



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:24 PM JST

PDB ID : 7W3E / pdb_00007w3e
Title : Bovine cytochrome c oxidase in CN-bound fully reduced state at 50 K
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2021-11-25
Resolution : 1.45 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

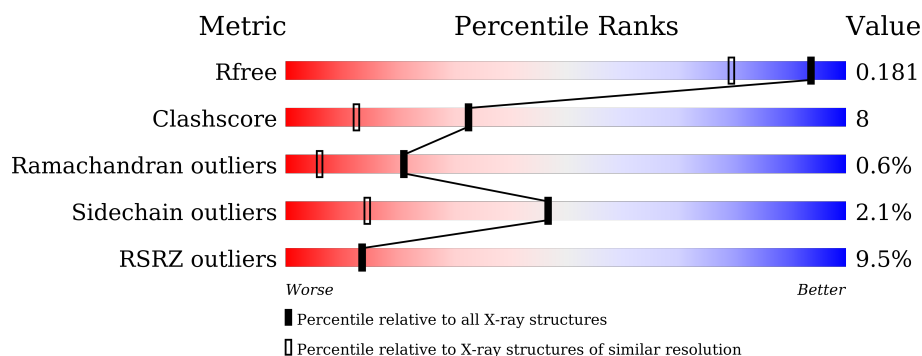
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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 of 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	2% 88% 12%
1	N	514	2% 89% 10%
2	B	227	12% 79% 19%
2	O	227	9% 80% 19%
3	C	259	3% 88% 12%
3	P	259	3% 90% 10%

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	104	
5	R	104	
6	F	93	
6	S	93	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	57	
10	W	57	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	41	
13	Z	41	

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
21	EDO	B	305	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 35109 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	34	0
			4162	2778	639	699	46			
1	N	514	Total	C	N	O	S	1	33	0
			4160	2776	639	698	47			

- 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	26	0
			2000	1306	302	372	20			
2	O	227	Total	C	N	O	S	0	26	0
			1999	1305	303	369	22			

- 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	7	0
			2125	1419	337	355	14			
3	P	259	Total	C	N	O	S	0	6	0
			2121	1417	339	351	14			

- 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	1	0
			1201	783	196	218	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1209	783	202	220	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	3	0
			720	445	128	142	5			
6	S	93	Total	C	N	O	S	0	4	0
			721	447	127	141	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	S	0	0	0
			642	413	122	106	1			
7	T	84	Total	C	N	O	S	0	2	0
			663	423	126	113	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	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	2	0
			389	253	65	68	3			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

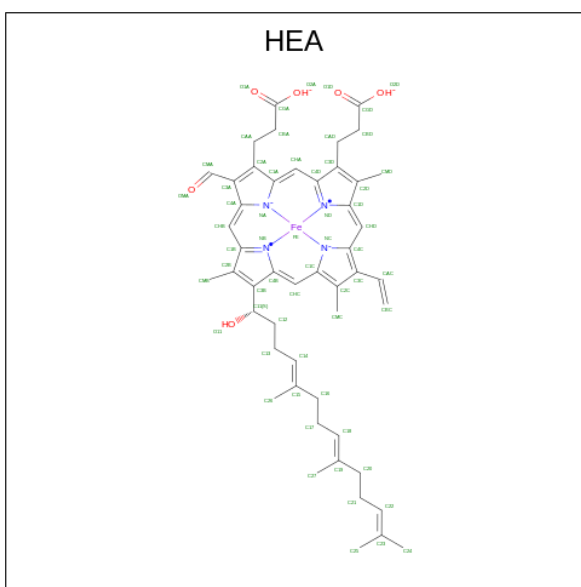
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	61	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	41	Total	C	N	O	0	1	0
			322	216	50	56			
13	Z	41	Total	C	N	O	0	0	0
			320	214	50	56			

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	
			79	67	1	4	7	0
14	A	1	Total	C	Fe	N	O	
			111	89	2	8	12	0
14	N	1	Total	C	Fe	N	O	
			79	67	1	4	7	0
14	N	1	Total	C	Fe	N	O	
			111	89	2	8	12	0

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

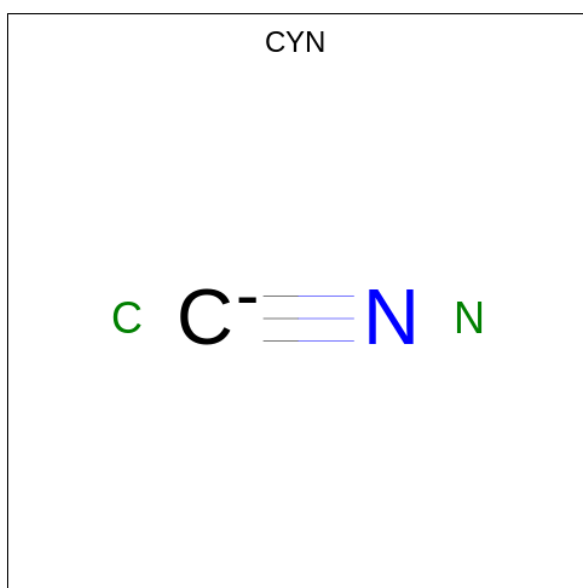
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

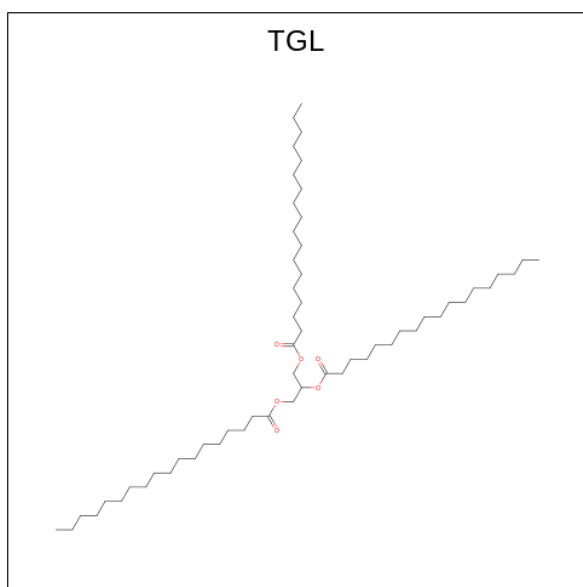
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		
17	P	1	Total	Na	0	0
			1	1		

- Molecule 18 is CYANIDE ION (CCD ID: CYN) (formula: CN).



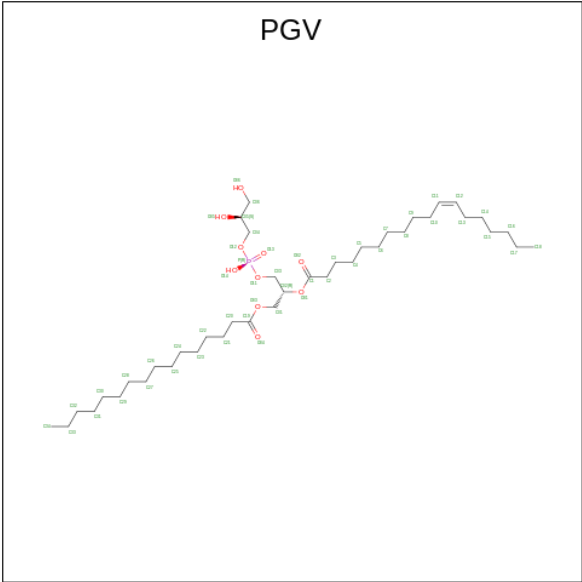
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	N	0	1
			4	2	2		
18	N	1	Total	C	N	0	1
			4	2	2		

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



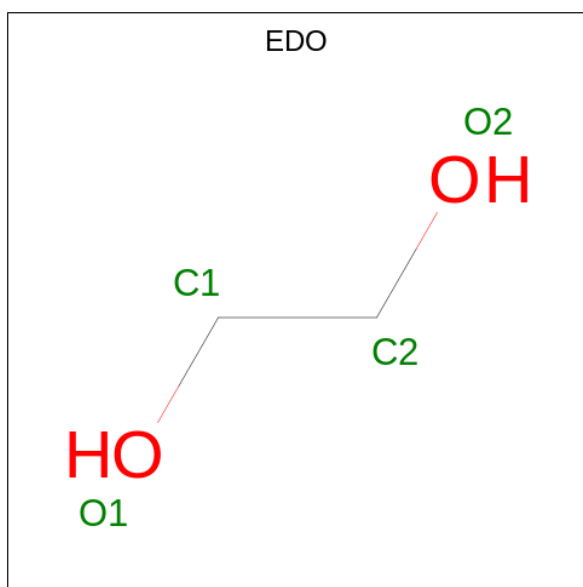
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	B	1	Total	C	O	0	0
			62	56	6		
19	D	1	Total	C	O	0	0
			48	42	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			46	37	8	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	C	1	Total	C	O	P	0	0
			47	36	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			45	34	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	Q	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: 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	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		

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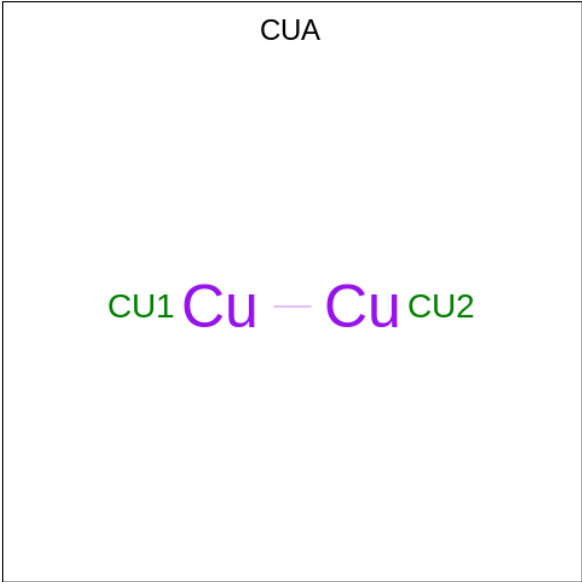
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	C	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4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

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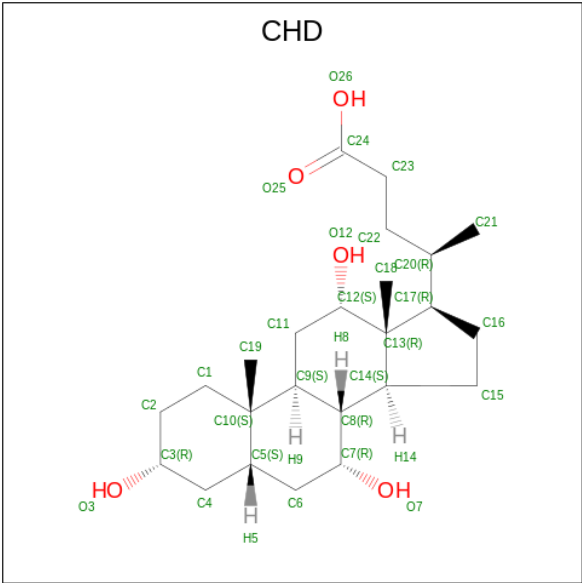
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4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

- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



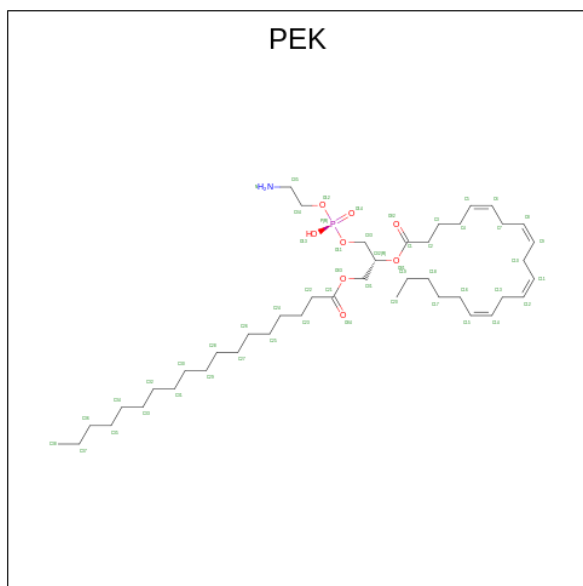
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 24 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



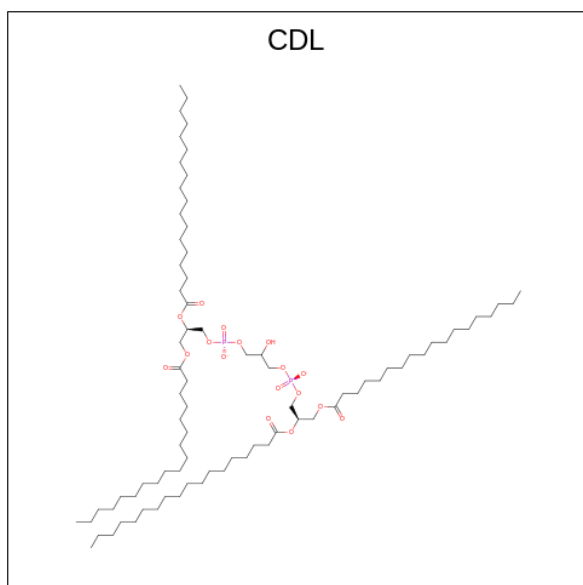
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
24	C	1	Total	C	O			0	0
			44	40	4				
24	P	1	Total	C	O			0	0
			22	20	2				
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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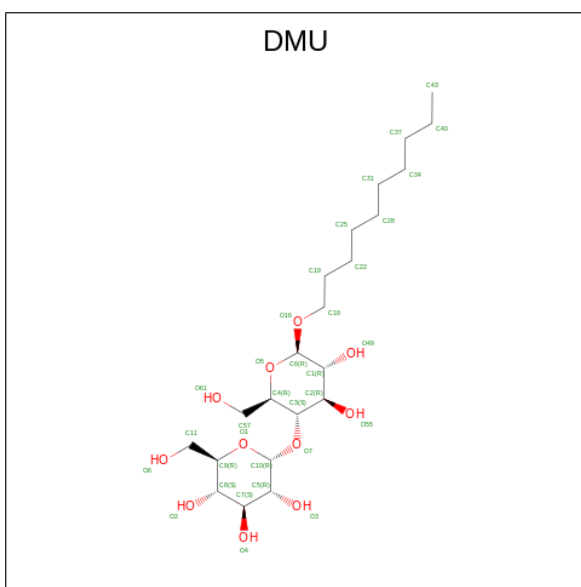
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	P	1	Total	C	O		0	0
			46	41	5			
24	T	1	Total	C	N	O	P	
			49	39	1	8	1	0

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			86	68	16	2		
25	G	1	Total	C	O	P	0	0
			89	71	16	2		
25	P	1	Total	C	O	P	0	0
			76	64	11	1		
25	T	1	Total	C	O	P	0	0
			80	63	15	2		
25	Y	1	Total	C	O	P	0	0
			87	68	17	2		

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



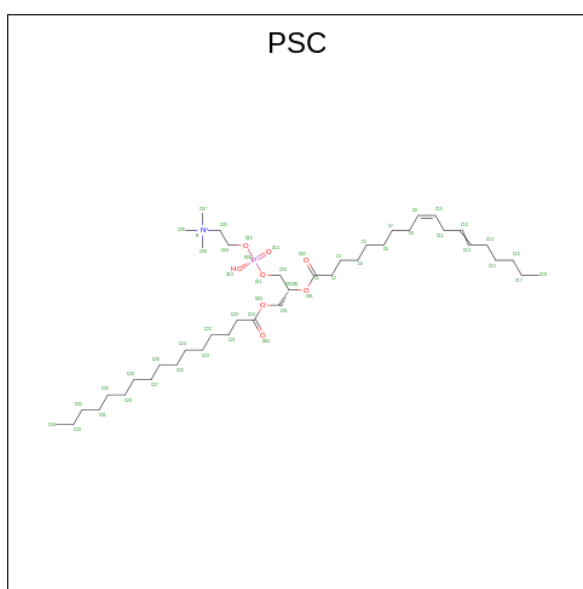
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total 33	C 22	O 11	0	0
26	G	1	Total 21	C 16	O 5	0	0
26	J	1	Total 33	C 22	O 11	0	0
26	K	1	Total 22	C 16	O 6	0	0
26	K	1	Total 22	C 16	O 6	0	0
26	K	1	Total 17	C 15	O 2	0	0
26	L	1	Total 18	C 12	O 6	0	0
26	M	1	Total 33	C 22	O 11	0	0
26	P	1	Total 33	C 22	O 11	0	0
26	P	1	Total 33	C 22	O 11	0	0
26	P	1	Total 33	C 22	O 11	0	0
26	P	1	Total 33	C 22	O 11	0	0
26	P	1	Total 22	C 16	O 6	0	0
26	X	1	Total 22	C 16	O 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	X	1	Total	C	O	0	0
			22	16	6		
26	X	1	Total	C	O	0	0
			22	16	6		
26	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 27 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).

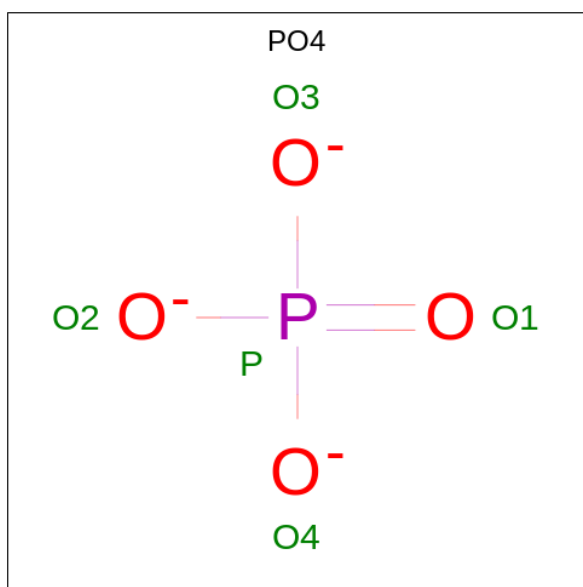


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
27	O	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 29 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	U	1	Total	O	P	0	0
			5	4	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	286	Total	O	0	3
			286	286		
30	B	245	Total	O	0	0
			245	245		
30	C	196	Total	O	0	0
			196	196		
30	D	250	Total	O	0	0
			250	250		
30	E	178	Total	O	0	0
			178	178		
30	F	177	Total	O	0	2
			177	177		
30	G	97	Total	O	0	0
			97	97		
30	H	111	Total	O	0	0
			111	111		
30	I	81	Total	O	0	0
			81	81		
30	J	63	Total	O	0	0
			63	63		
30	K	63	Total	O	0	0
			63	63		

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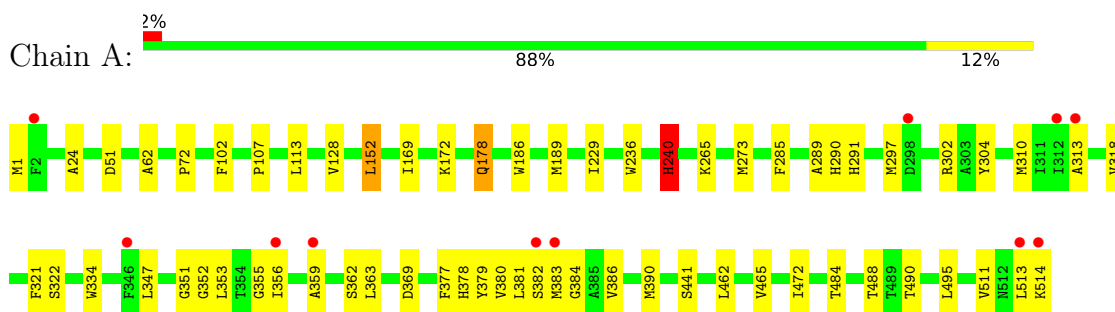
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	L	57	Total 57	O 57	0	0
30	M	46	Total 46	O 46	0	0
30	N	263	Total 263	O 263	0	1
30	O	204	Total 204	O 204	0	0
30	P	179	Total 179	O 179	0	0
30	Q	128	Total 128	O 128	0	0
30	R	131	Total 131	O 131	0	0
30	S	126	Total 126	O 126	0	0
30	T	78	Total 78	O 78	0	0
30	U	121	Total 121	O 121	0	0
30	V	68	Total 68	O 68	0	0
30	W	51	Total 51	O 51	0	0
30	X	50	Total 50	O 50	0	0
30	Y	48	Total 48	O 48	0	0
30	Z	30	Total 30	O 30	0	0

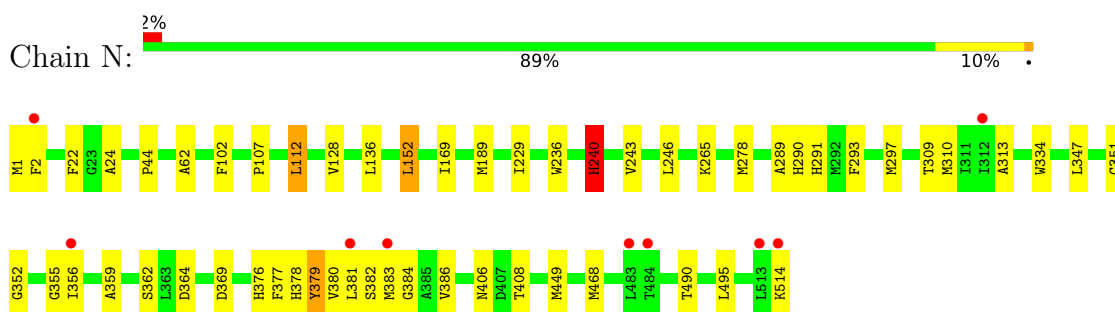
3 Residue-property plots [i](#)

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

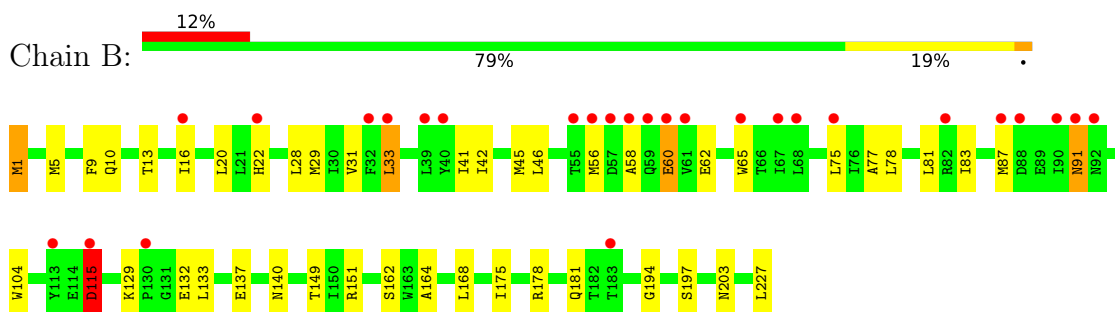
• Molecule 1: Cytochrome c oxidase subunit 1



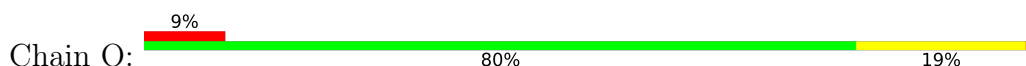
• Molecule 1: Cytochrome c oxidase subunit 1

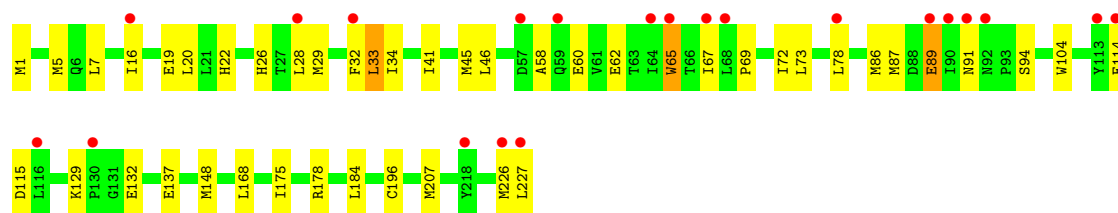


• Molecule 2: Cytochrome c oxidase subunit 2

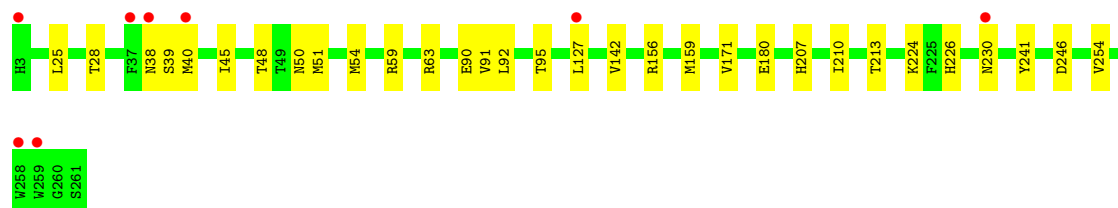
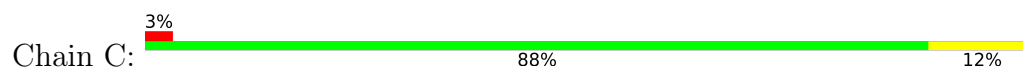


• Molecule 2: Cytochrome c oxidase subunit 2

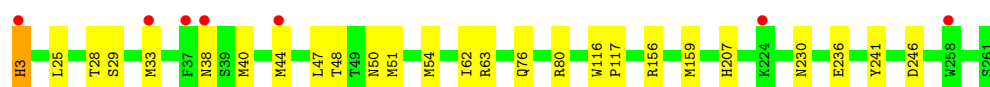
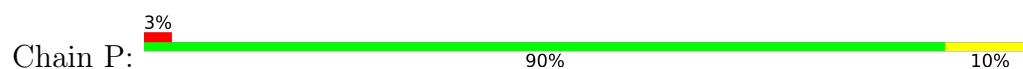




• Molecule 3: Cytochrome c oxidase subunit 3



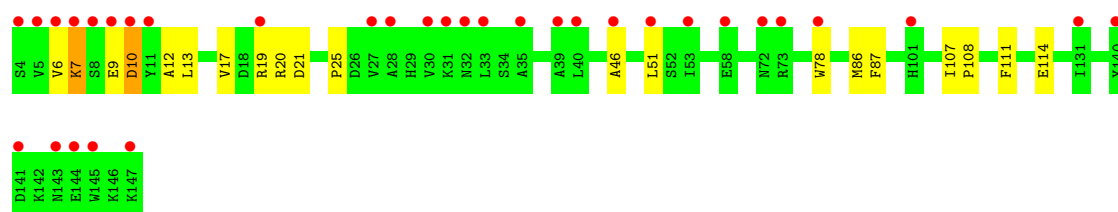
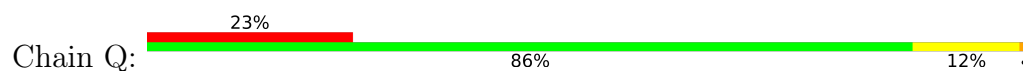
• Molecule 3: Cytochrome c oxidase subunit 3



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

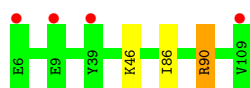


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

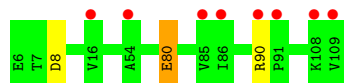


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

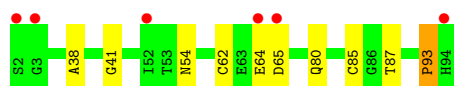
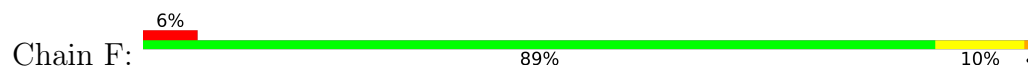




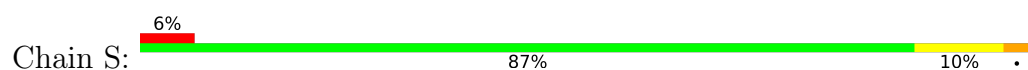
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



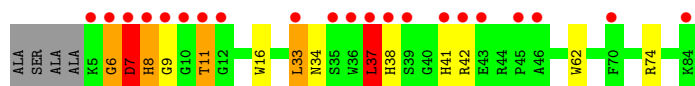
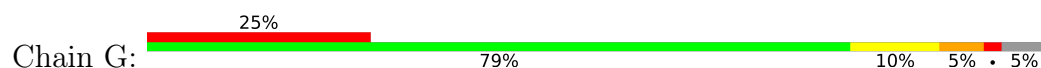
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



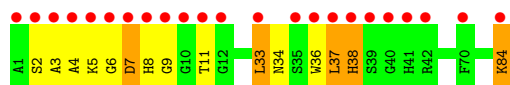
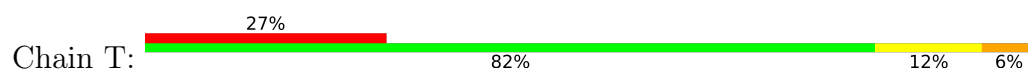
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



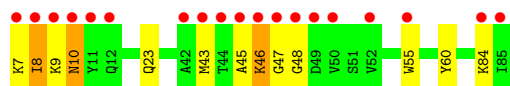
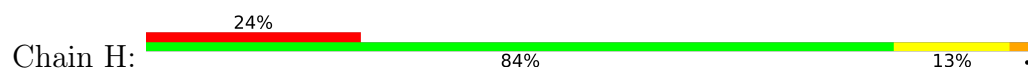
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



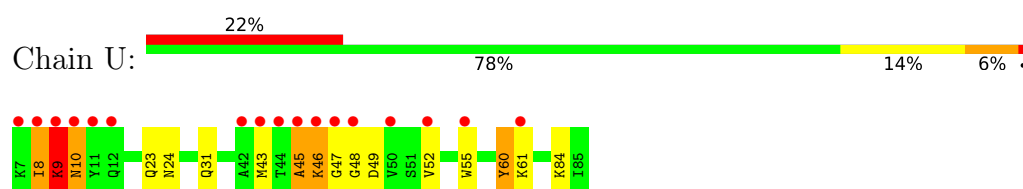
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



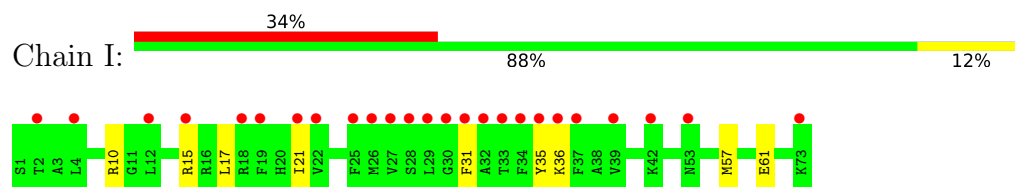
- Molecule 8: Cytochrome c oxidase subunit 6B1



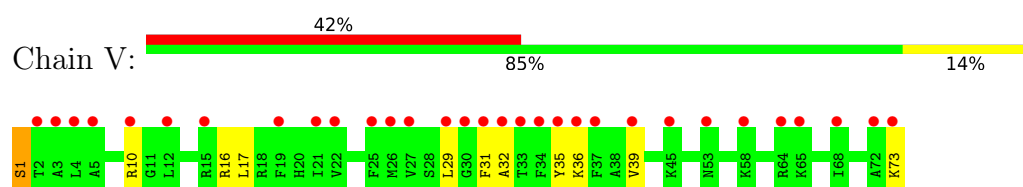
- Molecule 8: Cytochrome c oxidase subunit 6B1



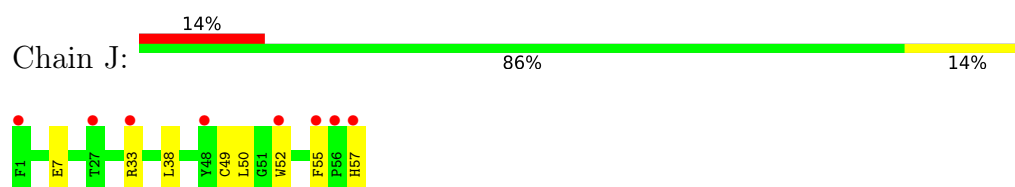
- Molecule 9: Cytochrome c oxidase subunit 6C



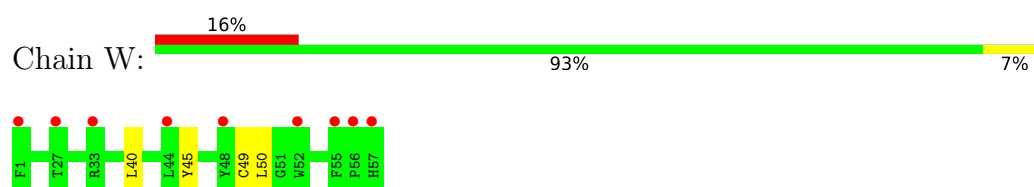
- Molecule 9: Cytochrome c oxidase subunit 6C



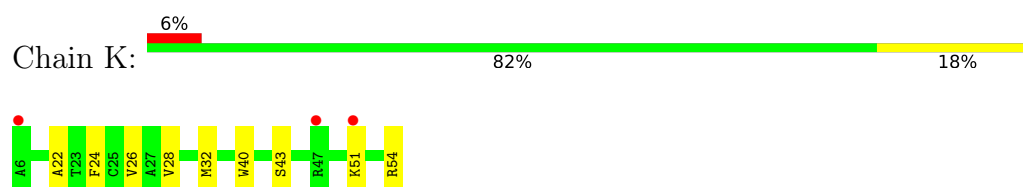
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



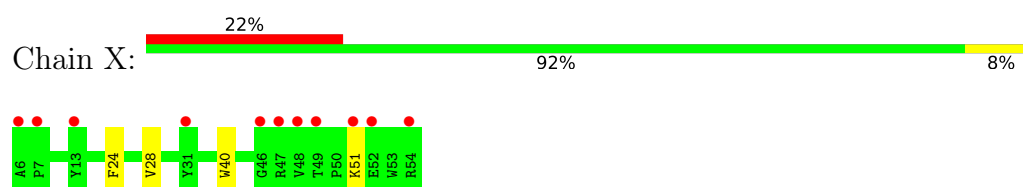
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



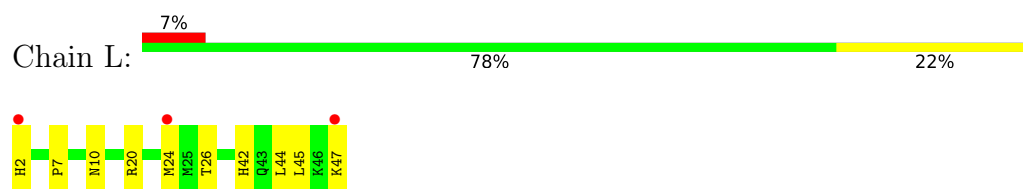
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



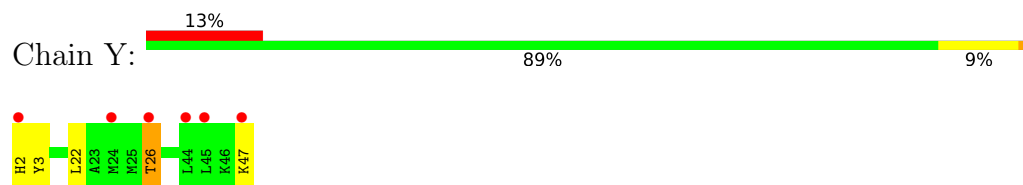
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



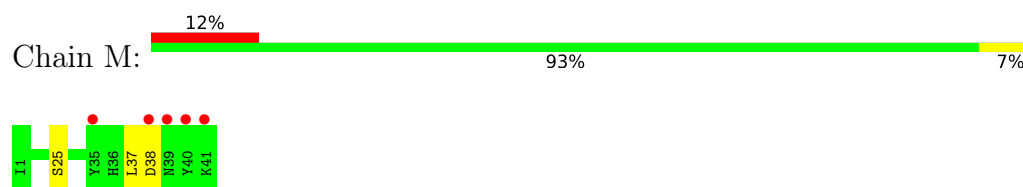
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



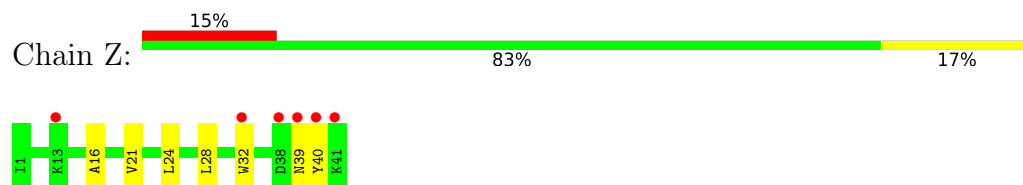
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	181.67Å 203.75Å 177.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.76 – 1.45 39.76 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.76-1.45) 99.8 (39.76-1.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.45Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.162 , 0.182 0.162 , 0.181	Depositor DCC
R_{free} test set	57695 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	35109	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: NA, CYN, CDL, PGV, SAC, PO4, PSC, ZN, CHD, PEK, HEA, MG, CUA, TGL, CU, FME, DMU, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.96	0/4449	1.01	5/6067 (0.1%)
1	N	0.88	1/4447 (0.0%)	0.93	3/6066 (0.0%)
2	B	0.84	0/2067	0.97	2/2815 (0.1%)
2	O	0.76	0/2065	0.89	1/2811 (0.0%)
3	C	0.82	0/2252	0.85	0/3077
3	P	0.82	0/2246	0.85	0/3068
4	D	0.80	0/1241	0.92	1/1674 (0.1%)
4	Q	0.60	0/1259	0.76	0/1697
5	E	0.89	0/860	0.90	0/1167
5	R	0.70	0/860	0.79	0/1167
6	F	0.93	0/751	1.11	2/1019 (0.2%)
6	S	0.83	0/758	0.98	0/1029
7	G	0.85	0/668	1.01	5/909 (0.6%)
7	T	0.73	0/699	0.90	0/950
8	H	0.79	0/682	0.98	0/921
8	U	0.73	0/682	0.90	0/921
9	I	0.70	0/605	0.83	0/802
9	V	0.63	0/605	0.79	0/802
10	J	0.63	0/462	0.77	0/625
10	W	0.59	0/462	0.76	0/625
11	K	0.86	0/414	0.87	0/566
11	X	0.60	0/399	0.74	0/546
12	L	0.88	0/393	0.96	0/526
12	Y	0.69	0/400	0.76	0/536
13	M	0.89	0/338	0.90	0/462
13	Z	0.73	0/330	0.75	0/451
All	All	0.82	1/30394 (0.0%)	0.91	19/41299 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	2
6	F	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	514	LYS	CE-NZ	5.10	1.64	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	CA-CB-CG	-8.67	105.13	113.80
1	A	240	HIS	CA-CB-CG	-7.62	106.17	113.80
4	D	133	GLY	N-CA-C	7.45	122.30	112.77
7	G	7	ASP	CA-C-N	6.14	133.26	121.54
7	G	7	ASP	C-N-CA	6.14	133.26	121.54
1	A	511	VAL	CA-C-N	-6.01	112.28	122.67
1	A	511	VAL	C-N-CA	-6.01	112.28	122.67
1	N	112	LEU	CD1-CG-CD2	-5.68	98.30	110.80
1	A	102	PHE	CA-CB-CG	-5.46	108.33	113.80
2	B	115[A]	ASP	CB-CA-C	5.41	120.77	111.68
2	B	115[B]	ASP	CB-CA-C	5.41	120.77	111.68
1	A	240	HIS	N-CA-CB	5.32	116.70	110.42
7	G	6	GLY	N-CA-C	5.28	125.70	113.18
7	G	8	HIS	N-CA-C	5.16	121.79	110.80
6	F	93	PRO	CA-C-N	5.10	130.88	121.70
6	F	93	PRO	C-N-CA	5.10	130.88	121.70
1	N	102	PHE	CA-CB-CG	-5.08	108.72	113.80
7	G	7	ASP	N-CA-C	5.07	121.60	110.80
2	O	65	TRP	CB-CA-C	-5.03	99.91	110.17

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	379	TYR	Mainchain

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Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
1	N	240	HIS	Sidechain
1	N	379	TYR	Mainchain

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	4162	0	4144	81	0
1	N	4160	0	4135	69	0
2	B	2000	0	2024	47	0
2	O	1999	0	2031	37	0
3	C	2125	0	2033	33	0
3	P	2121	0	2029	22	0
4	D	1201	0	1188	11	0
4	Q	1209	0	1197	17	0
5	E	842	0	838	2	0
5	R	842	0	838	5	0
6	F	720	0	698	7	0
6	S	721	0	702	12	0
7	G	642	0	606	7	0
7	T	663	0	626	15	0
8	H	662	0	623	13	0
8	U	662	0	623	21	0
9	I	601	0	613	7	0
9	V	601	0	613	10	0
10	J	451	0	446	8	0
10	W	451	0	446	3	0
11	K	389	0	372	10	0
11	X	385	0	366	4	0
12	L	380	0	380	9	0
12	Y	382	0	383	5	0
13	M	322	0	337	2	0
13	Z	320	0	334	5	0
14	A	190	0	138	16	0
14	N	190	0	138	18	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	4	0	0	0	0
18	N	4	0	0	0	0
19	A	63	0	110	10	0
19	B	62	0	105	6	0
19	D	48	0	77	7	0
19	O	126	0	220	14	0
20	A	46	0	69	7	0
20	C	149	0	217	8	0
20	N	51	0	76	4	0
20	P	96	0	138	1	0
20	Q	51	0	76	6	0
21	A	36	0	54	2	0
21	B	20	0	30	5	0
21	C	4	0	6	0	0
21	D	4	0	6	1	0
21	E	8	0	12	0	0
21	F	12	0	18	0	0
21	G	8	0	12	0	0
21	N	32	0	48	0	0
21	O	16	0	24	1	0
21	P	8	0	12	0	0
21	Q	4	0	6	0	0
21	R	4	0	6	0	0
21	S	28	0	42	3	0
21	T	8	0	12	0	0
21	U	4	0	6	3	0
21	Y	4	0	6	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	0	0
23	C	58	0	78	5	0
23	G	29	0	39	1	0
23	J	29	0	39	4	0
23	P	58	0	78	3	0
23	W	29	0	38	1	0
24	C	95	0	138	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	P	121	0	179	9	0
24	T	49	0	66	0	0
25	C	86	0	122	14	0
25	G	89	0	133	8	0
25	P	76	0	113	6	0
25	T	80	0	120	15	0
25	Y	87	0	127	4	0
26	C	33	0	42	5	0
26	G	21	0	30	2	0
26	J	33	0	42	3	0
26	K	61	0	84	2	0
26	L	18	0	20	3	0
26	M	33	0	42	0	0
26	P	154	0	199	8	0
26	X	66	0	93	5	0
26	Z	33	0	42	1	0
27	E	52	0	80	8	0
27	O	51	0	75	9	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	U	5	0	0	0	0
30	A	286	0	0	11	0
30	B	245	0	0	6	0
30	C	196	0	0	6	0
30	D	250	0	0	3	0
30	E	178	0	0	2	0
30	F	177	0	0	3	0
30	G	97	0	0	0	0
30	H	111	0	0	0	0
30	I	81	0	0	3	0
30	J	63	0	0	3	0
30	K	63	0	0	0	0
30	L	57	0	0	3	0
30	M	46	0	0	0	0
30	N	263	0	0	7	0
30	O	204	0	0	7	0
30	P	179	0	0	4	0
30	Q	128	0	0	3	0
30	R	131	0	0	3	0
30	S	126	0	0	4	0
30	T	78	0	0	1	0
30	U	121	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	V	68	0	0	1	0
30	W	51	0	0	0	0
30	X	50	0	0	0	0
30	Y	48	0	0	1	0
30	Z	30	0	0	1	0
All	All	35109	0	32347	504	0

