.58	1.58	1.50
28	N	601	CDL	C39-C38	-2.57	1.37	1.51
22	G	101	CHD	C11-C9	2.57	1.58	1.53
22	B	301	CHD	C11-C9	2.56	1.58	1.53
14	A	602[B]	HEA	C3A-CMA	2.55	1.52	1.46
22	C	301	CHD	C11-C9	2.55	1.58	1.53
28	P	304	CDL	C39-C38	-2.54	1.37	1.51
22	P	301	CHD	C11-C9	2.52	1.57	1.53
28	T	103	CDL	CB3-CB4	2.52	1.58	1.50
22	P	301	CHD	C10-C9	2.50	1.60	1.56
14	A	602[B]	HEA	C3A-C2A	-2.48	1.36	1.40
22	C	307	CHD	C16-C17	2.48	1.59	1.54
28	P	304	CDL	PB2-OB2	2.48	1.69	1.59
14	A	602[A]	HEA	O11-C11	2.46	1.48	1.42
28	P	304	CDL	O1-C1	2.44	1.50	1.43
20	A	609	PGV	C01-C02	2.43	1.58	1.50
20	P	303	PGV	O03-C19	2.41	1.40	1.33
25	Z	102	DMU	O16-C6	2.38	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	102	PEK	C3-C2	2.35	1.60	1.52
22	P	301	CHD	C8-C7	2.34	1.57	1.53
19	L	101	TGL	OC1-CC1	2.34	1.29	1.22
22	P	305	CHD	C20-C17	2.33	1.58	1.54
28	T	103	CDL	CB6-CB4	2.31	1.57	1.50
21	B	305	EDO	O1-C1	2.30	1.54	1.42
21	A	613	EDO	O2-C2	2.28	1.53	1.42
14	N	603[A]	HEA	C3C-C2C	-2.26	1.37	1.40
28	N	601	CDL	PB2-OB5	2.26	1.68	1.59
22	C	307	CHD	C4-C3	2.24	1.56	1.51
22	C	301	CHD	C13-C12	-2.24	1.51	1.54
22	C	301	CHD	C8-C7	2.22	1.57	1.53
14	N	602	HEA	CMD-C2D	2.22	1.56	1.51
20	A	609	PGV	O01-C1	2.21	1.40	1.34
20	A	610	PGV	P-O13	2.21	1.58	1.50
22	G	101	CHD	C2-C3	2.21	1.56	1.51
28	C	306	CDL	OB2-CB2	2.21	1.53	1.44
27	T	102	PEK	C3-C4	2.20	1.61	1.52
22	P	305	CHD	C11-C9	2.18	1.57	1.53
21	N	615	EDO	O2-C2	2.17	1.53	1.42
19	N	610	TGL	OC1-CC1	-2.17	1.16	1.22
28	P	304	CDL	CA3-CA4	2.17	1.57	1.50
14	A	601	HEA	C16-C17	-2.14	1.46	1.53
20	N	609	PGV	O01-C1	2.13	1.40	1.34
19	Y	101	TGL	CG3-CG2	2.13	1.57	1.50
19	Y	101	TGL	CB2-CB1	2.12	1.56	1.50
28	C	306	CDL	OB6-CB4	-2.12	1.41	1.46
25	L	102	DMU	O16-C6	2.09	1.43	1.40
20	A	609	PGV	O03-C01	2.09	1.49	1.45
20	A	609	PGV	C3-C2	2.08	1.59	1.52
27	T	102	PEK	C05-C04	2.07	1.58	1.50
22	C	307	CHD	C20-C17	2.07	1.58	1.54
22	P	301	CHD	C16-C17	2.07	1.58	1.54
22	C	301	CHD	C2-C3	2.07	1.56	1.51
20	N	609	PGV	O06-C06	2.07	1.51	1.42
14	N	603[A]	HEA	C1C-CHC	2.07	1.46	1.41
27	C	308	PEK	C01-C02	2.06	1.57	1.50
27	T	102	PEK	O01-C1	2.05	1.40	1.34
19	D	201	TGL	OC1-CC1	2.05	1.28	1.22
14	A	602[A]	HEA	C20-C19	2.04	1.55	1.51
27	C	304	PEK	P-O13	-2.03	1.45	1.55
19	L	101	TGL	CB2-CB1	2.01	1.56	1.50

All (580) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	305	CHD	C23-C22-C20	-17.48	91.17	114.72
22	C	307	CHD	C23-C22-C20	-15.64	93.65	114.72
27	T	102	PEK	C2-C3-C4	14.82	139.64	113.23
19	D	201	TGL	OG2-CB1-CB2	-10.77	88.29	111.50
22	J	101	CHD	C14-C8-C9	-10.23	95.67	109.71
19	A	608	TGL	OG2-CB1-CB2	9.81	132.64	111.50
22	W	101	CHD	C17-C13-C12	9.42	126.27	117.67
22	C	301	CHD	C23-C22-C20	-9.03	102.56	114.72
19	N	610	TGL	OG2-CB1-CB2	8.76	130.37	111.50
28	T	103	CDL	OB6-CB5-C51	8.68	130.21	111.50
22	W	101	CHD	C11-C12-C13	8.51	119.98	111.24
19	L	101	TGL	OG2-CB1-CB2	8.36	129.52	111.50
19	Q	201	TGL	OG2-CB1-CB2	-8.17	93.89	111.50
22	W	101	CHD	C18-C13-C12	-8.00	100.92	109.07
19	D	201	TGL	OG2-CB1-OB1	7.97	142.97	123.70
25	C	311	DMU	O16-C6-C1	7.86	120.58	108.30
14	N	603[A]	HEA	C13-C12-C11	-7.79	102.65	114.35
19	Y	101	TGL	OG2-CB1-CB2	7.63	127.94	111.50
19	L	101	TGL	CG2-OG2-CB1	7.54	136.35	117.79
14	N	603[A]	HEA	OMA-CMA-C3A	-7.53	108.50	124.91
19	A	608	TGL	OG3-CC1-OC1	-7.48	104.71	123.59
25	C	311	DMU	O7-C10-C5	7.48	127.48	108.10
28	N	601	CDL	OB6-CB5-C51	7.30	127.23	111.50
27	T	102	PEK	O01-C1-O02	-7.16	106.40	123.70
27	G	102	PEK	O01-C1-C2	7.15	126.91	111.50
14	N	603[A]	HEA	CAD-CBD-CGD	-7.14	100.69	112.67
20	G	103	PGV	O01-C1-C2	6.92	126.41	111.50
19	L	101	TGL	OG3-CG3-CG2	6.90	128.53	108.43
22	C	307	CHD	C22-C23-C24	-6.83	98.92	113.59
22	W	101	CHD	C13-C17-C20	6.80	127.61	119.50
22	P	305	CHD	C16-C17-C20	6.74	122.58	112.15
21	A	615	EDO	O2-C2-C1	-6.74	63.40	111.91
22	J	101	CHD	C15-C14-C8	6.64	127.61	118.33
14	N	602	HEA	C1B-C2B-C3B	-6.63	102.39	107.00
27	C	308	PEK	O01-C1-C2	6.62	125.77	111.50
25	C	310	DMU	O16-C6-C1	6.47	118.40	108.30
22	W	101	CHD	C14-C13-C12	6.46	113.42	107.40
14	N	602	HEA	C13-C14-C15	-6.38	112.30	127.66
22	C	307	CHD	C21-C20-C17	6.36	122.65	112.92
14	A	602[B]	HEA	CAA-CBA-CGA	-6.20	102.27	112.67
27	T	101	PEK	O01-C1-C2	6.14	124.74	111.50
24	O	302	PSC	O01-C1-C2	6.06	124.57	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	103	PGV	O03-C19-C20	6.05	130.89	111.91
22	J	101	CHD	C18-C13-C12	-6.01	102.95	109.07
14	A	601	HEA	CAD-CBD-CGD	-5.95	102.69	112.67
22	P	301	CHD	C23-C22-C20	-5.94	106.72	114.72
19	D	201	TGL	CB3-CB2-CB1	5.81	134.75	113.62
25	P	308	DMU	O16-C6-C1	5.80	117.35	108.30
28	C	306	CDL	OA6-CA5-C11	5.75	123.90	111.50
27	P	307	PEK	O01-C1-C2	5.71	123.82	111.50
25	P	308	DMU	O7-C10-C5	5.71	122.89	108.10
14	A	601	HEA	C13-C12-C11	-5.68	105.82	114.35
14	A	602[B]	HEA	CBA-CAA-C2A	-5.63	102.11	112.48
14	N	603[B]	HEA	CAA-CBA-CGA	-5.62	103.24	112.67
14	A	601	HEA	C13-C14-C15	-5.58	114.23	127.66
25	C	310	DMU	C10-O1-C9	-5.54	102.82	113.69
22	J	101	CHD	C11-C12-C13	5.53	116.92	111.24
19	A	608	TGL	OG2-CG2-CG3	5.52	128.40	108.40
22	P	305	CHD	C14-C13-C12	5.48	112.50	107.40
25	P	308	DMU	C18-O16-C6	-5.46	104.78	113.84
24	B	303	PSC	O01-C1-C2	5.45	123.25	111.50
14	A	602[A]	HEA	OMA-CMA-C3A	-5.38	113.19	124.91
22	W	101	CHD	C14-C8-C7	5.38	118.94	111.81
19	Y	101	TGL	CG2-OG2-CB1	5.35	130.97	117.79
14	A	602[B]	HEA	C27-C19-C20	5.35	124.28	115.27
22	P	305	CHD	C6-C7-C8	5.35	117.19	111.48
22	C	307	CHD	C6-C7-C8	5.33	117.17	111.48
19	A	608	TGL	OG3-CC1-CC2	5.17	128.15	111.91
22	C	301	CHD	C22-C20-C17	-5.17	99.60	110.28
22	C	307	CHD	C16-C17-C20	5.16	120.13	112.15
28	P	304	CDL	OA6-CA5-C11	5.12	122.54	111.50
25	C	310	DMU	O7-C10-C5	5.10	121.31	108.10
28	T	103	CDL	OA6-CA5-C11	5.09	122.48	111.50
20	Z	101	PGV	O01-C1-C2	5.09	122.48	111.50
24	B	303	PSC	O01-C1-O02	-5.08	111.44	123.70
22	W	101	CHD	C17-C13-C14	-5.05	95.00	100.09
25	C	311	DMU	O3-C5-C10	5.05	122.31	110.05
20	C	309	PGV	O03-C19-C20	5.05	127.74	111.91
22	P	305	CHD	C13-C17-C20	-5.03	113.49	119.50
22	C	307	CHD	C15-C14-C13	5.02	108.48	103.55
22	B	301	CHD	C16-C17-C20	-4.99	104.42	112.15
25	P	306	DMU	O16-C6-C1	4.92	115.99	108.30
22	J	101	CHD	C11-C9-C10	4.91	118.80	113.73
22	P	301	CHD	C22-C20-C17	-4.90	100.17	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	610	TGL	OG3-CC1-CC2	4.85	127.14	111.91
14	A	602[A]	HEA	C27-C19-C20	4.85	123.42	115.27
22	J	101	CHD	C15-C14-C13	4.82	108.28	103.55
22	P	305	CHD	C15-C14-C8	4.82	125.06	118.33
20	A	610	PGV	C02-O01-C1	4.81	129.63	117.79
22	J	101	CHD	C14-C8-C7	4.79	118.16	111.81
28	C	306	CDL	OA2-PA1-OA3	4.77	127.70	109.07
20	A	610	PGV	C3-C2-C1	4.66	130.57	113.62
25	C	302	DMU	C10-C5-C7	-4.65	100.31	110.00
14	N	603[A]	HEA	C1B-C2B-C3B	-4.64	103.77	107.00
22	J	101	CHD	C17-C13-C14	-4.60	95.45	100.09
22	G	101	CHD	C11-C12-C13	4.59	115.95	111.24
14	A	602[A]	HEA	C13-C12-C11	-4.57	107.48	114.35
28	P	304	CDL	OB8-CB7-C71	4.56	126.22	111.91
25	P	309	DMU	O16-C6-C1	4.56	115.42	108.30
28	N	601	CDL	CB4-OB6-CB5	4.55	129.00	117.79
25	P	308	DMU	C10-O1-C9	-4.50	104.86	113.69
14	A	602[B]	HEA	C13-C12-C11	-4.49	107.60	114.35
22	P	301	CHD	C21-C20-C22	-4.48	103.34	110.36
25	C	310	DMU	C10-C5-C7	-4.47	100.69	110.00
19	Q	201	TGL	CG2-OG2-CB1	-4.46	106.80	117.79
22	C	301	CHD	C5-C4-C3	-4.46	106.20	112.76
22	C	301	CHD	C1-C2-C3	-4.45	104.76	110.47
22	C	301	CHD	C22-C23-C24	-4.44	104.05	113.59
19	Q	201	TGL	OG2-CB1-OB1	4.40	134.33	123.70
19	D	201	TGL	OG1-CA1-CA2	4.39	125.69	111.91
19	A	608	TGL	CG3-OG3-CC1	4.39	133.37	117.12
20	C	309	PGV	C02-O01-C1	4.37	128.54	117.79
25	L	102	DMU	O5-C4-C3	4.36	118.95	109.75
22	C	307	CHD	C5-C6-C7	4.36	119.28	114.46
22	W	101	CHD	C6-C5-C4	-4.35	106.18	111.19
14	N	603[A]	HEA	CAA-CBA-CGA	-4.34	105.39	112.67
22	J	101	CHD	C16-C17-C13	4.34	107.81	103.55
22	C	307	CHD	C15-C14-C8	4.33	124.39	118.33
19	L	101	TGL	OC1-CC1-CC2	-4.33	106.84	123.73
19	Y	101	TGL	OG3-CG3-CG2	4.31	120.98	108.43
22	G	101	CHD	C23-C22-C20	-4.30	108.94	114.72
22	P	305	CHD	C19-C10-C9	-4.29	105.27	111.18
22	W	101	CHD	C9-C11-C12	4.29	119.97	114.30
14	N	602	HEA	C25-C23-C24	-4.29	105.13	114.60
27	G	102	PEK	O03-C21-C22	4.29	125.36	111.91
25	M	101	DMU	C18-O16-C6	-4.24	106.80	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603[A]	HEA	C26-C15-C16	4.24	122.41	115.27
25	P	308	DMU	O49-C1-C2	-4.24	100.55	110.35
14	N	602	HEA	C12-C13-C14	4.22	123.38	112.23
27	C	304	PEK	C24-C23-C22	-4.21	98.04	113.19
28	N	601	CDL	CB6-OB8-CB7	4.20	132.68	117.12
27	T	102	PEK	O03-C21-C22	4.20	125.08	111.91
20	A	610	PGV	O01-C1-O02	4.19	133.82	123.70
27	T	102	PEK	O02-C1-C2	4.18	140.05	123.73
22	C	307	CHD	C17-C13-C12	-4.17	113.86	117.67
22	J	101	CHD	C17-C13-C12	4.15	121.46	117.67
22	J	101	CHD	C21-C20-C22	4.13	116.83	110.36
19	N	610	TGL	OG1-CA1-CA2	4.12	124.85	111.91
14	N	602	HEA	CAA-CBA-CGA	-4.12	105.77	112.67
14	A	602[B]	HEA	CMD-C2D-C3D	4.09	132.66	124.94
22	J	101	CHD	C16-C15-C14	-4.09	97.02	105.13
22	P	301	CHD	C9-C11-C12	-4.08	108.91	114.30
14	A	601	HEA	CBD-CAD-C3D	-4.07	104.99	112.49
14	A	602[A]	HEA	CAD-CBD-CGD	-4.05	105.88	112.67
19	Y	101	TGL	OG3-CC1-CC2	4.03	124.56	111.91
22	C	307	CHD	C4-C5-C10	4.02	116.92	112.66
22	C	307	CHD	C14-C13-C12	4.01	111.14	107.40
22	J	101	CHD	C14-C13-C12	4.01	111.14	107.40
19	Y	101	TGL	OG2-CB1-OB1	-3.98	114.09	123.70
19	L	101	TGL	CG3-OG3-CC1	3.97	131.84	117.12
20	N	609	PGV	O03-C19-O04	-3.96	113.59	123.59
25	L	102	DMU	O3-C5-C10	3.92	119.58	110.05
22	B	301	CHD	C19-C10-C1	-3.92	101.95	108.26
25	Z	102	DMU	C6-O5-C4	3.92	121.37	113.69
27	C	308	PEK	O03-C21-C22	3.91	124.19	111.91
22	B	301	CHD	C23-C22-C20	-3.91	109.46	114.72
14	N	602	HEA	C27-C19-C20	3.90	121.83	115.27
19	D	201	TGL	CG1-OG1-CA1	3.88	131.48	117.12
20	A	610	PGV	C4-C3-C2	-3.87	99.26	113.19
14	A	601	HEA	C3C-C4C-NC	3.87	114.22	109.21
22	P	305	CHD	C17-C13-C12	-3.86	114.14	117.67
20	C	309	PGV	C01-O03-C19	3.85	131.39	117.12
24	B	303	PSC	O03-C19-C20	3.85	123.98	111.91
25	C	302	DMU	O2-C8-C7	-3.83	101.49	110.35
14	A	602[B]	HEA	C26-C15-C16	3.82	121.70	115.27
14	N	603[B]	HEA	OMA-CMA-C3A	-3.81	116.60	124.91
28	C	306	CDL	PA1-OA2-CA2	3.81	143.99	121.68
28	T	103	CDL	OB6-CB4-CB3	3.79	122.12	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	101	CHD	C22-C20-C17	3.78	118.09	110.28
27	G	102	PEK	O01-C1-O02	-3.78	114.57	123.70
22	B	301	CHD	C22-C23-C24	-3.78	105.47	113.59
19	L	101	TGL	OG2-CG2-CG3	3.76	122.02	108.40
22	C	301	CHD	C16-C17-C13	-3.75	99.87	103.55
14	N	602	HEA	CMB-C2B-C3B	3.75	132.03	124.69
19	A	608	TGL	OG2-CB1-OB1	-3.74	114.67	123.70
14	N	603[B]	HEA	C13-C12-C11	-3.73	108.74	114.35
19	N	610	TGL	OG3-CC1-OC1	-3.73	114.17	123.59
20	A	610	PGV	O03-C19-C20	3.72	123.60	111.91
22	P	301	CHD	C10-C9-C8	-3.72	107.82	111.82
22	C	307	CHD	C13-C17-C20	-3.71	115.06	119.50
14	A	601	HEA	C17-C18-C19	-3.71	118.73	127.66
22	P	305	CHD	C11-C9-C8	3.71	116.30	110.88
22	J	101	CHD	C10-C9-C8	3.70	115.79	111.82
14	N	603[A]	HEA	CBA-CAA-C2A	-3.69	105.67	112.48
20	G	103	PGV	O04-C19-C20	-3.67	109.40	123.73
19	Q	201	TGL	OG1-CA1-CA2	3.65	123.36	111.91
22	P	305	CHD	O7-C7-C6	-3.65	100.89	109.94
28	N	601	CDL	OA6-CA5-C11	3.64	119.35	111.50
14	A	601	HEA	C1B-C2B-C3B	-3.63	104.47	107.00
19	L	101	TGL	OB1-CB1-CB2	-3.62	109.59	123.73
20	N	609	PGV	O03-C19-C20	3.61	123.25	111.91
19	A	608	TGL	CG3-CG2-CG1	-3.60	103.27	111.79
14	A	602[A]	HEA	C12-C13-C14	-3.59	102.77	112.23
19	L	101	TGL	OG3-CC1-OC1	3.56	132.59	123.59
28	P	304	CDL	PA1-OA2-CA2	3.56	142.57	121.68
28	T	103	CDL	OA8-CA7-C31	3.56	123.07	111.91
28	N	601	CDL	OA8-CA7-C31	3.56	123.07	111.91
19	Y	101	TGL	CA4-CA3-CA2	-3.55	100.42	113.19
22	P	305	CHD	C21-C20-C17	3.55	118.35	112.92
20	C	305	PGV	C30-C29-C28	-3.54	96.45	114.42
19	D	201	TGL	CC3-CC2-CC1	-3.54	100.75	113.62
22	C	301	CHD	C11-C9-C10	-3.53	110.08	113.73
20	C	305	PGV	O03-C19-O04	-3.52	114.70	123.59
22	G	101	CHD	C1-C2-C3	-3.52	105.95	110.47
22	J	101	CHD	C6-C5-C10	3.52	116.39	112.66
28	P	304	CDL	OA8-CA7-C31	3.51	122.92	111.91
14	N	602	HEA	C4B-C3B-C2B	3.50	109.31	106.87
19	N	610	TGL	OG2-CB1-OB1	-3.49	115.27	123.70
25	C	310	DMU	C7-C8-C9	3.49	116.46	110.24
25	L	102	DMU	O16-C6-C1	-3.49	102.86	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	309	PGV	O01-C1-C2	3.48	119.01	111.50
25	C	311	DMU	C18-O16-C6	3.48	119.60	113.84
14	N	602	HEA	CBD-CAD-C3D	-3.47	106.08	112.49
27	P	307	PEK	O03-C21-O04	-3.47	114.84	123.59
22	J	101	CHD	C5-C4-C3	3.45	117.83	112.76
14	A	602[B]	HEA	CMC-C2C-C1C	-3.45	123.16	128.46
28	C	306	CDL	PB2-OB2-CB2	3.44	141.85	121.68
20	P	303	PGV	O01-C1-O02	-3.43	115.41	123.70
19	D	201	TGL	CG3-OG3-CC1	3.42	129.78	117.12
22	P	301	CHD	C1-C10-C5	3.41	112.81	107.77
19	Q	201	TGL	OG3-CC1-OC1	-3.40	115.00	123.59
14	N	602	HEA	CAD-CBD-CGD	-3.38	106.99	112.67
22	P	305	CHD	C5-C4-C3	-3.37	107.81	112.76
14	A	601	HEA	C4B-C3B-C2B	3.37	109.22	106.87
28	P	304	CDL	OA8-CA6-CA4	3.36	118.23	108.43
27	C	308	PEK	O03-C21-O04	-3.36	115.12	123.59
28	C	306	CDL	O1-C1-CA2	-3.35	97.79	109.56
22	C	301	CHD	O3-C3-C2	-3.35	101.64	110.16
27	T	101	PEK	O03-C21-C22	3.35	122.41	111.91
22	C	301	CHD	C5-C6-C7	3.34	118.15	114.46
22	W	101	CHD	C4-C5-C10	3.34	116.20	112.66
27	C	308	PEK	O01-C1-O02	-3.34	115.64	123.70
25	M	101	DMU	C22-C19-C18	-3.33	98.72	113.49
14	A	601	HEA	OMA-CMA-C3A	-3.33	117.66	124.91
14	A	602[A]	HEA	CMC-C2C-C3C	3.33	130.90	124.68
22	W	101	CHD	C1-C10-C5	3.32	112.68	107.77
22	P	301	CHD	C9-C8-C7	3.32	115.84	111.88
22	W	101	CHD	C11-C9-C10	3.30	117.13	113.73
14	N	602	HEA	OMA-CMA-C3A	-3.30	117.72	124.91
22	P	305	CHD	C15-C14-C13	3.30	106.79	103.55
19	L	101	TGL	OG1-CA1-CA2	3.29	122.25	111.91
28	P	304	CDL	C54-C53-C52	-3.29	97.74	114.42
25	P	308	DMU	O3-C5-C10	3.28	118.02	110.05
22	B	301	CHD	C18-C13-C12	-3.27	105.73	109.07
25	C	311	DMU	O16-C18-C19	3.27	121.02	109.56
20	Z	101	PGV	O01-C1-O02	-3.27	115.81	123.70
28	P	304	CDL	OA2-PA1-OA3	3.26	121.80	109.07
20	P	303	PGV	C22-C21-C20	-3.26	101.49	113.19
20	N	609	PGV	O01-C1-O02	-3.25	115.85	123.70
14	A	602[B]	HEA	C20-C19-C18	-3.24	114.56	121.12
28	T	103	CDL	OB6-CB5-OB7	-3.24	115.87	123.70
20	Z	101	PGV	O03-C19-C20	3.24	122.07	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C9-C8-C7	3.24	115.75	111.88
19	L	101	TGL	C26-C25-C24	-3.24	98.00	114.42
14	N	602	HEA	C3C-C4C-NC	3.23	113.38	109.21
20	C	309	PGV	O04-C19-C20	-3.22	111.17	123.73
25	C	302	DMU	C7-C8-C9	3.22	115.98	110.24
14	N	603[B]	HEA	O11-C11-C3B	-3.22	102.72	112.00
25	L	102	DMU	O7-C10-C5	3.22	116.43	108.10
20	A	610	PGV	C03-C02-C01	-3.21	104.18	111.79
22	G	101	CHD	C16-C17-C20	-3.21	107.18	112.15
27	T	102	PEK	O03-C21-O04	-3.21	115.50	123.59
14	N	602	HEA	C20-C21-C22	-3.17	101.47	111.88
25	L	102	DMU	C57-C4-C3	-3.16	104.12	113.33
22	W	101	CHD	C19-C10-C1	-3.16	103.16	108.26
20	A	609	PGV	O03-C19-C20	3.16	121.83	111.91
22	B	301	CHD	C1-C10-C9	3.16	116.31	111.35
20	G	103	PGV	C03-C02-C01	-3.15	104.33	111.79
22	C	301	CHD	C6-C7-C8	-3.14	108.12	111.48
28	N	601	CDL	OA8-CA7-OA9	-3.14	115.68	123.59
28	C	306	CDL	CA6-OA8-CA7	3.12	128.69	117.12
14	N	602	HEA	C16-C15-C14	3.11	127.41	121.12
22	C	301	CHD	C21-C20-C17	-3.10	108.17	112.92
22	W	101	CHD	C15-C14-C8	3.04	122.58	118.33
22	C	301	CHD	C2-C1-C10	3.03	117.98	112.78
25	P	306	DMU	O16-C18-C19	3.03	120.18	109.56
20	Z	101	PGV	C01-O03-C19	3.02	128.32	117.12
14	A	602[B]	HEA	C17-C18-C19	-3.02	120.39	127.66
28	C	306	CDL	OB8-CB7-C71	3.02	121.38	111.91
14	N	603[B]	HEA	CBA-CAA-C2A	-3.01	106.94	112.48
22	C	307	CHD	C14-C8-C9	-3.01	105.58	109.71
20	A	609	PGV	O01-C02-C01	-2.99	97.59	108.40
24	B	303	PSC	O03-C19-O04	-2.98	116.06	123.59
28	T	103	CDL	OB8-CB7-C71	2.96	121.21	111.91
22	C	307	CHD	C1-C10-C5	2.96	112.15	107.77
28	C	306	CDL	CB4-OB6-CB5	-2.96	110.50	117.79
27	C	308	PEK	C01-O03-C21	2.96	128.07	117.12
22	J	101	CHD	C1-C2-C3	2.95	114.26	110.47
21	H	101	EDO	O1-C1-C2	-2.95	90.72	111.91
20	Z	101	PGV	C4-C3-C2	2.94	123.78	113.19
22	P	305	CHD	C6-C5-C4	-2.94	107.80	111.19
22	J	101	CHD	C18-C13-C14	2.94	115.82	111.21
28	C	306	CDL	C73-C72-C71	-2.94	102.62	113.19
19	A	608	TGL	OB1-CB1-CB2	-2.94	112.28	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	305	CHD	C6-C5-C10	2.93	115.77	112.66
27	T	101	PEK	O01-C1-O02	-2.93	116.62	123.70
22	C	307	CHD	O7-C7-C6	-2.92	102.69	109.94
22	G	101	CHD	C5-C4-C3	-2.92	108.47	112.76
28	T	103	CDL	C83-C82-C81	2.92	129.24	114.42
19	Q	201	TGL	OG3-CC1-CC2	2.92	121.06	111.91
28	C	306	CDL	CB2-C1-CA2	2.91	121.36	112.79
28	P	304	CDL	OB8-CB7-OB9	-2.90	116.28	123.59
22	P	301	CHD	C14-C13-C12	2.89	110.09	107.40
25	L	102	DMU	O5-C6-O16	2.88	116.81	109.97
14	A	601	HEA	CMC-C2C-C3C	2.88	130.07	124.68
20	A	610	PGV	C01-O03-C19	2.88	127.78	117.12
25	C	311	DMU	O5-C6-O16	2.87	116.77	109.97
22	B	301	CHD	C22-C20-C17	2.87	116.21	110.28
19	L	101	TGL	CB6-CB5-CB4	-2.86	99.91	114.42
22	B	301	CHD	O12-C12-C13	-2.86	106.20	111.03
14	N	603[A]	HEA	C12-C13-C14	-2.85	104.69	112.23
25	C	310	DMU	O55-C2-C1	2.85	116.94	110.35
22	W	101	CHD	C6-C7-C8	2.85	114.53	111.48
27	G	102	PEK	O03-C21-O04	-2.84	116.41	123.59
22	G	101	CHD	C11-C9-C8	2.84	115.04	110.88
25	C	311	DMU	O3-C5-C7	2.83	116.89	110.35
22	P	301	CHD	C19-C10-C1	-2.82	103.72	108.26
27	G	102	PEK	O03-C01-C02	2.82	116.64	108.43
19	Q	201	TGL	OG1-CA1-OA1	-2.82	116.48	123.59
25	P	308	DMU	O7-C3-C4	-2.81	101.75	109.45
22	W	101	CHD	C19-C10-C5	-2.80	105.61	110.36
14	A	601	HEA	CMB-C2B-C3B	2.80	130.17	124.69
25	P	308	DMU	C10-C5-C7	-2.79	104.19	110.00
20	A	609	PGV	O03-C19-O04	-2.79	116.56	123.59
28	C	306	CDL	C39-C38-C37	2.78	128.56	114.42
28	N	601	CDL	C80-C79-C78	2.77	128.51	114.42
27	T	102	PEK	C24-C23-C22	-2.77	103.23	113.19
28	T	103	CDL	CB6-OB8-CB7	2.77	127.37	117.12
28	P	304	CDL	OA6-CA5-OA7	-2.77	117.01	123.70
25	C	302	DMU	C10-O1-C9	2.76	119.11	113.69
22	B	301	CHD	C11-C9-C10	-2.76	110.88	113.73
22	P	305	CHD	C1-C10-C9	2.76	115.70	111.35
28	T	103	CDL	C23-C22-C21	2.76	128.44	114.42
22	C	301	CHD	C9-C11-C12	-2.75	110.66	114.30
19	L	101	TGL	C25-C24-C23	-2.74	100.50	114.42
20	C	305	PGV	C21-C20-C19	-2.74	103.65	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	307	CHD	C11-C9-C10	-2.74	110.91	113.73
25	C	302	DMU	C18-O16-C6	-2.73	109.31	113.84
25	P	308	DMU	O4-C7-C8	2.73	116.66	110.35
25	P	308	DMU	O5-C6-O16	-2.73	103.51	109.97
22	W	101	CHD	C2-C1-C10	2.73	117.45	112.78
25	C	310	DMU	O5-C4-C57	2.72	113.21	106.44
14	N	603[A]	HEA	C17-C18-C19	2.72	134.22	127.66
28	P	304	CDL	CB4-OB6-CB5	-2.72	111.09	117.79
14	A	601	HEA	CMC-C2C-C1C	-2.72	124.28	128.46
14	A	602[B]	HEA	CMC-C2C-C3C	2.72	129.77	124.68
14	N	603[A]	HEA	CMC-C2C-C3C	2.72	129.77	124.68
22	J	101	CHD	C23-C22-C20	2.71	118.38	114.72
28	N	601	CDL	OB7-CB5-C51	-2.71	113.15	123.73
28	C	306	CDL	OA4-PA1-OA2	-2.71	95.17	107.75
28	P	304	CDL	OB2-PB2-OB3	2.69	119.60	109.07
24	O	302	PSC	O01-C1-O02	-2.69	117.20	123.70
22	B	301	CHD	C2-C1-C10	-2.69	108.17	112.78
19	L	101	TGL	OG3-CC1-CC2	2.69	120.33	111.91
22	J	101	CHD	C9-C10-C5	2.68	112.35	108.58
22	C	301	CHD	C21-C20-C22	-2.68	106.16	110.36
28	T	103	CDL	OB8-CB6-CB4	2.68	116.23	108.43
20	N	609	PGV	O12-P-O13	2.67	119.49	109.07
28	C	306	CDL	OA8-CA7-C31	2.67	120.28	111.91
22	G	101	CHD	C19-C10-C1	-2.66	103.97	108.26
19	D	201	TGL	OG1-CA1-OA1	-2.66	116.88	123.59
25	Z	102	DMU	O49-C1-C2	-2.65	104.21	110.35
27	T	101	PEK	C01-O03-C21	2.65	126.95	117.12
22	P	305	CHD	O3-C3-C4	-2.65	104.57	109.85
14	A	602[B]	HEA	CAD-C3D-C2D	2.64	134.84	127.25
27	C	304	PEK	C2-C3-C4	-2.64	108.52	113.23
20	P	303	PGV	C27-C26-C25	-2.64	101.04	114.42
25	C	302	DMU	C57-C4-C3	2.63	120.99	113.33
22	P	305	CHD	C16-C17-C13	2.63	106.14	103.55
27	T	101	PEK	C02-O01-C1	2.63	124.27	117.79
22	C	301	CHD	C16-C17-C20	-2.63	108.08	112.15
22	G	101	CHD	C21-C20-C17	-2.62	108.91	112.92
19	N	610	TGL	CG3-OG3-CC1	2.62	126.83	117.12
28	T	103	CDL	C80-C79-C78	2.62	127.72	114.42
14	A	601	HEA	C20-C21-C22	-2.61	103.29	111.88
22	P	305	CHD	C19-C10-C1	-2.61	104.05	108.26
14	N	603[B]	HEA	C27-C19-C20	2.61	119.66	115.27
22	C	301	CHD	C15-C14-C8	-2.61	114.69	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	306	CDL	C13-C12-C11	-2.59	103.87	113.19
28	N	601	CDL	C62-C61-C60	2.58	127.51	114.42
19	N	610	TGL	OG1-CA1-OA1	-2.57	117.10	123.59
28	C	306	CDL	C42-C41-C40	2.57	127.47	114.42
14	N	603[A]	HEA	C20-C21-C22	-2.56	103.47	111.88
27	C	308	PEK	P-O12-C04	-2.56	109.00	121.59
25	C	302	DMU	O55-C2-C3	2.55	116.71	109.94
22	P	305	CHD	C22-C23-C24	-2.55	108.11	113.59
14	A	602[B]	HEA	O11-C11-C3B	-2.54	104.67	112.00
14	A	602[A]	HEA	C26-C15-C16	2.54	119.54	115.27
28	T	103	CDL	OB7-CB5-C51	-2.53	113.88	123.73
19	Y	101	TGL	C26-C25-C24	-2.52	101.65	114.42
14	A	602[B]	HEA	C4B-C3B-C2B	-2.51	105.11	106.87
27	C	304	PEK	O03-C21-O04	-2.51	117.26	123.59
19	Y	101	TGL	C20-CA9-CA8	-2.51	101.70	114.42
27	C	304	PEK	O11-P-O14	-2.51	99.28	109.07
20	G	103	PGV	C21-C20-C19	-2.50	104.51	113.62
22	C	301	CHD	C15-C16-C17	2.50	110.09	105.13
27	C	308	PEK	O01-C02-C01	2.50	117.45	108.40
28	N	601	CDL	O1-C1-CA2	-2.50	100.81	109.56
25	M	101	DMU	C10-O1-C9	2.49	118.58	113.69
25	Z	102	DMU	O4-C7-C5	-2.49	104.58	110.35
25	Z	102	DMU	C10-O7-C3	-2.49	111.80	117.96
14	A	602[A]	HEA	C1B-C2B-C3B	-2.49	105.27	107.00
28	T	103	CDL	CB4-OB6-CB5	2.48	123.91	117.79
28	C	306	CDL	C76-C75-C74	-2.48	101.86	114.42
25	P	308	DMU	C7-C8-C9	2.47	114.65	110.24
20	A	609	PGV	C30-C29-C28	2.47	126.96	114.42
22	B	301	CHD	O3-C3-C4	-2.46	104.94	109.85
25	C	302	DMU	C25-C22-C19	-2.46	101.93	114.42
22	P	305	CHD	C19-C10-C5	2.46	114.54	110.36
21	P	310	EDO	O2-C2-C1	2.44	129.49	111.91
25	L	102	DMU	C1-C2-C3	2.44	115.26	109.68
25	M	101	DMU	C28-C25-C22	-2.44	102.03	114.42
22	P	301	CHD	O3-C3-C2	-2.44	103.95	110.16
22	C	307	CHD	C19-C10-C5	-2.44	106.22	110.36
20	G	103	PGV	O02-C1-C2	-2.44	114.21	123.73
14	A	601	HEA	CMD-C2D-C3D	2.44	129.54	124.94
28	P	304	CDL	C83-C82-C81	2.44	126.79	114.42
22	B	301	CHD	C16-C17-C13	2.43	105.94	103.55
27	T	102	PEK	C02-O01-C1	2.43	123.78	117.79
19	A	608	TGL	OG1-CA1-CA2	2.43	119.54	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	601	CDL	C60-C59-C58	2.43	126.77	114.42
22	B	301	CHD	C13-C17-C20	-2.42	116.61	119.50
27	C	304	PEK	O03-C01-C02	-2.42	101.40	108.43
19	N	610	TGL	OB1-CB1-CB2	-2.41	114.31	123.73
19	A	608	TGL	CG1-OG1-CA1	2.41	126.03	117.12
20	C	305	PGV	O01-C1-O02	-2.40	117.89	123.70
28	N	601	CDL	OB8-CB7-C71	2.40	119.44	111.91
28	P	304	CDL	C39-C38-C37	2.40	126.61	114.42
22	W	101	CHD	C23-C22-C20	-2.40	111.49	114.72
24	O	302	PSC	C29-C28-C27	-2.39	102.27	114.42
25	L	102	DMU	C8-C7-C5	-2.39	106.65	110.82
25	C	311	DMU	C8-C7-C5	-2.39	106.66	110.82
19	N	610	TGL	CG3-CG2-CG1	-2.38	106.15	111.79
28	T	103	CDL	C19-C18-C17	2.38	126.51	114.42
25	C	310	DMU	O7-C10-O1	2.38	117.32	110.67
25	M	101	DMU	O49-C1-C6	-2.37	104.28	110.05
19	N	610	TGL	CB3-CB2-CB1	-2.37	105.00	113.62
19	Y	101	TGL	CB4-CB3-CB2	2.37	121.70	113.19
27	C	304	PEK	O01-C02-C01	-2.37	99.83	108.40
28	T	103	CDL	OA8-CA7-OA9	-2.37	117.62	123.59
19	L	101	TGL	C20-CA9-CA8	-2.36	102.42	114.42
28	P	304	CDL	C57-C56-C55	-2.36	102.42	114.42
27	P	307	PEK	C03-C02-C01	-2.36	106.20	111.79
22	P	305	CHD	C14-C8-C9	-2.36	106.47	109.71
22	J	101	CHD	C2-C1-C10	2.36	116.83	112.78
19	N	610	TGL	OG1-CG1-CG2	2.36	115.29	108.43
28	T	103	CDL	C43-C42-C41	2.34	126.31	114.42
25	L	102	DMU	C2-C3-C4	2.34	116.28	110.93
27	C	304	PEK	O04-C21-C22	2.33	132.83	123.73
28	P	304	CDL	C40-C39-C38	2.33	126.25	114.42
25	C	311	DMU	O5-C4-C3	2.33	114.66	109.75
22	B	301	CHD	O7-C7-C6	2.33	115.72	109.94
25	P	309	DMU	C1-C2-C3	2.32	114.97	109.68
14	A	601	HEA	C12-C13-C14	2.32	118.35	112.23
28	N	601	CDL	C23-C22-C21	2.32	126.18	114.42
27	P	307	PEK	O03-C21-C22	2.32	119.17	111.91
28	N	601	CDL	CA6-OA8-CA7	2.31	125.66	117.12
20	C	305	PGV	O01-C1-C2	2.31	116.47	111.50
28	P	304	CDL	C19-C18-C17	2.30	126.12	114.42
25	C	310	DMU	O4-C7-C5	-2.30	105.02	110.35
22	J	101	CHD	C22-C23-C24	-2.30	108.64	113.59
27	T	101	PEK	O03-C01-C02	2.30	115.13	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	307	PEK	C35-C34-C33	2.30	126.08	114.42
28	N	601	CDL	OB8-CB7-OB9	-2.29	117.80	123.59
20	C	305	PGV	O14-P-O13	2.29	123.58	112.24
27	P	307	PEK	O01-C1-O02	-2.29	118.16	123.70
14	A	601	HEA	CMB-C2B-C1B	-2.29	124.94	128.46
28	N	601	CDL	C72-C71-CB7	2.29	121.94	113.62
25	C	302	DMU	O1-C9-C8	2.28	113.84	109.69
24	B	303	PSC	O03-C01-C02	2.28	115.08	108.43
22	C	301	CHD	C19-C10-C9	-2.28	108.04	111.18
14	A	602[A]	HEA	CAD-C3D-C2D	2.28	133.80	127.25
14	A	602[A]	HEA	CBD-CAD-C3D	-2.27	108.30	112.49
28	T	103	CDL	CB6-CB4-CB3	-2.27	106.42	111.79
14	A	601	HEA	C20-C19-C18	2.27	125.71	121.12
20	C	309	PGV	C21-C20-C19	-2.27	105.36	113.62
25	L	102	DMU	O1-C9-C11	2.27	112.08	106.44
19	L	101	TGL	CB5-CB4-CB3	2.27	125.94	114.42
20	P	303	PGV	O14-P-O13	2.27	123.45	112.24
22	B	301	CHD	C14-C8-C9	2.26	112.82	109.71
24	O	302	PSC	C28-C27-C26	-2.26	102.94	114.42
21	H	101	EDO	O2-C2-C1	-2.26	95.63	111.91
20	N	609	PGV	O02-C1-C2	2.26	132.54	123.73
22	C	307	CHD	C16-C17-C13	2.26	105.77	103.55
25	P	306	DMU	C8-C7-C5	2.25	114.76	110.82
14	A	601	HEA	O11-C11-C3B	-2.24	105.54	112.00
14	A	601	HEA	CAA-CBA-CGA	-2.24	108.92	112.67
22	C	307	CHD	C22-C20-C17	-2.23	105.68	110.28
22	P	301	CHD	C22-C23-C24	-2.23	108.80	113.59
24	B	303	PSC	C4-C3-C2	2.23	121.19	113.19
25	C	311	DMU	C10-C5-C7	2.23	114.63	110.00
22	C	301	CHD	C11-C12-C13	2.22	113.53	111.24
28	C	306	CDL	OA6-CA5-OA7	-2.22	118.33	123.70
28	N	601	CDL	C83-C82-C81	2.22	125.70	114.42
19	D	201	TGL	CB5-CB4-CB3	2.22	125.69	114.42
22	P	301	CHD	C14-C8-C7	-2.22	108.86	111.81
20	C	309	PGV	O01-C02-C01	2.22	116.43	108.40
28	C	306	CDL	OA6-CA4-CA6	2.20	116.38	108.40
28	N	601	CDL	C82-C81-C80	2.20	125.59	114.42
14	A	602[B]	HEA	C26-C15-C14	-2.20	118.04	123.68
25	M	101	DMU	O2-C8-C7	-2.20	105.27	110.35
22	J	101	CHD	C19-C10-C5	-2.20	106.64	110.36
14	A	601	HEA	C27-C19-C18	-2.19	118.05	123.68
24	B	303	PSC	C01-O03-C19	2.19	125.23	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	609	PGV	C34-C33-C32	-2.19	96.81	113.42
28	N	601	CDL	C43-C42-C41	2.19	125.52	114.42
20	P	303	PGV	O03-C19-O04	-2.19	118.08	123.59
22	J	101	CHD	C6-C5-C4	-2.18	108.68	111.19
25	C	302	DMU	O1-C9-C11	2.18	111.86	106.44
19	L	101	TGL	CA4-CA3-CA2	-2.18	105.35	113.19
14	N	602	HEA	C27-C19-C18	-2.18	118.10	123.68
28	P	304	CDL	OB8-CB6-CB4	2.17	114.76	108.43
14	N	603[A]	HEA	CMC-C2C-C1C	-2.17	125.12	128.46
28	T	103	CDL	CB2-C1-CA2	-2.17	106.41	112.79
28	P	304	CDL	C56-C55-C54	2.16	125.41	114.42
27	C	308	PEK	C02-O01-C1	2.16	123.12	117.79
25	P	308	DMU	O5-C4-C57	2.16	111.80	106.44
25	C	302	DMU	O4-C7-C8	2.16	115.33	110.35
21	S	103	EDO	O1-C1-C2	-2.15	96.40	111.91
20	C	305	PGV	C4-C3-C2	-2.15	105.45	113.19
28	T	103	CDL	C59-C58-C57	2.15	125.34	114.42
14	A	602[A]	HEA	C20-C19-C18	-2.15	116.77	121.12
25	P	308	DMU	C10-O7-C3	2.15	123.27	117.96
28	T	103	CDL	OB8-CB7-OB9	-2.15	118.18	123.59
20	C	309	PGV	O03-C01-C02	2.15	114.68	108.43
22	C	301	CHD	C16-C15-C14	-2.14	100.89	105.13
22	P	301	CHD	C2-C1-C10	-2.14	109.12	112.78
28	N	601	CDL	OA6-CA5-OA7	-2.14	118.54	123.70
27	C	308	PEK	O03-C01-C02	2.13	114.63	108.43
27	T	101	PEK	O03-C21-O04	-2.13	118.22	123.59
28	T	103	CDL	C58-C57-C56	-2.13	103.63	114.42
14	N	603[B]	HEA	C3C-C4C-NC	2.12	111.96	109.21
27	C	304	PEK	C02-O01-C1	-2.12	112.57	117.79
20	Z	101	PGV	O01-C02-C01	2.12	116.07	108.40
28	T	103	CDL	C42-C41-C40	2.11	125.16	114.42
14	N	603[A]	HEA	C26-C15-C14	-2.11	118.26	123.68
19	L	101	TGL	C22-C21-C20	-2.11	103.70	114.42
20	Z	101	PGV	O03-C19-O04	-2.11	118.26	123.59
28	T	103	CDL	C63-C62-C61	2.11	125.12	114.42
20	A	610	PGV	O02-C1-C2	-2.10	115.53	123.73
22	W	101	CHD	O12-C12-C13	2.10	114.58	111.03
14	N	603[B]	HEA	C20-C19-C18	-2.10	116.87	121.12
25	C	311	DMU	C10-O7-C3	-2.10	112.77	117.96
25	C	302	DMU	O3-C5-C10	2.10	115.14	110.05
19	D	201	TGL	OG3-CC1-OC1	-2.10	118.30	123.59
19	A	608	TGL	C33-C19-C18	2.10	125.06	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	303	PGV	C03-C02-C01	-2.09	106.83	111.79
28	C	306	CDL	C43-C42-C41	2.09	125.04	114.42
22	J	101	CHD	C1-C10-C5	2.09	110.85	107.77
25	P	309	DMU	C6-C1-C2	2.08	114.34	110.00
19	N	610	TGL	CC4-CC3-CC2	2.08	120.68	113.19
22	J	101	CHD	C4-C3-C2	2.08	113.04	110.55
14	A	602[B]	HEA	CAD-CBD-CGD	-2.08	109.18	112.67
22	P	301	CHD	C11-C9-C10	-2.08	111.58	113.73
22	P	301	CHD	C5-C4-C3	-2.07	109.72	112.76
22	G	101	CHD	C21-C20-C22	2.07	113.61	110.36
28	T	103	CDL	C62-C61-C60	2.07	124.92	114.42
22	J	101	CHD	C4-C5-C10	2.06	114.85	112.66
19	D	201	TGL	OC1-CC1-CC2	2.06	131.78	123.73
19	Q	201	TGL	OB1-CB1-CB2	2.06	131.75	123.73
22	C	301	CHD	C18-C13-C12	2.06	111.16	109.07
25	Z	102	DMU	C18-O16-C6	-2.06	110.43	113.84
14	N	603[A]	HEA	CMB-C2B-C3B	2.05	128.71	124.69
28	P	304	CDL	C23-C22-C21	2.05	124.84	114.42
25	C	302	DMU	O1-C10-C5	-2.05	106.02	110.35
28	T	103	CDL	C40-C39-C38	2.04	124.80	114.42
22	G	101	CHD	C13-C17-C20	-2.04	117.06	119.50
22	J	101	CHD	C5-C6-C7	-2.04	112.21	114.46
22	P	301	CHD	C6-C5-C10	2.04	114.82	112.66
25	C	302	DMU	O55-C2-C1	-2.04	105.64	110.35
20	P	303	PGV	O02-C1-C2	2.03	131.67	123.73
19	Y	101	TGL	CA7-CA6-CA5	-2.03	104.11	114.42
19	Y	101	TGL	CG3-OG3-CC1	2.02	124.59	117.12
28	C	306	CDL	C40-C39-C38	2.02	124.66	114.42
20	P	303	PGV	C3-C2-C1	-2.01	106.30	113.62
14	N	603[B]	HEA	C17-C18-C19	2.01	132.51	127.66
25	L	102	DMU	C6-C1-C2	2.01	114.18	110.00
22	C	307	CHD	C11-C9-C8	2.01	113.81	110.88
14	N	603[B]	HEA	C13-C14-C15	2.01	132.49	127.66
22	P	301	CHD	C5-C6-C7	2.00	116.67	114.46