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

All (504) 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)
6:S:94:HIS:HE1	21:S:108:EDO:H22	1.28	0.96
1:A:390[B]:MET:HE1	14:A:601[B]:HEA:H242	1.48	0.95
8:U:24:ASN:HD21	21:U:101:EDO:H21	1.31	0.93
10:J:50:LEU:HB2	26:J:101:DMU:H20	1.51	0.93
1:A:347:LEU:HD22	1:A:383[A]:MET:SD	2.10	0.91
1:A:356:ILE:HD13	14:A:602[C]:HEA:HMB1	1.54	0.87
1:A:347:LEU:HD13	1:A:383[A]:MET:HB3	1.57	0.86
6:S:94:HIS:NE2	30:S:201:HOH:O	2.11	0.83
1:N:356:ILE:HA	14:N:602[C]:HEA:HMB2	1.62	0.82
2:O:26:HIS:HA	2:O:29[C]:MET:HE3	1.62	0.81
20:Q:201:PGV:H22	20:Q:201:PGV:H011	1.64	0.79
7:G:11:THR:HG23	7:G:16:TRP:HE1	1.48	0.79
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.62	0.79
2:B:10:GLN:H	21:B:305:EDO:C1	1.98	0.77
12:Y:2:HIS:N	30:Y:201:HOH:O	2.17	0.77
1:N:359:ALA:HA	14:N:602[C]:HEA:OMA	1.86	0.75
10:J:55:PHE:HE1	26:L:101:DMU:H29	1.52	0.75
1:A:289:ALA:HB1	1:A:297[B]:MET:HE1	1.68	0.74
19:A:607:TGL:HC32	12:L:20:ARG:HH12	1.51	0.73
2:B:10:GLN:H	21:B:305:EDO:H12	1.53	0.73
19:A:607:TGL:HC41	30:A:933:HOH:O	1.88	0.72
4:D:100:LYS:HE3	30:D:344:HOH:O	1.89	0.71
5:E:46:LYS:NZ	30:E:301:HOH:O	2.23	0.71
1:A:347:LEU:HB3	1:A:383[A]:MET:HB3	1.71	0.71
1:N:347:LEU:HD13	1:N:383[A]:MET:HB3	1.72	0.71
1:A:347:LEU:CB	1:A:383[A]:MET:HB3	2.22	0.69
27:E:201:PSC:H42	27:E:201:PSC:H262	1.73	0.69
23:P:309:CHD:H231	30:P:547:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:94:HIS:CE1	21:S:108:EDO:H22	2.20	0.68
1:A:347:LEU:CD1	1:A:383[A]:MET:HB3	2.23	0.68
10:J:55:PHE:CE1	26:L:101:DMU:H29	2.28	0.68
1:A:386:VAL:HG21	14:A:601[A]:HEA:H261	1.76	0.68
19:A:607:TGL:HC22	19:A:607:TGL:HC82	1.77	0.67
1:N:356:ILE:HD13	14:N:602[C]:HEA:CMB	2.26	0.66
2:B:33[C]:LEU:HD22	30:B:624:HOH:O	1.96	0.65
1:N:24:ALA:HB2	14:N:601[A]:HEA:H253	1.79	0.65
1:N:356:ILE:HD13	14:N:602[C]:HEA:HMB3	1.79	0.65
1:N:352:GLY:O	14:N:602[C]:HEA:H121	1.98	0.64
1:N:362:SER:OG	2:O:87[A]:MET:HE2	1.97	0.64
8:U:23:GLN:NE2	30:U:201:HOH:O	2.30	0.64
1:N:309:THR:O	30:N:702:HOH:O	2.15	0.64
1:A:169[B]:ILE:HD11	1:A:189[B]:MET:HE1	1.80	0.64
1:N:386:VAL:HG21	14:N:601[A]:HEA:H261	1.80	0.63
24:P:305:PEK:C38	25:T:102:CDL:H273	2.29	0.63
1:A:352:GLY:O	14:A:602[C]:HEA:H121	1.99	0.63
2:B:42[A]:ILE:HG21	19:D:201:TGL:H232	1.79	0.63
3:C:51[A]:MET:HE1	20:C:306:PGV:H161	1.80	0.63
3:C:63:ARG:HE	25:C:308:CDL:CA2	2.12	0.63
1:N:359:ALA:HB2	14:N:602[C]:HEA:HMB1	1.81	0.63
19:A:607:TGL:HC51	19:A:607:TGL:CC1	2.30	0.62
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.29	0.62
1:A:347:LEU:HD13	1:A:383[A]:MET:CB	2.28	0.62
20:N:607:PGV:H343	24:P:304:PEK:H381	1.81	0.62
19:O:302:TGL:HG32	30:O:577:HOH:O	1.99	0.61
8:U:23:GLN:NE2	30:U:202:HOH:O	2.31	0.60
3:C:54[A]:MET:HE1	20:C:306:PGV:H152	1.82	0.60
1:N:334:TRP:CH2	2:O:46[A]:LEU:HD13	2.36	0.60
1:A:359:ALA:HA	14:A:602[C]:HEA:OMA	2.02	0.60
19:O:302:TGL:H181	30:O:567:HOH:O	2.00	0.60
3:C:213:THR:HG23	25:C:308:CDL:H771	1.83	0.60
19:B:301:TGL:HC61	30:I:170:HOH:O	2.01	0.60
1:N:136[B]:LEU:HD11	30:T:267:HOH:O	2.03	0.59
2:O:22:HIS:HB3	30:V:160:HOH:O	2.01	0.59
19:O:302:TGL:HG31	30:Q:352:HOH:O	2.00	0.59
1:A:514:LYS:HE2	30:F:223:HOH:O	2.00	0.59
30:A:809:HOH:O	27:E:201:PSC:H31	2.02	0.59
1:A:334:TRP:CH2	2:B:46[A]:LEU:HD13	2.37	0.59
2:B:10:GLN:HG3	21:B:305:EDO:H11	1.84	0.59
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229[B]:ILE:HD12	2:B:178:ARG:NH1	2.19	0.58
2:O:33[C]:LEU:HD21	9:V:32:ALA:HB2	1.85	0.58
8:U:24:ASN:HD21	21:U:101:EDO:C2	2.13	0.58
20:N:607:PGV:H183	24:P:304:PEK:H342	1.85	0.58
25:T:102:CDL:HA62	25:T:102:CDL:H352	1.86	0.58
1:A:347:LEU:HB3	1:A:383[A]:MET:CB	2.34	0.57
12:L:26:THR:OG1	30:L:201:HOH:O	2.16	0.57
30:A:927:HOH:O	8:H:23:GLN:HG2	2.03	0.57
1:A:302[B]:ARG:HH12	2:B:87:MET:HE1	1.69	0.57
2:B:22:HIS:HB3	30:I:166:HOH:O	2.04	0.57
3:C:91:VAL:O	3:C:95[B]:THR:HG23	2.04	0.57
2:B:83:ILE:O	2:B:87:MET:HG3	2.05	0.57
14:N:602[A]:HEA:HMB2	30:N:702:HOH:O	2.04	0.57
3:P:63:ARG:HE	25:P:308:CDL:CA2	2.16	0.57
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.87	0.57
1:A:313:ALA:HB2	1:A:356:ILE:HD11	1.87	0.57
1:N:356:ILE:CA	14:N:602[C]:HEA:HMB2	2.34	0.57
6:S:80[B]:GLN:NE2	30:S:203:HOH:O	2.38	0.56
7:G:62:TRP:HB2	26:G:105:DMU:H5	1.86	0.56
8:U:45:ALA:O	8:U:47:GLY:N	2.39	0.56
11:X:40:TRP:CD1	26:X:103:DMU:H9	2.40	0.56
1:A:356:ILE:HD13	14:A:602[C]:HEA:CMB	2.32	0.56
2:B:129:LYS:HE3	30:B:569:HOH:O	2.06	0.56
1:A:51[A]:ASP:OD2	1:A:441:SER:OG	2.21	0.56
1:A:353:LEU:HB3	2:B:31[A]:VAL:HG13	1.88	0.56
25:P:308:CDL:H521	25:P:308:CDL:HB62	1.88	0.56
3:C:40:MET:SD	26:G:105:DMU:H11	2.46	0.56
1:A:290[A]:HIS:CD2	1:A:291:HIS:CD2	2.95	0.55
20:A:608:PGV:H212	30:A:981:HOH:O	2.05	0.55
26:P:310:DMU:H10	26:P:311:DMU:H12	1.89	0.55
1:A:24:ALA:HB2	14:A:601[A]:HEA:H253	1.87	0.55
1:N:112:LEU:HG	30:N:904:HOH:O	2.05	0.55
1:N:468:MET:HG3	30:N:930:HOH:O	2.06	0.55
2:O:104:TRP:HB2	21:O:307:EDO:H22	1.88	0.55
3:C:39:SER:OG	26:C:311:DMU:H29	2.05	0.55
11:X:24:PHE:O	11:X:28:VAL:HG23	2.07	0.55
1:A:310[A]:MET:HE1	2:B:77:ALA:HB2	1.88	0.55
1:N:377:PHE:CD1	14:N:602[C]:HEA:HBD2	2.41	0.55
12:L:42:HIS:HB2	26:L:101:DMU:H6	1.89	0.55
1:A:513:LEU:O	30:A:702:HOH:O	2.18	0.55
2:O:67:ILE:HD11	30:O:588:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:SD	1:A:322[B]:SER:OG	2.63	0.55
1:A:514:LYS:HD2	30:F:212:HOH:O	2.07	0.55
1:A:236:TRP:CH2	14:A:602[A]:HEA:HBD1	2.42	0.54
30:A:703:HOH:O	2:B:203:ASN:ND2	2.41	0.54
3:C:171:VAL:HG22	25:C:308:CDL:H852	1.89	0.54
8:H:55:TRP:H	8:U:46:LYS:HZ3	1.56	0.54
3:C:90[B]:GLU:OE2	20:C:305:PGV:H321	2.07	0.54
1:N:347:LEU:CD1	1:N:383[A]:MET:HB3	2.36	0.54
1:N:449[A]:MET:SD	2:O:5:MET:HG2	2.48	0.54
6:S:22:LEU:HD12	30:S:298:HOH:O	2.07	0.54
1:N:112:LEU:HD23	1:N:112:LEU:C	2.32	0.54
1:A:356:ILE:CD1	14:A:602[C]:HEA:HMB1	2.33	0.53
19:B:301:TGL:H111	19:B:301:TGL:HA72	1.90	0.53
8:U:43:MET:HE3	8:U:49:ASP:N	2.23	0.53
19:O:301:TGL:HA22	19:O:301:TGL:H162	1.90	0.53
1:A:322[B]:SER:HB2	30:A:718:HOH:O	2.08	0.53
1:A:484[A]:THR:HG22	30:A:921:HOH:O	2.08	0.53
2:B:56:MET:HA	27:E:201:PSC:H211	1.90	0.53
10:J:52:TRP:O	10:J:57:HIS:HE1	1.92	0.53
2:O:58:ALA:O	2:O:62:GLU:HG3	2.08	0.53
2:O:129:LYS:NZ	30:O:405:HOH:O	2.39	0.53
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.91	0.53
3:C:50:ASN:ND2	3:C:54[A]:MET:HE2	2.24	0.53
2:O:65:TRP:HE1	27:O:304:PSC:H12	1.74	0.52
8:U:43:MET:HE3	8:U:48:GLY:HA3	1.91	0.52
2:B:78:LEU:HD23	25:T:102:CDL:H342	1.92	0.52
24:C:303:PEK:H322	20:C:305:PGV:C18	2.39	0.52
12:L:24:MET:HG3	30:L:227:HOH:O	2.09	0.52
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.92	0.52
3:C:224:LYS:HD3	25:C:308:CDL:HB31	1.90	0.52
7:T:38:HIS:HD1	7:T:38:HIS:N	2.06	0.52
26:P:312:DMU:H11	10:W:49:CYS:HB3	1.92	0.52
27:O:304:PSC:H061	5:R:8:ASP:OD1	2.09	0.52
8:U:31:GLN:NE2	30:U:203:HOH:O	2.36	0.52
1:A:169[B]:ILE:CD1	1:A:189[B]:MET:HE1	2.39	0.52
2:B:227:LEU:HD21	30:B:535:HOH:O	2.08	0.52
19:A:607:TGL:HG31	30:A:926:HOH:O	2.10	0.52
8:H:45:ALA:C	8:H:47:GLY:H	2.18	0.51
8:U:8:ILE:HG13	8:U:8:ILE:O	2.10	0.51
5:R:90:ARG:NH2	30:R:301:HOH:O	2.28	0.51
2:B:81:LEU:HD12	25:T:102:CDL:H371	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.51
2:B:29[C]:MET:HE1	30:B:406:HOH:O	2.10	0.51
1:A:169[B]:ILE:HD11	1:A:189[B]:MET:CE	2.41	0.51
1:N:169[A]:ILE:HG13	1:N:189[A]:MET:HE1	1.93	0.51
7:G:33:LEU:O	7:G:37:LEU:HB2	2.11	0.51
25:G:101:CDL:H131	25:G:101:CDL:OB4	2.11	0.51
7:T:38:HIS:NE2	25:T:102:CDL:H112	2.25	0.50
1:A:334:TRP:HH2	2:B:46[A]:LEU:HD13	1.76	0.50
1:A:488:THR:HB	1:A:495[B]:LEU:HG	1.93	0.50
3:P:40[B]:MET:HE2	3:P:44:MET:HE3	1.93	0.50
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	1.93	0.50
2:B:10:GLN:CG	21:B:305:EDO:H11	2.42	0.50
3:C:226:HIS:CE1	25:C:308:CDL:HB32	2.46	0.50
10:J:49:CYS:HB3	26:J:101:DMU:H11	1.94	0.50
30:N:919:HOH:O	20:Q:201:PGV:H032	2.10	0.50
8:H:8:ILE:HG12	8:H:8:ILE:O	2.10	0.50
9:I:35:TYR:C	9:I:35:TYR:CD2	2.90	0.50
3:P:62:ILE:HD12	25:P:308:CDL:H522	1.93	0.50
4:D:82:VAL:HG12	4:D:86:MET:HE2	1.94	0.50
1:A:113:LEU:HB2	19:A:607:TGL:H323	1.93	0.49
19:O:302:TGL:HB21	4:Q:78:TRP:CA	2.42	0.49
1:N:229[B]:ILE:HD12	2:O:178:ARG:NH1	2.27	0.49
27:E:201:PSC:H12	27:E:201:PSC:C34	2.43	0.49
6:S:64:GLU:O	6:S:65:ASP:HB2	2.13	0.49
1:A:362:SER:HB3	2:B:20:LEU:HD21	1.94	0.49
7:T:38:HIS:N	7:T:38:HIS:ND1	2.60	0.49
3:C:254:VAL:CG2	25:G:101:CDL:H652	2.42	0.49
8:U:43:MET:HE3	8:U:49:ASP:H	1.77	0.49
1:A:334:TRP:CZ2	2:B:46[A]:LEU:HB3	2.47	0.49
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.53	0.49
1:A:377:PHE:HA	1:A:380[A]:VAL:HG22	1.93	0.49
7:G:38:HIS:HE1	25:G:101:CDL:H122	1.77	0.49
19:O:302:TGL:H312	4:Q:86:MET:HG2	1.94	0.49
10:J:7:GLU:HG3	30:J:239:HOH:O	2.12	0.49
19:O:302:TGL:H342	9:V:16:ARG:HE	1.78	0.49
11:K:40:TRP:CD1	26:K:103:DMU:H12	2.48	0.49
1:N:290[A]:HIS:CD2	1:N:291:HIS:CD2	3.01	0.49
30:A:776:HOH:O	12:L:7:PRO:HG3	2.12	0.48
3:C:207:HIS:HD2	3:C:241:TYR:OH	1.96	0.48
19:D:201:TGL:HG32	30:D:440:HOH:O	2.13	0.48
1:A:462:LEU:O	1:A:465[B]:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:THR:HB	2:B:168:LEU:HD23	1.95	0.48
3:C:226:HIS:HE1	25:C:308:CDL:HB32	1.76	0.48
9:I:31:PHE:CD1	9:I:31:PHE:C	2.90	0.48
4:D:31:LYS:HE2	30:D:384:HOH:O	2.12	0.48
25:G:101:CDL:H421	1:N:310[B]:MET:HG3	1.95	0.48
1:N:243:VAL:HG11	14:N:602[C]:HEA:HMD2	1.94	0.48
1:N:334:TRP:CE3	19:O:302:TGL:HA31	2.48	0.48
8:U:47:GLY:HA2	30:U:268:HOH:O	2.13	0.48
1:N:310[B]:MET:HB2	2:O:73:LEU:HD22	1.95	0.48
4:Q:87:PHE:CD2	20:Q:201:PGV:H141	2.47	0.48
1:A:178[B]:GLN:HE21	7:T:7:ASP:HB2	1.78	0.48
1:A:390[B]:MET:CE	14:A:601[B]:HEA:H242	2.33	0.48
7:T:37:LEU:HD23	25:T:102:CDL:H381	1.95	0.48
26:X:101:DMU:H11	26:X:102:DMU:H12	1.96	0.48
1:N:376:HIS:CE1	1:N:380[C]:VAL:HG11	2.48	0.48
1:N:378:HIS:HA	1:N:382[C]:SER:HB2	1.96	0.48
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.49	0.48
1:N:236:TRP:CH2	14:N:602[A]:HEA:HBD1	2.48	0.48
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.94	0.48
1:A:304:TYR:HD1	25:T:102:CDL:HB32	1.79	0.48
20:A:608:PGV:C3	20:A:608:PGV:H011	2.44	0.48
6:F:87[A]:THR:HG21	30:F:315:HOH:O	2.14	0.48
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.96	0.48
2:O:28[C]:LEU:HG	2:O:32[C]:PHE:CE2	2.49	0.48
20:P:307:PGV:H241	20:P:307:PGV:H272	1.63	0.48
1:A:169[B]:ILE:HD12	7:T:9:GLY:H	1.79	0.47
10:W:40:LEU:HD12	23:W:101:CHD:H183	1.95	0.47
27:E:201:PSC:H12	27:E:201:PSC:H343	1.96	0.47
30:N:902:HOH:O	24:P:304:PEK:H382	2.14	0.47
3:P:48:THR:HG23	25:P:308:CDL:H392	1.96	0.47
25:Y:101:CDL:HB61	25:Y:101:CDL:H111	1.96	0.47
2:B:41[A]:ILE:O	2:B:45[A]:MET:HG2	2.14	0.47
3:C:48:THR:HG23	25:C:308:CDL:H412	1.96	0.47
1:N:334:TRP:CZ2	2:O:46[A]:LEU:HB3	2.50	0.47
19:O:302:TGL:H192	9:V:16:ARG:HH21	1.78	0.47
1:A:273:MET:HE2	30:A:718:HOH:O	2.14	0.47
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.15	0.47
23:J:102:CHD:H111	23:J:102:CHD:H193	1.45	0.47
20:A:608:PGV:H321	20:A:608:PGV:H141	1.95	0.47
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.96	0.47
2:O:45[C]:MET:HE1	9:V:17:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:O:304:PSC:H071	9:V:10:ARG:HH21	1.79	0.47
3:C:210:ILE:HD13	20:C:306:PGV:H302	1.96	0.47
23:J:102:CHD:H211	23:J:102:CHD:H231	1.66	0.47
1:N:229[B]:ILE:HD11	2:O:175:ILE:HD13	1.96	0.47
1:N:347:LEU:CB	1:N:383[A]:MET:HB3	2.45	0.47
1:N:406:ASN:HD21	20:Q:201:PGV:H21	1.80	0.47
1:N:408:THR:HB	20:Q:201:PGV:H51	1.96	0.47
8:U:24:ASN:ND2	21:U:101:EDO:H21	2.14	0.47
11:X:40:TRP:CD1	26:X:103:DMU:H14	2.49	0.47
19:B:301:TGL:H111	19:B:301:TGL:H142	1.63	0.47
3:C:39:SER:HB2	26:C:311:DMU:O61	2.15	0.47
8:H:7:LYS:HD2	8:U:46:LYS:HG2	1.97	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.95	0.47
2:B:5[A]:MET:HE2	11:K:43:SER:HB2	1.97	0.47
2:O:19:GLU:HG3	2:O:86[A]:MET:HE1	1.97	0.47
2:B:164:ALA:O	2:B:194:GLY:HA3	2.14	0.47
23:C:309:CHD:H161	30:C:589:HOH:O	2.14	0.47
4:D:86:MET:CE	11:K:22:ALA:HB2	2.45	0.47
1:N:313:ALA:HB2	1:N:356:ILE:HD11	1.95	0.47
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.96	0.47
3:P:50:ASN:ND2	3:P:54[A]:MET:HE2	2.30	0.47
5:R:90:ARG:NH1	30:R:303:HOH:O	2.48	0.47
6:S:94:HIS:HE1	21:S:108:EDO:C2	2.14	0.47
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.13	0.46
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.97	0.46
14:A:601[A]:HEA:H122	14:A:601[A]:HEA:H262	1.98	0.46
2:B:31[A]:VAL:CG1	19:B:301:TGL:HB72	2.44	0.46
2:B:140:ASN:HB3	30:B:517:HOH:O	2.15	0.46
2:O:114:GLU:HG3	2:O:227:LEU:HD21	1.97	0.46
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.67	0.46
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.96	0.46
23:C:309:CHD:H162	23:C:309:CHD:H231	1.97	0.46
5:E:86:ILE:O	5:E:90:ARG:HG2	2.15	0.46
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.98	0.46
1:N:310[A]:MET:HB3	2:O:73:LEU:HD22	1.98	0.46
2:O:168:LEU:HD13	2:O:184:LEU:HG	1.97	0.46
5:R:80:GLU:H	5:R:80:GLU:CD	2.23	0.46
25:T:102:CDL:H402	25:T:102:CDL:H161	1.97	0.46
19:O:302:TGL:H362	30:R:394:HOH:O	2.14	0.46
24:P:304:PEK:H161	24:P:304:PEK:H132	1.72	0.46
7:T:37:LEU:CD2	25:T:102:CDL:H381	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229[A]:ILE:HD11	2:B:175:ILE:HD13	1.97	0.46
4:Q:19[A]:ARG:HD2	4:Q:21[A]:ASP:OD1	2.15	0.46
1:A:321:PHE:CD2	2:B:65:TRP:HB2	2.51	0.46
3:C:142:VAL:HG21	25:G:101:CDL:H822	1.97	0.46
6:F:64:GLU:O	6:F:65:ASP:HB2	2.16	0.46
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.15	0.46
7:T:37:LEU:C	7:T:38:HIS:HD1	2.24	0.46
27:E:201:PSC:H252	27:E:201:PSC:H221	1.27	0.46
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.45	0.46
7:T:38:HIS:NE2	25:T:102:CDL:C11	2.79	0.46
19:A:607:TGL:HC42	30:L:238:HOH:O	2.16	0.46
3:C:156:ARG:HE	23:C:309:CHD:C24	2.28	0.46
2:B:28[C]:LEU:HD12	2:B:28[C]:LEU:HA	1.80	0.45
25:G:101:CDL:H151	25:G:101:CDL:H182	1.54	0.45
1:N:310[B]:MET:HE2	1:N:310[B]:MET:HB3	1.68	0.45
27:O:304:PSC:C07	9:V:10:ARG:HH21	2.30	0.45
3:P:38:ASN:O	26:P:310:DMU:H32	2.17	0.45
6:S:19:GLU:HG2	30:S:308:HOH:O	2.16	0.45
2:B:115[B]:ASP:OD1	30:B:401:HOH:O	2.21	0.45
1:N:347:LEU:HB3	1:N:383[A]:MET:HB3	1.98	0.45
27:O:304:PSC:H31	30:O:550:HOH:O	2.16	0.45
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.16	0.45
23:J:102:CHD:H213	30:J:237:HOH:O	2.16	0.45
1:N:362:SER:HA	2:O:87[A]:MET:HE1	1.99	0.45
2:O:41[A]:ILE:O	2:O:45[A]:MET:HG2	2.16	0.45
27:O:304:PSC:C01	27:O:304:PSC:H212	2.46	0.45
1:N:152[B]:LEU:HD11	3:P:28:THR:HG21	1.99	0.45
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.97	0.45
26:P:315:DMU:H13	26:P:315:DMU:H18	1.56	0.45
6:S:54:ASN:HD22	6:S:54:ASN:C	2.23	0.45
9:V:31:PHE:C	9:V:31:PHE:CD1	2.93	0.45
1:A:178[B]:GLN:NE2	7:T:8:HIS:O	2.50	0.45
3:C:51[A]:MET:CE	20:C:306:PGV:H161	2.47	0.45
1:A:186:TRP:HH2	7:T:7:ASP:HB3	1.80	0.45
1:A:285:PHE:CD2	7:T:3:ALA:O	2.69	0.45
7:G:34:ASN:HD22	25:G:101:CDL:H142	1.82	0.45
3:C:38:ASN:HA	30:C:410:HOH:O	2.17	0.45
25:C:308:CDL:H561	25:C:308:CDL:H532	1.75	0.45
7:G:41:HIS:HB3	7:G:74:ARG:NH1	2.32	0.45
8:H:46:LYS:HZ3	8:U:55:TRP:H	1.65	0.45
1:N:290[C]:HIS:HB2	1:N:293:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:356:ILE:HD13	14:N:602[C]:HEA:HMB2	1.98	0.45
3:P:29:SER:HB2	26:P:312:DMU:H21	1.99	0.45
26:P:310:DMU:H7	26:P:311:DMU:H8	1.98	0.45
20:Q:201:PGV:H311	13:Z:16:ALA:HA	1.98	0.45
26:X:103:DMU:H11	26:X:103:DMU:O49	2.17	0.45
1:A:347:LEU:CG	1:A:383[A]:MET:HB3	2.47	0.45
19:D:201:TGL:HA41	19:D:201:TGL:HB51	1.99	0.45
1:N:2:PHE:CZ	25:Y:101:CDL:H721	2.51	0.45
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.98	0.45
19:O:301:TGL:HC32	30:O:569:HOH:O	2.16	0.45
27:O:304:PSC:C07	9:V:10:ARG:HE	2.30	0.45
8:U:60:TYR:CD1	8:U:60:TYR:C	2.95	0.45
1:N:379:TYR:CZ	1:N:383[A]:MET:HE1	2.52	0.44
3:P:51[A]:MET:HE1	30:P:557:HOH:O	2.17	0.44
5:R:80:GLU:CD	5:R:80:GLU:N	2.75	0.44
25:T:102:CDL:H451	25:T:102:CDL:H422	1.68	0.44
26:X:103:DMU:H9	26:X:103:DMU:H14	1.58	0.44
3:C:246:ASP:HB2	30:C:491:HOH:O	2.17	0.44
12:L:26:THR:HG23	13:M:25:SER:CB	2.47	0.44
2:B:60:GLU:H	2:B:60:GLU:HG3	1.48	0.44
4:D:121:LYS:NZ	21:D:202:EDO:O2	2.51	0.44
1:N:22:PHE:HA	25:Y:101:CDL:H791	1.98	0.44
1:A:236:TRP:HH2	14:A:602[A]:HEA:HBD1	1.80	0.44
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.77	0.44
12:Y:47:LYS:HE3	12:Y:47:LYS:HB3	1.71	0.44
1:A:113:LEU:HB2	19:A:607:TGL:H302	2.00	0.44
4:D:78:TRP:CA	19:D:201:TGL:HB22	2.48	0.44
12:Y:2:HIS:CG	12:Y:3:TYR:H	2.35	0.44
27:E:201:PSC:H51	9:I:17:LEU:HD23	2.00	0.44
3:P:246:ASP:HB2	30:P:510:HOH:O	2.18	0.44
1:A:321:PHE:CD1	27:E:201:PSC:H341	2.53	0.44
1:A:378:HIS:HA	1:A:382[C]:SER:HB2	2.00	0.44
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.52	0.44
19:B:301:TGL:H221	19:B:301:TGL:H252	1.56	0.44
30:N:719:HOH:O	19:O:302:TGL:HB31	2.18	0.44
3:C:180:GLU:HG3	30:C:401:HOH:O	2.18	0.44
8:H:43:MET:HE1	8:U:43:MET:HE1	1.99	0.44
4:Q:46:ALA:HB3	30:Q:353:HOH:O	2.16	0.44
1:N:229[A]:ILE:HD11	2:O:175:ILE:HD13	1.99	0.43
20:A:608:PGV:H011	20:A:608:PGV:H31	2.00	0.43
8:H:7:LYS:HG2	8:H:8:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:41[C]:ILE:O	2:O:45[C]:MET:HG2	2.17	0.43
4:Q:9:GLU:HG2	4:Q:12:ALA:HB3	2.00	0.43
1:A:318:VAL:O	1:A:322[B]:SER:OG	2.36	0.43
24:C:303:PEK:H322	20:C:305:PGV:H183	1.99	0.43
8:H:9:LYS:O	8:H:10:ASN:ND2	2.52	0.43
1:N:152[B]:LEU:CD1	3:P:28:THR:HG21	2.48	0.43
24:P:305:PEK:H381	25:T:102:CDL:H273	2.00	0.43
7:G:38:HIS:CE1	25:G:101:CDL:H122	2.52	0.43
2:O:34[C]:ILE:HD11	2:O:72:ILE:HG21	2.01	0.43
2:O:89:GLU:O	2:O:91:ASN:ND2	2.52	0.43
3:P:156:ARG:HE	23:P:309:CHD:C24	2.31	0.43
12:Y:26[B]:THR:HG21	13:Z:21:VAL:HG12	2.00	0.43
20:C:307:PGV:H241	20:C:307:PGV:H272	1.50	0.43
9:V:1:SAC:HA	9:V:1:SAC:H2A1	1.73	0.43
2:B:58:ALA:O	2:B:62:GLU:HG3	2.18	0.43
8:H:46:LYS:HD3	8:U:52:VAL:HA	2.00	0.43
27:O:304:PSC:H212	27:O:304:PSC:H22	2.00	0.43
25:T:102:CDL:H382	25:T:102:CDL:H141	2.01	0.43
2:B:42[A]:ILE:HG22	19:D:201:TGL:H251	1.99	0.43
1:A:355:GLY:O	14:A:602[C]:HEA:HMB3	2.18	0.43
23:C:309:CHD:H183	23:C:309:CHD:H20	1.88	0.43
11:K:24:PHE:O	11:K:28[B]:VAL:HG23	2.18	0.43
1:N:364:ASP:OD1	14:N:602[A]:HEA:O1A	2.37	0.43
1:A:351:GLY:HA3	1:A:380[C]:VAL:HB	2.01	0.43
1:A:472:ILE:HG21	19:A:607:TGL:HA91	2.00	0.43
24:C:303:PEK:H203	24:C:303:PEK:H171	1.89	0.43
26:C:311:DMU:H2	26:J:101:DMU:O3	2.19	0.43
23:J:102:CHD:H191	23:J:102:CHD:H8	1.88	0.43
3:P:33:MET:HE3	26:P:312:DMU:O16	2.18	0.43
3:P:246:ASP:HB2	30:P:497:HOH:O	2.19	0.43
4:Q:114:GLU:CD	11:X:51:LYS:HE2	2.44	0.43
25:T:102:CDL:H832	25:T:102:CDL:H801	1.83	0.43
1:A:513:LEU:O	1:A:514:LYS:HB2	2.18	0.43
4:Q:7:LYS:HB3	4:Q:10:ASP:OD1	2.19	0.43
1:A:172:LYS:HZ2	1:A:178[A]:GLN:HE22	1.66	0.42
2:B:91:ASN:HB3	2:B:149:THR:HG21	2.00	0.42
9:I:15:ARG:HD3	30:I:160:HOH:O	2.19	0.42
7:T:36:TRP:CG	7:T:36:TRP:O	2.71	0.42
1:A:152[B]:LEU:CD1	3:C:28:THR:HG21	2.49	0.42
14:A:602[A]:HEA:HHA	14:A:602[A]:HEA:HAD2	1.77	0.42
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:240:HIS:CD2	1:N:240:HIS:C	2.97	0.42
20:N:607:PGV:H343	24:P:304:PEK:C38	2.47	0.42
3:C:224:LYS:CD	25:C:308:CDL:HB31	2.49	0.42
8:H:45:ALA:O	8:H:47:GLY:N	2.53	0.42
25:P:308:CDL:H521	25:P:308:CDL:OB9	2.19	0.42
6:S:10:GLU:OE2	6:S:25:ARG:NH2	2.46	0.42
1:A:240:HIS:CD2	1:A:240:HIS:C	2.98	0.42
24:C:303:PEK:H201	30:C:563:HOH:O	2.19	0.42
11:K:54:ARG:HE	11:K:54:ARG:HB3	1.64	0.42
3:P:116:TRP:HA	3:P:117:PRO:C	2.44	0.42
25:T:102:CDL:HA62	25:T:102:CDL:H311	1.70	0.42
21:A:615:EDO:H12	2:B:58:ALA:HB3	2.02	0.42
2:B:16:ILE:HD12	2:B:87:MET:HG2	2.01	0.42
3:P:156:ARG:HE	23:P:309:CHD:C23	2.32	0.42
26:C:311:DMU:H26	10:J:38:LEU:HD23	2.00	0.42
12:L:45:LEU:HD23	12:L:45:LEU:HA	1.89	0.42
24:P:304:PEK:H31	24:P:304:PEK:H71	2.01	0.42
3:C:92:LEU:O	3:C:95[B]:THR:OG1	2.28	0.42
9:I:57:MET:O	9:I:61:GLU:HG2	2.19	0.42
1:N:378:HIS:O	1:N:383[C]:MET:HG2	2.20	0.42
1:A:321:PHE:HB3	2:B:65:TRP:CE3	2.55	0.42
2:B:9:PHE:HA	21:B:305:EDO:H12	2.01	0.42
27:O:304:PSC:H292	27:O:304:PSC:H261	1.51	0.42
4:Q:17:VAL:O	4:Q:25:PRO:HG3	2.19	0.42
20:A:608:PGV:H142	20:A:608:PGV:H301	2.02	0.41
3:C:45:ILE:HD13	26:C:311:DMU:H21	2.02	0.41
3:C:246:ASP:HB2	30:C:521:HOH:O	2.20	0.41
25:C:308:CDL:H162	25:C:308:CDL:H361	2.02	0.41
25:C:308:CDL:H312	25:C:308:CDL:HA61	1.89	0.41
12:L:44:LEU:O	12:L:47:LYS:HD2	2.19	0.41
1:N:347:LEU:HB3	1:N:383[A]:MET:CB	2.50	0.41
8:U:9:LYS:HA	8:U:9:LYS:HD3	1.49	0.41
19:B:301:TGL:HA92	19:B:301:TGL:HA62	1.82	0.41
1:N:355:GLY:O	14:N:602[C]:HEA:CHB	2.68	0.41
19:O:302:TGL:HB21	4:Q:78:TRP:HB3	2.02	0.41
9:V:35:TYR:CZ	9:V:39:VAL:HG11	2.55	0.41
1:A:377:PHE:CD2	14:A:602[C]:HEA:HBD2	2.55	0.41
1:N:309:THR:HG22	14:N:602[C]:HEA:HMB1	2.03	0.41
6:S:37:LYS:HD2	6:S:37:LYS:HA	1.80	0.41
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.92	0.41
2:O:86[A]:MET:HE2	2:O:86[A]:MET:HB2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:80[A]:ARG:NH2	3:P:236:GLU:OE1	2.49	0.41
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	2.61	0.41
8:H:9:LYS:HA	8:H:9:LYS:HD2	1.76	0.41
1:N:246:LEU:HB3	1:N:381[C]:LEU:HD11	2.03	0.41
4:Q:20[A]:ARG:HG2	30:Q:360:HOH:O	2.20	0.41
13:Z:28:LEU:HD23	26:Z:101:DMU:H7	2.02	0.41
1:N:289:ALA:HB1	1:N:297[A]:MET:HE1	2.02	0.41
20:A:608:PGV:H51	20:A:608:PGV:H22	1.97	0.41
21:A:617:EDO:H11	12:L:10:ASN:HD22	1.85	0.41
1:N:362:SER:HB3	2:O:20:LEU:HD21	2.03	0.41
4:Q:19[A]:ARG:CD	4:Q:21[A]:ASP:OD1	2.69	0.41
13:Z:24:LEU:HD23	13:Z:24:LEU:HA	1.91	0.41
10:J:33:ARG:HD3	30:J:232:HOH:O	2.20	0.41
2:O:16:ILE:HD12	2:O:16:ILE:HG23	1.71	0.41
12:Y:22:LEU:O	12:Y:26[B]:THR:HG23	2.20	0.41
1:A:152[B]:LEU:HD11	3:C:28:THR:HG21	2.01	0.41
2:B:162:SER:HB3	2:B:197:SER:C	2.46	0.41
25:C:308:CDL:HB62	25:C:308:CDL:H522	2.03	0.41
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.56	0.41
1:N:351:GLY:HA3	1:N:380[C]:VAL:HB	2.03	0.41
4:Q:107:ILE:HB	4:Q:108:PRO:CD	2.50	0.41
7:T:84:LYS:H	7:T:84:LYS:NZ	2.19	0.41
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.86	0.41
30:E:351:HOH:O	9:I:10:ARG:HG2	2.21	0.41
2:O:94[B]:SER:OG	2:O:148:MET:HE2	2.21	0.41
25:P:308:CDL:H402	25:P:308:CDL:H431	1.93	0.41
3:C:51[A]:MET:SD	25:C:308:CDL:H621	2.61	0.40
11:K:24:PHE:O	11:K:28[A]:VAL:HG12	2.21	0.40
2:O:7:LEU:HD11	19:O:301:TGL:H161	2.04	0.40
26:P:310:DMU:H17	10:W:45:TYR:CG	2.56	0.40
4:Q:7:LYS:HG2	4:Q:13:LEU:HD12	2.04	0.40
7:T:33:LEU:O	7:T:34:ASN:C	2.64	0.40
8:U:9:LYS:HA	30:U:264:HOH:O	2.20	0.40
20:N:607:PGV:C18	24:P:304:PEK:H322	2.51	0.40
8:U:9:LYS:O	8:U:10:ASN:HB2	2.21	0.40
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.03	0.40
23:G:102:CHD:H12	23:G:102:CHD:H212	2.02	0.40
30:O:459:HOH:O	4:Q:21[B]:ASP:HB2	2.20	0.40
20:A:608:PGV:H202	20:A:608:PGV:H232	1.74	0.40
23:C:309:CHD:H112	23:C:309:CHD:H12A	1.86	0.40
3:P:3:HIS:CD2	3:P:3:HIS:N	2.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:101:CDL:OB9	25:Y:101:CDL:H122	2.21	0.40
1:A:113:LEU:HB2	19:A:607:TGL:C30	2.52	0.40
1:A:377:PHE:CD2	14:A:602[A]:HEA:HAD1	2.57	0.40
3:C:59:ARG:HB2	25:C:308:CDL:H512	2.04	0.40
4:D:114:GLU:OE1	11:K:51:LYS:NZ	2.51	0.40
11:K:26:VAL:HG13	26:K:101:DMU:H11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	550/514 (107%)	531 (96%)	17 (3%)	2 (0%)	30	11
1	N	549/514 (107%)	532 (97%)	15 (3%)	2 (0%)	30	11
2	B	251/227 (111%)	246 (98%)	5 (2%)	0	100	100
2	O	251/227 (111%)	245 (98%)	6 (2%)	0	100	100
3	C	264/259 (102%)	260 (98%)	4 (2%)	0	100	100
3	P	263/259 (102%)	257 (98%)	6 (2%)	0	100	100
4	D	143/144 (99%)	140 (98%)	3 (2%)	0	100	100
4	Q	145/144 (101%)	141 (97%)	2 (1%)	2 (1%)	9	1
5	E	102/104 (98%)	102 (100%)	0	0	100	100
5	R	102/104 (98%)	102 (100%)	0	0	100	100
6	F	94/93 (101%)	92 (98%)	2 (2%)	0	100	100
6	S	95/93 (102%)	93 (98%)	2 (2%)	0	100	100
7	G	78/84 (93%)	71 (91%)	2 (3%)	5 (6%)	1	0
7	T	84/84 (100%)	73 (87%)	7 (8%)	4 (5%)	2	0
8	H	77/79 (98%)	70 (91%)	4 (5%)	3 (4%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	U	77/79 (98%)	69 (90%)	4 (5%)	4 (5%)	1	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	55/57 (96%)	55 (100%)	0	0	100	100
10	W	55/57 (96%)	55 (100%)	0	0	100	100
11	K	49/49 (100%)	48 (98%)	1 (2%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
12	Y	45/46 (98%)	44 (98%)	1 (2%)	0	100	100
13	M	40/41 (98%)	39 (98%)	1 (2%)	0	100	100
13	Z	39/41 (95%)	39 (100%)	0	0	100	100
All	All	3641/3540 (103%)	3533 (97%)	86 (2%)	22 (1%)	21	6

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384[A]	GLY
1	A	384[B]	GLY
7	G	7	ASP
7	G	8	HIS
8	H	10	ASN
1	N	384[A]	GLY
1	N	384[B]	GLY
7	T	4	ALA
8	U	45	ALA
7	G	37	LEU
8	H	48	GLY
4	Q	7	LYS
7	T	7	ASP
8	U	9	LYS
8	U	46	LYS
8	H	46	LYS
4	Q	6	VAL
7	T	5	LYS
8	U	10	ASN
7	G	9	GLY
7	T	6	GLY
7	G	6	GLY

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	463/426 (109%)	455 (98%)	8 (2%)	53	21
1	N	462/426 (108%)	458 (99%)	4 (1%)	70	46
2	B	236/210 (112%)	229 (97%)	7 (3%)	36	7
2	O	236/210 (112%)	229 (97%)	7 (3%)	36	7
3	C	231/224 (103%)	228 (99%)	3 (1%)	61	31
3	P	230/224 (103%)	226 (98%)	4 (2%)	53	21
4	D	129/128 (101%)	128 (99%)	1 (1%)	73	50
4	Q	131/128 (102%)	129 (98%)	2 (2%)	57	25
5	E	91/91 (100%)	90 (99%)	1 (1%)	65	38
5	R	91/91 (100%)	90 (99%)	1 (1%)	65	38
6	F	81/78 (104%)	77 (95%)	4 (5%)	22	2
6	S	82/78 (105%)	78 (95%)	4 (5%)	22	2
7	G	65/68 (96%)	60 (92%)	5 (8%)	12	1
7	T	68/68 (100%)	62 (91%)	6 (9%)	9	0
8	H	71/71 (100%)	68 (96%)	3 (4%)	26	3
8	U	71/71 (100%)	66 (93%)	5 (7%)	14	1
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	19
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	1
10	J	48/48 (100%)	48 (100%)	0	100	100
10	W	48/48 (100%)	47 (98%)	1 (2%)	47	14
11	K	41/39 (105%)	41 (100%)	0	100	100
11	X	39/39 (100%)	39 (100%)	0	100	100
12	L	39/39 (100%)	38 (97%)	1 (3%)	40	10
12	Y	40/39 (103%)	38 (95%)	2 (5%)	22	2
13	M	36/35 (103%)	35 (97%)	1 (3%)	38	8
13	Z	35/35 (100%)	34 (97%)	1 (3%)	37	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3178/3028 (105%)	3103 (98%)	75 (2%)	47 12

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	A	152[A]	LEU
1	A	152[B]	LEU
1	A	178[A]	GLN
1	A	178[B]	GLN
1	A	363[A]	LEU
1	A	363[B]	LEU
1	A	369	ASP
2	B	33[A]	LEU
2	B	33[C]	LEU
2	B	60	GLU
2	B	75	LEU
2	B	91	ASN
2	B	115[A]	ASP
2	B	115[B]	ASP
3	C	127	LEU
3	C	159	MET
3	C	230	ASN
4	D	4	SER
5	E	90	ARG
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	80[A]	GLN
6	F	80[B]	GLN
7	G	7	ASP
7	G	11	THR
7	G	33	LEU
7	G	37	LEU
7	G	42	ARG
8	H	8	ILE
8	H	60	TYR
8	H	84	LYS
9	I	36	LYS
12	L	2	HIS
13	M	38	ASP
1	N	128	VAL
1	N	152[A]	LEU

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Mol	Chain	Res	Type
1	N	152[B]	LEU
1	N	369	ASP
2	O	33[A]	LEU
2	O	33[C]	LEU
2	O	60	GLU
2	O	78	LEU
2	O	89	GLU
2	O	115	ASP
2	O	226	MET
3	P	3	HIS
3	P	76	GLN
3	P	159	MET
3	P	230	ASN
4	Q	10	ASP
4	Q	51	LEU
5	R	80	GLU
6	S	54	ASN
6	S	80[A]	GLN
6	S	80[B]	GLN
6	S	94	HIS
7	T	2	SER
7	T	11	THR
7	T	33	LEU
7	T	37	LEU
7	T	38	HIS
7	T	84	LYS
8	U	8	ILE
8	U	9	LYS
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	29	LEU
9	V	36	LYS
9	V	73	LYS
10	W	50	LEU
12	Y	26[A]	THR
12	Y	26[B]	THR
13	Z	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
2	B	181	GLN
2	B	203	ASN
3	C	50	ASN
3	C	68	GLN
4	D	76	ASN
4	D	119	GLN
5	E	94	ASN
7	G	34	ASN
8	H	10	ASN
8	H	23	GLN
8	H	28	ASN
8	H	32	ASN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	170	ASN
2	O	91	ASN
2	O	181	GLN
3	P	3	HIS
3	P	50	ASN
3	P	56	GLN
3	P	68	GLN
3	P	76	GLN
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
6	S	94	HIS
7	T	34	ASN
7	T	41	HIS
8	U	24	ASN
8	U	28	ASN
8	U	32	ASN
9	V	8	GLN
9	V	53	ASN
11	X	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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
2	FME	O	1	2	8,9,10	0.78	0	7,9,11	1.09	1 (14%)
1	FME	N	1	1	8,9,10	0.46	0	7,9,11	1.83	2 (28%)
2	FME	B	1	2	8,9,10	1.34	1 (12%)	7,9,11	1.12	0
1	FME	A	1	1	8,9,10	1.09	0	7,9,11	2.41	5 (71%)
9	SAC	V	1	9	7,8,9	0.65	0	8,9,11	0.94	1 (12%)
9	SAC	I	1	9	7,8,9	0.72	0	8,9,11	1.04	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	5/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-
9	SAC	I	1	9	-	5/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CB-CG	2.48	1.61	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CE-SD-CG	3.66	112.98	100.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CE-SD-CG	3.50	112.42	100.40
1	A	1	FME	CA-N-CN	-3.37	117.64	122.82
1	N	1	FME	O-C-CA	-2.44	118.37	124.78
1	A	1	FME	CG-CB-CA	-2.33	106.47	112.95
1	A	1	FME	O-C-CA	-2.30	118.74	124.78
2	O	1	FME	O-C-CA	-2.23	118.93	124.78
9	V	1	SAC	O-C-CA	-2.18	119.06	124.78
1	A	1	FME	O1-CN-N	-2.09	119.75	125.27

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	CB-CA-N-CN
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	O-C-CA-CB
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	C-CA-CB-OG
9	I	1	SAC	N-CA-CB-OG
1	N	1	FME	CB-CG-SD-CE
9	V	1	SAC	N-CA-CB-OG
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	CA-CB-CG-SD
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	1	0
9	V	1	SAC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 10 are monoatomic - leaving 118 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	A	601[A]	-	66,67,67	1.73	17 (25%)	78,103,103	1.88	17 (21%)
24	PEK	T	101	-	48,48,52	1.20	2 (4%)	51,53,57	1.56	9 (17%)
21	EDO	G	104	-	3,3,3	0.63	0	2,2,2	0.60	0
24	PEK	P	304	-	52,52,52	0.56	0	55,57,57	1.17	3 (5%)
21	EDO	C	310	-	3,3,3	0.90	0	2,2,2	0.25	0
19	TGL	A	607	-	62,62,62	1.22	3 (4%)	65,65,65	2.02	18 (27%)
23	CHD	P	301	-	32,32,32	0.93	2 (6%)	51,51,51	1.47	8 (15%)
22	CUA	B	302	2	0,1,1	-	-	-	-	-
26	DMU	G	105	-	21,21,34	1.24	2 (9%)	24,25,45	2.11	7 (29%)
19	TGL	O	302	-	62,62,62	1.12	4 (6%)	65,65,65	1.10	4 (6%)
26	DMU	J	101	-	34,34,34	0.95	1 (2%)	45,45,45	1.47	8 (17%)
26	DMU	M	101	-	34,34,34	0.65	1 (2%)	45,45,45	1.38	9 (20%)
23	CHD	C	309	-	32,32,32	0.91	0	51,51,51	2.52	13 (25%)
21	EDO	S	105	-	3,3,3	0.98	0	2,2,2	0.88	0
21	EDO	B	305	-	3,3,3	0.91	0	2,2,2	1.48	1 (50%)
21	EDO	N	614	-	3,3,3	0.79	0	2,2,2	0.44	0
21	EDO	O	305	-	3,3,3	0.79	0	2,2,2	0.75	0
26	DMU	P	311	-	34,34,34	0.80	1 (2%)	45,45,45	1.23	6 (13%)
26	DMU	X	103	-	22,22,34	1.18	1 (4%)	27,27,45	1.69	7 (25%)
21	EDO	E	203	-	3,3,3	0.48	0	2,2,2	0.59	0
21	EDO	Q	202	-	3,3,3	0.60	0	2,2,2	0.14	0
21	EDO	A	610	-	3,3,3	1.08	0	2,2,2	1.03	0
23	CHD	B	303	-	32,32,32	0.82	1 (3%)	51,51,51	1.91	17 (33%)
21	EDO	A	616	-	3,3,3	0.81	0	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	P	306	-	44,44,50	0.82	2 (4%)	47,50,56	1.12	3 (6%)
26	DMU	K	102	-	22,22,34	1.45	5 (22%)	27,27,45	1.78	6 (22%)
21	EDO	A	617	-	3,3,3	0.70	0	2,2,2	0.71	0
23	CHD	W	101	-	32,32,32	0.87	0	51,51,51	2.36	18 (35%)
27	PSC	O	304	-	50,50,51	1.24	3 (6%)	56,58,59	1.98	11 (19%)
21	EDO	A	612	-	3,3,3	0.33	0	2,2,2	1.09	0
20	PGV	A	608	-	45,45,50	1.18	4 (8%)	49,50,56	1.44	6 (12%)
22	CUA	O	303	2	0,1,1	-	-	-	-	-
20	PGV	C	305	-	50,50,50	0.79	0	53,56,56	0.87	0
20	PGV	C	306	-	50,50,50	0.85	2 (4%)	53,56,56	0.90	2 (3%)
21	EDO	N	613	-	3,3,3	0.64	0	2,2,2	0.54	0
21	EDO	O	306	-	3,3,3	0.81	0	2,2,2	0.20	0
21	EDO	S	107	-	3,3,3	0.66	0	2,2,2	0.68	0
25	CDL	T	102	-	79,79,99	1.36	9 (11%)	84,89,111	1.57	18 (21%)
23	CHD	P	309	-	32,32,32	0.78	0	51,51,51	1.87	12 (23%)
21	EDO	N	615	-	3,3,3	0.62	0	2,2,2	0.50	0
20	PGV	Q	201	-	50,50,50	1.02	2 (4%)	53,56,56	1.53	8 (15%)
18	CYN	A	606[C]	15	0,1,1	-	-	-	-	-
14	HEA	N	601[A]	-	66,67,67	1.73	17 (25%)	78,103,103	2.37	22 (28%)
21	EDO	N	612	-	3,3,3	0.49	0	2,2,2	0.35	0
26	DMU	X	101	-	22,22,34	1.56	2 (9%)	27,27,45	1.99	9 (33%)
26	DMU	P	316	-	22,22,34	1.20	2 (9%)	27,27,45	2.22	9 (33%)
21	EDO	F	103	-	3,3,3	0.88	0	2,2,2	0.28	0
21	EDO	A	615	-	3,3,3	0.35	0	2,2,2	0.67	0
25	CDL	Y	101	-	86,86,99	1.35	10 (11%)	92,98,111	1.23	8 (8%)
21	EDO	A	614	-	3,3,3	0.73	0	2,2,2	0.57	0
23	CHD	G	102	-	32,32,32	0.80	1 (3%)	51,51,51	1.51	7 (13%)
29	PO4	U	102	-	4,4,4	0.58	0	6,6,6	0.70	0
21	EDO	N	609	-	3,3,3	0.28	0	2,2,2	0.55	0
24	PEK	C	303	-	50,50,52	0.75	2 (4%)	53,55,57	1.05	4 (7%)
21	EDO	B	306	-	3,3,3	0.79	0	2,2,2	0.51	0
21	EDO	G	103	-	3,3,3	0.72	0	2,2,2	0.56	0
20	PGV	N	607	-	50,50,50	1.10	6 (12%)	53,56,56	1.26	5 (9%)
21	EDO	S	104	-	3,3,3	0.65	0	2,2,2	0.98	0
21	EDO	Y	102	-	3,3,3	0.48	0	2,2,2	0.06	0
21	EDO	N	610	-	3,3,3	0.34	0	2,2,2	1.04	0
21	EDO	N	608	-	3,3,3	0.79	0	2,2,2	0.65	0
14	HEA	N	602[C]	1	66,67,67	1.84	20 (30%)	78,103,103	2.15	30 (38%)
21	EDO	F	104	-	3,3,3	0.76	0	2,2,2	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DMU	P	312	-	34,34,34	0.80	1 (2%)	45,45,45	1.25	4 (8%)
21	EDO	P	314	-	3,3,3	0.39	0	2,2,2	1.36	0
20	PGV	C	307	-	46,46,50	1.27	2 (4%)	49,52,56	1.83	9 (18%)
21	EDO	T	103	-	3,3,3	0.83	0	2,2,2	0.83	0
14	HEA	A	601[B]	-	66,67,67	1.75	16 (24%)	78,103,103	1.81	15 (19%)
19	TGL	D	201	-	47,47,62	1.71	5 (10%)	50,50,65	1.27	8 (16%)
24	PEK	P	305	-	45,45,52	1.21	2 (4%)	47,47,57	1.57	4 (8%)
21	EDO	S	103	-	3,3,3	0.65	0	2,2,2	0.18	0
18	CYN	A	606[A]	15	0,1,1	-	-	-	-	-
14	HEA	A	602[A]	1	66,67,67	1.82	19 (28%)	78,103,103	2.20	30 (38%)
21	EDO	O	308	-	3,3,3	0.56	0	2,2,2	0.56	0
21	EDO	T	104	-	3,3,3	0.56	0	2,2,2	0.28	0
26	DMU	P	315	-	34,34,34	1.05	3 (8%)	45,45,45	1.92	12 (26%)
21	EDO	N	611	-	3,3,3	0.65	0	2,2,2	0.86	0
21	EDO	U	101	-	3,3,3	0.65	0	2,2,2	0.38	0
14	HEA	N	602[A]	1	66,67,67	1.79	18 (27%)	78,103,103	2.35	33 (42%)
26	DMU	K	101	-	22,22,34	1.27	1 (4%)	27,27,45	1.61	7 (25%)
14	HEA	A	602[C]	1	66,67,67	1.76	20 (30%)	78,103,103	2.35	36 (46%)
21	EDO	B	307	-	3,3,3	0.49	0	2,2,2	0.42	0
18	CYN	N	606[C]	15	0,1,1	-	-	-	-	-
21	EDO	F	102	-	3,3,3	0.89	0	2,2,2	0.55	0
21	EDO	A	611	-	3,3,3	0.29	0	2,2,2	0.51	0
21	EDO	O	307	-	3,3,3	0.58	0	2,2,2	0.51	0
26	DMU	Z	101	-	34,34,34	0.51	0	45,45,45	1.18	4 (8%)
26	DMU	X	102	-	22,22,34	1.35	3 (13%)	27,27,45	1.39	5 (18%)
21	EDO	A	613	-	3,3,3	0.78	0	2,2,2	0.28	0
23	CHD	J	102	-	32,32,32	0.89	1 (3%)	51,51,51	2.70	22 (43%)
21	EDO	B	308	-	3,3,3	1.24	0	2,2,2	0.73	0
21	EDO	D	202	-	3,3,3	0.47	0	2,2,2	0.53	0
21	EDO	A	609	-	3,3,3	0.42	0	2,2,2	0.32	0
26	DMU	P	310	-	34,34,34	0.53	0	45,45,45	1.31	5 (11%)
21	EDO	S	106	-	3,3,3	0.68	0	2,2,2	0.52	0
24	PEK	C	304	-	43,43,52	1.16	2 (4%)	44,44,57	1.41	5 (11%)
21	EDO	P	313	-	3,3,3	0.84	0	2,2,2	0.48	0
23	CHD	C	301	-	32,32,32	1.10	2 (6%)	51,51,51	1.67	10 (19%)
19	TGL	O	301	-	62,62,62	1.11	3 (4%)	65,65,65	1.40	7 (10%)
21	EDO	R	201	-	3,3,3	0.61	0	2,2,2	0.60	0
25	CDL	C	308	-	84,84,99	1.41	13 (15%)	91,94,111	1.59	17 (18%)
21	EDO	S	102	-	3,3,3	0.72	0	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	B	304	-	3,3,3	0.71	0	2,2,2	0.47	0
21	EDO	S	108	-	3,3,3	0.68	0	2,2,2	0.57	0
27	PSC	E	201	-	51,51,51	1.21	3 (5%)	57,59,59	1.83	7 (12%)
18	CYN	N	606[A]	15	0,1,1	-	-	-	-	-
26	DMU	L	101	-	18,18,34	1.21	1 (5%)	23,23,45	1.56	3 (13%)
21	EDO	E	202	-	3,3,3	0.65	0	2,2,2	0.40	0
25	CDL	P	308	-	71,74,99	1.60	10 (14%)	72,78,111	1.63	10 (13%)
20	PGV	P	307	-	50,50,50	1.06	2 (4%)	53,56,56	1.60	7 (13%)
25	CDL	G	101	-	87,87,99	1.43	13 (14%)	91,97,111	1.52	10 (10%)
26	DMU	K	103	-	17,17,34	0.65	0	17,18,45	1.20	1 (5%)
19	TGL	B	301	-	61,61,62	1.18	3 (4%)	64,64,65	1.61	9 (14%)
26	DMU	C	311	-	34,34,34	0.86	0	45,45,45	1.83	12 (26%)
14	HEA	N	601[B]	-	66,67,67	1.75	17 (25%)	78,103,103	2.34	24 (30%)
24	PEK	P	303	-	21,21,52	1.11	1 (4%)	21,21,57	1.26	3 (14%)

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	A	601[A]	-	-	8/36/76/76	-
24	PEK	T	101	-	-	18/52/52/56	-
21	EDO	G	104	-	-	0/1/1/1	-
24	PEK	P	304	-	-	8/56/56/56	-
21	EDO	C	310	-	-	0/1/1/1	-
19	TGL	A	607	-	-	31/65/65/65	-
23	CHD	P	301	-	-	1/9/74/74	0/4/4/4
26	DMU	G	105	-	-	6/13/29/59	0/1/1/2
19	TGL	O	302	-	-	26/65/65/65	-
26	DMU	J	101	-	-	5/19/59/59	0/2/2/2
26	DMU	M	101	-	-	5/19/59/59	0/2/2/2
23	CHD	C	309	-	-	6/9/74/74	0/4/4/4
21	EDO	S	105	-	-	0/1/1/1	-
21	EDO	B	305	-	-	1/1/1/1	-
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	O	305	-	-	0/1/1/1	-
26	DMU	P	311	-	-	7/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DMU	X	103	-	-	7/13/33/59	0/1/1/2
21	EDO	E	203	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	1/1/1/1	-
23	CHD	B	303	-	-	2/9/74/74	0/4/4/4
21	EDO	A	610	-	-	0/1/1/1	-
21	EDO	A	616	-	-	0/1/1/1	-
20	PGV	P	306	-	-	8/49/49/55	-
26	DMU	K	102	-	-	8/13/33/59	0/1/1/2
21	EDO	A	617	-	-	1/1/1/1	-
23	CHD	W	101	-	-	5/9/74/74	0/4/4/4
27	PSC	O	304	-	-	24/54/54/55	-
21	EDO	A	612	-	-	0/1/1/1	-
20	PGV	A	608	-	-	18/47/47/55	-
20	PGV	C	305	-	-	7/55/55/55	-
20	PGV	C	306	-	-	12/55/55/55	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	O	306	-	-	0/1/1/1	-
21	EDO	S	107	-	-	1/1/1/1	-
25	CDL	T	102	-	-	30/87/87/110	-
23	CHD	P	309	-	-	5/9/74/74	0/4/4/4
21	EDO	N	615	-	-	0/1/1/1	-
20	PGV	Q	201	-	-	14/55/55/55	-
14	HEA	N	601[A]	-	-	4/36/76/76	-
21	EDO	N	612	-	-	0/1/1/1	-
26	DMU	X	101	-	-	5/13/33/59	0/1/1/2
26	DMU	P	316	-	-	7/13/33/59	0/1/1/2
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	A	615	-	-	0/1/1/1	-
25	CDL	Y	101	-	-	39/97/97/110	-
21	EDO	A	614	-	-	0/1/1/1	-
23	CHD	G	102	-	-	2/9/74/74	0/4/4/4
21	EDO	N	609	-	-	0/1/1/1	-
24	PEK	C	303	-	-	14/54/54/56	-
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	G	103	-	-	0/1/1/1	-
20	PGV	N	607	-	-	4/55/55/55	-
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	Y	102	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	N	608	-	-	0/1/1/1	-
14	HEA	N	602[C]	1	-	8/36/76/76	-
21	EDO	F	104	-	-	0/1/1/1	-
26	DMU	P	312	-	-	5/19/59/59	0/2/2/2
21	EDO	P	314	-	-	1/1/1/1	-
20	PGV	C	307	-	-	18/51/51/55	-
21	EDO	T	103	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	-	5/36/76/76	-
19	TGL	D	201	-	-	19/50/50/65	-
24	PEK	P	305	-	-	22/47/47/56	-
21	EDO	S	103	-	-	0/1/1/1	-
14	HEA	A	602[A]	1	-	8/36/76/76	-
21	EDO	O	308	-	-	0/1/1/1	-
21	EDO	T	104	-	-	0/1/1/1	-
26	DMU	P	315	-	-	10/19/59/59	0/2/2/2
21	EDO	N	611	-	-	0/1/1/1	-
21	EDO	U	101	-	-	1/1/1/1	-
14	HEA	N	602[A]	1	-	9/36/76/76	-
26	DMU	K	101	-	-	4/13/33/59	0/1/1/2
14	HEA	A	602[C]	1	-	7/36/76/76	-
21	EDO	B	307	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	A	611	-	-	0/1/1/1	-
21	EDO	O	307	-	-	0/1/1/1	-
26	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
26	DMU	X	102	-	-	9/13/33/59	0/1/1/2
21	EDO	A	613	-	-	0/1/1/1	-
23	CHD	J	102	-	-	7/9/74/74	0/4/4/4
21	EDO	B	308	-	-	0/1/1/1	-
21	EDO	D	202	-	-	1/1/1/1	-
21	EDO	A	609	-	-	0/1/1/1	-
26	DMU	P	310	-	-	9/19/59/59	0/2/2/2
21	EDO	S	106	-	-	1/1/1/1	-
24	PEK	C	304	-	-	22/43/43/56	-
21	EDO	P	313	-	-	0/1/1/1	-
23	CHD	C	301	-	-	2/9/74/74	0/4/4/4
19	TGL	O	301	-	-	33/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	R	201	-	-	0/1/1/1	-
25	CDL	C	308	-	-	35/90/90/110	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	B	304	-	-	0/1/1/1	-
21	EDO	S	108	-	-	1/1/1/1	-
27	PSC	E	201	-	-	28/55/55/55	-
26	DMU	L	101	-	-	2/9/29/59	0/1/1/2
21	EDO	E	202	-	-	0/1/1/1	-
25	CDL	P	308	-	-	23/73/77/110	-
20	PGV	P	307	-	-	14/55/55/55	-
25	CDL	G	101	-	-	31/94/94/110	-
26	DMU	K	103	-	-	4/11/19/59	0/1/1/2
19	TGL	B	301	-	-	33/64/64/65	-
26	DMU	C	311	-	-	7/19/59/59	0/2/2/2
14	HEA	N	601[B]	-	-	5/36/76/76	-
24	PEK	P	303	-	-	7/19/19/56	-

All (283) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	7.11	1.43	1.22
19	A	607	TGL	OG2-CB1	5.83	1.50	1.34
20	C	307	PGV	O03-C19	5.83	1.50	1.33
25	P	308	CDL	OA8-CA7	5.78	1.50	1.33
19	D	201	TGL	OG2-CB1	5.70	1.50	1.34
27	E	201	PSC	O01-C1	5.42	1.49	1.34
24	T	101	PEK	O03-C21	5.42	1.49	1.33
24	P	305	PEK	O01-C1	5.32	1.49	1.34
20	P	307	PGV	O03-C19	5.32	1.48	1.33
25	G	101	CDL	OA6-CA5	5.23	1.49	1.34
27	O	304	PSC	O01-C1	5.21	1.49	1.34
19	O	301	TGL	OG2-CB1	5.18	1.48	1.34
25	P	308	CDL	OA6-CA5	5.11	1.48	1.34
24	C	304	PEK	O01-C1	5.05	1.48	1.33
19	B	301	TGL	OG2-CB1	5.01	1.48	1.34
20	A	608	PGV	O03-C19	5.00	1.48	1.33
25	P	308	CDL	OB6-CB5	5.00	1.47	1.33
19	A	607	TGL	OG3-CC1	4.96	1.47	1.33
14	A	602[A]	HEA	CHA-C1A	4.96	1.48	1.38
24	P	305	PEK	O03-C21	4.95	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	101	CDL	OA8-CA7	4.91	1.47	1.33
25	Y	101	CDL	OA6-CA5	4.90	1.48	1.34
24	P	303	PEK	O01-C1	4.89	1.47	1.30
25	P	308	CDL	OB8-CB7	4.88	1.47	1.33
14	N	602[C]	HEA	CHA-C1A	4.87	1.47	1.38
25	T	102	CDL	OB8-CB7	4.83	1.47	1.33
20	C	307	PGV	O01-C1	4.82	1.47	1.34
25	T	102	CDL	OA6-CA5	4.80	1.47	1.34
25	C	308	CDL	OA8-CA7	4.76	1.47	1.33
26	X	101	DMU	O16-C6	4.75	1.48	1.40
19	O	302	TGL	OG1-CA1	4.75	1.47	1.33
24	C	304	PEK	O03-C21	4.73	1.47	1.33
25	G	101	CDL	OB8-CB7	4.72	1.47	1.33
25	Y	101	CDL	OB8-CB7	4.68	1.47	1.33
19	B	301	TGL	OG1-CA1	4.68	1.47	1.33
14	A	601[A]	HEA	C1A-C2A	-4.63	1.37	1.45
14	A	601[B]	HEA	C1A-C2A	-4.63	1.37	1.45
20	Q	201	PGV	O03-C19	4.63	1.46	1.33
19	D	201	TGL	OG1-CA1	4.56	1.46	1.33
19	O	302	TGL	OG2-CB1	4.54	1.47	1.34
24	T	101	PEK	O01-C1	4.46	1.46	1.34
27	O	304	PSC	O03-C19	4.43	1.46	1.33
19	A	607	TGL	OG1-CA1	4.41	1.46	1.33
25	Y	101	CDL	OB6-CB5	4.38	1.46	1.34
19	B	301	TGL	OG3-CC1	4.35	1.46	1.33
14	N	602[A]	HEA	C4D-C3D	-4.35	1.37	1.45
14	A	602[C]	HEA	CHA-C1A	4.31	1.46	1.38
20	Q	201	PGV	O01-C1	4.28	1.46	1.34
14	N	602[A]	HEA	CHB-C4A	4.24	1.46	1.38
14	A	602[A]	HEA	CHB-C4A	4.23	1.46	1.38
19	O	301	TGL	OG3-CC1	4.20	1.45	1.33
27	E	201	PSC	O03-C19	4.15	1.45	1.33
19	O	301	TGL	OG1-CA1	4.10	1.45	1.33
25	C	308	CDL	OA6-CA5	4.06	1.45	1.34
19	D	201	TGL	OG3-CC1	4.00	1.45	1.33
19	O	302	TGL	OG3-CC1	3.93	1.44	1.33
14	N	602[A]	HEA	C3A-C4A	-3.90	1.39	1.46
14	A	602[A]	HEA	C4D-C3D	-3.90	1.38	1.45
14	N	601[A]	HEA	C3A-C4A	-3.88	1.39	1.46
14	N	601[B]	HEA	C3A-C4A	-3.88	1.39	1.46
14	N	601[A]	HEA	C1A-C2A	-3.87	1.38	1.45
14	N	601[B]	HEA	C1A-C2A	-3.87	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	307	PGV	O01-C1	3.87	1.45	1.34
14	N	602[C]	HEA	CHD-C1D	3.85	1.46	1.38
20	A	608	PGV	O01-C1	3.85	1.45	1.34
25	C	308	CDL	C79-C78	-3.79	1.30	1.51
14	N	602[A]	HEA	CHC-C1C	3.78	1.47	1.39
25	T	102	CDL	OA8-CA7	3.77	1.44	1.33
26	J	101	DMU	O16-C6	3.77	1.46	1.40
26	K	101	DMU	O16-C6	3.74	1.46	1.40
25	C	308	CDL	OB8-CB7	3.74	1.44	1.33
20	N	607	PGV	O01-C02	-3.73	1.37	1.46
14	A	601[A]	HEA	C1D-ND	-3.70	1.33	1.40
14	A	601[B]	HEA	C1D-ND	-3.70	1.33	1.40
14	A	602[C]	HEA	CHD-C4C	3.69	1.47	1.39
27	E	201	PSC	C13-C12	3.67	1.53	1.31
26	X	102	DMU	O16-C6	3.66	1.46	1.40
14	N	601[A]	HEA	C4B-NB	-3.62	1.34	1.40
14	N	601[B]	HEA	C4B-NB	-3.62	1.34	1.40
14	N	602[A]	HEA	O11-C11	3.61	1.50	1.42
26	L	101	DMU	O16-C6	3.60	1.46	1.40
27	O	304	PSC	C13-C12	3.60	1.52	1.31
14	N	602[C]	HEA	C1B-C2B	-3.59	1.37	1.44
25	Y	101	CDL	OA8-CA7	3.59	1.43	1.33
25	C	308	CDL	C82-C81	-3.56	1.31	1.51
14	N	601[A]	HEA	CHB-C4A	3.56	1.45	1.38
14	N	601[B]	HEA	CHB-C4A	3.56	1.45	1.38
14	A	601[A]	HEA	C1D-C2D	-3.55	1.37	1.44
14	A	601[B]	HEA	C1D-C2D	-3.55	1.37	1.44
14	N	602[A]	HEA	CHA-C1A	3.55	1.45	1.38
14	N	601[A]	HEA	C1D-ND	-3.53	1.34	1.40
14	N	601[B]	HEA	C1D-ND	-3.53	1.34	1.40
14	A	602[C]	HEA	CHD-C1D	3.48	1.45	1.38
25	C	308	CDL	OB6-CB5	3.45	1.44	1.34
14	A	602[C]	HEA	C1A-C2A	-3.45	1.39	1.45
25	C	308	CDL	C59-C58	-3.43	1.32	1.51
25	P	308	CDL	C79-C78	-3.42	1.32	1.51
26	K	102	DMU	O16-C6	3.42	1.46	1.40
25	P	308	CDL	C59-C58	-3.40	1.32	1.51
25	T	102	CDL	C42-C41	-3.34	1.32	1.51
25	P	308	CDL	C82-C81	-3.33	1.32	1.51
14	N	602[C]	HEA	FE-ND	3.30	2.05	1.94
25	T	102	CDL	C22-C21	-3.30	1.33	1.51
14	A	602[C]	HEA	C4A-NA	-3.28	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[A]	HEA	CHD-C1D	3.28	1.45	1.38
14	A	601[B]	HEA	CHD-C1D	3.28	1.45	1.38
25	Y	101	CDL	C79-C78	-3.27	1.33	1.51
25	T	102	CDL	C19-C18	-3.26	1.33	1.51
25	G	101	CDL	C62-C61	-3.26	1.33	1.51
14	N	602[C]	HEA	C3A-C4A	-3.26	1.40	1.46
14	N	601[B]	HEA	O11-C11	3.24	1.49	1.42
25	Y	101	CDL	C82-C81	-3.23	1.33	1.51
25	T	102	CDL	C82-C81	-3.21	1.33	1.51
14	A	602[A]	HEA	CHD-C1D	3.20	1.45	1.38
25	G	101	CDL	C19-C18	-3.19	1.33	1.51
14	N	602[C]	HEA	C4D-C3D	-3.19	1.39	1.45
14	A	602[C]	HEA	C3A-C4A	-3.19	1.40	1.46
14	A	602[A]	HEA	CHC-C1C	3.18	1.46	1.39
14	N	602[C]	HEA	CHC-C4B	3.18	1.45	1.38
14	A	602[A]	HEA	FE-NC	3.18	2.05	1.95
14	A	601[A]	HEA	CHB-C4A	3.17	1.44	1.38
14	A	601[B]	HEA	CHB-C4A	3.17	1.44	1.38
25	G	101	CDL	C22-C21	-3.16	1.33	1.51
14	A	602[A]	HEA	C1D-C2D	-3.15	1.38	1.44
25	G	101	CDL	C42-C41	-3.14	1.33	1.51
14	A	602[A]	HEA	C4B-C3B	-3.12	1.39	1.44
14	N	602[C]	HEA	C4B-C3B	-3.12	1.39	1.44
25	C	308	CDL	C62-C61	-3.11	1.34	1.51
25	G	101	CDL	C82-C81	-3.09	1.34	1.51
26	X	103	DMU	O16-C6	3.08	1.45	1.40
14	A	602[C]	HEA	CHB-C4A	3.07	1.44	1.38
14	N	602[C]	HEA	CHD-C4C	3.06	1.46	1.39
14	N	602[A]	HEA	CHD-C4C	3.05	1.46	1.39
25	T	102	CDL	C79-C78	-3.02	1.34	1.51
14	A	601[B]	HEA	O11-C11	3.01	1.49	1.42
14	A	602[A]	HEA	CHC-C4B	3.00	1.44	1.38
25	Y	101	CDL	C62-C61	-3.00	1.34	1.51
25	Y	101	CDL	C59-C58	-2.99	1.34	1.51
25	C	308	CDL	C39-C38	-2.98	1.34	1.51
25	Y	101	CDL	C22-C21	-2.97	1.34	1.51
25	G	101	CDL	C79-C78	-2.97	1.34	1.51
14	N	602[A]	HEA	CHC-C4B	2.96	1.44	1.38
14	N	601[A]	HEA	CHC-C4B	2.94	1.44	1.38
14	N	601[B]	HEA	CHC-C4B	2.94	1.44	1.38
25	T	102	CDL	C39-C38	-2.93	1.35	1.51
25	C	308	CDL	C42-C41	-2.92	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	312	DMU	O16-C6	2.90	1.45	1.40
25	P	308	CDL	C39-C38	-2.90	1.35	1.51
25	G	101	CDL	C39-C38	-2.89	1.35	1.51
25	P	308	CDL	C42-C41	-2.89	1.35	1.51
26	P	316	DMU	C3-C4	2.87	1.59	1.53
14	N	602[C]	HEA	C1D-ND	-2.86	1.35	1.40
14	N	602[A]	HEA	CHD-C1D	2.86	1.44	1.38
14	A	602[C]	HEA	C4B-C3B	-2.83	1.39	1.44
14	N	601[A]	HEA	C1D-C2D	-2.82	1.39	1.44
14	N	601[B]	HEA	C1D-C2D	-2.82	1.39	1.44
14	N	602[C]	HEA	C4B-NB	-2.81	1.35	1.40
14	N	601[A]	HEA	FE-ND	2.81	2.03	1.94
14	N	601[B]	HEA	FE-ND	2.81	2.03	1.94
25	Y	101	CDL	C19-C18	-2.79	1.35	1.51
24	C	303	PEK	O03-C21	2.77	1.41	1.33
14	A	602[A]	HEA	CHB-C1B	2.77	1.45	1.39
26	P	315	DMU	O16-C6	2.77	1.44	1.40
25	P	308	CDL	CA6-CA4	2.75	1.59	1.50
14	A	601[A]	HEA	CHD-C4C	2.72	1.45	1.39
14	A	601[B]	HEA	CHD-C4C	2.72	1.45	1.39
14	A	601[A]	HEA	C1C-C2C	-2.72	1.36	1.43
14	A	601[B]	HEA	C1C-C2C	-2.72	1.36	1.43
23	C	301	CHD	O25-C24	2.72	1.31	1.22
26	G	105	DMU	O16-C6	2.70	1.44	1.40
14	A	601[A]	HEA	O11-C11	2.70	1.48	1.42
14	A	602[A]	HEA	C18-C19	2.69	1.39	1.33
14	A	602[C]	HEA	C18-C19	2.69	1.39	1.33
14	N	602[C]	HEA	CHB-C4A	2.69	1.43	1.38
14	A	602[A]	HEA	CHD-C4C	2.69	1.45	1.39
14	N	602[C]	HEA	C1A-C2A	-2.68	1.40	1.45
26	K	102	DMU	C2-C1	2.68	1.59	1.52
14	A	602[C]	HEA	CHC-C4B	2.68	1.44	1.38
14	N	602[A]	HEA	CHB-C1B	2.68	1.45	1.39
20	A	608	PGV	O02-C1	2.66	1.30	1.22
14	A	602[C]	HEA	FE-ND	2.63	2.03	1.94
25	G	101	CDL	C58-C59	-2.61	1.33	1.51
14	N	601[A]	HEA	CHC-C1C	2.60	1.45	1.39
14	N	601[B]	HEA	CHC-C1C	2.60	1.45	1.39
14	A	602[C]	HEA	C4D-C3D	-2.59	1.40	1.45
20	P	306	PGV	P-O14	-2.58	1.43	1.55
14	A	601[A]	HEA	C1B-NB	-2.58	1.33	1.38
14	A	601[B]	HEA	C1B-NB	-2.58	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[C]	HEA	CHC-C1C	2.58	1.45	1.39
14	A	601[A]	HEA	CBD-CGD	2.55	1.56	1.50
14	A	601[B]	HEA	CBD-CGD	2.55	1.56	1.50
14	A	602[A]	HEA	FE-NB	2.54	2.02	1.94
26	P	316	DMU	O16-C6	2.53	1.44	1.40
14	N	601[A]	HEA	CHA-C1A	2.53	1.43	1.38
14	N	601[B]	HEA	CHA-C1A	2.53	1.43	1.38
20	N	607	PGV	O01-C1	2.52	1.41	1.34
14	A	602[A]	HEA	O11-C11	2.51	1.48	1.42
14	A	601[A]	HEA	FE-NB	2.50	2.02	1.94
14	A	601[B]	HEA	FE-NB	2.50	2.02	1.94
25	C	308	CDL	PB2-OB3	2.49	1.58	1.50
14	N	601[A]	HEA	CMD-C2D	2.47	1.56	1.50
14	N	601[B]	HEA	CMD-C2D	2.47	1.56	1.50
14	N	601[A]	HEA	C1B-C2B	-2.47	1.39	1.44
14	N	601[B]	HEA	C1B-C2B	-2.47	1.39	1.44
23	J	102	CHD	C13-C14	-2.46	1.51	1.55
14	N	602[C]	HEA	FE-NC	2.44	2.03	1.95
23	P	301	CHD	C23-C24	2.43	1.56	1.50
14	N	601[A]	HEA	C12-C11	-2.43	1.48	1.52
14	N	602[A]	HEA	FE-NB	2.42	2.02	1.94
14	N	602[C]	HEA	FE-NB	2.42	2.02	1.94
26	X	102	DMU	C3-C2	2.41	1.58	1.52
20	N	607	PGV	O03-C19	2.41	1.40	1.33
14	A	602[C]	HEA	C1B-C2B	-2.41	1.39	1.44
14	A	601[A]	HEA	C3A-C4A	-2.41	1.41	1.46
14	A	601[B]	HEA	C3A-C4A	-2.41	1.41	1.46
26	M	101	DMU	O16-C6	2.39	1.44	1.40
14	N	602[C]	HEA	FE-NA	2.36	2.03	1.95
14	N	602[A]	HEA	FE-ND	2.35	2.02	1.94
14	N	602[A]	HEA	C4B-C3B	-2.35	1.40	1.44
14	N	601[A]	HEA	O2D-CGD	-2.34	1.22	1.30
14	N	601[B]	HEA	O2D-CGD	-2.34	1.22	1.30
20	N	607	PGV	C01-C02	2.34	1.57	1.50
14	A	602[C]	HEA	C4B-NB	-2.33	1.36	1.40
14	N	602[C]	HEA	CHB-C1B	2.33	1.44	1.39
14	A	601[A]	HEA	C4D-C3D	-2.32	1.41	1.45
14	A	601[B]	HEA	C4D-C3D	-2.32	1.41	1.45
26	X	101	DMU	C3-C2	2.29	1.58	1.52
14	N	601[A]	HEA	O1D-CGD	2.25	1.29	1.22
14	N	601[B]	HEA	O1D-CGD	2.25	1.29	1.22
20	P	306	PGV	O01-C02	-2.24	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	105	DMU	C2-C1	2.23	1.55	1.52
20	C	306	PGV	O03-C01	2.23	1.50	1.45
14	N	602[C]	HEA	CMA-C3A	2.23	1.49	1.45
14	A	602[C]	HEA	C1D-C2D	-2.21	1.40	1.44
14	A	601[A]	HEA	C1B-C2B	-2.21	1.40	1.44
14	A	601[B]	HEA	C1B-C2B	-2.21	1.40	1.44
14	A	602[A]	HEA	C1A-C2A	-2.20	1.41	1.45
14	A	601[A]	HEA	CHA-C1A	2.20	1.42	1.38
14	A	601[B]	HEA	CHA-C1A	2.20	1.42	1.38
14	A	602[C]	HEA	FE-NA	2.20	2.02	1.95
23	B	303	CHD	C11-C9	2.18	1.57	1.53
26	P	315	DMU	C8-C9	2.17	1.57	1.53
14	N	601[A]	HEA	O1A-CGA	2.17	1.29	1.22
14	N	601[B]	HEA	O1A-CGA	2.17	1.29	1.22
24	C	303	PEK	O01-C1	2.16	1.40	1.34
14	N	602[A]	HEA	C4B-NB	-2.15	1.36	1.40
26	K	102	DMU	O55-C2	2.15	1.48	1.43
14	N	601[A]	HEA	CBD-CGD	2.14	1.55	1.50
14	N	601[B]	HEA	CBD-CGD	2.14	1.55	1.50
14	N	602[A]	HEA	C1D-C2D	-2.14	1.40	1.44
14	A	602[C]	HEA	CHC-C1C	2.13	1.44	1.39
25	G	101	CDL	CA6-CA4	2.12	1.57	1.50
14	A	602[A]	HEA	FE-NA	2.12	2.02	1.95
19	D	201	TGL	CB2-CB1	2.12	1.56	1.50
14	N	602[A]	HEA	CMA-C3A	2.12	1.49	1.45
26	P	315	DMU	C10-C5	2.10	1.58	1.52
26	X	102	DMU	O5-C6	2.10	1.47	1.41
14	A	602[C]	HEA	CHB-C1B	2.10	1.44	1.39
20	N	607	PGV	P-O12	-2.10	1.50	1.59
14	N	602[A]	HEA	C3B-C2B	2.09	1.39	1.34
26	P	311	DMU	O16-C6	2.09	1.43	1.40
14	A	602[A]	HEA	FE-ND	2.08	2.01	1.94
14	A	602[C]	HEA	CMA-C3A	2.07	1.49	1.45
25	C	308	CDL	OB6-CB4	-2.07	1.41	1.46
23	G	102	CHD	C10-C9	-2.06	1.52	1.56
20	A	608	PGV	O01-C02	-2.05	1.41	1.46
14	A	602[A]	HEA	C1B-C2B	-2.04	1.40	1.44
26	K	102	DMU	C3-C2	2.04	1.57	1.52
14	N	602[C]	HEA	C1C-NC	-2.03	1.35	1.39
23	P	301	CHD	O25-C24	2.03	1.28	1.22
14	A	602[A]	HEA	C1D-ND	-2.03	1.36	1.40
25	C	308	CDL	PB2-OB2	2.03	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[A]	HEA	C12-C11	-2.02	1.49	1.52
26	K	102	DMU	C3-C4	2.02	1.57	1.53
25	G	101	CDL	CA3-CA4	2.02	1.56	1.50
23	C	301	CHD	C18-C13	-2.02	1.51	1.54
14	N	602[A]	HEA	FE-NC	2.01	2.01	1.95
19	O	302	TGL	OB1-CB1	2.01	1.28	1.22
14	A	601[A]	HEA	CMC-C2C	2.01	1.55	1.50
14	A	601[B]	HEA	CMC-C2C	2.01	1.55	1.50
20	C	306	PGV	C03-C02	2.00	1.56	1.50
14	A	602[C]	HEA	O11-C11	2.00	1.47	1.42
20	N	607	PGV	O04-C19	-2.00	1.16	1.22

All (624) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	309	CHD	C23-C22-C20	-10.67	95.03	114.52
27	E	201	PSC	C03-C02-C01	-9.39	89.58	111.79
14	N	601[A]	HEA	C3C-C4C-NC	9.10	115.85	110.25
14	N	601[B]	HEA	C3C-C4C-NC	9.10	115.85	110.25
25	G	101	CDL	OA6-CA5-C11	8.69	130.24	111.50
23	W	101	CHD	C13-C17-C20	8.16	129.24	119.50
19	O	301	TGL	OG2-CB1-CB2	7.52	127.70	111.50
19	B	301	TGL	OG2-CB1-CB2	7.15	126.91	111.50
14	N	601[A]	HEA	C13-C12-C11	-7.03	103.78	114.35
27	O	304	PSC	O01-C1-C2	7.00	126.58	111.50
14	N	602[C]	HEA	CHD-C1D-ND	6.84	132.81	124.37
14	N	601[A]	HEA	C4C-NC-C1C	-6.76	98.73	105.35
14	N	601[B]	HEA	C4C-NC-C1C	-6.76	98.73	105.35
14	N	602[A]	HEA	CHA-C1A-NA	6.68	131.66	124.44
20	C	307	PGV	O03-C19-C20	6.65	132.79	111.91
27	O	304	PSC	C03-C02-C01	-6.58	96.23	111.79
20	P	307	PGV	O03-C19-C20	6.39	131.95	111.91
23	J	102	CHD	C16-C17-C20	6.34	121.96	112.15
19	A	607	TGL	OG2-CB1-CB2	6.25	124.97	111.50
20	Q	201	PGV	C02-O01-C1	-6.23	102.46	117.79
23	C	309	CHD	C21-C20-C17	6.22	122.44	112.92
23	J	102	CHD	C17-C13-C12	-6.17	112.03	117.67
23	J	102	CHD	C11-C9-C10	-6.15	107.39	113.73
27	E	201	PSC	O01-C1-C2	6.06	124.56	111.50
23	J	102	CHD	C19-C10-C9	-5.97	102.96	111.18
14	N	601[A]	HEA	C2A-C1A-NA	5.86	116.03	110.32
14	N	601[B]	HEA	C2A-C1A-NA	5.86	116.03	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	102	CDL	OA6-CA5-C11	5.83	124.06	111.50
14	A	601[A]	HEA	C13-C12-C11	-5.76	105.70	114.35
20	C	307	PGV	O01-C1-C2	5.73	123.85	111.50
14	A	601[A]	HEA	C2D-C1D-ND	5.62	116.50	109.84
14	A	601[B]	HEA	C2D-C1D-ND	5.62	116.50	109.84
26	G	105	DMU	C6-O5-C4	5.61	119.35	113.13
14	N	601[A]	HEA	C3A-C2A-C1A	-5.58	101.75	107.08
14	N	601[B]	HEA	C3A-C2A-C1A	-5.58	101.75	107.08
14	A	601[A]	HEA	C3C-C4C-NC	5.56	113.67	110.25
14	A	601[B]	HEA	C3C-C4C-NC	5.56	113.67	110.25
14	N	602[A]	HEA	CHB-C1B-NB	5.51	130.40	124.42
25	P	308	CDL	OB8-CB7-C71	5.48	129.11	111.91
19	A	607	TGL	CG2-OG2-CB1	5.44	131.18	117.79
14	A	602[C]	HEA	CHB-C4A-NA	5.42	130.30	124.44
26	X	101	DMU	O16-C6-C1	5.40	116.74	108.30
14	A	602[A]	HEA	C3C-C4C-NC	5.39	113.57	110.25
25	C	308	CDL	OB2-PB2-OB5	-5.37	92.43	106.73
14	A	602[C]	HEA	C13-C12-C11	-5.35	106.32	114.35
19	A	607	TGL	OG3-CC1-CC2	5.25	128.37	111.91
24	P	305	PEK	O03-C21-C22	5.22	128.31	111.91
14	A	602[C]	HEA	C17-C18-C19	-5.17	115.21	127.66
26	K	102	DMU	O16-C6-C1	5.06	116.20	108.30
20	A	608	PGV	C3-C2-C1	5.05	131.99	113.62
23	P	309	CHD	C15-C14-C13	5.03	108.48	103.55
23	P	309	CHD	C19-C10-C9	-4.98	104.31	111.18
23	W	101	CHD	C17-C13-C14	-4.88	95.17	100.09
14	A	601[B]	HEA	C17-C18-C19	-4.81	116.07	127.66
24	P	305	PEK	O01-C1-C2	4.72	121.68	111.50
23	C	301	CHD	C18-C13-C12	4.71	113.86	109.07
26	P	315	DMU	O7-C10-C5	4.69	120.27	108.10
24	T	101	PEK	O01-C1-C2	4.69	121.62	111.50
23	J	102	CHD	C13-C17-C20	-4.68	113.91	119.50
26	P	316	DMU	O5-C4-C3	4.64	118.13	109.69
14	N	602[C]	HEA	C4C-CHD-C1D	-4.64	115.33	126.34
23	C	309	CHD	C13-C17-C20	-4.64	113.96	119.50
14	A	601[A]	HEA	C2B-C1B-NB	4.62	115.42	109.88
14	A	601[B]	HEA	C2B-C1B-NB	4.62	115.42	109.88
24	T	101	PEK	O03-C01-C02	4.60	121.83	108.43
26	P	316	DMU	O16-C6-C1	4.59	115.47	108.30
14	A	602[C]	HEA	C3C-C2C-C1C	-4.59	101.62	107.16
27	O	304	PSC	C21-C20-C19	-4.58	96.97	113.62
25	P	308	CDL	OA8-CA6-CA4	4.57	121.74	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	101	DMU	C22-C19-C18	-4.50	93.54	113.49
14	N	602[A]	HEA	C1A-CHA-C4D	-4.48	116.39	126.06
23	C	309	CHD	C15-C14-C13	4.45	107.92	103.55
26	P	315	DMU	C6-C1-C2	4.42	119.21	110.00
14	N	602[A]	HEA	C4A-CHB-C1B	-4.42	116.52	126.06
14	N	602[A]	HEA	C3C-C4C-NC	4.40	112.96	110.25
26	C	311	DMU	O5-C6-C1	4.39	119.63	110.35
23	W	101	CHD	C1-C2-C3	4.34	116.04	110.47
14	N	602[C]	HEA	C1A-CHA-C4D	-4.34	116.70	126.06
14	N	602[A]	HEA	CHA-C4D-ND	4.33	129.12	124.42
14	A	602[A]	HEA	C17-C18-C19	4.31	138.04	127.66
23	W	101	CHD	C18-C13-C14	-4.30	104.48	111.21
24	P	305	PEK	C01-O03-C21	4.27	132.95	117.12
23	C	301	CHD	C6-C7-C8	-4.26	106.93	111.48
19	B	301	TGL	CG3-CG2-CG1	-4.26	101.71	111.79
24	C	304	PEK	O03-C21-C22	4.25	125.23	111.91
14	A	602[A]	HEA	C21-C20-C19	4.24	126.94	112.98
14	A	602[C]	HEA	C21-C20-C19	4.24	126.94	112.98
14	N	602[A]	HEA	CHD-C1D-ND	4.22	129.58	124.37
14	A	602[A]	HEA	C13-C14-C15	-4.21	117.51	127.66
23	W	101	CHD	C17-C13-C12	4.21	121.51	117.67
14	A	601[A]	HEA	C3C-C2C-C1C	4.20	112.23	107.16
14	A	601[B]	HEA	C3C-C2C-C1C	4.20	112.23	107.16
14	N	602[A]	HEA	CHB-C1B-C2B	-4.19	118.43	124.98
14	A	602[C]	HEA	C4C-CHD-C1D	-4.18	116.42	126.34
23	W	101	CHD	C6-C5-C4	-4.17	106.39	111.19
20	P	307	PGV	O01-C1-C2	4.16	120.47	111.50
23	P	309	CHD	C16-C17-C13	4.16	107.63	103.55
20	N	607	PGV	O01-C1-O02	-4.15	113.67	123.70
14	A	602[C]	HEA	OMA-CMA-C3A	-4.13	116.35	125.69
26	C	311	DMU	C18-O16-C6	-4.10	107.03	113.84
23	B	303	CHD	C17-C13-C14	4.07	104.20	100.09
14	A	602[A]	HEA	C27-C19-C20	4.06	122.11	115.27
14	A	602[C]	HEA	C27-C19-C20	4.06	122.11	115.27
14	A	601[A]	HEA	C1D-C2D-C3D	-4.06	102.69	106.96
14	A	601[B]	HEA	C1D-C2D-C3D	-4.06	102.69	106.96
24	P	305	PEK	O03-C21-O04	-4.06	113.36	123.59
14	N	601[B]	HEA	C17-C18-C19	-4.04	117.94	127.66
25	G	101	CDL	CB6-OB8-CB7	4.01	131.99	117.12
23	J	102	CHD	C15-C14-C8	4.01	123.94	118.33
25	P	308	CDL	OA8-CA7-C31	4.00	124.46	111.91
14	N	602[C]	HEA	CMD-C2D-C1D	-3.99	118.96	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	O	302	TGL	OG1-CA1-CA2	3.98	124.38	111.91
24	C	304	PEK	C01-O03-C21	3.97	129.76	116.92
19	A	607	TGL	OG1-CA1-CA2	3.95	124.29	111.91
25	Y	101	CDL	OA8-CA7-OA9	-3.91	113.73	123.59
23	G	102	CHD	C17-C13-C14	3.89	104.02	100.09
26	C	311	DMU	C6-C1-C2	3.89	118.09	110.00
26	G	105	DMU	O16-C6-C1	3.88	114.36	108.30
20	C	307	PGV	O03-C19-O04	-3.86	113.85	123.59
25	G	101	CDL	OA6-CA5-OA7	-3.85	114.39	123.70
14	N	601[B]	HEA	C27-C19-C20	3.84	121.73	115.27
26	X	101	DMU	C2-C3-C4	3.84	117.09	110.24
25	C	308	CDL	OA8-CA6-CA4	3.83	119.57	108.43
24	C	304	PEK	O03-C21-O04	-3.83	113.94	123.59
24	T	101	PEK	C03-C02-C01	3.83	120.84	111.79
23	C	309	CHD	C19-C10-C9	-3.82	105.92	111.18
14	A	602[A]	HEA	CHA-C4D-ND	3.82	128.57	124.42
14	N	601[A]	HEA	C2C-C1C-NC	3.81	115.89	110.08
14	N	601[B]	HEA	C2C-C1C-NC	3.81	115.89	110.08
26	K	101	DMU	C18-O16-C6	3.81	120.16	113.84
23	P	301	CHD	C11-C9-C10	-3.79	109.82	113.73
14	A	602[C]	HEA	CHA-C4D-C3D	-3.78	119.28	124.84
26	G	105	DMU	O5-C4-C57	3.77	112.88	106.83
23	B	303	CHD	C5-C4-C3	-3.75	107.25	112.76
23	J	102	CHD	C9-C8-C7	-3.75	107.39	111.88
14	A	602[A]	HEA	CHA-C1A-NA	3.75	128.49	124.44
23	W	101	CHD	C9-C11-C12	-3.74	109.37	114.30
14	N	602[C]	HEA	CHB-C4A-NA	3.73	128.48	124.44
26	P	316	DMU	C6-O5-C4	3.73	121.01	113.69
14	N	602[A]	HEA	CHA-C4D-C3D	-3.72	119.37	124.84
26	K	102	DMU	C2-C3-C4	3.72	116.88	110.24
20	C	307	PGV	C21-C20-C19	-3.72	100.11	113.62
23	B	303	CHD	C15-C14-C13	-3.71	99.92	103.55
19	B	301	TGL	OG1-CA1-CA2	3.71	123.54	111.91
27	O	304	PSC	O01-C1-O02	-3.70	114.75	123.70
23	B	303	CHD	C19-C10-C1	-3.68	102.33	108.26
26	L	101	DMU	C18-O16-C6	3.68	119.94	113.84
26	P	316	DMU	O49-C1-C2	3.65	118.78	110.35
20	Q	201	PGV	O01-C1-C2	3.63	119.33	111.50
26	P	315	DMU	C10-C5-C7	3.63	117.56	110.00
26	X	101	DMU	C3-C2-C1	3.63	117.15	110.82
23	J	102	CHD	C21-C20-C17	-3.61	107.39	112.92
14	A	602[A]	HEA	C4A-CHB-C1B	-3.60	118.28	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	102	CHD	C22-C20-C17	3.59	117.71	110.28
14	A	602[C]	HEA	CAD-C3D-C2D	3.59	134.57	127.88
20	A	608	PGV	P-O11-C03	3.59	128.19	118.30
26	P	315	DMU	C11-C9-C8	3.59	121.41	113.00
25	C	308	CDL	C52-C51-CB5	-3.59	100.57	113.62
26	X	101	DMU	C18-O16-C6	3.58	119.78	113.84
25	T	102	CDL	CB2-C1-CA2	-3.58	102.26	112.79
14	N	601[A]	HEA	C13-C14-C15	-3.57	119.05	127.66
24	P	303	PEK	O01-C1-C2	3.57	125.51	114.03
23	C	309	CHD	C16-C17-C20	3.57	117.67	112.15
24	T	101	PEK	C02-O01-C1	-3.57	109.01	117.79
14	A	602[A]	HEA	C4C-NC-C1C	-3.56	101.86	105.35
19	B	301	TGL	OG2-CG2-CG3	3.55	121.27	108.40
14	N	602[C]	HEA	CHC-C1C-NC	3.55	130.38	123.85
19	D	201	TGL	OG3-CC1-OC1	-3.55	114.63	123.59
23	J	102	CHD	C4-C3-C2	-3.55	106.32	110.55
26	X	103	DMU	C6-O5-C4	3.54	120.64	113.69
25	C	308	CDL	C78-C77-C76	-3.53	96.48	114.42
14	N	601[A]	HEA	CHC-C1C-NC	-3.52	117.36	123.85
14	N	601[B]	HEA	CHC-C1C-NC	-3.52	117.36	123.85
26	J	101	DMU	C18-O16-C6	3.52	119.67	113.84
20	P	307	PGV	O01-C1-O02	-3.52	115.20	123.70
25	Y	101	CDL	OB8-CB7-C71	3.51	122.93	111.91
20	Q	201	PGV	O03-C19-C20	3.49	122.87	111.91
14	N	601[B]	HEA	C13-C12-C11	-3.48	109.11	114.35
23	W	101	CHD	C18-C13-C17	3.47	116.65	111.21
14	N	602[C]	HEA	CHD-C1D-C2D	-3.46	117.12	126.73
23	P	309	CHD	C22-C23-C24	-3.45	103.35	112.51
19	O	302	TGL	OG1-CA1-OA1	-3.44	114.92	123.59
25	C	308	CDL	OA8-CA7-C31	3.43	122.67	111.91
14	N	602[C]	HEA	CHA-C4D-C3D	-3.43	119.80	124.84
25	P	308	CDL	OB8-CB7-OB9	-3.41	114.99	123.59
14	N	602[C]	HEA	C13-C12-C11	-3.41	109.23	114.35
23	B	303	CHD	C2-C1-C10	-3.39	106.96	112.78
27	E	201	PSC	C02-O01-C1	3.39	126.14	117.79
20	P	306	PGV	O01-C1-O02	-3.38	115.54	123.70
14	N	602[A]	HEA	C4C-CHD-C1D	-3.38	118.33	126.34
14	A	602[C]	HEA	C26-C15-C14	-3.37	115.02	123.68
23	P	301	CHD	C22-C20-C17	-3.36	103.35	110.28
14	N	601[A]	HEA	CAA-CBA-CGA	-3.36	106.38	113.60
14	N	601[B]	HEA	CAA-CBA-CGA	-3.36	106.38	113.60
19	A	607	TGL	CB9-CB8-CB7	-3.35	97.40	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	101	DMU	O61-C57-C4	3.34	122.75	111.29
14	N	602[C]	HEA	CHC-C1C-C2C	-3.34	117.81	127.24
23	G	102	CHD	C6-C5-C4	-3.34	107.35	111.19
14	N	602[C]	HEA	CHA-C1A-NA	3.33	128.05	124.44
23	P	309	CHD	O25-C24-C23	-3.32	112.40	123.08
26	P	315	DMU	O5-C6-C1	3.32	117.38	110.35
19	A	607	TGL	OG3-CC1-OC1	-3.32	115.21	123.59
26	P	315	DMU	O2-C8-C9	3.32	117.53	109.30
14	A	602[A]	HEA	C1D-C2D-C3D	-3.31	103.48	106.96
25	P	308	CDL	OA6-CA5-C11	3.31	118.63	111.50
14	N	602[A]	HEA	CMB-C2B-C3B	-3.31	124.04	130.34
14	A	602[A]	HEA	C1A-CHA-C4D	-3.30	118.93	126.06
23	P	301	CHD	C19-C10-C1	-3.30	102.94	108.26
26	P	316	DMU	C2-C3-C4	3.30	116.12	110.24
23	W	101	CHD	C9-C10-C5	3.29	113.21	108.58
26	G	105	DMU	O5-C6-C1	3.28	117.30	110.35
19	A	607	TGL	CA4-CA3-CA2	-3.28	101.39	113.19
26	P	316	DMU	C3-C2-C1	-3.28	105.09	110.82
14	N	602[A]	HEA	C4C-NC-C1C	-3.28	102.14	105.35
14	A	602[A]	HEA	C20-C19-C18	-3.28	114.48	121.12
14	A	602[C]	HEA	C20-C19-C18	-3.28	114.48	121.12
26	P	316	DMU	O55-C2-C1	3.27	117.90	110.35
23	J	102	CHD	C1-C2-C3	3.26	114.65	110.47
23	J	102	CHD	C18-C13-C12	3.26	112.39	109.07
14	N	602[A]	HEA	CHC-C1C-C2C	-3.25	118.06	127.24
25	T	102	CDL	CB6-CB4-CB3	-3.24	102.92	113.70
23	J	102	CHD	O3-C3-C4	3.23	116.28	109.85
14	A	602[C]	HEA	C3B-C4B-NB	3.22	113.66	109.84
26	K	103	DMU	C2-C3-C4	3.21	117.88	110.40
14	N	602[A]	HEA	CHB-C4A-NA	3.20	127.90	124.44
25	P	308	CDL	CA6-OA8-CA7	3.19	128.94	117.12
26	P	312	DMU	C6-O5-C4	3.19	119.95	113.69
14	N	602[A]	HEA	C1C-CHC-C4B	-3.18	118.80	126.34
19	O	301	TGL	OG1-CA1-CA2	3.17	121.87	111.91
23	G	102	CHD	C15-C14-C13	-3.15	100.46	103.55
19	A	607	TGL	C12-C11-C10	-3.15	98.42	114.42
25	T	102	CDL	CB6-OB8-CB7	3.14	127.06	116.92
23	P	309	CHD	C18-C13-C12	-3.14	105.87	109.07
26	L	101	DMU	O5-C4-C57	3.13	114.23	106.44
26	P	312	DMU	O55-C2-C1	-3.13	103.11	110.35
25	P	308	CDL	OB6-CB5-C51	3.12	121.70	111.91
25	Y	101	CDL	OB6-CB5-C51	3.12	118.23	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	309	CHD	C6-C5-C4	-3.11	107.61	111.19
14	N	601[A]	HEA	C4A-C3A-C2A	3.10	109.30	106.75
14	N	601[B]	HEA	C4A-C3A-C2A	3.10	109.30	106.75
14	N	602[C]	HEA	CHA-C4D-ND	3.10	127.78	124.42
14	A	601[A]	HEA	C13-C14-C15	-3.10	120.20	127.66
26	G	105	DMU	C18-O16-C6	-3.09	108.71	113.84
26	P	310	DMU	O3-C5-C7	-3.09	103.20	110.35
26	P	315	DMU	O4-C7-C5	3.09	117.49	110.35
23	B	303	CHD	C6-C5-C4	-3.08	107.64	111.19
14	N	601[A]	HEA	O2A-CGA-CBA	3.07	123.89	114.03
14	N	601[B]	HEA	O2A-CGA-CBA	3.07	123.89	114.03
14	A	602[A]	HEA	CHB-C1B-C2B	-3.07	120.19	124.98
20	P	307	PGV	O03-C19-O04	-3.05	115.89	123.59
14	N	602[C]	HEA	C3C-C4C-NC	-3.05	108.37	110.25
14	A	602[C]	HEA	CHB-C4A-C3A	-3.04	120.06	125.26
27	O	304	PSC	P-O11-C03	3.04	139.49	121.68
27	O	304	PSC	C28-C27-C26	-3.03	99.02	114.42
20	A	608	PGV	O03-C19-C20	3.03	121.41	111.91
20	P	307	PGV	O04-C19-C20	-3.03	111.92	123.73
23	J	102	CHD	C14-C13-C12	3.02	110.22	107.40
26	X	103	DMU	C3-C2-C1	3.02	116.09	110.82
26	P	312	DMU	C22-C19-C18	-3.02	100.12	113.49
14	N	602[C]	HEA	O2A-CGA-CBA	3.01	123.71	114.03
26	G	105	DMU	C3-C2-C1	3.01	115.06	110.69
19	O	301	TGL	CG3-CG2-CG1	-3.00	104.69	111.79
14	A	602[A]	HEA	C2D-C1D-ND	2.99	113.38	109.84
23	B	303	CHD	C4-C5-C10	-2.99	109.48	112.66
25	C	308	CDL	C53-C52-C51	-2.99	102.46	113.19
26	C	311	DMU	O1-C9-C11	2.97	113.82	106.44
25	C	308	CDL	OB4-PB2-OB3	2.96	122.27	110.68
26	Z	101	DMU	O61-C57-C4	-2.95	101.16	111.29
27	O	304	PSC	C02-O01-C1	2.95	125.05	117.79
19	B	301	TGL	CC3-CC2-CC1	-2.95	102.91	113.62
14	A	602[C]	HEA	C16-C15-C14	2.94	127.08	121.12
20	A	608	PGV	C01-O03-C19	2.94	128.02	117.12
14	N	602[C]	HEA	CAD-C3D-C2D	2.94	133.35	127.88
26	X	102	DMU	O5-C4-C57	2.93	113.73	106.44
19	A	607	TGL	C25-C24-C23	-2.93	99.54	114.42
23	J	102	CHD	C16-C17-C13	2.93	106.43	103.55
23	J	102	CHD	C10-C9-C8	-2.93	108.67	111.82
25	C	308	CDL	OA8-CA7-OA9	-2.92	116.21	123.59
26	K	101	DMU	O5-C4-C3	2.92	114.99	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	101	DMU	C6-O5-C4	2.91	119.40	113.69
26	M	101	DMU	O5-C6-O16	-2.91	103.09	109.97
14	N	602[A]	HEA	CHA-C1A-C2A	-2.90	120.24	124.94
25	C	308	CDL	PB2-OB5-CB3	2.90	126.28	118.30
14	A	602[C]	HEA	CHC-C1C-C2C	-2.89	119.07	127.24
14	A	602[A]	HEA	O1D-CGD-CBD	-2.89	113.79	123.08
26	C	311	DMU	C6-O5-C4	-2.88	108.03	113.69
23	W	101	CHD	C19-C10-C9	-2.88	107.22	111.18
26	K	101	DMU	C6-O5-C4	2.88	119.33	113.69
23	G	102	CHD	C4-C5-C10	-2.88	109.60	112.66
14	A	602[C]	HEA	CHD-C1D-ND	2.87	127.92	124.37
25	Y	101	CDL	OA8-CA7-C31	2.87	120.92	111.91
25	G	101	CDL	C39-C38-C37	2.86	128.93	114.42
14	A	602[C]	HEA	C3D-C4D-ND	2.85	113.12	110.36
26	X	102	DMU	O16-C6-C1	2.85	112.75	108.30
14	N	602[A]	HEA	CAA-C2A-C1A	2.84	130.25	124.89
23	C	301	CHD	C22-C23-C24	-2.83	104.99	112.51
25	Y	101	CDL	OA6-CA4-CA3	2.83	118.66	108.40
14	N	602[A]	HEA	CAD-C3D-C2D	2.83	133.15	127.88
23	J	102	CHD	C14-C8-C9	2.83	113.59	109.71
14	A	602[C]	HEA	CMB-C2B-C3B	-2.82	124.97	130.34
14	A	601[B]	HEA	C26-C15-C16	2.82	120.01	115.27
26	K	102	DMU	C3-C2-C1	2.82	115.74	110.82
23	B	303	CHD	C1-C10-C5	2.82	111.93	107.77
14	N	602[A]	HEA	C13-C12-C11	-2.82	110.12	114.35
14	A	602[A]	HEA	CMD-C2D-C1D	2.81	129.32	125.04
23	C	309	CHD	C11-C9-C10	-2.81	110.83	113.73
26	P	315	DMU	O1-C9-C8	2.81	114.79	109.69
14	A	602[C]	HEA	CHD-C4C-NC	2.81	129.01	123.85
26	C	311	DMU	O7-C10-C5	2.80	115.35	108.10
19	O	301	TGL	OG2-CG2-CG3	2.80	118.53	108.40
23	C	309	CHD	C9-C11-C12	-2.79	110.61	114.30
14	N	601[A]	HEA	O1D-CGD-CBD	-2.79	114.11	123.08
14	N	601[B]	HEA	O1D-CGD-CBD	-2.79	114.11	123.08
19	O	302	TGL	CG2-OG2-CB1	-2.79	110.92	117.79
26	X	103	DMU	O5-C6-C1	2.78	116.24	110.35
14	A	602[C]	HEA	CHA-C4D-ND	2.78	127.44	124.42
26	X	103	DMU	C18-O16-C6	-2.78	109.23	113.84
14	N	602[A]	HEA	O2D-CGD-O1D	2.78	130.22	123.30
25	G	101	CDL	OA8-CA6-CA4	2.77	116.51	108.43
26	P	310	DMU	C7-C8-C9	2.77	115.17	110.24
26	P	311	DMU	O3-C5-C10	2.77	116.77	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	101	CHD	C4-C5-C10	2.76	115.59	112.66
26	P	310	DMU	O16-C6-C1	-2.76	103.99	108.30
14	N	602[A]	HEA	C2C-C1C-NC	2.76	114.28	110.08
19	A	607	TGL	OG2-CG2-CG1	2.76	118.39	108.40
23	C	309	CHD	C17-C13-C12	-2.75	115.16	117.67
14	N	602[C]	HEA	C13-C14-C15	-2.75	121.04	127.66
23	P	309	CHD	C4-C3-C2	-2.75	107.27	110.55
14	A	602[A]	HEA	CHC-C4B-NB	2.74	127.75	124.37
14	N	602[A]	HEA	CAD-CBD-CGD	-2.74	107.71	113.60
25	C	308	CDL	C81-C80-C79	-2.73	100.59	114.42
24	T	101	PEK	O03-C21-C22	2.71	120.42	111.91
20	P	307	PGV	C21-C20-C19	-2.71	103.76	113.62
23	P	309	CHD	C5-C4-C3	-2.71	108.78	112.76
14	N	601[A]	HEA	C3B-C4B-NB	2.70	113.04	109.84
14	N	601[B]	HEA	C3B-C4B-NB	2.70	113.04	109.84
14	A	602[C]	HEA	C2C-C1C-NC	2.70	114.20	110.08
14	A	602[A]	HEA	CHD-C1D-C2D	-2.70	119.22	126.73
26	K	101	DMU	C2-C3-C4	2.70	115.06	110.24
23	B	303	CHD	O3-C3-C4	-2.70	104.47	109.85
23	W	101	CHD	O12-C12-C11	-2.70	103.63	109.12
14	N	602[A]	HEA	CMB-C2B-C1B	2.69	129.14	125.04
19	B	301	TGL	OG1-CA1-OA1	-2.69	116.80	123.59
14	A	602[A]	HEA	CAD-C3D-C4D	-2.69	119.96	124.66
27	O	304	PSC	C24-C23-C22	-2.69	100.79	114.42
14	A	602[A]	HEA	C4C-CHD-C1D	-2.68	119.98	126.34
14	A	602[A]	HEA	CHA-C4D-C3D	-2.68	120.90	124.84
20	C	307	PGV	O04-C19-C20	-2.67	113.30	123.73
24	C	304	PEK	O01-C1-C2	2.67	120.28	111.91
23	C	309	CHD	C4-C5-C10	2.67	115.49	112.66
25	T	102	CDL	OB5-CB3-CB4	2.67	117.88	108.99
23	C	301	CHD	C23-C22-C20	-2.66	109.66	114.52
20	C	307	PGV	O03-C01-C02	2.65	116.16	108.43
19	A	607	TGL	OG2-CB1-OB1	-2.64	117.32	123.70
26	P	315	DMU	O7-C10-O1	-2.64	103.29	110.67
23	C	301	CHD	C1-C2-C3	-2.63	107.10	110.47
14	A	601[A]	HEA	C21-C22-C23	-2.62	118.78	127.75
14	N	602[A]	HEA	CAD-C3D-C4D	-2.62	120.08	124.66
19	D	201	TGL	CG3-CG2-CG1	-2.62	105.59	111.79
26	K	102	DMU	O5-C4-C3	2.62	114.45	109.69
26	C	311	DMU	O61-C57-C4	-2.62	102.31	111.29
14	N	602[A]	HEA	C26-C15-C16	2.62	119.67	115.27
20	Q	201	PGV	O03-C19-O04	-2.61	117.00	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	O	301	TGL	OG2-CB1-OB1	-2.60	117.41	123.70
23	C	301	CHD	C17-C13-C12	-2.60	115.30	117.67
26	J	101	DMU	O5-C4-C57	2.59	112.89	106.44
24	P	303	PEK	O01-C1-O02	-2.59	116.84	123.30
20	A	608	PGV	C4-C3-C2	-2.59	103.87	113.19
14	A	602[A]	HEA	CAA-C2A-C1A	2.59	129.78	124.89
26	K	102	DMU	O55-C2-C1	2.59	116.33	110.35
23	J	102	CHD	C4-C5-C10	2.59	115.40	112.66
14	A	602[C]	HEA	C4A-CHB-C1B	-2.57	120.51	126.06
23	G	102	CHD	O3-C3-C4	-2.57	104.74	109.85
23	P	309	CHD	C13-C17-C20	-2.56	116.44	119.50
19	A	607	TGL	C26-C25-C24	-2.56	101.44	114.42
25	Y	101	CDL	C78-C77-C76	-2.56	101.44	114.42
23	P	301	CHD	C21-C20-C22	-2.56	106.36	110.36
23	J	102	CHD	C11-C9-C8	2.56	114.62	110.88
24	C	304	PEK	C24-C23-C22	2.55	122.37	113.19
25	T	102	CDL	PB2-OB5-CB3	-2.55	109.02	121.59
23	W	101	CHD	C22-C20-C17	2.55	115.56	110.28
14	N	601[A]	HEA	CHA-C1A-NA	-2.55	121.68	124.44
14	N	601[B]	HEA	CHA-C1A-NA	-2.55	121.68	124.44
23	B	303	CHD	O12-C12-C13	-2.55	106.73	111.03
19	D	201	TGL	OG3-CC1-CC2	2.54	118.05	111.38
23	C	301	CHD	C13-C17-C20	2.54	122.53	119.50
26	J	101	DMU	O49-C1-C6	2.54	116.22	110.05
27	O	304	PSC	C14-C13-C12	-2.53	105.29	124.73
23	P	301	CHD	C22-C23-C24	-2.53	105.80	112.51
26	X	101	DMU	O5-C4-C3	2.52	114.28	109.69
14	A	602[C]	HEA	CHD-C1D-C2D	-2.52	119.73	126.73
24	C	303	PEK	C14-C13-C12	2.52	124.43	112.02
14	N	601[A]	HEA	O2D-CGD-CBD	2.51	122.08	114.03
14	N	601[B]	HEA	O2D-CGD-CBD	2.51	122.08	114.03
20	N	607	PGV	C9-C10-C11	-2.50	98.09	112.43
25	C	308	CDL	CA4-OA6-CA5	-2.50	111.65	117.79
19	B	301	TGL	OB1-CB1-CB2	-2.49	114.00	123.73
23	B	303	CHD	C19-C10-C5	-2.49	106.14	110.36
26	G	105	DMU	C22-C19-C18	-2.49	102.46	113.49
26	P	311	DMU	O7-C10-C5	2.49	114.55	108.10
27	E	201	PSC	C08-N-C07	-2.48	102.59	108.97
14	N	602[C]	HEA	CHB-C4A-C3A	-2.48	121.02	125.26
14	N	601[A]	HEA	C3C-C2C-C1C	-2.48	104.17	107.16
14	N	601[B]	HEA	C3C-C2C-C1C	-2.48	104.17	107.16
26	M	101	DMU	C22-C19-C18	-2.48	102.51	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	607	TGL	OG3-CG3-CG2	2.47	115.64	108.43
14	A	602[C]	HEA	C1A-CHA-C4D	-2.47	120.72	126.06
27	E	201	PSC	O01-C1-O02	-2.47	117.73	123.70
26	X	101	DMU	O5-C6-C1	-2.47	105.12	110.35
14	N	601[A]	HEA	C4A-NA-C1A	-2.47	102.93	105.35
14	N	601[B]	HEA	C4A-NA-C1A	-2.47	102.93	105.35
19	A	607	TGL	CG3-CG2-CG1	-2.46	105.97	111.79
19	D	201	TGL	OG1-CG1-CG2	-2.46	101.27	108.43
19	A	607	TGL	CB6-CB5-CB4	-2.46	101.94	114.42
26	P	310	DMU	O1-C10-C5	2.46	115.55	110.35
23	J	102	CHD	C23-C22-C20	-2.45	110.04	114.52
23	G	102	CHD	C19-C10-C1	-2.45	104.32	108.26
26	X	102	DMU	O7-C3-C2	2.44	116.00	110.35
27	E	201	PSC	C07-N-C06	2.44	115.25	108.97
26	X	102	DMU	C28-C25-C22	-2.44	102.03	114.42
27	O	304	PSC	C25-C24-C23	-2.44	102.04	114.42
25	C	308	CDL	C43-C42-C41	2.44	126.80	114.42
20	P	306	PGV	C03-C02-C01	-2.43	106.03	111.79
14	A	602[A]	HEA	CHB-C1B-NB	2.43	127.06	124.42
26	K	101	DMU	C57-C4-C3	-2.43	107.31	113.00
26	M	101	DMU	C18-O16-C6	-2.43	109.81	113.84
26	C	311	DMU	O5-C4-C3	2.42	114.86	109.75
14	A	602[A]	HEA	CHD-C1D-ND	2.42	127.36	124.37
20	A	608	PGV	O14-P-O11	2.42	113.17	106.73
23	P	309	CHD	C14-C8-C9	-2.41	106.40	109.71
14	A	601[A]	HEA	CHA-C4D-ND	2.41	127.04	124.42
14	A	601[B]	HEA	CHA-C4D-ND	2.41	127.04	124.42
26	P	311	DMU	O16-C6-C1	2.41	112.06	108.30
25	Y	101	CDL	OA6-CA5-C11	2.40	116.67	111.50
20	N	607	PGV	C22-C21-C20	2.39	121.79	113.19
19	B	301	TGL	CB3-CB2-CB1	-2.39	104.92	113.62
14	A	601[A]	HEA	C1B-C2B-C3B	-2.39	103.94	106.80
14	A	601[B]	HEA	C1B-C2B-C3B	-2.39	103.94	106.80
14	N	602[C]	HEA	C1C-CHC-C4B	-2.39	120.68	126.34
14	N	602[C]	HEA	CHB-C1B-NB	2.39	127.01	124.42
14	N	602[C]	HEA	CHA-C1A-C2A	-2.38	121.07	124.94
14	A	601[A]	HEA	CHA-C4D-C3D	-2.38	121.34	124.84
14	A	601[B]	HEA	CHA-C4D-C3D	-2.38	121.34	124.84
14	A	602[C]	HEA	O1A-CGA-CBA	-2.38	115.43	123.08
14	A	602[A]	HEA	O1A-CGA-CBA	-2.38	115.44	123.08
19	D	201	TGL	OG1-CA1-CA2	2.38	119.37	111.91
25	T	102	CDL	OB4-PB2-OB3	2.38	123.99	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	102	CHD	C13-C14-C8	-2.38	111.70	114.74
23	W	101	CHD	C14-C13-C12	-2.37	105.20	107.40
23	C	309	CHD	C1-C2-C3	2.37	113.50	110.47
14	A	601[A]	HEA	CHA-C1A-NA	-2.37	121.88	124.44
14	A	601[B]	HEA	CHA-C1A-NA	-2.37	121.88	124.44
25	T	102	CDL	C15-C14-C13	-2.36	102.42	114.42
24	C	303	PEK	O11-P-O14	-2.36	99.83	109.07
25	T	102	CDL	C18-C17-C16	-2.36	102.45	114.42
26	X	101	DMU	O5-C4-C57	2.36	112.29	106.44
26	X	102	DMU	C2-C3-C4	2.36	114.44	110.24
14	N	602[C]	HEA	C3C-C2C-C1C	-2.35	104.32	107.16
25	G	101	CDL	C62-C61-C60	2.35	126.36	114.42
25	C	308	CDL	OA6-CA4-CA3	2.35	116.91	108.40
26	P	315	DMU	O7-C3-C4	-2.35	103.01	109.45
23	J	102	CHD	C5-C4-C3	-2.35	109.31	112.76
14	N	602[A]	HEA	CMD-C2D-C1D	2.34	128.61	125.04
26	M	101	DMU	O5-C6-C1	2.34	115.30	110.35
25	T	102	CDL	C85-C84-C83	2.33	126.27	114.42
14	A	602[A]	HEA	CHB-C4A-NA	2.33	126.96	124.44
26	J	101	DMU	O16-C6-C1	2.33	111.94	108.30
24	T	101	PEK	C3-C4-C5	-2.33	99.09	112.43
26	C	311	DMU	C10-O1-C9	2.32	118.25	113.69
26	K	102	DMU	C6-C1-C2	2.32	114.83	110.00
23	C	309	CHD	O7-C7-C8	2.32	114.61	109.43
23	P	301	CHD	C5-C6-C7	2.32	117.02	114.46
25	C	308	CDL	C76-C75-C74	-2.31	102.69	114.42
14	N	602[A]	HEA	CHC-C4B-NB	2.31	127.22	124.37
24	P	304	PEK	C11-C10-C9	-2.30	100.68	112.02
14	N	602[C]	HEA	CMD-C2D-C3D	2.30	132.37	126.12
14	A	602[C]	HEA	CAD-C3D-C4D	-2.30	120.64	124.66
14	N	601[A]	HEA	O2A-CGA-O1A	-2.30	117.58	123.30
14	N	601[B]	HEA	O2A-CGA-O1A	-2.30	117.58	123.30
14	N	602[A]	HEA	C2A-C1A-NA	-2.29	108.09	110.32
14	N	602[C]	HEA	OMA-CMA-C3A	-2.29	120.51	125.69
14	A	602[A]	HEA	O2A-CGA-CBA	2.29	121.37	114.03
25	P	308	CDL	OA9-CA7-C31	-2.28	114.83	123.73
14	A	601[A]	HEA	C1D-ND-C4D	-2.28	102.72	105.07
14	A	601[B]	HEA	C1D-ND-C4D	-2.28	102.72	105.07
20	C	307	PGV	C01-O03-C19	2.27	125.53	117.12
14	A	602[C]	HEA	C12-C13-C14	-2.27	106.24	112.23
19	O	301	TGL	OB1-CB1-CB2	-2.27	114.88	123.73
14	N	602[C]	HEA	C4A-CHB-C1B	-2.26	121.18	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	301	TGL	CG3-OG3-CC1	2.26	125.49	117.12
26	Z	101	DMU	C31-C28-C25	-2.26	102.96	114.42
20	Q	201	PGV	C01-O03-C19	2.26	125.47	117.12
20	Q	201	PGV	C5-C4-C3	-2.26	102.98	114.42
19	A	607	TGL	C20-CA9-CA8	-2.25	102.99	114.42
14	A	601[A]	HEA	O2D-CGD-O1D	2.25	128.91	123.30
14	A	601[B]	HEA	O2D-CGD-O1D	2.25	128.91	123.30
26	Z	101	DMU	O4-C7-C8	2.25	115.55	110.35
19	O	301	TGL	OG1-CA1-OA1	-2.25	117.92	123.59
14	A	601[A]	HEA	CHD-C1D-C2D	-2.24	120.50	126.73
14	A	601[B]	HEA	CHD-C1D-C2D	-2.24	120.50	126.73
14	N	601[A]	HEA	C4B-C3B-C2B	-2.24	103.58	107.41
14	N	601[B]	HEA	C4B-C3B-C2B	-2.24	103.58	107.41
23	W	101	CHD	C1-C10-C5	2.24	111.08	107.77
14	N	601[A]	HEA	CHA-C4D-ND	2.24	126.85	124.42
14	N	601[B]	HEA	CHA-C4D-ND	2.24	126.85	124.42
26	M	101	DMU	C6-C1-C2	-2.24	105.34	110.00
26	J	101	DMU	O1-C9-C11	2.24	112.00	106.44
20	Q	201	PGV	C8-C7-C6	-2.23	103.08	114.42
26	M	101	DMU	C31-C28-C25	-2.23	103.09	114.42
25	T	102	CDL	C17-C16-C15	-2.23	103.09	114.42
23	B	303	CHD	C22-C20-C17	2.23	114.89	110.28
20	N	607	PGV	C01-O03-C19	-2.23	108.86	117.12
23	B	303	CHD	C17-C13-C12	2.22	119.70	117.67
14	A	602[A]	HEA	C2B-C1B-NB	2.22	112.54	109.88
14	A	601[A]	HEA	C17-C18-C19	2.22	133.00	127.66
23	B	303	CHD	O12-C12-C11	2.22	113.64	109.12
26	C	311	DMU	O5-C6-O16	-2.21	104.73	109.97
23	C	301	CHD	C5-C4-C3	-2.21	109.51	112.76
24	T	101	PEK	P-O12-C04	2.21	132.47	121.59
24	C	303	PEK	C16-C15-C14	-2.21	107.78	124.73
23	W	101	CHD	O7-C7-C8	2.21	114.36	109.43
26	P	316	DMU	O49-C1-C6	2.21	115.41	110.05
26	P	315	DMU	C1-C2-C3	2.20	114.71	109.68
26	K	101	DMU	O5-C4-C57	2.20	111.91	106.44
26	X	103	DMU	O16-C6-C1	2.20	111.73	108.30
20	P	306	PGV	C27-C26-C25	-2.20	103.28	114.42
27	E	201	PSC	C25-C24-C23	-2.19	103.31	114.42
14	A	602[C]	HEA	C3C-C4C-NC	-2.19	108.90	110.25
23	B	303	CHD	C1-C10-C9	2.18	114.79	111.35
25	G	101	CDL	OA7-CA5-C11	-2.18	115.22	123.73
27	O	304	PSC	C08-N-C06	-2.18	103.36	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	316	DMU	O55-C2-C3	2.18	115.39	110.35
26	M	101	DMU	O2-C8-C9	-2.17	103.90	109.30
14	N	602[C]	HEA	CHD-C4C-NC	2.17	127.84	123.85
20	C	306	PGV	O01-C1-O02	-2.17	118.46	123.70
26	P	315	DMU	O3-C5-C7	-2.16	105.35	110.35
26	X	103	DMU	C2-C3-C4	2.16	114.10	110.24
26	K	101	DMU	O16-C6-C1	2.16	111.68	108.30
14	N	602[A]	HEA	O1A-CGA-CBA	-2.16	116.14	123.08
23	P	309	CHD	C22-C20-C17	-2.16	105.82	110.28
20	N	607	PGV	C30-C29-C28	2.16	125.38	114.42
25	C	308	CDL	OB5-PB2-OB3	2.16	112.52	106.47
19	A	607	TGL	C23-C22-C21	-2.15	103.49	114.42
19	O	302	TGL	OG2-CB1-CB2	2.15	116.14	111.50
14	A	602[C]	HEA	C13-C14-C15	-2.15	122.48	127.66
25	C	308	CDL	OA6-CA5-C11	2.15	116.13	111.50
23	C	301	CHD	C21-C20-C22	-2.14	107.00	110.36
26	P	310	DMU	O3-C5-C10	2.14	115.25	110.05
14	A	602[A]	HEA	CAA-CBA-CGA	-2.13	109.01	113.60
26	X	101	DMU	C6-O5-C4	2.13	117.88	113.69
24	P	304	PEK	O03-C21-C22	2.13	118.60	111.91
23	P	301	CHD	C9-C11-C12	-2.13	111.49	114.30
14	N	602[C]	HEA	O2A-CGA-O1A	-2.13	117.99	123.30
25	T	102	CDL	OB4-PB2-OB5	-2.13	97.87	107.75
14	N	602[C]	HEA	C3D-C4D-ND	2.13	112.42	110.36
14	A	602[C]	HEA	C2D-C1D-ND	2.12	112.35	109.84
14	N	602[A]	HEA	C3C-C2C-C1C	-2.12	104.60	107.16
24	C	303	PEK	C24-C23-C22	-2.12	105.57	113.19
14	N	602[C]	HEA	CMB-C2B-C3B	-2.11	126.31	130.34
14	N	601[B]	HEA	C27-C19-C18	-2.11	118.26	123.68
25	G	101	CDL	C61-C60-C59	-2.11	103.71	114.42
14	N	602[A]	HEA	C4A-NA-C1A	2.11	107.41	105.35
24	P	304	PEK	C7-C8-C9	-2.11	105.78	123.57
25	T	102	CDL	OA6-CA4-CA3	2.11	116.03	108.40
26	J	101	DMU	O49-C1-C2	-2.11	105.48	110.35
26	X	101	DMU	O7-C3-C2	2.11	115.22	110.35
14	A	601[A]	HEA	CHB-C1B-C2B	-2.11	121.69	124.98
14	A	601[B]	HEA	CHB-C1B-C2B	-2.11	121.69	124.98
26	X	103	DMU	C34-C31-C28	-2.10	103.78	114.42
20	Q	201	PGV	O01-C02-C03	2.10	116.00	108.40
26	P	311	DMU	C2-C3-C4	-2.09	106.12	110.93
25	P	308	CDL	CA4-OA6-CA5	2.09	122.94	117.79
21	B	305	EDO	O2-C2-C1	2.09	126.94	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601[A]	HEA	CHB-C4A-NA	2.09	126.70	124.44
14	N	601[B]	HEA	CHB-C4A-NA	2.09	126.70	124.44
14	N	602[C]	HEA	C4D-C3D-C2D	-2.09	103.86	106.90
24	P	303	PEK	C8-C7-C6	-2.08	101.76	112.02
25	C	308	CDL	OB8-CB6-CB4	-2.08	102.37	108.43
19	A	607	TGL	C22-C21-C20	-2.08	103.86	114.42
26	P	311	DMU	C10-O1-C9	-2.08	109.61	113.69
19	D	201	TGL	OG2-CG2-CG3	2.08	115.93	108.40
23	B	303	CHD	C21-C20-C17	-2.08	109.74	112.92
14	A	602[C]	HEA	CMC-C2C-C3C	2.07	131.59	126.59
26	P	312	DMU	O16-C18-C19	2.07	116.81	109.56
20	C	307	PGV	C26-C25-C24	-2.07	103.94	114.42
14	N	602[A]	HEA	CHC-C1C-NC	2.06	127.64	123.85
23	G	102	CHD	C13-C17-C20	-2.06	117.04	119.50
25	G	101	CDL	C85-C84-C83	2.05	124.84	114.42
26	M	101	DMU	O1-C9-C8	2.05	113.42	109.69
25	T	102	CDL	OA5-PA1-OA3	2.05	117.08	109.07
14	A	602[A]	HEA	C25-C23-C24	2.05	119.13	114.60
14	A	602[C]	HEA	C25-C23-C24	2.05	119.13	114.60
24	T	101	PEK	O01-C1-O02	-2.05	118.75	123.70
23	P	301	CHD	C6-C7-C8	-2.05	109.30	111.48
14	A	602[C]	HEA	O2A-CGA-CBA	2.05	120.60	114.03
26	M	101	DMU	O3-C5-C10	-2.05	105.08	110.05
14	A	602[C]	HEA	C4A-NA-C1A	2.04	107.35	105.35
25	G	101	CDL	C40-C39-C38	2.04	124.78	114.42
23	B	303	CHD	O7-C7-C6	2.03	114.99	109.94
26	C	311	DMU	O3-C5-C10	2.03	114.99	110.05
14	N	601[A]	HEA	CHD-C1D-ND	2.03	126.88	124.37
14	N	601[B]	HEA	CHD-C1D-ND	2.03	126.88	124.37
25	T	102	CDL	C83-C82-C81	2.03	124.74	114.42
25	Y	101	CDL	C52-C51-CB5	-2.03	106.23	113.62
20	C	306	PGV	O03-C19-O04	-2.03	118.47	123.59
26	P	311	DMU	C18-O16-C6	-2.03	110.48	113.84
23	W	101	CHD	C4-C3-C2	2.03	112.97	110.55
23	W	101	CHD	C15-C14-C13	2.03	105.54	103.55
19	D	201	TGL	CB4-CB3-CB2	-2.02	105.92	113.19
25	T	102	CDL	PB2-OB2-CB2	-2.02	109.82	121.68
23	P	309	CHD	C11-C9-C8	2.02	113.83	110.88
14	A	602[C]	HEA	C4B-NB-C1B	-2.02	102.99	105.07
20	P	307	PGV	O03-C01-C02	2.02	114.31	108.43
14	N	602[C]	HEA	C4C-NC-C1C	2.02	107.33	105.35
25	P	308	CDL	OB9-CB7-C71	-2.02	115.87	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	101	DMU	C18-O16-C6	2.01	117.18	113.84
14	N	602[A]	HEA	CHD-C1D-C2D	-2.01	121.15	126.73
23	C	301	CHD	C16-C17-C20	-2.01	109.04	112.15
24	T	101	PEK	C8-C7-C6	-2.01	102.15	112.02
26	C	311	DMU	C28-C25-C22	-2.00	104.25	114.42
25	T	102	CDL	C40-C39-C38	2.00	124.59	114.42
20	C	307	PGV	O01-C1-O02	-2.00	118.86	123.70
25	T	102	CDL	C19-C18-C17	2.00	124.59	114.42
19	D	201	TGL	OG1-CA1-OA1	-2.00	118.54	123.59

There are no chirality outliers.