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	603[B]	HEA	ND
14	N	603[B]	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NA

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Mol	Chain	Res	Type	Atom
14	A	601	HEA	NB
14	A	602[B]	HEA	ND
14	A	602[B]	HEA	NA
14	A	602[B]	HEA	NB
14	N	603[A]	HEA	ND
14	N	603[A]	HEA	NA
14	N	603[A]	HEA	NB
14	N	602	HEA	ND
14	N	602	HEA	NB
14	A	602[A]	HEA	ND
14	A	602[A]	HEA	NA
14	A	602[A]	HEA	NB

All (983) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	603[B]	HEA	C2D-C3D-CAD-CBD
14	N	603[B]	HEA	C4D-C3D-CAD-CBD
27	C	304	PEK	C10-C11-C12-C13
27	C	308	PEK	C04-O12-P-O14
27	C	308	PEK	O12-C04-C05-N
27	C	308	PEK	O02-C1-O01-C02
27	C	308	PEK	C2-C1-O01-C02
27	C	308	PEK	C12-C13-C14-C15
27	C	308	PEK	C13-C14-C15-C16
22	W	101	CHD	C13-C17-C20-C22
25	P	309	DMU	O5-C6-O16-C18
27	G	102	PEK	C03-O11-P-O14
27	G	102	PEK	O12-C04-C05-N
27	G	102	PEK	O02-C1-O01-C02
27	G	102	PEK	C2-C1-O01-C02
27	P	307	PEK	C03-O11-P-O13
27	P	307	PEK	C03-O11-P-O14
27	P	307	PEK	C04-O12-P-O14
27	P	307	PEK	C2-C1-O01-C02
27	P	307	PEK	C13-C14-C15-C16
20	Z	101	PGV	O02-C1-O01-C02
20	Z	101	PGV	C2-C1-O01-C02
20	Z	101	PGV	C20-C19-O03-C01
20	Z	101	PGV	C10-C11-C12-C13
27	T	101	PEK	O03-C01-C02-O01
27	T	101	PEK	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
27	T	101	PEK	C12-C13-C14-C15
14	A	602[B]	HEA	C2D-C3D-CAD-CBD
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
25	C	311	DMU	C1-C6-O16-C18
25	C	311	DMU	O5-C6-O16-C18
25	C	311	DMU	C19-C18-O16-C6
24	O	302	PSC	C03-O11-P-O12
24	O	302	PSC	O12-C04-C05-N
24	O	302	PSC	C2-C1-O01-C02
24	O	302	PSC	O04-C19-O03-C01
24	O	302	PSC	C20-C19-O03-C01
25	C	302	DMU	C19-C18-O16-C6
28	T	103	CDL	O1-C1-CA2-OA2
28	T	103	CDL	CA2-OA2-PA1-OA3
28	T	103	CDL	CA3-OA5-PA1-OA3
28	T	103	CDL	CA3-OA5-PA1-OA4
28	T	103	CDL	C1-CB2-OB2-PB2
19	Y	101	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	CG2-CG1-OG1-CA1
25	P	306	DMU	C1-C6-O16-C18
25	P	306	DMU	O5-C6-O16-C18
24	B	303	PSC	C03-O11-P-O13
24	B	303	PSC	C04-O12-P-O13
24	B	303	PSC	O12-C04-C05-N
24	B	303	PSC	O04-C19-O03-C01
24	B	303	PSC	C20-C19-O03-C01
20	G	103	PGV	C03-O11-P-O14
20	G	103	PGV	C04-O12-P-O11
20	G	103	PGV	C04-O12-P-O13
20	G	103	PGV	C04-O12-P-O14
20	G	103	PGV	O03-C01-C02-O01
20	G	103	PGV	O12-C04-C05-C06
20	G	103	PGV	O12-C04-C05-O05
20	A	610	PGV	C03-O11-P-O13
20	A	610	PGV	C03-O11-P-O14
20	A	610	PGV	O01-C02-C03-O11
20	A	610	PGV	C04-C05-C06-O06
20	A	610	PGV	C2-C1-O01-C02
19	L	101	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	OB1-CB1-OG2-CG2
19	L	101	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	OC1-CC1-OG3-CG3
28	P	304	CDL	CB2-OB2-PB2-OB3
28	P	304	CDL	CB2-OB2-PB2-OB4
28	P	304	CDL	CB2-OB2-PB2-OB5
28	P	304	CDL	CB3-OB5-PB2-OB3
28	P	304	CDL	CB3-OB5-PB2-OB4
20	C	309	PGV	C03-O11-P-O13
20	C	309	PGV	C03-O11-P-O14
20	C	309	PGV	C04-O12-P-O13
28	C	306	CDL	CA3-OA5-PA1-OA2
28	C	306	CDL	OA7-CA5-OA6-CA4
28	C	306	CDL	C11-CA5-OA6-CA4
28	C	306	CDL	C1-CB2-OB2-PB2
27	T	102	PEK	C9-C10-C11-C12
28	N	601	CDL	CA2-OA2-PA1-OA3
28	N	601	CDL	CA3-OA5-PA1-OA3
28	N	601	CDL	C11-CA5-OA6-CA4
28	N	601	CDL	CB2-OB2-PB2-OB3
28	N	601	CDL	CB3-OB5-PB2-OB4
28	N	601	CDL	OB6-CB4-CB6-OB8
25	C	310	DMU	C5-C10-O7-C3
25	L	102	DMU	C2-C3-O7-C10
20	Z	101	PGV	O04-C19-O03-C01
28	T	103	CDL	OA9-CA7-OA8-CA6
25	P	308	DMU	C5-C10-O7-C3
28	T	103	CDL	C31-CA7-OA8-CA6
19	Q	201	TGL	OC1-CC1-OG3-CG3
19	A	608	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	OA1-CA1-OG1-CG1
19	D	201	TGL	OC1-CC1-OG3-CG3
28	N	601	CDL	OA9-CA7-OA8-CA6
22	W	101	CHD	C13-C17-C20-C21
27	P	307	PEK	O02-C1-O01-C02
27	T	101	PEK	O02-C1-O01-C02
24	O	302	PSC	O02-C1-O01-C02
20	A	610	PGV	O02-C1-O01-C02
28	P	304	CDL	OB7-CB5-OB6-CB4
28	C	306	CDL	OB7-CB5-OB6-CB4
28	N	601	CDL	OA7-CA5-OA6-CA4
19	Q	201	TGL	CC2-CC1-OG3-CG3
19	A	608	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	CA2-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
22	W	101	CHD	C16-C17-C20-C21
25	L	102	DMU	O6-C11-C9-O1
28	T	103	CDL	C42-C43-C44-C45
27	G	102	PEK	C22-C21-O03-C01
19	D	201	TGL	CC2-CC1-OG3-CG3
28	N	601	CDL	C31-CA7-OA8-CA6
25	L	102	DMU	O6-C11-C9-C8
27	C	304	PEK	C13-C14-C15-C16
27	C	308	PEK	C4-C5-C6-C7
24	O	302	PSC	C11-C12-C13-C14
27	T	102	PEK	C4-C5-C6-C7
27	T	102	PEK	C10-C11-C12-C13
28	C	306	CDL	C76-C77-C78-C79
27	G	102	PEK	O04-C21-O03-C01
28	T	103	CDL	C79-C80-C81-C82
19	A	608	TGL	C21-C20-CA9-CA8
20	A	610	PGV	C20-C21-C22-C23
27	T	101	PEK	C22-C21-O03-C01
19	Y	101	TGL	CA2-CA1-OG1-CG1
28	T	103	CDL	C11-CA5-OA6-CA4
28	P	304	CDL	C51-CB5-OB6-CB4
28	C	306	CDL	C51-CB5-OB6-CB4
25	L	102	DMU	C3-C4-C57-O61
19	Y	101	TGL	OA1-CA1-OG1-CG1
24	O	302	PSC	C29-C30-C31-C32
25	C	302	DMU	C25-C28-C31-C34
19	D	201	TGL	C21-C22-C23-C24
24	B	303	PSC	C21-C22-C23-C24
19	L	101	TGL	CA9-C20-C21-C22
25	L	102	DMU	O5-C4-C57-O61
22	W	101	CHD	C16-C17-C20-C22
28	N	601	CDL	C81-C82-C83-C84
19	N	610	TGL	CC2-CC1-OG3-CG3
19	A	608	TGL	OB1-CB1-OG2-CG2
28	T	103	CDL	OA7-CA5-OA6-CA4
28	T	103	CDL	C60-C61-C62-C63
27	T	101	PEK	O04-C21-O03-C01
14	A	601	HEA	C15-C16-C17-C18
28	P	304	CDL	C81-C82-C83-C84
20	A	610	PGV	C20-C19-O03-C01
19	N	610	TGL	OC1-CC1-OG3-CG3
19	N	610	TGL	CB2-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
24	O	302	PSC	C20-C21-C22-C23
28	P	304	CDL	CB2-C1-CA2-OA2
28	P	304	CDL	CA2-C1-CB2-OB2
28	C	306	CDL	CB2-C1-CA2-OA2
22	P	305	CHD	C21-C20-C22-C23
19	A	608	TGL	CA2-CA1-OG1-CG1
19	N	610	TGL	CA2-CA1-OG1-CG1
22	C	307	CHD	C20-C22-C23-C24
28	T	103	CDL	C23-C24-C25-C26
22	C	307	CHD	C17-C20-C22-C23
28	T	103	CDL	O1-C1-CB2-OB2
28	P	304	CDL	O1-C1-CB2-OB2
28	C	306	CDL	O1-C1-CA2-OA2
19	A	608	TGL	CA1-CA2-CA3-CA4
19	N	610	TGL	CC1-CC2-CC3-CC4
25	P	309	DMU	C1-C6-O16-C18
27	P	307	PEK	O03-C01-C02-O01
28	T	103	CDL	OB6-CB4-CB6-OB8
19	N	610	TGL	OB1-CB1-OG2-CG2
28	N	601	CDL	CA5-C11-C12-C13
19	A	608	TGL	OA1-CA1-OG1-CG1
24	O	302	PSC	C22-C23-C24-C25
22	C	307	CHD	C21-C20-C22-C23
19	Y	101	TGL	C20-C21-C22-C23
27	T	101	PEK	C13-C14-C15-C16
24	O	302	PSC	C11-C10-C9-C8
20	A	609	PGV	C26-C27-C28-C29
27	P	307	PEK	C1-C2-C3-C4
20	Z	101	PGV	C19-C20-C21-C22
27	T	101	PEK	C21-C22-C23-C24
19	A	608	TGL	CB1-CB2-CB3-CB4
19	N	610	TGL	CA1-CA2-CA3-CA4
19	D	201	TGL	CA1-CA2-CA3-CA4
19	D	201	TGL	CB1-CB2-CB3-CB4
20	C	309	PGV	C1-C2-C3-C4
28	C	306	CDL	CA7-C31-C32-C33
28	C	306	CDL	CB5-C51-C52-C53
27	T	102	PEK	C1-C2-C3-C4
25	P	309	DMU	O16-C18-C19-C22
28	C	306	CDL	CB4-CB6-OB8-CB7
19	A	608	TGL	C24-C25-C26-C27
28	T	103	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
28	T	103	CDL	CB5-C51-C52-C53
21	C	318	EDO	O1-C1-C2-O2
21	J	102	EDO	O1-C1-C2-O2
21	H	102	EDO	O1-C1-C2-O2
21	N	613	EDO	O1-C1-C2-O2
19	N	610	TGL	OA1-CA1-OG1-CG1
20	A	610	PGV	O04-C19-O03-C01
19	Y	101	TGL	CC1-CC2-CC3-CC4
28	P	304	CDL	O1-C1-CA2-OA2
28	C	306	CDL	O1-C1-CB2-OB2
28	P	304	CDL	CB4-CB6-OB8-CB7
25	L	102	DMU	O16-C18-C19-C22
27	C	308	PEK	C7-C8-C9-C10
27	P	307	PEK	C4-C5-C6-C7
20	P	303	PGV	C10-C11-C12-C13
27	T	102	PEK	C13-C14-C15-C16
19	A	608	TGL	CB2-CB1-OG2-CG2
25	Z	102	DMU	O16-C18-C19-C22
27	C	308	PEK	C03-O11-P-O12
27	C	308	PEK	C04-O12-P-O11
27	G	102	PEK	C04-O12-P-O11
27	P	307	PEK	C03-O11-P-O12
20	Z	101	PGV	C03-O11-P-O12
20	Z	101	PGV	C04-O12-P-O11
27	T	101	PEK	C03-O11-P-O12
27	T	101	PEK	C04-O12-P-O11
28	T	103	CDL	CA3-OA5-PA1-OA2
28	T	103	CDL	CB2-OB2-PB2-OB5
24	B	303	PSC	C03-O11-P-O12
24	B	303	PSC	C04-O12-P-O11
20	G	103	PGV	C03-O11-P-O12
20	A	610	PGV	C03-O11-P-O12
28	P	304	CDL	CB3-OB5-PB2-OB2
20	C	309	PGV	C03-O11-P-O12
28	C	306	CDL	CB2-OB2-PB2-OB5
28	C	306	CDL	CB3-OB5-PB2-OB2
28	N	601	CDL	CB3-OB5-PB2-OB2
19	L	101	TGL	CA2-CA1-OG1-CG1
25	P	308	DMU	O6-C11-C9-O1
19	L	101	TGL	CC2-CC3-CC4-CC5
27	G	102	PEK	C29-C30-C31-C32
20	Z	101	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
28	T	103	CDL	C34-C35-C36-C37
19	Y	101	TGL	CA2-CA3-CA4-CA5
24	B	303	PSC	C2-C1-O01-C02
19	Q	201	TGL	CC9-C15-C16-C17
19	Q	201	TGL	C19-C33-C34-C35
19	N	610	TGL	CB7-CB8-CB9-C10
28	T	103	CDL	C13-C14-C15-C16
19	Y	101	TGL	CA3-CA4-CA5-CA6
19	Y	101	TGL	CB6-CB7-CB8-CB9
19	D	201	TGL	C17-C18-C19-C33
19	D	201	TGL	C18-C19-C33-C34
24	B	303	PSC	C20-C21-C22-C23
20	A	610	PGV	C14-C15-C16-C17
19	L	101	TGL	CA3-CA4-CA5-CA6
20	C	309	PGV	C13-C14-C15-C16
28	C	306	CDL	C57-C58-C59-C60
27	T	102	PEK	C26-C27-C28-C29
28	N	601	CDL	C60-C61-C62-C63
19	Q	201	TGL	C11-C10-CB9-CB8
19	A	608	TGL	CB4-CB5-CB6-CB7
19	A	608	TGL	C23-C24-C25-C26
19	N	610	TGL	CB6-CB7-CB8-CB9
19	N	610	TGL	CA9-C20-C21-C22
19	Y	101	TGL	CB3-CB4-CB5-CB6
20	C	309	PGV	C23-C24-C25-C26
25	M	101	DMU	C19-C22-C25-C28
20	Z	101	PGV	C01-C02-O01-C1
28	T	103	CDL	OB7-CB5-OB6-CB4
24	B	303	PSC	O02-C1-O01-C02
19	Q	201	TGL	CB4-CB5-CB6-CB7
27	P	307	PEK	C33-C34-C35-C36
24	O	302	PSC	C24-C25-C26-C27
20	Z	101	PGV	C02-C03-O11-P
27	T	101	PEK	C10-C11-C12-C13
27	G	102	PEK	C24-C25-C26-C27
19	A	608	TGL	C12-C13-C14-C29
24	O	302	PSC	C25-C26-C27-C28
28	T	103	CDL	C21-C22-C23-C24
20	C	305	PGV	C14-C15-C16-C17
20	G	103	PGV	C24-C25-C26-C27
20	A	610	PGV	C21-C22-C23-C24
19	N	610	TGL	CA6-CA7-CA8-CA9

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Mol	Chain	Res	Type	Atoms
28	T	103	CDL	C71-C72-C73-C74
25	C	310	DMU	O16-C18-C19-C22
19	L	101	TGL	C12-C13-C14-C29
28	P	304	CDL	C61-C62-C63-C64
27	P	307	PEK	C21-C22-C23-C24
25	C	302	DMU	C1-C6-O16-C18
19	Q	201	TGL	CA6-CA7-CA8-CA9
19	N	610	TGL	CA4-CA5-CA6-CA7
28	T	103	CDL	C22-C23-C24-C25
28	T	103	CDL	C51-C52-C53-C54
19	Y	101	TGL	CB5-CB6-CB7-CB8
19	Y	101	TGL	CA9-C20-C21-C22
19	D	201	TGL	CC5-CC6-CC7-CC8
20	C	305	PGV	C7-C8-C9-C10
28	P	304	CDL	C43-C44-C45-C46
19	Q	201	TGL	C10-C11-C12-C13
19	A	608	TGL	CA4-CA5-CA6-CA7
20	G	103	PGV	C13-C14-C15-C16
19	L	101	TGL	CB3-CB4-CB5-CB6
20	C	309	PGV	C6-C7-C8-C9
28	N	601	CDL	C14-C15-C16-C17
28	P	304	CDL	CB5-C51-C52-C53
27	C	308	PEK	C28-C29-C30-C31
19	A	608	TGL	CA2-CA3-CA4-CA5
19	A	608	TGL	C10-C11-C12-C13
19	A	608	TGL	C20-C21-C22-C23
28	T	103	CDL	C41-C42-C43-C44
19	Y	101	TGL	CA5-CA6-CA7-CA8
19	Y	101	TGL	CC4-CC5-CC6-CC7
28	N	601	CDL	C35-C36-C37-C38
27	C	304	PEK	C26-C27-C28-C29
27	C	308	PEK	C25-C26-C27-C28
19	A	608	TGL	CA3-CA4-CA5-CA6
19	N	610	TGL	C16-C15-CC9-CC8
25	P	308	DMU	C19-C22-C25-C28
20	G	103	PGV	C04-C05-C06-O06
20	C	309	PGV	C04-C05-C06-O06
25	C	302	DMU	C18-C19-C22-C25
28	T	103	CDL	C51-CB5-OB6-CB4
27	G	102	PEK	C30-C31-C32-C33
20	Z	101	PGV	C2-C3-C4-C5
27	T	101	PEK	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
24	O	302	PSC	C5-C6-C7-C8
28	T	103	CDL	C17-C18-C19-C20
20	C	305	PGV	C12-C13-C14-C15
20	G	103	PGV	C12-C13-C14-C15
19	A	608	TGL	CB9-C10-C11-C12
19	D	201	TGL	C16-C15-CC9-CC8
28	P	304	CDL	C40-C41-C42-C43
28	C	306	CDL	C42-C43-C44-C45
25	L	102	DMU	C31-C34-C37-C40
28	N	601	CDL	C42-C43-C44-C45
28	N	601	CDL	C59-C60-C61-C62
25	C	302	DMU	O5-C6-O16-C18
22	P	305	CHD	C17-C20-C22-C23
19	Q	201	TGL	CC5-CC6-CC7-CC8
28	N	601	CDL	C21-C22-C23-C24
28	N	601	CDL	C41-C42-C43-C44
28	P	304	CDL	C22-C23-C24-C25
28	P	304	CDL	C23-C24-C25-C26
28	P	304	CDL	C57-C58-C59-C60
19	N	610	TGL	CA3-CA4-CA5-CA6
22	J	101	CHD	C20-C22-C23-C24
19	Q	201	TGL	C12-C13-C14-C29
19	N	610	TGL	CB9-C10-C11-C12
19	N	610	TGL	C13-C14-C29-C30
19	D	201	TGL	CC6-CC7-CC8-CC9
28	P	304	CDL	C77-C78-C79-C80
27	C	304	PEK	C16-C17-C18-C19
19	A	608	TGL	CC6-CC7-CC8-CC9
25	C	311	DMU	C31-C34-C37-C40
19	N	610	TGL	CC9-C15-C16-C17
28	C	306	CDL	C11-C12-C13-C14
28	C	306	CDL	C72-C73-C74-C75
28	N	601	CDL	C79-C80-C81-C82
19	A	608	TGL	CA5-CA6-CA7-CA8
19	A	608	TGL	CA7-CA8-CA9-C20
19	Y	101	TGL	CC3-CC4-CC5-CC6
20	C	305	PGV	C10-C11-C12-C13
20	A	610	PGV	C10-C11-C12-C13
27	C	304	PEK	C34-C35-C36-C37
20	Z	101	PGV	C4-C5-C6-C7
19	N	610	TGL	CC4-CC5-CC6-CC7
28	C	306	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
28	C	306	CDL	C61-C62-C63-C64
27	T	102	PEK	C30-C31-C32-C33
27	T	102	PEK	C33-C34-C35-C36
28	N	601	CDL	C13-C14-C15-C16
25	C	310	DMU	C19-C22-C25-C28
28	C	306	CDL	C59-C60-C61-C62
20	A	610	PGV	O05-C05-C06-O06
20	C	309	PGV	O05-C05-C06-O06
27	G	102	PEK	C25-C26-C27-C28
28	T	103	CDL	C19-C20-C21-C22
20	P	303	PGV	C7-C8-C9-C10
19	D	201	TGL	C10-C11-C12-C13
20	G	103	PGV	C7-C8-C9-C10
28	P	304	CDL	C31-C32-C33-C34
28	N	601	CDL	C18-C19-C20-C21
28	N	601	CDL	C62-C63-C64-C65
20	Z	101	PGV	C12-C13-C14-C15
20	C	309	PGV	C12-C13-C14-C15
27	T	102	PEK	C15-C16-C17-C18
19	Q	201	TGL	CA2-CA3-CA4-CA5
28	P	304	CDL	C82-C83-C84-C85
25	C	311	DMU	C18-C19-C22-C25
28	C	306	CDL	C62-C63-C64-C65
20	P	303	PGV	C11-C12-C13-C14
28	P	304	CDL	C11-C12-C13-C14
20	C	309	PGV	C30-C31-C32-C33
19	L	101	TGL	OA1-CA1-OG1-CG1
28	T	103	CDL	CA2-C1-CB2-OB2
28	T	103	CDL	C18-C19-C20-C21
28	T	103	CDL	C73-C74-C75-C76
25	Z	102	DMU	C25-C28-C31-C34
24	B	303	PSC	C22-C23-C24-C25
27	G	102	PEK	C22-C23-C24-C25
28	C	306	CDL	C43-C44-C45-C46
28	C	306	CDL	C53-C54-C55-C56
28	T	103	CDL	C14-C15-C16-C17
21	N	611	EDO	O1-C1-C2-O2
21	D	206	EDO	O1-C1-C2-O2
21	C	319	EDO	O1-C1-C2-O2
21	R	202	EDO	O1-C1-C2-O2
21	D	204	EDO	O1-C1-C2-O2
21	N	614	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
21	D	203	EDO	O1-C1-C2-O2
21	P	310	EDO	O1-C1-C2-O2
21	C	317	EDO	O1-C1-C2-O2
21	P	313	EDO	O1-C1-C2-O2
21	A	615	EDO	O1-C1-C2-O2
21	N	622	EDO	O1-C1-C2-O2
19	Q	201	TGL	C13-C14-C29-C30
27	G	102	PEK	C32-C33-C34-C35
27	G	102	PEK	C33-C34-C35-C36
19	N	610	TGL	C11-C10-CB9-CB8
28	T	103	CDL	C81-C82-C83-C84
19	Y	101	TGL	C10-C11-C12-C13
28	N	601	CDL	C31-C32-C33-C34
28	P	304	CDL	C20-C21-C22-C23
28	P	304	CDL	C60-C61-C62-C63
28	C	306	CDL	C12-C13-C14-C15
19	Q	201	TGL	CB2-CB3-CB4-CB5
20	Z	101	PGV	C27-C28-C29-C30
19	L	101	TGL	CA6-CA7-CA8-CA9
28	N	601	CDL	C71-C72-C73-C74
20	C	309	PGV	C28-C29-C30-C31
28	C	306	CDL	C64-C65-C66-C67
27	P	307	PEK	C10-C11-C12-C13
24	B	303	PSC	C11-C10-C9-C8
27	G	102	PEK	C23-C24-C25-C26
20	G	103	PGV	C22-C23-C24-C25
27	C	308	PEK	C2-C3-C4-C5
20	P	303	PGV	C12-C13-C14-C15
19	Q	201	TGL	OB1-CB1-OG2-CG2
28	N	601	CDL	OB7-CB5-OB6-CB4
20	A	609	PGV	C28-C29-C30-C31
20	N	609	PGV	C27-C28-C29-C30
19	N	610	TGL	CA7-CA8-CA9-C20
28	T	103	CDL	C59-C60-C61-C62
28	P	304	CDL	C16-C17-C18-C19
19	Q	201	TGL	CB9-C10-C11-C12
19	N	610	TGL	CC6-CC7-CC8-CC9
28	T	103	CDL	C12-C13-C14-C15
19	Y	101	TGL	C11-C12-C13-C14
19	L	101	TGL	C10-C11-C12-C13
25	P	309	DMU	C19-C22-C25-C28
27	P	307	PEK	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
27	T	101	PEK	C27-C28-C29-C30
24	O	302	PSC	C2-C3-C4-C5
24	O	302	PSC	C3-C4-C5-C6
19	Q	201	TGL	CB2-CB1-OG2-CG2
28	N	601	CDL	C51-CB5-OB6-CB4
27	C	308	PEK	O01-C02-C03-O11
28	C	306	CDL	OB5-CB3-CB4-OB6
20	P	303	PGV	C24-C25-C26-C27
19	D	201	TGL	C16-C17-C18-C19
28	C	306	CDL	C58-C59-C60-C61
28	C	306	CDL	C73-C74-C75-C76
28	N	601	CDL	C34-C35-C36-C37
27	T	102	PEK	C3-C4-C5-C6
27	P	307	PEK	C26-C27-C28-C29
25	Z	102	DMU	C28-C31-C34-C37
20	G	103	PGV	C29-C30-C31-C32
20	N	609	PGV	C29-C30-C31-C32
19	N	610	TGL	C21-C20-CA9-CA8
28	T	103	CDL	C16-C17-C18-C19
25	Z	102	DMU	C19-C22-C25-C28
19	D	201	TGL	C21-C20-CA9-CA8
28	N	601	CDL	C77-C78-C79-C80
20	Z	101	PGV	C11-C10-C9-C8
25	P	306	DMU	O6-C11-C9-C8
19	Y	101	TGL	C16-C17-C18-C19
19	D	201	TGL	CA6-CA7-CA8-CA9
20	A	609	PGV	C10-C11-C12-C13
24	B	303	PSC	C3-C4-C5-C6
28	C	306	CDL	C82-C83-C84-C85
19	Q	201	TGL	C17-C18-C19-C33
20	N	609	PGV	C30-C31-C32-C33
19	Q	201	TGL	C22-C23-C24-C25
20	N	609	PGV	C14-C15-C16-C17
25	L	102	DMU	C19-C22-C25-C28
28	N	601	CDL	C43-C44-C45-C46
27	G	102	PEK	C03-O11-P-O12
28	N	601	CDL	CA3-OA5-PA1-OA2
20	A	610	PGV	C13-C14-C15-C16
19	Y	101	TGL	CA1-CA2-CA3-CA4
28	C	306	CDL	C22-C23-C24-C25
20	Z	101	PGV	C01-C02-C03-O11
27	T	101	PEK	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
20	A	610	PGV	C01-C02-C03-O11
20	C	309	PGV	C01-C02-C03-O11
25	M	101	DMU	C28-C31-C34-C37
19	L	101	TGL	C21-C22-C23-C24
24	B	303	PSC	C4-C5-C6-C7
20	N	609	PGV	C23-C24-C25-C26
19	Y	101	TGL	C12-C13-C14-C29
20	C	305	PGV	C20-C21-C22-C23
20	C	309	PGV	C7-C8-C9-C10
27	T	102	PEK	C2-C3-C4-C5
28	C	306	CDL	CA5-C11-C12-C13
19	D	201	TGL	C11-C10-CB9-CB8
28	T	103	CDL	C80-C81-C82-C83
19	Y	101	TGL	C21-C20-CA9-CA8
28	P	304	CDL	C80-C81-C82-C83
24	B	303	PSC	C25-C26-C27-C28
19	L	101	TGL	C11-C10-CB9-CB8
27	P	307	PEK	O03-C01-C02-C03
20	Z	101	PGV	O03-C01-C02-C03
24	O	302	PSC	O03-C01-C02-C03
28	T	103	CDL	CB3-CB4-CB6-OB8
19	Y	101	TGL	OG1-CG1-CG2-CG3
19	D	201	TGL	OG1-CG1-CG2-CG3
28	P	304	CDL	CA3-CA4-CA6-OA8
28	N	601	CDL	CA3-CA4-CA6-OA8
28	N	601	CDL	C54-C55-C56-C57
28	N	601	CDL	C64-C65-C66-C67
27	C	304	PEK	C4-C5-C6-C7
27	C	308	PEK	C35-C36-C37-C38
28	C	306	CDL	C36-C37-C38-C39
20	A	610	PGV	C15-C16-C17-C18
20	A	609	PGV	C31-C32-C33-C34
20	G	103	PGV	C3-C4-C5-C6
20	Z	101	PGV	C14-C15-C16-C17
24	B	303	PSC	C15-C16-C17-C18
20	G	103	PGV	O05-C05-C06-O06
22	J	101	CHD	C16-C17-C20-C22
20	N	609	PGV	C12-C13-C14-C15
20	G	103	PGV	C11-C10-C9-C8
24	O	302	PSC	C31-C32-C33-C34
27	C	304	PEK	C17-C18-C19-C20
25	C	311	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
20	G	103	PGV	C31-C32-C33-C34
19	L	101	TGL	CG1-CG2-OG2-CB1
19	L	101	TGL	C11-C12-C13-C14
24	O	302	PSC	C23-C24-C25-C26
19	Q	201	TGL	CA4-CA5-CA6-CA7
19	D	201	TGL	CA4-CA5-CA6-CA7
25	L	102	DMU	C34-C37-C40-C43
27	T	102	PEK	C34-C35-C36-C37
28	N	601	CDL	C72-C73-C74-C75
19	Y	101	TGL	C18-C19-C33-C34
21	A	617	EDO	O1-C1-C2-O2
21	O	304	EDO	O1-C1-C2-O2
21	L	103	EDO	O1-C1-C2-O2
20	P	303	PGV	C1-C2-C3-C4
28	T	103	CDL	C58-C59-C60-C61
20	C	309	PGV	O03-C01-C02-O01
28	T	103	CDL	C75-C76-C77-C78
22	P	305	CHD	C20-C22-C23-C24
27	P	307	PEK	C35-C36-C37-C38
27	T	101	PEK	C17-C18-C19-C20
20	C	305	PGV	C15-C16-C17-C18
19	L	101	TGL	CC6-CC7-CC8-CC9
28	N	601	CDL	C20-C21-C22-C23
27	C	308	PEK	C26-C27-C28-C29
19	L	101	TGL	C25-C26-C27-C28
22	C	307	CHD	C16-C17-C20-C22
19	A	608	TGL	C25-C26-C27-C28
25	L	102	DMU	C25-C28-C31-C34
27	C	304	PEK	C7-C8-C9-C10
27	C	308	PEK	C10-C11-C12-C13
28	P	304	CDL	C39-C40-C41-C42
28	P	304	CDL	C74-C75-C76-C77
19	A	608	TGL	CB5-CB6-CB7-CB8
28	T	103	CDL	C82-C83-C84-C85
28	P	304	CDL	OA5-CA3-CA4-CA6
28	C	306	CDL	OB5-CB3-CB4-CB6
28	P	304	CDL	C51-C52-C53-C54
28	N	601	CDL	C11-C12-C13-C14
27	T	101	PEK	O12-C04-C05-N
19	Q	201	TGL	C20-C21-C22-C23
27	C	304	PEK	C23-C24-C25-C26
25	P	309	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
28	C	306	CDL	C77-C78-C79-C80
24	O	302	PSC	C26-C27-C28-C29
25	C	302	DMU	C19-C22-C25-C28
28	C	306	CDL	C63-C64-C65-C66
20	C	305	PGV	C1-C2-C3-C4
27	T	101	PEK	C26-C27-C28-C29
20	N	609	PGV	C13-C14-C15-C16
19	D	201	TGL	CC7-CC8-CC9-C15
27	C	308	PEK	C32-C33-C34-C35
20	G	103	PGV	C19-C20-C21-C22
19	Y	101	TGL	C29-C30-C31-C32
20	Z	101	PGV	C05-C04-O12-P
25	L	102	DMU	C19-C18-O16-C6
19	Q	201	TGL	C16-C17-C18-C19
24	O	302	PSC	C27-C28-C29-C30
28	T	103	CDL	C64-C65-C66-C67
19	N	610	TGL	CB1-CB2-CB3-CB4
20	C	309	PGV	C22-C23-C24-C25
27	T	102	PEK	C23-C24-C25-C26
19	Q	201	TGL	OG1-CG1-CG2-CG3
28	T	103	CDL	CA3-CA4-CA6-OA8
28	P	304	CDL	CB3-CB4-CB6-OB8
20	C	309	PGV	O03-C01-C02-C03
28	C	306	CDL	CB3-CB4-CB6-OB8
28	C	306	CDL	C37-C38-C39-C40
19	L	101	TGL	C20-C21-C22-C23
25	C	311	DMU	O1-C10-O7-C3
20	N	609	PGV	C31-C32-C33-C34
19	Y	101	TGL	C11-C10-CB9-CB8
19	L	101	TGL	CB7-CB8-CB9-C10
28	N	601	CDL	C33-C34-C35-C36
27	C	308	PEK	C11-C12-C13-C14
27	G	102	PEK	C6-C7-C8-C9
27	G	102	PEK	C11-C10-C9-C8
27	G	102	PEK	C11-C12-C13-C14
27	G	102	PEK	C12-C13-C14-C15
27	P	307	PEK	C04-O12-P-O11
27	P	307	PEK	C9-C10-C11-C12
27	P	307	PEK	C12-C13-C14-C15
27	T	101	PEK	C11-C10-C9-C8
27	T	101	PEK	C9-C10-C11-C12
24	B	303	PSC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	B	303	PSC	C10-C11-C12-C13
27	T	102	PEK	C12-C13-C14-C15
20	C	309	PGV	C21-C22-C23-C24
20	N	609	PGV	C28-C29-C30-C31
28	P	304	CDL	OA5-CA3-CA4-OA6
28	C	306	CDL	OA5-CA3-CA4-OA6
20	A	609	PGV	C11-C10-C9-C8
20	N	609	PGV	C11-C10-C9-C8
20	A	610	PGV	C11-C10-C9-C8
19	L	101	TGL	CC1-CC2-CC3-CC4
19	L	101	TGL	C29-C30-C31-C32
19	A	608	TGL	CA6-CA7-CA8-CA9
28	N	601	CDL	C17-C18-C19-C20
27	G	102	PEK	C28-C29-C30-C31
27	G	102	PEK	O03-C01-C02-O01
20	Z	101	PGV	O03-C01-C02-O01
28	C	306	CDL	OA6-CA4-CA6-OA8
19	Q	201	TGL	CB5-CB6-CB7-CB8
27	P	307	PEK	C30-C31-C32-C33
22	J	101	CHD	C13-C17-C20-C22
25	P	306	DMU	C22-C25-C28-C31
28	C	306	CDL	C84-C85-C86-C87
28	N	601	CDL	C58-C59-C60-C61
19	A	608	TGL	C29-C30-C31-C32
25	M	101	DMU	C31-C34-C37-C40
22	P	305	CHD	C16-C17-C20-C22
24	O	302	PSC	C13-C14-C15-C16
20	C	309	PGV	C5-C6-C7-C8
19	A	608	TGL	C13-C14-C29-C30
20	C	305	PGV	C24-C25-C26-C27
21	G	104	EDO	O1-C1-C2-O2
21	A	611	EDO	O1-C1-C2-O2
19	Y	101	TGL	CC5-CC6-CC7-CC8
20	A	609	PGV	C23-C24-C25-C26
25	P	309	DMU	C28-C31-C34-C37
19	Q	201	TGL	CC2-CC3-CC4-CC5
19	N	610	TGL	C20-C21-C22-C23
27	G	102	PEK	O03-C21-C22-C23
20	Z	101	PGV	C29-C30-C31-C32
19	Y	101	TGL	CA6-CA7-CA8-CA9
19	L	101	TGL	C14-C29-C30-C31
27	P	307	PEK	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	G	102	PEK	C3-C4-C5-C6
27	T	102	PEK	C17-C18-C19-C20
27	C	304	PEK	C35-C36-C37-C38
25	P	308	DMU	C25-C28-C31-C34
19	Y	101	TGL	C22-C23-C24-C25
24	O	302	PSC	C01-C02-O01-C1
19	D	201	TGL	CG3-CG2-OG2-CB1
19	Q	201	TGL	C15-C16-C17-C18
20	A	610	PGV	C29-C30-C31-C32
25	C	311	DMU	O16-C18-C19-C22
19	L	101	TGL	C15-C16-C17-C18
24	B	303	PSC	C6-C7-C8-C9
28	P	304	CDL	CA5-C11-C12-C13
27	T	101	PEK	O03-C01-C02-C03
20	P	303	PGV	C02-C03-O11-P
19	D	201	TGL	CG1-CG2-CG3-OG3
20	G	103	PGV	O03-C01-C02-C03
19	L	101	TGL	OG1-CG1-CG2-CG3
20	C	309	PGV	C02-C03-O11-P
28	C	306	CDL	C1-CA2-OA2-PA1
28	C	306	CDL	CA4-CA3-OA5-PA1
28	C	306	CDL	CA3-CA4-CA6-OA8
28	N	601	CDL	CB3-CB4-CB6-OB8
28	P	304	CDL	C56-C57-C58-C59
20	C	305	PGV	C27-C28-C29-C30
20	A	609	PGV	C30-C31-C32-C33
25	C	310	DMU	C25-C28-C31-C34
27	T	101	PEK	C30-C31-C32-C33
19	A	608	TGL	OG1-CG1-CG2-OG2
19	N	610	TGL	OG2-CG2-CG3-OG3
19	D	201	TGL	OG2-CG2-CG3-OG3
28	P	304	CDL	OB6-CB4-CB6-OB8
28	C	306	CDL	OB6-CB4-CB6-OB8
28	N	601	CDL	OA6-CA4-CA6-OA8
25	C	310	DMU	C28-C31-C34-C37
20	G	103	PGV	C23-C24-C25-C26
19	L	101	TGL	C22-C23-C24-C25
20	P	303	PGV	C11-C10-C9-C8
27	C	308	PEK	C29-C30-C31-C32
22	J	101	CHD	C21-C20-C22-C23
28	T	103	CDL	C24-C25-C26-C27
19	L	101	TGL	C21-C20-CA9-CA8