All (737) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C12-C11-C3B-C2B
14	A	601[B]	HEA	C14-C15-C16-C17
14	A	601[B]	HEA	C26-C15-C16-C17
14	A	602[C]	HEA	C2A-C3A-CMA-OMA
14	A	602[C]	HEA	C4A-C3A-CMA-OMA
14	A	602[C]	HEA	C4D-C3D-CAD-CBD
14	N	601[A]	HEA	C12-C11-C3B-C2B
14	N	601[B]	HEA	C14-C15-C16-C17
14	N	601[B]	HEA	C26-C15-C16-C17
14	N	602[A]	HEA	C2A-C3A-CMA-OMA
14	N	602[C]	HEA	C2A-C3A-CMA-OMA
14	N	602[C]	HEA	C4A-C3A-CMA-OMA
14	N	602[C]	HEA	C4D-C3D-CAD-CBD
19	A	607	TGL	OB1-CB1-OG2-CG2
19	B	301	TGL	OG1-CG1-CG2-OG2
19	O	301	TGL	OG1-CG1-CG2-OG2
19	O	302	TGL	CB2-CB1-OG2-CG2
20	A	608	PGV	C03-O11-P-O13
20	A	608	PGV	C03-O11-P-O14
20	A	608	PGV	C2-C1-O01-C02
20	A	608	PGV	O04-C19-O03-C01
20	A	608	PGV	C20-C19-O03-C01
20	C	307	PGV	C03-O11-P-O13
20	P	307	PGV	C10-C11-C12-C13
20	Q	201	PGV	C2-C1-O01-C02
20	Q	201	PGV	O04-C19-O03-C01
20	Q	201	PGV	C20-C19-O03-C01
23	J	102	CHD	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
23	J	102	CHD	C16-C17-C20-C22
23	J	102	CHD	C20-C22-C23-C24
24	C	304	PEK	C4-C5-C6-C7
24	P	305	PEK	C2-C1-O01-C02
24	P	305	PEK	C12-C13-C14-C15
24	P	305	PEK	C13-C14-C15-C16
24	T	101	PEK	C03-O11-P-O12
24	T	101	PEK	C03-O11-P-O13
24	T	101	PEK	C03-O11-P-O14
24	T	101	PEK	C2-C1-O01-C02
25	C	308	CDL	CA3-OA5-PA1-OA3
25	C	308	CDL	OA7-CA5-OA6-CA4
25	C	308	CDL	OA9-CA7-OA8-CA6
25	C	308	CDL	C31-CA7-OA8-CA6
25	C	308	CDL	CB3-OB5-PB2-OB2
25	C	308	CDL	CB3-OB5-PB2-OB3
25	C	308	CDL	CB3-OB5-PB2-OB4
25	G	101	CDL	OA9-CA7-OA8-CA6
25	G	101	CDL	C31-CA7-OA8-CA6
25	G	101	CDL	C1-CB2-OB2-PB2
25	G	101	CDL	CB3-OB5-PB2-OB2
25	G	101	CDL	CB3-OB5-PB2-OB3
25	G	101	CDL	CB3-OB5-PB2-OB4
25	G	101	CDL	OB6-CB4-CB6-OB8
25	T	102	CDL	CA3-OA5-PA1-OA4
25	T	102	CDL	OA9-CA7-OA8-CA6
25	T	102	CDL	C31-CA7-OA8-CA6
25	Y	101	CDL	CA3-OA5-PA1-OA4
25	Y	101	CDL	CB2-OB2-PB2-OB3
25	Y	101	CDL	CB3-OB5-PB2-OB3
26	C	311	DMU	C1-C6-O16-C18
26	G	105	DMU	C3-C4-C57-O61
26	G	105	DMU	O5-C4-C57-O61
26	G	105	DMU	C19-C18-O16-C6
26	K	101	DMU	C1-C6-O16-C18
26	K	102	DMU	C19-C18-O16-C6
26	P	316	DMU	O5-C6-O16-C18
26	X	102	DMU	C1-C6-O16-C18
26	X	103	DMU	C1-C6-O16-C18
26	X	103	DMU	O5-C6-O16-C18
26	X	103	DMU	C19-C18-O16-C6
27	E	201	PSC	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
27	E	201	PSC	O02-C1-O01-C02
27	E	201	PSC	C2-C1-O01-C02
27	O	304	PSC	C04-O12-P-O14
27	O	304	PSC	O02-C1-O01-C02
27	O	304	PSC	C2-C1-O01-C02
24	C	304	PEK	O04-C21-O03-C01
24	P	305	PEK	O04-C21-O03-C01
24	T	101	PEK	O04-C21-O03-C01
25	C	308	CDL	OB9-CB7-OB8-CB6
25	P	308	CDL	OA9-CA7-OA8-CA6
25	Y	101	CDL	OA9-CA7-OA8-CA6
24	C	304	PEK	C22-C21-O03-C01
24	P	305	PEK	C22-C21-O03-C01
25	C	308	CDL	C71-CB7-OB8-CB6
25	P	308	CDL	C31-CA7-OA8-CA6
25	Y	101	CDL	C31-CA7-OA8-CA6
20	C	307	PGV	O04-C19-O03-C01
20	P	307	PGV	O04-C19-O03-C01
23	J	102	CHD	C16-C17-C20-C21
19	D	201	TGL	OB1-CB1-OG2-CG2
19	O	302	TGL	OB1-CB1-OG2-CG2
20	A	608	PGV	O02-C1-O01-C02
20	Q	201	PGV	O02-C1-O01-C02
24	P	305	PEK	O02-C1-O01-C02
20	C	307	PGV	C20-C19-O03-C01
20	P	307	PGV	C20-C19-O03-C01
27	O	304	PSC	C20-C19-O03-C01
19	A	607	TGL	CB2-CB1-OG2-CG2
23	J	102	CHD	C13-C17-C20-C22
14	A	602[C]	HEA	C2D-C3D-CAD-CBD
14	N	602[C]	HEA	C2D-C3D-CAD-CBD
19	B	301	TGL	CC2-CC1-OG3-CG3
19	O	301	TGL	CC2-CC1-OG3-CG3
24	T	101	PEK	C22-C21-O03-C01
27	E	201	PSC	C20-C19-O03-C01
20	C	307	PGV	C10-C11-C12-C13
24	T	101	PEK	O02-C1-O01-C02
19	B	301	TGL	OC1-CC1-OG3-CG3
27	O	304	PSC	O04-C19-O03-C01
19	B	301	TGL	C11-C12-C13-C14
19	A	607	TGL	CC2-CC3-CC4-CC5
26	P	311	DMU	O5-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
26	P	316	DMU	O5-C4-C57-O61
25	C	308	CDL	C11-CA5-OA6-CA4
26	K	102	DMU	O5-C4-C57-O61
26	P	312	DMU	O6-C11-C9-O1
27	E	201	PSC	O04-C19-O03-C01
25	P	308	CDL	C37-C38-C39-C40
19	O	301	TGL	OC1-CC1-OG3-CG3
26	X	102	DMU	O5-C4-C57-O61
26	K	101	DMU	O5-C6-O16-C18
26	K	102	DMU	O5-C6-O16-C18
20	P	306	PGV	C28-C29-C30-C31
26	P	316	DMU	C3-C4-C57-O61
23	P	309	CHD	C17-C20-C22-C23
25	P	308	CDL	OB6-CB4-CB6-OB8
19	D	201	TGL	CB2-CB1-OG2-CG2
26	P	315	DMU	C3-C4-C57-O61
19	O	302	TGL	CA9-C20-C21-C22
27	O	304	PSC	C20-C21-C22-C23
25	T	102	CDL	CA2-C1-CB2-OB2
25	Y	101	CDL	C17-C18-C19-C20
26	P	311	DMU	C3-C4-C57-O61
14	A	602[A]	HEA	C2D-C3D-CAD-CBD
25	T	102	CDL	OA5-CA3-CA4-OA6
23	C	309	CHD	C21-C20-C22-C23
27	E	201	PSC	C1-C2-C3-C4
26	C	311	DMU	O5-C4-C57-O61
26	P	311	DMU	O6-C11-C9-O1
23	P	309	CHD	C21-C20-C22-C23
24	C	304	PEK	C1-C2-C3-C4
24	C	303	PEK	C7-C8-C9-C10
24	C	304	PEK	C7-C8-C9-C10
24	C	304	PEK	C13-C14-C15-C16
26	X	102	DMU	C3-C4-C57-O61
23	W	101	CHD	C13-C17-C20-C22
19	B	301	TGL	CC1-CC2-CC3-CC4
20	C	306	PGV	C19-C20-C21-C22
20	P	307	PGV	C19-C20-C21-C22
24	P	305	PEK	C1-C2-C3-C4
25	P	308	CDL	CB5-C51-C52-C53
20	C	305	PGV	C26-C27-C28-C29
23	C	309	CHD	C17-C20-C22-C23
25	C	308	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
25	P	308	CDL	OA7-CA5-OA6-CA4
27	E	201	PSC	C04-C05-N-C06
27	E	201	PSC	C04-C05-N-C07
19	O	301	TGL	CA1-CA2-CA3-CA4
19	O	302	TGL	CC9-C15-C16-C17
26	K	102	DMU	O16-C18-C19-C22
23	P	309	CHD	C20-C22-C23-C24
26	X	103	DMU	O16-C18-C19-C22
26	P	315	DMU	O5-C4-C57-O61
26	K	101	DMU	C3-C4-C57-O61
26	P	310	DMU	O6-C11-C9-C8
26	C	311	DMU	O5-C6-O16-C18
25	T	102	CDL	C11-C12-C13-C14
26	X	101	DMU	O16-C18-C19-C22
20	C	307	PGV	O12-C04-C05-O05
25	G	101	CDL	O1-C1-CA2-OA2
24	C	304	PEK	O02-C1-O01-C02
20	A	608	PGV	C19-C20-C21-C22
26	J	101	DMU	O16-C18-C19-C22
26	P	312	DMU	O16-C18-C19-C22
24	P	304	PEK	C7-C8-C9-C10
24	P	305	PEK	C10-C11-C12-C13
27	E	201	PSC	C11-C10-C9-C8
25	C	308	CDL	C80-C81-C82-C83
25	P	308	CDL	C11-CA5-OA6-CA4
20	P	307	PGV	C03-O11-P-O12
25	G	101	CDL	CA2-OA2-PA1-OA5
25	G	101	CDL	CA3-OA5-PA1-OA2
25	T	102	CDL	CA3-OA5-PA1-OA2
25	Y	101	CDL	CA3-OA5-PA1-OA2
27	E	201	PSC	C03-O11-P-O12
27	O	304	PSC	C04-O12-P-O11
19	D	201	TGL	CC2-CC1-OG3-CG3
24	C	304	PEK	C2-C1-O01-C02
23	W	101	CHD	C16-C17-C20-C21
23	W	101	CHD	C13-C17-C20-C21
26	P	311	DMU	O16-C18-C19-C22
25	G	101	CDL	CB2-C1-CA2-OA2
26	X	101	DMU	O5-C4-C57-O61
27	O	304	PSC	C04-C05-N-C06
26	C	311	DMU	O6-C11-C9-O1
25	P	308	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	CA9-C20-C21-C22
19	B	301	TGL	C22-C23-C24-C25
20	A	608	PGV	C20-C21-C22-C23
26	X	103	DMU	O5-C4-C57-O61
25	C	308	CDL	C51-CB5-OB6-CB4
19	A	607	TGL	CC3-CC4-CC5-CC6
19	B	301	TGL	CC4-CC5-CC6-CC7
19	O	301	TGL	C10-C11-C12-C13
20	P	306	PGV	C7-C8-C9-C10
25	C	308	CDL	C82-C83-C84-C85
19	A	607	TGL	C13-C14-C29-C30
19	A	607	TGL	C20-C21-C22-C23
19	O	302	TGL	C21-C22-C23-C24
24	C	303	PEK	C22-C23-C24-C25
24	C	303	PEK	C26-C27-C28-C29
25	C	308	CDL	OB7-CB5-OB6-CB4
25	P	308	CDL	OB7-CB5-OB6-CB4
24	P	304	PEK	C4-C5-C6-C7
24	P	304	PEK	C10-C11-C12-C13
24	T	101	PEK	C4-C5-C6-C7
25	G	101	CDL	C15-C16-C17-C18
26	K	102	DMU	C3-C4-C57-O61
25	T	102	CDL	O1-C1-CB2-OB2
25	Y	101	CDL	O1-C1-CB2-OB2
19	A	607	TGL	C21-C22-C23-C24
19	O	301	TGL	CC3-CC4-CC5-CC6
19	O	301	TGL	C20-C21-C22-C23
26	P	315	DMU	C1-C6-O16-C18
19	A	607	TGL	CA3-CA4-CA5-CA6
19	D	201	TGL	CA3-CA4-CA5-CA6
20	C	306	PGV	C20-C21-C22-C23
24	C	303	PEK	C28-C29-C30-C31
19	D	201	TGL	CA7-CA8-CA9-C20
26	K	103	DMU	O16-C18-C19-C22
26	P	310	DMU	C25-C28-C31-C34
19	B	301	TGL	CA5-CA6-CA7-CA8
19	O	302	TGL	CB9-C10-C11-C12
20	C	307	PGV	C2-C3-C4-C5
19	A	607	TGL	C22-C23-C24-C25
19	B	301	TGL	CA4-CA5-CA6-CA7
19	B	301	TGL	CB6-CB7-CB8-CB9
20	C	306	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	C	308	CDL	C60-C61-C62-C63
25	Y	101	CDL	C20-C21-C22-C23
19	B	301	TGL	C10-C11-C12-C13
19	B	301	TGL	C20-C21-C22-C23
19	O	301	TGL	CA9-C20-C21-C22
19	O	302	TGL	CA6-CA7-CA8-CA9
26	X	102	DMU	C28-C31-C34-C37
27	O	304	PSC	C04-C05-N-C07
26	P	310	DMU	O5-C6-O16-C18
26	P	315	DMU	O5-C6-O16-C18
26	X	102	DMU	O5-C6-O16-C18
19	O	301	TGL	C16-C15-CC9-CC8
19	O	302	TGL	C11-C10-CB9-CB8
19	O	302	TGL	C11-C12-C13-C14
19	O	302	TGL	C16-C15-CC9-CC8
19	O	302	TGL	CC5-CC6-CC7-CC8
26	P	316	DMU	C22-C25-C28-C31
26	C	311	DMU	O6-C11-C9-C8
25	G	101	CDL	C58-C59-C60-C61
25	T	102	CDL	C16-C17-C18-C19
24	P	304	PEK	C22-C23-C24-C25
19	O	301	TGL	CC2-CC3-CC4-CC5
26	P	310	DMU	O16-C18-C19-C22
19	D	201	TGL	C23-C24-C25-C26
19	O	301	TGL	C16-C17-C18-C19
24	C	303	PEK	C13-C14-C15-C16
19	A	607	TGL	C10-C11-C12-C13
19	B	301	TGL	C12-C13-C14-C29
19	B	301	TGL	CC5-CC6-CC7-CC8
14	A	602[A]	HEA	C4D-C3D-CAD-CBD
25	T	102	CDL	C34-C35-C36-C37
27	O	304	PSC	C28-C29-C30-C31
19	D	201	TGL	OC1-CC1-OG3-CG3
26	P	315	DMU	C25-C28-C31-C34
26	K	102	DMU	C19-C22-C25-C28
26	X	102	DMU	C18-C19-C22-C25
25	C	308	CDL	C59-C60-C61-C62
26	P	316	DMU	C19-C22-C25-C28
19	D	201	TGL	CB9-C10-C11-C12
25	T	102	CDL	C37-C38-C39-C40
25	Y	101	CDL	C57-C58-C59-C60
20	C	305	PGV	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	CC4-CC5-CC6-CC7
27	O	304	PSC	C04-C05-N-C08
21	B	305	EDO	O1-C1-C2-O2
25	P	308	CDL	C43-C44-C45-C46
26	Z	101	DMU	C28-C31-C34-C37
19	O	302	TGL	CC2-CC1-OG3-CG3
19	B	301	TGL	C21-C20-CA9-CA8
19	A	607	TGL	C11-C10-CB9-CB8
19	A	607	TGL	CA2-CA1-OG1-CG1
26	P	315	DMU	C22-C25-C28-C31
19	B	301	TGL	CB9-C10-C11-C12
20	C	305	PGV	C29-C30-C31-C32
26	Z	101	DMU	C22-C25-C28-C31
19	O	301	TGL	CB2-CB1-OG2-CG2
20	C	307	PGV	C2-C1-O01-C02
25	G	101	CDL	C82-C83-C84-C85
19	O	301	TGL	CA3-CA4-CA5-CA6
24	C	304	PEK	C10-C11-C12-C13
27	O	304	PSC	C11-C10-C9-C8
26	L	101	DMU	C3-C4-C57-O61
25	G	101	CDL	C60-C61-C62-C63
26	J	101	DMU	C28-C31-C34-C37
20	C	307	PGV	O02-C1-O01-C02
27	O	304	PSC	C5-C6-C7-C8
25	C	308	CDL	C77-C78-C79-C80
20	C	307	PGV	C02-C03-O11-P
20	P	307	PGV	C02-C03-O11-P
25	Y	101	CDL	C51-C52-C53-C54
24	T	101	PEK	C01-C02-C03-O11
25	T	102	CDL	OA5-CA3-CA4-CA6
20	C	307	PGV	O12-C04-C05-C06
25	Y	101	CDL	CA2-C1-CB2-OB2
19	O	301	TGL	OB1-CB1-OG2-CG2
19	A	607	TGL	CC9-C15-C16-C17
20	Q	201	PGV	C20-C21-C22-C23
26	M	101	DMU	C19-C22-C25-C28
19	B	301	TGL	CC6-CC7-CC8-CC9
20	C	307	PGV	C20-C21-C22-C23
27	E	201	PSC	C5-C6-C7-C8
19	A	607	TGL	OA1-CA1-OG1-CG1
19	O	302	TGL	OC1-CC1-OG3-CG3
26	X	102	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
24	P	305	PEK	O03-C01-C02-C03
25	Y	101	CDL	C60-C61-C62-C63
19	O	301	TGL	C14-C29-C30-C31
25	G	101	CDL	C37-C38-C39-C40
19	B	301	TGL	C11-C10-CB9-CB8
19	A	607	TGL	CB1-CB2-CB3-CB4
25	Y	101	CDL	C64-C65-C66-C67
26	Z	101	DMU	C25-C28-C31-C34
19	O	301	TGL	CA6-CA7-CA8-CA9
25	T	102	CDL	C20-C21-C22-C23
20	C	307	PGV	O05-C05-C06-O06
20	A	608	PGV	C11-C10-C9-C8
19	O	301	TGL	C13-C14-C29-C30
26	Z	101	DMU	C34-C37-C40-C43
20	A	608	PGV	C15-C16-C17-C18
26	P	312	DMU	O6-C11-C9-C8
19	B	301	TGL	CC3-CC4-CC5-CC6
26	J	101	DMU	C34-C37-C40-C43
26	P	316	DMU	O16-C18-C19-C22
26	P	315	DMU	O6-C11-C9-O1
20	A	608	PGV	C10-C11-C12-C13
24	C	303	PEK	C4-C5-C6-C7
24	C	303	PEK	C10-C11-C12-C13
24	P	304	PEK	C13-C14-C15-C16
27	E	201	PSC	C04-C05-N-C08
25	T	102	CDL	C77-C78-C79-C80
26	M	101	DMU	C28-C31-C34-C37
14	N	602[A]	HEA	C4D-C3D-CAD-CBD
25	C	308	CDL	C41-C42-C43-C44
25	G	101	CDL	C81-C82-C83-C84
26	P	310	DMU	C1-C6-O16-C18
20	A	608	PGV	O03-C01-C02-O01
19	A	607	TGL	C23-C24-C25-C26
19	A	607	TGL	C14-C29-C30-C31
27	E	201	PSC	C20-C21-C22-C23
27	E	201	PSC	O03-C19-C20-C21
20	P	307	PGV	C1-C2-C3-C4
20	A	608	PGV	C7-C8-C9-C10
25	G	101	CDL	C77-C78-C79-C80
19	D	201	TGL	CA6-CA7-CA8-CA9
25	C	308	CDL	C51-C52-C53-C54
20	C	306	PGV	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	G	101	CDL	C57-C58-C59-C60
26	P	315	DMU	C4-C3-O7-C10
27	E	201	PSC	C19-C20-C21-C22
20	P	307	PGV	C20-C21-C22-C23
25	C	308	CDL	C38-C39-C40-C41
26	X	102	DMU	C19-C22-C25-C28
20	C	305	PGV	C10-C11-C12-C13
20	Q	201	PGV	C10-C11-C12-C13
20	A	608	PGV	C01-C02-C03-O11
20	Q	201	PGV	C01-C02-C03-O11
25	C	308	CDL	OA5-CA3-CA4-CA6
25	G	101	CDL	C80-C81-C82-C83
26	P	316	DMU	C25-C28-C31-C34
19	O	301	TGL	CB1-CB2-CB3-CB4
19	B	301	TGL	CA3-CA4-CA5-CA6
25	Y	101	CDL	CA7-C31-C32-C33
25	C	308	CDL	C40-C41-C42-C43
20	P	307	PGV	O12-C04-C05-O05
19	O	301	TGL	C25-C26-C27-C28
27	O	304	PSC	C24-C25-C26-C27
25	G	101	CDL	CA7-C31-C32-C33
26	X	103	DMU	C25-C28-C31-C34
26	K	103	DMU	C19-C18-O16-C6
26	P	310	DMU	C22-C25-C28-C31
24	C	304	PEK	C35-C36-C37-C38
19	B	301	TGL	OG1-CG1-CG2-CG3
19	O	301	TGL	OG1-CG1-CG2-CG3
19	O	302	TGL	C10-C11-C12-C13
20	P	306	PGV	C24-C25-C26-C27
20	N	607	PGV	C10-C11-C12-C13
24	T	101	PEK	C7-C8-C9-C10
26	K	103	DMU	C19-C22-C25-C28
19	O	302	TGL	C17-C18-C19-C33
14	A	602[A]	HEA	C2A-C3A-CMA-OMA
20	C	307	PGV	C03-O11-P-O12
24	C	303	PEK	C6-C7-C8-C9
24	C	303	PEK	C9-C10-C11-C12
24	C	303	PEK	C11-C12-C13-C14
24	C	304	PEK	C5-C6-C7-C8
24	C	304	PEK	C6-C7-C8-C9
24	C	304	PEK	C11-C10-C9-C8
24	C	304	PEK	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	C	304	PEK	C11-C12-C13-C14
24	C	304	PEK	C12-C13-C14-C15
24	P	303	PEK	C5-C6-C7-C8
24	P	303	PEK	C6-C7-C8-C9
24	P	303	PEK	C11-C10-C9-C8
24	P	303	PEK	C11-C12-C13-C14
24	P	303	PEK	C12-C13-C14-C15
24	P	305	PEK	C5-C6-C7-C8
24	P	305	PEK	C6-C7-C8-C9
24	P	305	PEK	C11-C10-C9-C8
24	P	305	PEK	C9-C10-C11-C12
24	P	305	PEK	C11-C12-C13-C14
24	T	101	PEK	C5-C6-C7-C8
24	T	101	PEK	C11-C10-C9-C8
24	T	101	PEK	C9-C10-C11-C12
24	T	101	PEK	C12-C13-C14-C15
25	Y	101	CDL	CB2-OB2-PB2-OB5
27	E	201	PSC	C9-C10-C11-C12
27	E	201	PSC	C10-C11-C12-C13
27	O	304	PSC	C9-C10-C11-C12
27	O	304	PSC	C10-C11-C12-C13
19	B	301	TGL	CB3-CB4-CB5-CB6
20	A	608	PGV	O01-C02-C03-O11
24	T	101	PEK	O01-C02-C03-O11
25	C	308	CDL	C39-C40-C41-C42
25	Y	101	CDL	C76-C77-C78-C79
19	A	607	TGL	C21-C20-CA9-CA8
25	G	101	CDL	C38-C39-C40-C41
25	Y	101	CDL	C77-C78-C79-C80
19	B	301	TGL	CB7-CB8-CB9-C10
19	D	201	TGL	C21-C20-CA9-CA8
20	Q	201	PGV	O03-C01-C02-O01
27	E	201	PSC	C24-C25-C26-C27
19	A	607	TGL	CC6-CC7-CC8-CC9
25	G	101	CDL	CA2-C1-CB2-OB2
26	X	101	DMU	C19-C22-C25-C28
19	B	301	TGL	OB1-CB1-OG2-CG2
25	G	101	CDL	C11-C12-C13-C14
20	P	306	PGV	C02-C03-O11-P
25	C	308	CDL	C36-C37-C38-C39
27	O	304	PSC	C22-C23-C24-C25
21	A	617	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	CB5-CB6-CB7-CB8
19	B	301	TGL	CB5-CB6-CB7-CB8
24	C	303	PEK	C17-C18-C19-C20
26	K	103	DMU	C18-C19-C22-C25
14	N	602[A]	HEA	C2D-C3D-CAD-CBD
26	P	310	DMU	C28-C31-C34-C37
25	P	308	CDL	OA5-CA3-CA4-CA6
24	P	305	PEK	C2-C3-C4-C5
26	J	101	DMU	C18-C19-C22-C25
23	C	309	CHD	C20-C22-C23-C24
20	A	608	PGV	C03-O11-P-O12
25	P	308	CDL	CA7-C31-C32-C33
19	B	301	TGL	CC7-CC8-CC9-C15
25	C	308	CDL	C13-C14-C15-C16
19	A	607	TGL	CG1-CG2-OG2-CB1
19	D	201	TGL	CB4-CB5-CB6-CB7
25	P	308	CDL	C41-C42-C43-C44
19	A	607	TGL	OG1-CG1-CG2-CG3
19	O	302	TGL	CG1-CG2-CG3-OG3
20	C	306	PGV	C02-C03-O11-P
25	Y	101	CDL	CA3-CA4-CA6-OA8
25	C	308	CDL	CA7-C31-C32-C33
25	Y	101	CDL	OA7-CA5-OA6-CA4
19	O	301	TGL	C24-C25-C26-C27
26	G	105	DMU	C1-C6-O16-C18
26	P	311	DMU	C1-C6-O16-C18
19	A	607	TGL	OG1-CG1-CG2-OG2
19	B	301	TGL	OG2-CG2-CG3-OG3
19	O	301	TGL	OG2-CG2-CG3-OG3
25	Y	101	CDL	OA6-CA4-CA6-OA8
25	Y	101	CDL	OB6-CB4-CB6-OB8
19	O	301	TGL	CC5-CC6-CC7-CC8
25	P	308	CDL	C82-C83-C84-C85
20	C	306	PGV	C24-C25-C26-C27
24	C	303	PEK	C27-C28-C29-C30
27	E	201	PSC	C23-C24-C25-C26
19	B	301	TGL	CC2-CC3-CC4-CC5
25	P	308	CDL	C58-C59-C60-C61
25	T	102	CDL	CB3-OB5-PB2-OB2
19	A	607	TGL	CA2-CA3-CA4-CA5
24	C	303	PEK	C25-C26-C27-C28
25	C	308	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	CB6-CB7-CB8-CB9
26	P	315	DMU	C19-C22-C25-C28
20	P	307	PGV	C03-O11-P-O13
25	G	101	CDL	CA2-OA2-PA1-OA3
25	G	101	CDL	CA3-OA5-PA1-OA3
27	E	201	PSC	C03-O11-P-O14
27	O	304	PSC	C04-O12-P-O13
19	D	201	TGL	CA9-C20-C21-C22
27	E	201	PSC	C22-C23-C24-C25
26	P	315	DMU	C2-C3-O7-C10
20	N	607	PGV	C23-C24-C25-C26
26	P	312	DMU	C18-C19-C22-C25
19	B	301	TGL	C16-C15-CC9-CC8
19	D	201	TGL	C11-C10-CB9-CB8
25	Y	101	CDL	C72-C71-CB7-OB8
27	O	304	PSC	O03-C19-C20-C21
14	N	602[A]	HEA	C4A-C3A-CMA-OMA
19	B	301	TGL	CG1-CG2-CG3-OG3
19	O	301	TGL	CB7-CB8-CB9-C10
19	O	301	TGL	CG1-CG2-CG3-OG3
20	A	608	PGV	O03-C01-C02-C03
27	E	201	PSC	O12-C04-C05-N
27	O	304	PSC	O03-C01-C02-C03
27	O	304	PSC	O12-C04-C05-N
19	O	302	TGL	OG2-CG2-CG3-OG3
24	P	305	PEK	O03-C01-C02-O01
27	O	304	PSC	O03-C01-C02-O01
24	P	305	PEK	C4-C5-C6-C7
19	D	201	TGL	CB7-CB8-CB9-C10
20	C	306	PGV	C13-C14-C15-C16
26	P	310	DMU	O6-C11-C9-O1
26	K	102	DMU	C22-C25-C28-C31
25	T	102	CDL	C80-C81-C82-C83
25	Y	101	CDL	C59-C60-C61-C62
20	Q	201	PGV	C01-C02-O01-C1
26	X	103	DMU	C3-C4-C57-O61
25	C	308	CDL	OA5-CA3-CA4-OA6
14	A	601[A]	HEA	C27-C19-C20-C21
19	O	301	TGL	CC6-CC7-CC8-CC9
21	P	314	EDO	O1-C1-C2-O2
21	S	107	EDO	O1-C1-C2-O2
20	C	307	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	B	301	TGL	CB2-CB1-OG2-CG2
25	Y	101	CDL	C11-CA5-OA6-CA4
26	P	311	DMU	O5-C6-O16-C18
25	Y	101	CDL	C18-C19-C20-C21
27	E	201	PSC	C7-C8-C9-C10
25	C	308	CDL	CA3-OA5-PA1-OA2
25	T	102	CDL	CB2-OB2-PB2-OB5
25	Y	101	CDL	CA2-OA2-PA1-OA5
25	Y	101	CDL	CB3-OB5-PB2-OB2
27	E	201	PSC	C04-O12-P-O11
26	Z	101	DMU	O6-C11-C9-C8
25	Y	101	CDL	CB3-CB4-CB6-OB8
24	P	305	PEK	C14-C15-C16-C17
19	D	201	TGL	CB3-CB4-CB5-CB6
25	P	308	CDL	C55-C56-C57-C58
25	P	308	CDL	CA5-C11-C12-C13
20	C	305	PGV	C11-C12-C13-C14
20	N	607	PGV	C11-C12-C13-C14
24	P	305	PEK	C3-C4-C5-C6
19	B	301	TGL	CA6-CA7-CA8-CA9
26	C	311	DMU	C3-C4-C57-O61
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
14	N	602[C]	HEA	CAA-CBA-CGA-O2A
19	A	607	TGL	OG1-CA1-CA2-CA3
25	T	102	CDL	C14-C15-C16-C17
25	T	102	CDL	C81-C82-C83-C84
23	C	309	CHD	C22-C23-C24-O26
14	A	601[A]	HEA	C16-C17-C18-C19
25	Y	101	CDL	C22-C23-C24-C25
25	T	102	CDL	OB5-CB3-CB4-CB6
20	C	307	PGV	C9-C10-C11-C12
25	T	102	CDL	C42-C43-C44-C45
23	W	101	CHD	C22-C23-C24-O25
19	D	201	TGL	CB5-CB6-CB7-CB8
19	O	301	TGL	C12-C13-C14-C29
25	T	102	CDL	CB3-CB4-CB6-OB8
26	L	101	DMU	C1-C6-O16-C18
23	B	303	CHD	C22-C23-C24-O25
23	G	102	CHD	C22-C23-C24-O25
25	T	102	CDL	C1-CB2-OB2-PB2
27	E	201	PSC	O04-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
19	O	301	TGL	CA7-CA8-CA9-C20
25	P	308	CDL	C34-C35-C36-C37
23	J	102	CHD	C22-C23-C24-O26
20	Q	201	PGV	C12-C13-C14-C15
21	S	108	EDO	O1-C1-C2-O2
26	K	101	DMU	O5-C4-C57-O61
20	C	306	PGV	C15-C16-C17-C18
26	G	105	DMU	C28-C31-C34-C37
23	B	303	CHD	C22-C23-C24-O26
14	N	602[A]	HEA	CAD-CBD-CGD-O1D
19	A	607	TGL	C11-C12-C13-C14
26	K	102	DMU	C28-C31-C34-C37
25	C	308	CDL	C58-C59-C60-C61
23	J	102	CHD	C22-C23-C24-O25
19	A	607	TGL	CC5-CC6-CC7-CC8
14	N	601[A]	HEA	CAD-CBD-CGD-O1D
14	N	601[B]	HEA	CAD-CBD-CGD-O1D
19	O	302	TGL	CB5-CB6-CB7-CB8
24	P	303	PEK	C9-C10-C11-C12
24	P	304	PEK	C11-C12-C13-C14
24	T	101	PEK	C6-C7-C8-C9
24	T	101	PEK	C11-C12-C13-C14
19	O	302	TGL	CB4-CB5-CB6-CB7
14	N	602[C]	HEA	CAA-CBA-CGA-O1A
23	G	102	CHD	C22-C23-C24-O26
23	W	101	CHD	C22-C23-C24-O26
20	C	306	PGV	C10-C11-C12-C13
20	P	306	PGV	C20-C21-C22-C23
26	J	101	DMU	C31-C34-C37-C40
19	O	302	TGL	CA5-CA6-CA7-CA8
25	Y	101	CDL	C53-C54-C55-C56
14	A	602[C]	HEA	CAA-CBA-CGA-O2A
24	P	305	PEK	C7-C8-C9-C10
14	N	602[A]	HEA	CAD-CBD-CGD-O2D
14	A	602[A]	HEA	CAD-CBD-CGD-O1D
25	Y	101	CDL	C12-C11-CA5-OA6
19	O	302	TGL	C20-C21-C22-C23
19	O	301	TGL	CC7-CC8-CC9-C15
25	P	308	CDL	C73-C74-C75-C76
20	Q	201	PGV	C2-C3-C4-C5
25	Y	101	CDL	C71-C72-C73-C74
26	X	102	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
20	P	306	PGV	C9-C10-C11-C12
24	P	304	PEK	C14-C15-C16-C17
27	E	201	PSC	C12-C13-C14-C15
14	A	602[A]	HEA	CAD-CBD-CGD-O2D
14	N	602[A]	HEA	CAA-CBA-CGA-O1A
23	P	309	CHD	C22-C23-C24-O26
21	Q	202	EDO	O1-C1-C2-O2
21	S	106	EDO	O1-C1-C2-O2
25	T	102	CDL	C12-C13-C14-C15
14	A	602[C]	HEA	C26-C15-C16-C17
14	N	602[C]	HEA	C26-C15-C16-C17
14	A	602[C]	HEA	CAA-CBA-CGA-O1A
25	T	102	CDL	C32-C33-C34-C35
20	P	307	PGV	C6-C7-C8-C9
27	E	201	PSC	C21-C22-C23-C24
14	A	602[A]	HEA	CAA-CBA-CGA-O1A
19	O	301	TGL	C17-C18-C19-C33
26	M	101	DMU	C22-C25-C28-C31
26	C	311	DMU	C22-C25-C28-C31
25	C	308	CDL	C52-C51-CB5-OB6
14	A	602[A]	HEA	C26-C15-C16-C17
14	A	601[A]	HEA	C18-C19-C20-C21
25	G	101	CDL	C12-C11-CA5-OA6
24	C	304	PEK	C14-C15-C16-C17
24	P	303	PEK	C3-C4-C5-C6
14	N	601[A]	HEA	CAD-CBD-CGD-O2D
14	N	601[B]	HEA	CAD-CBD-CGD-O2D
20	Q	201	PGV	C03-C02-O01-C1
25	C	308	CDL	C37-C38-C39-C40
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
14	N	602[A]	HEA	C26-C15-C16-C17
14	N	602[C]	HEA	C14-C15-C16-C17
20	C	307	PGV	C13-C14-C15-C16
26	X	101	DMU	C22-C25-C28-C31
20	C	306	PGV	C05-C04-O12-P
20	Q	201	PGV	O03-C01-C02-C03
20	C	307	PGV	C7-C8-C9-C10
19	B	301	TGL	C21-C22-C23-C24
19	O	301	TGL	CB6-CB7-CB8-CB9
14	N	602[A]	HEA	CAA-CBA-CGA-O2A
23	C	309	CHD	C22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	CA2-CA3-CA4-CA5
26	P	311	DMU	C34-C37-C40-C43
19	D	201	TGL	OG2-CB1-CB2-CB3
23	P	301	CHD	C22-C23-C24-O25
23	P	309	CHD	C22-C23-C24-O25
25	T	102	CDL	C13-C14-C15-C16
24	C	304	PEK	O01-C1-C2-C3
25	C	308	CDL	C81-C82-C83-C84
20	C	305	PGV	C11-C10-C9-C8
25	T	102	CDL	C40-C41-C42-C43
26	Z	101	DMU	O16-C18-C19-C22
25	Y	101	CDL	C32-C31-CA7-OA8
19	O	302	TGL	CC1-CC2-CC3-CC4
24	T	101	PEK	C26-C27-C28-C29
23	C	301	CHD	C22-C23-C24-O25
20	Q	201	PGV	C11-C12-C13-C14
25	Y	101	CDL	C31-C32-C33-C34
25	P	308	CDL	C81-C82-C83-C84
23	C	309	CHD	C16-C17-C20-C22
26	M	101	DMU	C34-C37-C40-C43
26	G	105	DMU	C34-C37-C40-C43
19	O	302	TGL	CA7-CA8-CA9-C20
20	C	306	PGV	C11-C12-C13-C14
14	A	602[A]	HEA	CAA-CBA-CGA-O2A
19	O	301	TGL	C15-C16-C17-C18
26	M	101	DMU	O6-C11-C9-C8
20	A	608	PGV	C23-C24-C25-C26
20	P	306	PGV	C30-C31-C32-C33
26	P	310	DMU	C19-C22-C25-C28
27	O	304	PSC	C12-C13-C14-C15
24	C	304	PEK	C2-C3-C4-C5
20	P	307	PGV	C2-C3-C4-C5
20	C	307	PGV	C24-C25-C26-C27
25	P	308	CDL	C36-C37-C38-C39
24	P	305	PEK	C32-C33-C34-C35
25	G	101	CDL	C12-C11-CA5-OA7
19	A	607	TGL	C16-C15-CC9-CC8
24	C	304	PEK	C31-C32-C33-C34
24	C	304	PEK	O02-C1-C2-C3
24	P	304	PEK	C27-C28-C29-C30
25	Y	101	CDL	C74-C75-C76-C77
25	C	308	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
26	P	312	DMU	C25-C28-C31-C34
14	A	601[A]	HEA	CAA-CBA-CGA-O2A
14	A	601[B]	HEA	CAA-CBA-CGA-O2A
20	P	307	PGV	C9-C10-C11-C12
25	Y	101	CDL	C32-C31-CA7-OA9
19	O	302	TGL	OG2-CB1-CB2-CB3
14	N	601[A]	HEA	CAA-CBA-CGA-O2A
14	N	601[B]	HEA	CAA-CBA-CGA-O2A
25	G	101	CDL	C20-C21-C22-C23
21	D	202	EDO	O1-C1-C2-O2
21	U	101	EDO	O1-C1-C2-O2
20	P	307	PGV	C12-C13-C14-C15
19	O	302	TGL	C16-C17-C18-C19
24	C	304	PEK	C3-C4-C5-C6
25	P	308	CDL	CA3-CA4-OA6-CA5
27	E	201	PSC	C03-C02-O01-C1
25	G	101	CDL	OB9-CB7-OB8-CB6
25	T	102	CDL	C17-C18-C19-C20
23	C	301	CHD	C22-C23-C24-O26
24	P	305	PEK	C21-C22-C23-C24
26	X	101	DMU	C18-C19-C22-C25
20	C	306	PGV	C9-C10-C11-C12
27	O	304	PSC	C7-C8-C9-C10
24	C	303	PEK	C16-C17-C18-C19
25	Y	101	CDL	C58-C59-C60-C61
25	T	102	CDL	C32-C31-CA7-OA8
20	P	306	PGV	C1-C2-C3-C4
14	A	601[A]	HEA	O11-C11-C3B-C2B
19	O	301	TGL	C22-C23-C24-C25
20	N	607	PGV	C28-C29-C30-C31
19	O	302	TGL	OG3-CC1-CC2-CC3
25	Y	101	CDL	C52-C51-CB5-OB6
19	D	201	TGL	OG3-CC1-CC2-CC3
25	T	102	CDL	C32-C31-CA7-OA9
20	C	305	PGV	O03-C19-C20-C21
25	P	308	CDL	C80-C81-C82-C83
25	G	101	CDL	C63-C64-C65-C66

There are no ring outliers.

55 monomers are involved in 223 short contacts:

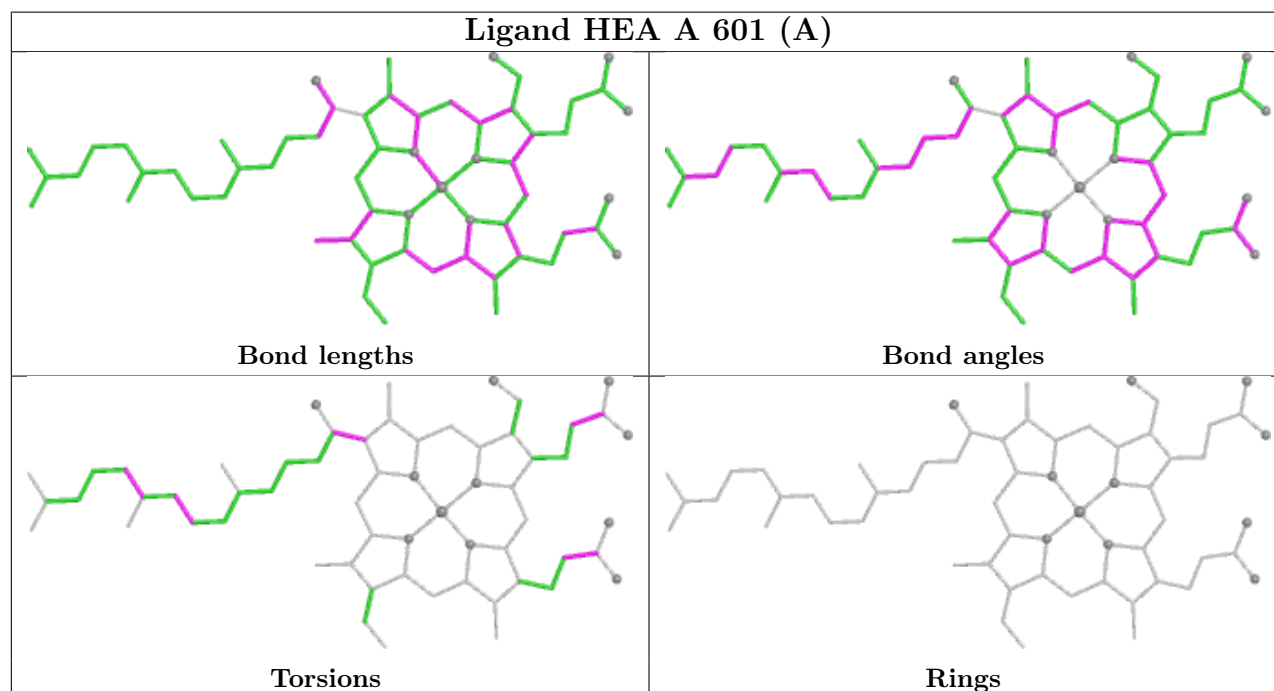
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601[A]	HEA	3	0
24	P	304	PEK	7	0
19	A	607	TGL	10	0
26	G	105	DMU	2	0
19	O	302	TGL	11	0
26	J	101	DMU	3	0
23	C	309	CHD	5	0
21	B	305	EDO	5	0
26	P	311	DMU	2	0
26	X	103	DMU	4	0
21	A	617	EDO	1	0
23	W	101	CHD	1	0
27	O	304	PSC	9	0
20	A	608	PGV	7	0
20	C	305	PGV	3	0
20	C	306	PGV	4	0
25	T	102	CDL	15	0
23	P	309	CHD	3	0
20	Q	201	PGV	6	0
14	N	601[A]	HEA	3	0
26	X	101	DMU	1	0
21	A	615	EDO	1	0
25	Y	101	CDL	4	0
23	G	102	CHD	1	0
24	C	303	PEK	4	0
20	N	607	PGV	4	0
14	N	602[C]	HEA	12	0
26	P	312	DMU	3	0
20	C	307	PGV	1	0
14	A	601[B]	HEA	2	0
19	D	201	TGL	7	0
24	P	305	PEK	2	0
14	A	602[A]	HEA	4	0
26	P	315	DMU	1	0
21	U	101	EDO	3	0
14	N	602[A]	HEA	3	0
26	K	101	DMU	1	0
14	A	602[C]	HEA	7	0
21	O	307	EDO	1	0
26	Z	101	DMU	1	0
26	X	102	DMU	1	0
23	J	102	CHD	4	0
21	D	202	EDO	1	0

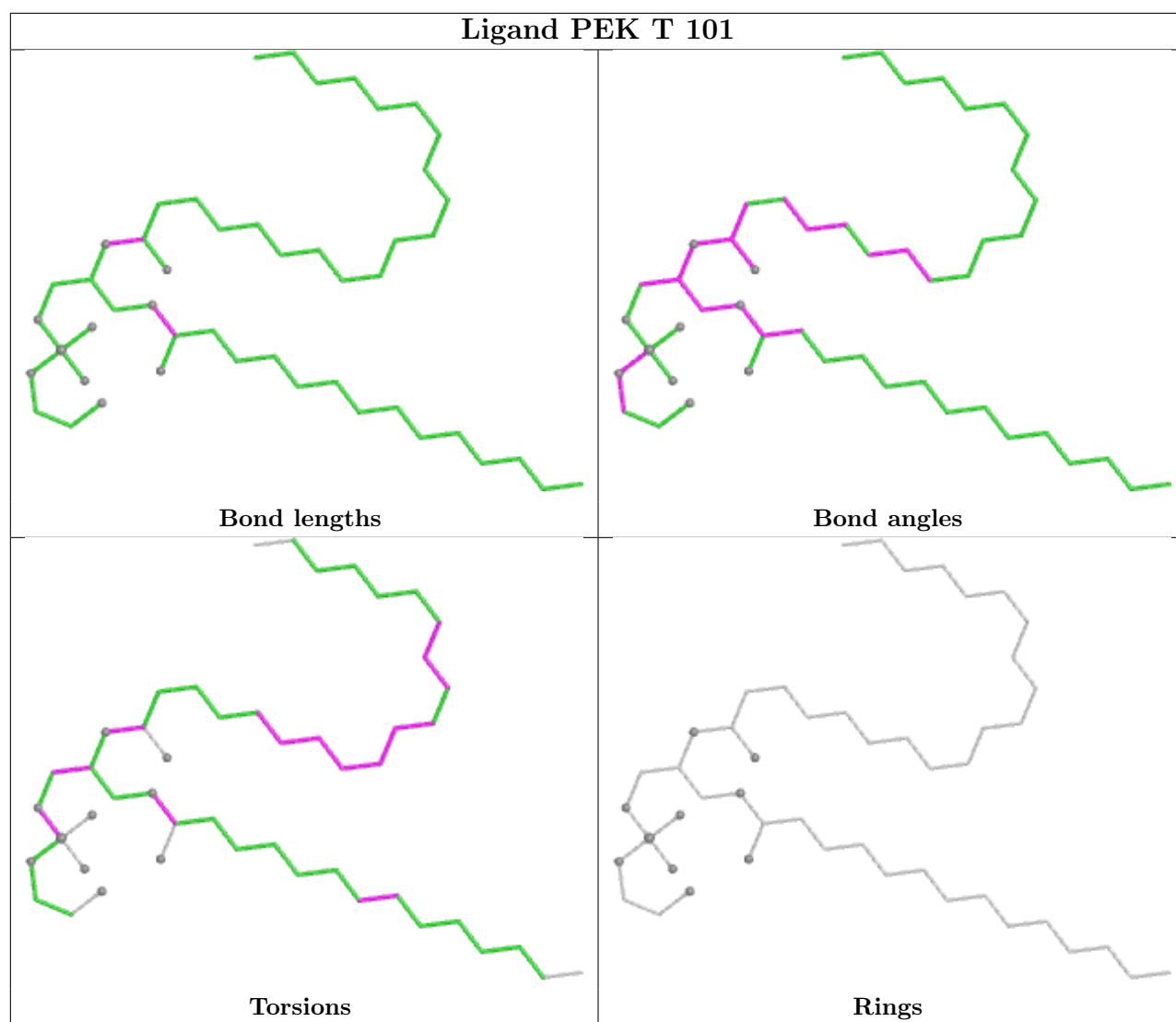
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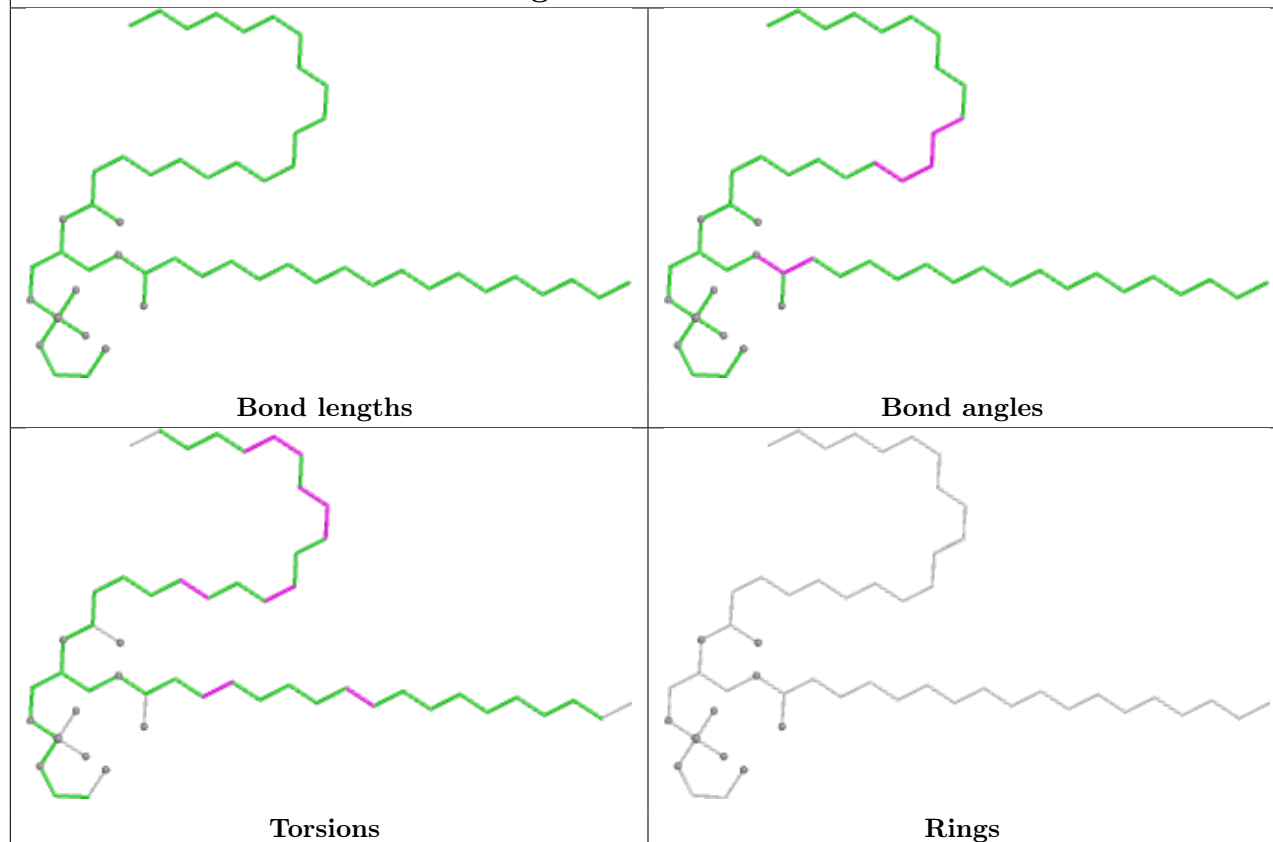
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	P	310	DMU	4	0
19	O	301	TGL	3	0
25	C	308	CDL	14	0
21	S	108	EDO	3	0
27	E	201	PSC	8	0
26	L	101	DMU	3	0
25	P	308	CDL	6	0
20	P	307	PGV	1	0
25	G	101	CDL	8	0
26	K	103	DMU	1	0
19	B	301	TGL	6	0
26	C	311	DMU	5	0

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.

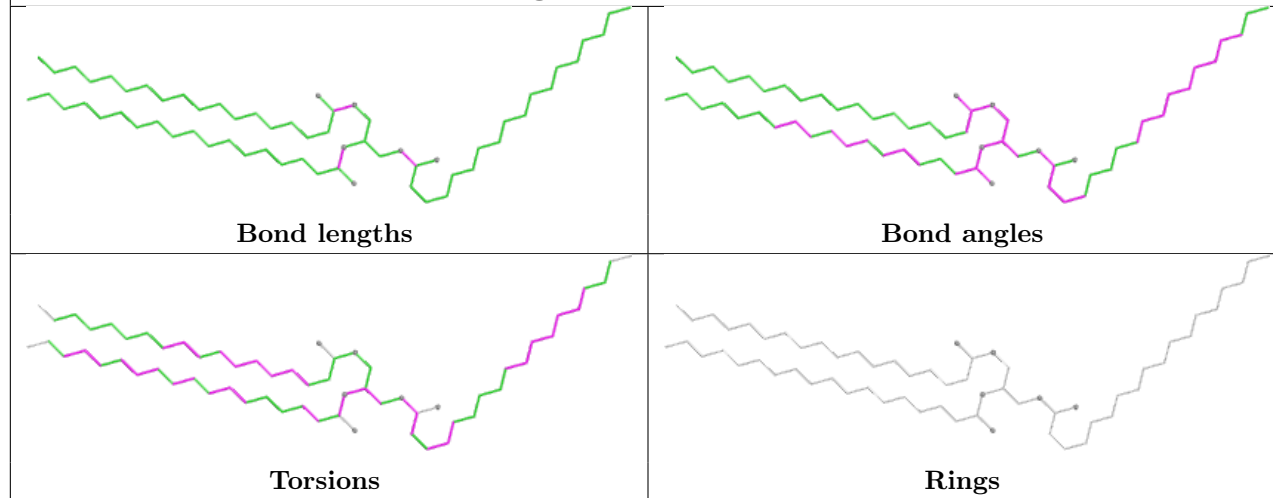


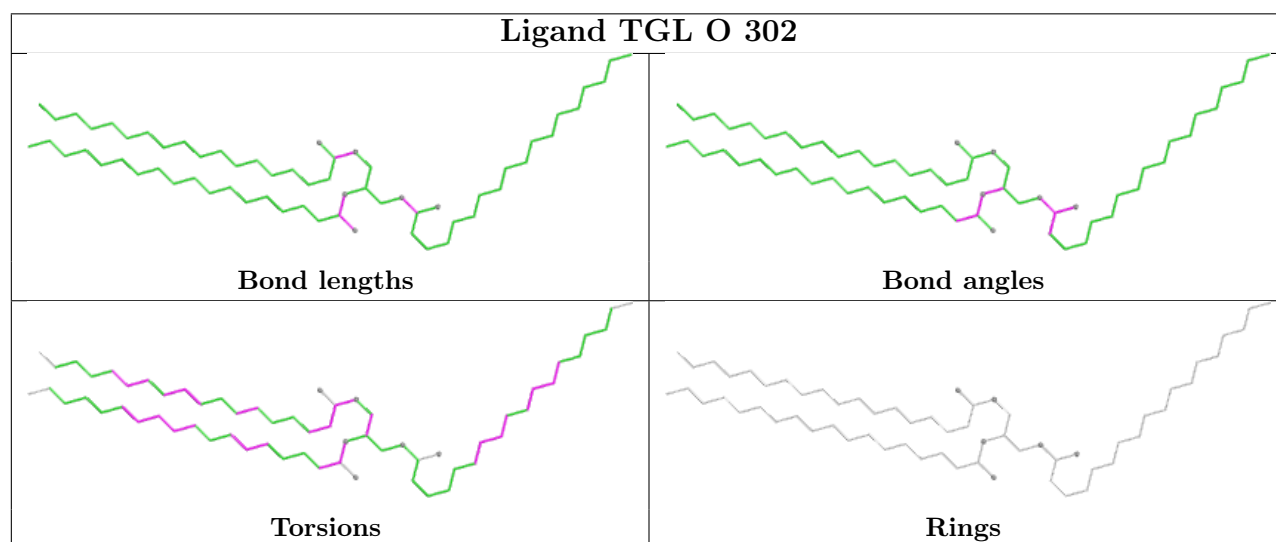
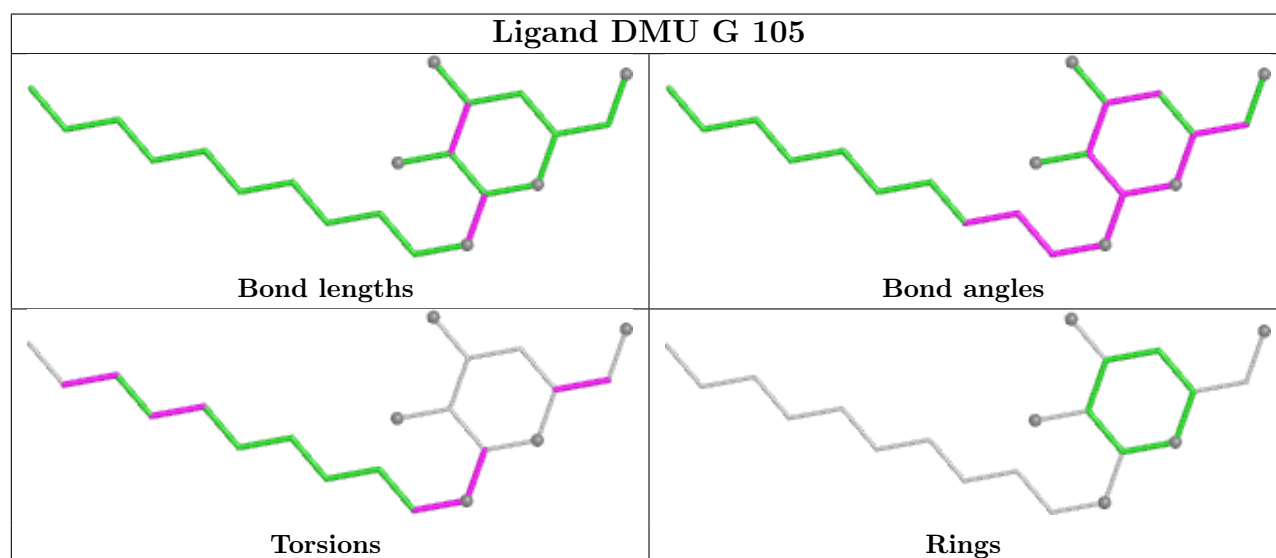
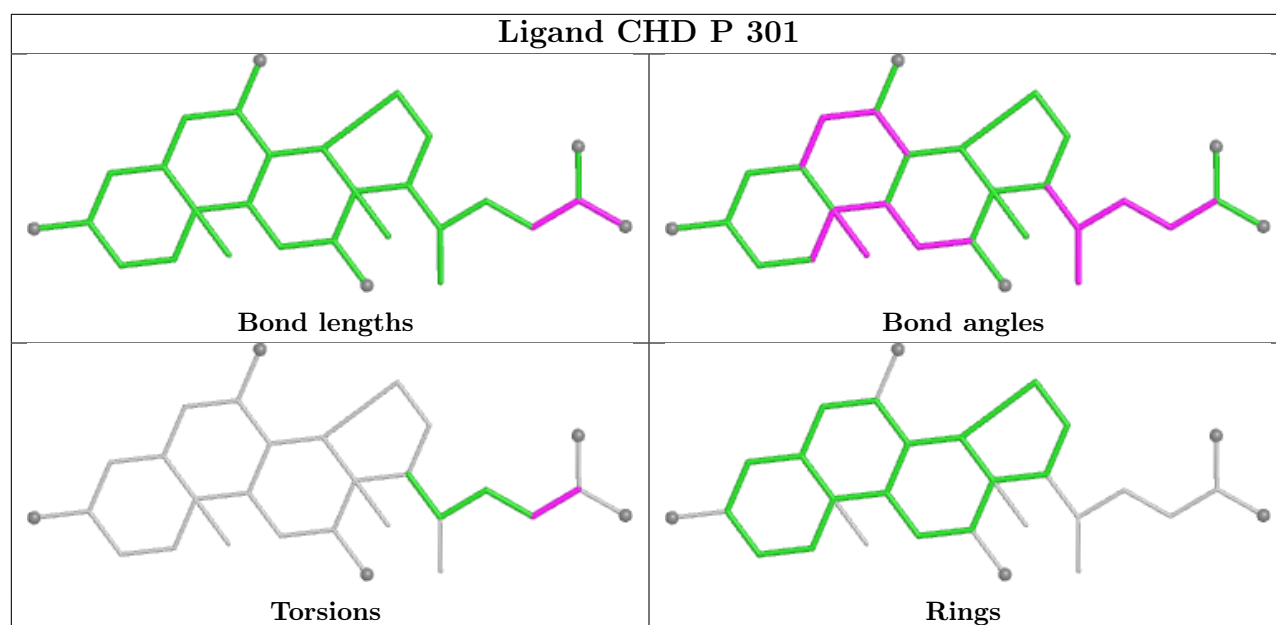


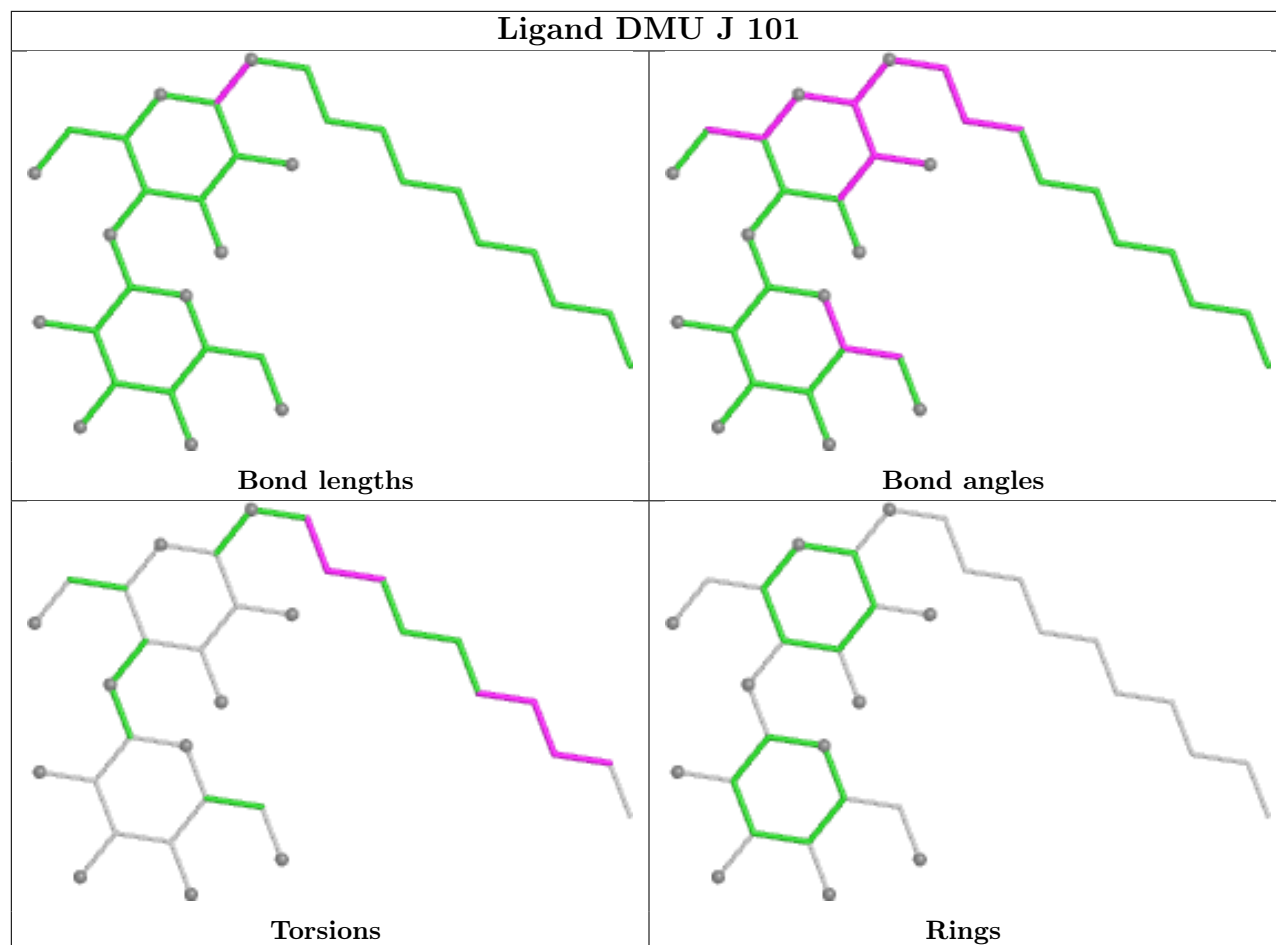
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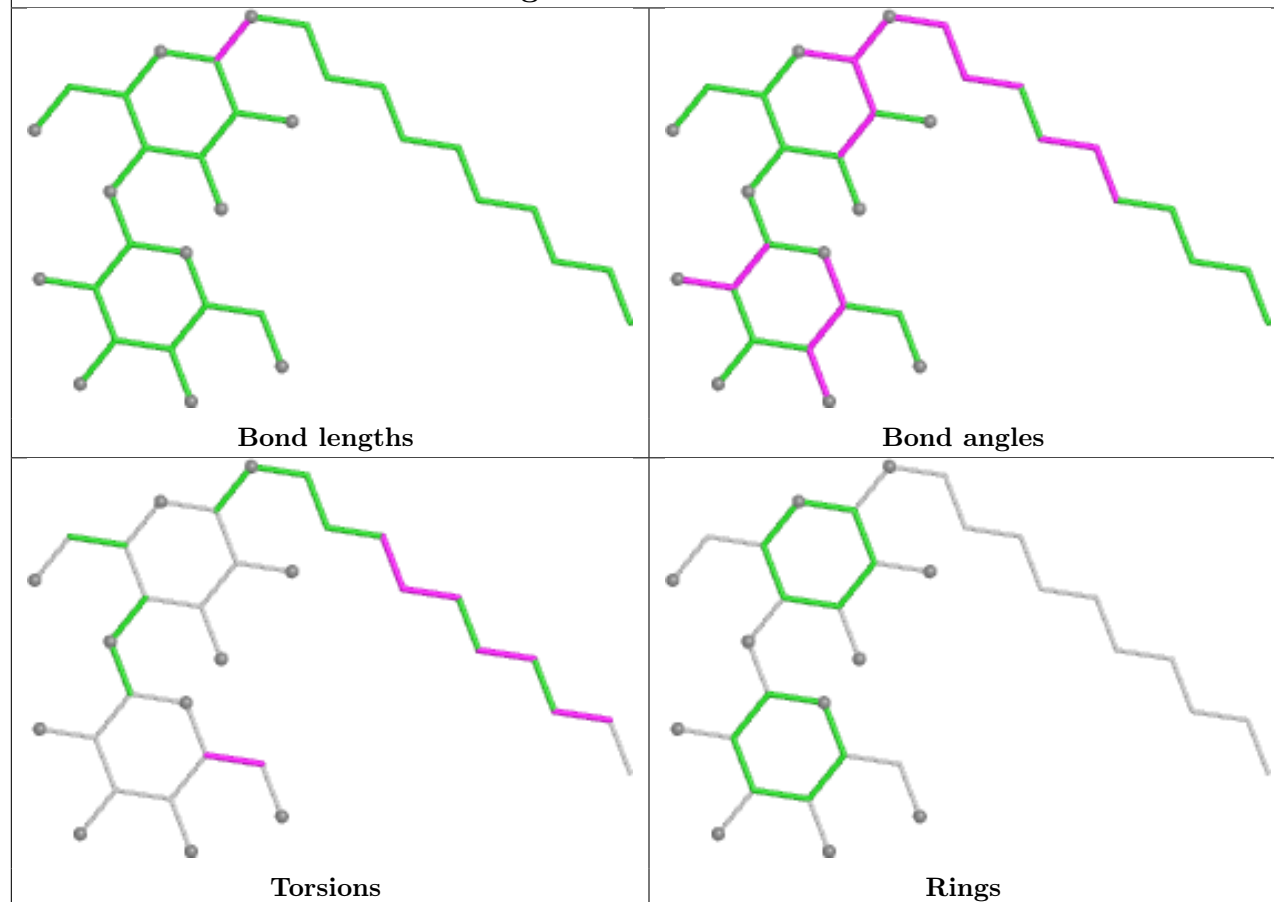
Ligand TGL A 607



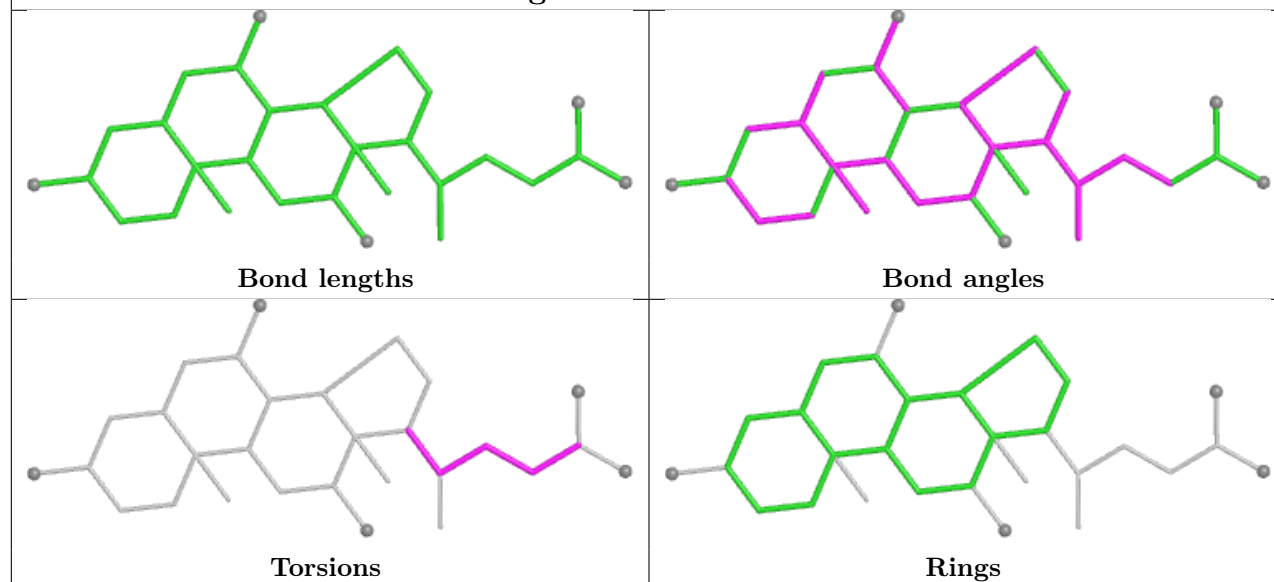


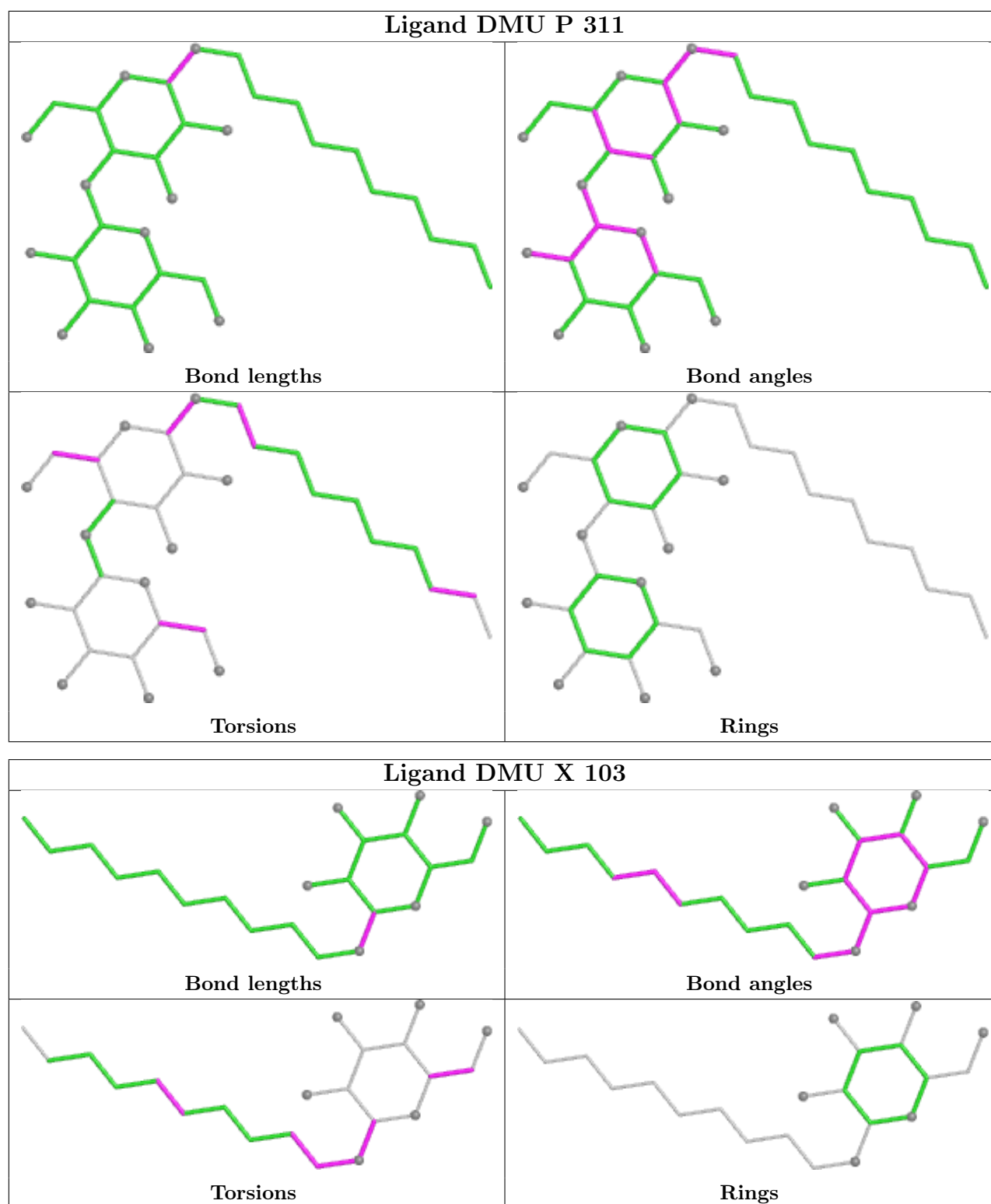


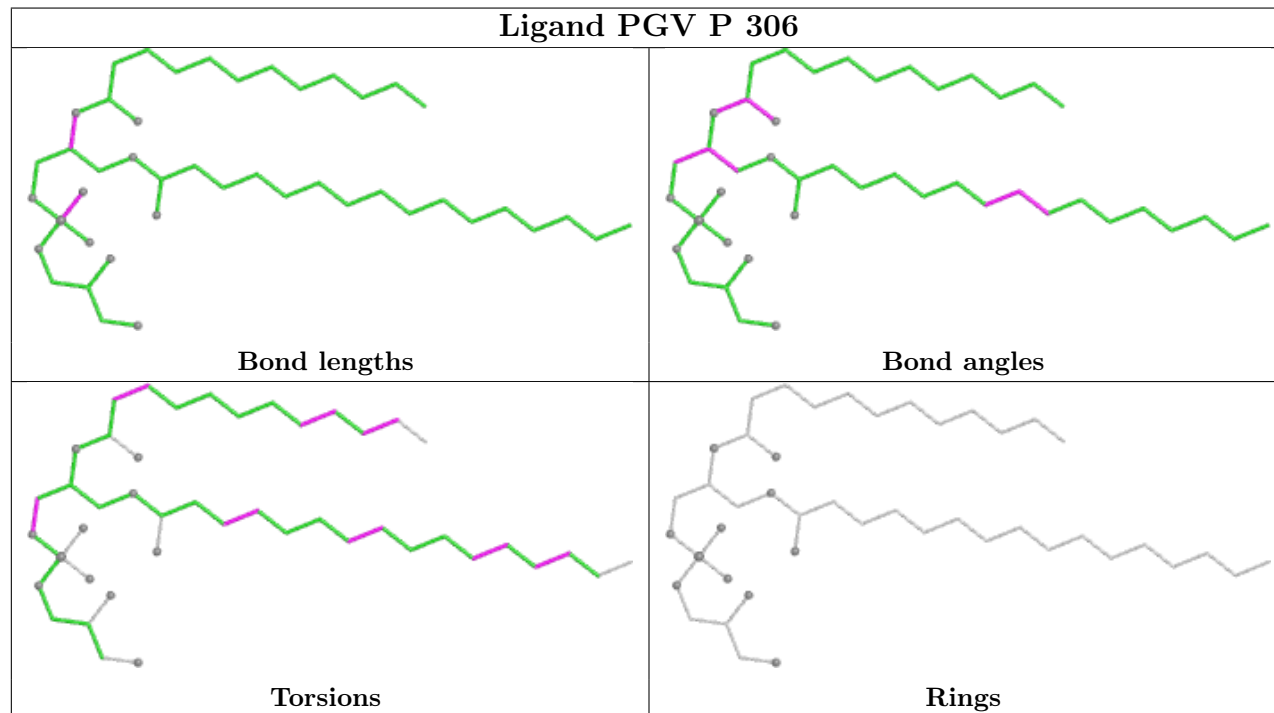
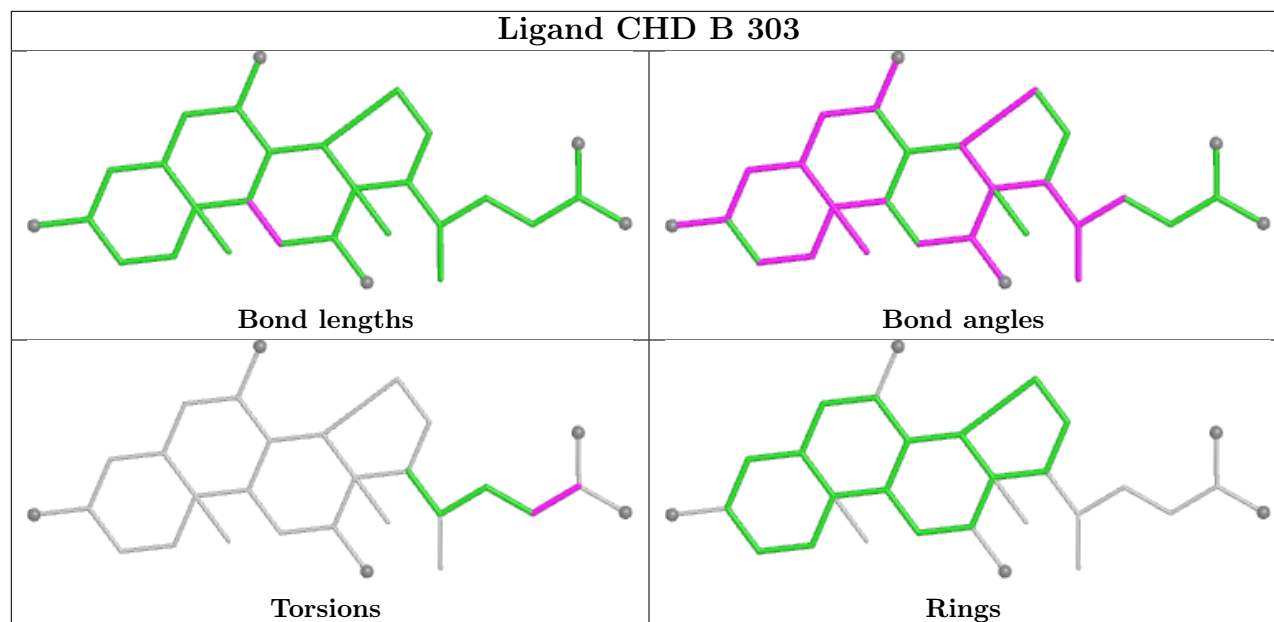
Ligand DMU M 101

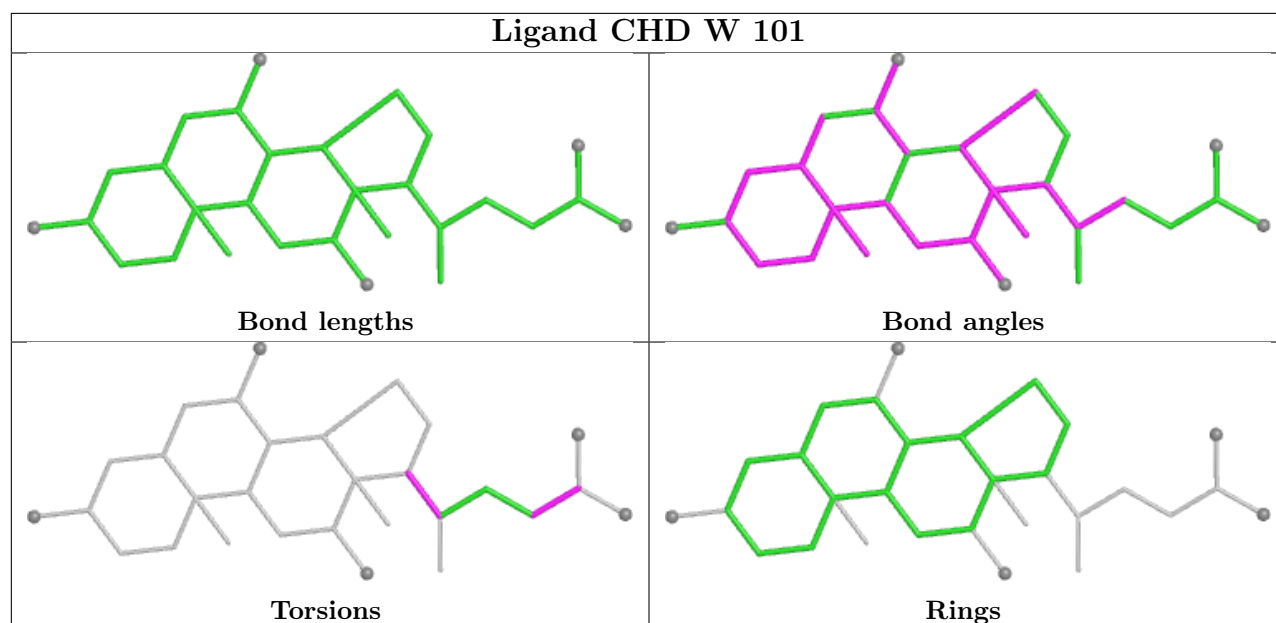
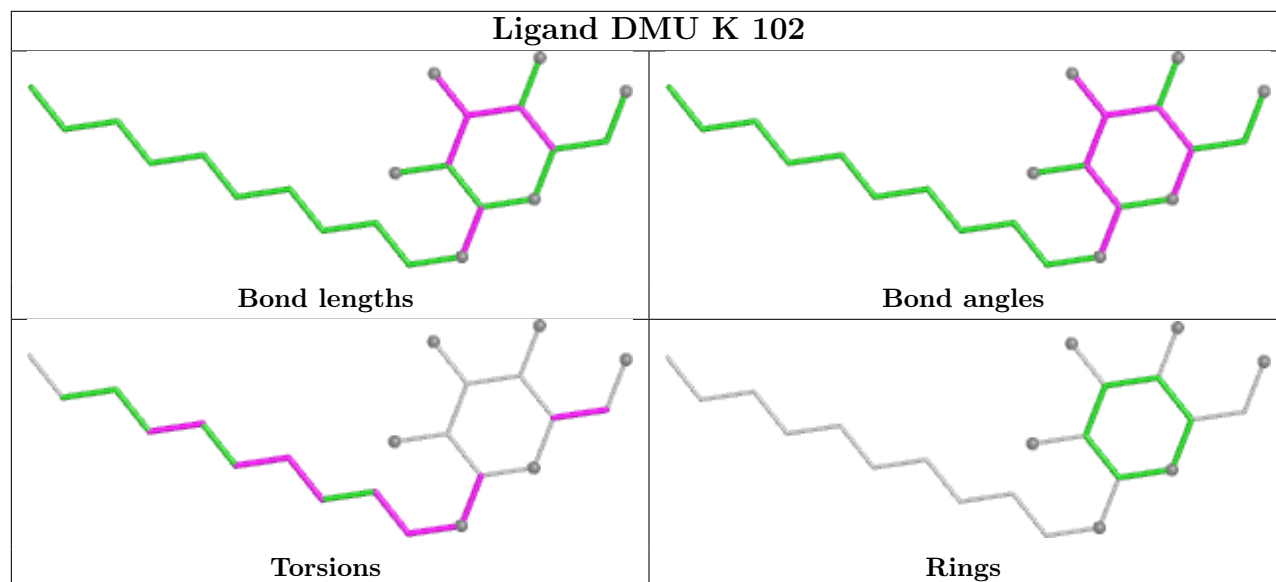


Ligand CHD C 309

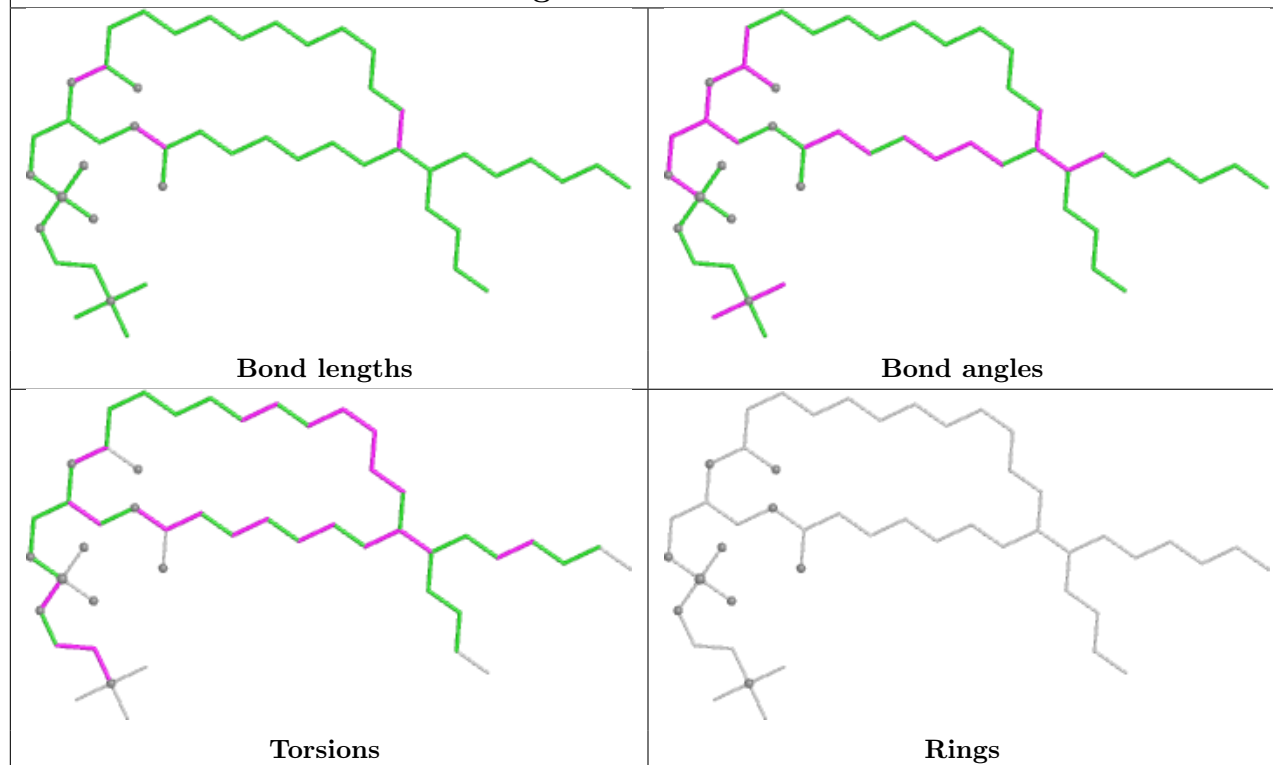




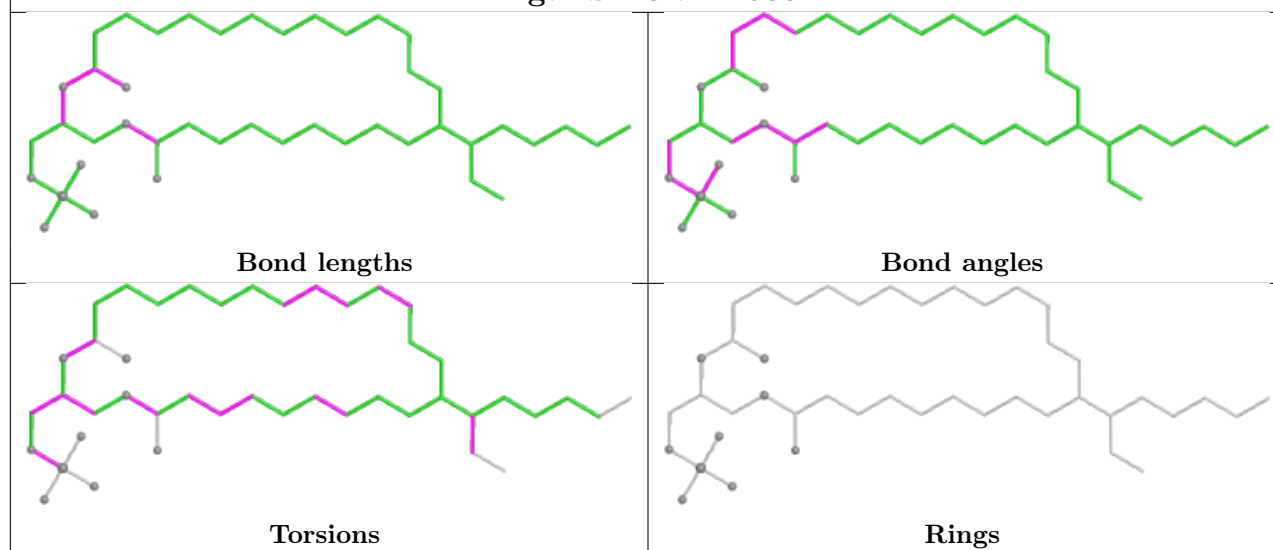


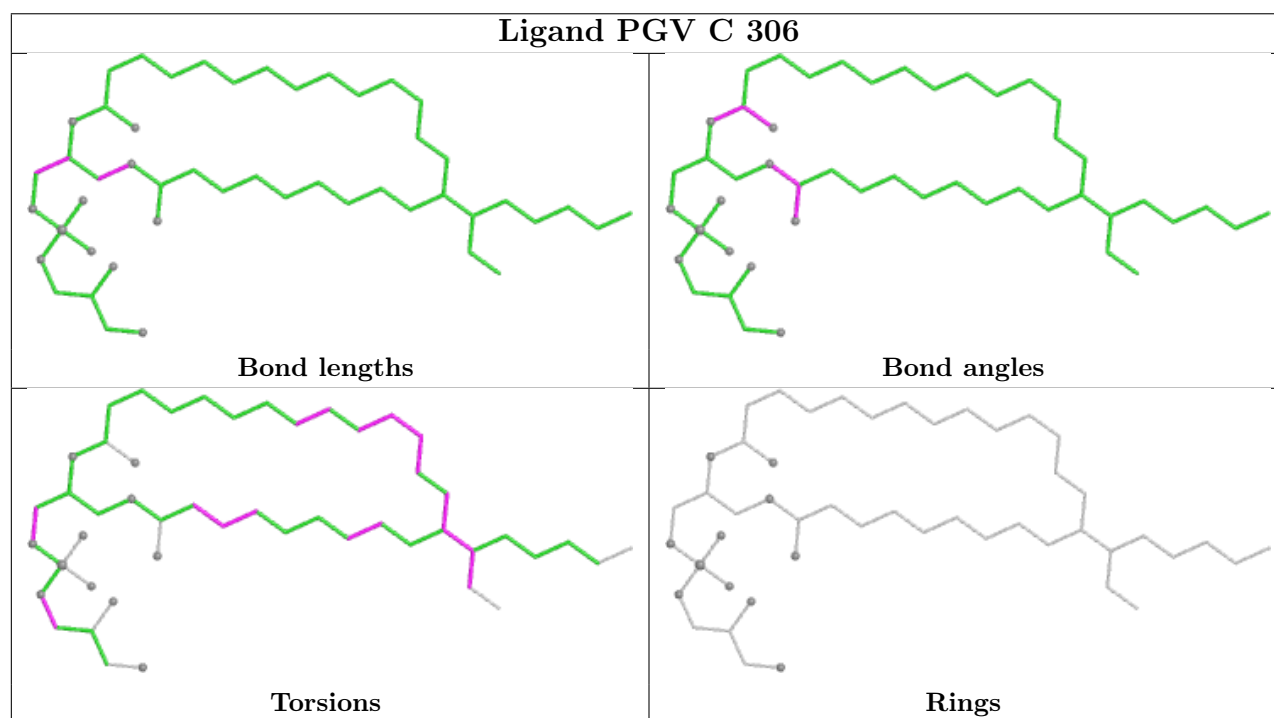
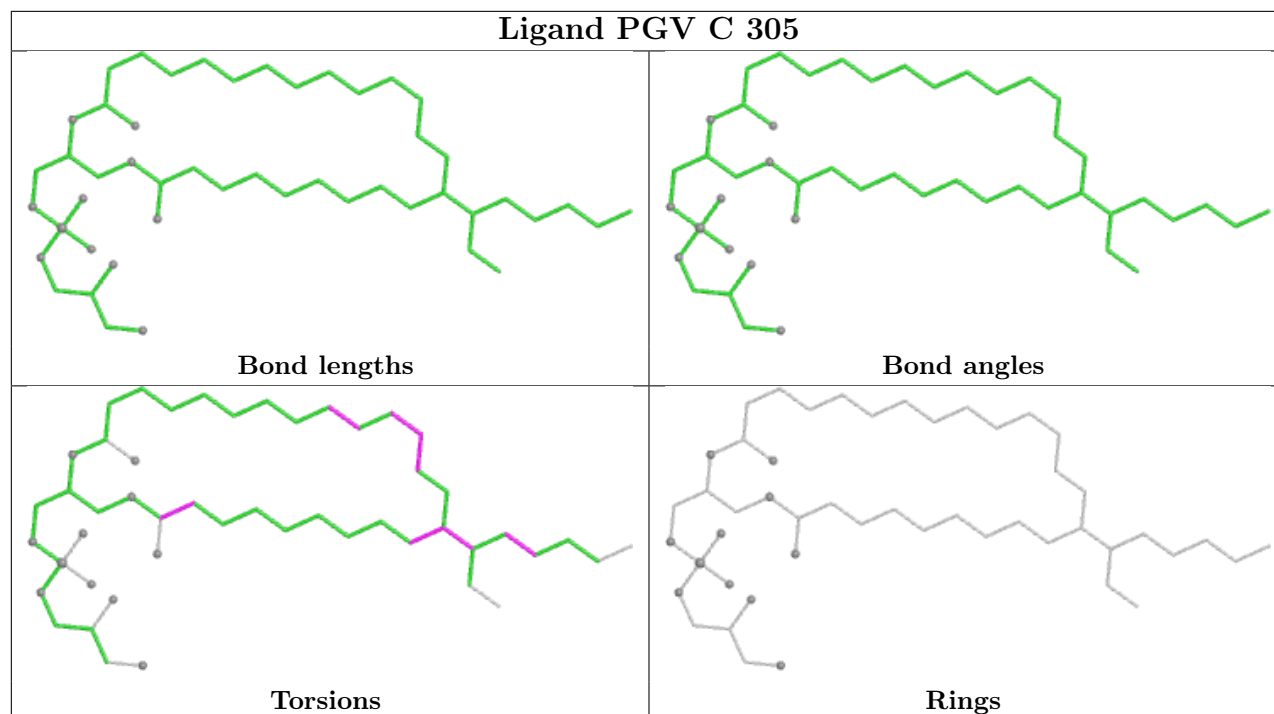


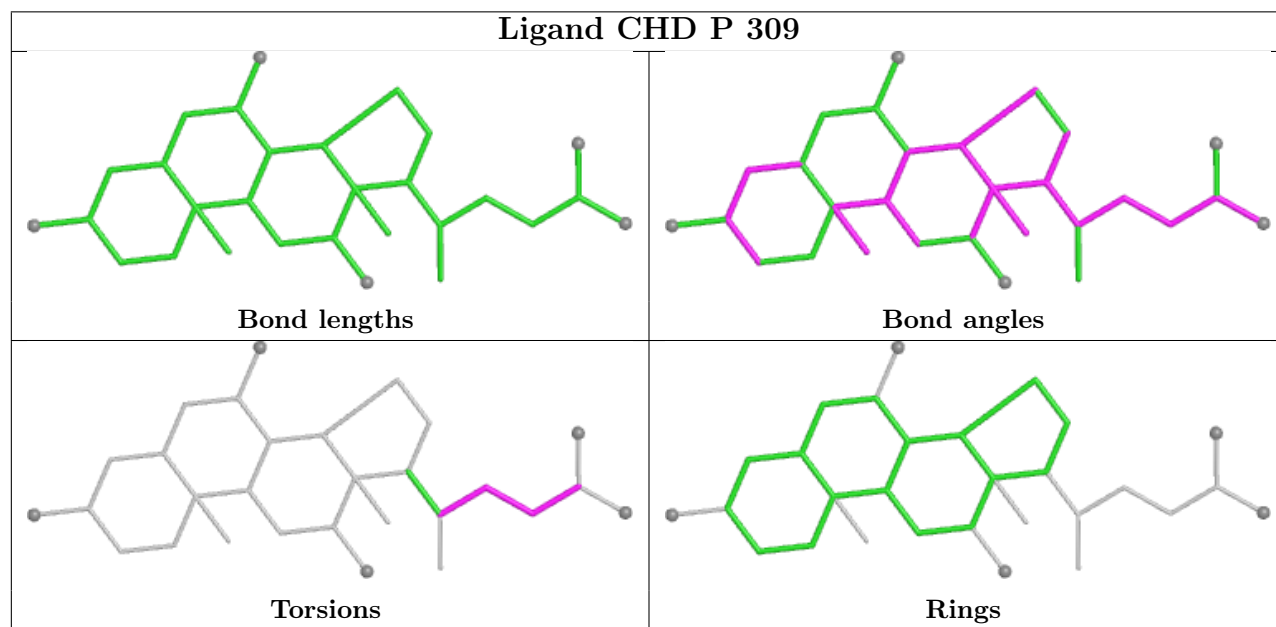
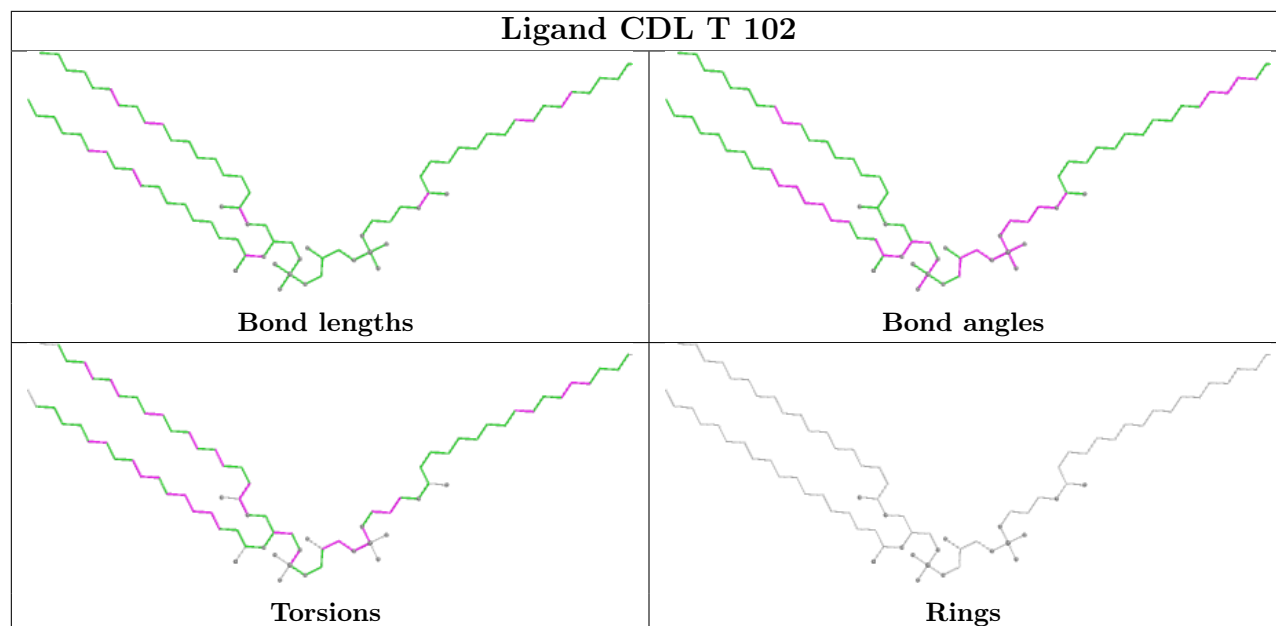
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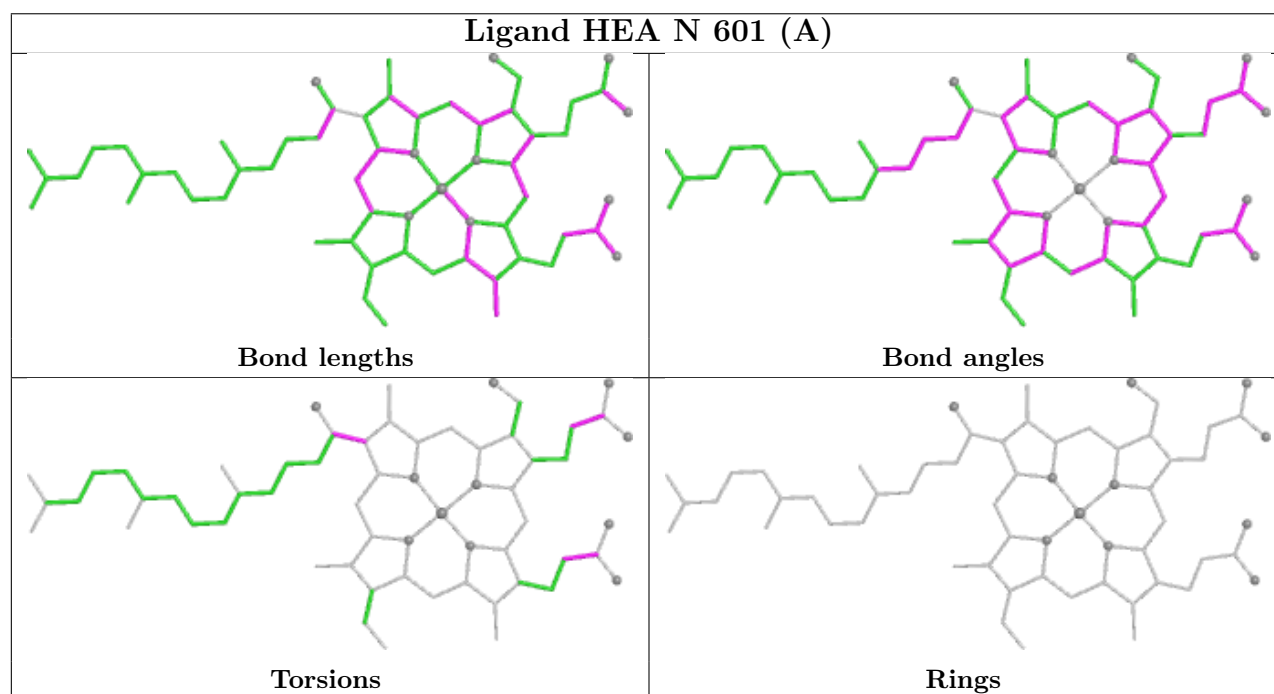
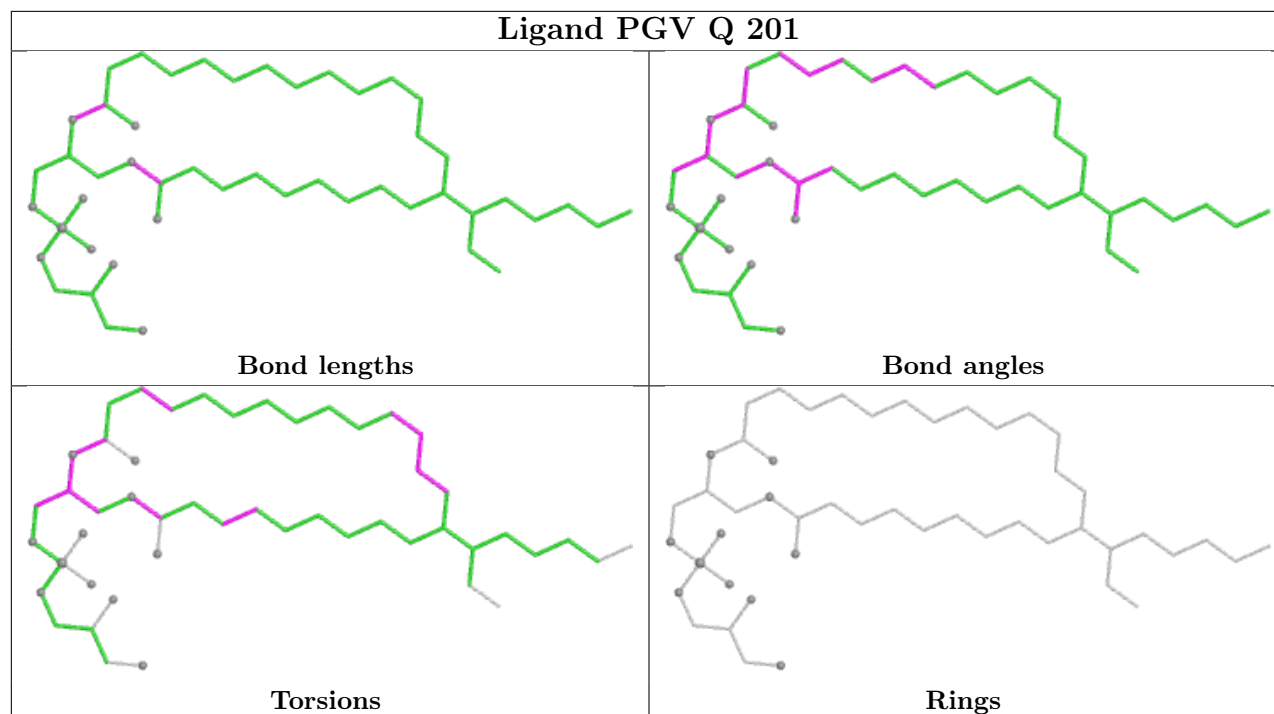


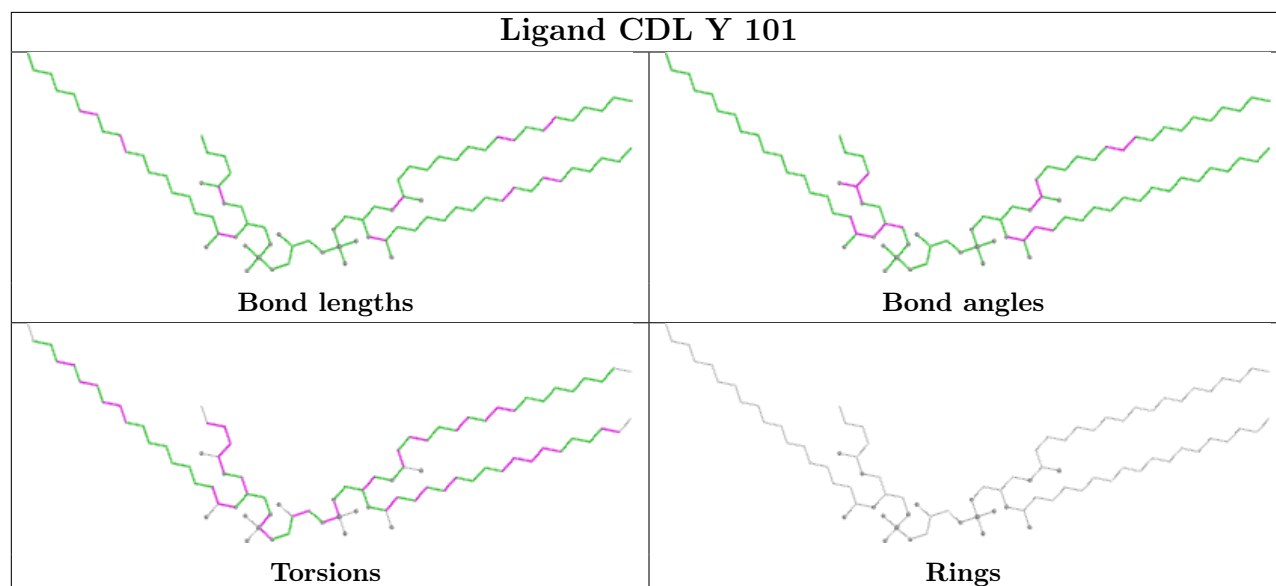
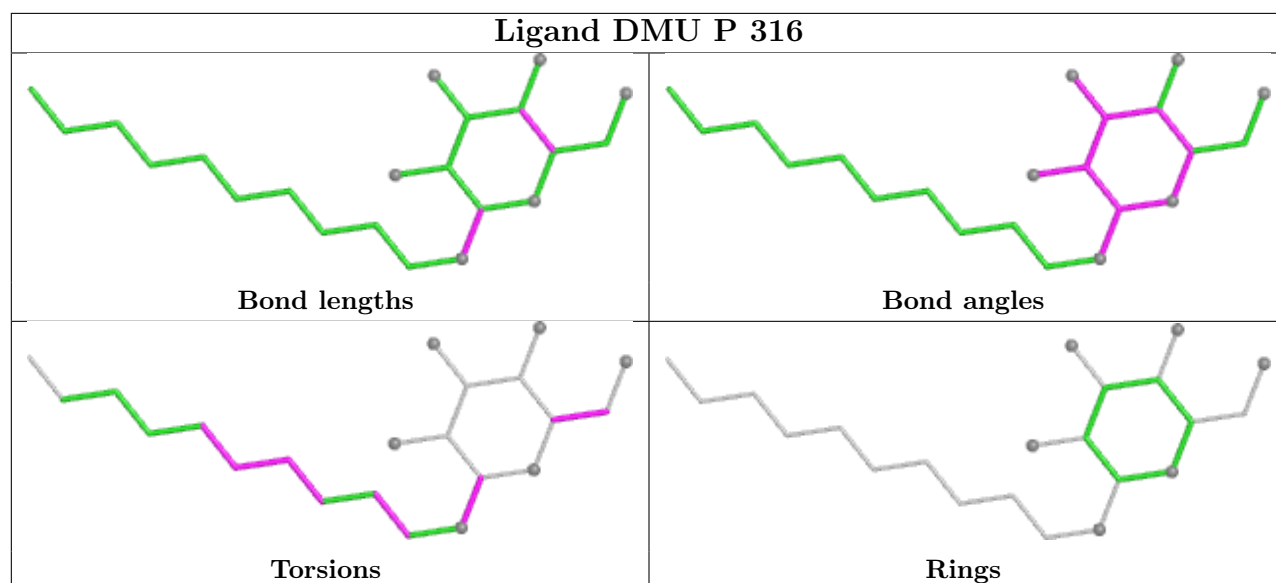
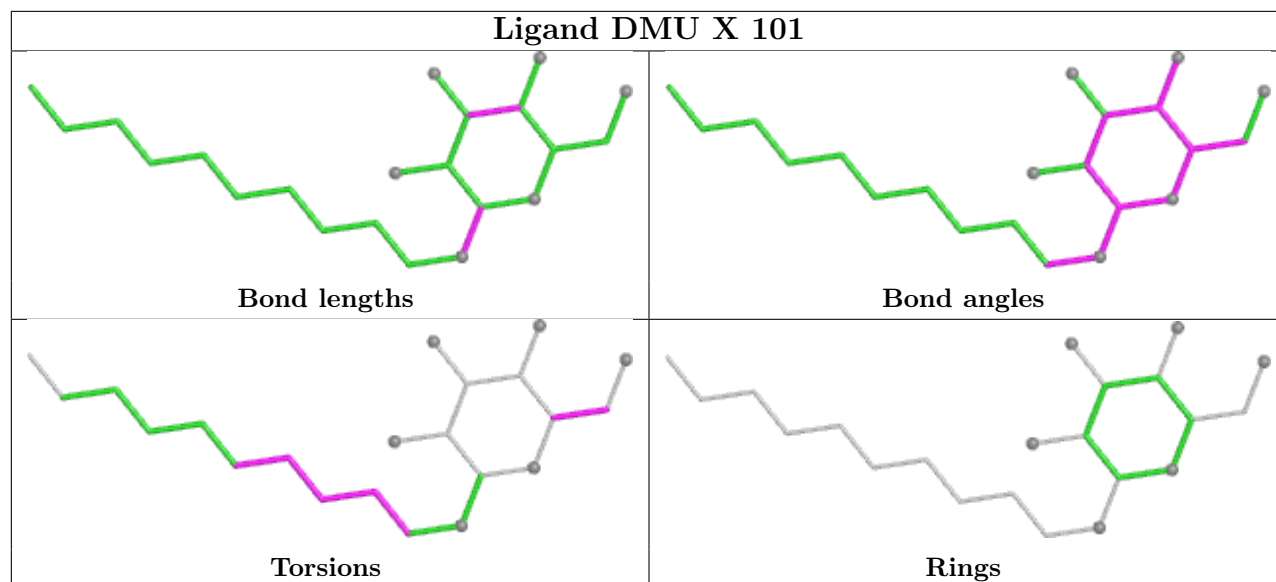
Ligand PGV A 608

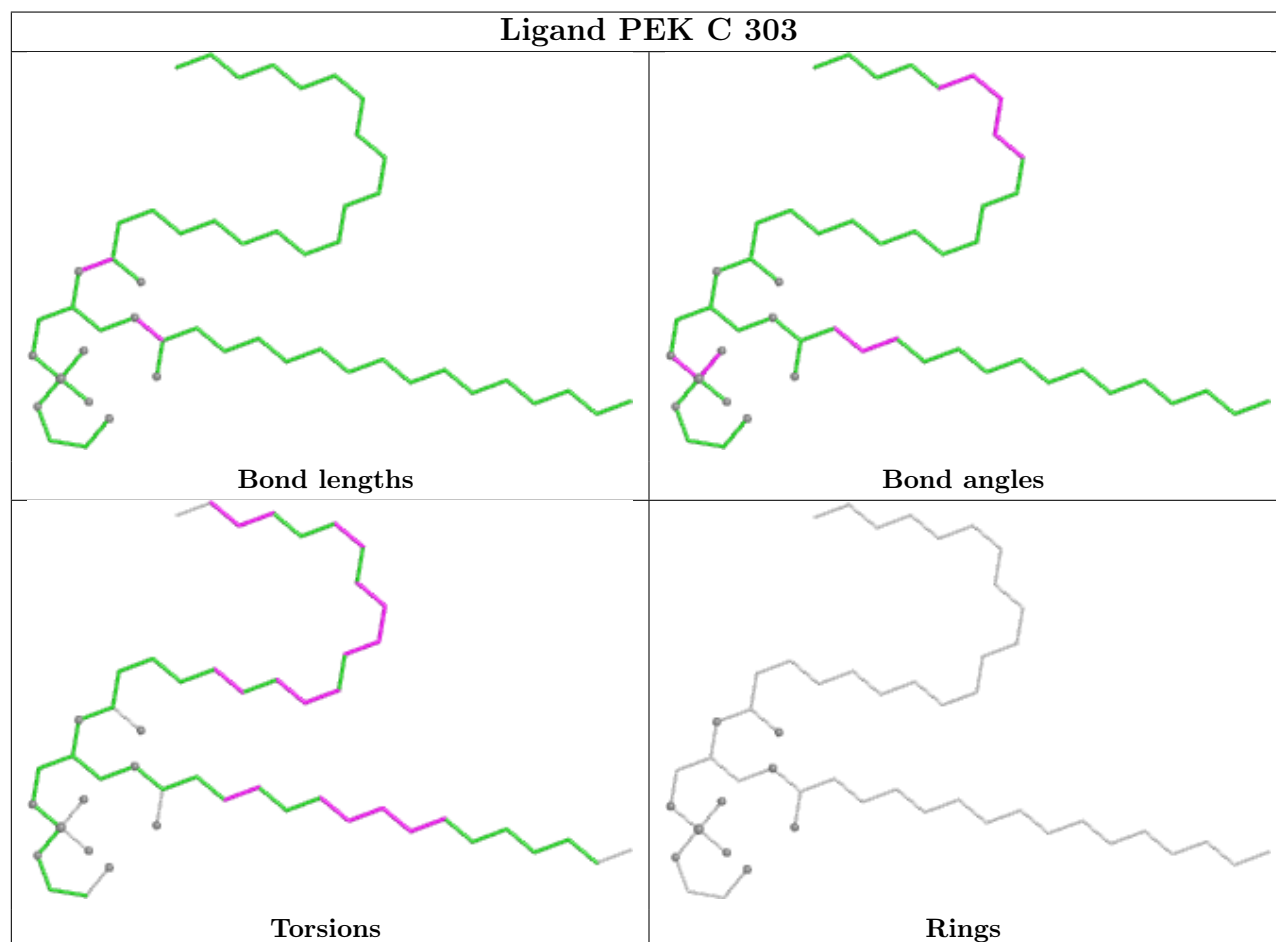
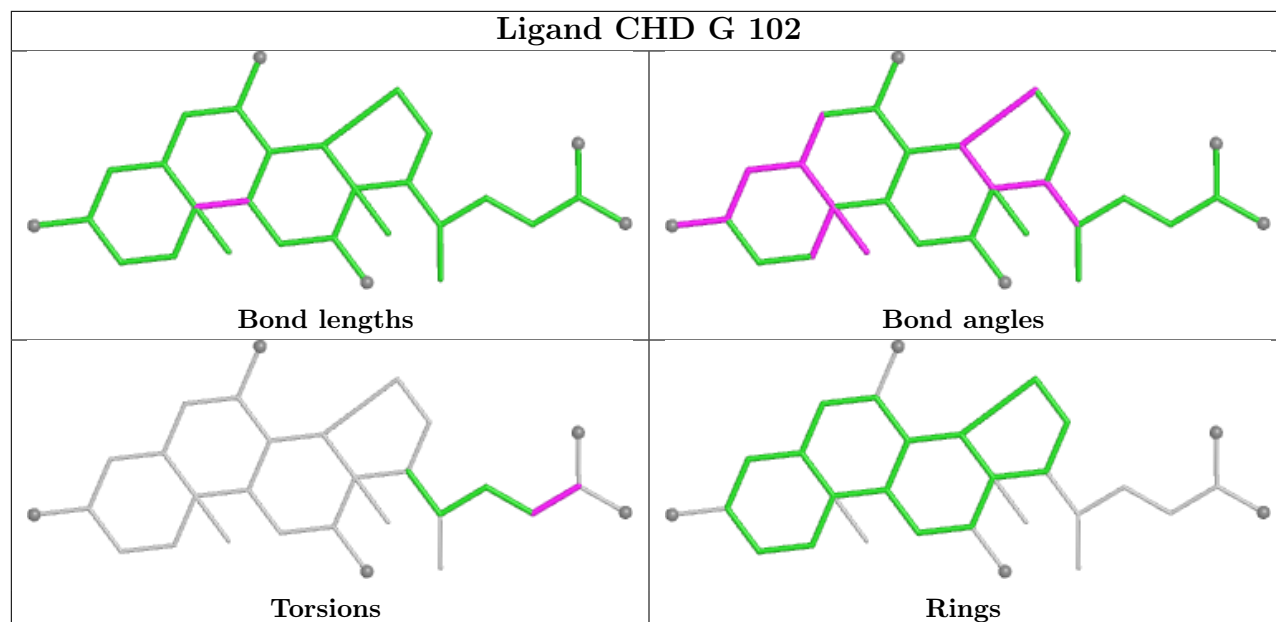


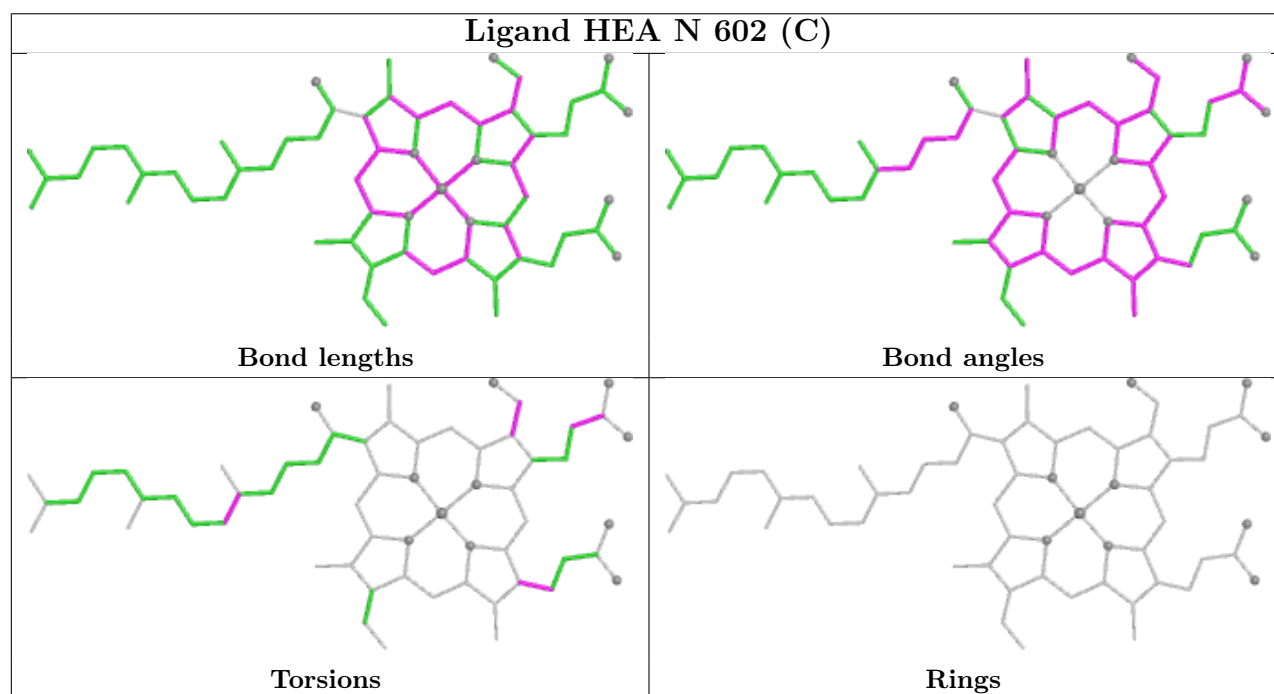
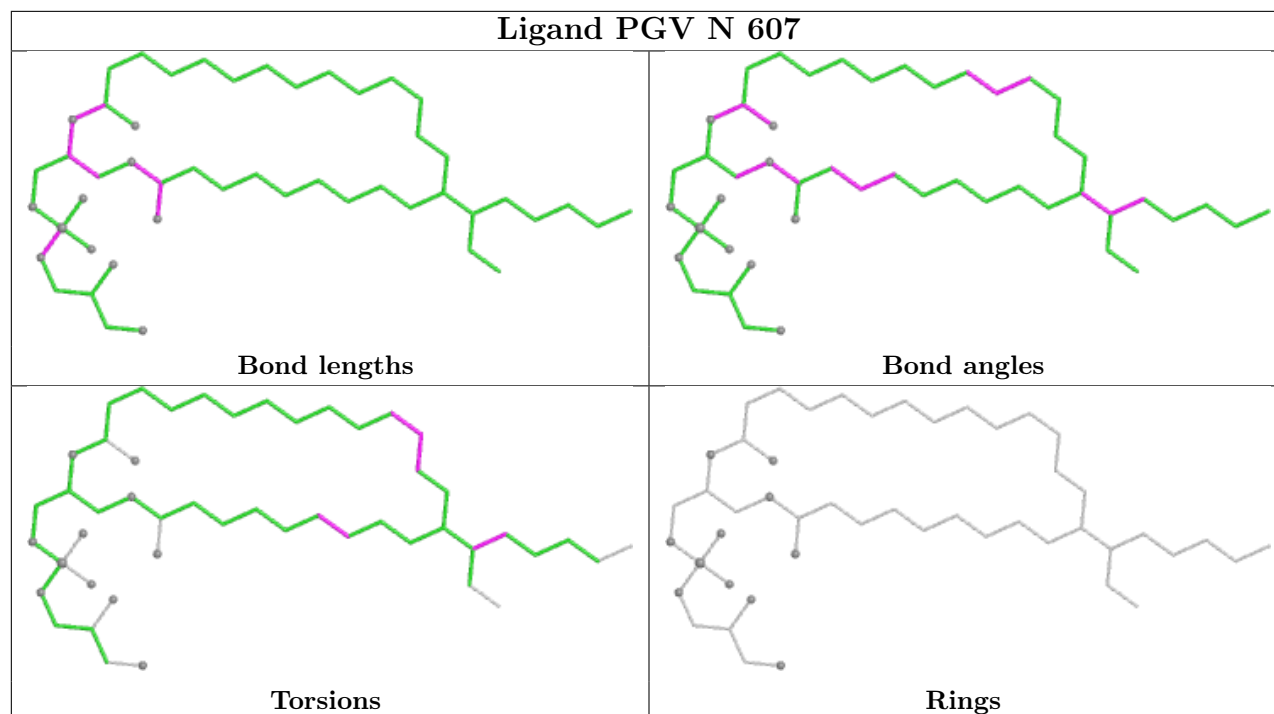