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Mol	Chain	Res	Type	Atoms
24	O	302	PSC	C15-C16-C17-C18
19	A	608	TGL	CC9-C15-C16-C17
28	T	103	CDL	CA2-OA2-PA1-OA5
28	P	304	CDL	CA3-OA5-PA1-OA2
20	C	309	PGV	C04-O12-P-O11
28	N	601	CDL	CA2-OA2-PA1-OA5
28	N	601	CDL	CB2-OB2-PB2-OB5
28	C	306	CDL	C17-C18-C19-C20
20	G	103	PGV	C02-C03-O11-P
20	A	610	PGV	C05-C04-O12-P
19	D	201	TGL	C12-C13-C14-C29
27	C	308	PEK	C03-O11-P-O14
27	G	102	PEK	C03-O11-P-O13
27	G	102	PEK	C04-O12-P-O14
20	Z	101	PGV	C03-O11-P-O13
20	Z	101	PGV	C04-O12-P-O14
27	T	101	PEK	C03-O11-P-O14
27	T	101	PEK	C04-O12-P-O14
24	O	302	PSC	C03-O11-P-O13
28	T	103	CDL	CA2-OA2-PA1-OA4
28	T	103	CDL	CB2-OB2-PB2-OB4
28	C	306	CDL	CA3-OA5-PA1-OA3
28	C	306	CDL	CB2-OB2-PB2-OB3
28	C	306	CDL	CB2-OB2-PB2-OB4
28	C	306	CDL	CB3-OB5-PB2-OB3
25	P	308	DMU	C28-C31-C34-C37
20	C	305	PGV	C28-C29-C30-C31
20	A	610	PGV	C31-C32-C33-C34
28	T	103	CDL	C71-CB7-OB8-CB6
27	C	308	PEK	C01-C02-C03-O11
28	C	306	CDL	OA5-CA3-CA4-CA6
27	C	304	PEK	C28-C29-C30-C31
19	Y	101	TGL	C15-C16-C17-C18
19	L	101	TGL	CB5-CB6-CB7-CB8
21	R	205	EDO	O1-C1-C2-O2
19	Q	201	TGL	CC4-CC5-CC6-CC7
27	G	102	PEK	C7-C8-C9-C10
20	N	609	PGV	C15-C16-C17-C18
24	B	303	PSC	C05-C04-O12-P
19	D	201	TGL	OG2-CB1-CB2-CB3
24	O	302	PSC	C28-C29-C30-C31
20	C	309	PGV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
22	W	101	CHD	C17-C20-C22-C23
28	C	306	CDL	C35-C36-C37-C38
28	N	601	CDL	CB7-C71-C72-C73
28	N	601	CDL	C55-C56-C57-C58
28	C	306	CDL	CA2-C1-CB2-OB2
20	G	103	PGV	C2-C3-C4-C5
28	C	306	CDL	C74-C75-C76-C77
28	N	601	CDL	C16-C17-C18-C19
20	Z	101	PGV	O01-C02-C03-O11
27	T	101	PEK	O01-C02-C03-O11
20	C	309	PGV	O01-C02-C03-O11
28	T	103	CDL	OB9-CB7-OB8-CB6
20	G	103	PGV	C4-C5-C6-C7
20	G	103	PGV	C1-C2-C3-C4
28	T	103	CDL	C11-C12-C13-C14
19	A	608	TGL	OG1-CG1-CG2-CG3
14	A	602[A]	HEA	C2D-C3D-CAD-CBD
14	A	602[A]	HEA	C4D-C3D-CAD-CBD
19	Q	201	TGL	OG2-CG2-CG3-OG3
24	O	302	PSC	O03-C01-C02-O01
19	Y	101	TGL	OG1-CG1-CG2-OG2
19	D	201	TGL	OG1-CG1-CG2-OG2
19	L	101	TGL	OG1-CG1-CG2-OG2
28	P	304	CDL	OA6-CA4-CA6-OA8
28	T	103	CDL	C74-C75-C76-C77
19	D	201	TGL	C25-C26-C27-C28
27	C	308	PEK	C34-C35-C36-C37
24	O	302	PSC	C02-C03-O11-P
20	C	305	PGV	C02-C03-O11-P
28	C	306	CDL	C31-CA7-OA8-CA6
27	G	102	PEK	C26-C27-C28-C29
28	C	306	CDL	C40-C41-C42-C43
28	N	601	CDL	C57-C58-C59-C60
28	T	103	CDL	C38-C39-C40-C41
22	J	101	CHD	C16-C17-C20-C21
27	G	102	PEK	C35-C36-C37-C38
19	L	101	TGL	C24-C25-C26-C27
28	C	306	CDL	OA9-CA7-OA8-CA6
27	T	102	PEK	C16-C17-C18-C19
25	P	308	DMU	O16-C18-C19-C22
19	Y	101	TGL	CC2-CC3-CC4-CC5
19	D	201	TGL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	C	304	PEK	C29-C30-C31-C32
21	U	101	EDO	O1-C1-C2-O2
21	A	614	EDO	O1-C1-C2-O2
21	R	203	EDO	O1-C1-C2-O2
28	C	306	CDL	C56-C57-C58-C59
27	P	307	PEK	O01-C1-C2-C3
22	C	307	CHD	C16-C17-C20-C21
28	T	103	CDL	OA6-CA4-CA6-OA8
19	Q	201	TGL	C29-C30-C31-C32
19	L	101	TGL	CC7-CC8-CC9-C15
24	O	302	PSC	C04-O12-P-O11
20	A	610	PGV	C04-O12-P-O11
28	P	304	CDL	CA2-OA2-PA1-OA5
27	G	102	PEK	O03-C01-C02-C03
19	L	101	TGL	CG1-CG2-CG3-OG3
19	A	608	TGL	C11-C10-CB9-CB8
19	N	610	TGL	C24-C25-C26-C27
28	P	304	CDL	C72-C73-C74-C75
19	Q	201	TGL	OG1-CA1-CA2-CA3
28	T	103	CDL	C52-C51-CB5-OB6
24	B	303	PSC	C31-C32-C33-C34
28	P	304	CDL	CA4-CA3-OA5-PA1
20	Z	101	PGV	C5-C6-C7-C8
27	C	308	PEK	C14-C15-C16-C17
28	T	103	CDL	C56-C57-C58-C59
27	G	102	PEK	C4-C5-C6-C7
28	C	306	CDL	C51-C52-C53-C54
28	N	601	CDL	C83-C84-C85-C86
19	Q	201	TGL	CC7-CC8-CC9-C15
28	N	601	CDL	C61-C62-C63-C64
19	N	610	TGL	CC5-CC6-CC7-CC8
28	P	304	CDL	OB9-CB7-OB8-CB6
19	N	610	TGL	CA2-CA3-CA4-CA5
19	N	610	TGL	C12-C13-C14-C29
20	G	103	PGV	C6-C7-C8-C9
28	C	306	CDL	C31-C32-C33-C34
19	L	101	TGL	OG1-CA1-CA2-CA3
19	Y	101	TGL	C24-C25-C26-C27
20	P	303	PGV	C05-C04-O12-P
25	C	302	DMU	C22-C25-C28-C31
27	T	101	PEK	C24-C25-C26-C27
19	D	201	TGL	CB7-CB8-CB9-C10

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Mol	Chain	Res	Type	Atoms
21	C	320	EDO	O1-C1-C2-O2
21	A	619	EDO	O1-C1-C2-O2
20	Z	101	PGV	C13-C14-C15-C16
27	C	308	PEK	C24-C25-C26-C27
25	P	309	DMU	C31-C34-C37-C40
19	D	201	TGL	CC9-C15-C16-C17
24	O	302	PSC	C14-C15-C16-C17
19	L	101	TGL	C16-C15-CC9-CC8
25	L	102	DMU	C4-C3-O7-C10
27	C	308	PEK	C6-C7-C8-C9
27	P	307	PEK	C11-C10-C9-C8
27	T	102	PEK	C5-C6-C7-C8
27	G	102	PEK	C31-C32-C33-C34
19	N	610	TGL	CB2-CB3-CB4-CB5
20	Z	101	PGV	C20-C21-C22-C23
19	D	201	TGL	CB2-CB1-OG2-CG2
22	J	101	CHD	C13-C17-C20-C21
14	N	602	HEA	C26-C15-C16-C17
27	C	308	PEK	C1-C2-C3-C4
28	T	103	CDL	C76-C77-C78-C79
28	C	306	CDL	C21-C22-C23-C24
19	D	201	TGL	OB1-CB1-OG2-CG2
28	P	304	CDL	C78-C79-C80-C81
19	Q	201	TGL	CB1-CB2-CB3-CB4
27	P	307	PEK	C2-C3-C4-C5
19	N	610	TGL	CC2-CC3-CC4-CC5
20	C	309	PGV	C4-C5-C6-C7
19	N	610	TGL	C33-C34-C35-C36
19	D	201	TGL	CB3-CB4-CB5-CB6
19	L	101	TGL	CC3-CC4-CC5-CC6
20	C	309	PGV	C24-C25-C26-C27
19	Q	201	TGL	OG2-CB1-CB2-CB3
27	T	102	PEK	O03-C21-C22-C23
19	N	610	TGL	CG1-CG2-CG3-OG3
21	D	205	EDO	O1-C1-C2-O2
21	E	204	EDO	O1-C1-C2-O2
21	Q	203	EDO	O1-C1-C2-O2
21	A	622	EDO	O1-C1-C2-O2
21	R	206	EDO	O1-C1-C2-O2
21	N	612	EDO	O1-C1-C2-O2
21	S	103	EDO	O1-C1-C2-O2
22	C	301	CHD	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
28	P	304	CDL	C38-C39-C40-C41
14	N	603[B]	HEA	C26-C15-C16-C17
19	N	610	TGL	OG3-CC1-CC2-CC3
27	T	102	PEK	C2-C1-O01-C02
19	A	608	TGL	CC4-CC5-CC6-CC7
19	N	610	TGL	C22-C23-C24-C25
28	T	103	CDL	C72-C73-C74-C75
28	P	304	CDL	C13-C14-C15-C16
28	P	304	CDL	C42-C43-C44-C45
20	A	609	PGV	O03-C19-C20-C21
27	P	307	PEK	C27-C28-C29-C30
22	C	307	CHD	C13-C17-C20-C22
25	C	310	DMU	C18-C19-C22-C25
28	C	306	CDL	C44-C45-C46-C47
19	Y	101	TGL	OG1-CA1-CA2-CA3
24	B	303	PSC	O01-C1-C2-C3
20	Z	101	PGV	C15-C16-C17-C18
27	T	102	PEK	C25-C26-C27-C28
20	P	303	PGV	C22-C23-C24-C25
28	P	304	CDL	C71-CB7-OB8-CB6
28	T	103	CDL	CB2-C1-CA2-OA2
20	A	610	PGV	C24-C25-C26-C27
28	P	304	CDL	C35-C36-C37-C38
28	C	306	CDL	OB9-CB7-OB8-CB6
19	Y	101	TGL	CC7-CC8-CC9-C15
20	C	305	PGV	C13-C14-C15-C16
24	O	302	PSC	C7-C8-C9-C10
19	Q	201	TGL	OG3-CC1-CC2-CC3
14	A	601	HEA	C26-C15-C16-C17
28	N	601	CDL	C44-C45-C46-C47
25	P	306	DMU	O6-C11-C9-O1
28	P	304	CDL	C76-C77-C78-C79
20	P	303	PGV	C21-C22-C23-C24
28	P	304	CDL	C84-C85-C86-C87
20	G	103	PGV	C25-C26-C27-C28
19	A	608	TGL	OG3-CC1-CC2-CC3
24	B	303	PSC	C12-C13-C14-C15
28	P	304	CDL	C44-C45-C46-C47
27	T	101	PEK	O03-C21-C22-C23
19	N	610	TGL	OG1-CA1-CA2-CA3
28	T	103	CDL	C55-C56-C57-C58
19	D	201	TGL	OG1-CA1-CA2-CA3

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Mol	Chain	Res	Type	Atoms
20	Z	101	PGV	C9-C10-C11-C12
27	T	101	PEK	C3-C4-C5-C6
20	G	103	PGV	C9-C10-C11-C12
20	A	610	PGV	O03-C01-C02-C03
28	T	103	CDL	OB5-CB3-CB4-OB6
20	G	103	PGV	O01-C02-C03-O11
28	P	304	CDL	OB5-CB3-CB4-OB6
28	C	306	CDL	C71-CB7-OB8-CB6
19	A	608	TGL	C14-C29-C30-C31
21	A	621	EDO	O1-C1-C2-O2
21	C	315	EDO	O1-C1-C2-O2
21	E	203	EDO	O1-C1-C2-O2
21	A	612	EDO	O1-C1-C2-O2
21	C	313	EDO	O1-C1-C2-O2
27	T	102	PEK	O01-C1-C2-C3
27	C	308	PEK	C17-C18-C19-C20
25	P	308	DMU	O6-C11-C9-C8
20	G	103	PGV	C14-C15-C16-C17
20	N	609	PGV	O03-C19-C20-C21
24	B	303	PSC	O03-C19-C20-C21
19	N	610	TGL	C21-C22-C23-C24
19	Q	201	TGL	C24-C25-C26-C27
24	B	303	PSC	C14-C15-C16-C17
19	D	201	TGL	OG3-CC1-CC2-CC3
19	D	201	TGL	C20-C21-C22-C23
24	O	302	PSC	O03-C19-C20-C21
20	N	609	PGV	C11-C12-C13-C14
24	B	303	PSC	C7-C8-C9-C10
20	C	305	PGV	C9-C10-C11-C12
20	C	305	PGV	C11-C12-C13-C14
14	N	602	HEA	C14-C15-C16-C17
19	D	201	TGL	OA1-CA1-CA2-CA3
20	A	610	PGV	C28-C29-C30-C31
19	Q	201	TGL	OC1-CC1-CC2-CC3
19	D	201	TGL	OC1-CC1-CC2-CC3
19	Q	201	TGL	CG1-CG2-CG3-OG3
19	N	610	TGL	C10-C11-C12-C13
25	P	306	DMU	C19-C22-C25-C28
28	C	306	CDL	C79-C80-C81-C82
27	T	102	PEK	O02-C1-O01-C02
20	C	309	PGV	C19-C20-C21-C22
19	A	608	TGL	OC1-CC1-CC2-CC3

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Mol	Chain	Res	Type	Atoms
20	G	103	PGV	C30-C31-C32-C33
25	Z	102	DMU	C31-C34-C37-C40
20	A	610	PGV	C04-O12-P-O13
28	P	304	CDL	CA3-OA5-PA1-OA3
20	G	103	PGV	C26-C27-C28-C29
27	T	101	PEK	O04-C21-C22-C23
27	T	102	PEK	O02-C1-C2-C3
27	P	307	PEK	C01-C02-C03-O11
24	O	302	PSC	O04-C19-C20-C21
21	D	202	EDO	O1-C1-C2-O2
21	A	618	EDO	O1-C1-C2-O2
21	N	616	EDO	O1-C1-C2-O2
21	G	105	EDO	O1-C1-C2-O2
21	B	305	EDO	O1-C1-C2-O2
21	E	201	EDO	O1-C1-C2-O2
28	N	601	CDL	C73-C74-C75-C76
27	G	102	PEK	O04-C21-C22-C23
19	A	608	TGL	CA9-C20-C21-C22
19	L	101	TGL	C13-C14-C29-C30
19	Q	201	TGL	CG3-CG2-OG2-CB1
27	T	101	PEK	C03-C02-O01-C1
19	D	201	TGL	CG1-CG2-OG2-CB1
27	G	102	PEK	C21-C22-C23-C24
28	T	103	CDL	C32-C33-C34-C35
28	C	306	CDL	C12-C11-CA5-OA6
19	L	101	TGL	C23-C24-C25-C26
28	C	306	CDL	C78-C79-C80-C81
28	N	601	CDL	C36-C37-C38-C39
24	B	303	PSC	O04-C19-C20-C21
14	N	602	HEA	C27-C19-C20-C21
28	C	306	CDL	C12-C11-CA5-OA7
28	C	306	CDL	C52-C51-CB5-OB6
20	Z	101	PGV	O03-C19-C20-C21

There are no ring outliers.

79 monomers are involved in 470 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	603[B]	HEA	12	0
21	N	618	EDO	6	0
19	Q	201	TGL	10	0
22	C	301	CHD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	304	PEK	8	0
27	C	308	PEK	11	0
21	O	305	EDO	1	0
21	D	202	EDO	7	0
21	D	206	EDO	2	0
14	A	601	HEA	6	0
21	P	312	EDO	1	0
22	W	101	CHD	9	0
21	A	621	EDO	5	0
21	C	315	EDO	1	0
25	P	309	DMU	1	0
27	G	102	PEK	10	0
27	P	307	PEK	10	0
20	A	609	PGV	6	0
20	Z	101	PGV	12	0
21	D	204	EDO	2	0
21	R	202	EDO	1	0
22	C	307	CHD	6	0
21	A	618	EDO	3	0
27	T	101	PEK	4	0
18	A	607	AZI	6	0
21	R	205	EDO	1	0
22	P	301	CHD	1	0
19	A	608	TGL	3	0
21	C	316	EDO	2	0
14	A	602[B]	HEA	11	0
25	C	311	DMU	1	0
18	N	607	AZI	1	0
18	N	608	AZI	6	0
20	N	609	PGV	2	0
19	N	610	TGL	8	0
24	O	302	PSC	12	0
18	A	606	AZI	2	0
22	J	101	CHD	2	0
21	A	622	EDO	1	0
21	A	617	EDO	1	0
14	N	603[A]	HEA	8	0
25	C	302	DMU	12	0
21	H	102	EDO	1	0
21	O	304	EDO	1	0
21	D	203	EDO	4	0
14	N	602	HEA	7	0

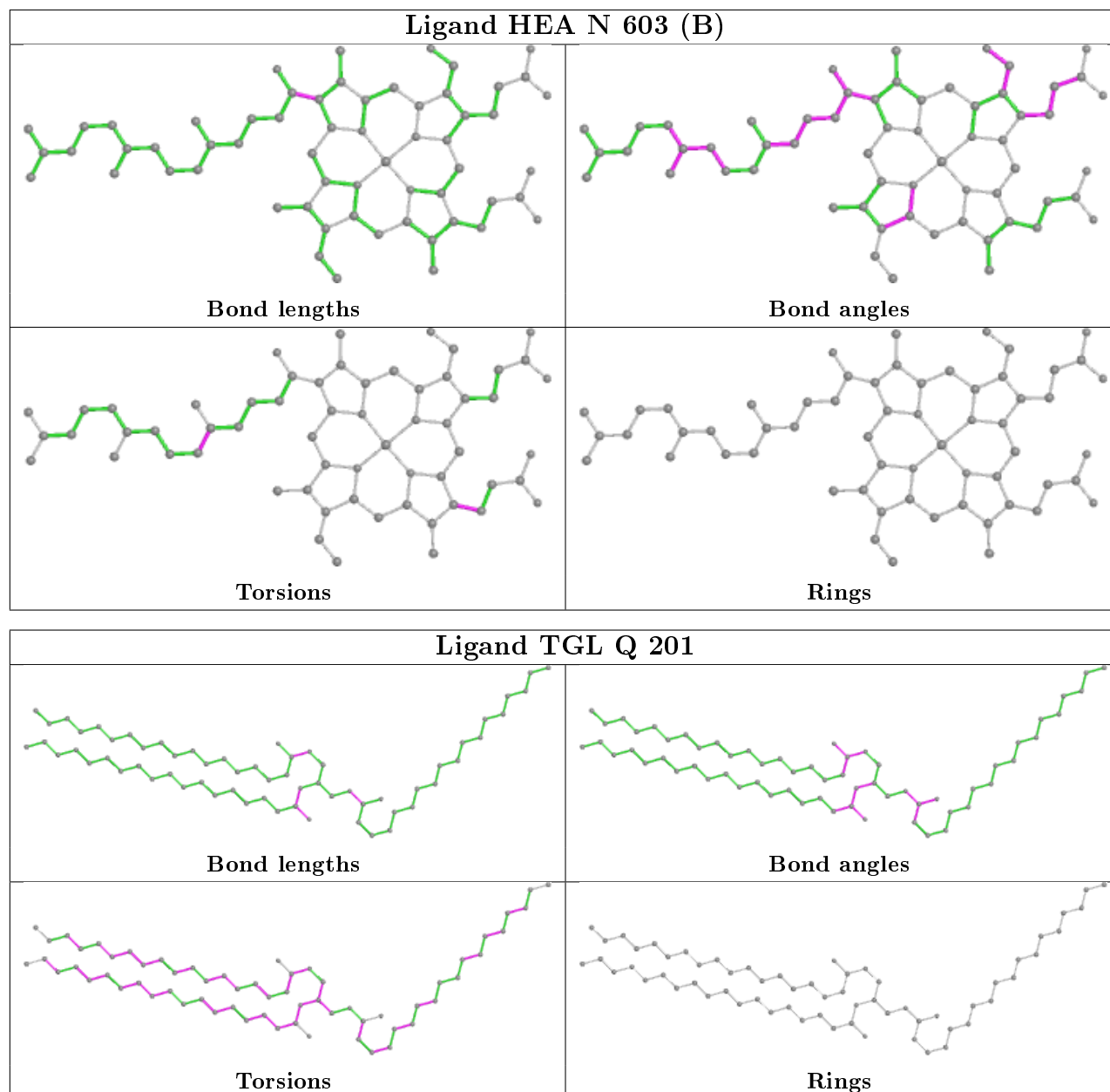
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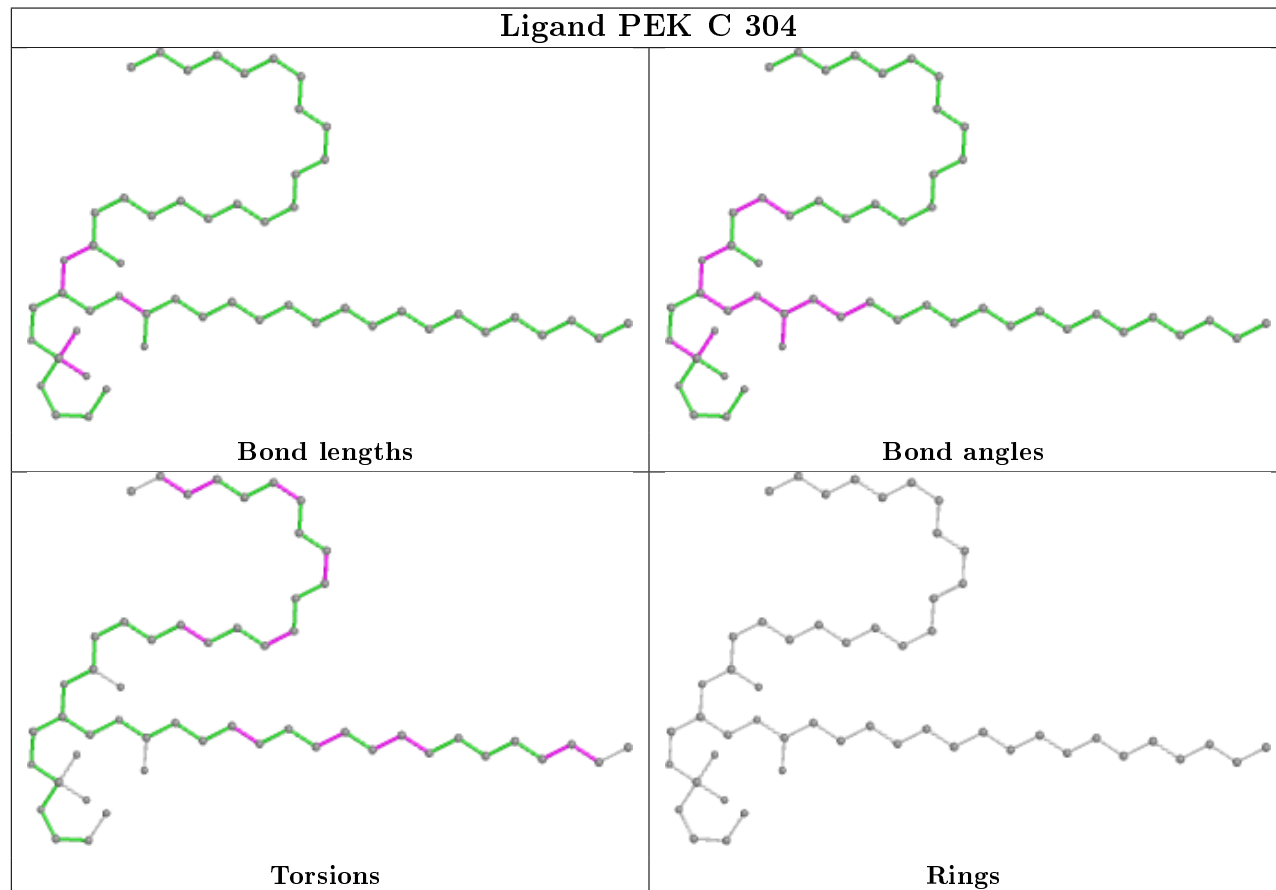
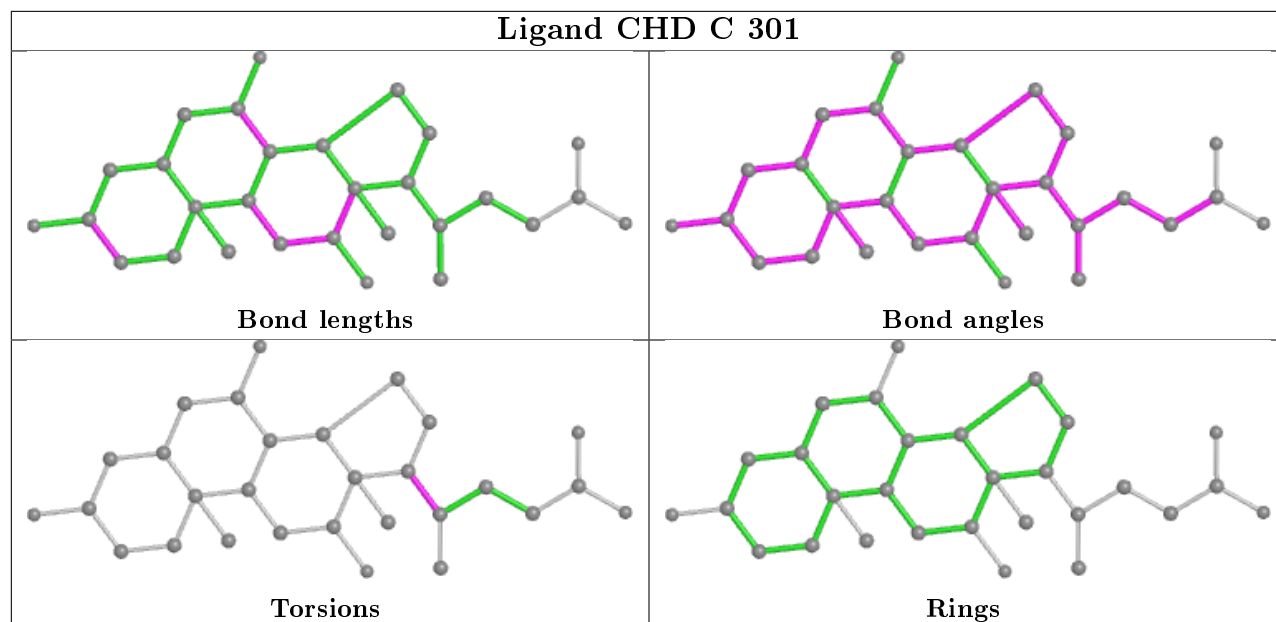
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	T	103	CDL	20	0
21	H	101	EDO	3	0
25	C	310	DMU	5	0
21	A	613	EDO	2	0
19	Y	101	TGL	13	0
20	P	303	PGV	3	0
19	D	201	TGL	21	0
25	P	306	DMU	16	0
22	P	305	CHD	6	0
21	C	317	EDO	1	0
21	G	104	EDO	1	0
25	P	308	DMU	1	0
24	B	303	PSC	23	0
20	C	305	PGV	3	0
20	G	103	PGV	4	0
21	N	612	EDO	3	0
21	A	619	EDO	2	0
20	A	610	PGV	7	0
14	A	602[A]	HEA	10	0
19	L	101	TGL	4	0
28	P	304	CDL	25	0
21	N	621	EDO	6	0
20	C	309	PGV	8	0
21	A	615	EDO	6	0
22	G	101	CHD	1	0
21	F	105	EDO	5	0
28	C	306	CDL	30	0
21	N	613	EDO	1	0
25	L	102	DMU	5	0
27	T	102	PEK	4	0
25	M	101	DMU	1	0
21	N	622	EDO	7	0
28	N	601	CDL	15	0

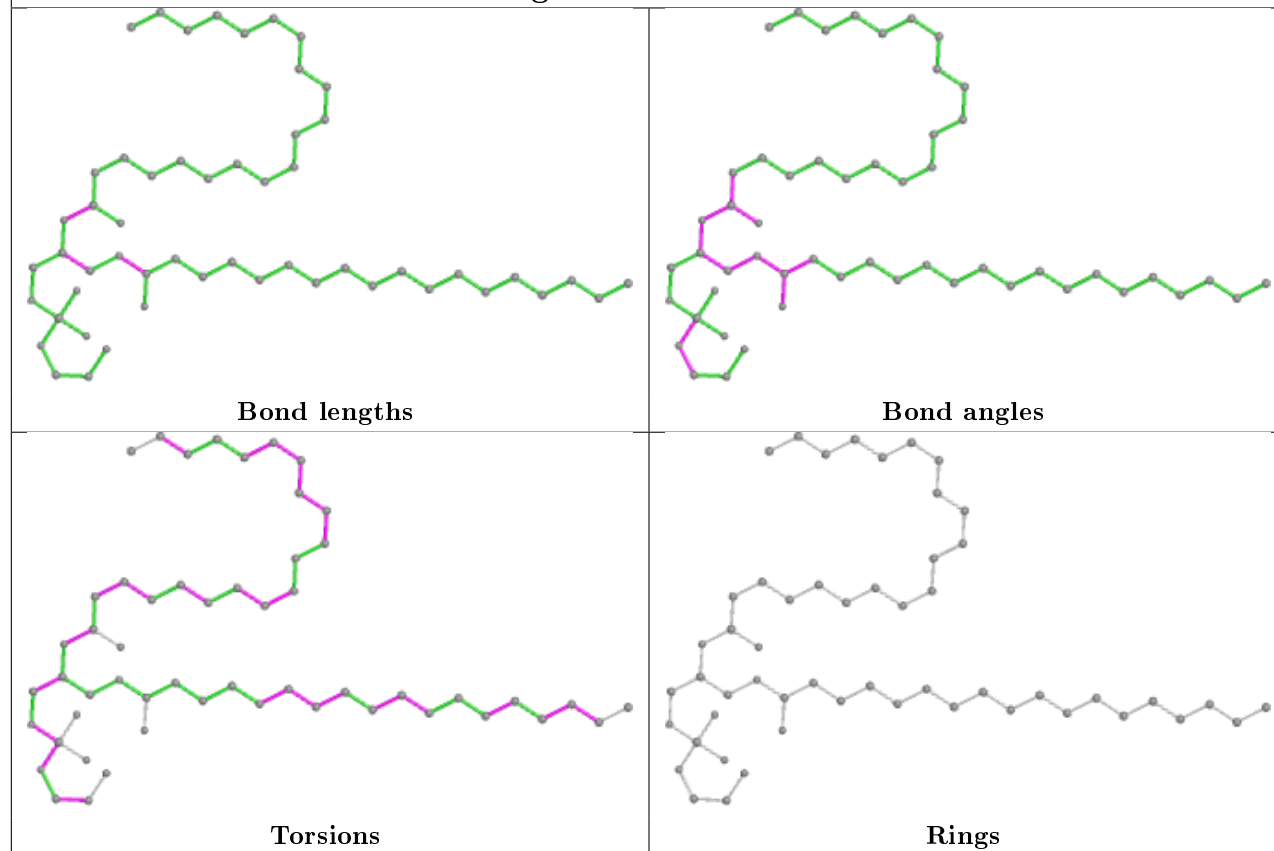
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

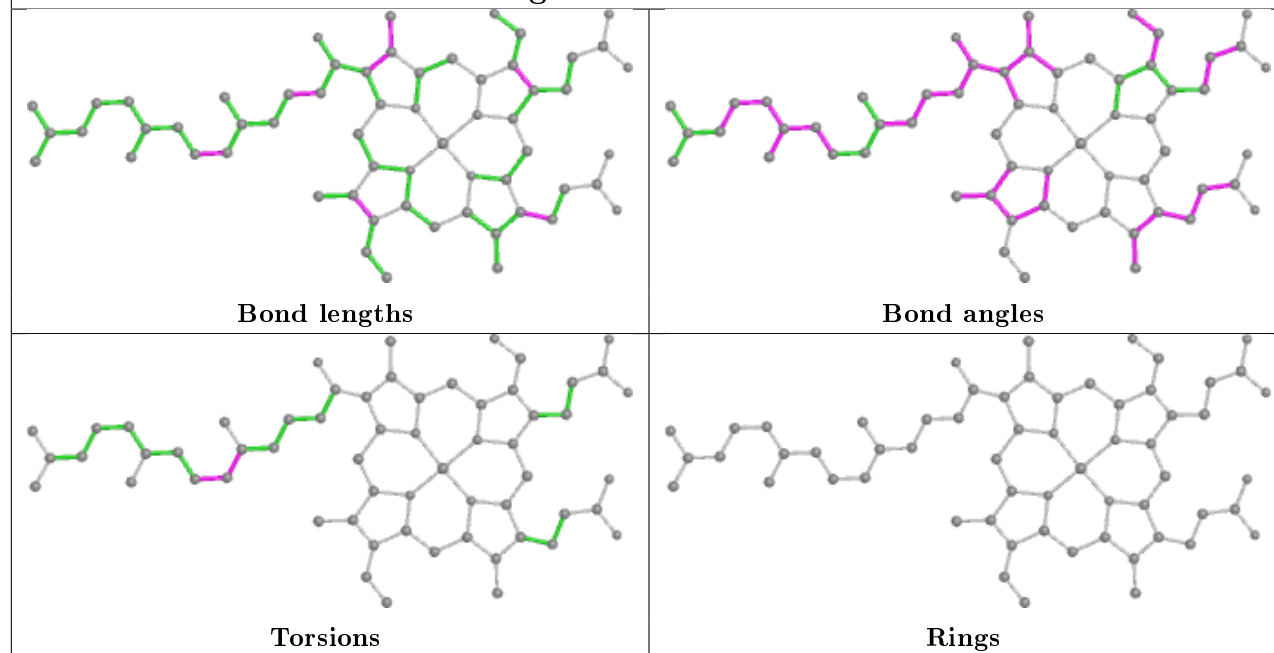


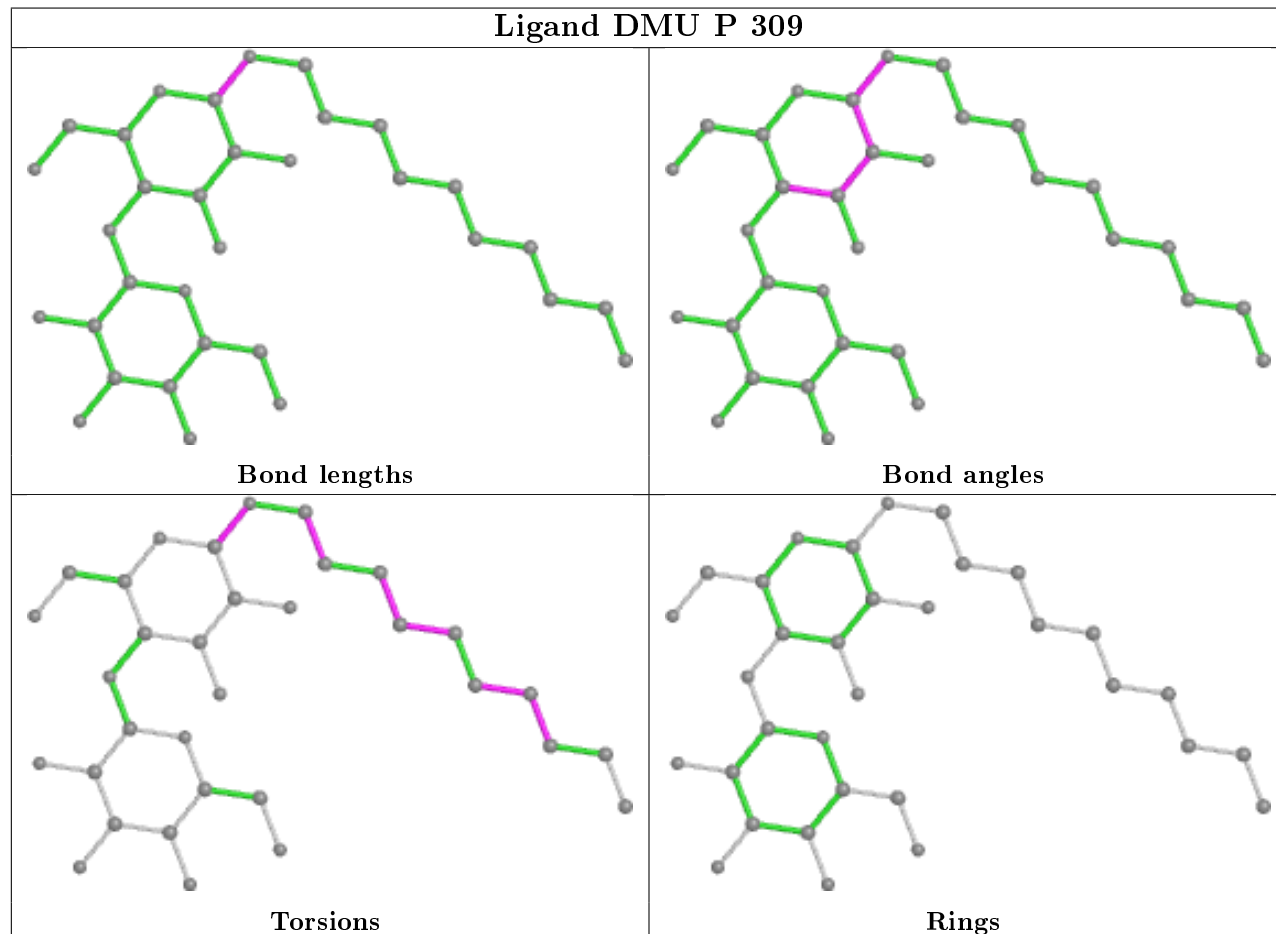
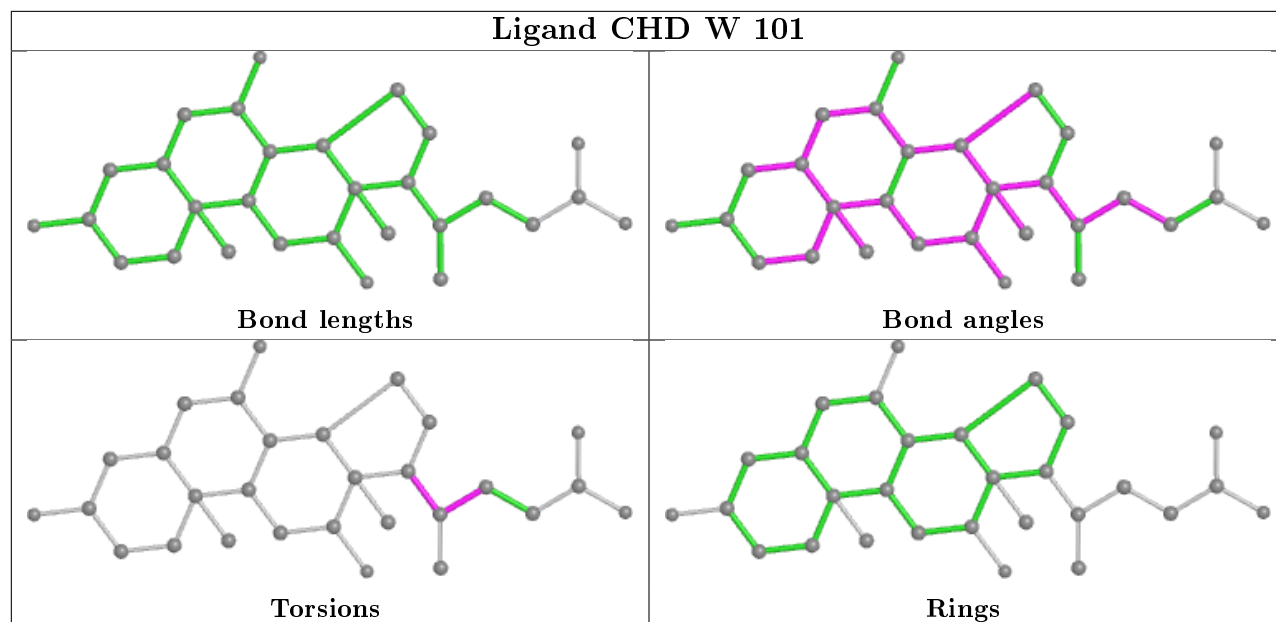