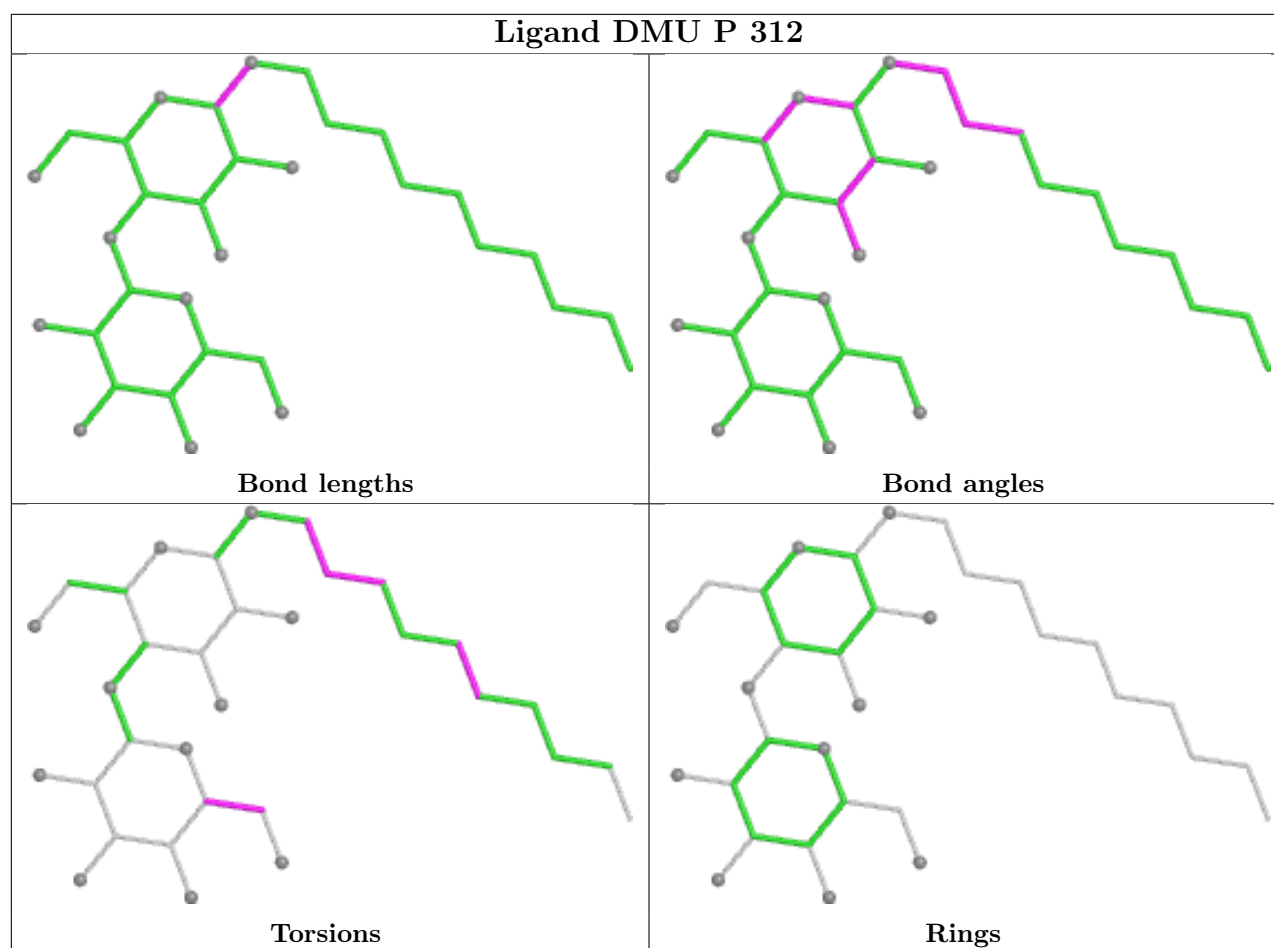


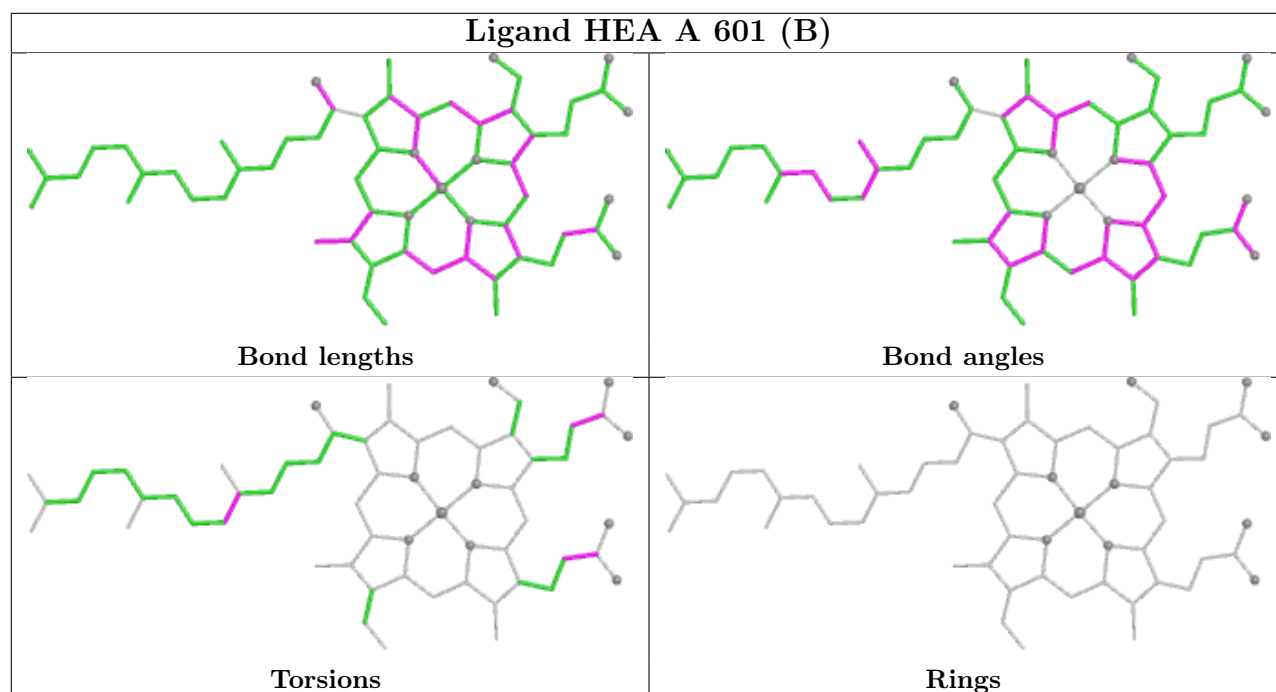
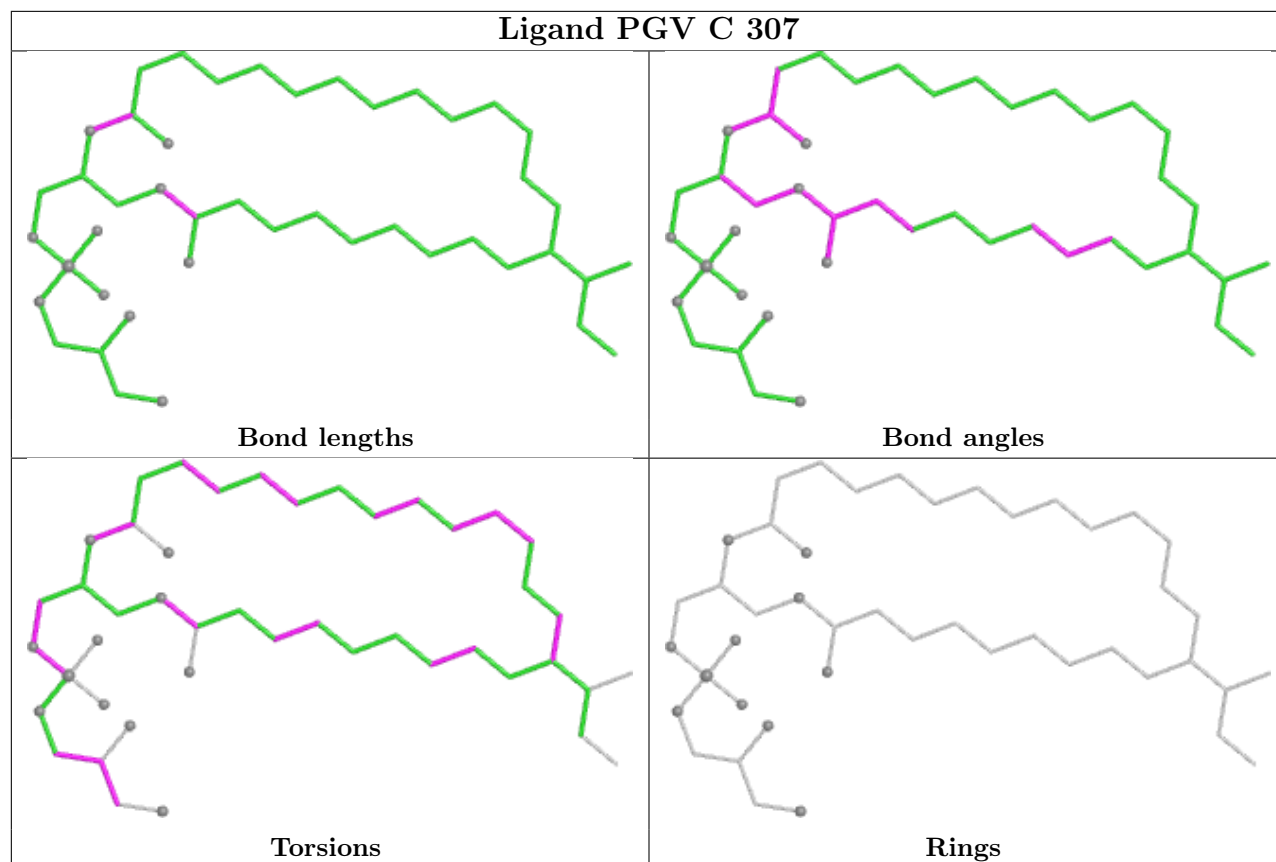


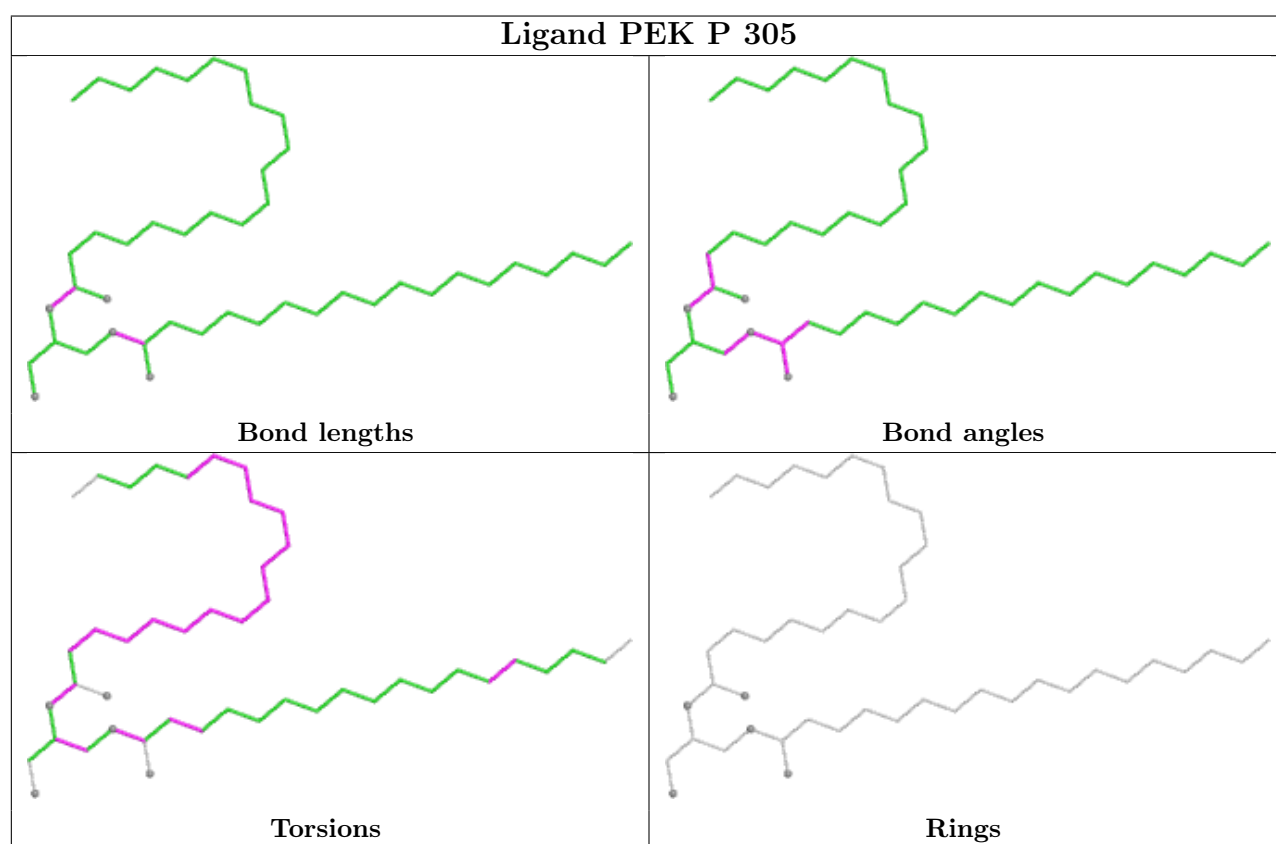
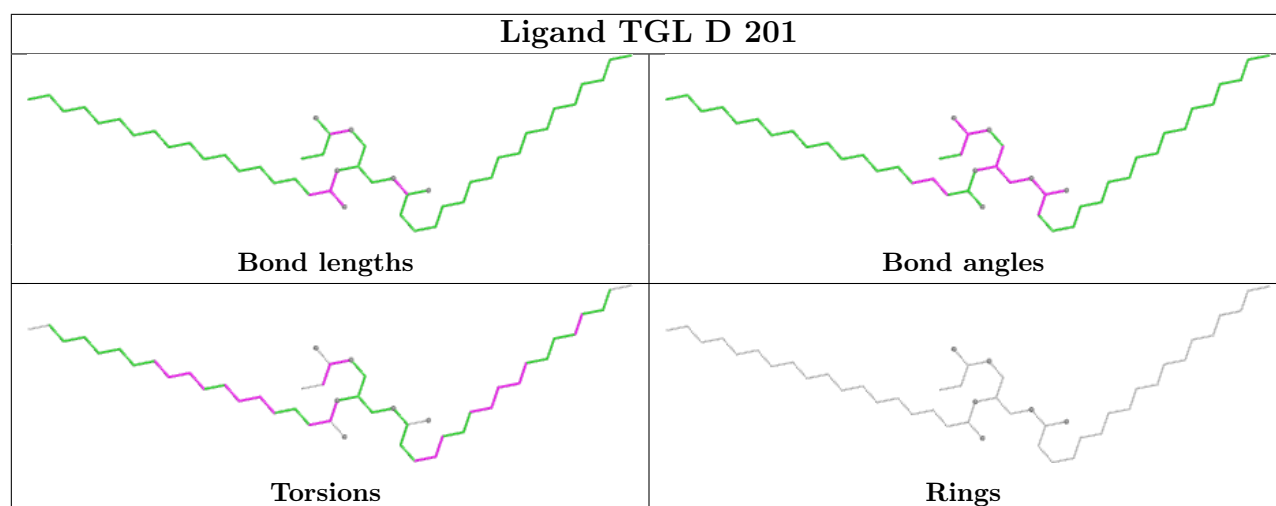




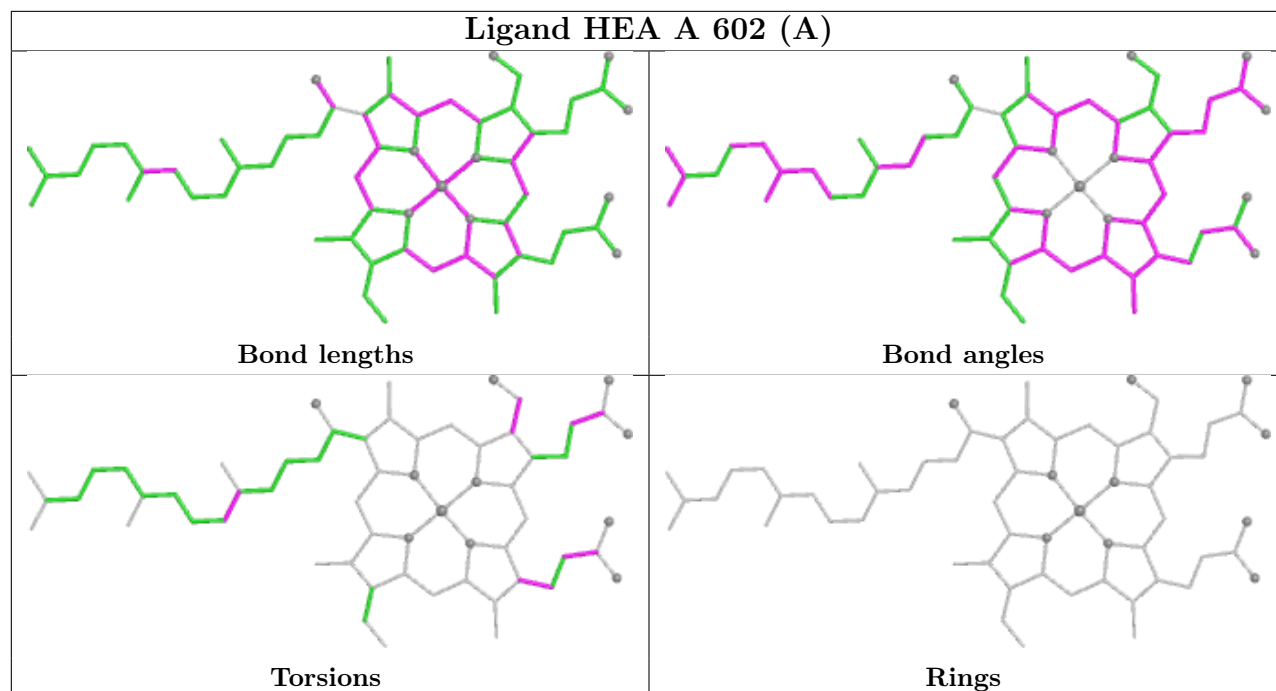




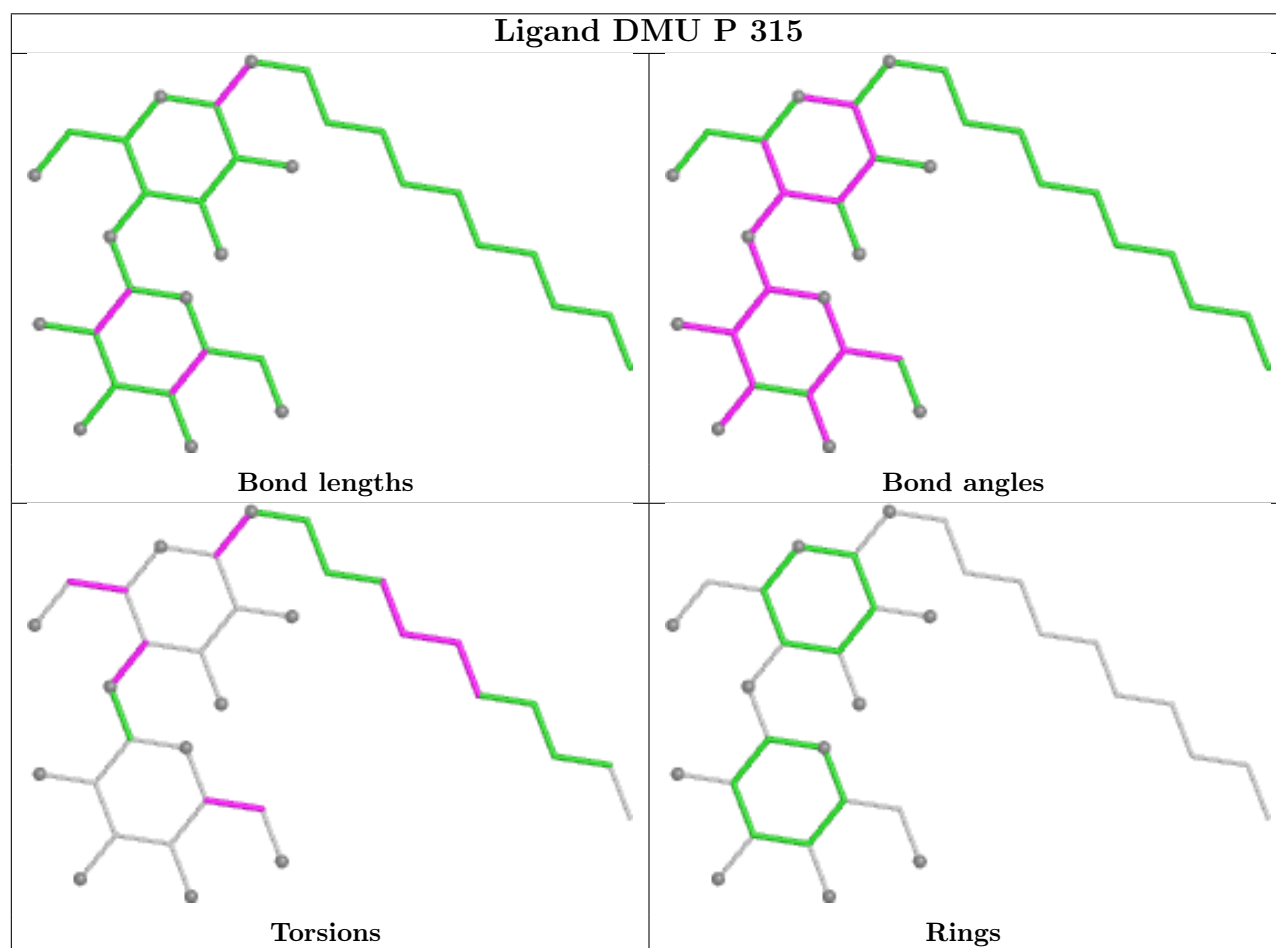


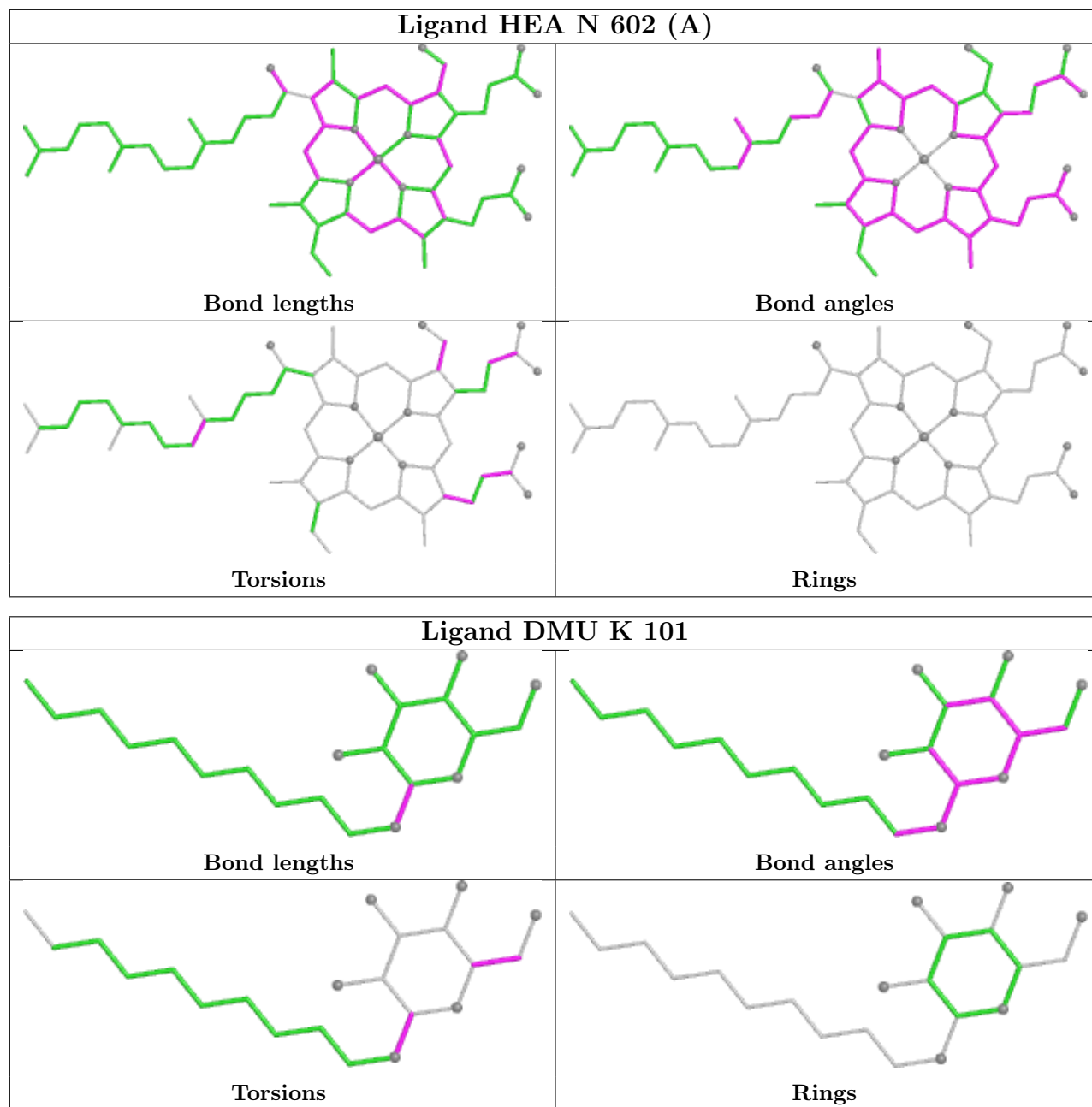


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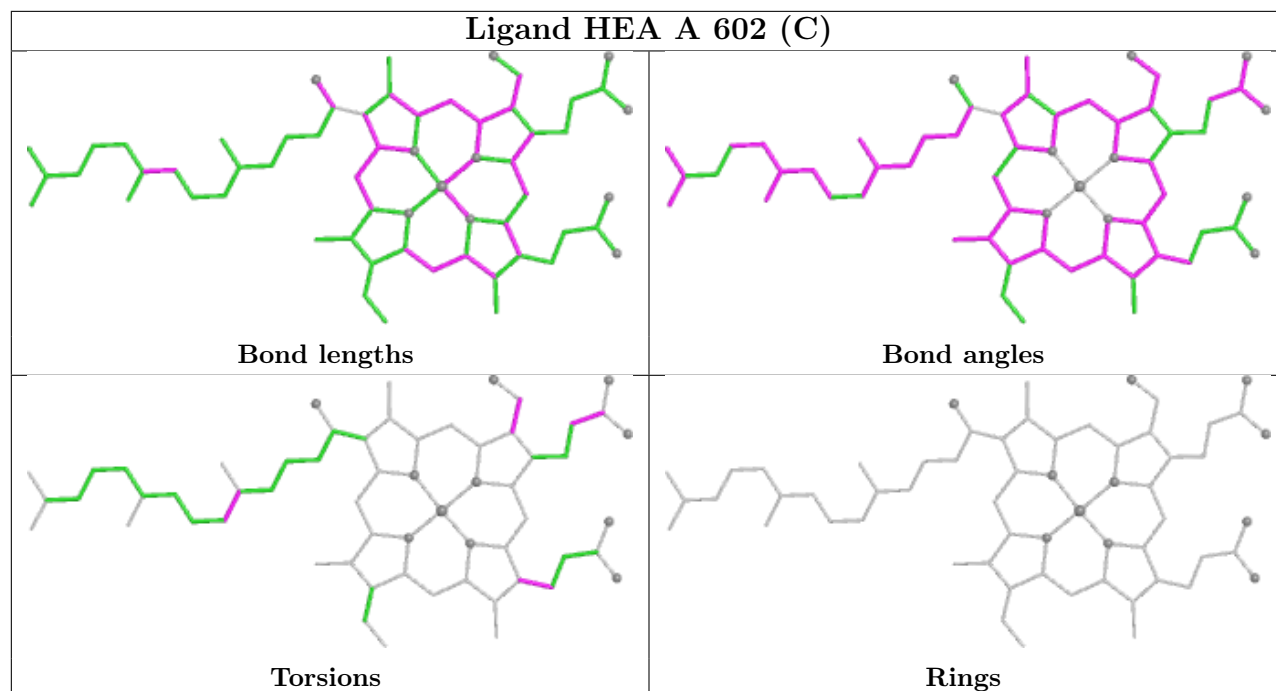


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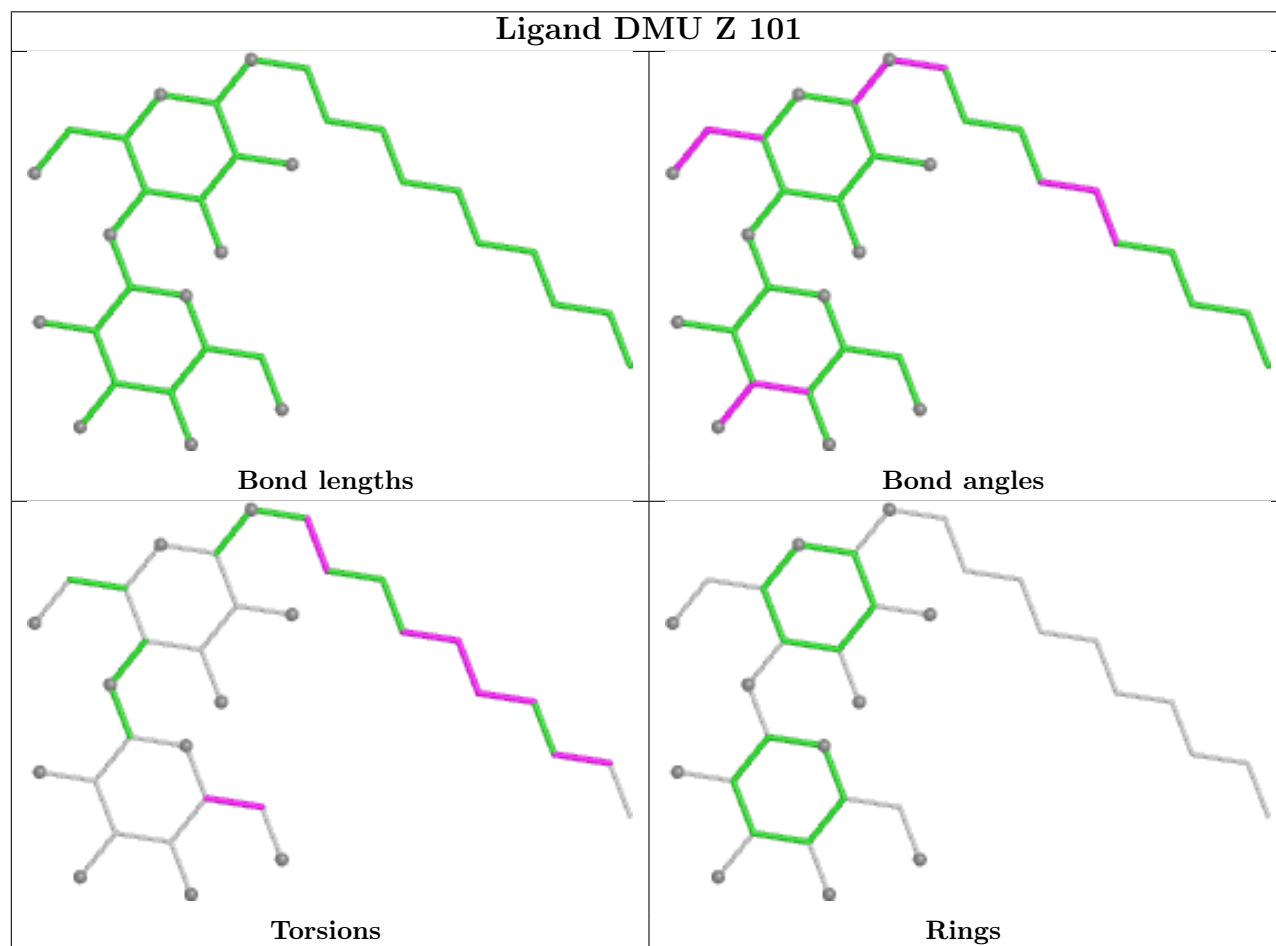


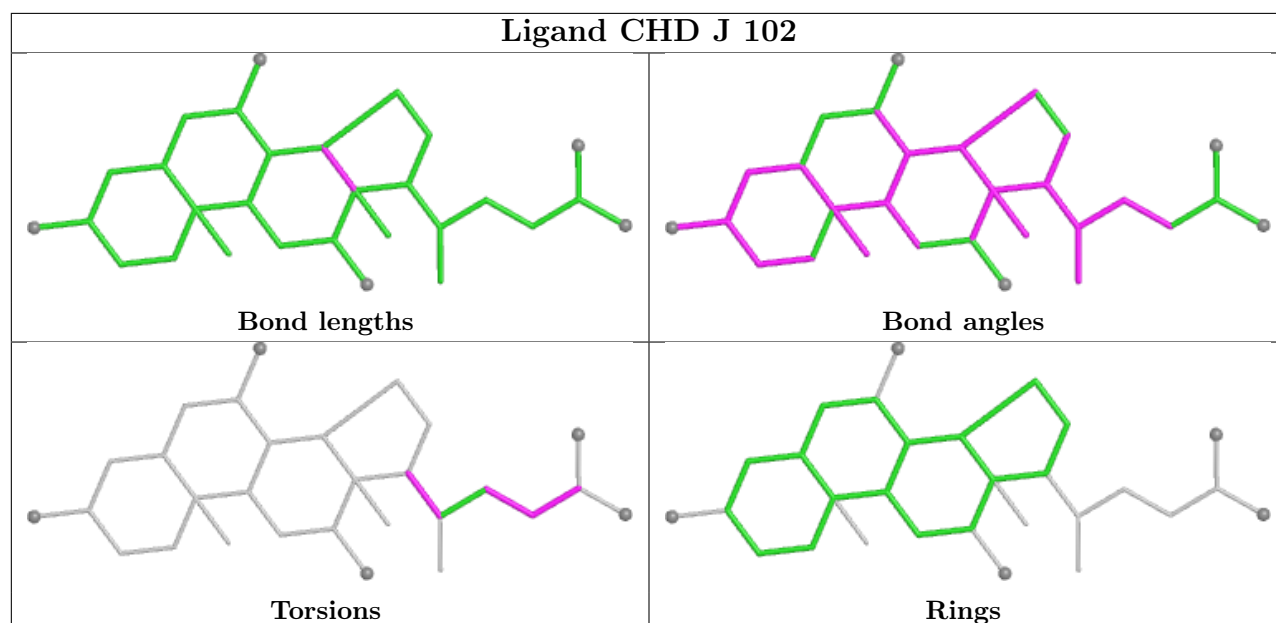
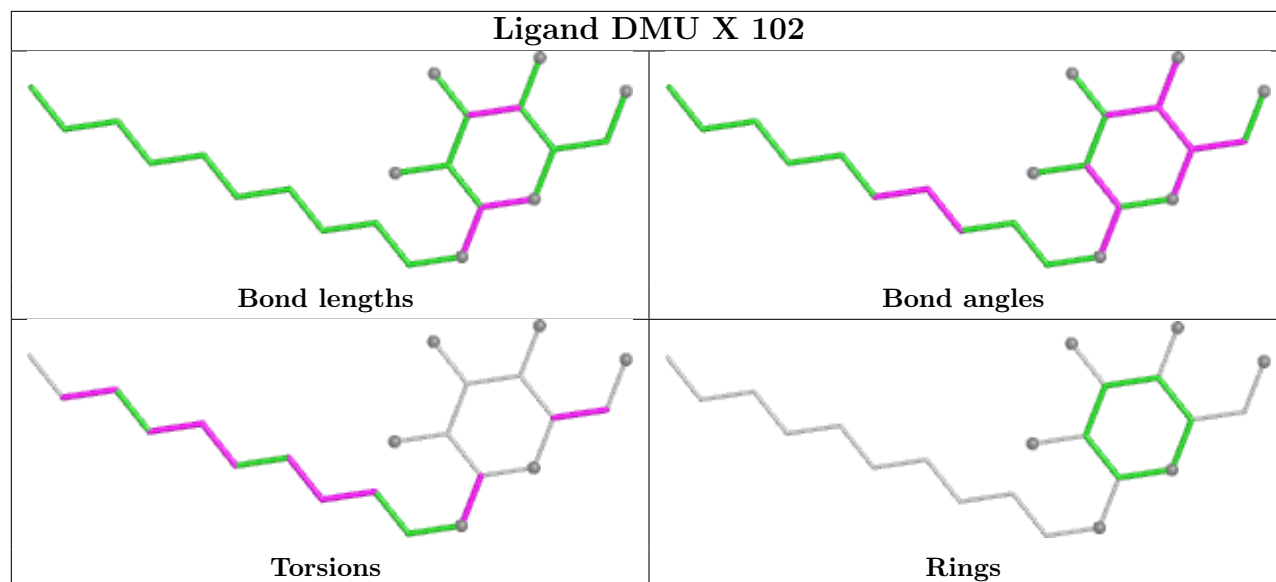


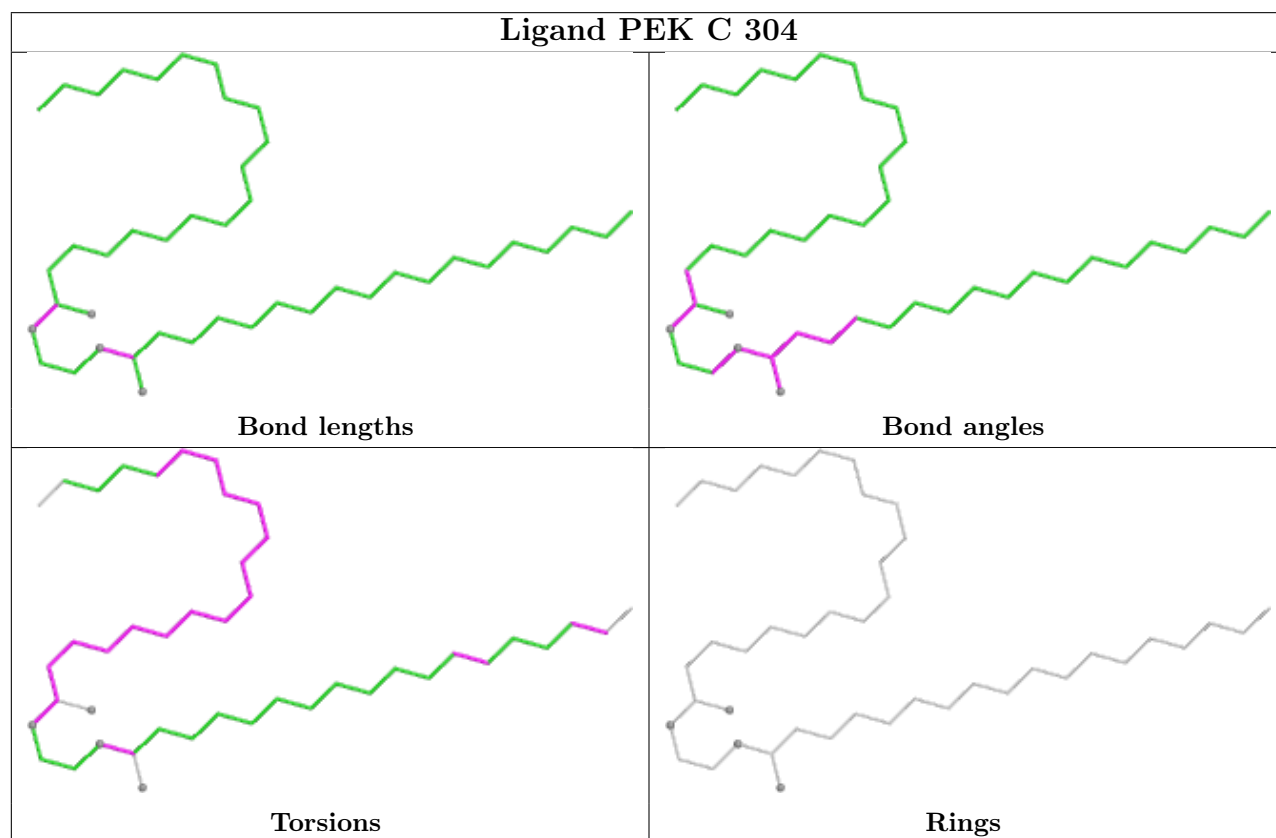
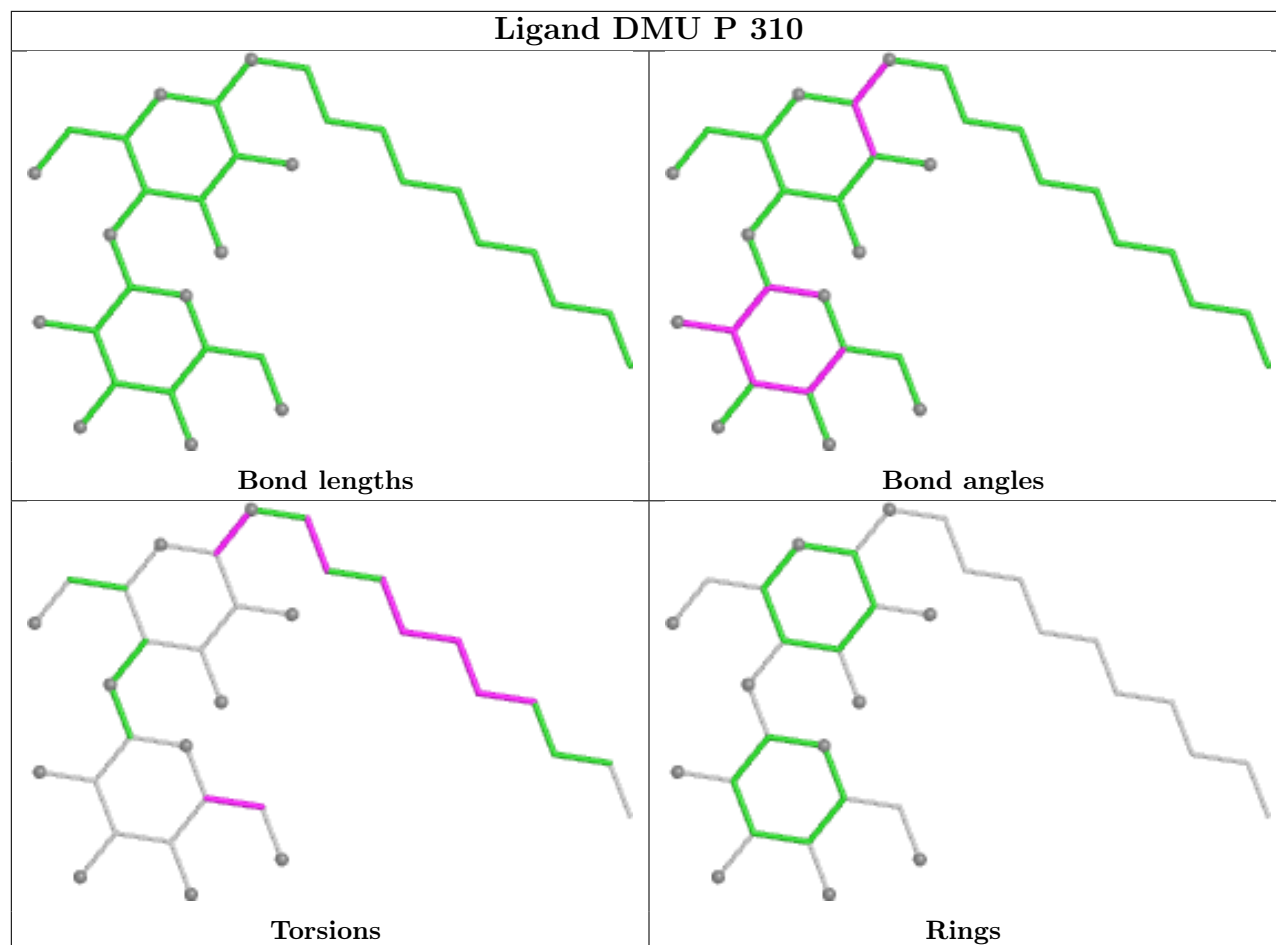
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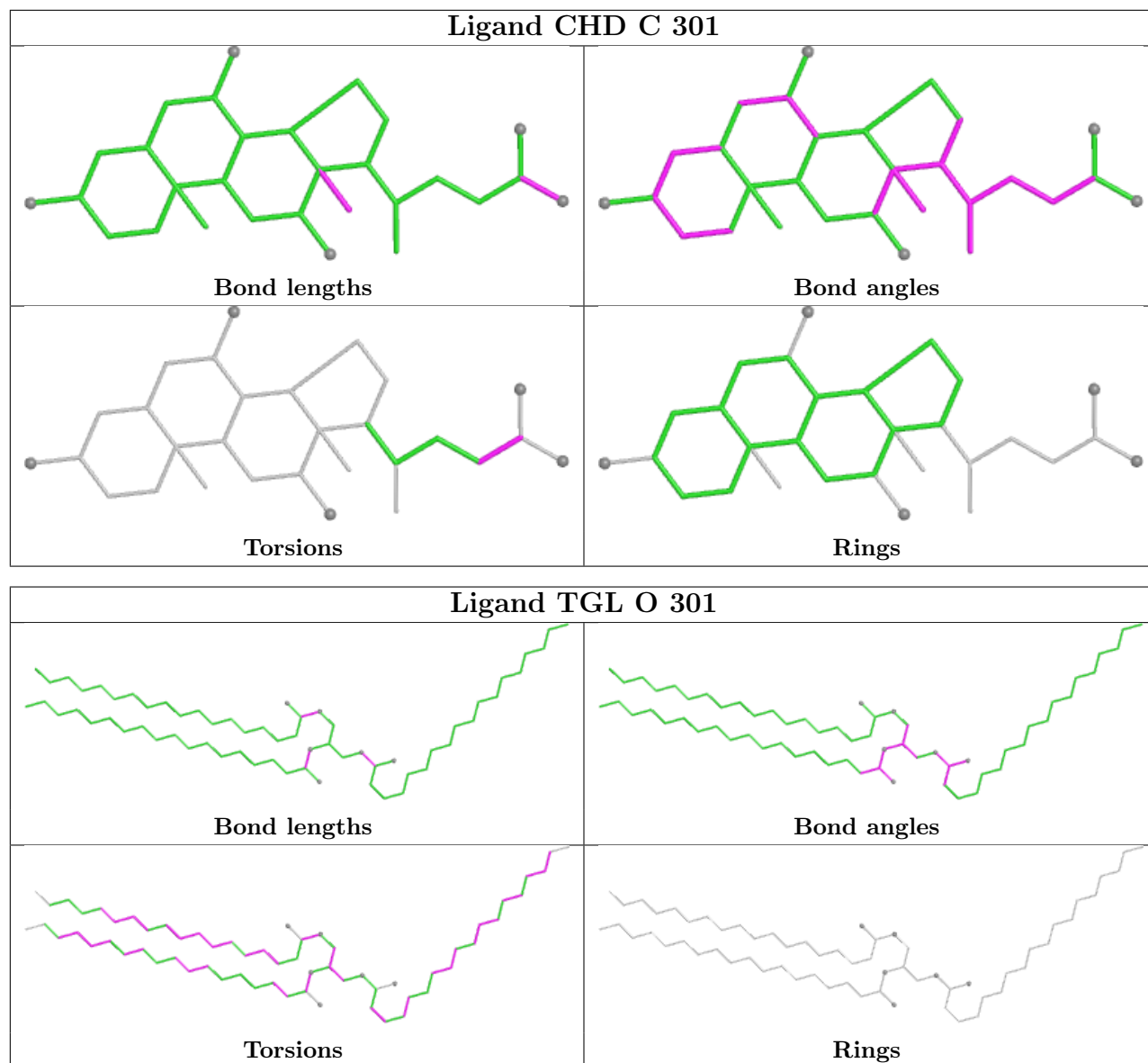


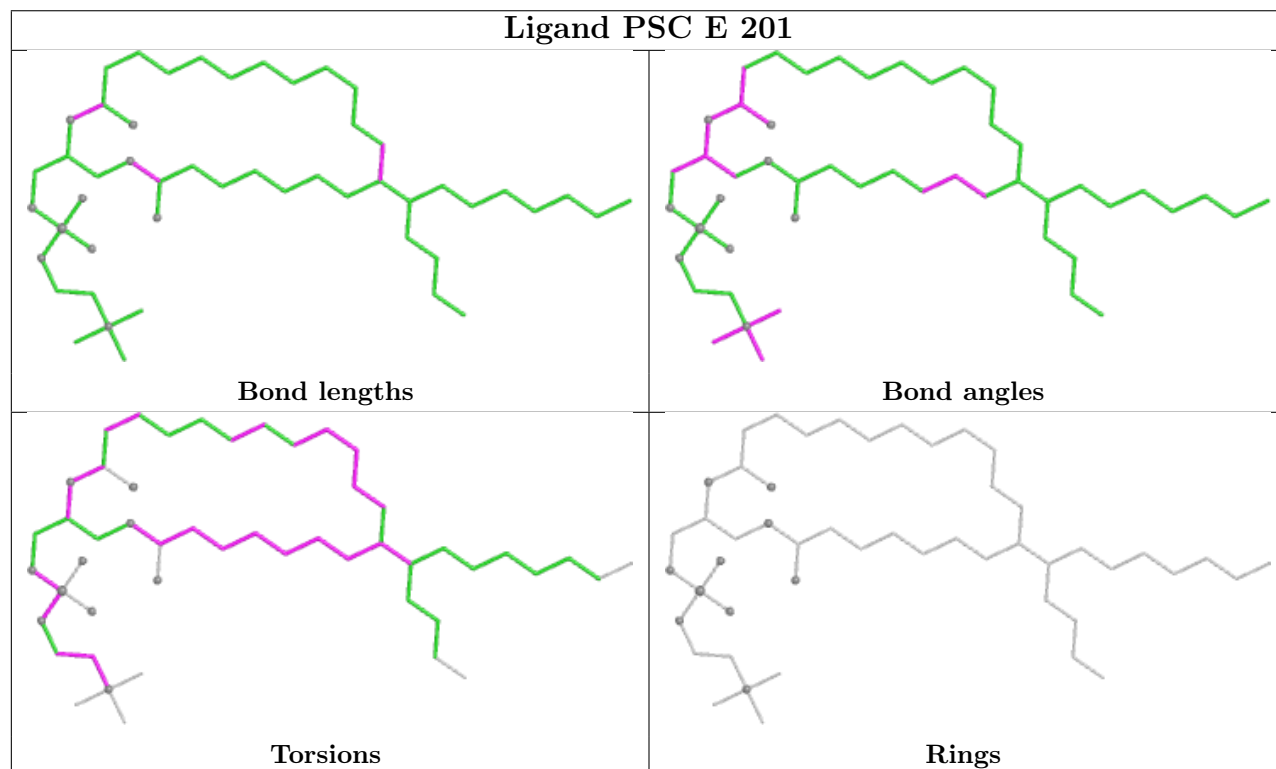
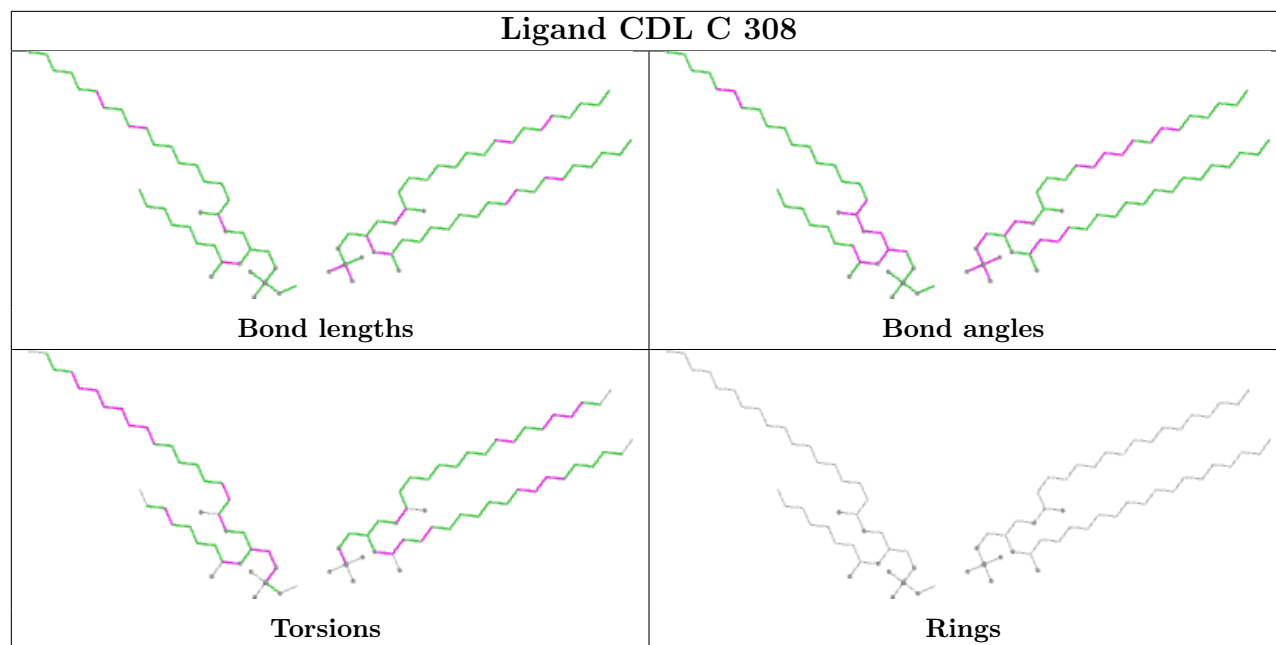
Ligand DMU Z 101

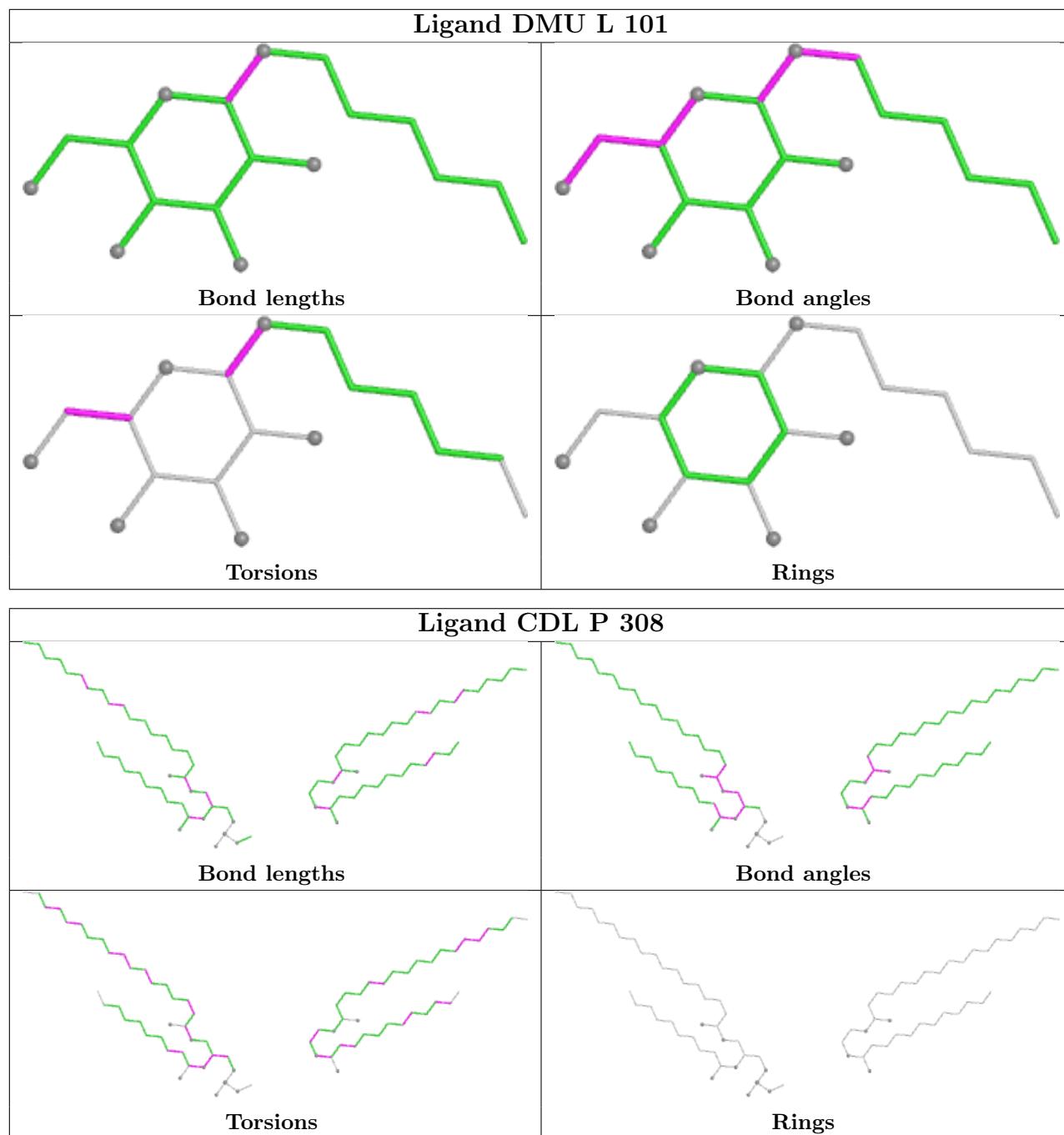


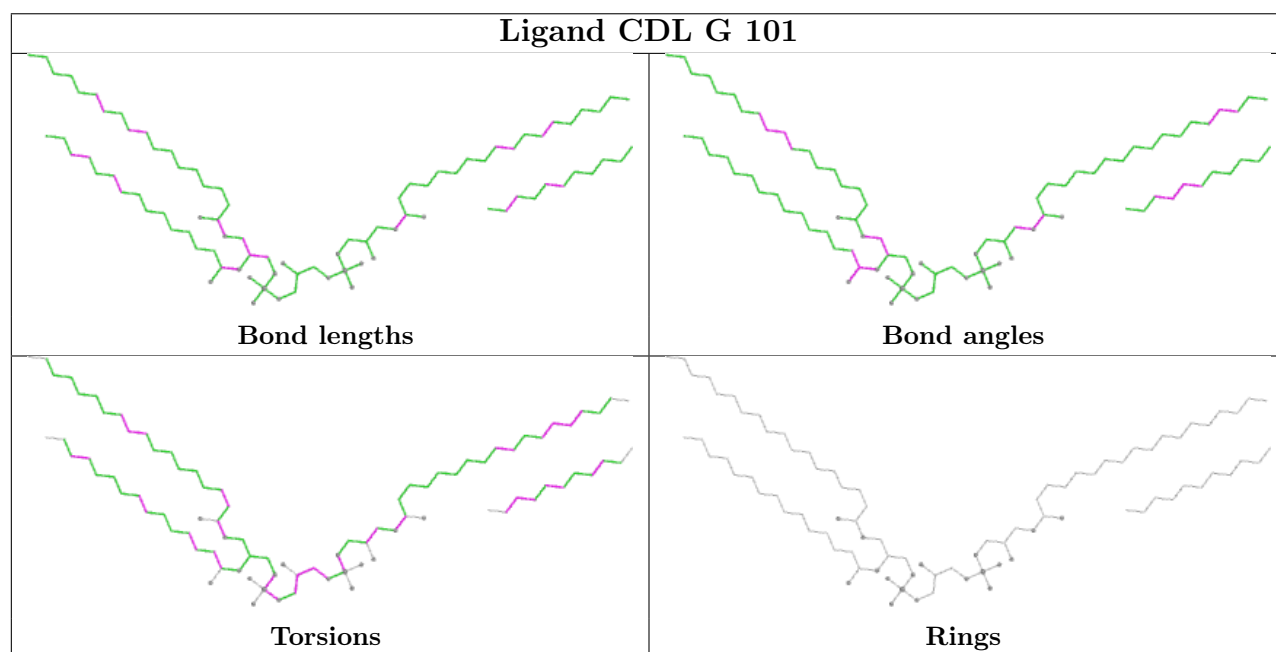
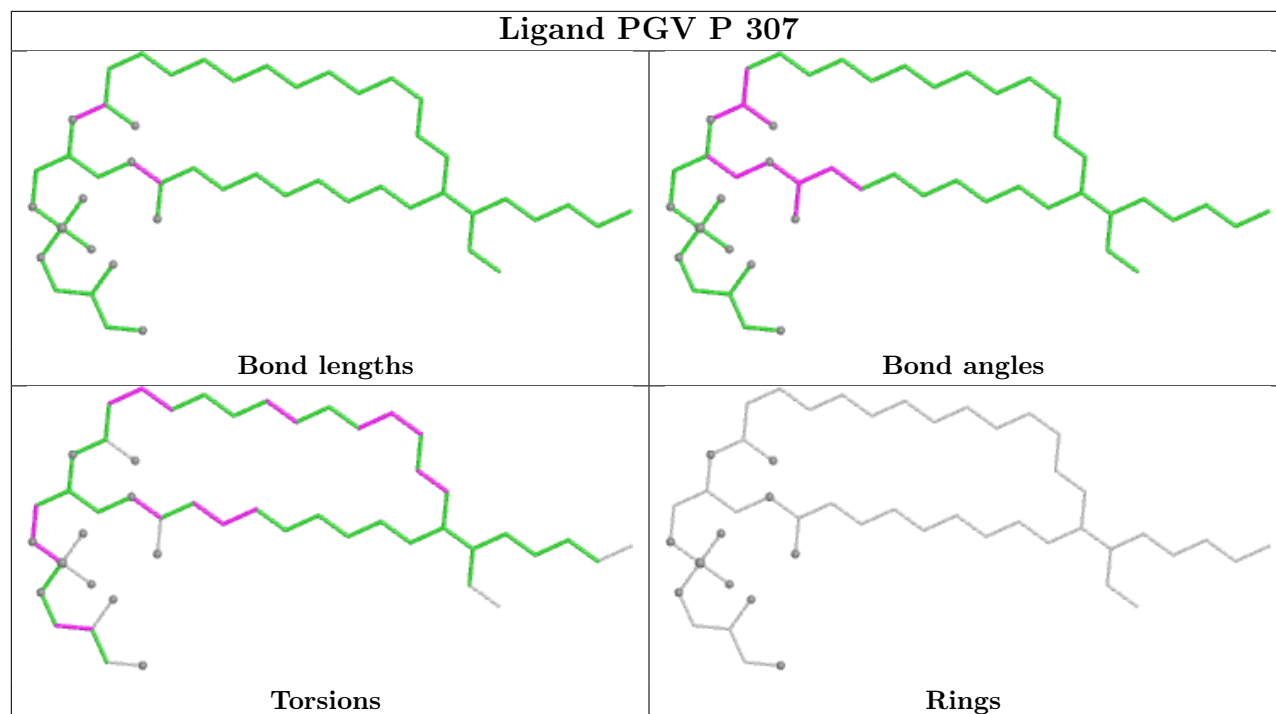


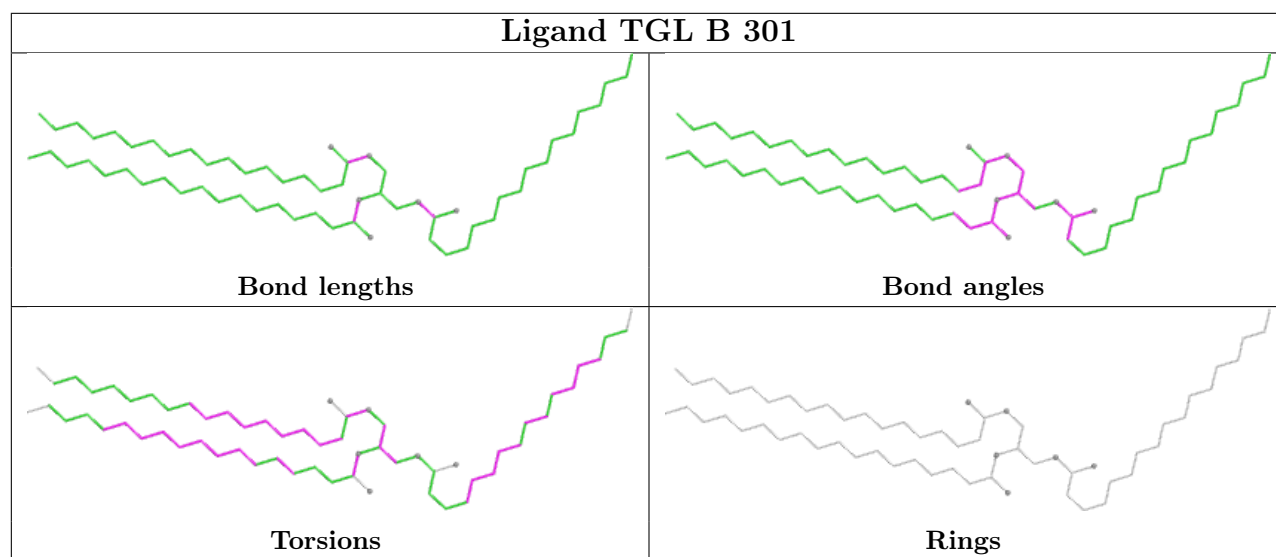
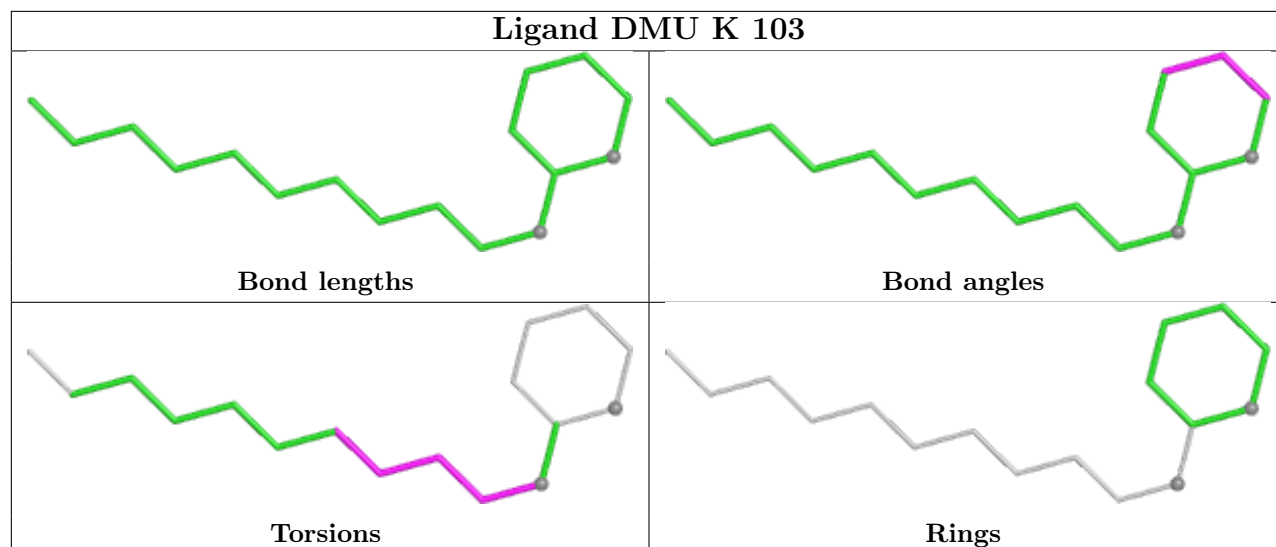


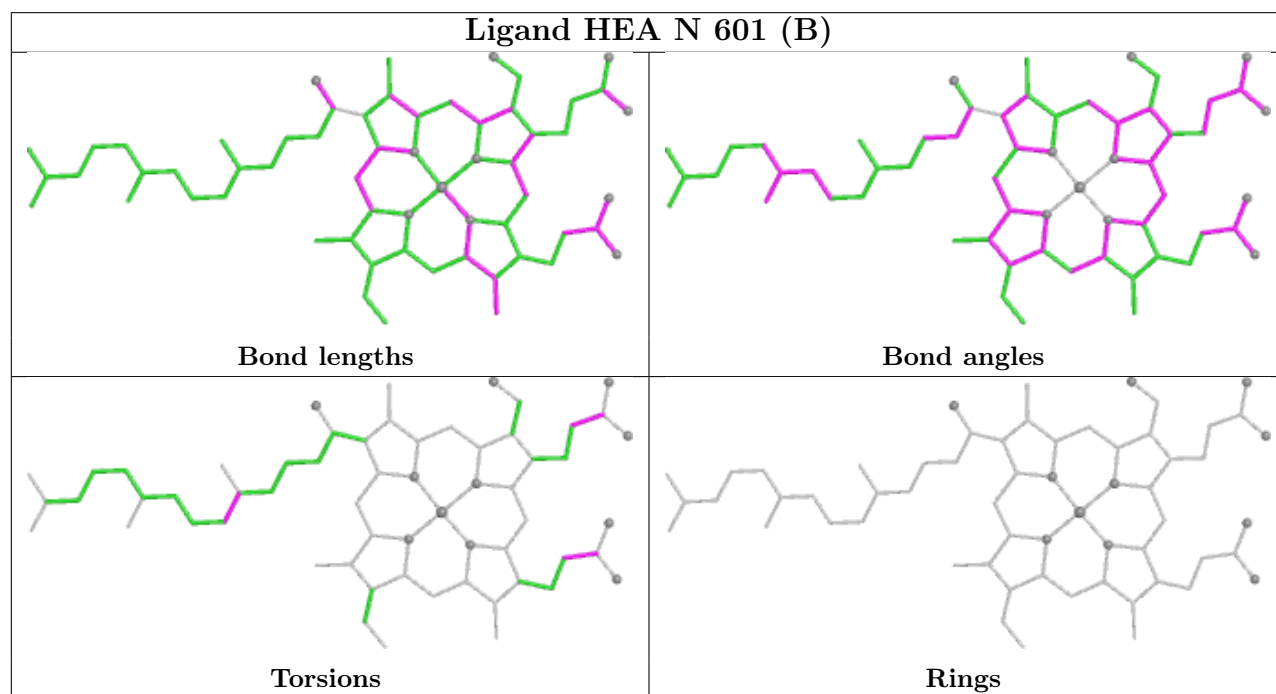
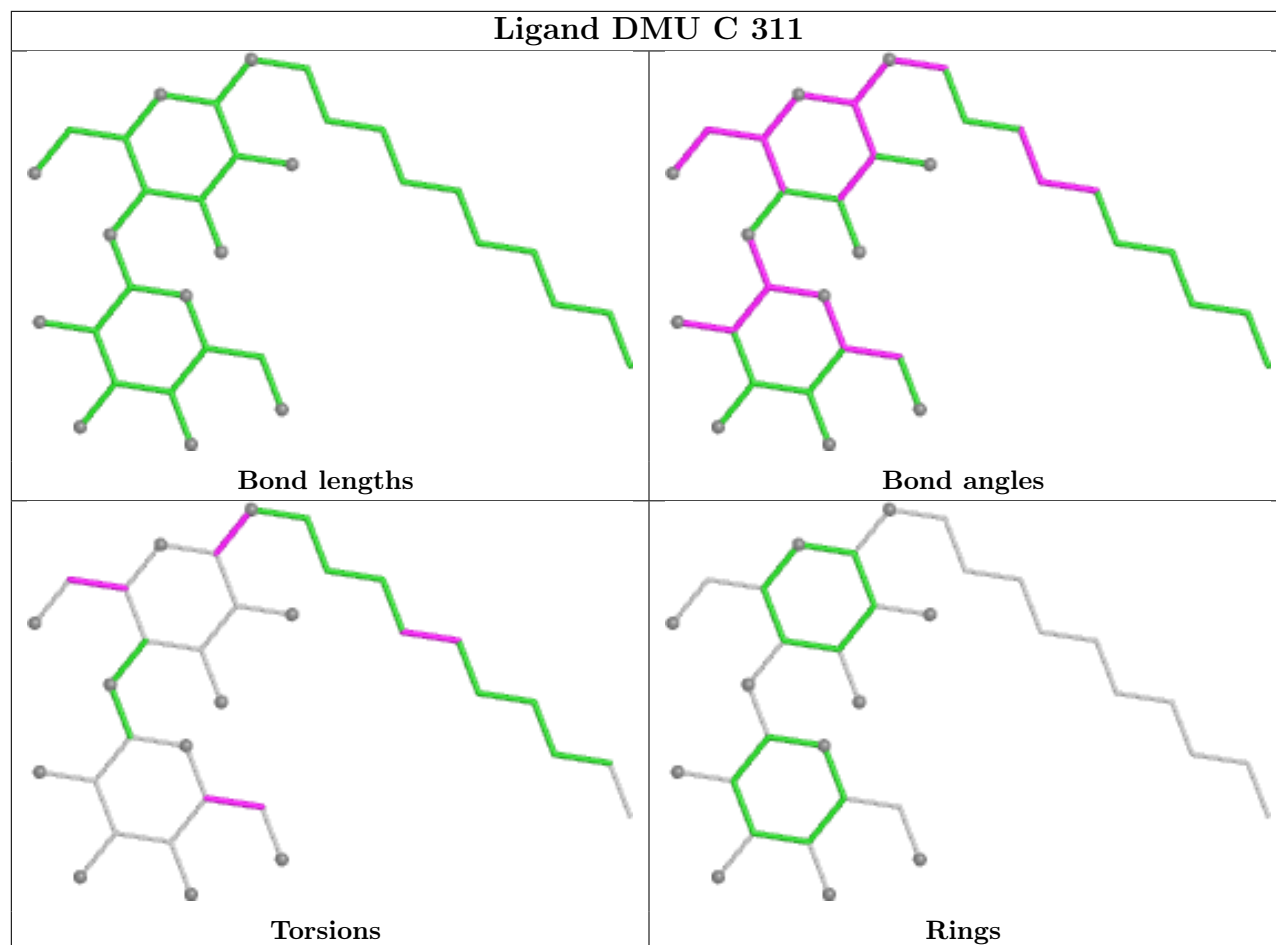


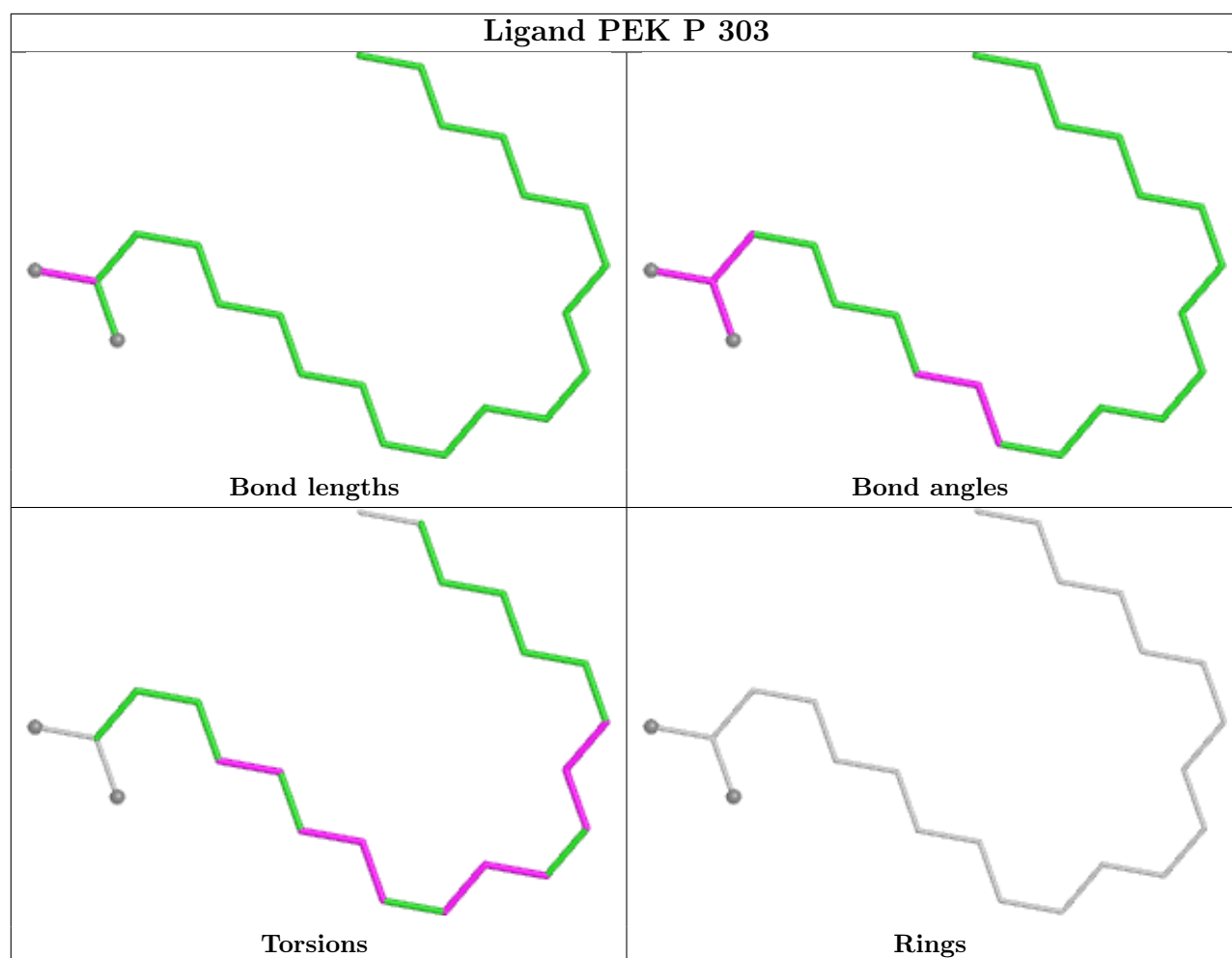












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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%)	-0.14	11 (2%) 63 66	7, 24, 33, 97	34 (6%)
1	N	513/514 (99%)	-0.06	9 (1%) 67 70	8, 27, 35, 81	33 (6%)
2	B	226/227 (99%)	0.57	27 (11%) 9 9	15, 30, 65, 117	26 (11%)
2	O	226/227 (99%)	0.56	21 (9%) 14 14	16, 35, 72, 110	26 (11%)
3	C	259/259 (100%)	0.11	8 (3%) 51 54	18, 28, 42, 81	7 (2%)
3	P	259/259 (100%)	0.13	7 (2%) 56 58	21, 28, 45, 110	6 (2%)
4	D	144/144 (100%)	0.45	7 (4%) 35 36	21, 33, 63, 101	1 (0%)
4	Q	144/144 (100%)	1.32	33 (22%) 2 2	30, 46, 97, 205	3 (2%)
5	E	104/104 (100%)	0.57	4 (3%) 44 47	26, 33, 61, 88	0
5	R	104/104 (100%)	0.98	8 (7%) 19 19	30, 39, 67, 97	0
6	F	93/93 (100%)	0.59	6 (6%) 25 24	21, 31, 63, 111	3 (3%)
6	S	93/93 (100%)	0.61	6 (6%) 25 24	24, 31, 63, 108	4 (4%)
7	G	80/84 (95%)	1.34	21 (26%) 1 1	26, 37, 97, 117	0
7	T	84/84 (100%)	1.54	23 (27%) 1 1	25, 38, 125, 148	2 (2%)
8	H	79/79 (100%)	1.15	19 (24%) 2 2	27, 37, 112, 130	0
8	U	79/79 (100%)	1.22	17 (21%) 2 2	31, 43, 132, 178	0
9	I	72/73 (98%)	1.88	25 (34%) 1 1	30, 46, 114, 194	0
9	V	72/73 (98%)	1.93	31 (43%) 0 1	30, 56, 98, 182	0
10	J	57/57 (100%)	0.83	8 (14%) 6 7	28, 37, 78, 102	0
10	W	57/57 (100%)	1.00	9 (15%) 5 5	28, 39, 80, 144	0
11	K	49/49 (100%)	0.71	3 (6%) 27 26	25, 37, 59, 72	2 (4%)
11	X	49/49 (100%)	1.23	11 (22%) 2 2	36, 47, 84, 104	0
12	L	46/46 (100%)	0.35	3 (6%) 25 24	24, 29, 50, 115	0
12	Y	46/46 (100%)	0.72	6 (13%) 7 8	29, 34, 69, 209	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	41/41 (100%)	0.54	5 (12%) 8 8	23, 29, 58, 81	1 (2%)
13	Z	41/41 (100%)	1.10	6 (14%) 6 6	33, 38, 77, 122	0
All	All	3530/3540 (99%)	0.50	334 (9%) 14 13	7, 31, 76, 209	149 (4%)

All (334) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	29	LEU	12.5
4	Q	5	VAL	11.4
7	T	3	ALA	11.1
6	F	2	SER	8.3
3	P	3	HIS	8.1
9	I	25	PHE	8.1
8	H	8	ILE	7.9
7	G	36	TRP	7.8
4	D	4	SER	7.7
7	T	5	LYS	7.7
6	S	94	HIS	7.6
4	Q	6	VAL	7.6
8	U	45	ALA	7.4
7	T	7	ASP	7.2
9	I	32	ALA	7.2
6	F	3	GLY	7.1
8	U	8	ILE	7.1
9	V	3	ALA	6.7
4	Q	8	SER	6.7
7	T	8	HIS	6.6
2	O	113	TYR	6.5
7	T	11	THR	6.4
12	Y	2	HIS	6.4
8	U	46	LYS	6.2
7	T	10	GLY	6.1
2	B	90	ILE	6.0
9	I	30	GLY	6.0
8	H	46	LYS	5.9
6	F	94	HIS	5.8
9	V	37	PHE	5.8
13	Z	40	TYR	5.6
7	G	8	HIS	5.5
10	J	1	PHE	5.5
6	S	3	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	61	VAL	5.5
7	G	37	LEU	5.4
2	O	90	ILE	5.4
9	I	37	PHE	5.4
8	U	44	THR	5.4
9	I	34	PHE	5.3
7	G	5	LYS	5.3
10	W	57	HIS	5.2
7	T	9	GLY	5.2
7	G	10	GLY	5.1
9	I	2	THR	5.1
9	I	33	THR	5.1
9	V	2	THR	5.1
2	B	58	ALA	5.1
13	M	40	TYR	5.1
1	A	312	ILE	5.1
12	L	2	HIS	5.0
7	G	7	ASP	4.9
7	T	38	HIS	4.9
5	R	109	VAL	4.9
7	T	1	ALA	4.8
11	K	6	ALA	4.8
7	T	36	TRP	4.8
6	S	93	PRO	4.8
2	B	59	GLN	4.7
9	V	34	PHE	4.7
2	O	227	LEU	4.7
2	B	113	TYR	4.6
7	G	11	THR	4.6
9	V	30	GLY	4.6
9	I	31	PHE	4.6
7	T	40	GLY	4.6
9	V	29	LEU	4.6
8	H	45	ALA	4.5
9	I	22	VAL	4.4
2	B	65	TRP	4.4
12	Y	47	LYS	4.4
4	Q	7	LYS	4.4
7	T	37	LEU	4.3
9	V	35	TYR	4.3
9	I	35	TYR	4.3
9	I	27	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
8	U	47	GLY	4.2
4	Q	35	ALA	4.2
11	X	6	ALA	4.2
8	H	47	GLY	4.2
1	N	312	ILE	4.2
2	B	57	ASP	4.2
9	I	73	LYS	4.2
10	W	52	TRP	4.1
3	P	37	PHE	4.1
4	D	5	VAL	4.1
1	N	513	LEU	4.1
1	A	514	LYS	4.1
13	Z	39	ASN	4.1
8	U	7	LYS	4.0
1	N	514	LYS	4.0
5	E	109	VAL	4.0
7	G	9	GLY	3.9
10	W	55	PHE	3.9
2	B	16	ILE	3.9
9	I	21	ILE	3.9
13	Z	41	LYS	3.9
2	B	87	MET	3.9
9	V	65	LYS	3.9
1	A	382[A]	SER	3.9
4	Q	4	SER	3.9
7	T	39	SER	3.9
4	Q	33	LEU	3.9
8	U	10	ASN	3.9
7	T	12	GLY	3.8
4	Q	10	ASP	3.8
13	Z	38	ASP	3.8
2	B	91	ASN	3.8
8	H	42	ALA	3.8
7	T	2	SER	3.8
9	V	31	PHE	3.8
6	S	2	SER	3.8
12	L	47	LYS	3.7
12	Y	24	MET	3.7
8	U	50	VAL	3.6
7	T	6	GLY	3.6
9	V	32	ALA	3.6
3	P	44	MET	3.6

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Mol	Chain	Res	Type	RSRZ
8	U	42	ALA	3.6
8	U	52	VAL	3.6
9	V	33	THR	3.5
8	H	48	GLY	3.5
11	X	7	PRO	3.5
4	Q	140	TYR	3.5
7	T	84	LYS	3.5
7	G	6	GLY	3.4
9	V	15	ARG	3.4
9	I	19	PHE	3.4
2	B	60	GLU	3.4
8	H	44	THR	3.4
2	O	130	PRO	3.4
9	V	5	ALA	3.4
8	H	10	ASN	3.3
10	W	48	TYR	3.3
8	H	55	TRP	3.3
8	U	61	LYS	3.3
8	H	50	VAL	3.3
3	C	37	PHE	3.3
2	O	68	LEU	3.3
7	T	4	ALA	3.3
1	A	356	ILE	3.3
8	U	9	LYS	3.3
2	B	68	LEU	3.2
4	Q	51	LEU	3.2
7	T	42	ARG	3.2
10	J	57	HIS	3.2
10	W	56	PRO	3.2
7	G	33	LEU	3.2
7	T	33	LEU	3.2
11	X	52	GLU	3.2
4	Q	30	VAL	3.2
8	H	9	LYS	3.1
13	M	39	ASN	3.1
4	D	7	LYS	3.1
2	O	218	TYR	3.1
7	G	38	HIS	3.1
10	J	56	PRO	3.1
2	O	32[A]	PHE	3.1
9	V	25	PHE	3.1
4	Q	28	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	O	92	ASN	3.0
3	C	3	HIS	3.0
9	I	28	SER	3.0
2	O	65	TRP	3.0
2	B	22	HIS	3.0
5	E	6	GLU	3.0
9	V	27	VAL	3.0
1	N	484	THR	3.0
7	G	84	LYS	3.0
11	X	49	THR	3.0
8	U	55	TRP	3.0
8	H	85	ILE	2.9
11	X	54	ARG	2.9
7	G	12	GLY	2.9
7	G	35	SER	2.9
5	R	90	ARG	2.9
2	O	116	LEU	2.9
1	A	383[A]	MET	2.9
10	W	1	PHE	2.9
6	F	64	GLU	2.9
7	G	39	SER	2.9
4	D	73	ARG	2.8
1	N	2	PHE	2.8
9	V	19	PHE	2.8
4	Q	53	ILE	2.8
5	R	86	ILE	2.8
2	O	226	MET	2.8
5	R	85	VAL	2.8
2	B	32[A]	PHE	2.8
10	J	52	TRP	2.8
13	Z	32	TRP	2.8
1	N	381[A]	LEU	2.8
9	V	39	VAL	2.8
12	L	24	MET	2.8
13	M	41	LYS	2.8
2	B	183	THR	2.8
8	U	11	TYR	2.8
2	O	78	LEU	2.8
2	B	67	ILE	2.7
9	V	73	LYS	2.7
2	O	114	GLU	2.7
9	I	53	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	513	LEU	2.7
3	C	38	ASN	2.7
2	O	91	ASN	2.6
3	P	258	TRP	2.6
8	U	48	GLY	2.6
11	K	47	ARG	2.6
9	I	39	VAL	2.6
9	V	22	VAL	2.6
4	Q	31	LYS	2.6
8	H	84	LYS	2.6
2	O	59	GLN	2.6
9	V	21	ILE	2.6
9	V	68	ILE	2.6
1	A	346	PHE	2.6
3	P	33	MET	2.6
9	I	26	MET	2.6
10	J	27	THR	2.5
4	Q	40	LEU	2.5
7	G	41	HIS	2.5
2	B	55	THR	2.5
4	Q	143	ASN	2.5
8	U	43	MET	2.5
6	F	65	ASP	2.5
3	C	127	LEU	2.5
4	Q	11	TYR	2.5
9	V	4	LEU	2.5
7	G	70	PHE	2.5
4	Q	32	ASN	2.5
1	N	383[A]	MET	2.5
4	Q	46	ALA	2.4
11	X	46	GLY	2.4
2	B	56	MET	2.4
5	E	39	TYR	2.4
9	V	53	ASN	2.4
10	W	44	LEU	2.4
12	Y	44	LEU	2.4
12	Y	45	LEU	2.4
2	B	115[A]	ASP	2.4
11	X	48	VAL	2.4
4	Q	147	LYS	2.4
8	U	12	GLN	2.4
11	X	51	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	40	MET	2.4
7	G	45	PRO	2.4
11	X	13	TYR	2.4
10	W	27	THR	2.4
1	A	2	PHE	2.4
10	J	55	PHE	2.4
2	O	89	GLU	2.4
4	Q	73	ARG	2.4
9	I	12	LEU	2.4
12	Y	26[A]	THR	2.4
5	R	91	PRO	2.3
2	B	75	LEU	2.3
1	A	298[A]	ASP	2.3
2	O	57	ASP	2.3
13	M	38	ASP	2.3
1	A	313	ALA	2.3
9	I	36	LYS	2.3
9	V	36	LYS	2.3
13	Z	13	LYS	2.3
7	T	41	HIS	2.3
9	V	72	ALA	2.3
7	T	70	PHE	2.3
2	B	130	PRO	2.3
9	I	18	ARG	2.3
11	X	47	ARG	2.3
4	Q	145	TRP	2.3
4	D	147	LYS	2.3
9	I	42	LYS	2.3
9	V	58	LYS	2.3
2	B	39[A]	LEU	2.3
7	T	35	SER	2.3
10	J	48	TYR	2.3
4	Q	39	ALA	2.2
7	G	42	ARG	2.2
9	V	10	ARG	2.2
10	J	33	ARG	2.2
10	W	33	ARG	2.2
6	S	43	LYS	2.2
8	H	7	LYS	2.2
4	Q	72	ASN	2.2
2	B	82	ARG	2.2
6	S	65	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	Q	58	GLU	2.2
9	V	26	MET	2.2
4	D	74	SER	2.2
2	O	16	ILE	2.2
4	Q	9	GLU	2.2
5	E	9	GLU	2.2
7	G	43	GLU	2.2
1	A	359	ALA	2.2
5	R	108	LYS	2.2
4	Q	101	HIS	2.2
4	Q	131	ILE	2.1
4	Q	27	VAL	2.1
8	H	52	VAL	2.1
4	Q	19[A]	ARG	2.1
9	I	15	ARG	2.1
2	O	28[A]	LEU	2.1
7	G	46	ALA	2.1
8	H	12	GLN	2.1
3	C	230	ASN	2.1
13	M	35	TYR	2.1
9	V	45	LYS	2.1
2	B	88	ASP	2.1
8	H	43	MET	2.1
1	N	483	LEU	2.1
2	B	33[A]	LEU	2.1
9	I	4	LEU	2.1
2	B	40[A]	TYR	2.1
2	O	67	ILE	2.1
6	F	52	ILE	2.1
8	H	11	TYR	2.1
9	V	64	ARG	2.1
4	Q	141	ASP	2.1
5	R	16	VAL	2.0
5	R	54	ALA	2.0
9	V	12	LEU	2.0
1	N	356	ILE	2.0
2	O	64	ILE	2.0
11	X	31	TYR	2.0
3	P	224	LYS	2.0
11	K	51	LYS	2.0
3	C	258	TRP	2.0
3	C	259	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
4	Q	78	TRP	2.0
4	Q	144	GLU	2.0
2	B	92	ASN	2.0
3	P	38	ASN	2.0
8	H	49	ASP	2.0
4	D	102	TYR	2.0

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

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
9	SAC	V	1	9/10	0.29	0.22	261,280,298,300	0
9	SAC	I	1	9/10	0.52	0.25	123,141,157,179	0
1	FME	N	1	10/11	0.93	0.13	35,42,79,80	0
1	FME	A	1	10/11	0.93	0.12	34,45,69,100	0
2	FME	O	1	10/11	0.96	0.12	34,36,42,117	0
2	FME	B	1	10/11	0.97	0.09	27,30,35,81	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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
26	DMU	X	101	22/33	0.63	0.21	49,75,84,89	0
26	DMU	K	101	22/33	0.65	0.21	40,67,83,84	0
26	DMU	P	311	33/33	0.67	0.19	57,85,99,101	0
26	DMU	X	103	22/33	0.68	0.19	61,72,82,86	0
26	DMU	K	102	22/33	0.71	0.18	46,73,82,87	0
26	DMU	K	103	17/33	0.72	0.22	55,70,77,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	S	108	4/4	0.73	0.16	49,55,62,64	0
26	DMU	X	102	22/33	0.73	0.17	62,71,84,89	0
24	PEK	T	101	49/53	0.73	0.22	47,76,117,205	0
26	DMU	P	315	33/33	0.74	0.18	41,67,84,90	0
25	CDL	T	102	80/100	0.74	0.24	42,78,116,206	0
26	DMU	C	311	33/33	0.74	0.19	53,68,90,99	0
23	CHD	W	101	29/29	0.74	0.18	60,74,91,109	0
25	CDL	G	101	89/100	0.75	0.24	51,77,107,188	0
26	DMU	P	316	22/33	0.77	0.18	50,68,84,87	0
27	PSC	E	201	52/52	0.77	0.24	45,77,123,221	0
20	PGV	P	307	51/51	0.78	0.22	42,75,109,197	0
19	TGL	O	301	63/63	0.78	0.20	37,74,90,106	0
20	PGV	C	307	47/51	0.78	0.22	39,73,103,206	0
24	PEK	C	304	44/53	0.78	0.24	47,74,99,130	0
26	DMU	G	105	21/33	0.78	0.19	53,70,81,87	0
24	PEK	P	305	46/53	0.79	0.23	48,75,102,117	0
26	DMU	L	101	18/33	0.79	0.18	46,65,84,84	0
20	PGV	Q	201	51/51	0.79	0.22	47,72,111,195	0
25	CDL	Y	101	87/100	0.80	0.21	38,78,116,159	0
26	DMU	P	310	33/33	0.80	0.17	61,75,97,110	0
23	CHD	J	102	29/29	0.80	0.17	50,74,103,112	0
25	CDL	P	308	76/100	0.81	0.23	31,74,108,157	0
26	DMU	P	312	33/33	0.81	0.17	38,75,97,106	0
29	PO4	U	102	5/5	0.81	0.14	53,58,65,65	0
19	TGL	O	302	63/63	0.82	0.22	49,71,97,104	0
27	PSC	O	304	51/52	0.82	0.23	43,74,116,204	0
19	TGL	B	301	62/63	0.82	0.19	28,65,88,98	0
20	PGV	A	608	46/51	0.83	0.22	33,67,110,193	0
19	TGL	D	201	48/63	0.83	0.21	30,59,91,127	0
23	CHD	P	309	29/29	0.83	0.14	47,59,82,103	0
25	CDL	C	308	86/100	0.83	0.20	29,73,103,171	0
21	EDO	S	107	4/4	0.83	0.18	52,58,59,63	0
26	DMU	J	101	33/33	0.84	0.15	31,70,97,106	0
24	PEK	P	303	22/53	0.84	0.19	51,60,86,98	0
23	CHD	C	309	29/29	0.85	0.12	45,58,84,85	0
21	EDO	S	104	4/4	0.86	0.16	43,45,55,57	0
19	TGL	A	607	63/63	0.86	0.22	32,62,96,123	0
21	EDO	T	104	4/4	0.88	0.16	37,44,47,59	0
26	DMU	Z	101	33/33	0.89	0.13	38,46,63,74	0
21	EDO	A	613	4/4	0.89	0.17	39,39,41,56	0
21	EDO	B	308	4/4	0.90	0.14	31,34,38,43	0
17	NA	C	302	1/1	0.91	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	F	103	4/4	0.91	0.13	36,36,40,55	0
21	EDO	A	616	4/4	0.91	0.12	38,38,40,41	0
21	EDO	Y	102	4/4	0.91	0.16	53,55,61,65	0
21	EDO	N	612	4/4	0.92	0.12	42,42,45,46	0
21	EDO	P	314	4/4	0.92	0.15	47,58,60,61	0
21	EDO	B	306	4/4	0.92	0.16	29,45,56,75	0
21	EDO	A	614	4/4	0.92	0.14	37,39,42,46	0
21	EDO	A	610	4/4	0.92	0.11	29,29,30,31	0
21	EDO	G	104	4/4	0.92	0.14	42,62,72,77	0
21	EDO	U	101	4/4	0.92	0.18	35,37,62,63	0
21	EDO	N	610	4/4	0.92	0.15	31,50,52,52	0
21	EDO	O	307	4/4	0.93	0.14	35,42,48,60	0
21	EDO	O	308	4/4	0.93	0.13	38,46,48,51	0
21	EDO	B	305	4/4	0.93	0.13	30,31,38,43	0
21	EDO	E	203	4/4	0.93	0.13	49,50,54,58	0
21	EDO	S	106	4/4	0.93	0.14	40,49,50,52	0
26	DMU	M	101	33/33	0.93	0.11	33,39,56,71	0
21	EDO	O	306	4/4	0.94	0.10	34,36,42,46	0
21	EDO	B	304	4/4	0.94	0.12	35,39,40,43	0
21	EDO	A	615	4/4	0.94	0.14	32,48,68,71	0
17	NA	P	302	1/1	0.94	0.09	38,38,38,38	0
21	EDO	Q	202	4/4	0.94	0.14	30,49,53,65	0
21	EDO	A	617	4/4	0.94	0.14	31,37,41,65	0
21	EDO	D	202	4/4	0.94	0.11	42,45,53,61	0
21	EDO	N	615	4/4	0.94	0.11	38,39,40,43	0
21	EDO	O	305	4/4	0.94	0.09	29,30,31,31	0
21	EDO	A	612	4/4	0.95	0.12	41,53,56,68	0
24	PEK	C	303	51/53	0.95	0.14	27,43,85,92	0
21	EDO	N	611	4/4	0.95	0.09	37,38,41,44	0
20	PGV	N	607	51/51	0.95	0.12	22,29,75,83	0
24	PEK	P	304	53/53	0.95	0.14	28,46,85,94	0
21	EDO	N	614	4/4	0.95	0.10	38,41,41,41	0
21	EDO	N	608	4/4	0.95	0.08	28,29,30,31	0
21	EDO	T	103	4/4	0.95	0.10	31,31,36,37	0
21	EDO	B	307	4/4	0.96	0.08	25,25,26,28	0
20	PGV	C	305	51/51	0.96	0.11	22,28,72,81	0
21	EDO	R	201	4/4	0.96	0.08	38,40,41,43	0
21	EDO	N	609	4/4	0.96	0.07	26,27,29,30	0
21	EDO	S	105	4/4	0.96	0.08	28,30,31,33	0
21	EDO	C	310	4/4	0.96	0.09	29,30,30,31	0
23	CHD	C	301	29/29	0.96	0.07	25,30,35,36	0
23	CHD	P	301	29/29	0.97	0.06	27,30,34,35	0

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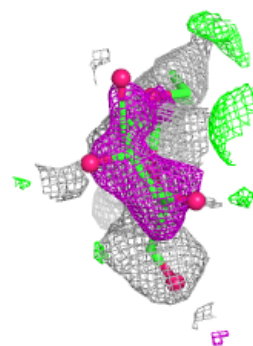
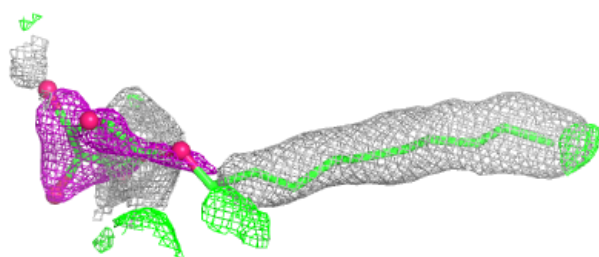
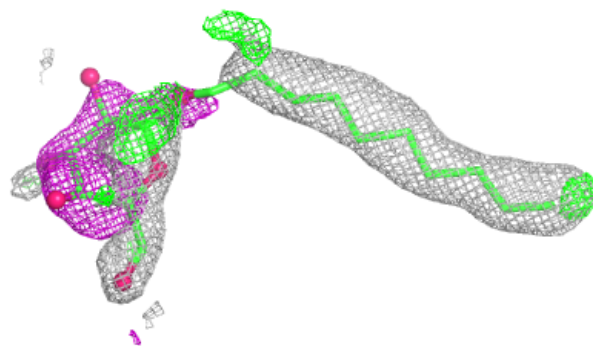
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	CYN	N	606[A]	2/2	0.97	0.12	26,26,26,28	2
21	EDO	S	103	4/4	0.97	0.07	33,34,37,38	0
18	CYN	N	606[C]	2/2	0.97	0.12	20,20,20,24	2
20	PGV	C	306	51/51	0.97	0.11	23,29,83,91	0
21	EDO	N	613	4/4	0.97	0.08	32,34,35,39	0
14	HEA	A	602[A]	60/60	0.97	0.08	17,22,37,43	51
21	EDO	E	202	4/4	0.97	0.06	36,37,39,40	0
17	NA	N	605	1/1	0.97	0.07	29,29,29,29	0
20	PGV	P	306	45/51	0.97	0.09	24,29,58,76	0
21	EDO	G	103	4/4	0.97	0.07	30,32,33,36	0
14	HEA	A	602[C]	60/60	0.97	0.08	16,21,37,43	51
23	CHD	B	303	29/29	0.97	0.07	26,29,38,54	0
21	EDO	P	313	4/4	0.97	0.08	33,35,38,38	0
18	CYN	A	606[A]	2/2	0.97	0.19	24,24,24,25	2
23	CHD	G	102	29/29	0.97	0.07	26,29,33,41	0
18	CYN	A	606[C]	2/2	0.97	0.19	17,17,17,18	2
21	EDO	S	102	4/4	0.98	0.06	24,24,24,26	0
14	HEA	N	602[C]	60/60	0.98	0.07	19,24,35,39	51
21	EDO	F	104	4/4	0.98	0.07	31,31,31,32	0
21	EDO	A	609	4/4	0.98	0.07	29,33,34,38	0
14	HEA	N	602[A]	60/60	0.98	0.07	19,23,35,39	51
14	HEA	A	601[C]	43/60	0.99	0.07	19,21,23,28	1
14	HEA	A	601[A]	60/60	0.99	0.07	12,22,31,33	18
21	EDO	A	611	4/4	0.99	0.05	23,24,24,27	0
16	MG	A	604	1/1	0.99	0.03	22,22,22,22	0
17	NA	A	605	1/1	0.99	0.07	25,25,25,25	0
14	HEA	A	601[B]	60/60	0.99	0.07	19,22,30,46	18
14	HEA	N	601[A]	60/60	0.99	0.06	21,25,32,35	18
14	HEA	N	601[B]	60/60	0.99	0.06	23,25,34,44	18
14	HEA	N	601[C]	43/60	0.99	0.06	23,25,27,28	1
28	ZN	F	101	1/1	0.99	0.03	29,29,29,29	0
28	ZN	S	101	1/1	0.99	0.03	28,28,28,28	0
21	EDO	F	102	4/4	0.99	0.05	23,24,24,25	0
15	CU	N	603	1/1	1.00	0.02	25,25,25,25	0
15	CU	A	603	1/1	1.00	0.02	23,23,23,23	0
22	CUA	B	302	2/2	1.00	0.01	24,24,24,24	0
22	CUA	O	303	2/2	1.00	0.02	27,27,27,28	0
16	MG	N	604	1/1	1.00	0.05	23,23,23,23	0

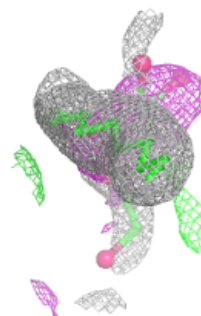
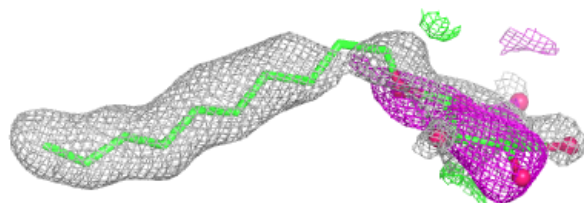
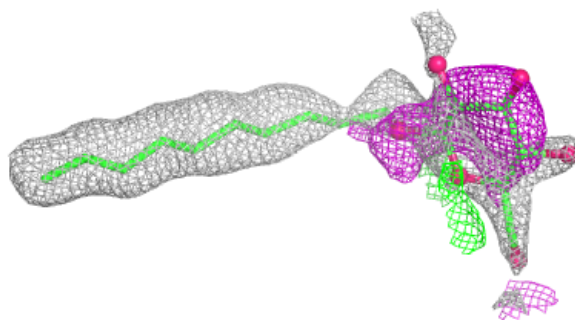
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DMU X 101:

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

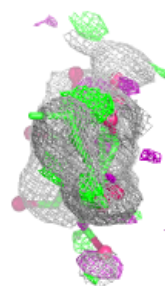
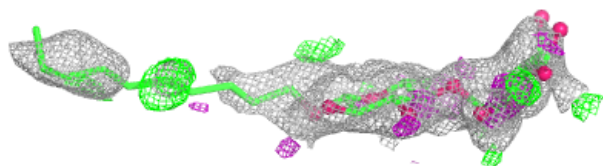
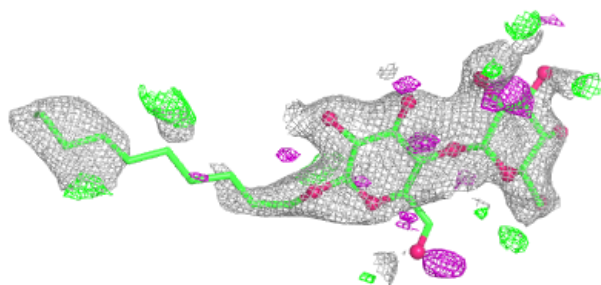
**Electron density around DMU K 101:**

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

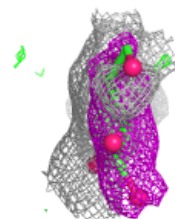
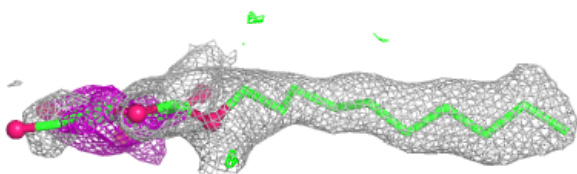
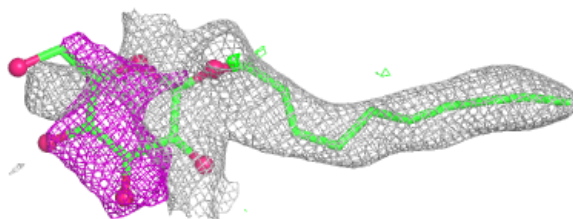


Electron density around DMU P 311:

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

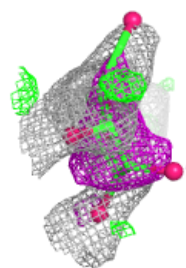
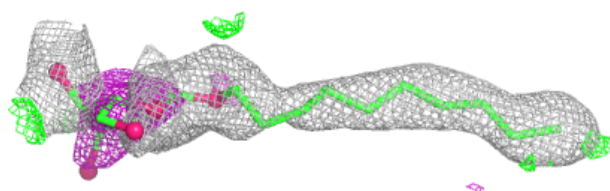
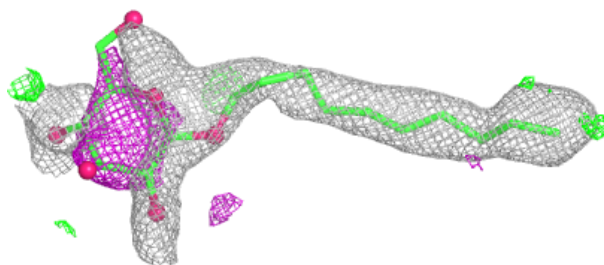
**Electron density around DMU X 103:**

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

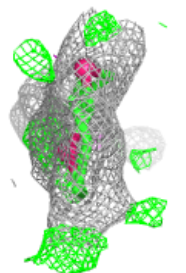
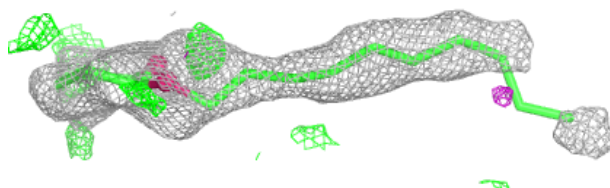
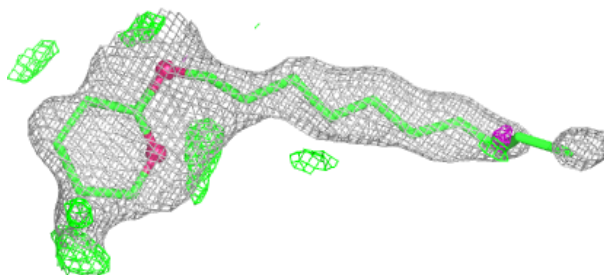


Electron density around DMU K 102:

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

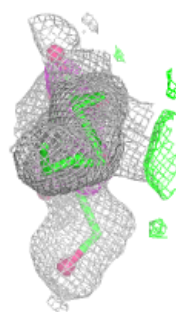
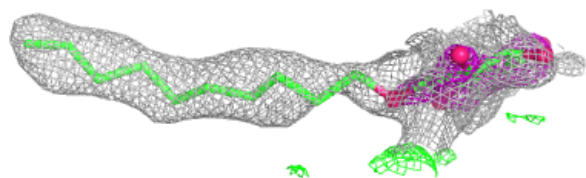
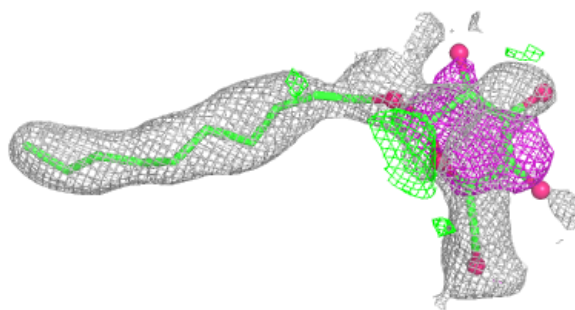
**Electron density around DMU K 103:**

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



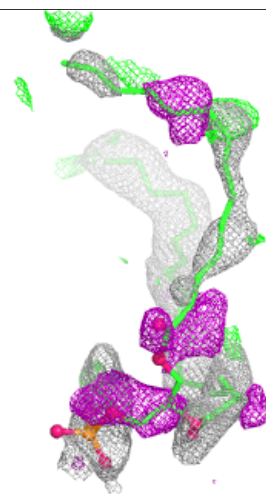
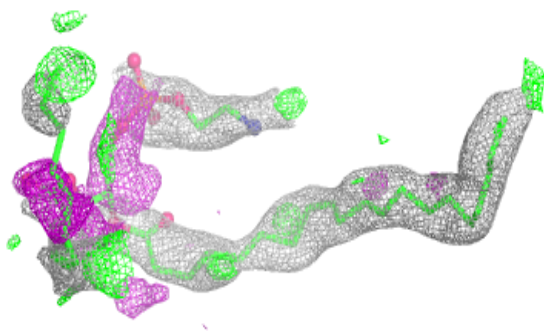
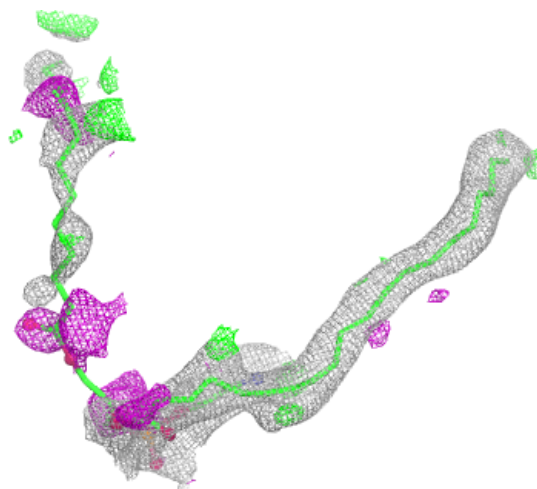
Electron density around DMU X 102:

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



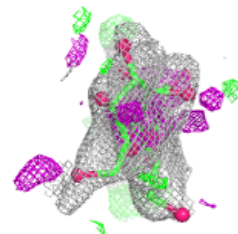
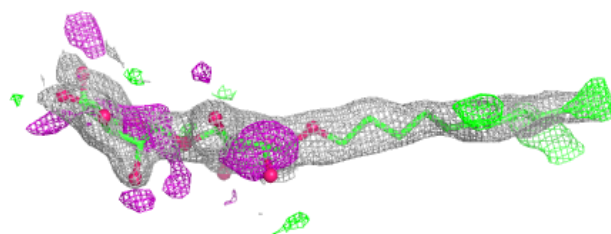
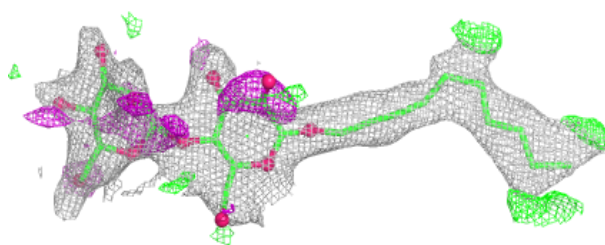
Electron density around PEK T 101:

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

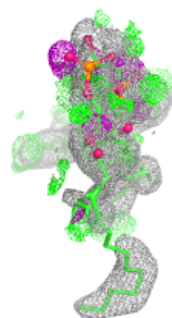
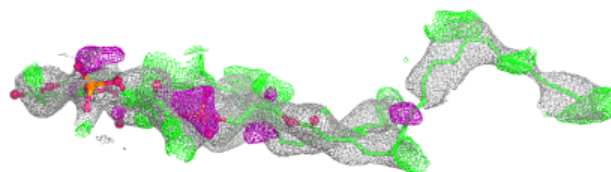
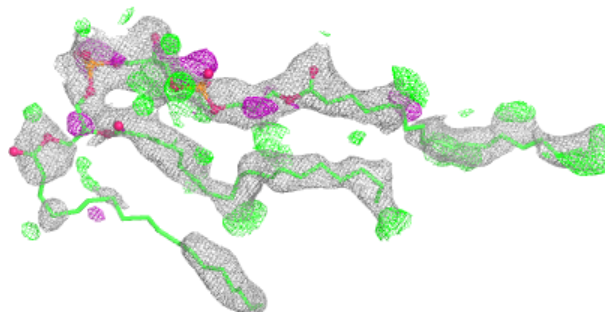


Electron density around DMU P 315:

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

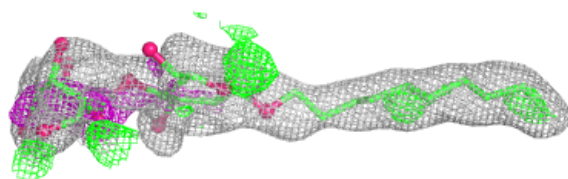
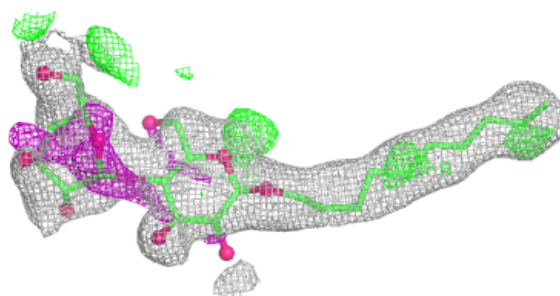
**Electron density around CDL T 102:**

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

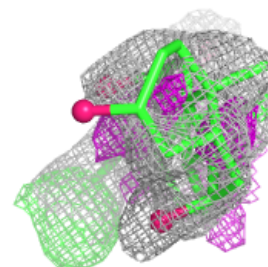
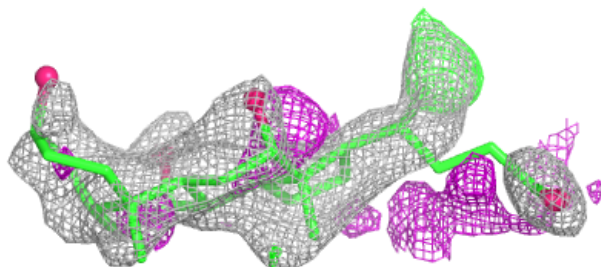
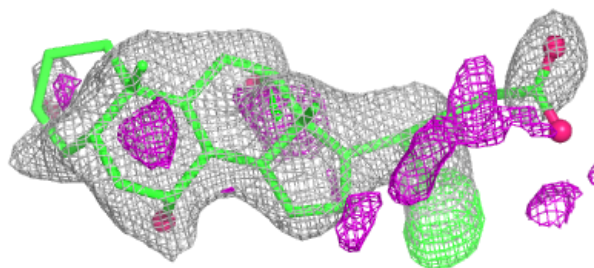


Electron density around DMU C 311:

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

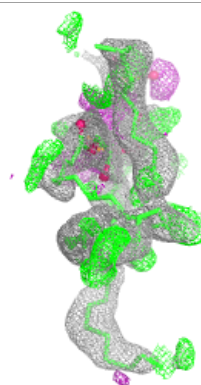
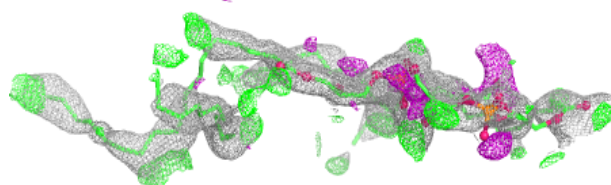
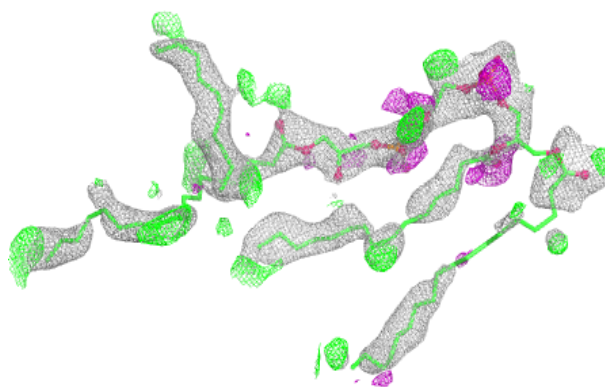
**Electron density around CHD W 101:**

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

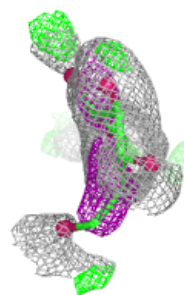
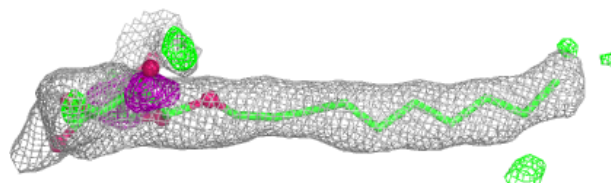
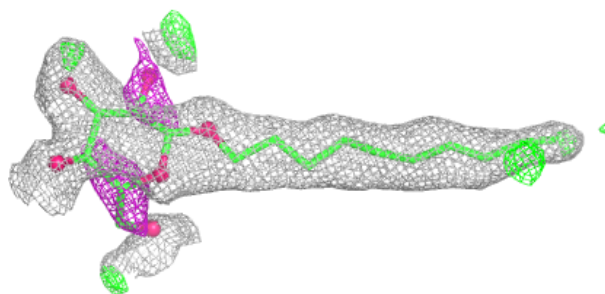


Electron density around CDL G 101:

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

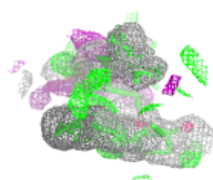
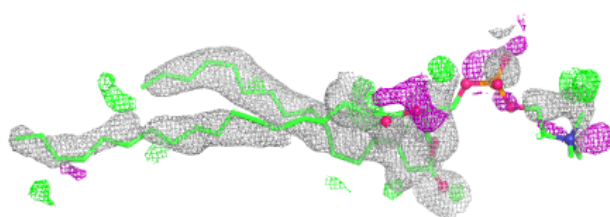
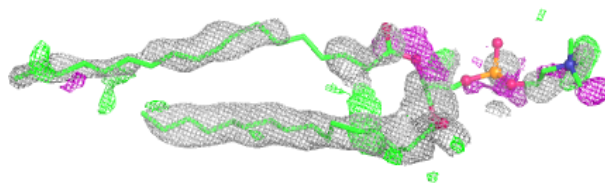
**Electron density around DMU P 316:**

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

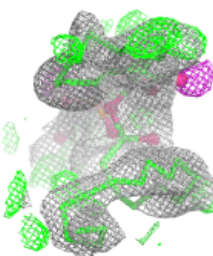
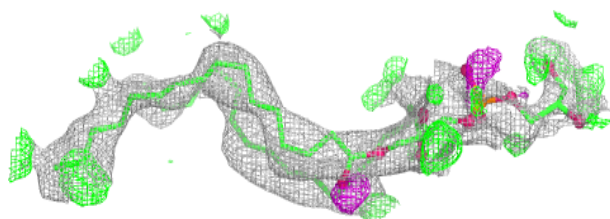
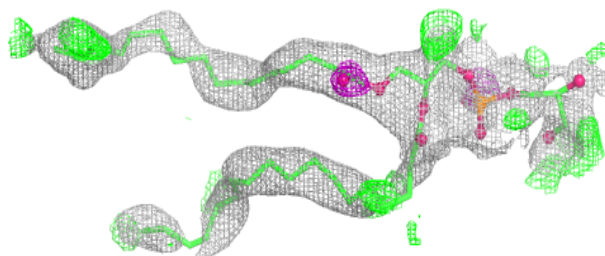


Electron density around PSC E 201:

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

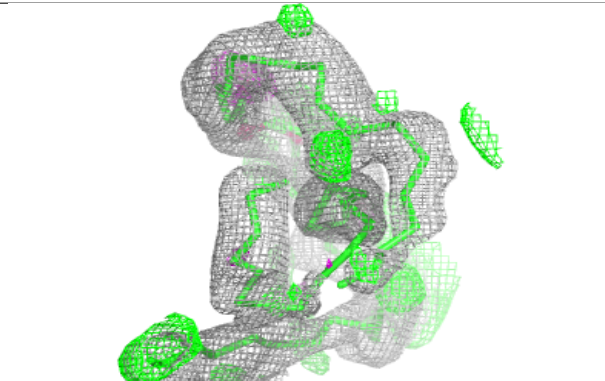
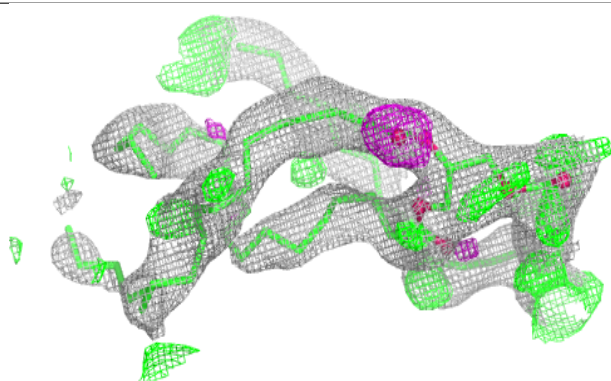
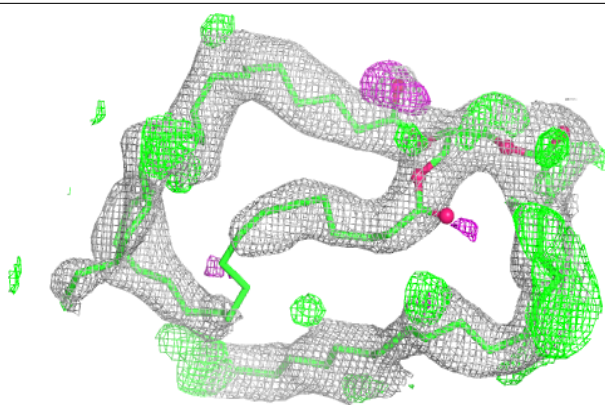
**Electron density around PGV P 307:**

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

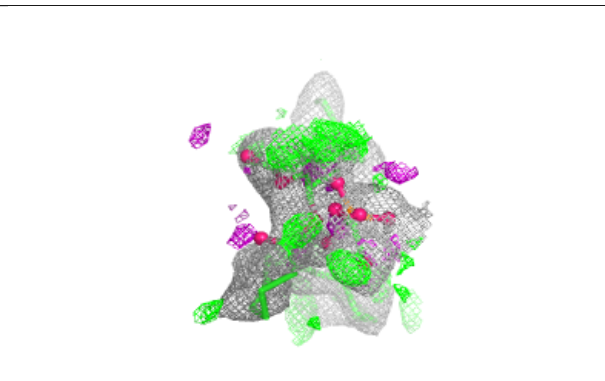
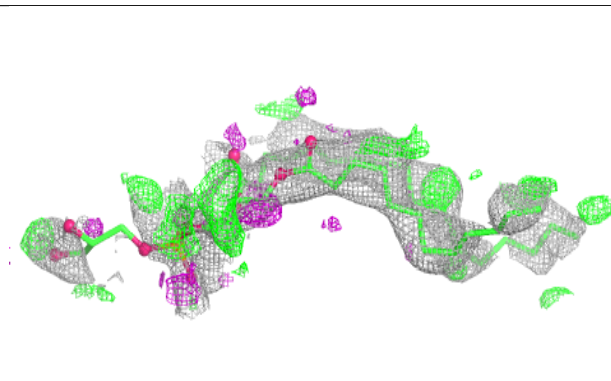
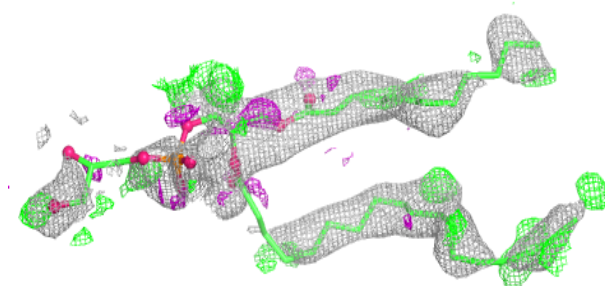