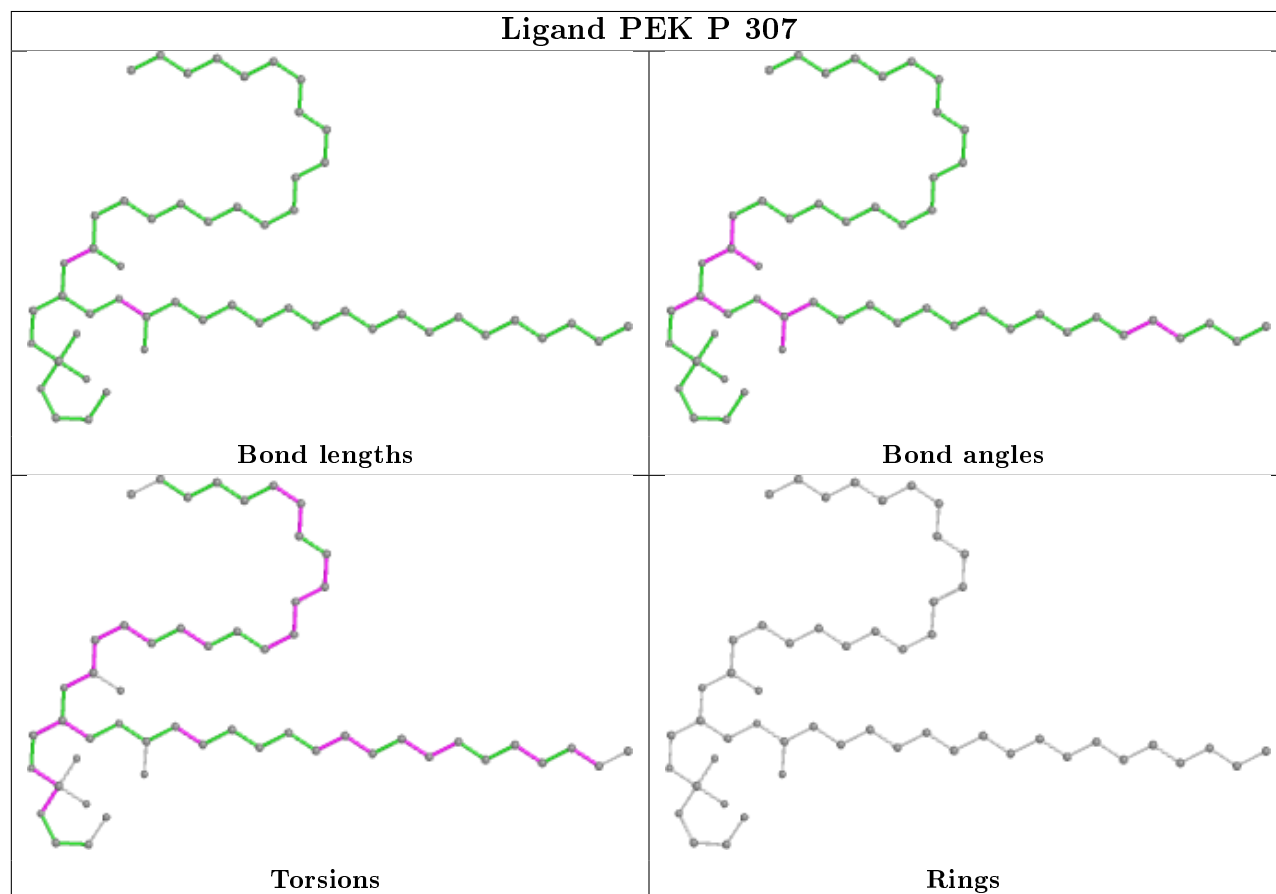
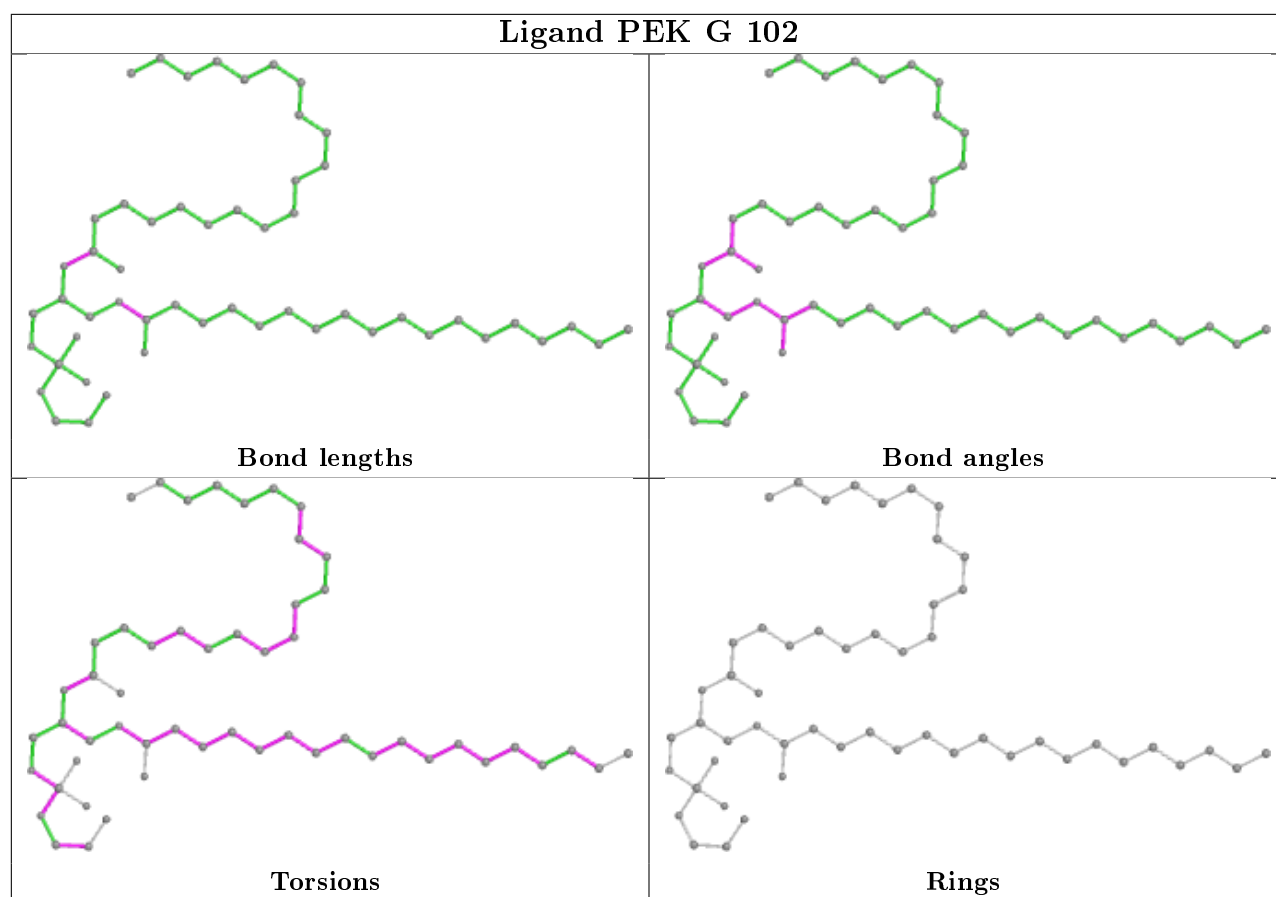
Ligand PEK C 308

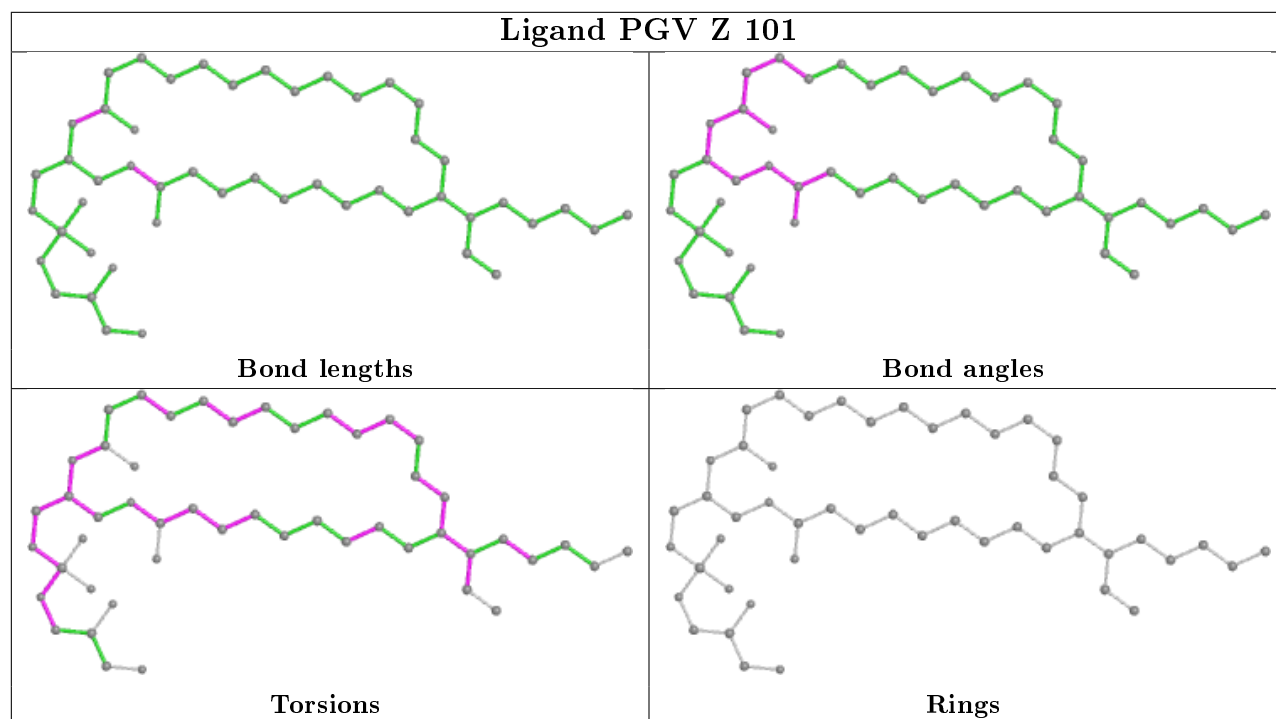
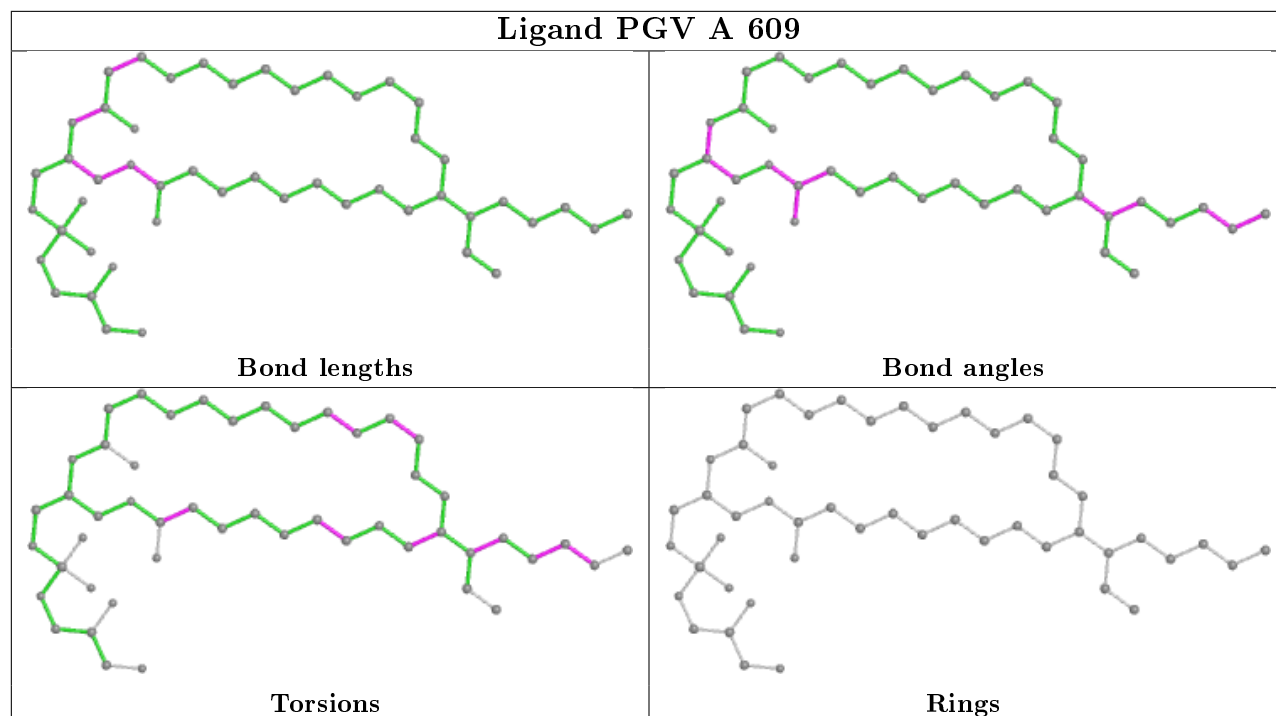


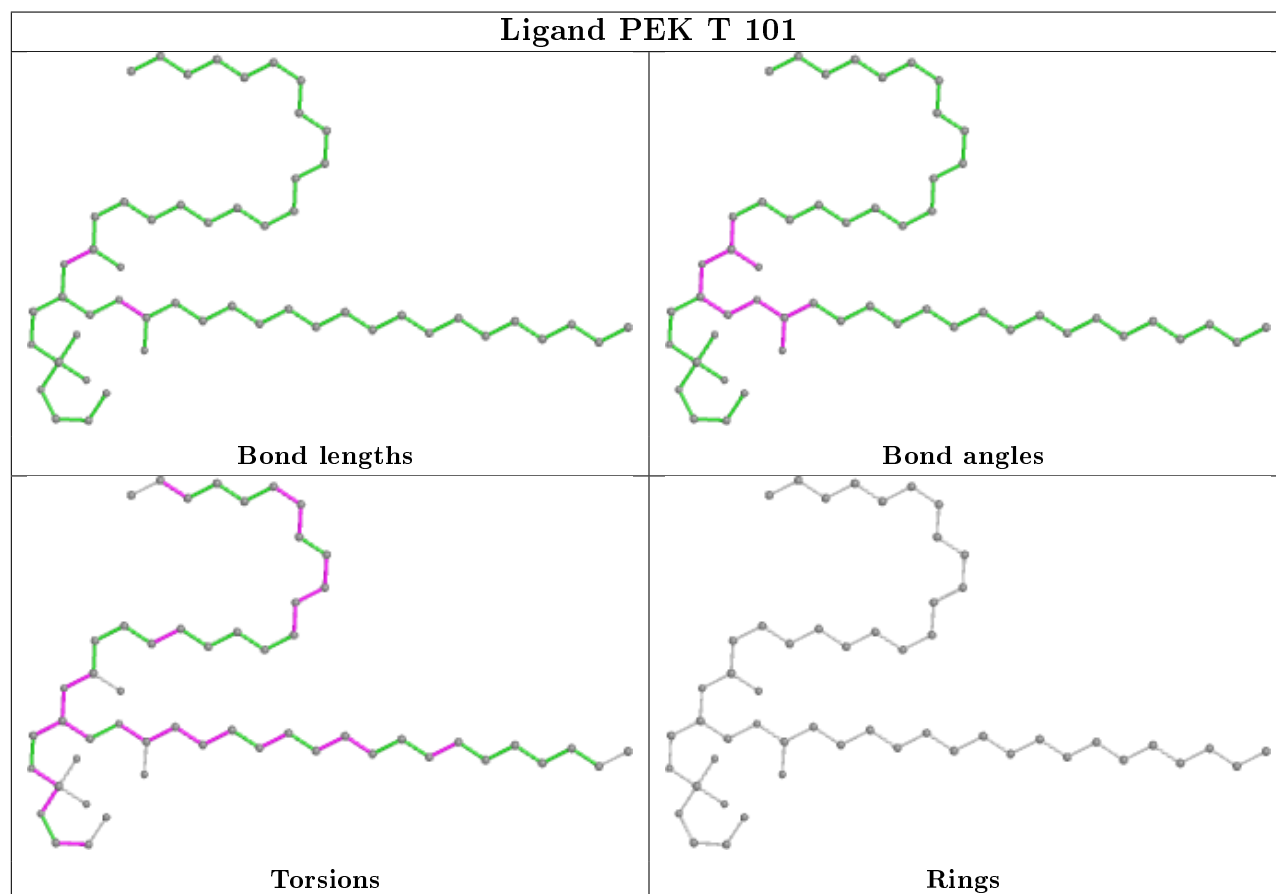
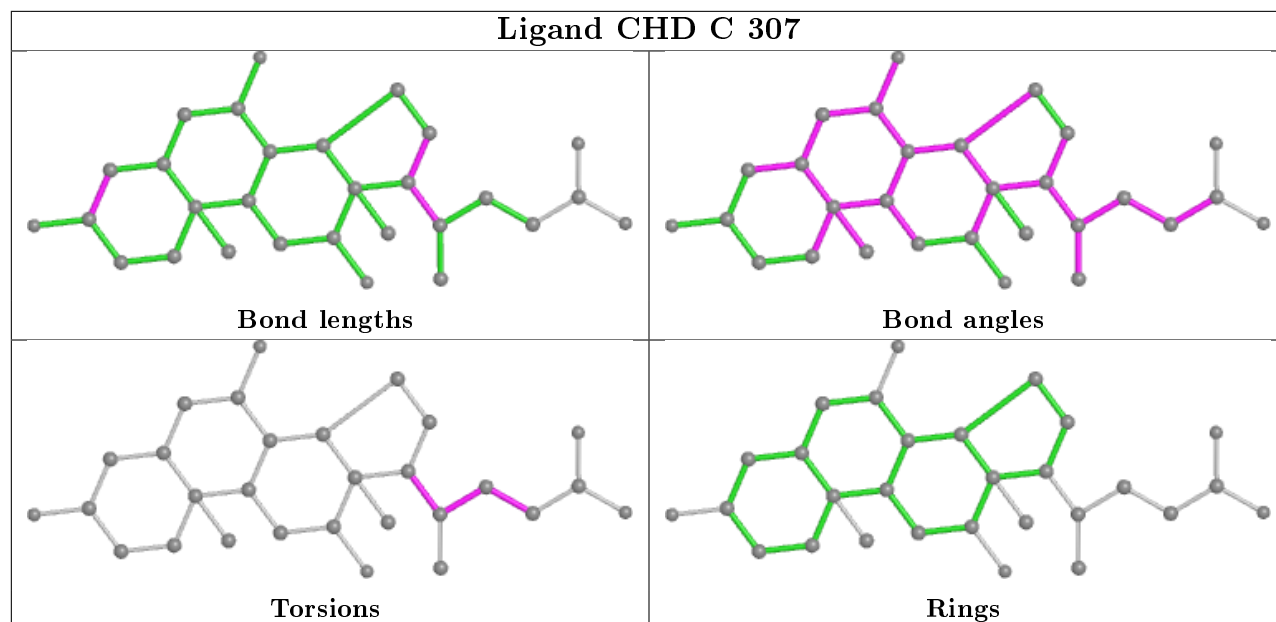
Ligand HEA A 601

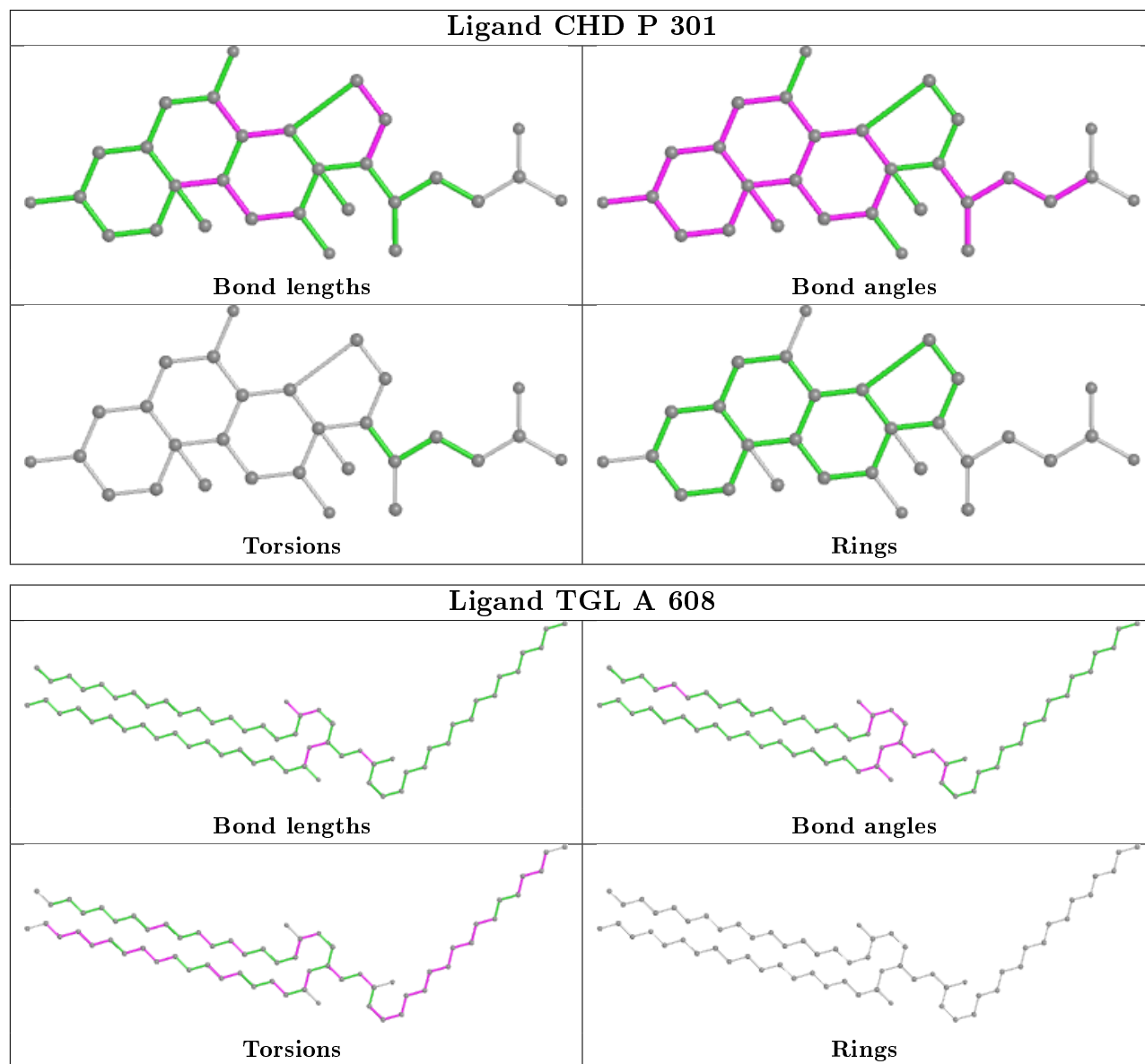




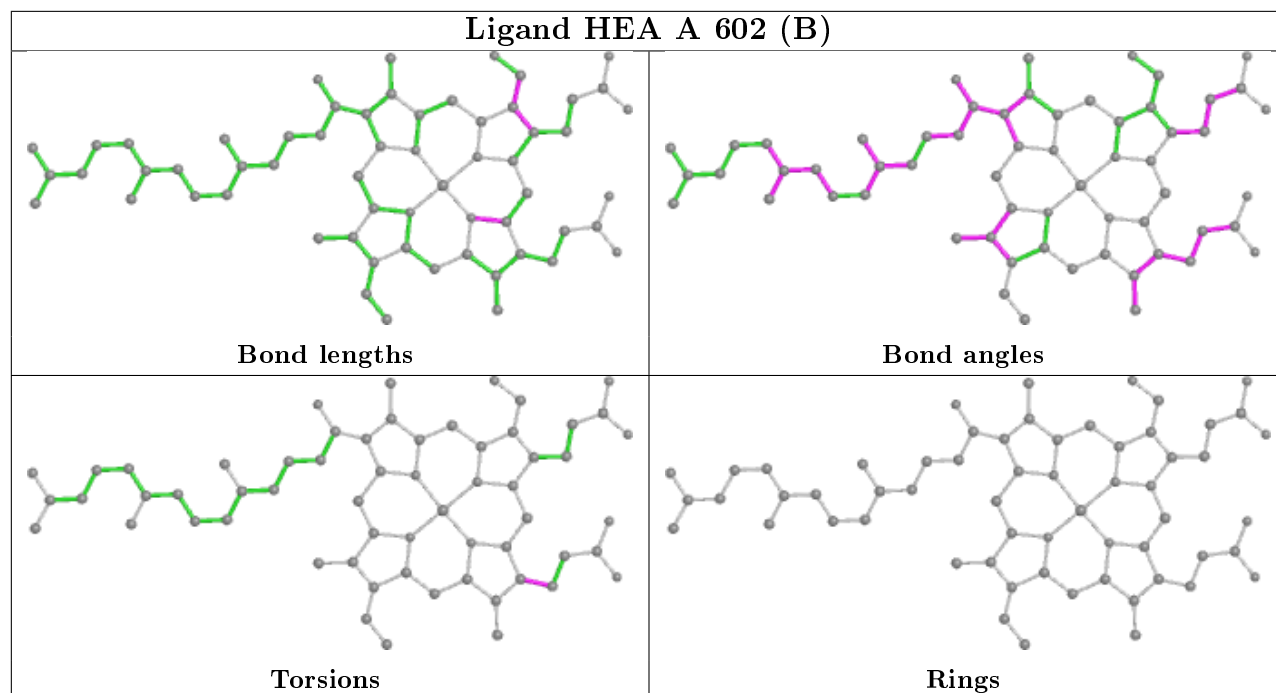




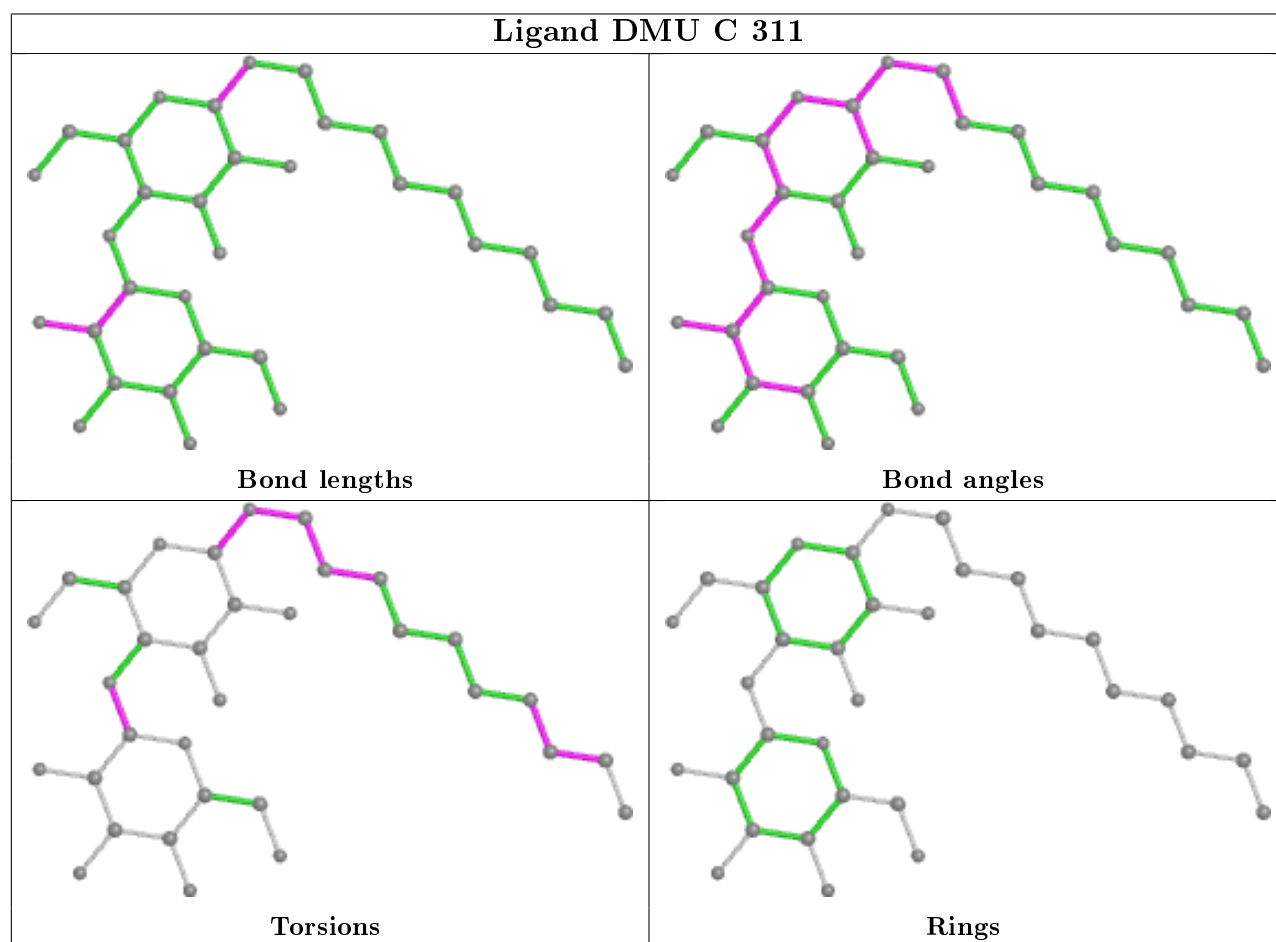


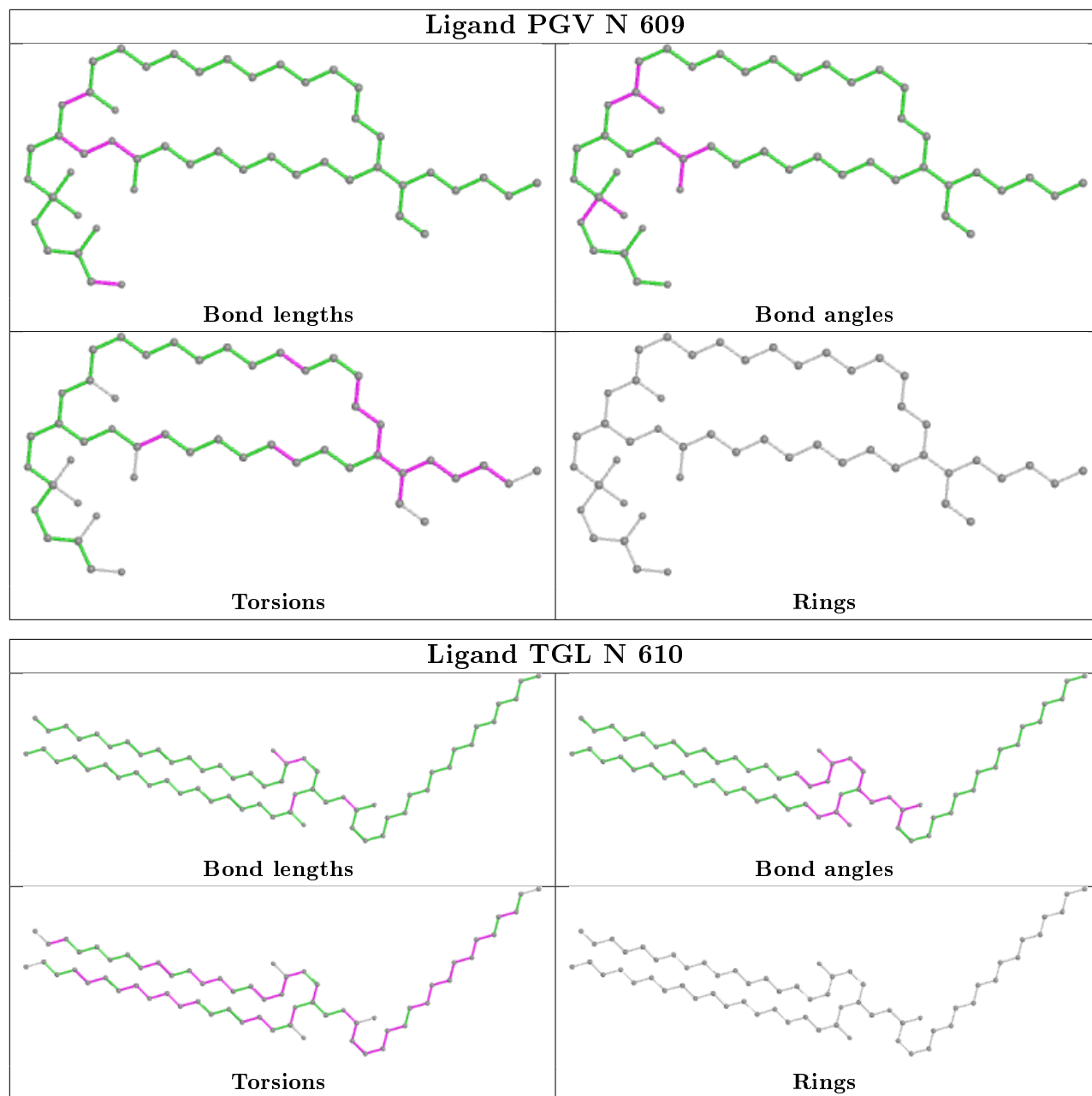


Ligand HEA A 602 (B)

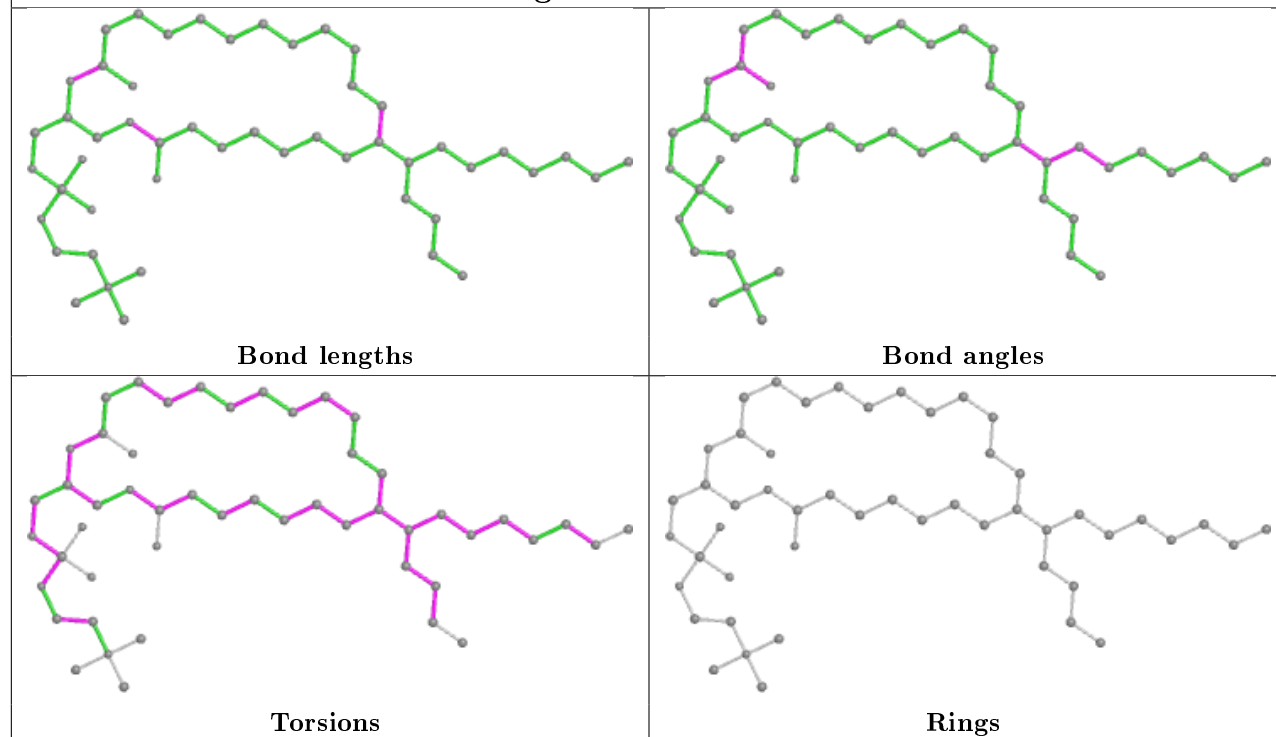


Ligand DMU C 311

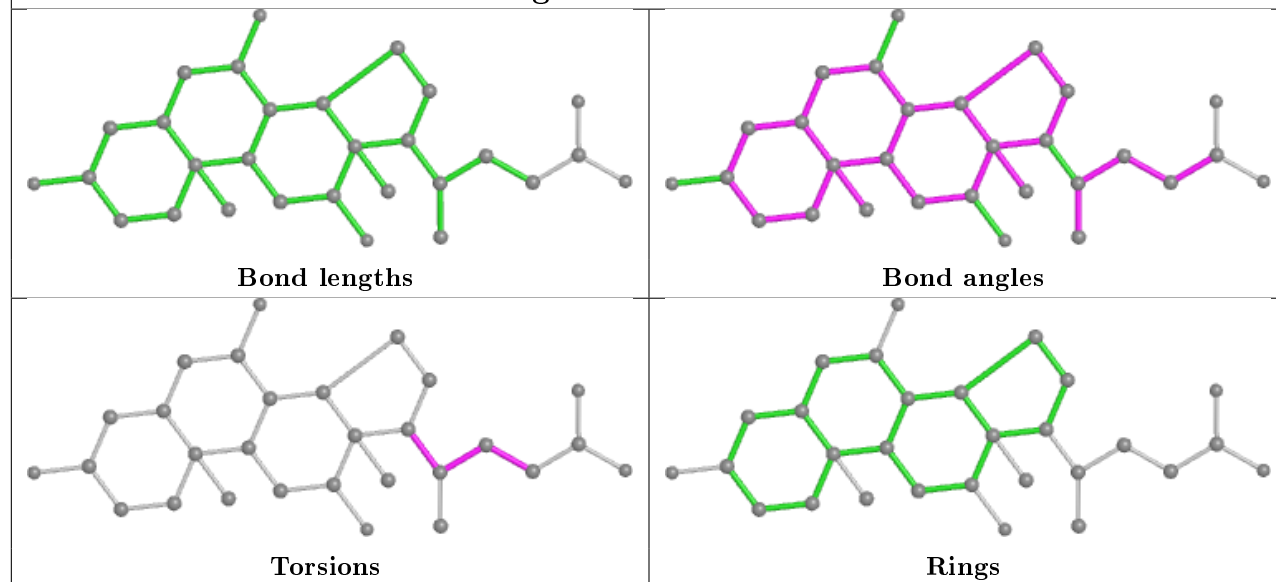


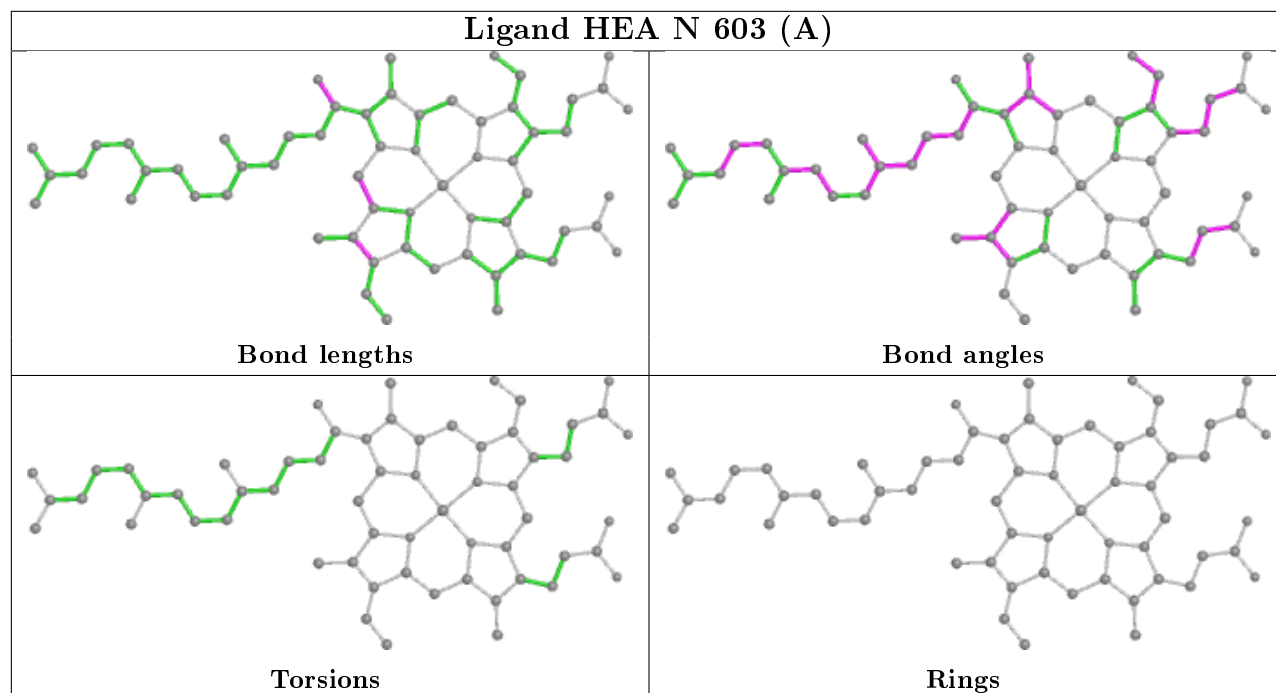
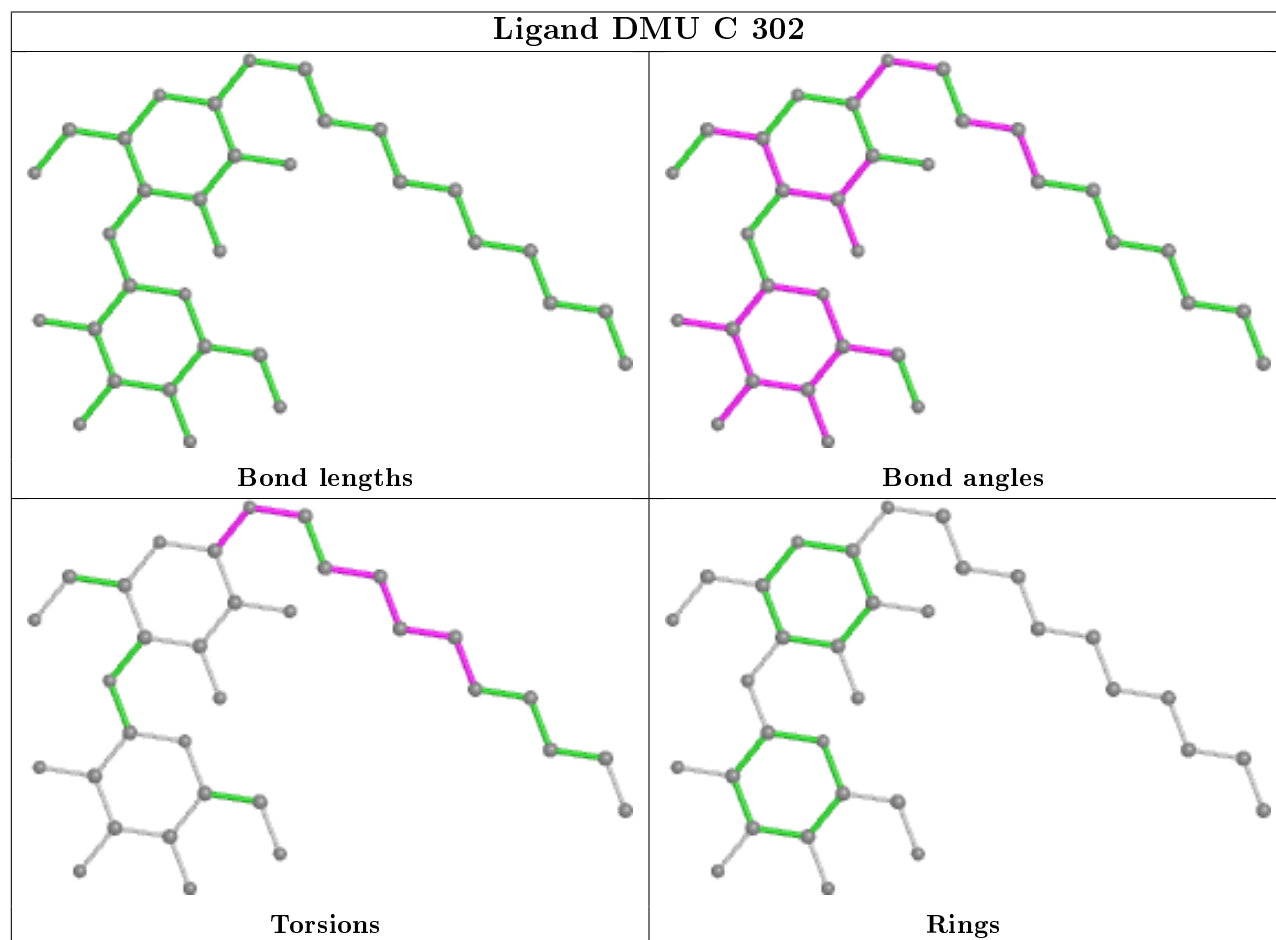