Electron density around TGL O 301:

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

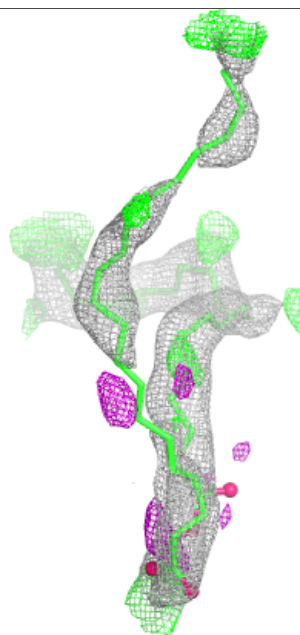
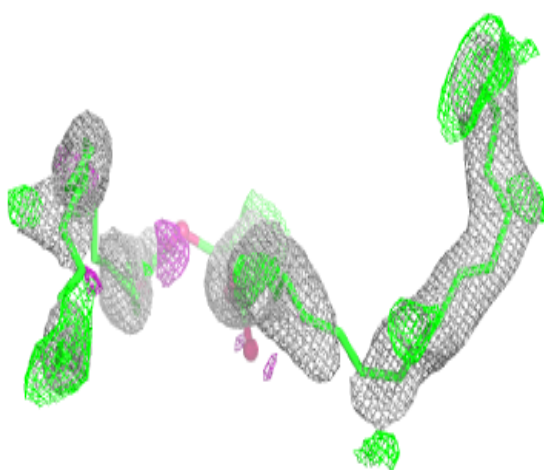
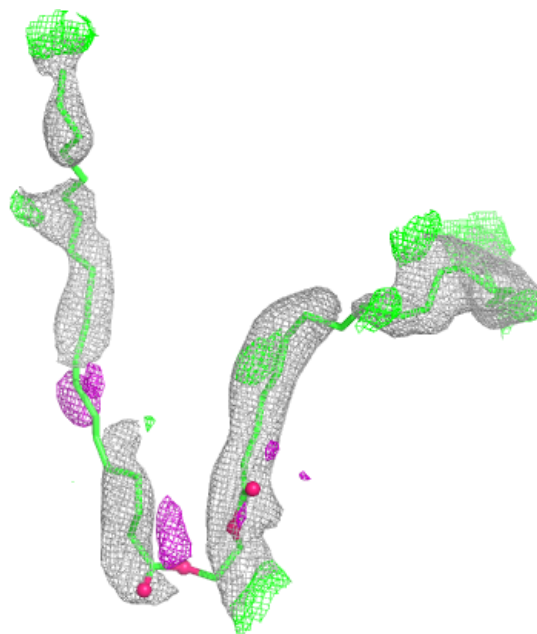
**Electron density around PGV C 307:**

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



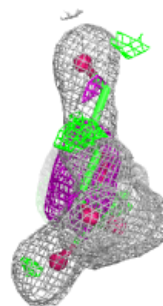
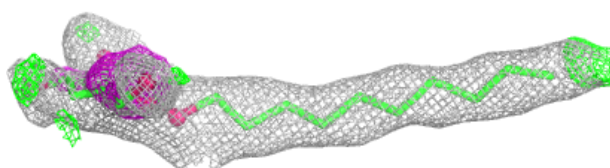
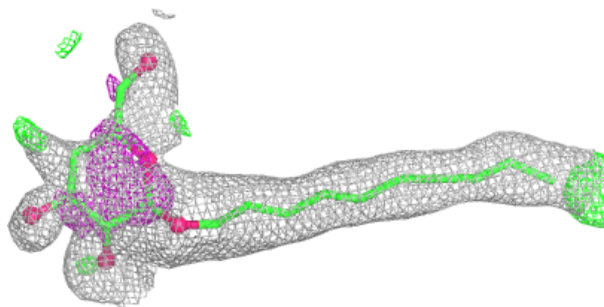
Electron density around PEK C 304:

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



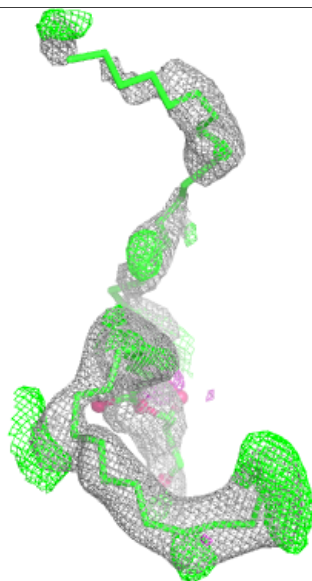
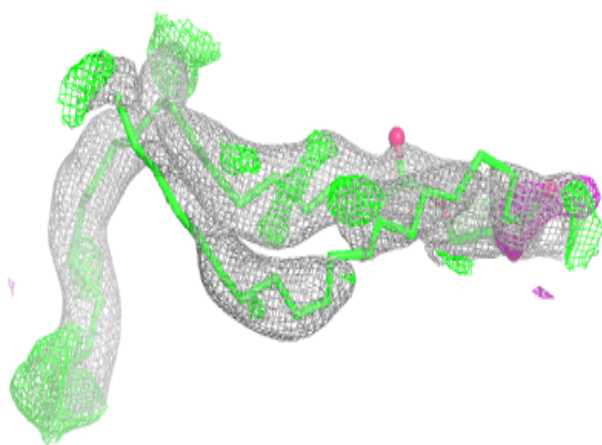
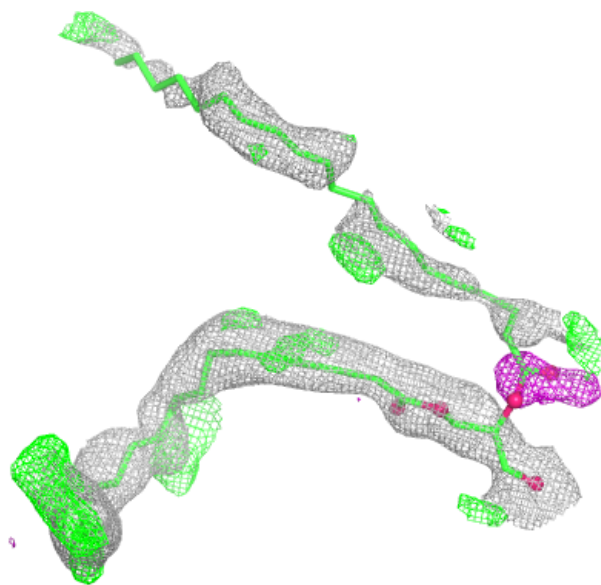
Electron density around DMU G 105:

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



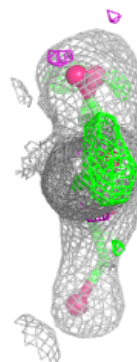
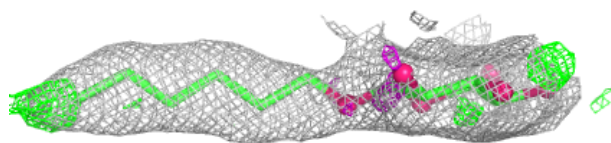
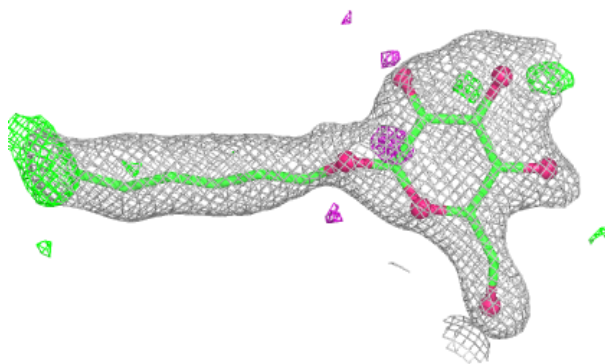
Electron density around PEK P 305:

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

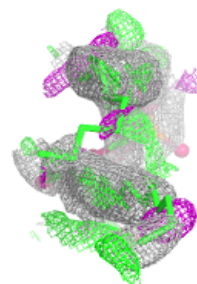
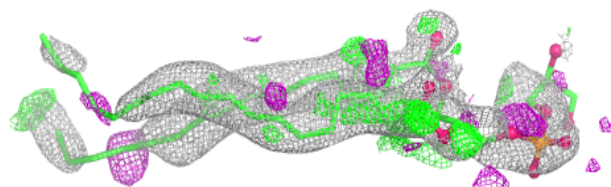
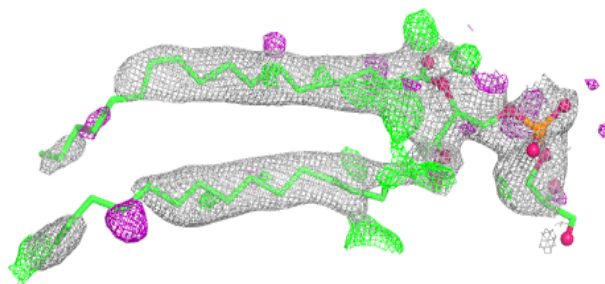


Electron density around DMU L 101:

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

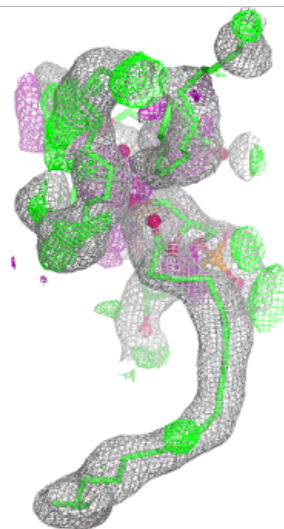
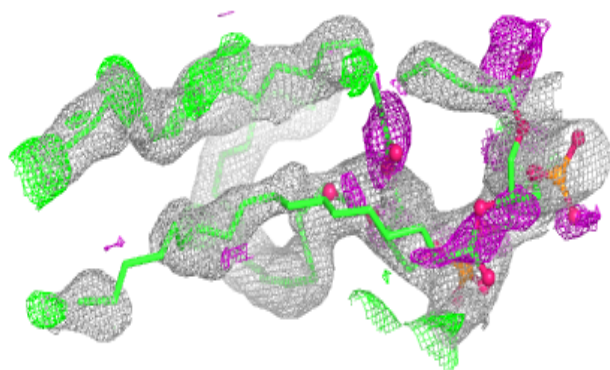
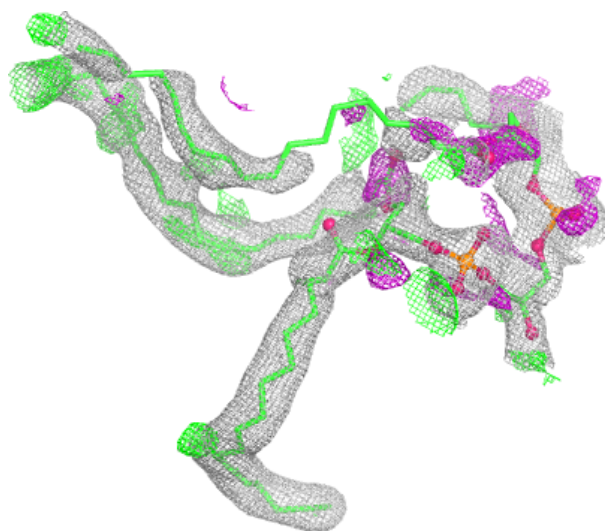
**Electron density around PGV Q 201:**

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



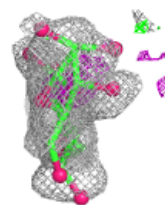
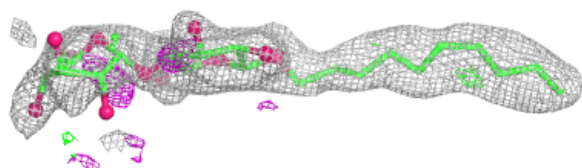
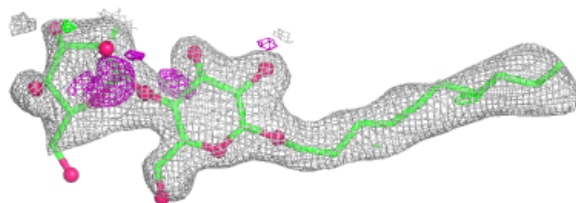
Electron density around CDL Y 101:

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

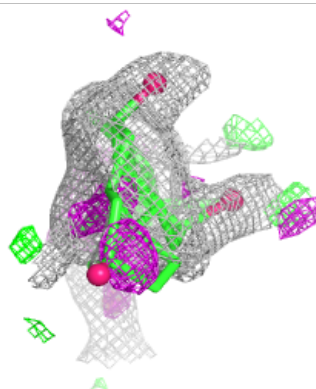
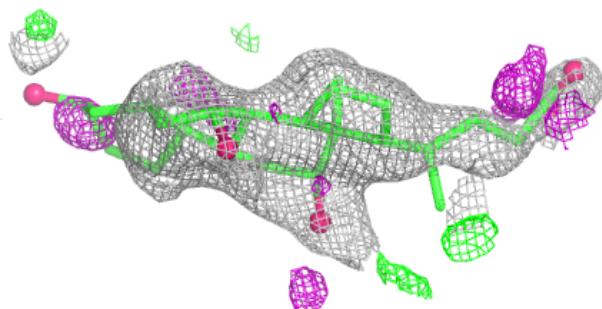
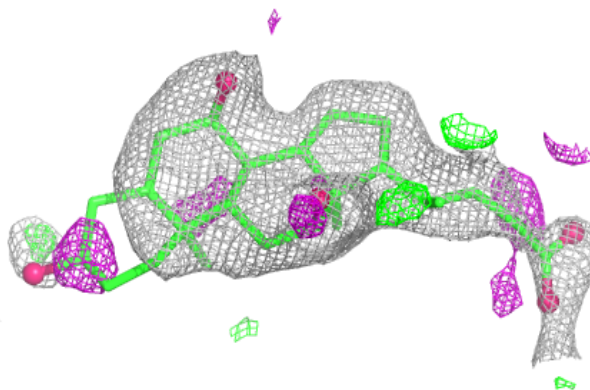


Electron density around DMU P 310:

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

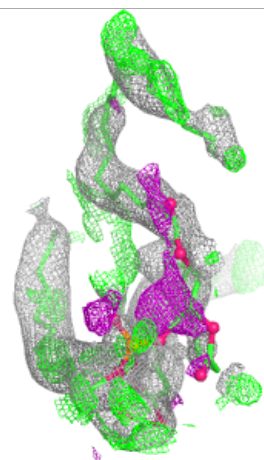
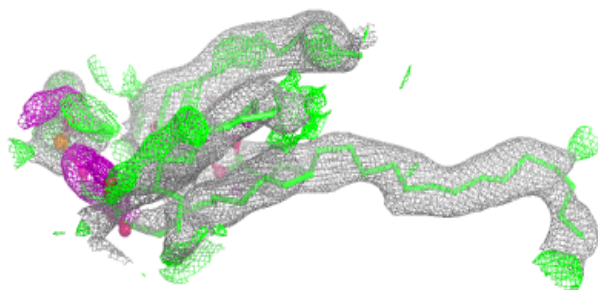
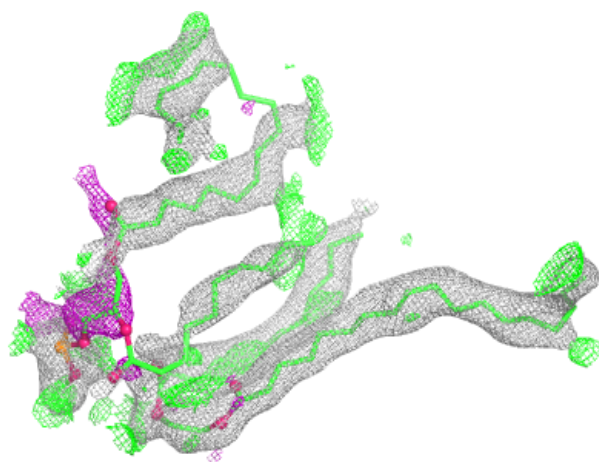
**Electron density around CHD J 102:**

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



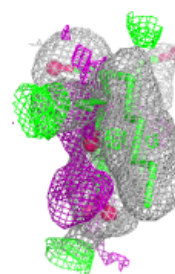
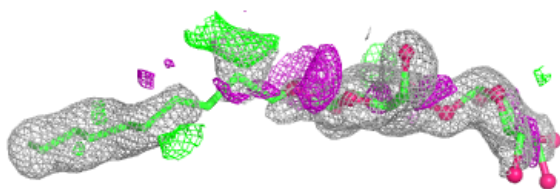
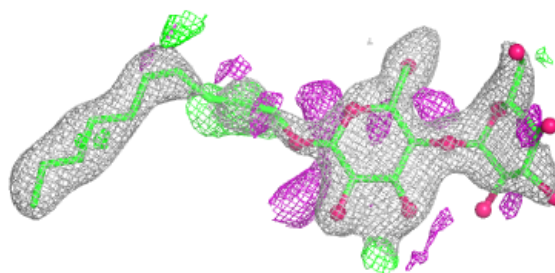
Electron density around CDL P 308:

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

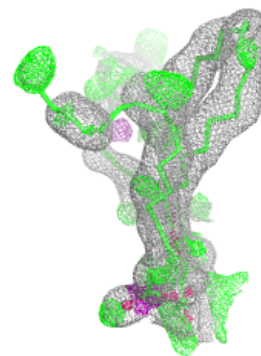
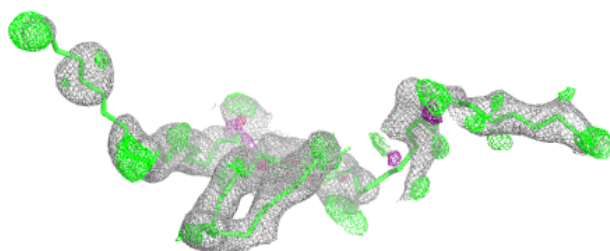
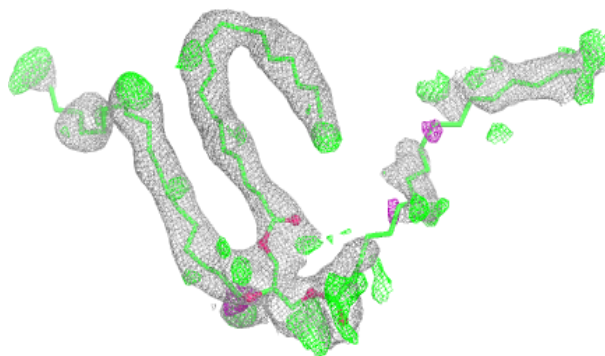


Electron density around DMU P 312:

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

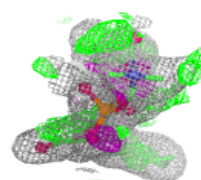
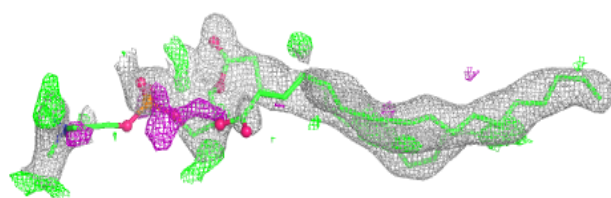
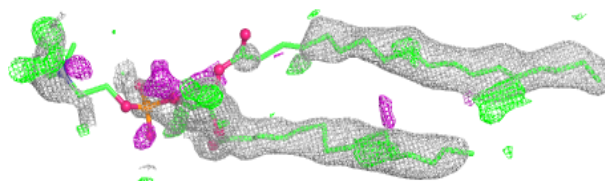
**Electron density around TGL O 302:**

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

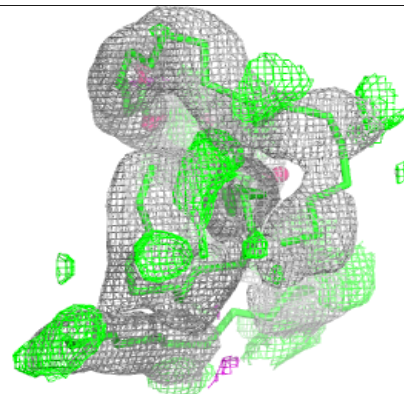
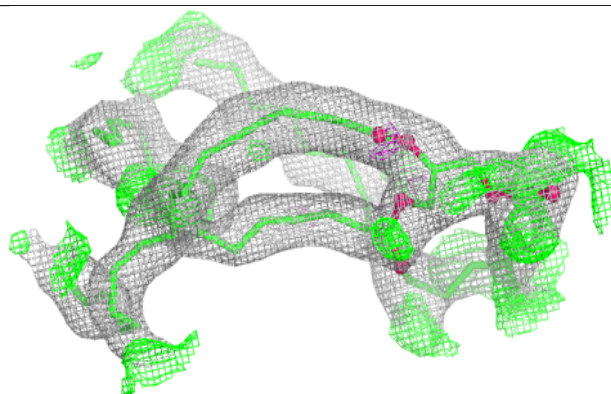
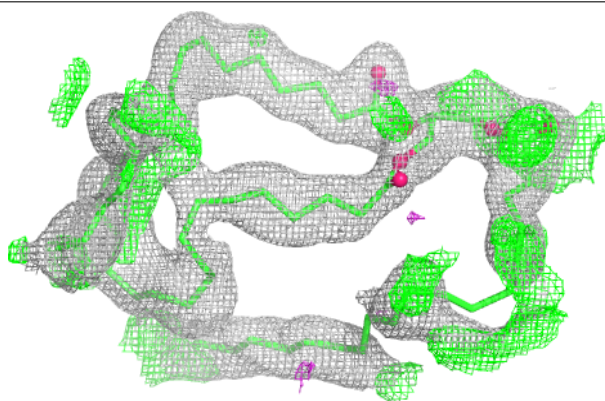


Electron density around PSC O 304:

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

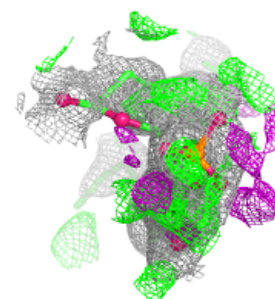
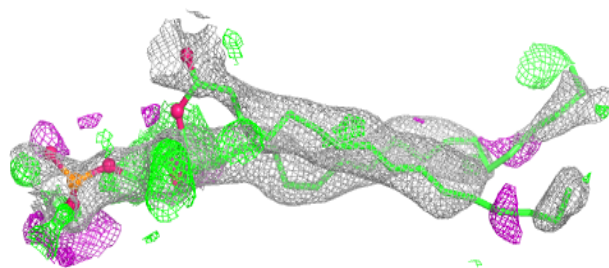
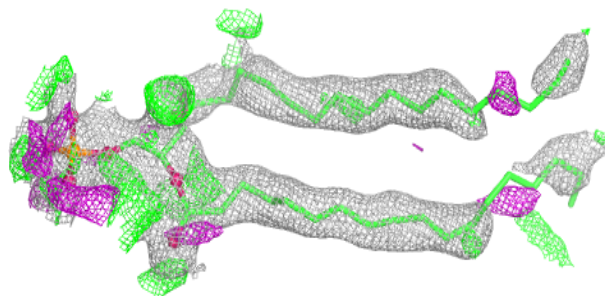
**Electron density around TGL B 301:**

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



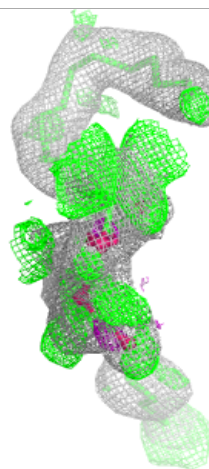
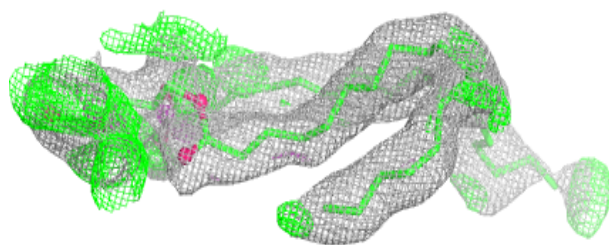
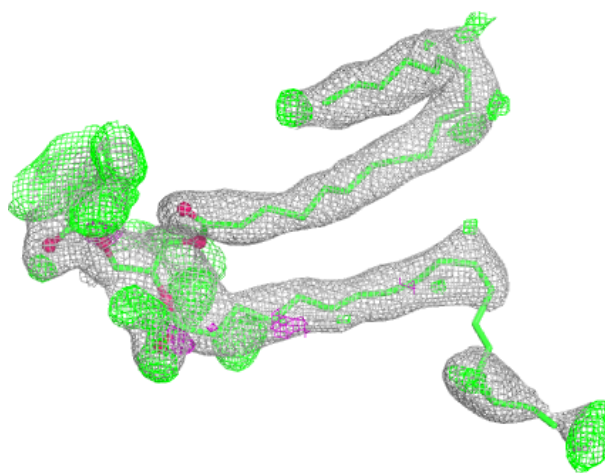
Electron density around PGV A 608:

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



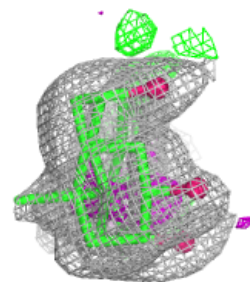
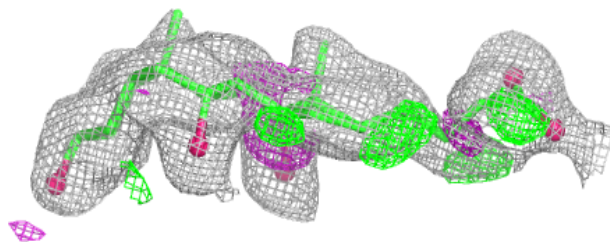
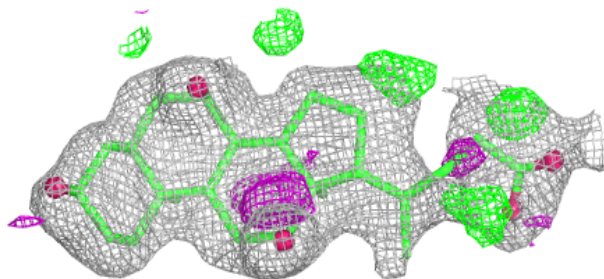
Electron density around TGL D 201:

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



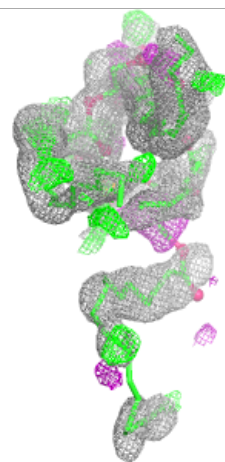
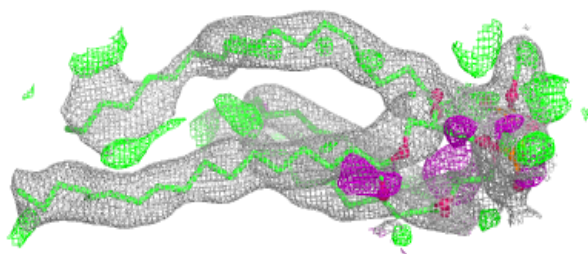
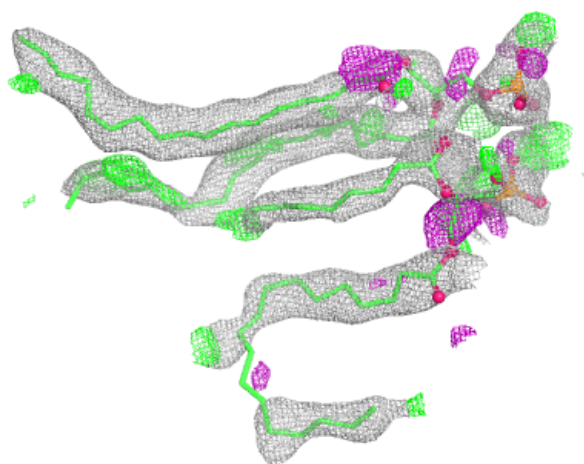
Electron density around CHD P 309:

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



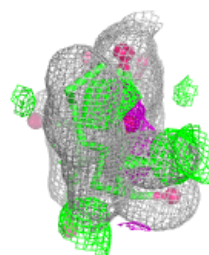
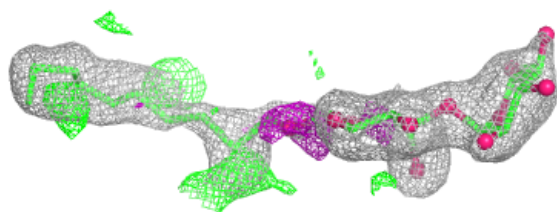
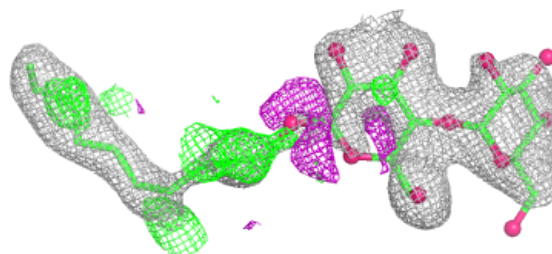
Electron density around CDL C 308:

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

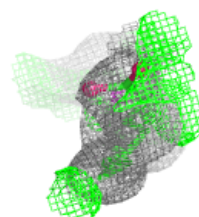
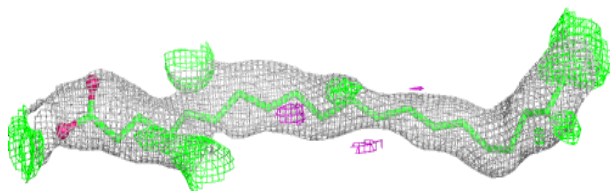
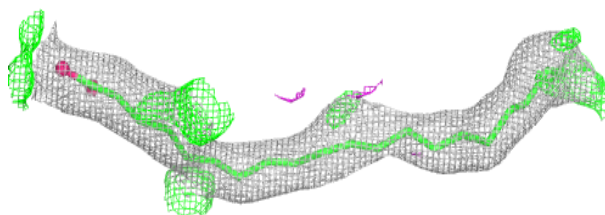


Electron density around DMU J 101:

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

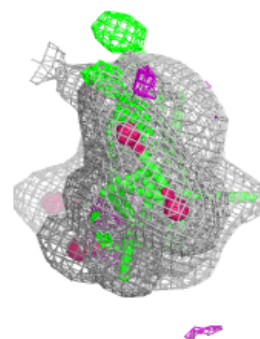
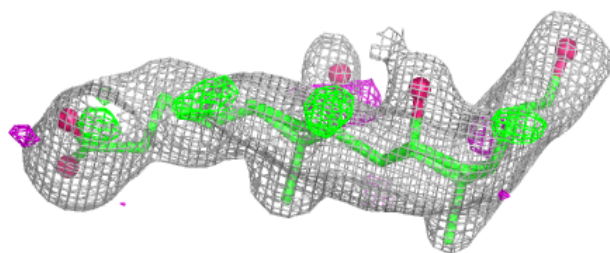
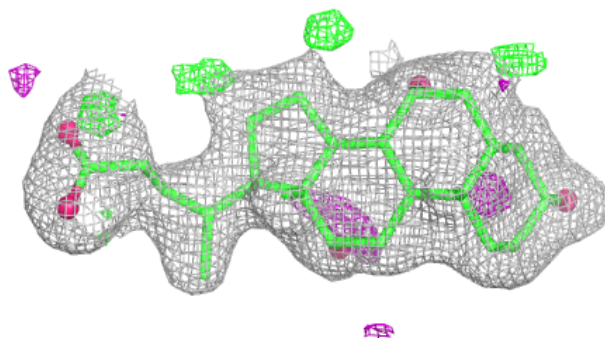
**Electron density around PEK P 303:**

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



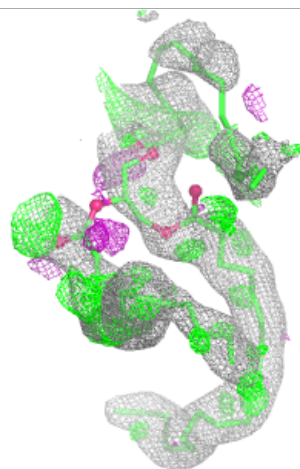
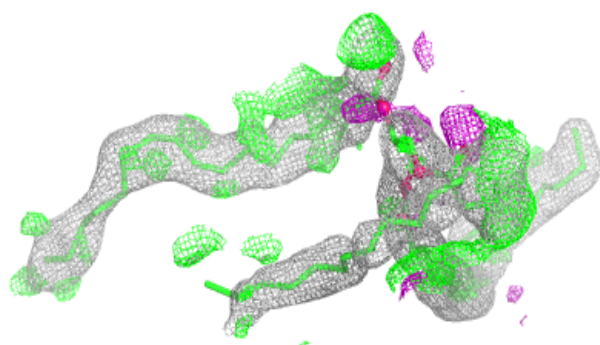
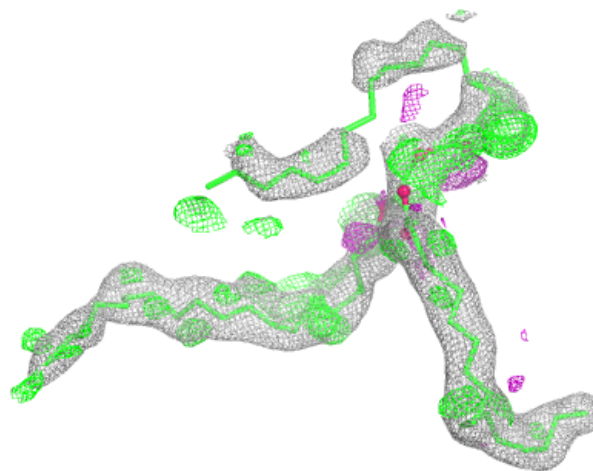
Electron density around CHD C 309:

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



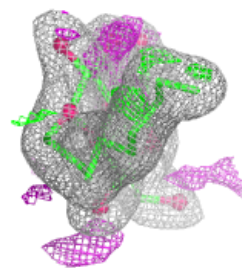
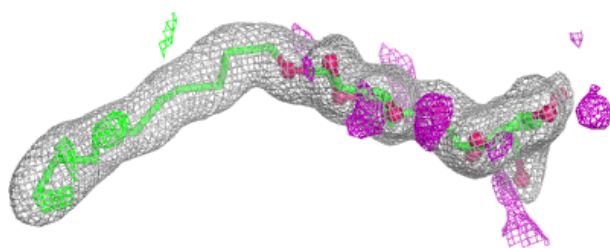
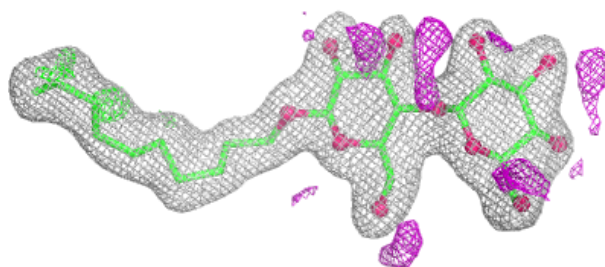
Electron density around TGL A 607:

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

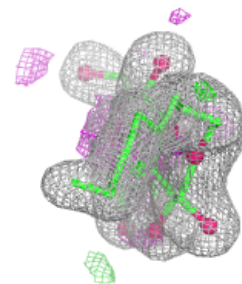
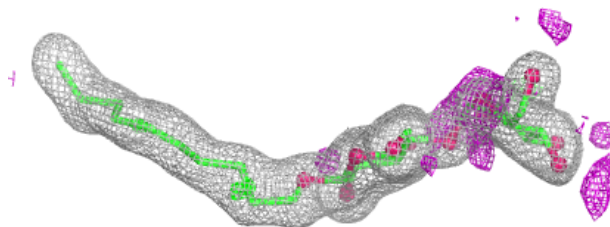
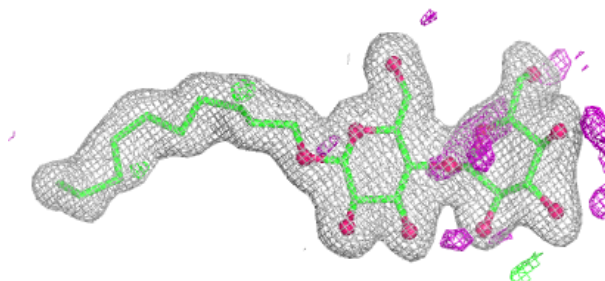


Electron density around DMU Z 101:

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

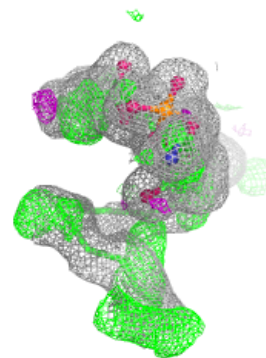
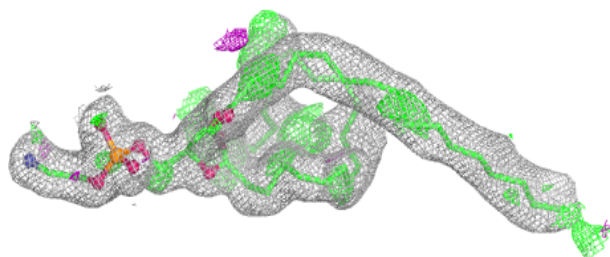
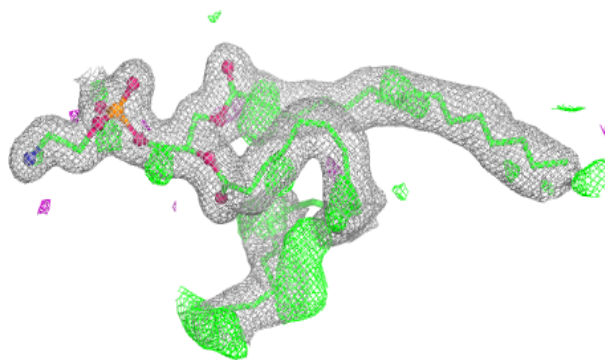
**Electron density around DMU M 101:**

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

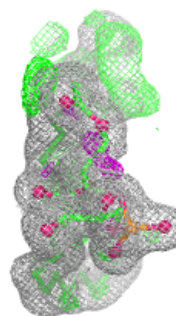
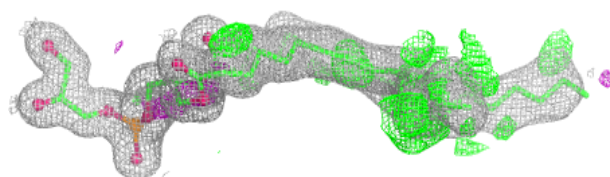
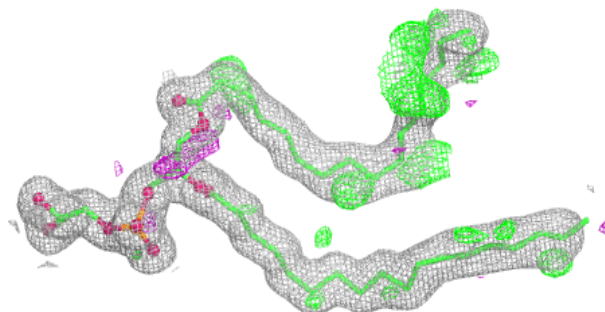


Electron density around PEK C 303:

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

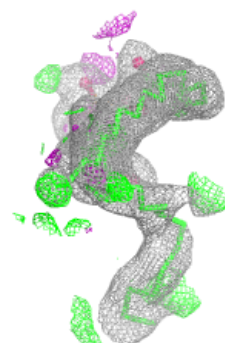
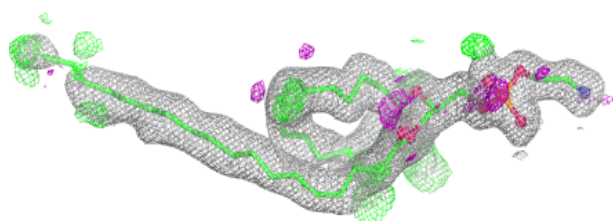
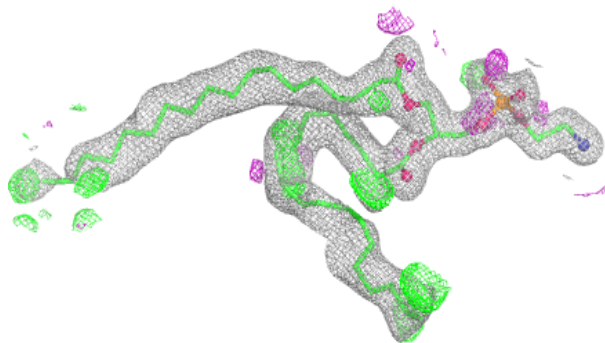
**Electron density around PGV N 607:**

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

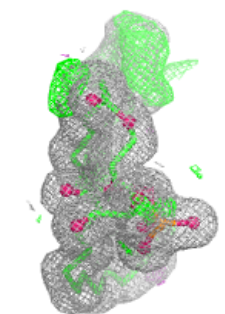
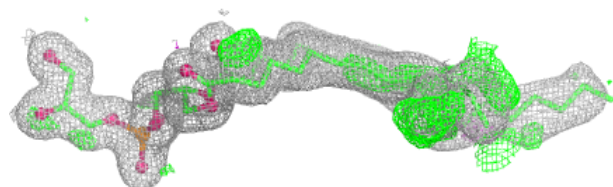
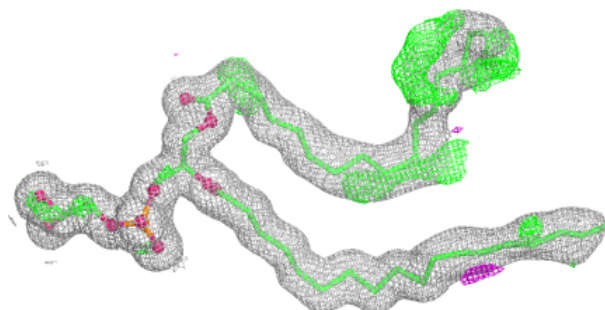


Electron density around PEK P 304:

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

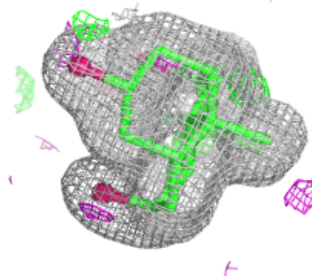
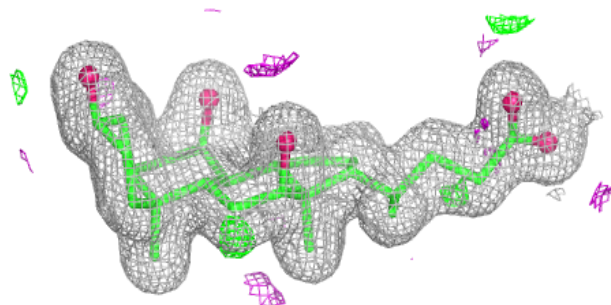
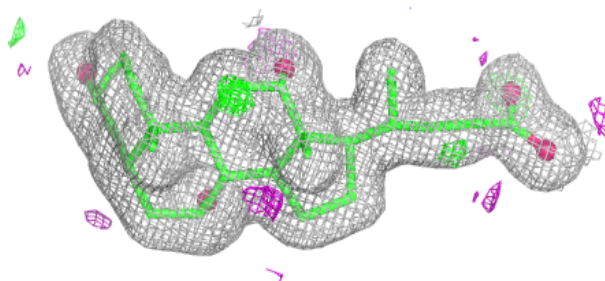
**Electron density around PGV C 305:**

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

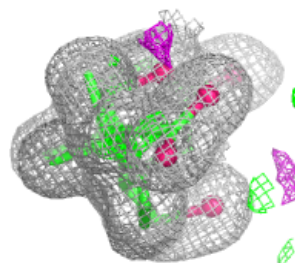
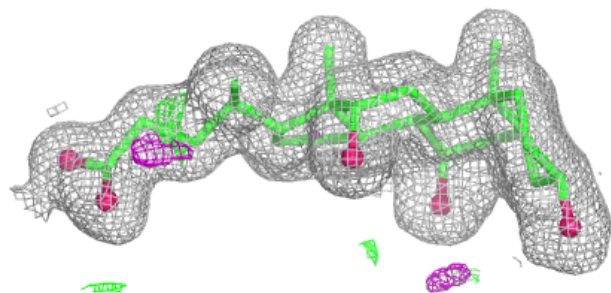
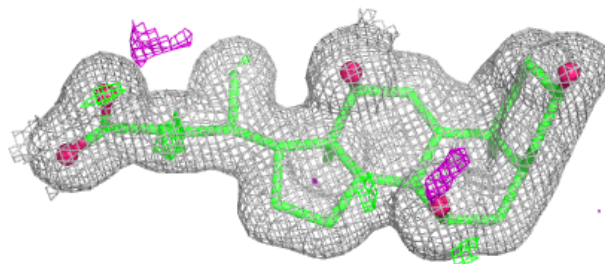


Electron density around CHD C 301:

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

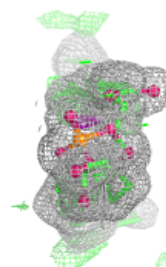
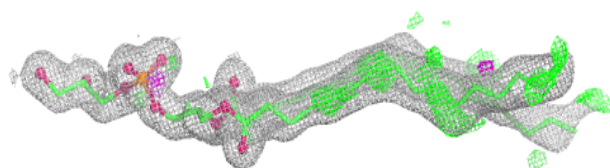
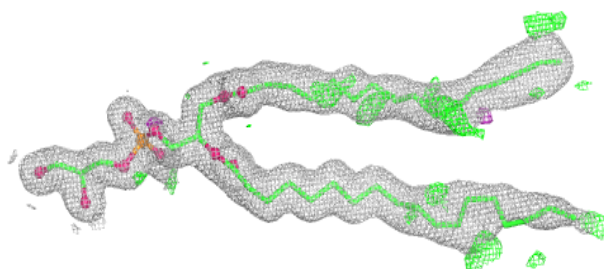
**Electron density around CHD P 301:**

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

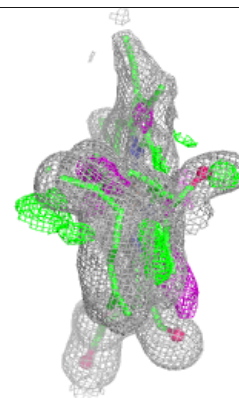
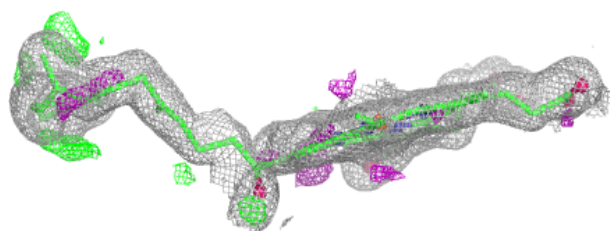
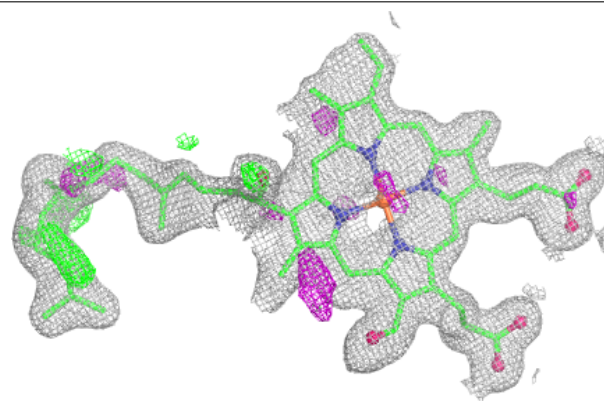


Electron density around PGV C 306:

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

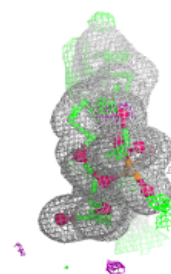
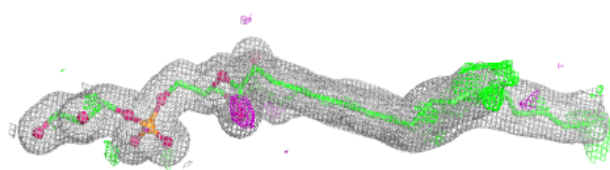
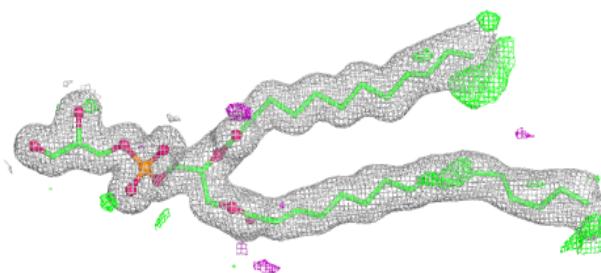
**Electron density around HEA A 602 (A):**

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

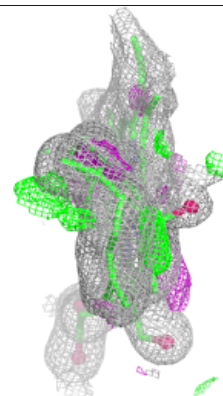
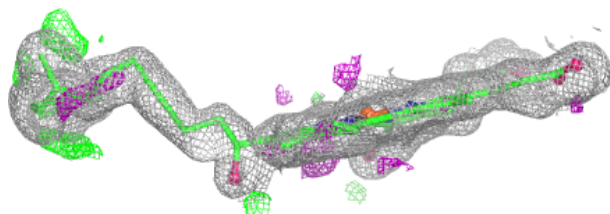
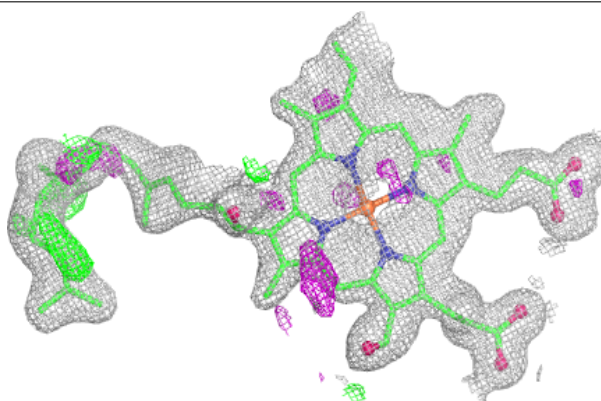


Electron density around PGV P 306:

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

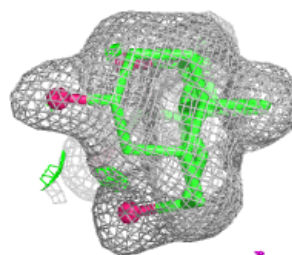
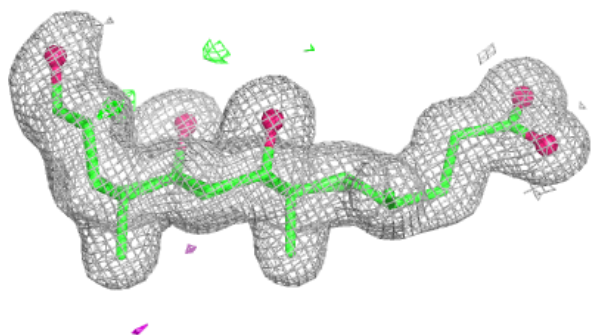
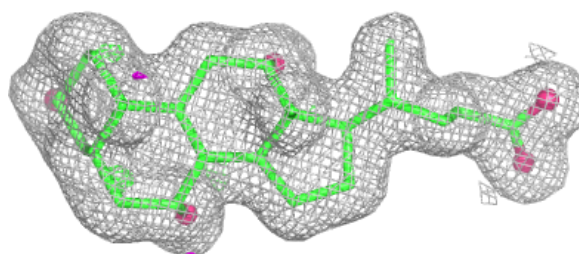
**Electron density around HEA A 602 (C):**

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

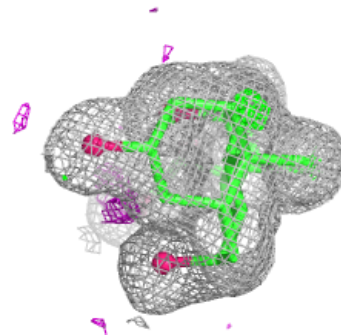
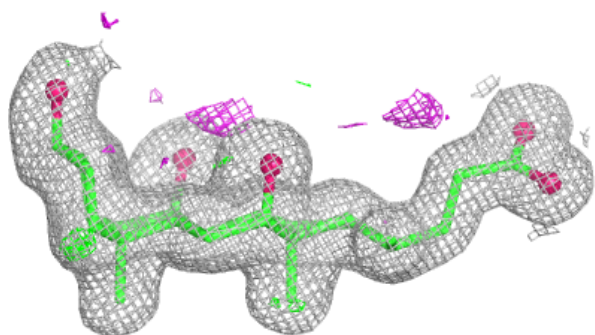
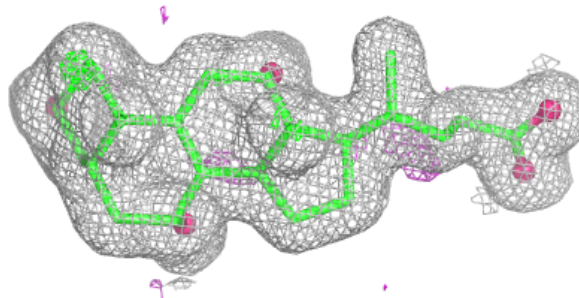


Electron density around CHD B 303:

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

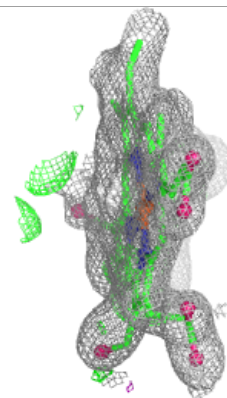
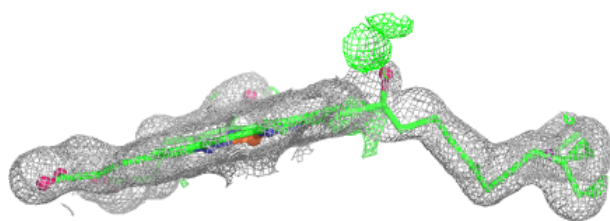
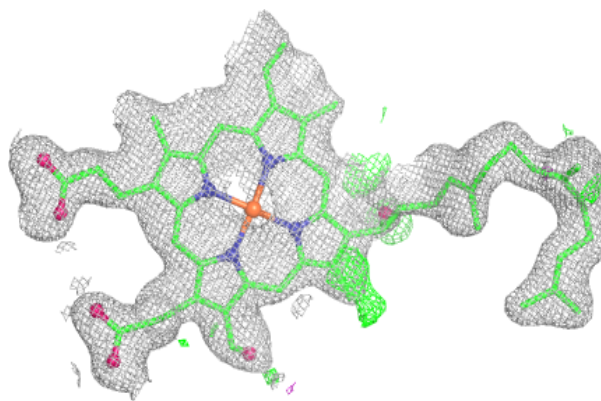
**Electron density around CHD G 102:**

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

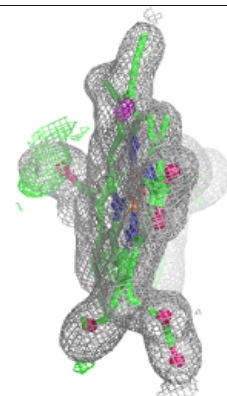
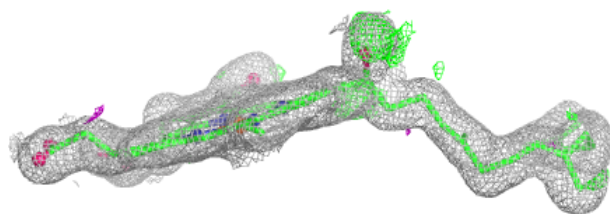
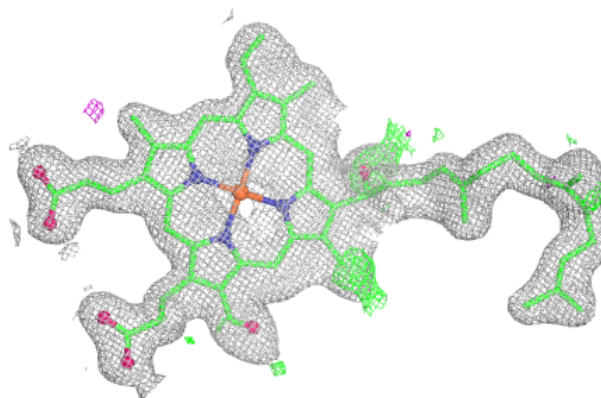


Electron density around HEA N 602 (C):

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

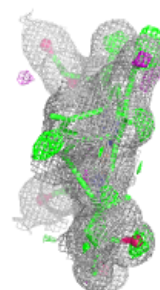
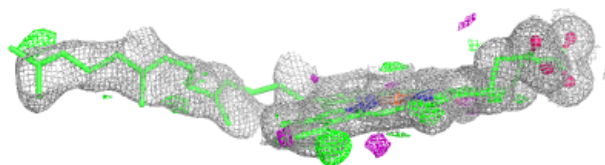
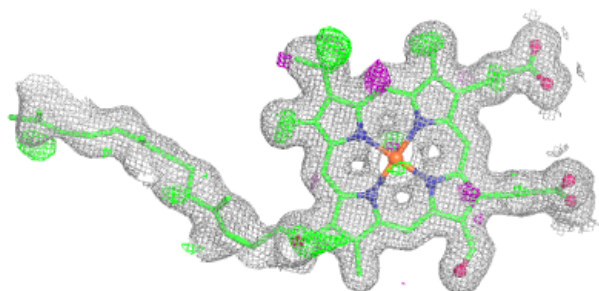
**Electron density around HEA N 602 (A):**

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

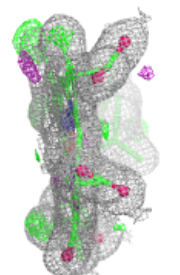
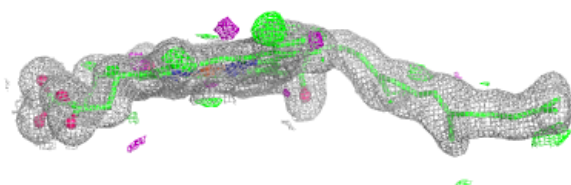
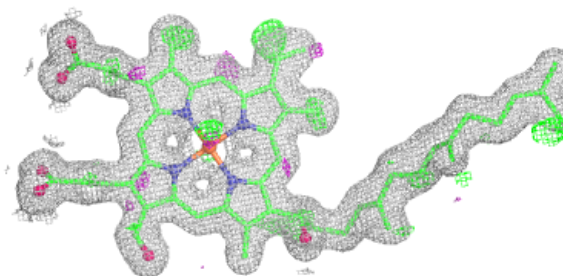


Electron density around HEA A 601 (A):

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

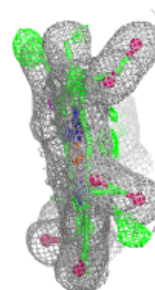
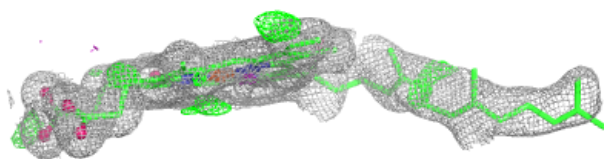
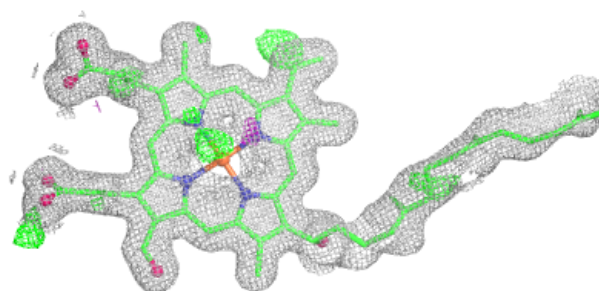
**Electron density around HEA A 601 (B):**

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

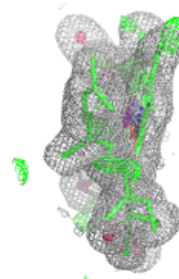
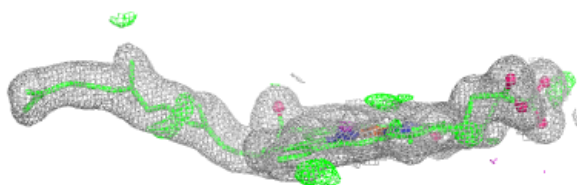
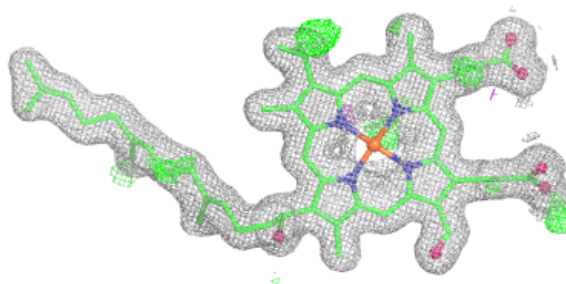


Electron density around HEA N 601 (A):

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

**Electron density around HEA N 601 (B):**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.