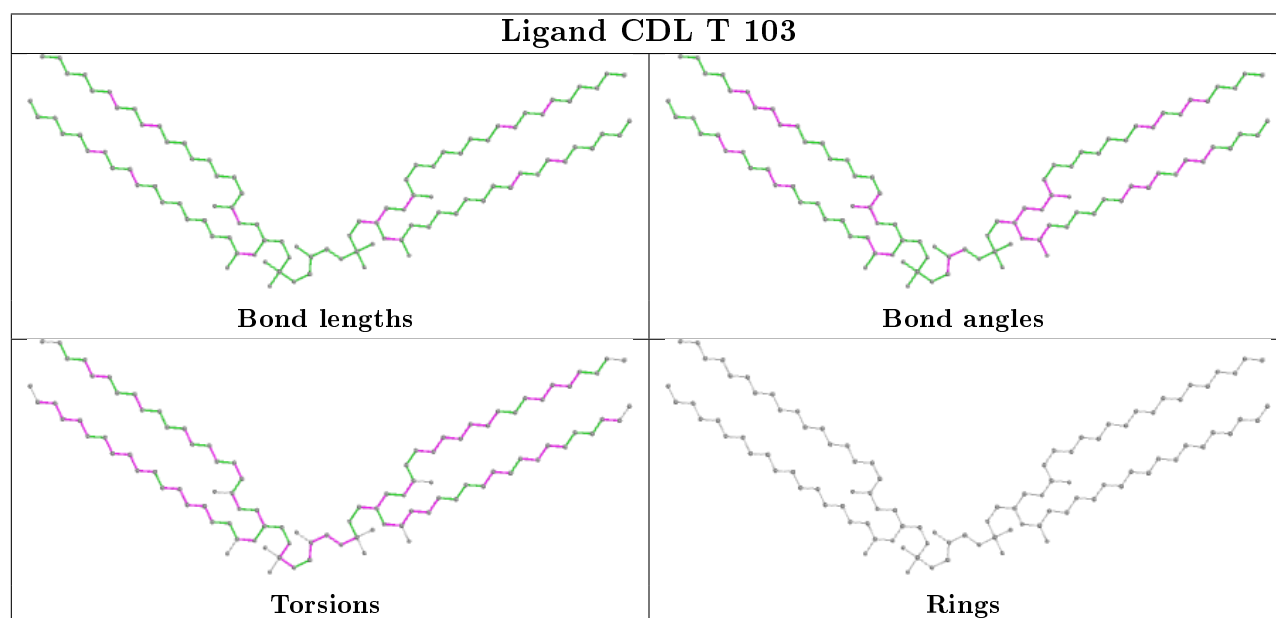
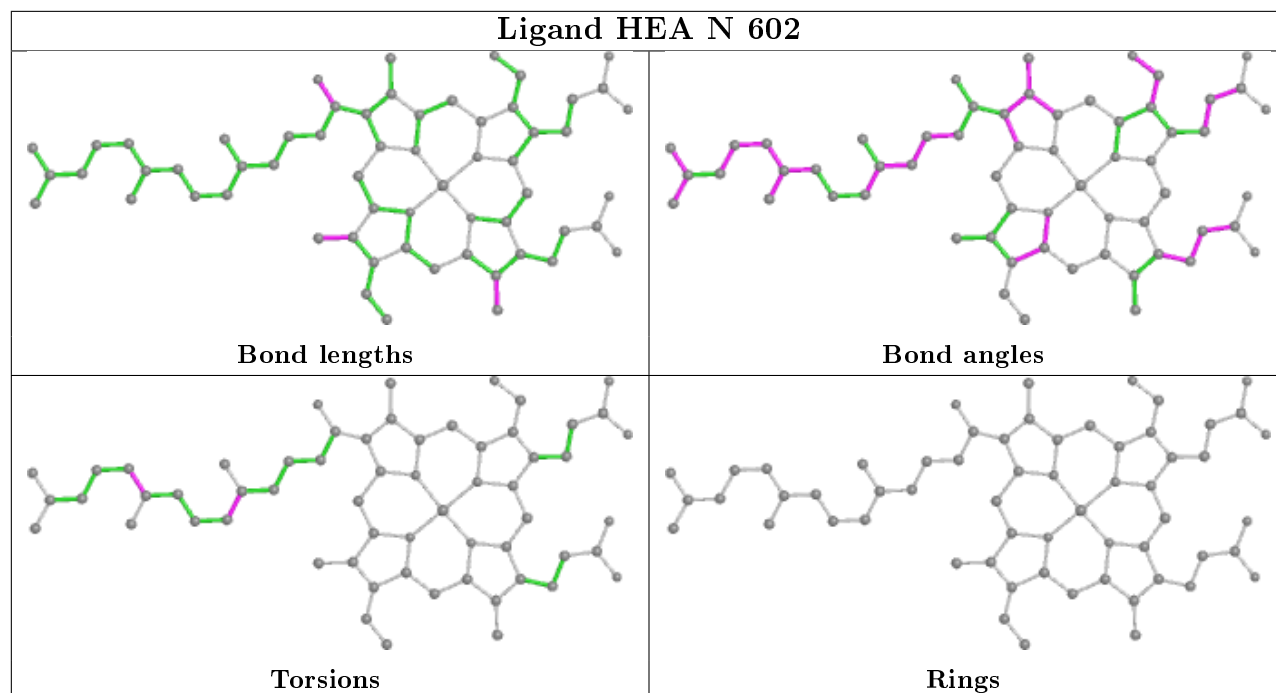
Ligand PSC O 302

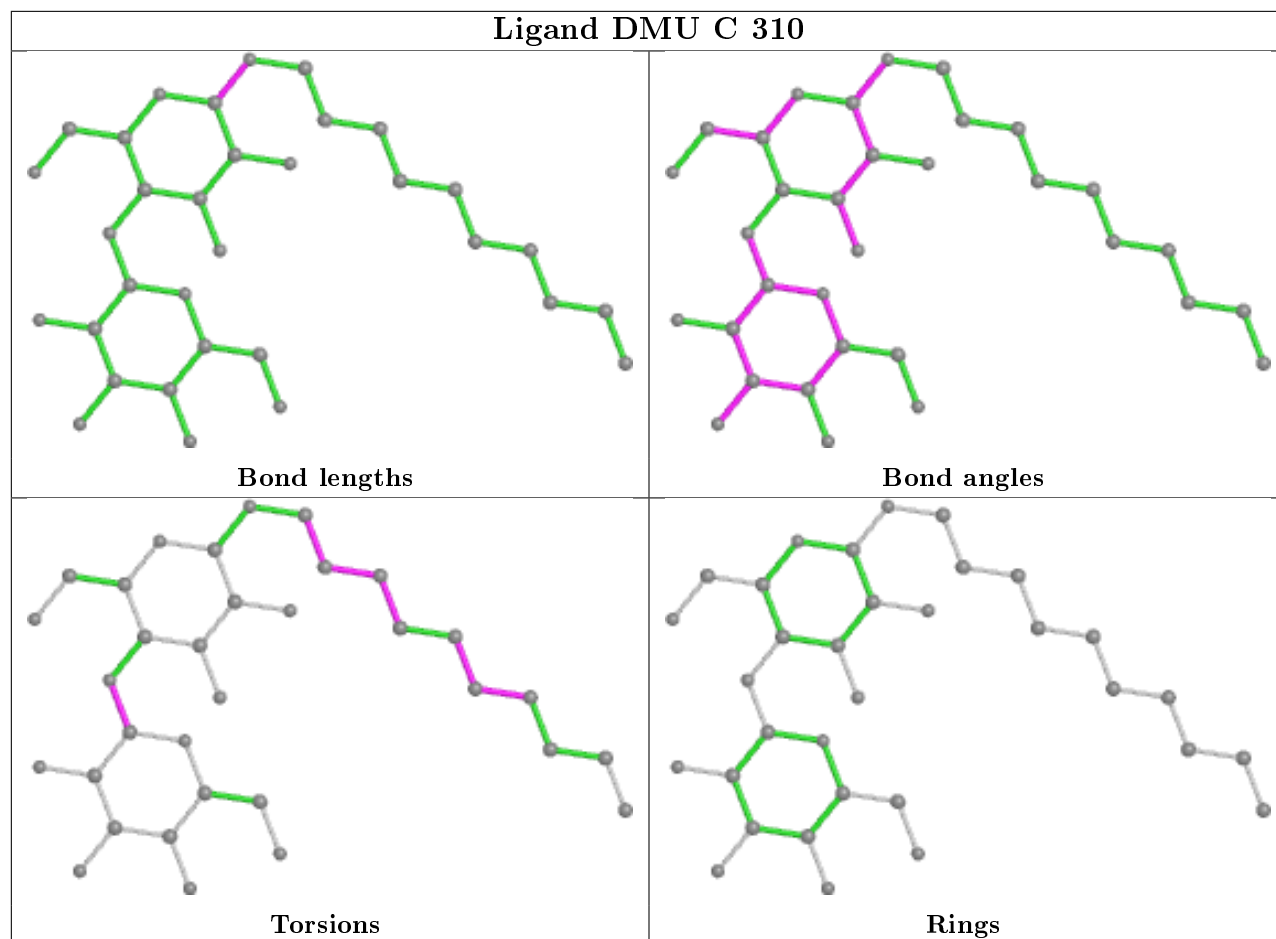


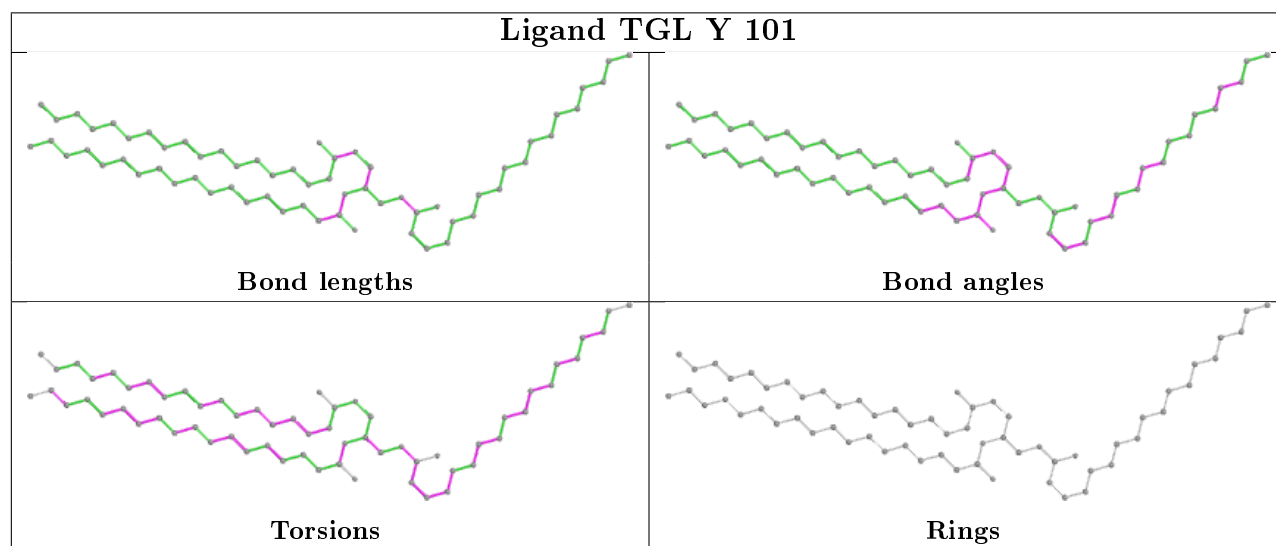
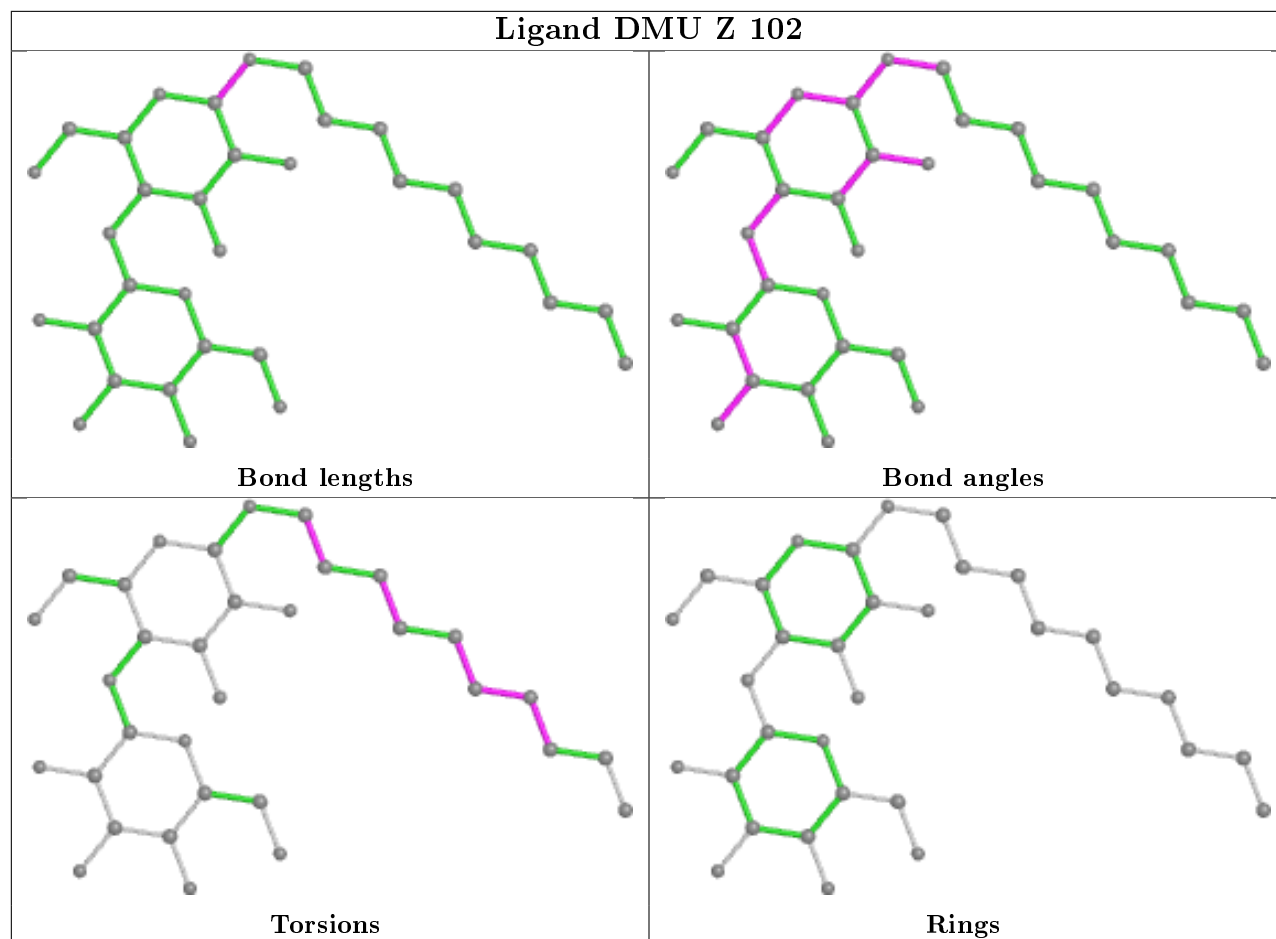
Ligand CHD J 101



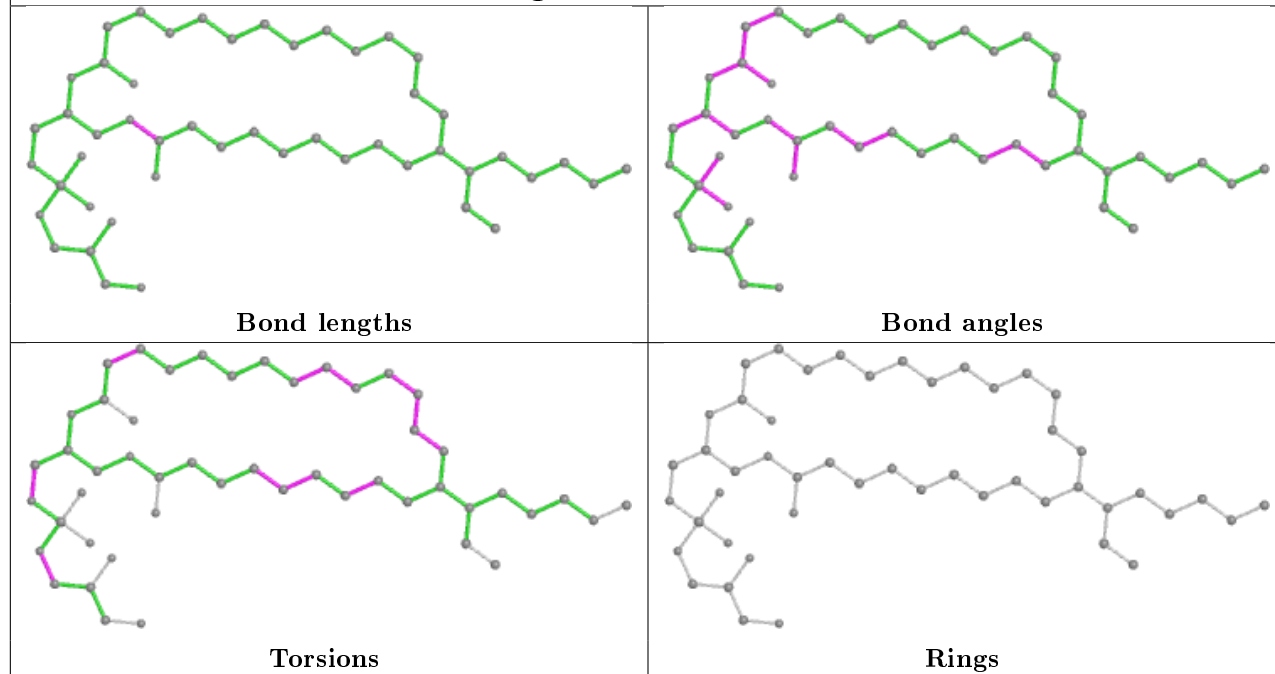
Ligand HEA N 603 (A)**Ligand DMU C 302**



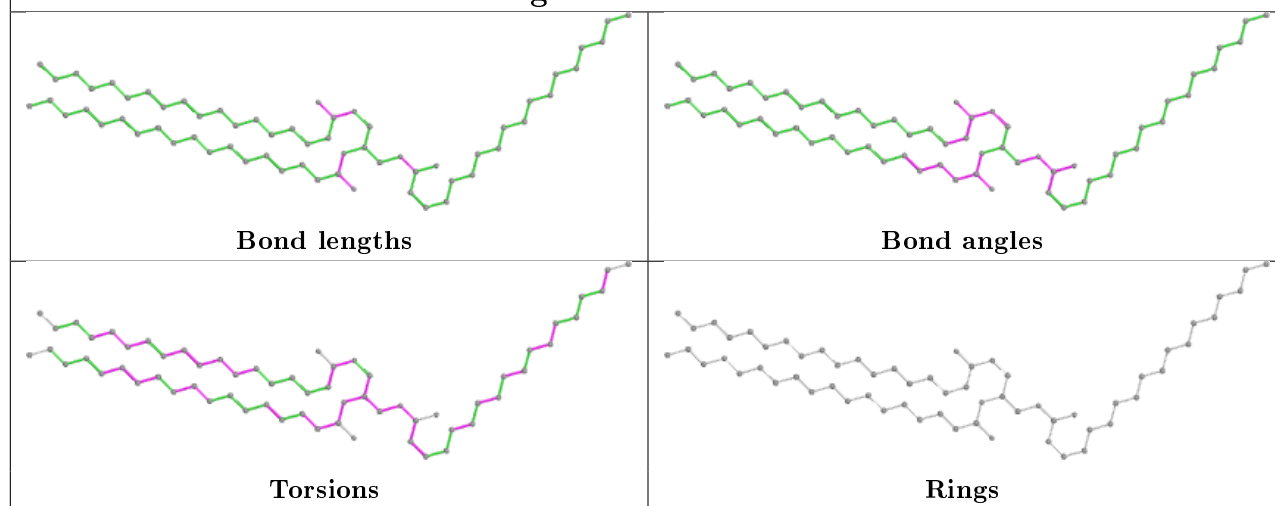




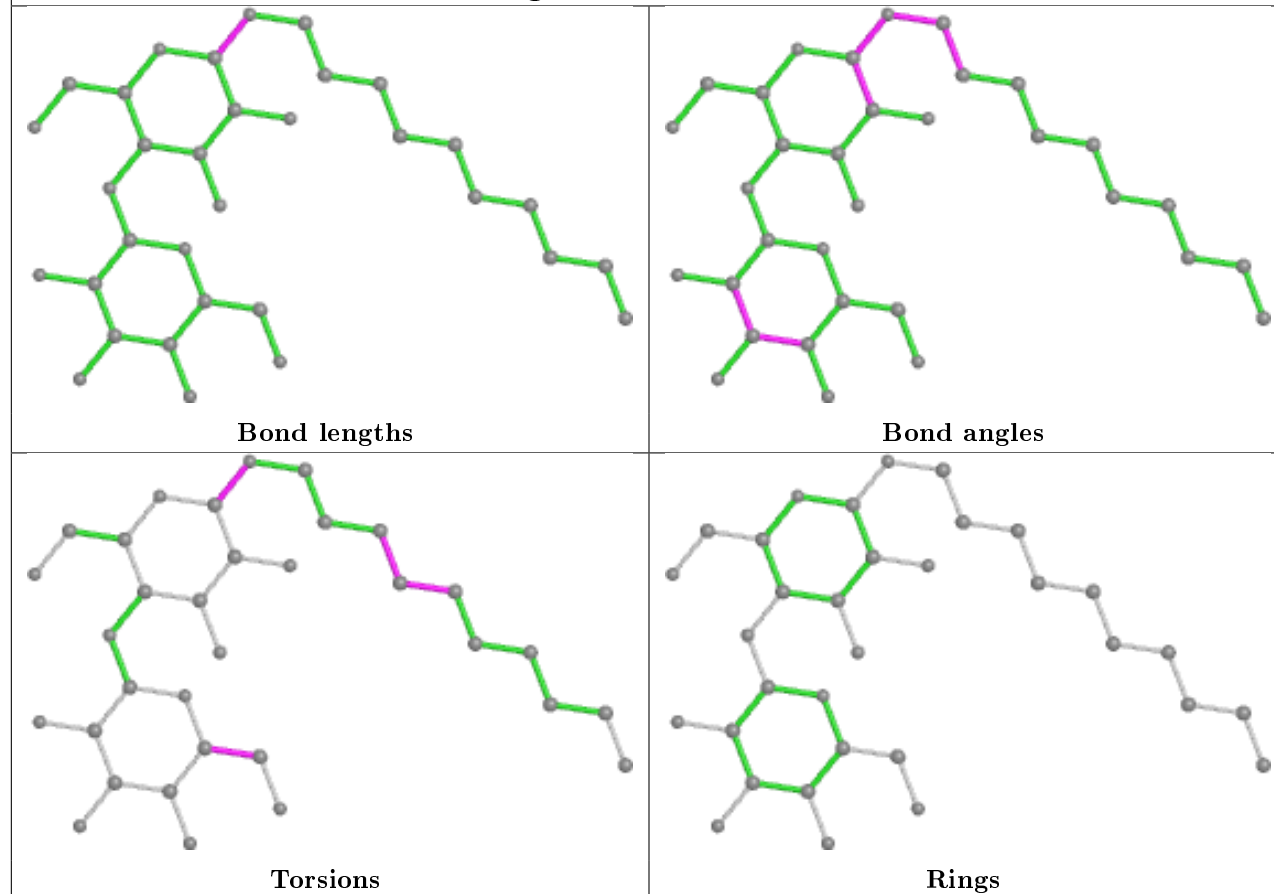
Ligand PGV P 303



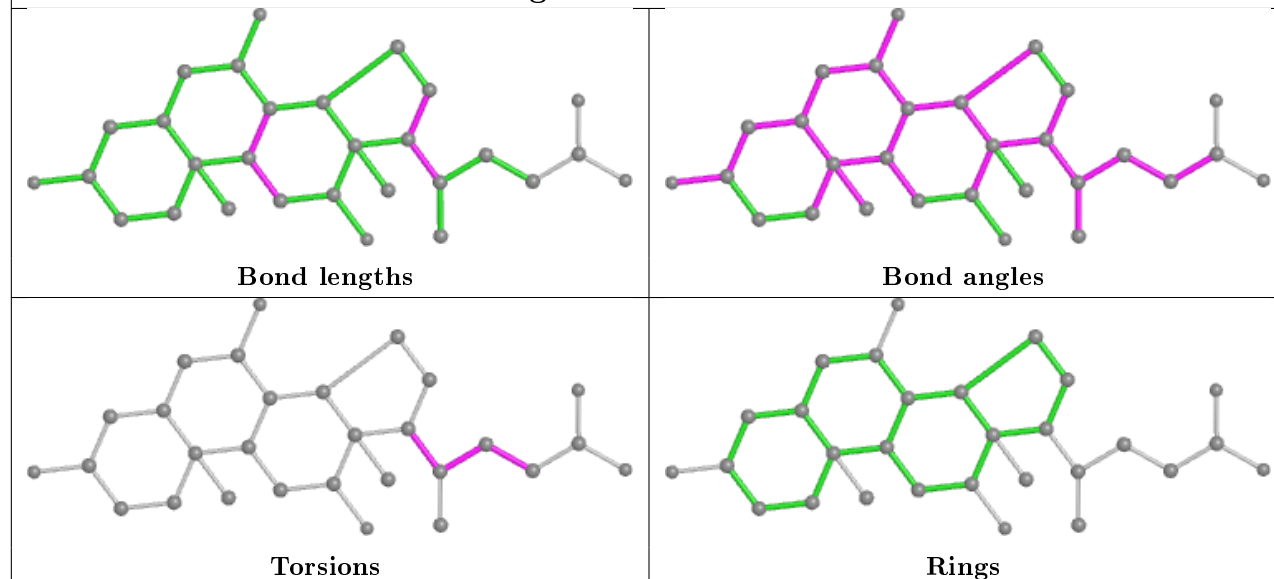
Ligand TGL D 201

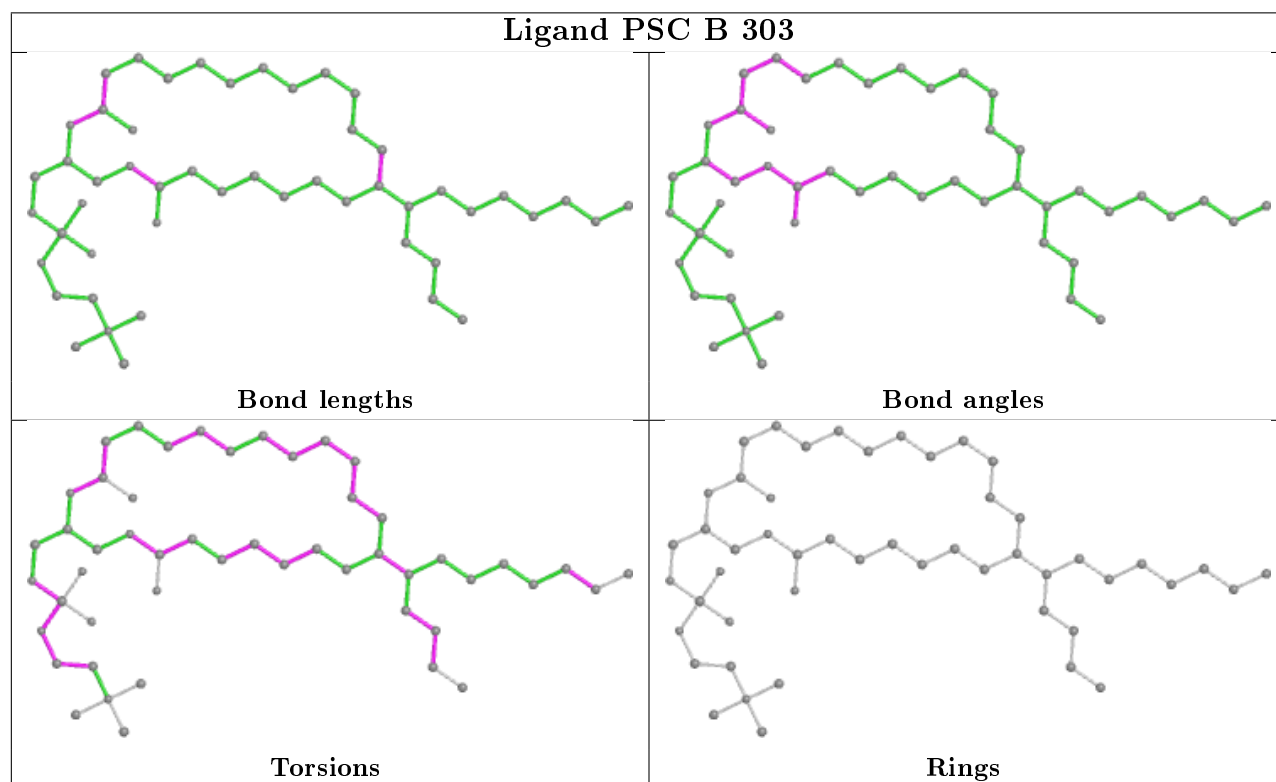
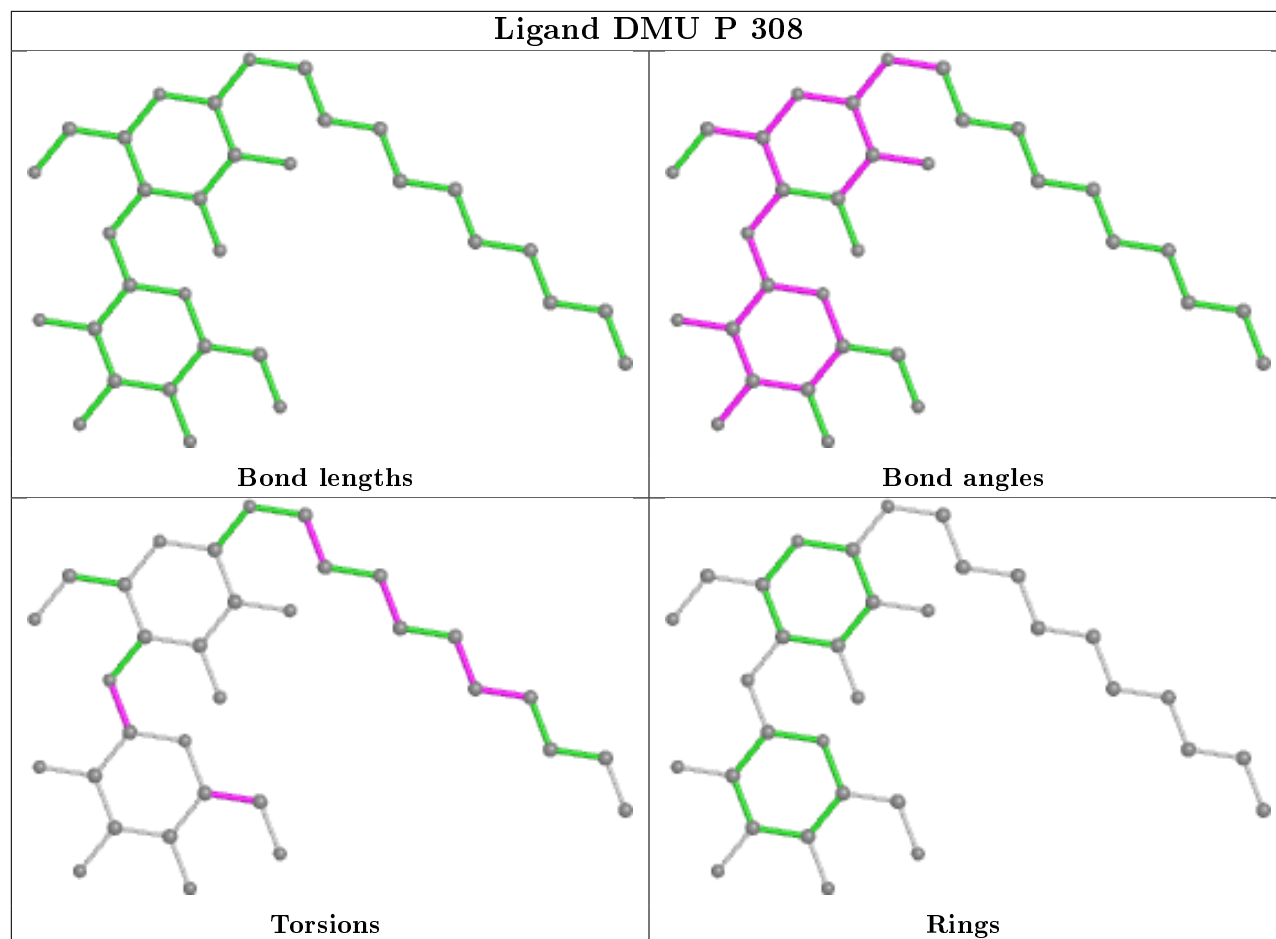


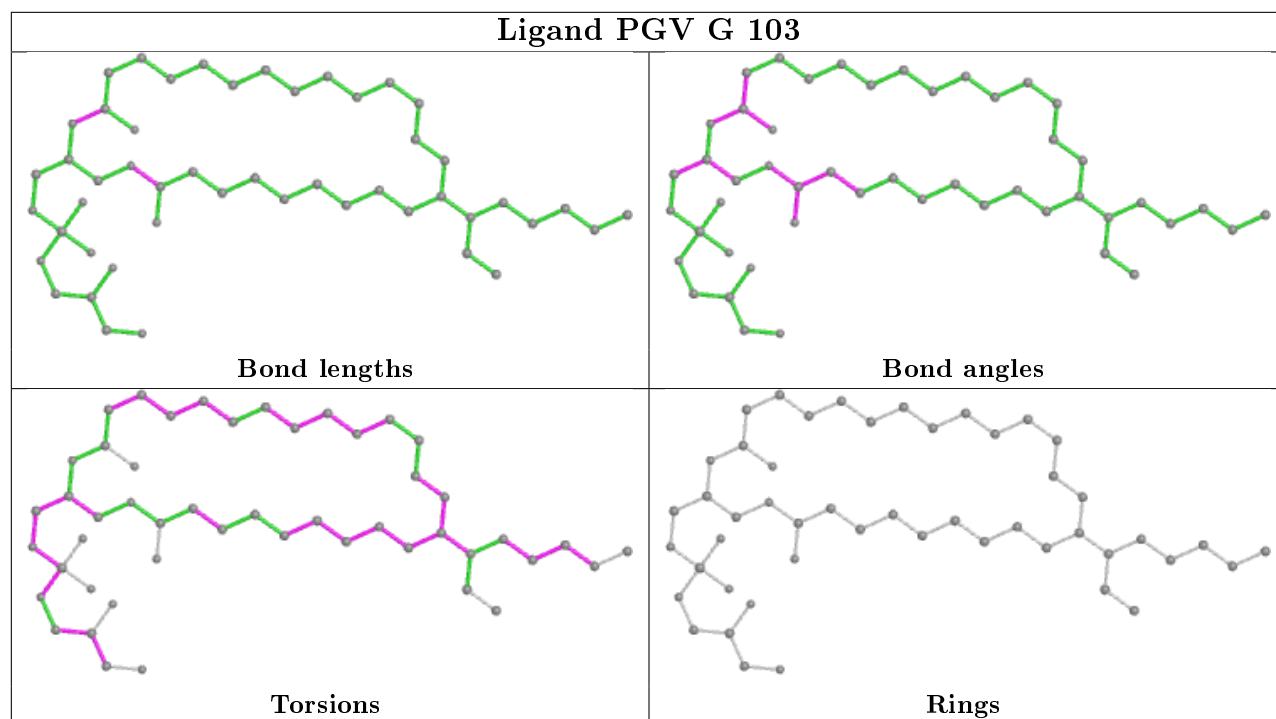
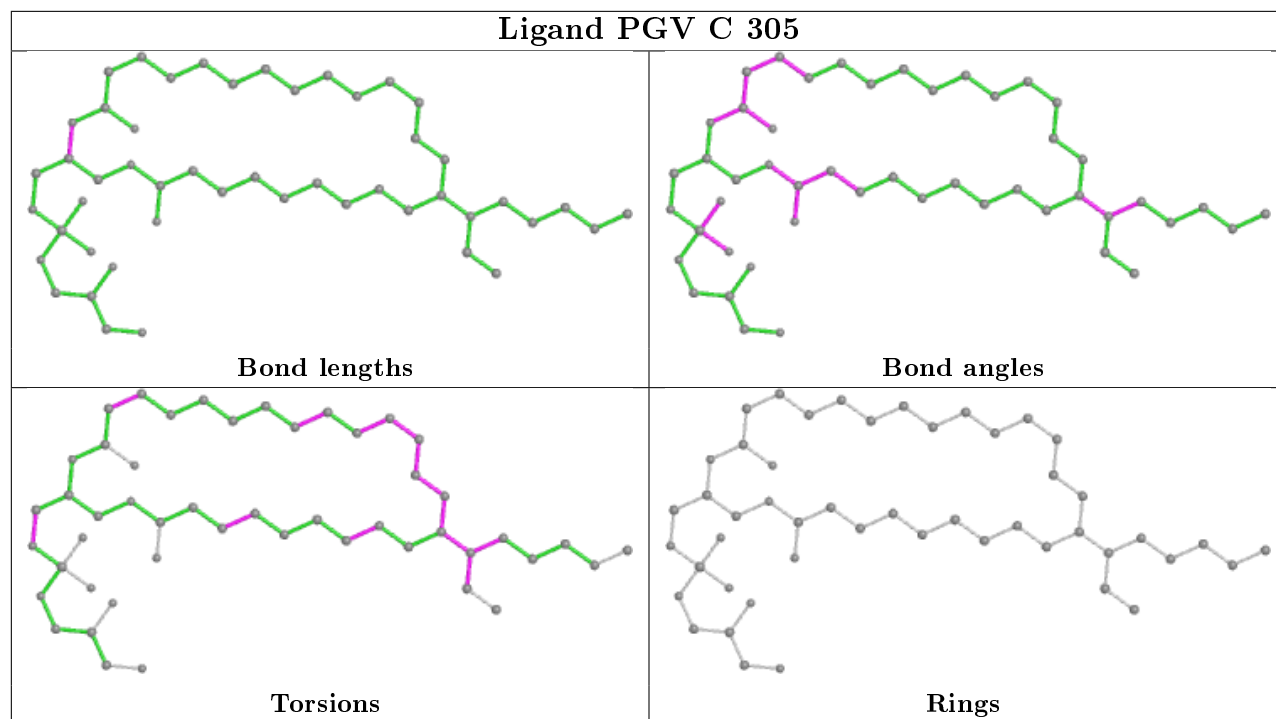
Ligand DMU P 306

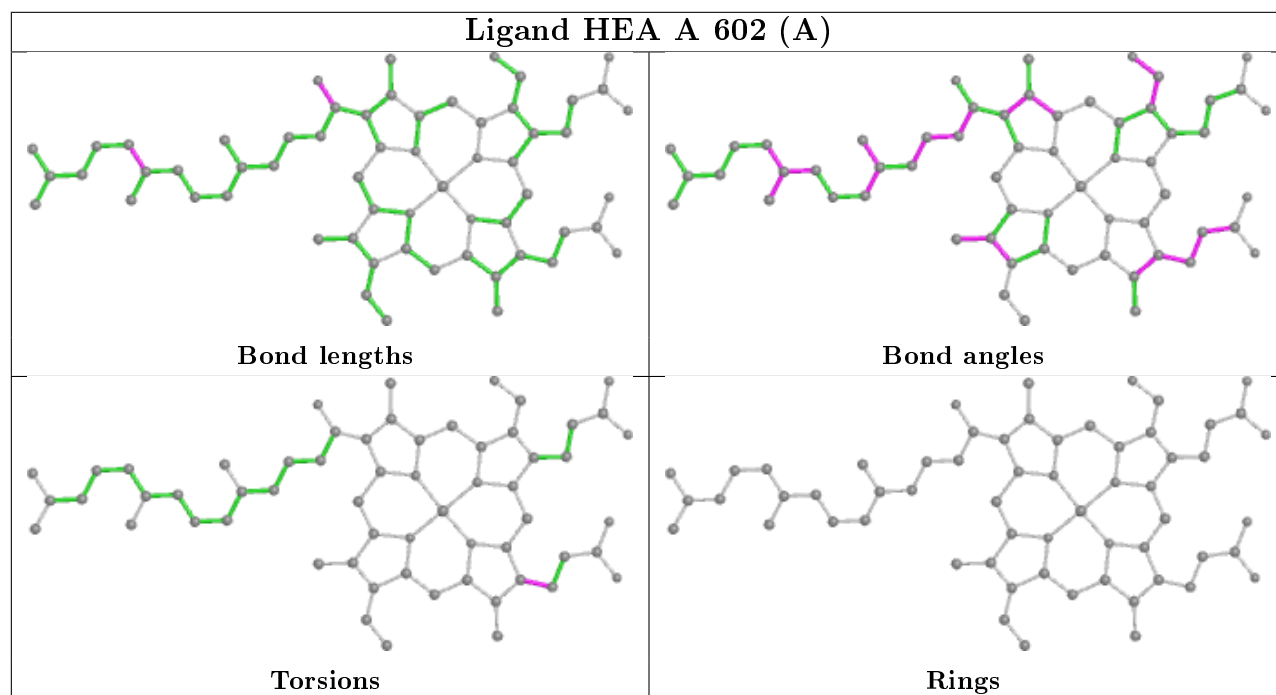
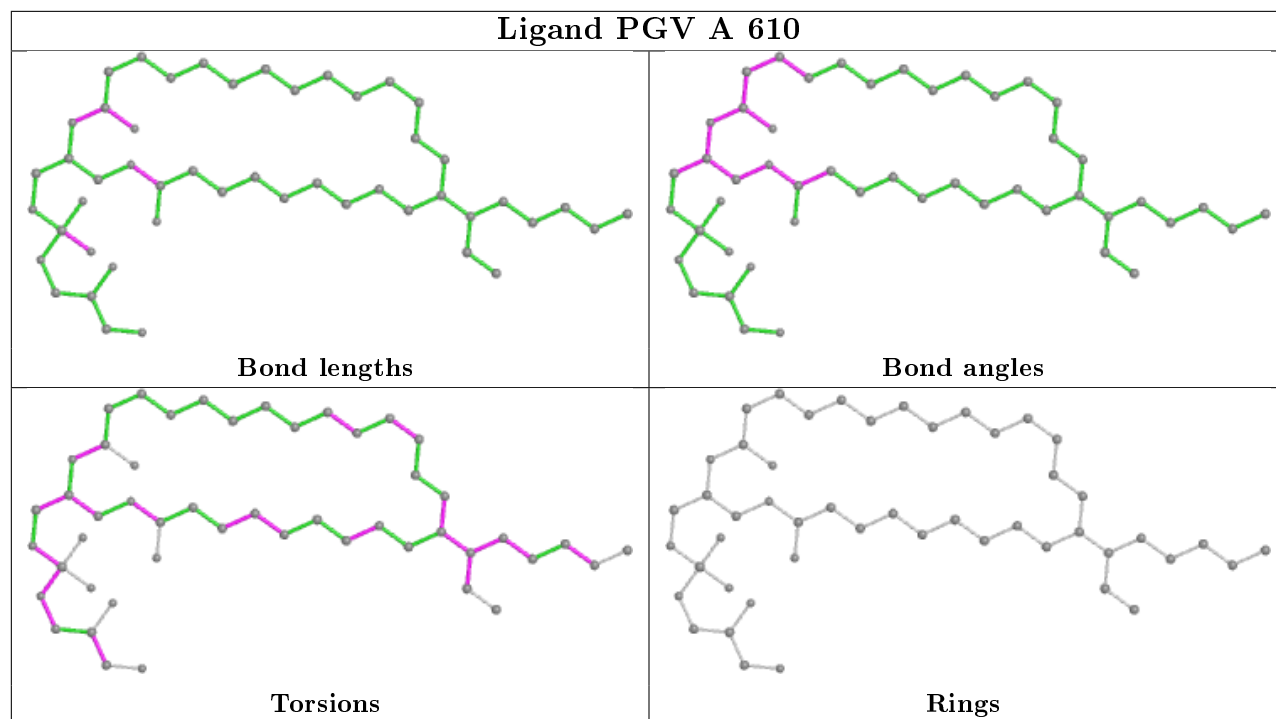


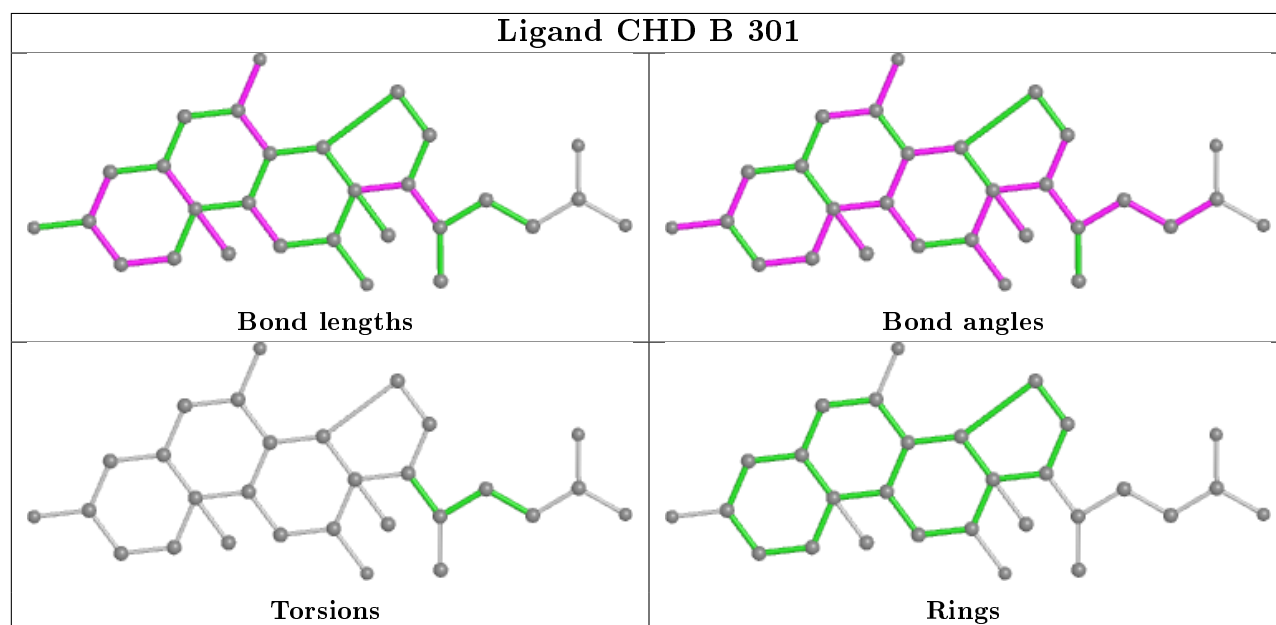
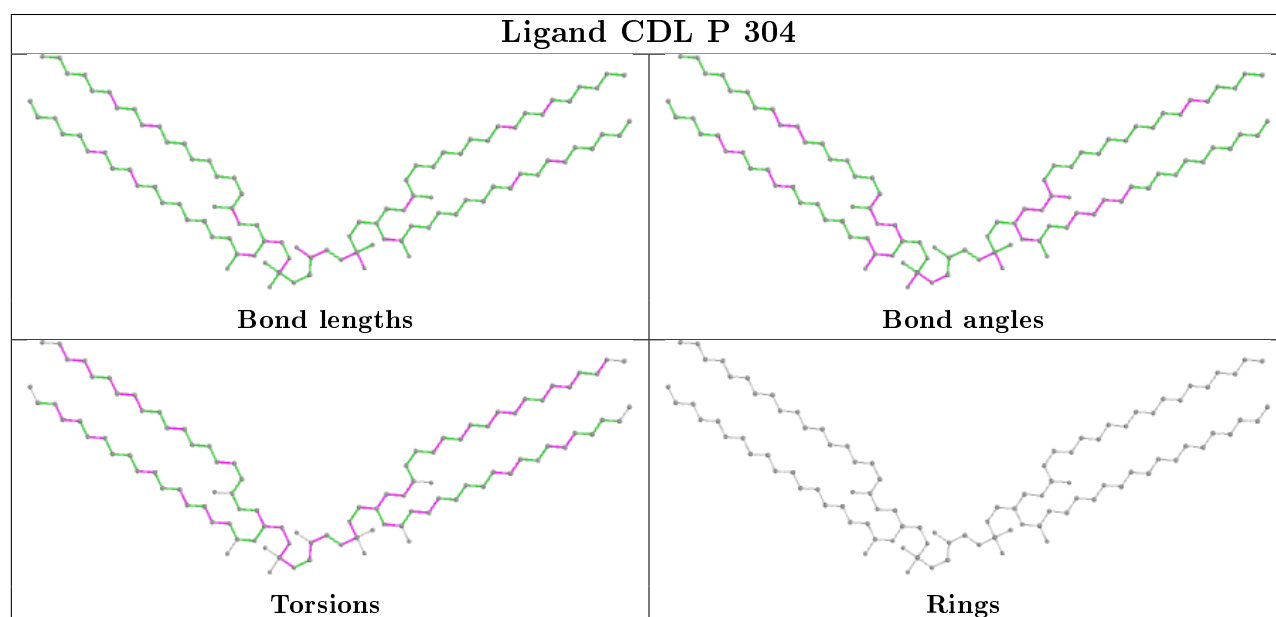
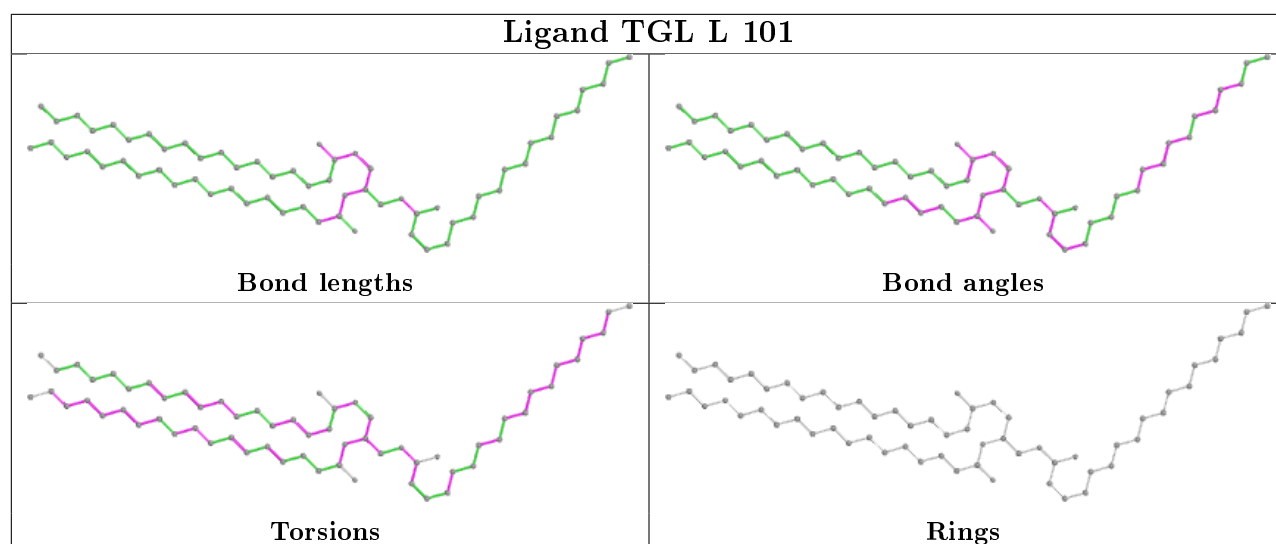
Ligand CHD P 305

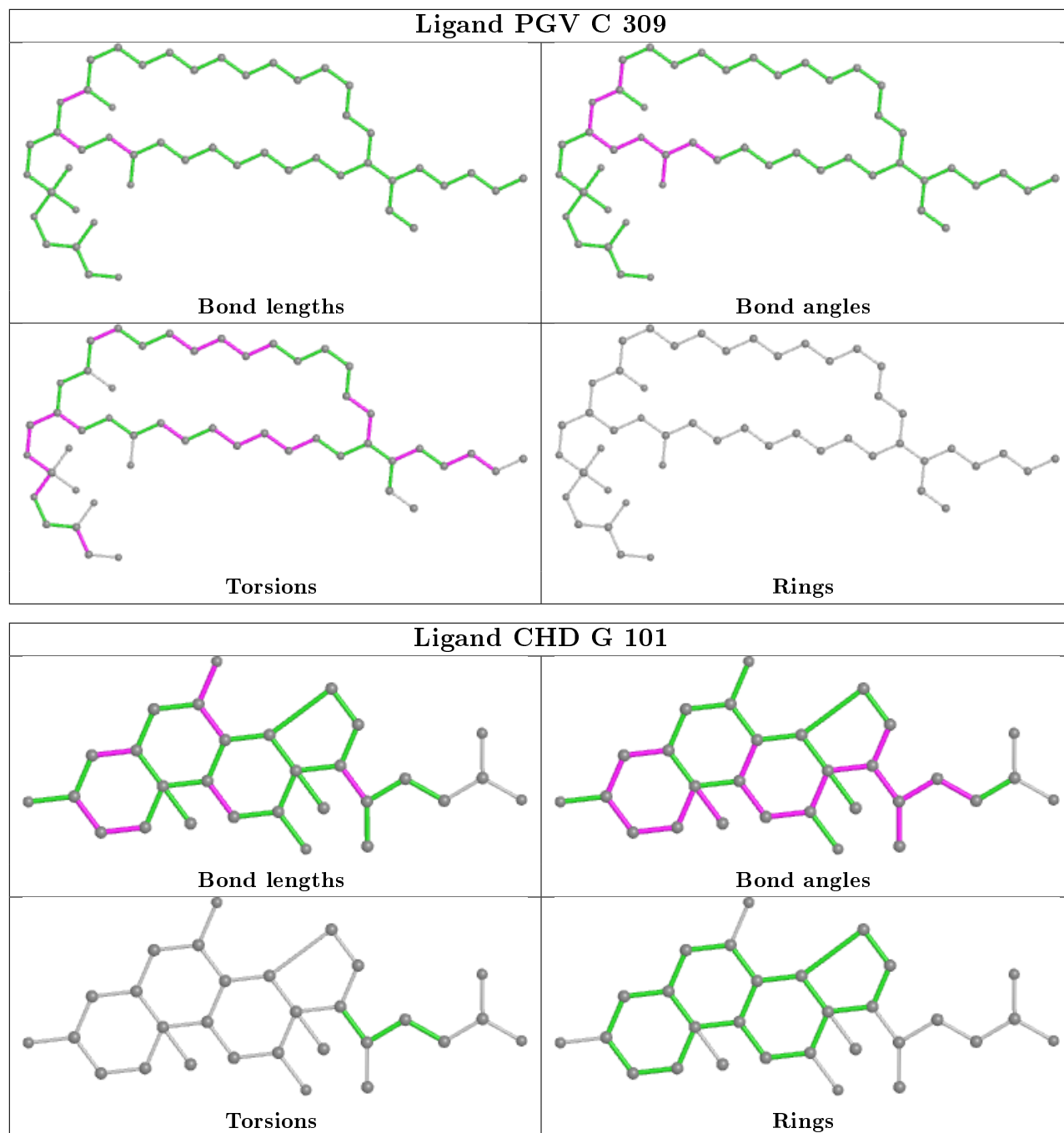


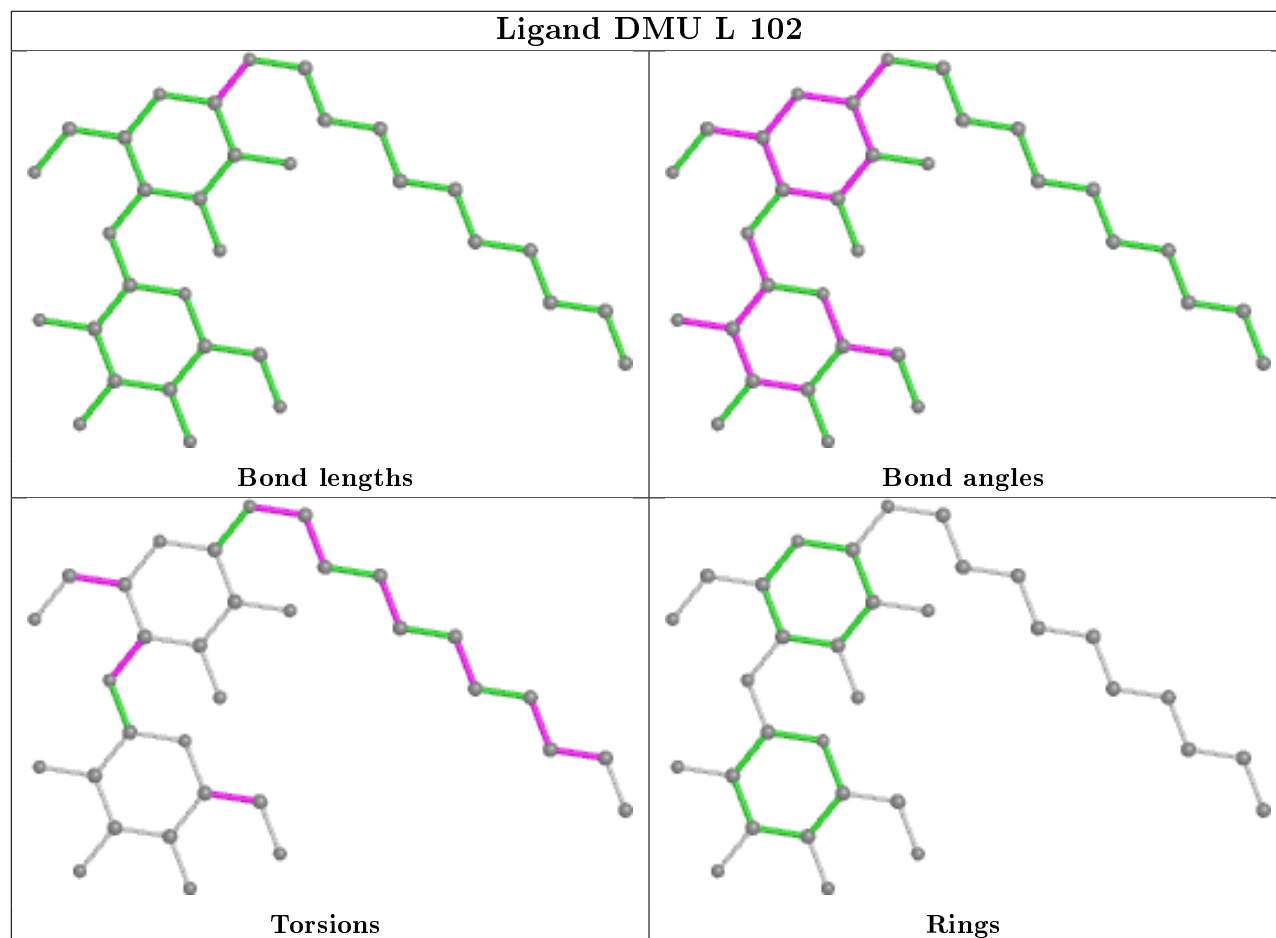
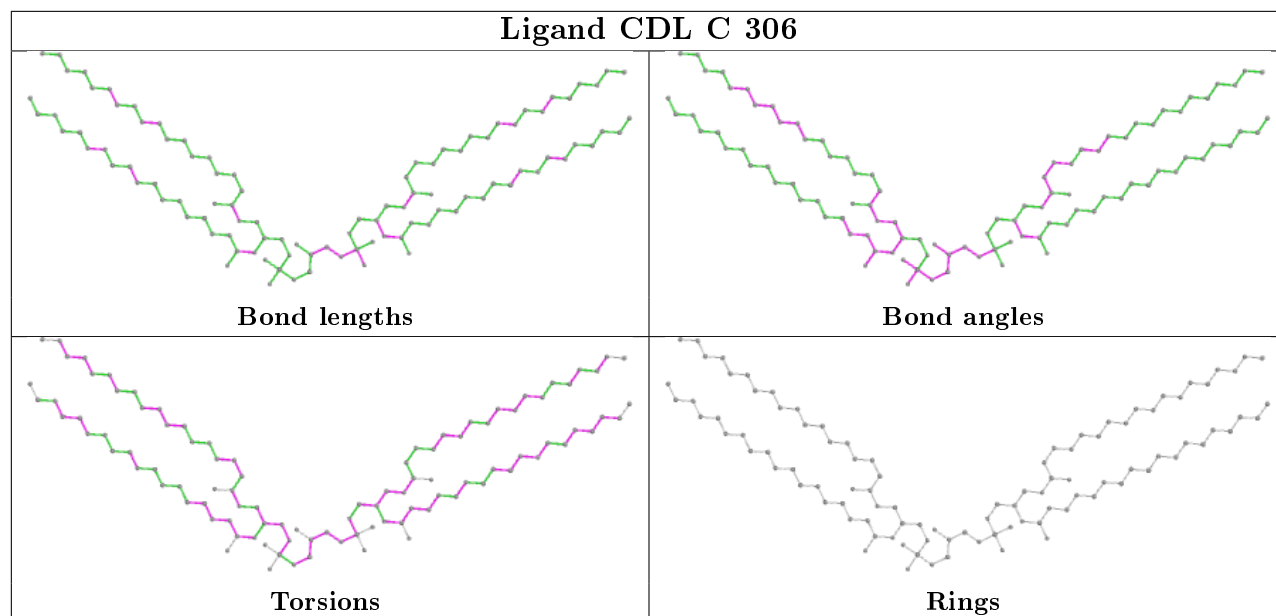


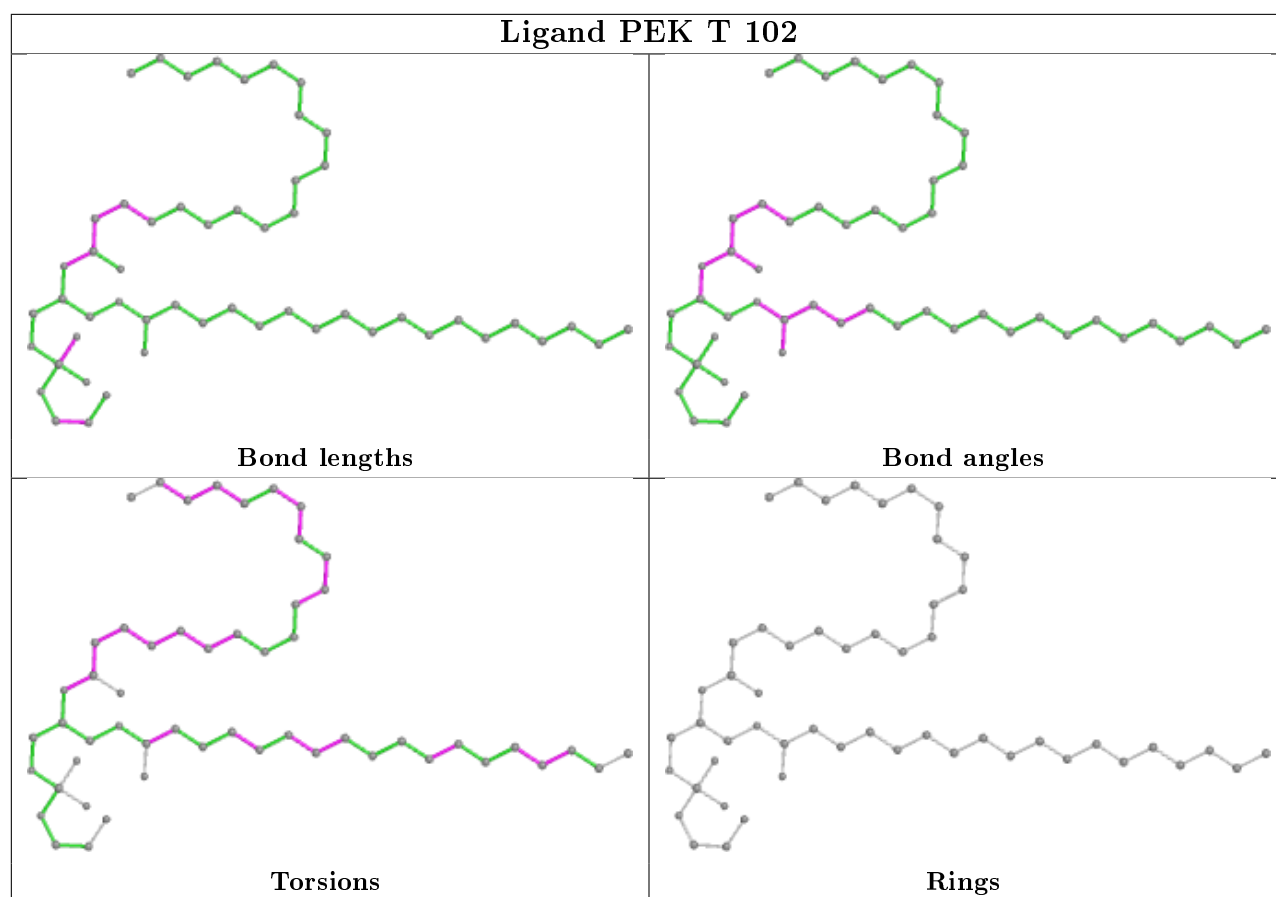


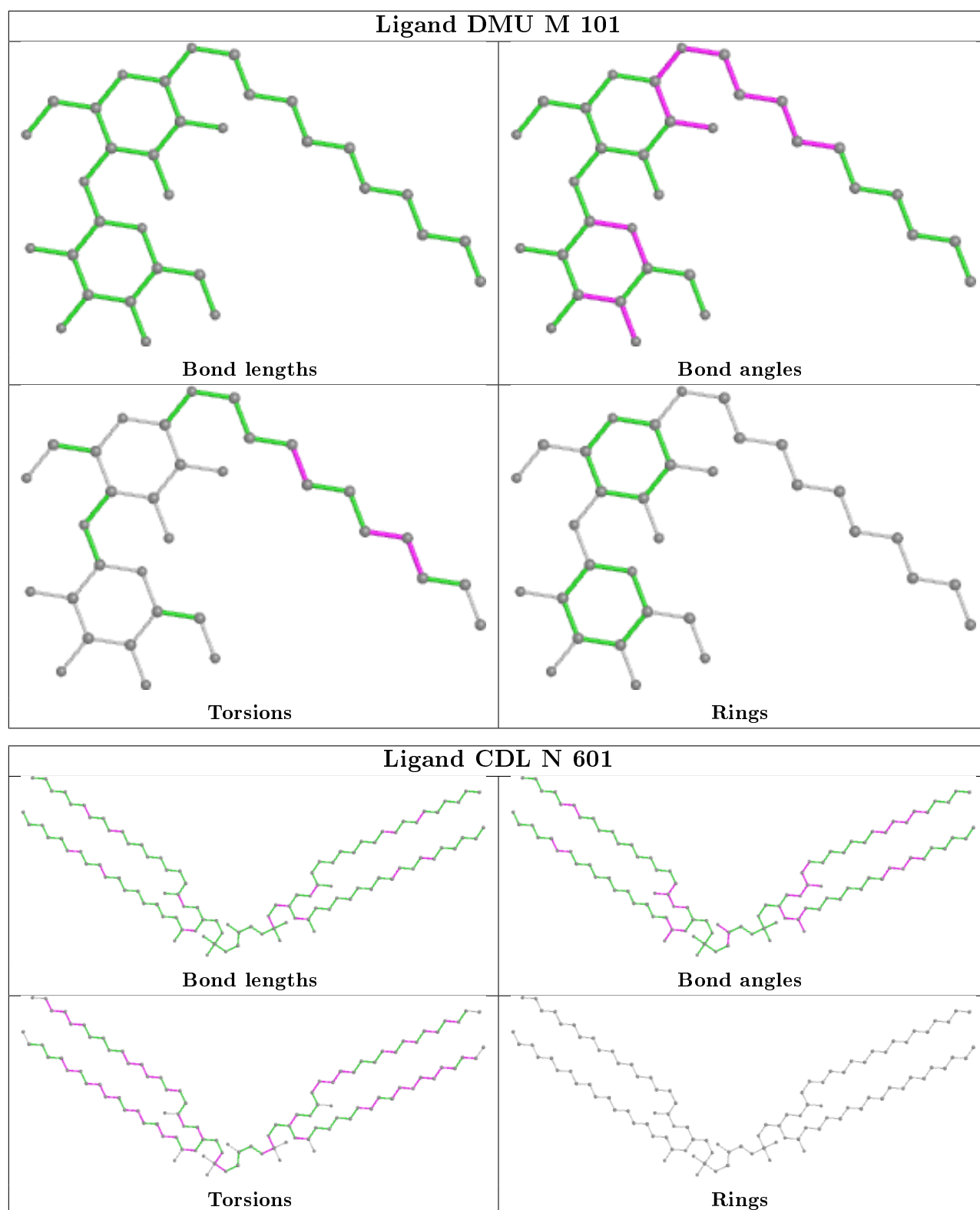












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	0.12	1 (0%) 95 94	25, 30, 38, 76	0
1	N	513/514 (99%)	-0.02	1 (0%) 95 94	27, 35, 44, 77	0
2	B	226/227 (99%)	0.10	1 (0%) 92 92	28, 38, 57, 78	0
2	O	226/227 (99%)	0.08	3 (1%) 77 78	34, 45, 69, 89	0
3	C	259/261 (99%)	0.06	1 (0%) 92 92	26, 33, 45, 84	0
3	P	259/261 (99%)	0.02	2 (0%) 86 86	28, 35, 46, 72	0
4	D	144/147 (97%)	-0.09	1 (0%) 87 88	30, 39, 60, 82	0
4	Q	144/147 (97%)	0.51	8 (5%) 24 23	39, 53, 78, 152	0
5	E	105/109 (96%)	-0.07	2 (1%) 66 66	31, 38, 63, 113	0
5	R	105/109 (96%)	-0.04	2 (1%) 66 66	38, 46, 65, 120	0
6	F	98/98 (100%)	0.54	7 (7%) 16 15	30, 41, 95, 147	0
6	S	98/98 (100%)	0.73	8 (8%) 11 11	31, 42, 104, 148	0
7	G	83/85 (97%)	0.90	15 (18%) 1 1	32, 43, 113, 127	0
7	T	83/85 (97%)	0.84	15 (18%) 1 1	31, 43, 101, 133	0
8	H	79/85 (92%)	0.30	8 (10%) 7 6	35, 45, 91, 104	0
8	U	79/85 (92%)	0.30	5 (6%) 20 19	39, 50, 102, 116	0
9	I	72/73 (98%)	0.43	5 (6%) 16 16	35, 49, 85, 92	0
9	V	72/73 (98%)	0.41	5 (6%) 16 16	36, 58, 83, 102	0
10	J	58/59 (98%)	0.37	4 (6%) 16 16	34, 44, 70, 107	0
10	W	58/59 (98%)	0.40	4 (6%) 16 16	37, 48, 72, 125	0
11	K	49/56 (87%)	0.01	1 (2%) 65 64	38, 45, 59, 65	0
11	X	49/56 (87%)	0.34	4 (8%) 11 11	48, 55, 77, 82	0
12	L	46/47 (97%)	0.07	1 (2%) 62 61	31, 37, 56, 86	0
12	Y	46/47 (97%)	0.12	1 (2%) 62 61	38, 45, 68, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.28	4 (9%) 8 8	32, 36, 71, 103	0
13	Z	43/46 (93%)	0.34	4 (9%) 8 8	43, 50, 83, 142	0
All	All	3550/3614 (98%)	0.18	113 (3%) 47 45	25, 38, 71, 152	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	22.1
6	F	98	HIS	13.5
4	Q	6	VAL	12.8
4	Q	4	SER	12.6
6	F	97	ALA	12.2
7	G	3	ALA	11.2
6	S	98	HIS	11.2
6	F	1	ALA	11.1
4	Q	5	VAL	10.8
6	S	96	LEU	9.9
7	T	3	ALA	9.7
10	W	58	LYS	9.3
10	J	58	LYS	8.5
13	Z	43	SER	8.0
7	G	2	SER	7.6
6	S	2	SER	7.1
6	S	94	HIS	7.0
6	S	1	ALA	6.9
6	F	96	LEU	6.9
9	I	37	PHE	6.8
5	R	5	HIS	6.5
6	F	2	SER	6.3
4	Q	8	SER	6.3
6	F	95	GLN	5.8
5	R	109	VAL	5.6
7	G	42	ARG	5.5
7	T	40	GLY	4.9
9	V	37	PHE	4.8
8	U	8	ILE	4.8
13	M	42	LYS	4.7
8	U	7	LYS	4.7
7	T	36	TRP	4.6
7	T	8	HIS	4.6
7	G	10	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
13	Z	42	LYS	4.5
5	E	109	VAL	4.5
7	T	42	ARG	4.4
2	O	113	TYR	4.4
6	S	93	PRO	4.4
7	T	2	SER	4.4
6	S	95	GLN	4.3
7	T	10	GLY	4.3
8	H	46	LYS	4.2
7	G	40	GLY	4.2
7	T	39	SER	4.1
7	T	1	ALA	4.1
7	G	1	ALA	4.1
7	G	6	GLY	4.1
11	X	6	ALA	4.1
3	P	3	HIS	4.0
7	T	5	LYS	3.9
7	G	5	LYS	3.9
11	X	7	PRO	3.9
9	I	25	PHE	3.9
9	I	29	LEU	3.8
9	I	30	GLY	3.8
12	Y	47	LYS	3.6
9	V	25	PHE	3.6
4	Q	7	LYS	3.5
7	G	8	HIS	3.5
8	H	8	ILE	3.4
7	G	37	LEU	3.4
7	G	36	TRP	3.3
10	W	57	HIS	3.3
5	E	5	HIS	3.3
7	T	7	ASP	3.3
9	V	29	LEU	3.2
8	U	44	THR	3.1
9	I	33	THR	3.1
11	X	13	TYR	3.1
10	J	57	HIS	3.0
10	J	1	PHE	3.0
7	T	6	GLY	3.0
8	H	45	ALA	2.9
7	T	9	GLY	2.9
4	Q	147	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	O	91	ASN	2.9
4	Q	10	ASP	2.9
8	U	46	LYS	2.8
7	G	7	ASP	2.8
7	T	4	ALA	2.7
6	F	94	HIS	2.7
1	N	311[A]	ILE	2.7
2	O	227	LEU	2.7
8	H	44	THR	2.6
7	G	4	ALA	2.6
8	U	10	ASN	2.6
12	L	2	HIS	2.6
7	G	84	LYS	2.6
4	Q	87[A]	PHE	2.6
13	M	40	TYR	2.6
13	M	43	SER	2.5
9	V	30	GLY	2.5
7	T	41	HIS	2.4
9	V	34	PHE	2.4
13	Z	40	TYR	2.4
3	P	33[A]	MET	2.4
4	D	4	SER	2.4
7	G	41	HIS	2.4
13	M	39	ASN	2.3
10	W	52	TRP	2.3
11	K	47	ARG	2.3
8	H	47	GLY	2.2
13	Z	39	ASN	2.2
1	A	311[A]	ILE	2.2
3	C	33[A]	MET	2.1
10	W	56	PRO	2.1
2	B	16[A]	ILE	2.1
8	H	48	GLY	2.1
10	J	52	TRP	2.1
11	X	52	GLU	2.0
8	H	7	LYS	2.0
8	H	43	MET	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.45	0.38	92,121,130,132	0
7	TPO	T	11	11/12	0.51	0.31	109,118,139,142	0
9	SAC	V	1	9/10	0.68	0.22	101,116,124,132	0
9	SAC	I	1	9/10	0.85	0.24	70,80,87,89	0
1	FME	N	1	10/11	0.96	0.13	47,56,74,79	0
1	FME	A	1	10/11	0.97	0.14	41,50,81,95	0
2	FME	B	1	10/11	0.98	0.13	33,35,45,66	0
2	FME	O	1	10/11	0.98	0.13	41,42,54,65	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	EDO	C	319	4/4	0.20	0.85	81,98,105,107	0
21	EDO	Q	203	4/4	0.47	0.23	81,81,88,91	0
22	CHD	W	101	29/29	0.53	0.37	69,124,145,148	0
22	CHD	J	101	29/29	0.55	0.42	99,135,149,150	0
21	EDO	D	207	4/4	0.60	0.17	62,66,70,75	0
25	DMU	C	311	33/33	0.61	0.22	56,82,119,129	0
25	DMU	L	102	33/33	0.63	0.25	54,93,139,139	0
21	EDO	A	619	4/4	0.65	0.37	50,57,58,83	0
28	CDL	T	103	100/100	0.66	0.32	54,88,145,159	0
27	PEK	T	101	53/53	0.66	0.35	51,87,154,155	0
25	DMU	C	302	33/33	0.67	0.34	35,79,111,124	0
24	PSC	B	303	52/52	0.71	0.33	42,85,156,156	0
21	EDO	A	620	4/4	0.71	0.24	64,64,67,70	0
28	CDL	N	601	100/100	0.72	0.32	57,90,140,159	0
27	PEK	G	102	53/53	0.74	0.29	52,95,154,154	0
28	CDL	P	304	100/100	0.74	0.31	43,87,119,134	0
19	TGL	Q	201	63/63	0.74	0.21	52,76,98,109	0
21	EDO	C	318	4/4	0.74	0.35	58,86,90,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	PEK	P	307	53/53	0.75	0.25	45,78,128,145	0
21	EDO	O	305	4/4	0.76	0.12	67,74,79,79	0
27	PEK	C	308	53/53	0.76	0.24	49,80,136,148	0
25	DMU	P	306	33/33	0.77	0.29	47,79,120,123	0
21	EDO	F	105	4/4	0.77	0.22	69,74,77,78	0
21	EDO	C	313	4/4	0.78	0.14	77,84,85,95	0
24	PSC	O	302	52/52	0.78	0.33	48,84,160,160	0
20	PGV	C	309	51/51	0.78	0.20	45,78,121,151	0
20	PGV	G	103	51/51	0.79	0.25	53,83,119,139	0
21	EDO	D	203	4/4	0.80	0.44	55,61,73,93	0
21	EDO	N	611	4/4	0.81	0.17	72,73,74,76	0
21	EDO	H	102	4/4	0.81	0.14	68,73,79,94	0
28	CDL	C	306	100/100	0.81	0.28	40,80,115,128	0
25	DMU	C	310	33/33	0.81	0.26	56,82,112,121	0
19	TGL	Y	101	63/63	0.81	0.28	48,78,110,148	0
21	EDO	A	617	4/4	0.82	0.26	49,53,56,62	0
20	PGV	Z	101	51/51	0.82	0.31	51,83,138,144	0
21	EDO	G	104	4/4	0.83	0.27	56,67,71,89	0
21	EDO	R	201	4/4	0.83	0.29	57,61,66,72	0
19	TGL	L	101	63/63	0.83	0.20	36,64,99,119	0
25	DMU	P	309	33/33	0.84	0.23	65,87,106,112	0
19	TGL	N	610	63/63	0.84	0.24	52,82,110,122	0
21	EDO	D	204	4/4	0.84	0.32	65,69,81,85	0
20	PGV	A	610	51/51	0.84	0.26	36,72,112,121	0
25	DMU	P	308	33/33	0.84	0.20	55,78,101,105	0
21	EDO	C	315	4/4	0.84	0.32	60,75,77,79	0
26	UNX	C	303	1/1	0.85	0.16	28,28,28,28	0
19	TGL	D	201	63/63	0.85	0.21	37,67,90,97	0
21	EDO	L	103	4/4	0.85	0.16	71,75,76,99	0
21	EDO	P	313	4/4	0.86	0.24	54,62,70,73	0
21	EDO	U	101	4/4	0.86	0.14	66,70,70,84	0
22	CHD	P	305	29/29	0.86	0.22	53,65,71,76	0
21	EDO	C	317	4/4	0.86	0.15	68,69,71,84	0
21	EDO	E	203	4/4	0.86	0.27	50,59,66,70	0
21	EDO	A	612	4/4	0.86	0.18	52,61,65,67	0
21	EDO	C	314	4/4	0.86	0.13	60,64,67,85	0
21	EDO	A	616	4/4	0.86	0.18	46,47,50,50	0
19	TGL	A	608	63/63	0.87	0.19	43,79,109,121	0
21	EDO	A	623	4/4	0.87	0.26	55,57,62,63	0
25	DMU	Z	102	33/33	0.88	0.15	50,60,75,78	0
21	EDO	N	622	4/4	0.88	0.32	55,58,81,101	0
21	EDO	R	205	4/4	0.89	0.45	57,58,61,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CHD	C	307	29/29	0.89	0.21	52,65,72,75	0
21	EDO	B	305	4/4	0.89	0.19	35,45,53,55	0
21	EDO	A	614	4/4	0.90	0.16	59,69,74,83	0
26	UNX	P	302	1/1	0.90	0.21	28,28,28,28	0
21	EDO	J	102	4/4	0.90	0.27	52,75,78,81	0
21	EDO	H	101	4/4	0.91	0.11	54,57,67,73	0
21	EDO	R	202	4/4	0.91	0.12	61,67,72,78	0
21	EDO	E	201	4/4	0.92	0.12	43,46,56,58	0
21	EDO	A	615	4/4	0.92	0.15	25,30,31,46	0
21	EDO	E	205	4/4	0.92	0.23	60,63,68,78	0
21	EDO	N	618	4/4	0.92	0.55	60,63,67,70	0
21	EDO	V	101	4/4	0.92	0.18	62,68,74,75	0
21	EDO	N	617	4/4	0.92	0.12	50,53,53,57	0
21	EDO	S	103	4/4	0.92	0.24	44,56,72,72	0
21	EDO	P	312	4/4	0.92	0.33	52,60,72,75	0
16	MG	N	605	1/1	0.93	0.08	35,35,35,35	0
21	EDO	P	310	4/4	0.93	0.15	36,42,48,59	0
21	EDO	A	613	4/4	0.93	0.14	35,37,39,41	0
21	EDO	O	304	4/4	0.93	0.15	63,67,67,83	0
21	EDO	A	618	4/4	0.93	0.40	43,68,78,83	0
21	EDO	N	612	4/4	0.93	0.25	36,41,53,64	0
21	EDO	D	202	4/4	0.93	0.57	44,51,52,68	0
25	DMU	M	101	33/33	0.94	0.12	43,50,62,73	0
21	EDO	R	203	4/4	0.94	0.23	53,63,69,73	0
21	EDO	R	206	4/4	0.94	0.20	47,52,58,63	0
21	EDO	N	621	4/4	0.94	0.20	48,51,51,71	0
21	EDO	N	614	4/4	0.95	0.14	56,59,66,69	0
21	EDO	D	206	4/4	0.95	0.19	54,62,67,73	0
21	EDO	F	104	4/4	0.95	0.23	50,52,62,64	0
21	EDO	F	103	4/4	0.95	0.13	40,41,42,45	0
21	EDO	A	621	4/4	0.96	0.45	38,52,62,68	0
21	EDO	E	204	4/4	0.96	0.10	43,44,47,50	0
22	CHD	C	301	29/29	0.96	0.10	30,33,37,40	0
27	PEK	T	102	53/53	0.96	0.15	34,51,84,97	0
21	EDO	N	615	4/4	0.96	0.12	38,39,43,47	0
21	EDO	T	104	4/4	0.96	0.16	39,41,42,49	0
21	EDO	N	619	4/4	0.96	0.18	50,53,59,62	0
21	EDO	Q	202	4/4	0.96	0.14	62,66,69,69	0
21	EDO	C	320	4/4	0.97	0.16	37,45,48,63	0
21	EDO	A	622	4/4	0.97	0.24	37,45,60,64	0
21	EDO	N	613	4/4	0.97	0.17	42,49,49,54	0
27	PEK	C	304	53/53	0.97	0.15	32,49,84,106	0

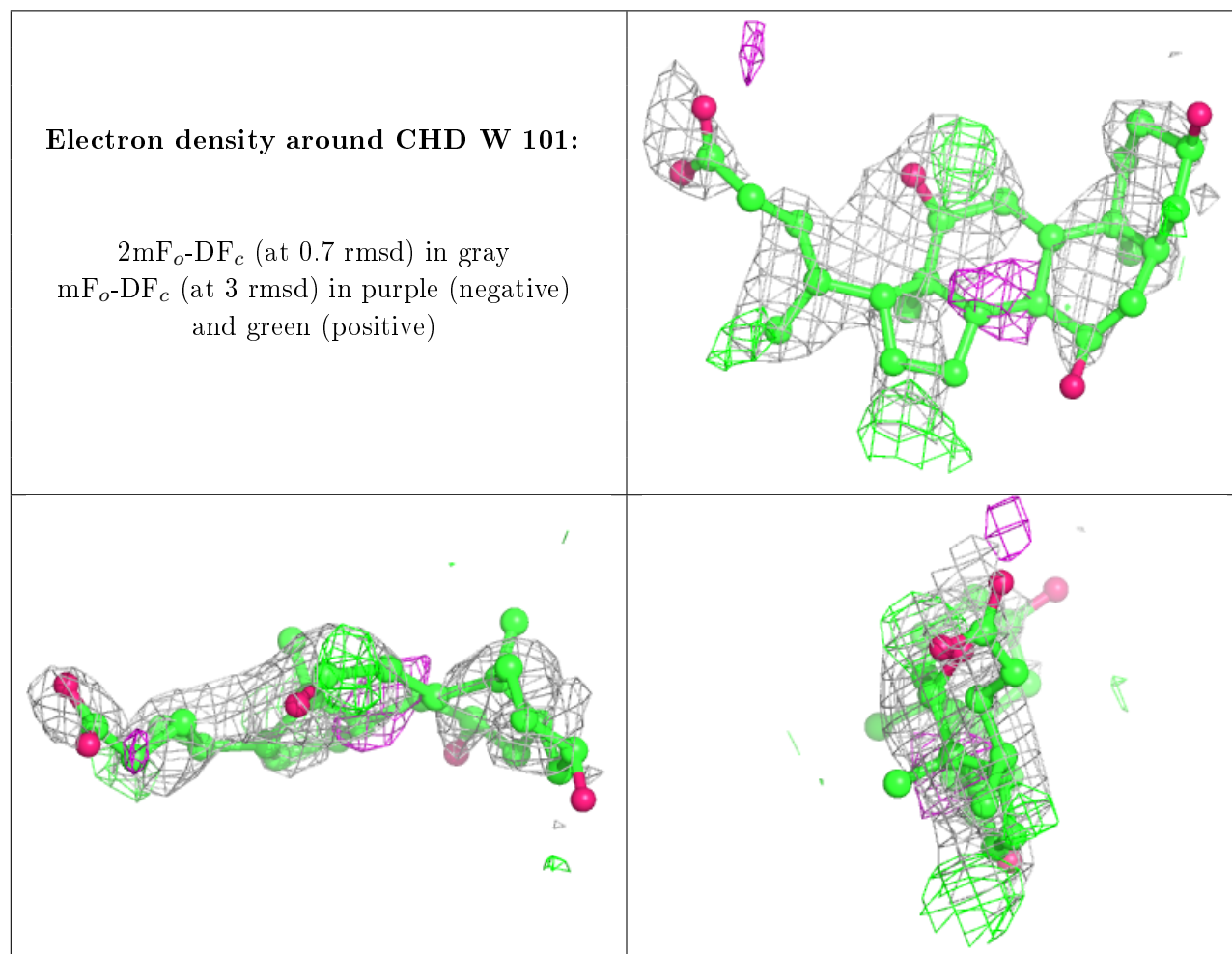
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	EDO	R	204	4/4	0.97	0.17	45,49,49,50	0
21	EDO	D	205	4/4	0.97	0.15	40,41,58,58	0
22	CHD	P	301	29/29	0.97	0.08	31,36,39,46	0
21	EDO	A	611	4/4	0.97	0.18	39,44,46,56	0
21	EDO	C	316	4/4	0.97	0.23	41,61,67,70	0
20	PGV	C	305	51/51	0.98	0.13	29,38,92,108	0
21	EDO	P	311	4/4	0.98	0.21	44,44,47,48	0
22	CHD	G	101	29/29	0.98	0.11	32,34,38,43	0
22	CHD	B	301	29/29	0.98	0.12	29,33,36,44	0
21	EDO	E	202	4/4	0.98	0.13	44,46,46,48	0
18	AZI	A	607	3/3	0.98	0.18	34,34,37,37	0
20	PGV	A	609	51/51	0.98	0.14	27,38,69,73	0
21	EDO	N	616	4/4	0.98	0.12	34,37,38,39	0
18	AZI	N	608	3/3	0.98	0.12	39,39,39,41	0
21	EDO	O	303	4/4	0.98	0.20	41,41,42,44	0
21	EDO	S	102	4/4	0.98	0.14	33,34,36,36	0
14	HEA	N	602	60/60	0.98	0.12	28,34,56,65	0
20	PGV	N	609	51/51	0.98	0.13	30,40,71,77	0
21	EDO	B	304	4/4	0.98	0.14	32,33,38,40	0
21	EDO	N	620	4/4	0.98	0.15	49,59,67,73	0
21	EDO	C	312	4/4	0.98	0.10	42,42,45,45	0
21	EDO	G	105	4/4	0.98	0.09	35,38,42,44	0
14	HEA	A	602[B]	60/60	0.99	0.15	21,26,35,39	60
17	NA	A	605	1/1	0.99	0.09	32,32,32,32	0
14	HEA	A	601	60/60	0.99	0.12	23,28,49,51	0
14	HEA	N	603[A]	60/60	0.99	0.14	24,27,33,35	60
18	AZI	N	607	3/3	0.99	0.12	39,39,40,42	0
18	AZI	A	606	3/3	0.99	0.16	33,33,36,36	0
16	MG	A	604	1/1	0.99	0.09	28,28,28,28	0
14	HEA	N	603[B]	60/60	0.99	0.14	26,33,45,47	60
14	HEA	A	602[A]	60/60	0.99	0.15	21,27,31,36	60
17	NA	N	606	1/1	0.99	0.06	39,39,39,39	0
20	PGV	P	303	51/51	0.99	0.14	31,40,77,86	0
23	CUA	O	301	2/2	0.99	0.16	36,36,36,36	0
21	EDO	F	102	4/4	0.99	0.10	29,31,31,33	0
29	ZN	S	101	1/1	1.00	0.14	38,38,38,38	0
15	CU	A	603	1/1	1.00	0.17	30,30,30,30	0
23	CUA	B	302	2/2	1.00	0.18	30,30,30,31	0
29	ZN	F	101	1/1	1.00	0.15	36,36,36,36	0
15	CU	N	604	1/1	1.00	0.18	33,33,33,33	0

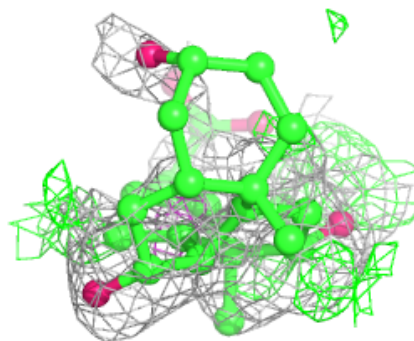
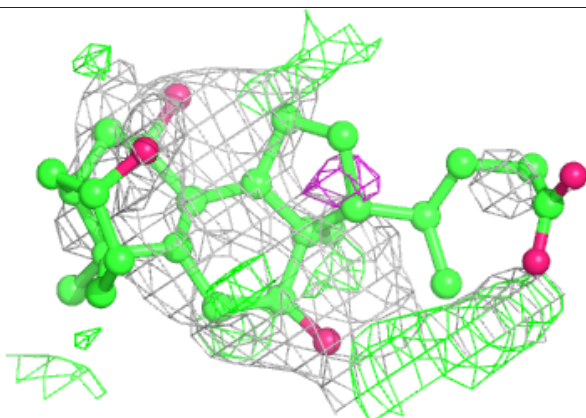
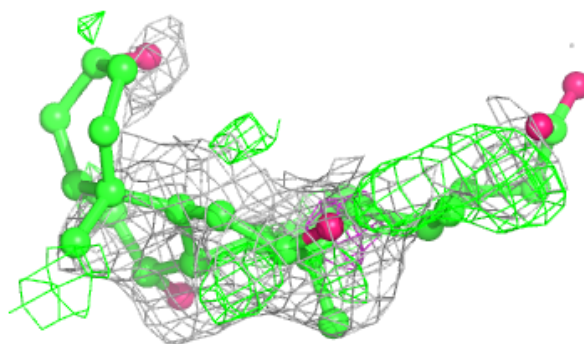
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

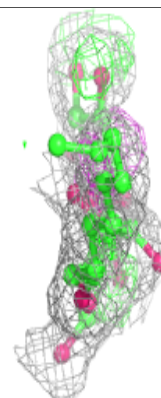
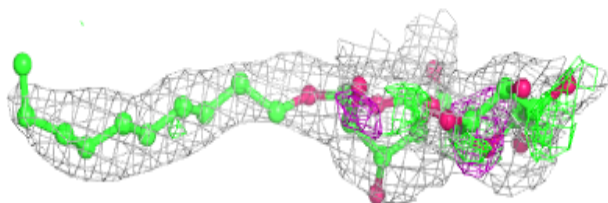
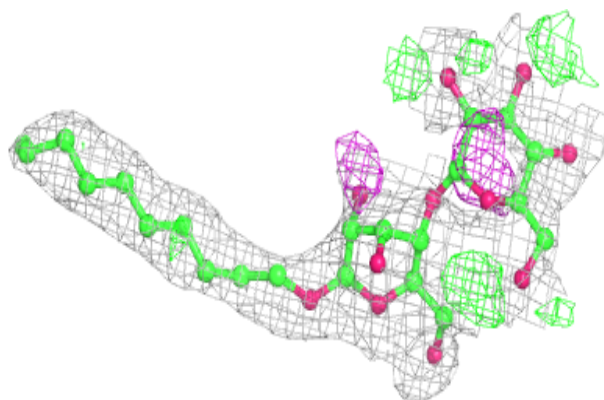


Electron density around CHD J 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

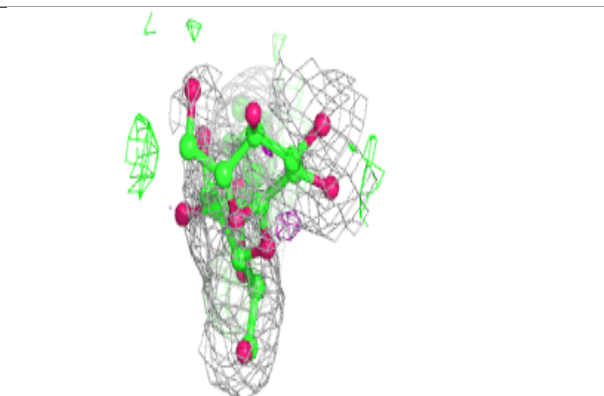
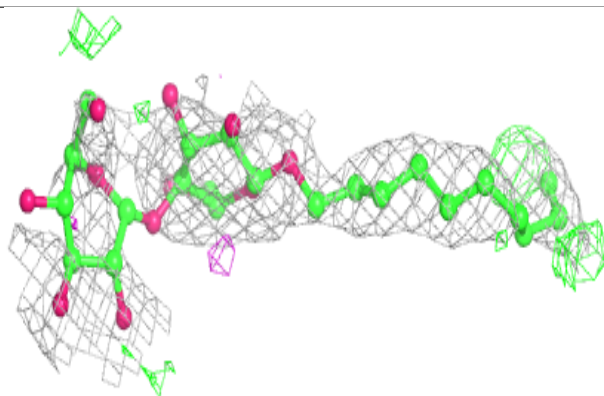
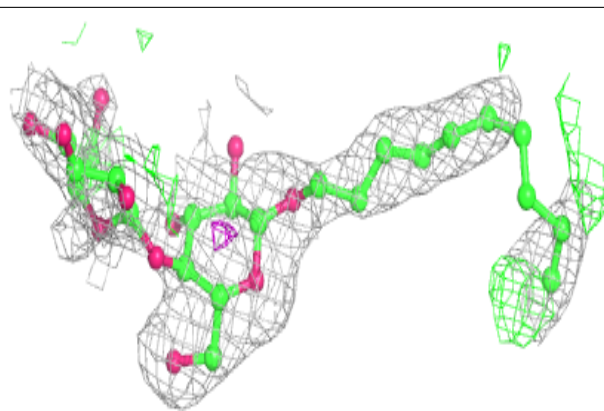
**Electron density around DMU C 311:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

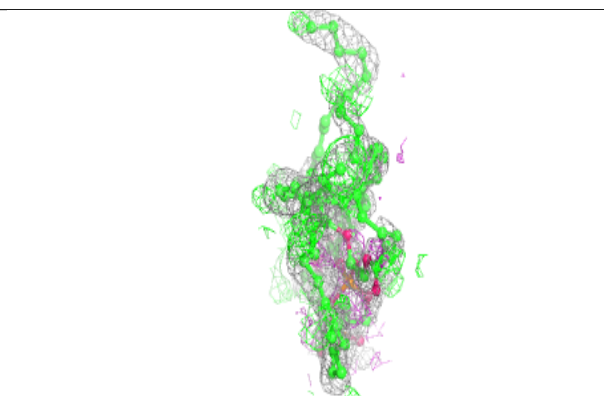
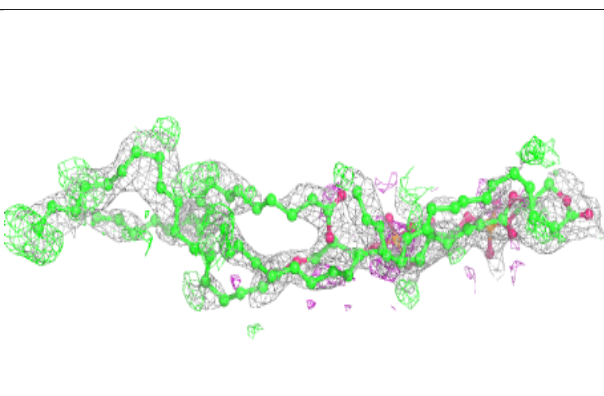
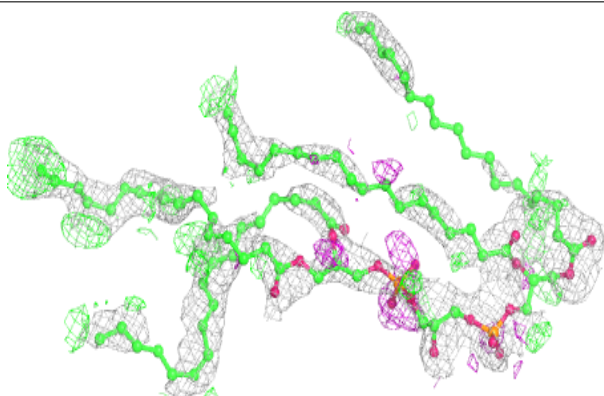


Electron density around DMU L 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

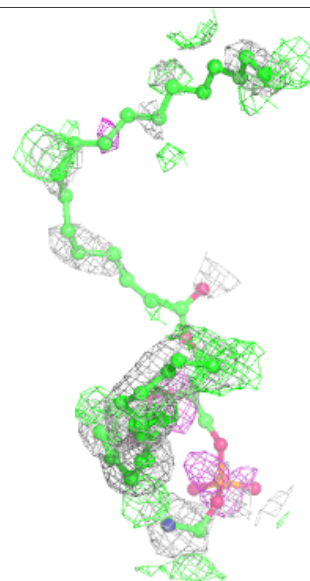
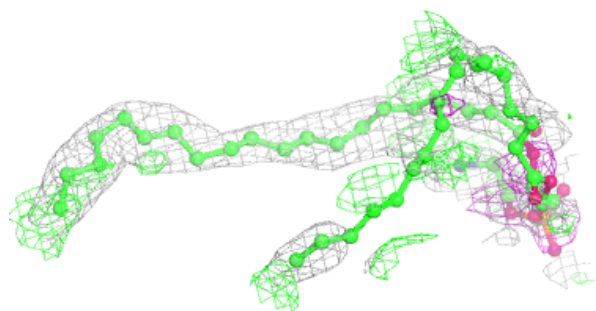
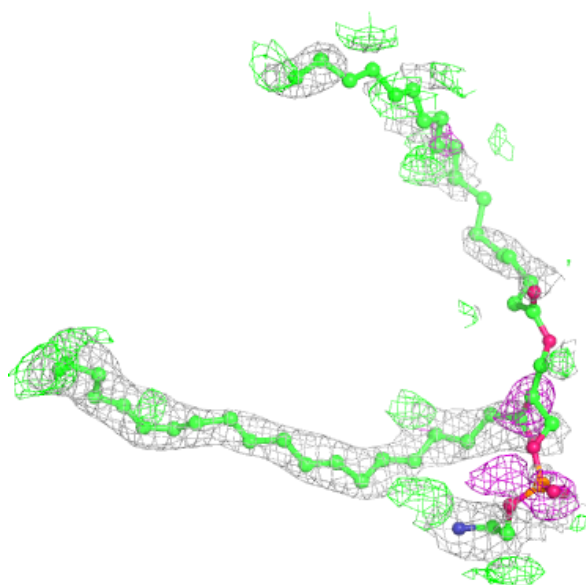
**Electron density around CDL T 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



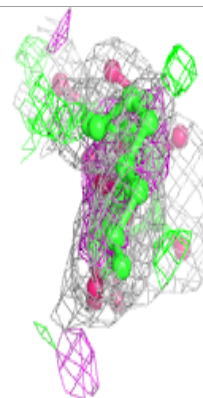
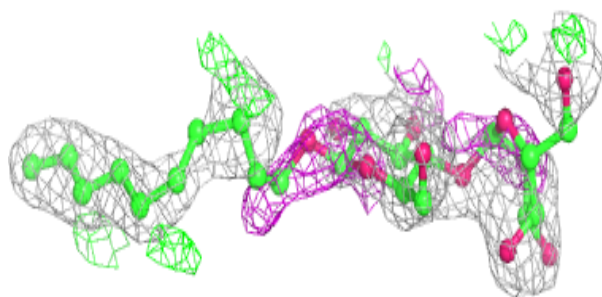
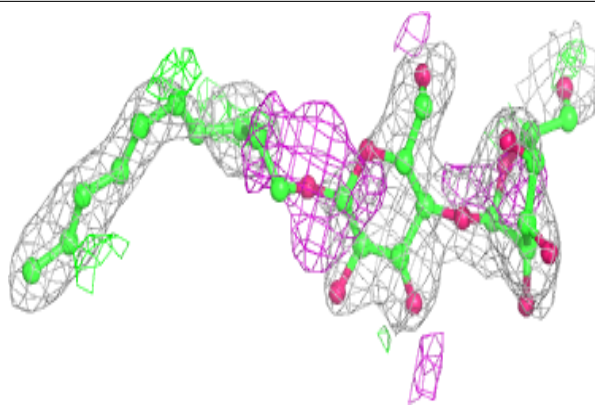
Electron density around PEK T 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

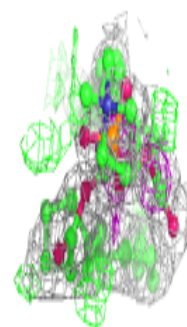
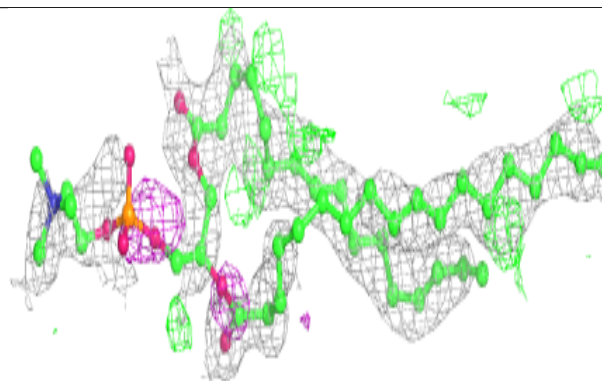
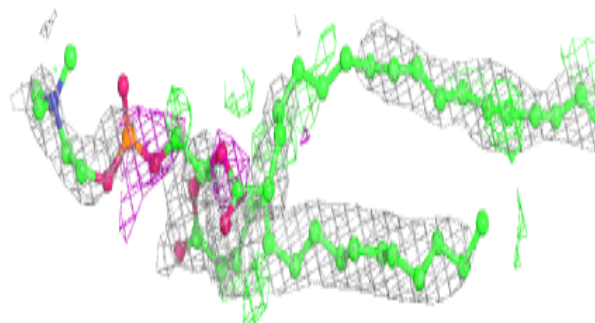


Electron density around DMU C 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

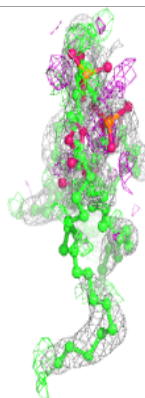
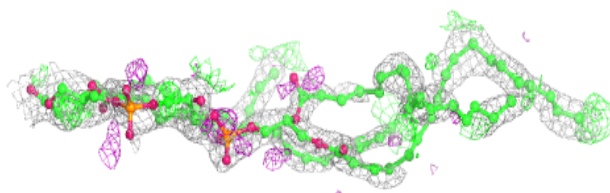
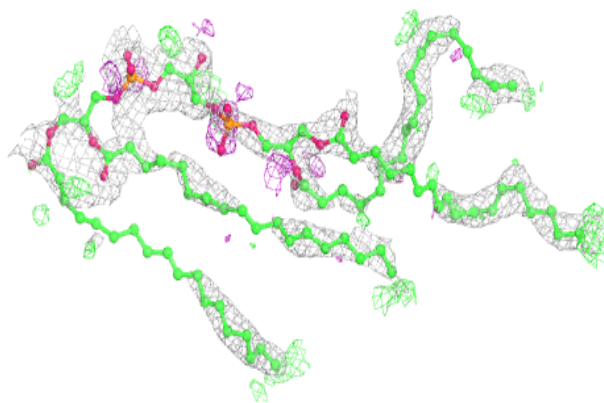
**Electron density around PSC B 303:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



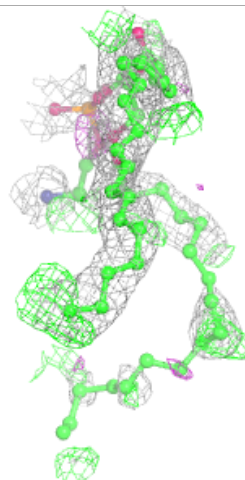
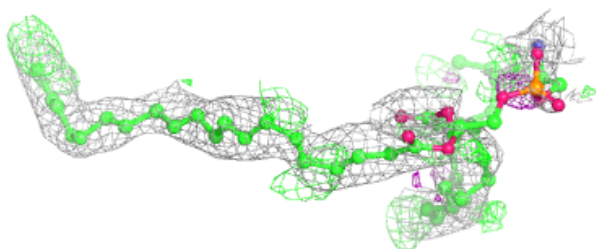
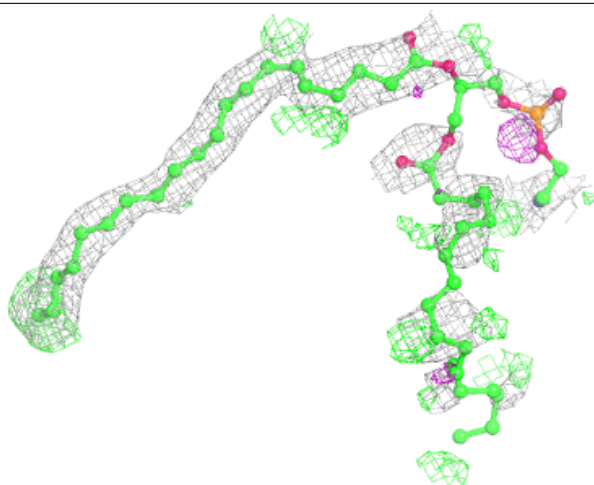
Electron density around CDL N 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



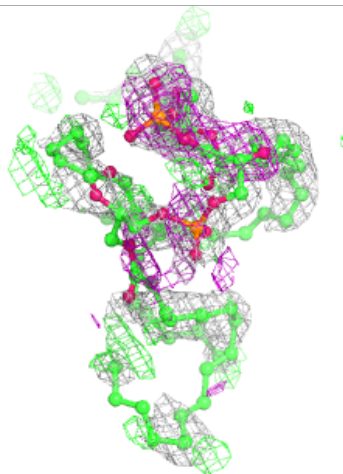
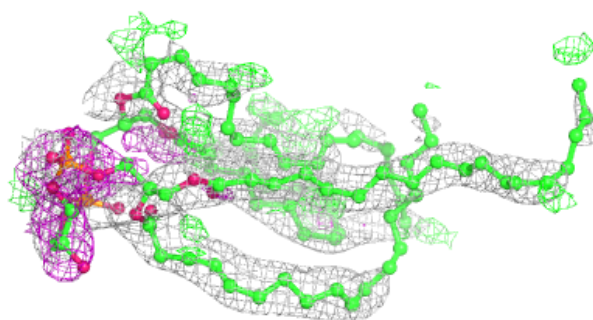
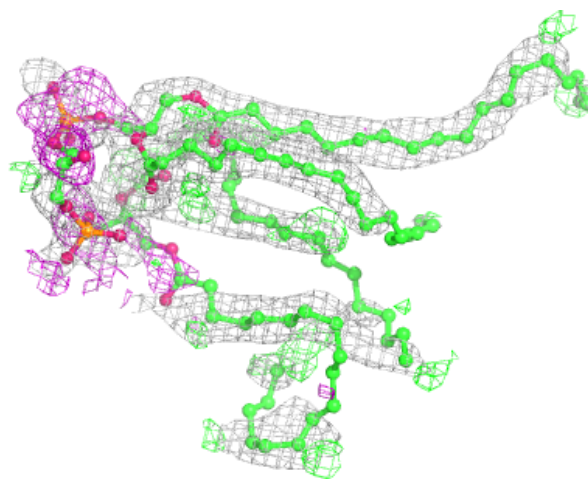
Electron density around PEK G 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



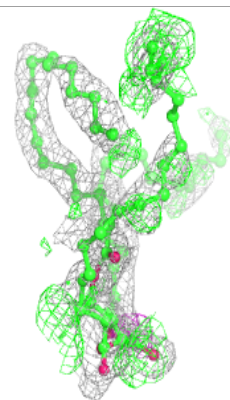
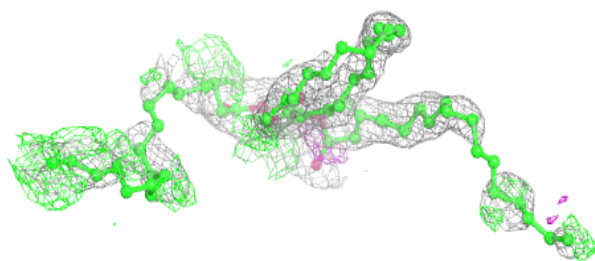
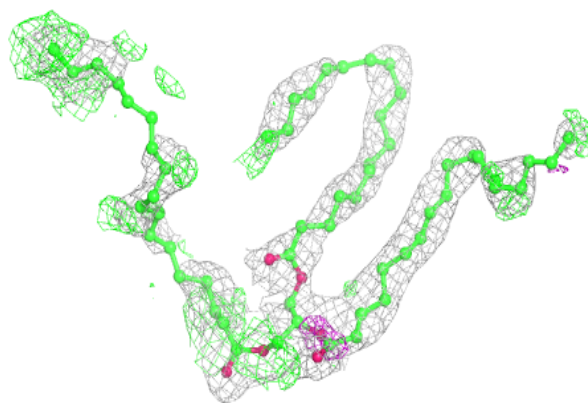
Electron density around CDL P 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

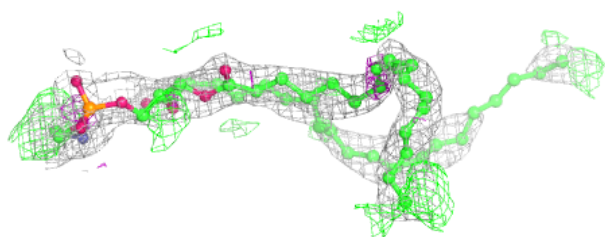
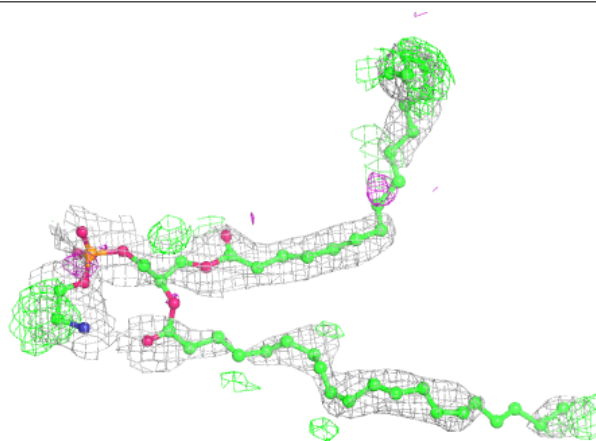


Electron density around TGL Q 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

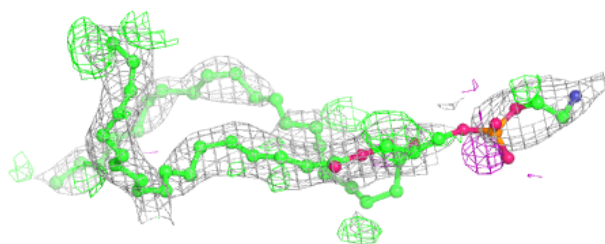
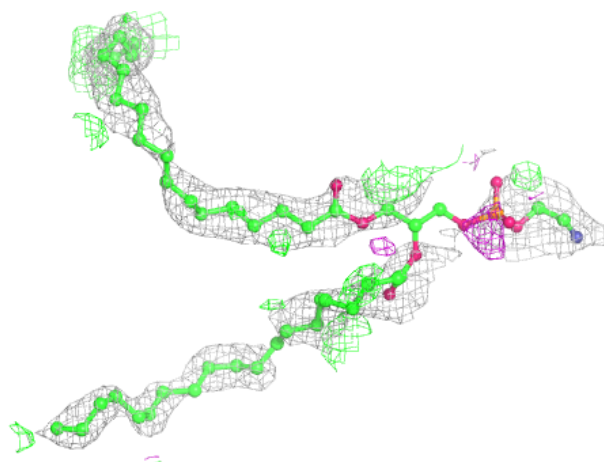
**Electron density around PEK P 307:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



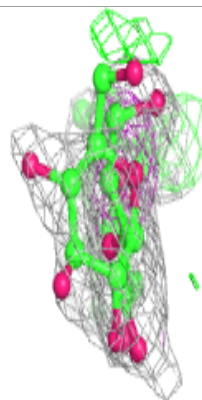
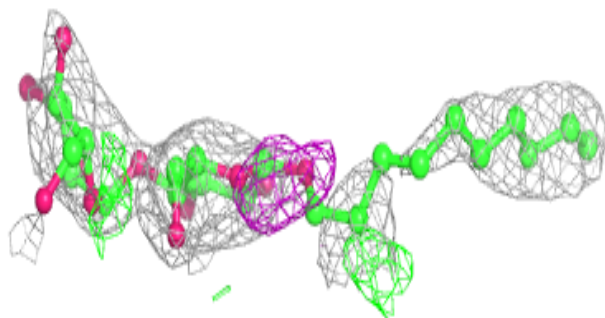
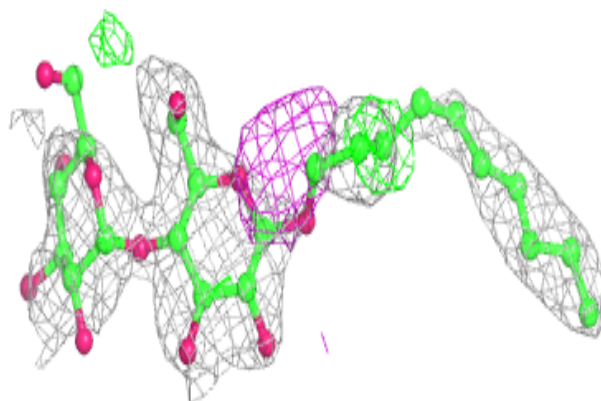
Electron density around PEK C 308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

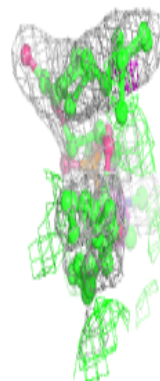
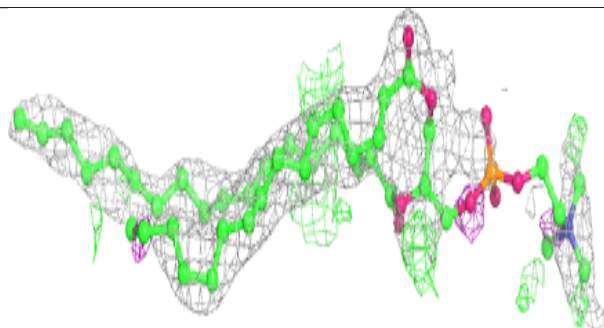
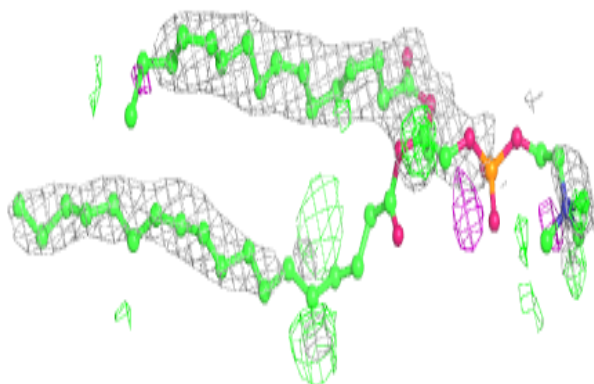


Electron density around DMU P 306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

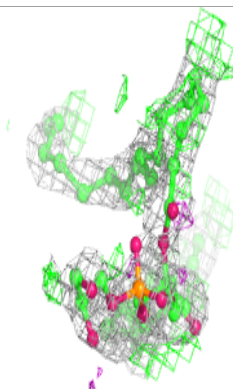
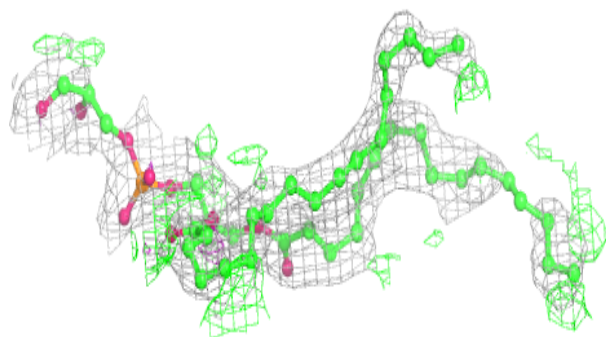
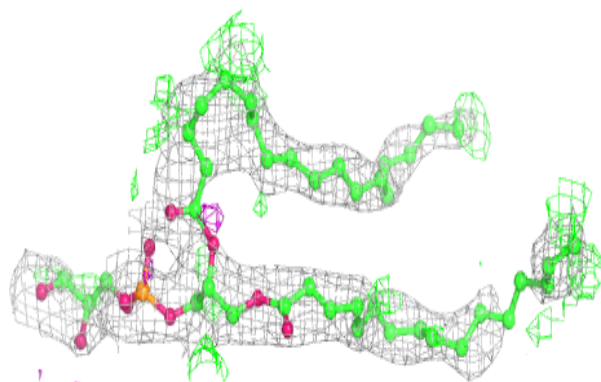
**Electron density around PSC O 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

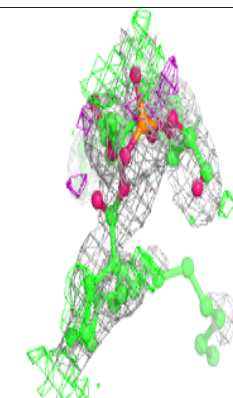
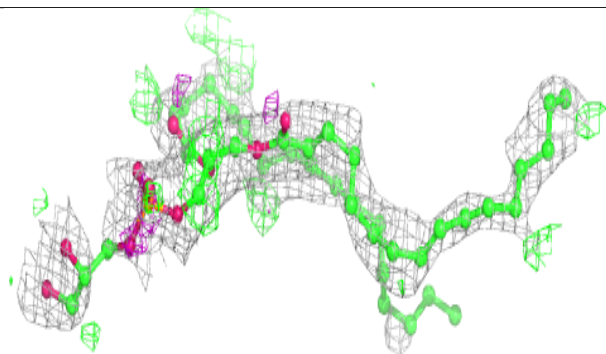
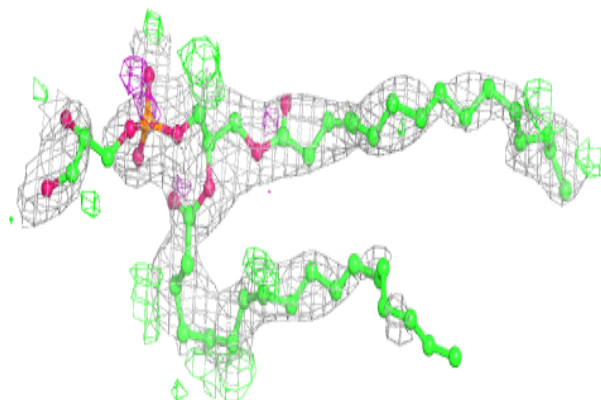


Electron density around PGV C 309:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

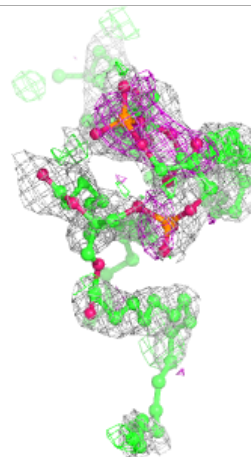
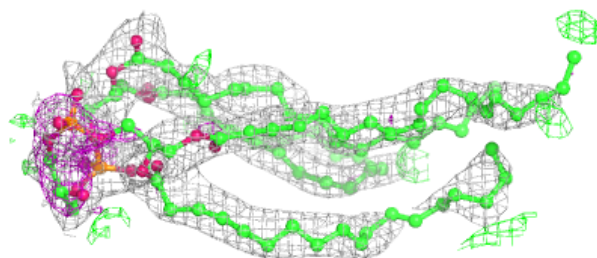
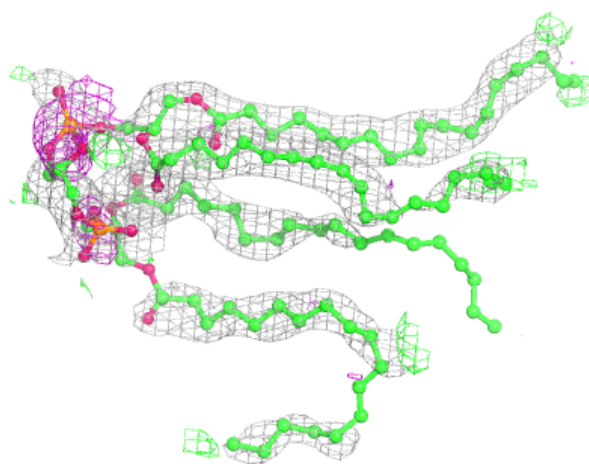
**Electron density around PGV G 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



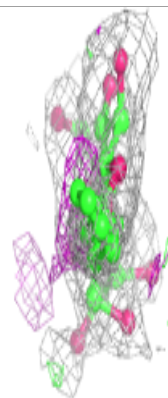
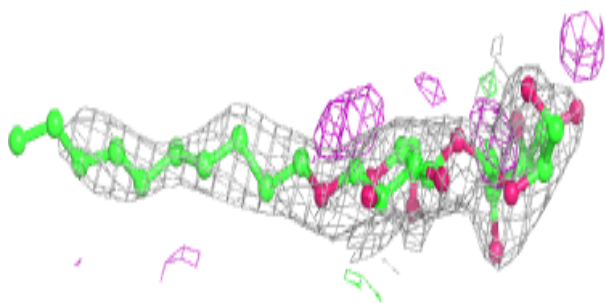
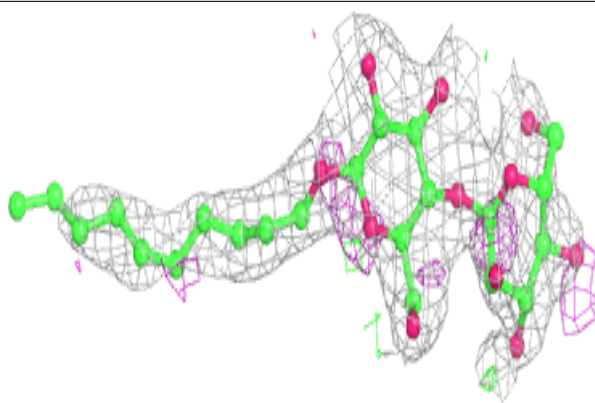
Electron density around CDL C 306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

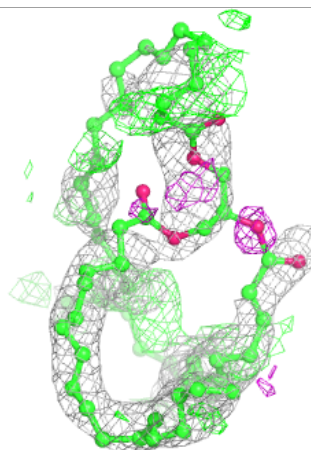
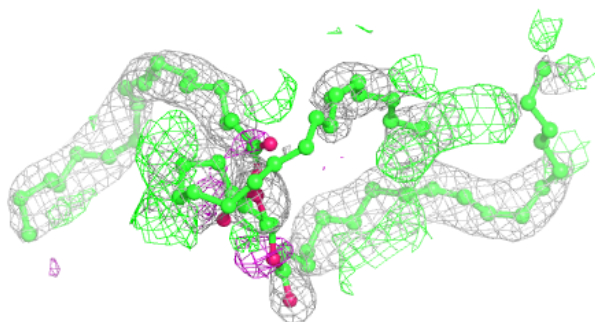
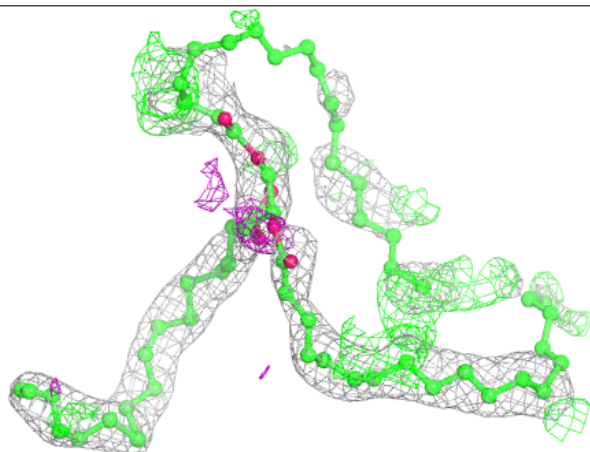


Electron density around DMU C 310:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

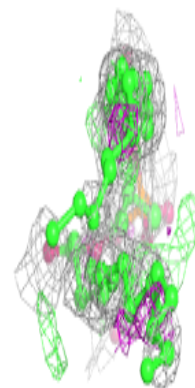
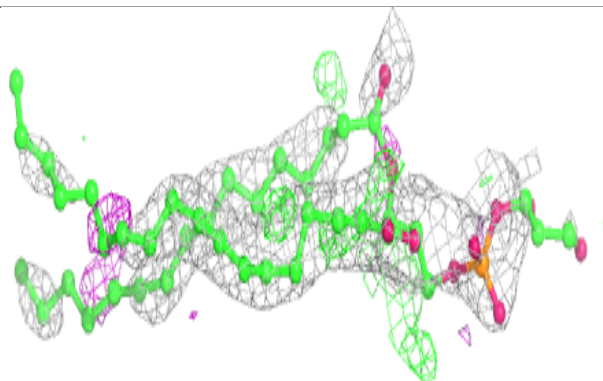
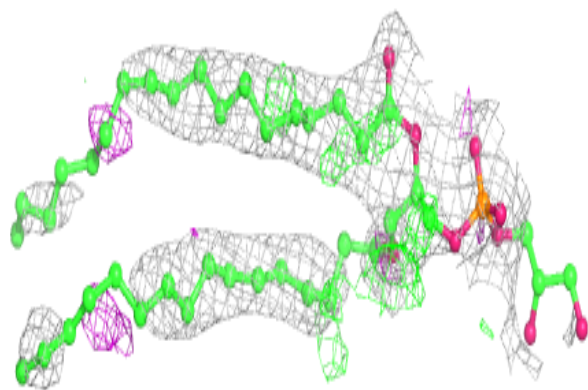
**Electron density around TGL Y 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



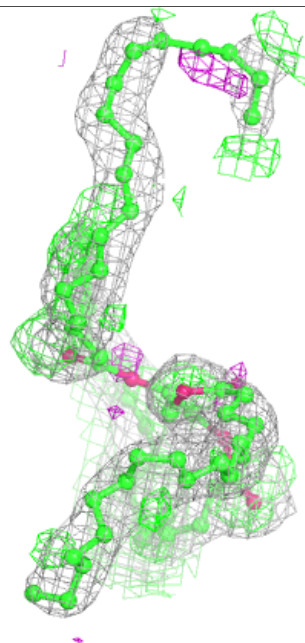
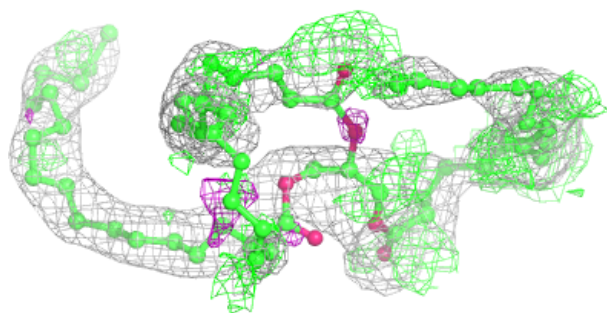
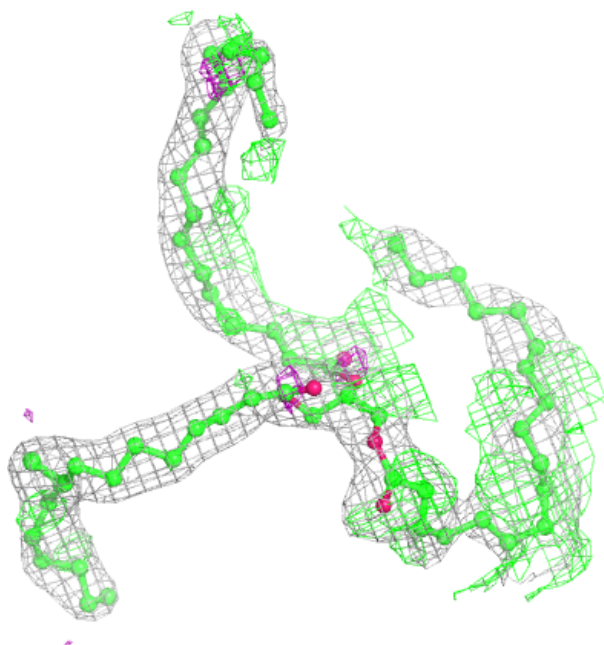
Electron density around PGV Z 101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



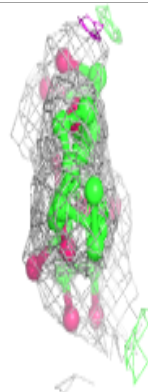
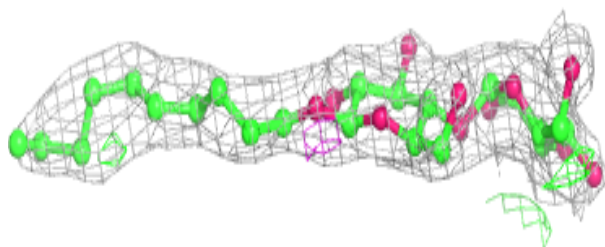
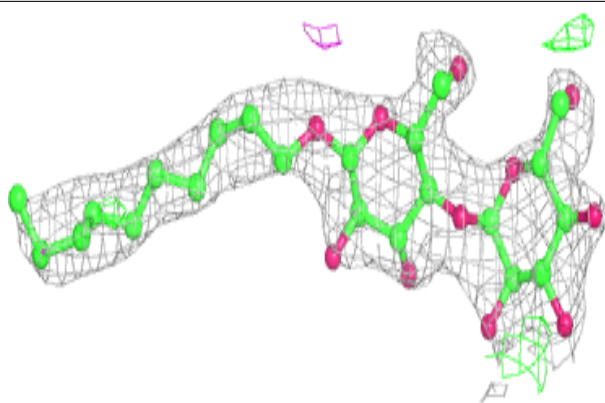
Electron density around TGL L 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

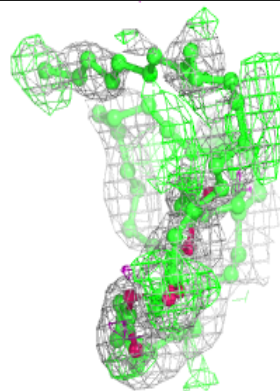
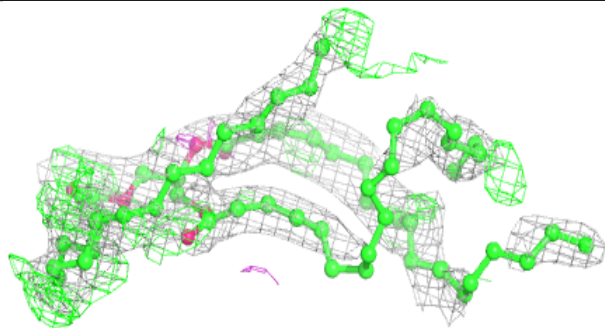
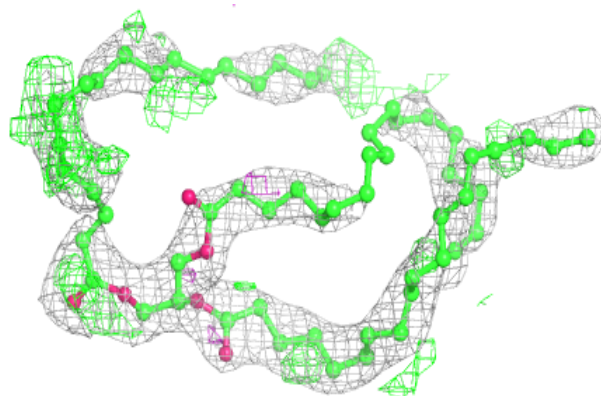


Electron density around DMU P 309:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

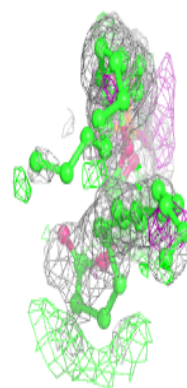
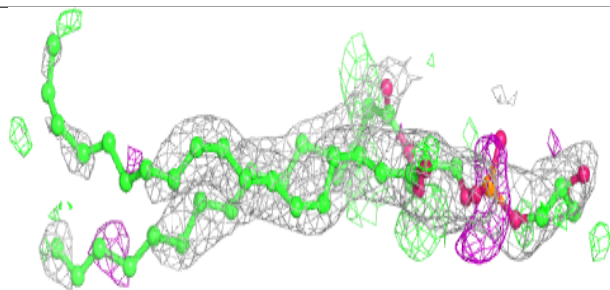
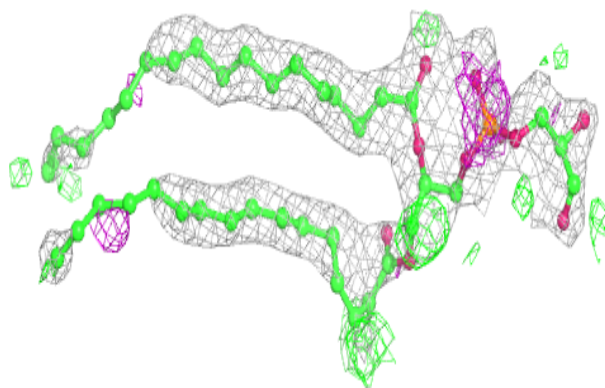
**Electron density around TGL N 610:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

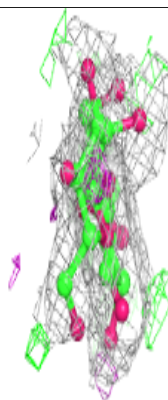
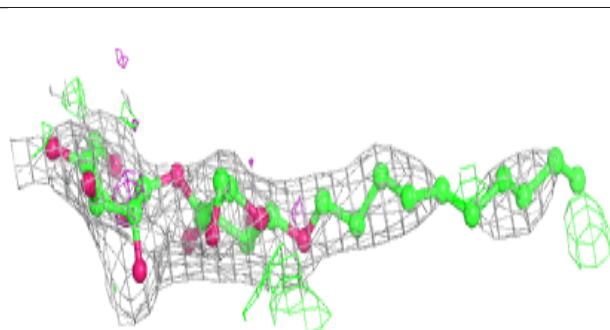
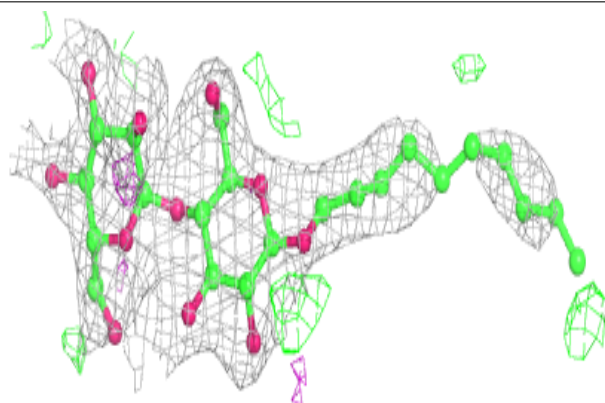


Electron density around PGV A 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

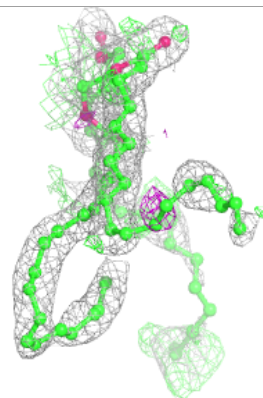
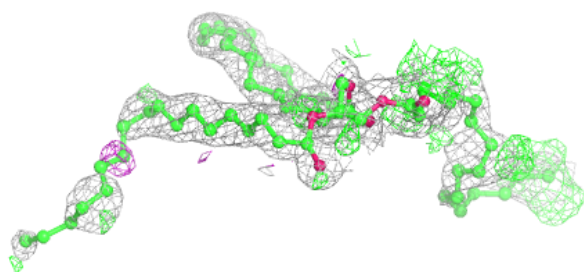
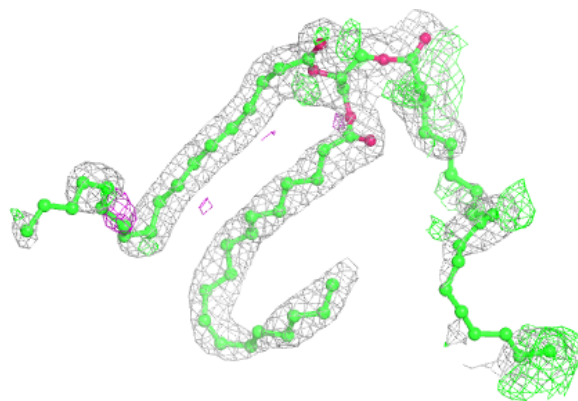
**Electron density around DMU P 308:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

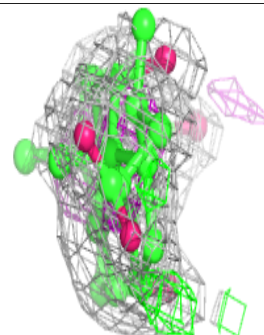
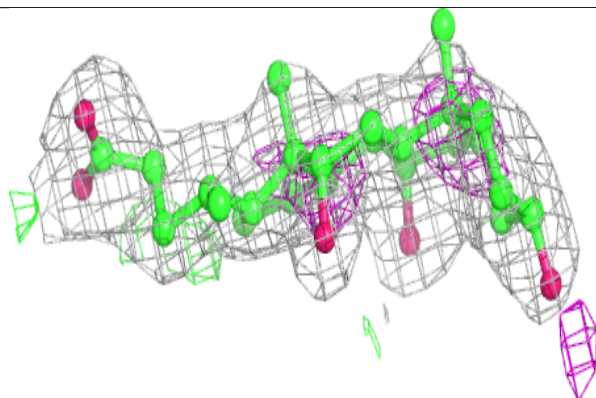
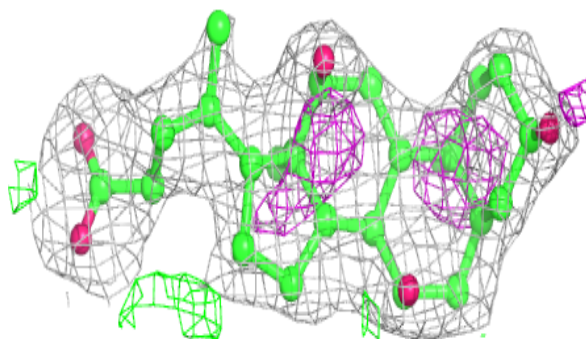


Electron density around TGL D 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

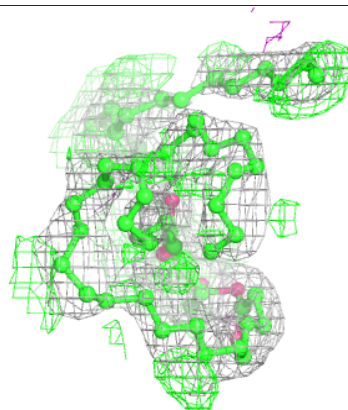
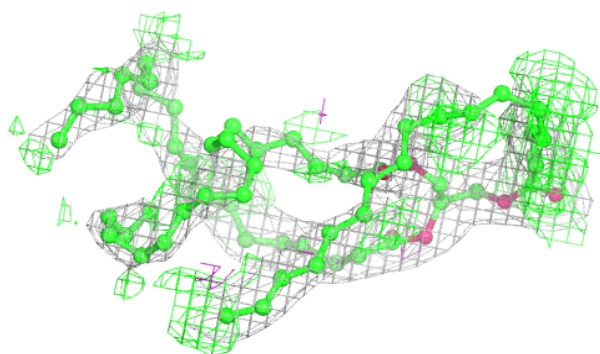
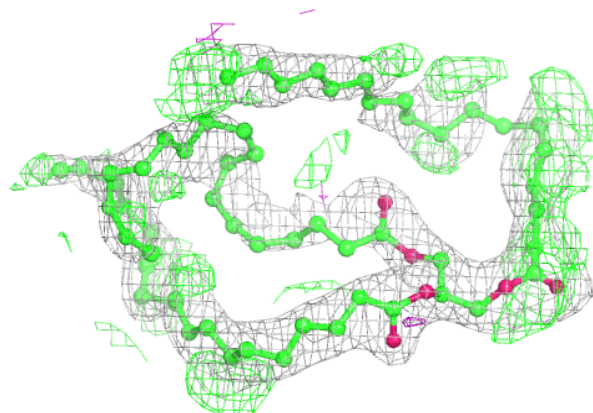
**Electron density around CHD P 305:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

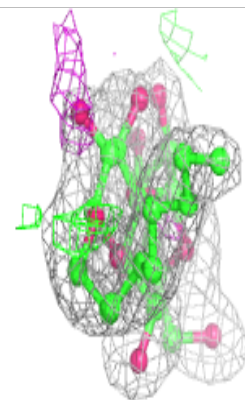
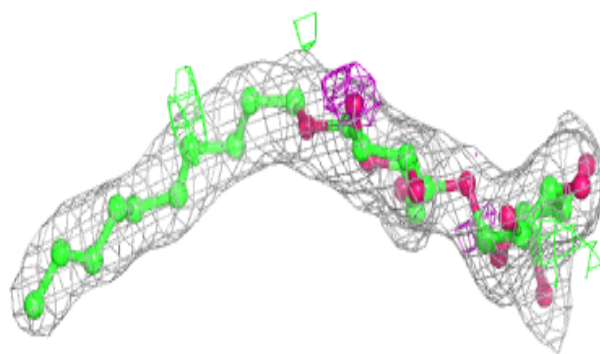
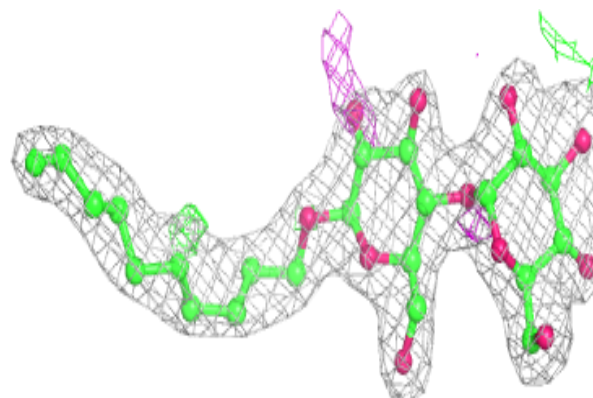


Electron density around TGL A 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

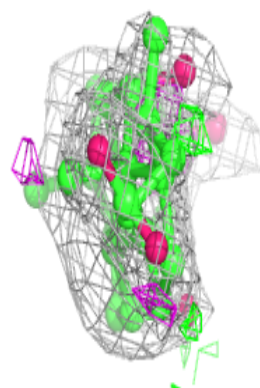
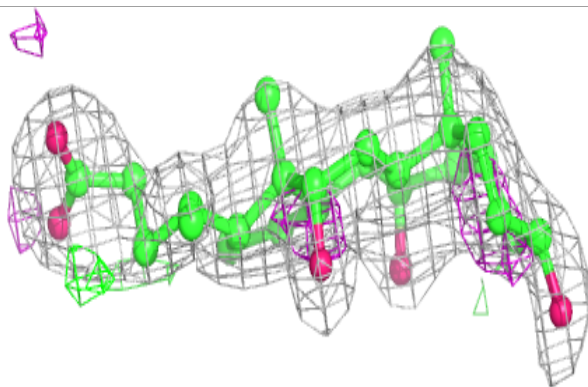
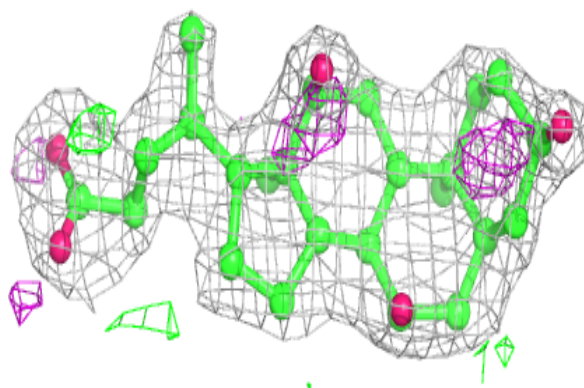
**Electron density around DMU Z 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

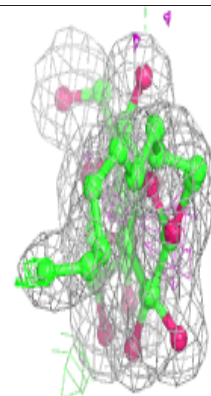
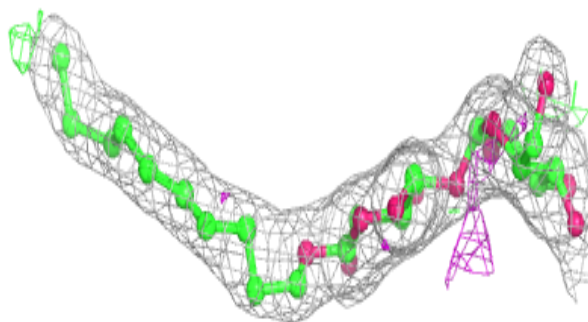
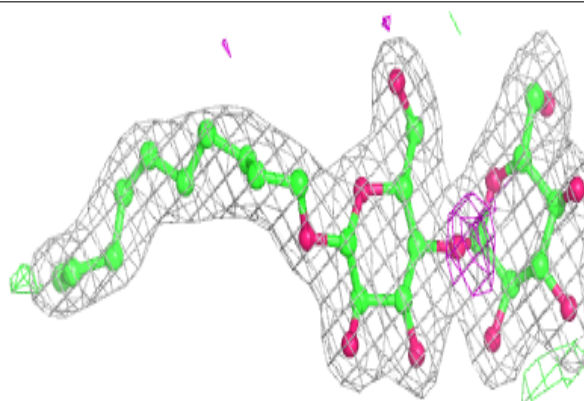


Electron density around CHD C 307:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

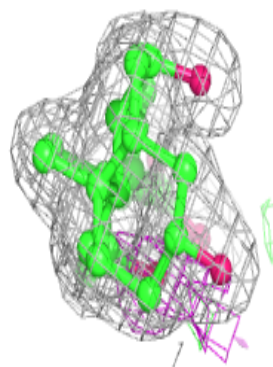
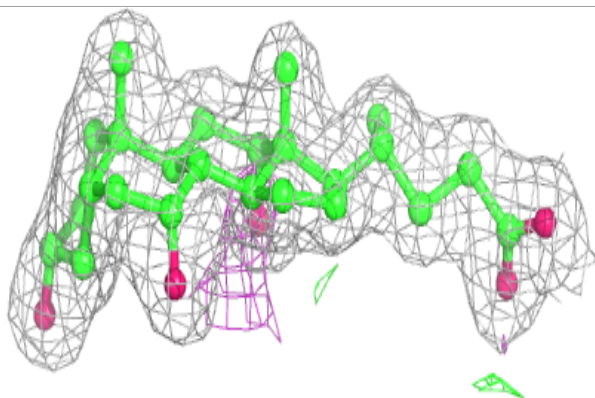
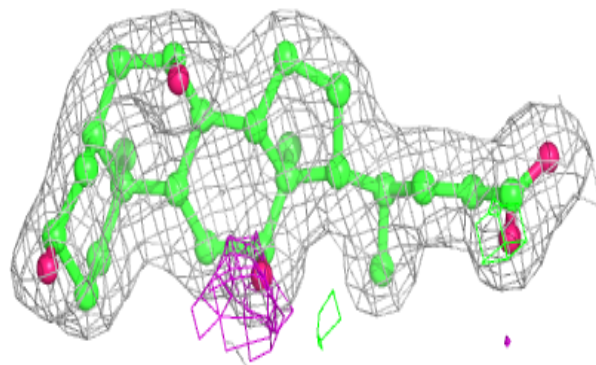
**Electron density around DMU M 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

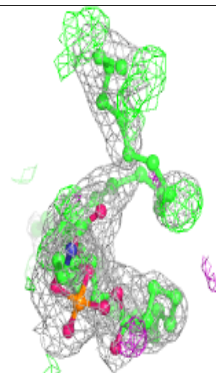
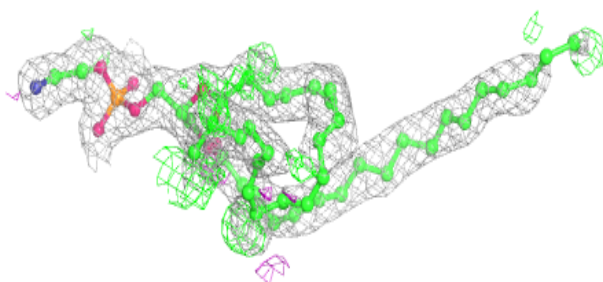
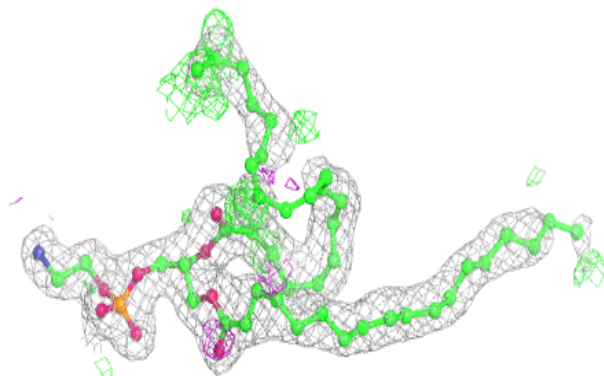


Electron density around CHD C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

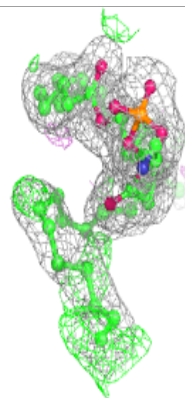
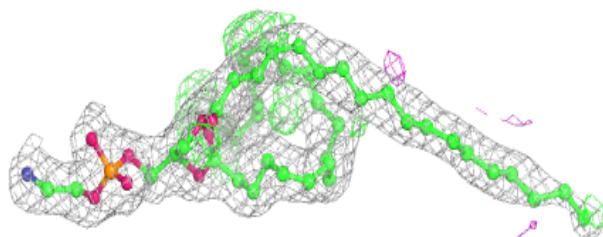
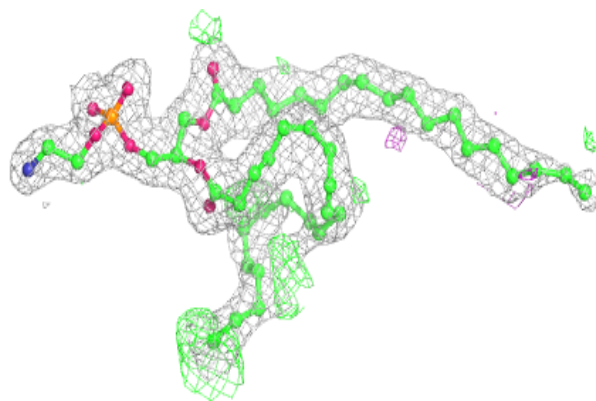
**Electron density around PEK T 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

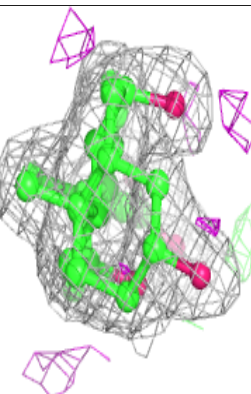
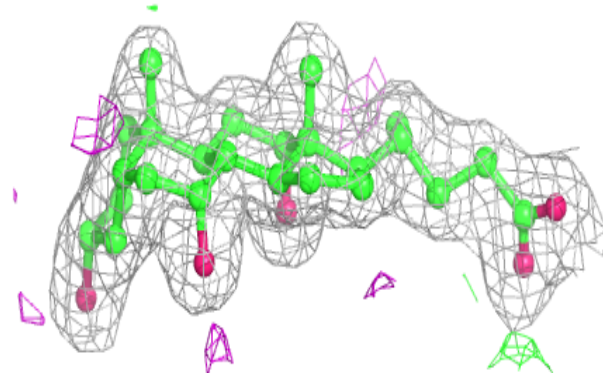
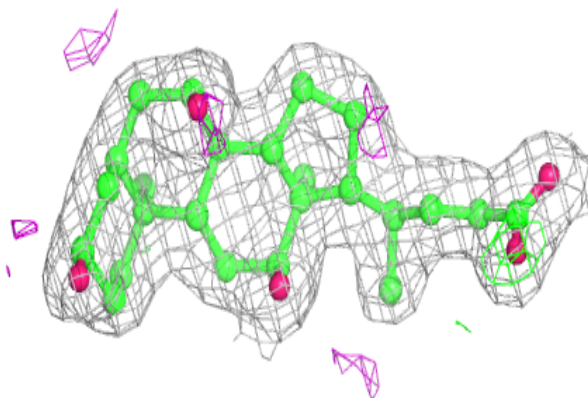


Electron density around PEK C 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

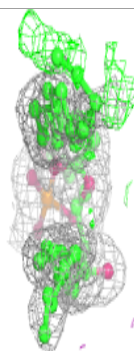
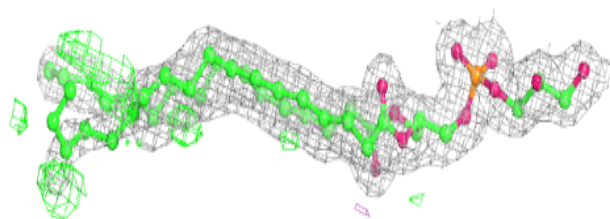
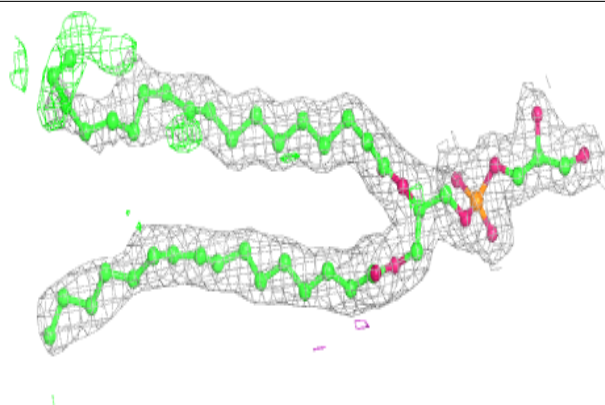
**Electron density around CHD P 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

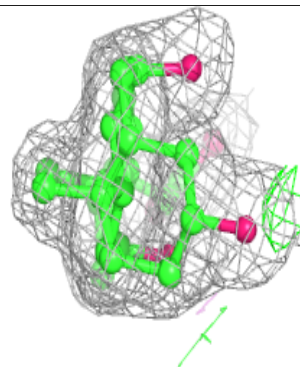
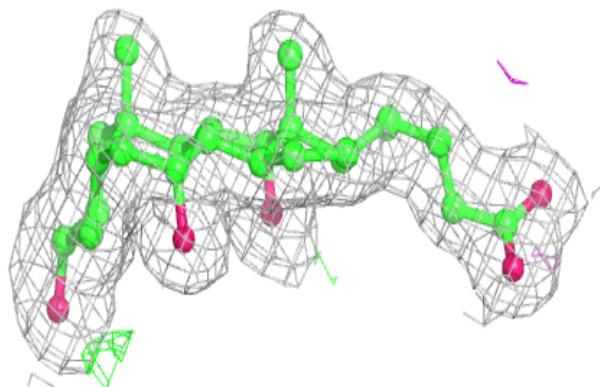
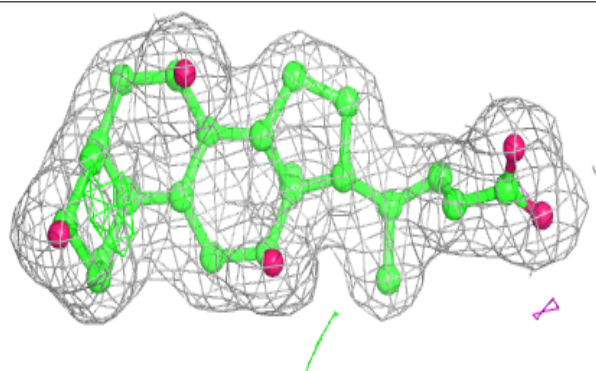


Electron density around PGV C 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

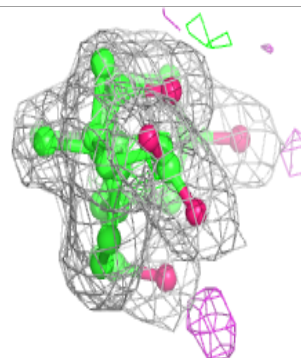
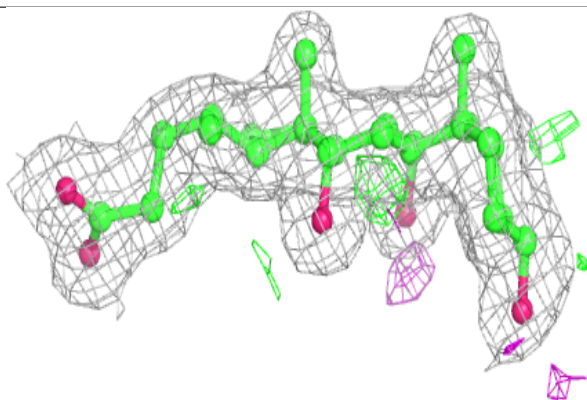
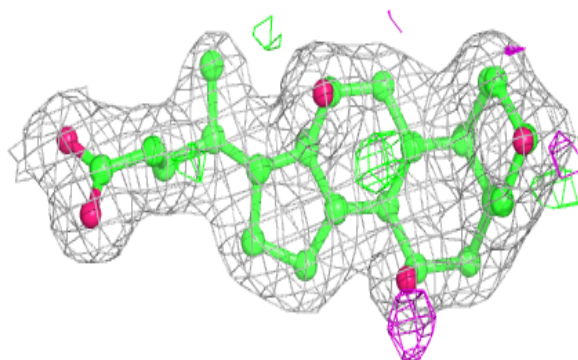
**Electron density around CHD G 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

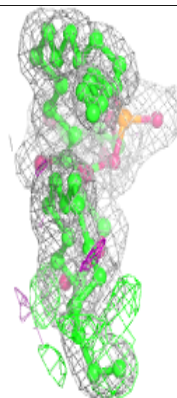
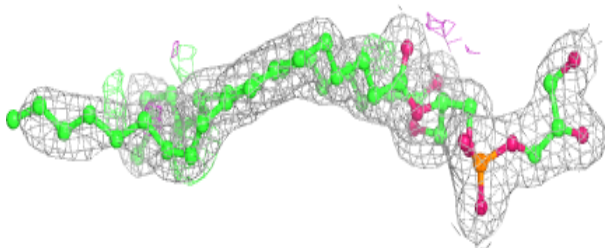
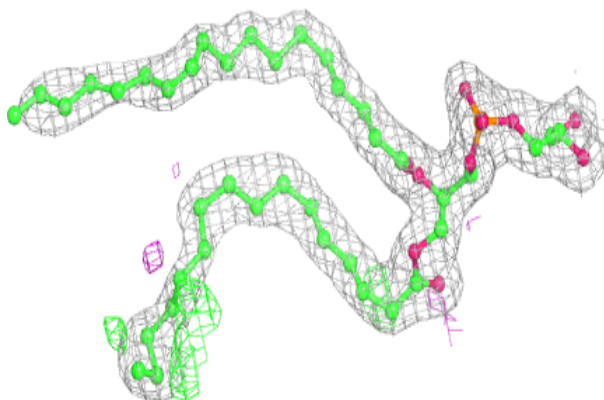


Electron density around CHD B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

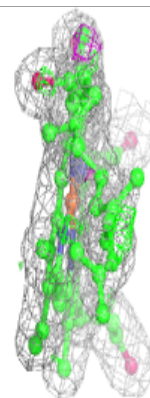
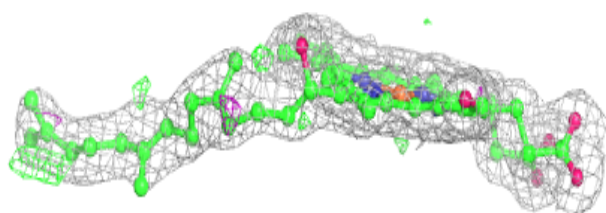
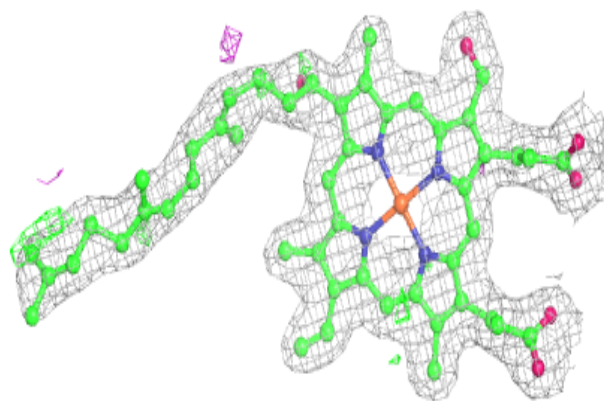
**Electron density around PGV A 609:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

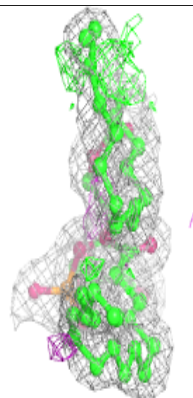
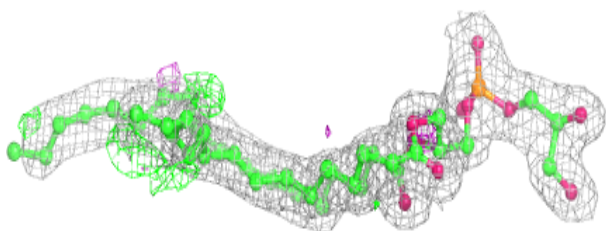
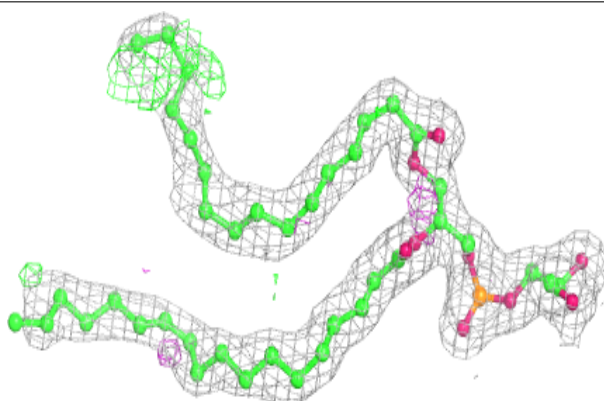


Electron density around HEA N 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

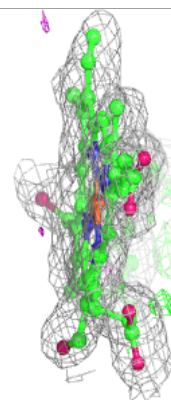
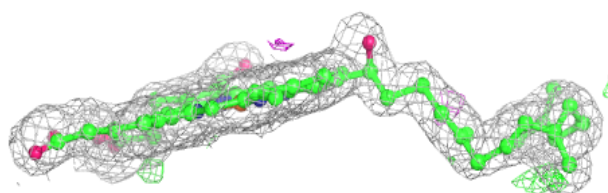
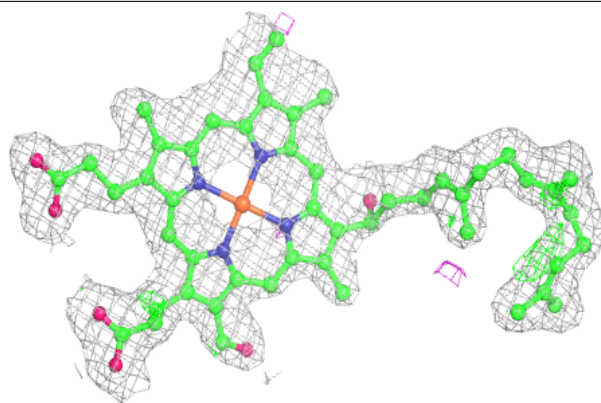
**Electron density around PGV N 609:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

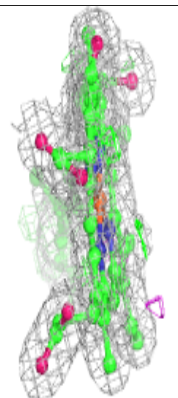
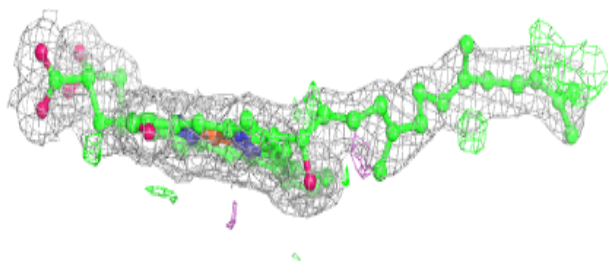
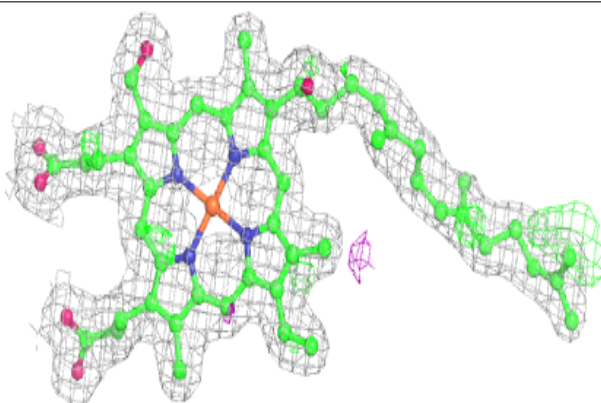


Electron density around HEA A 602 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

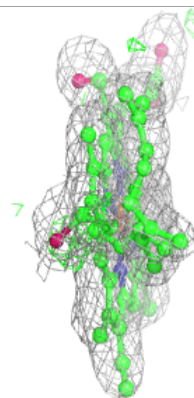
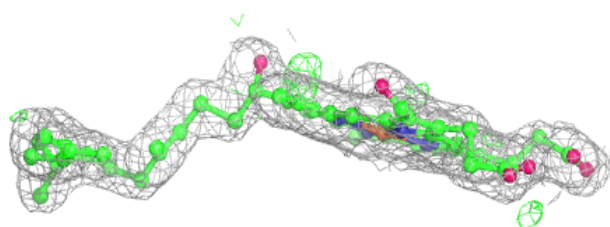
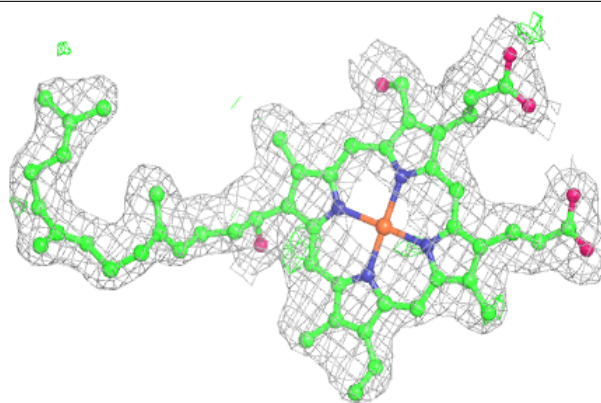
**Electron density around HEA A 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

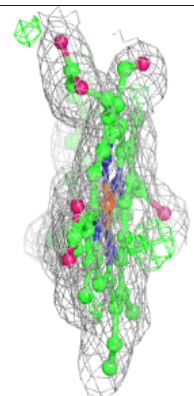
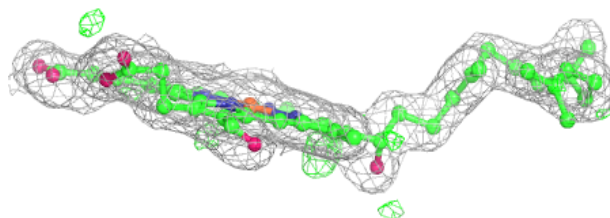
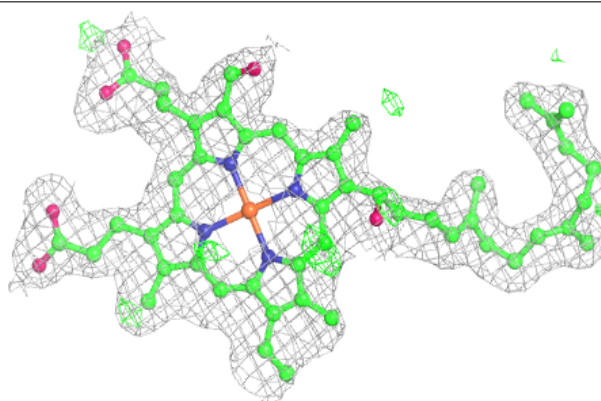


Electron density around HEA N 603 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

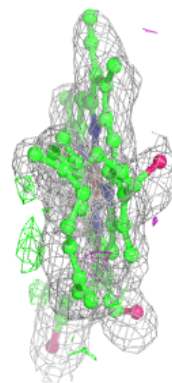
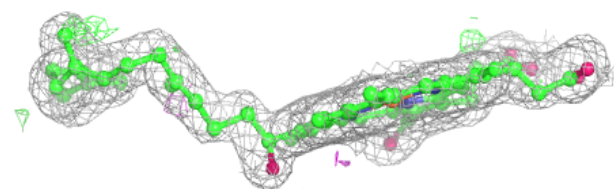
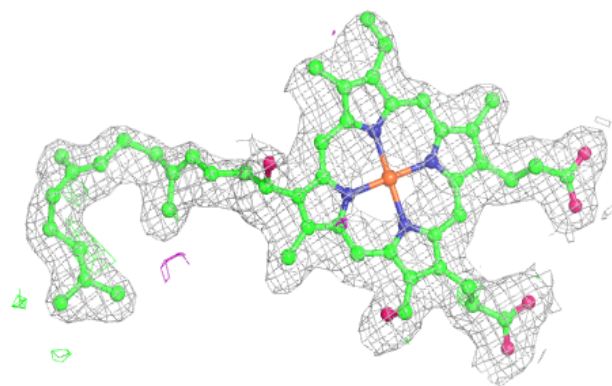
**Electron density around HEA N 603 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

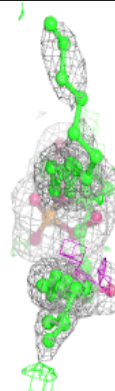
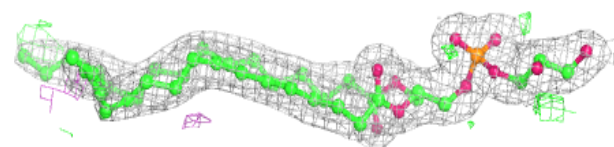
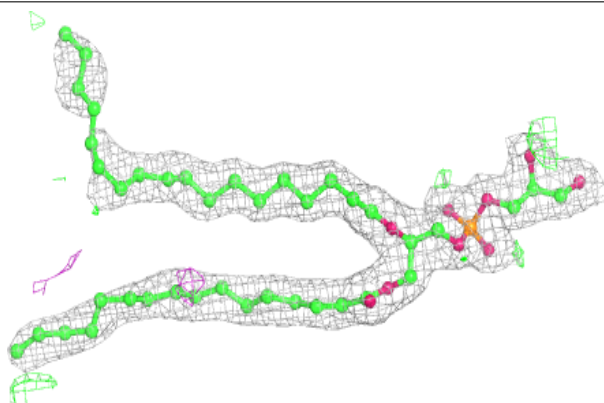


Electron density around HEA A 602 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PGV P 303:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.