



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:42 AM UTC

PDB ID : 5XDX / pdb_00005xdx
Title : Bovine heart cytochrome c oxidase in the reduced state with pH 7.3 at 1.99 angstrom resolution
Authors : Luo, F.J.; Shimada, A.; Hagimoto, N.; Shimada, S.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2017-03-30
Resolution : 1.99 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	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

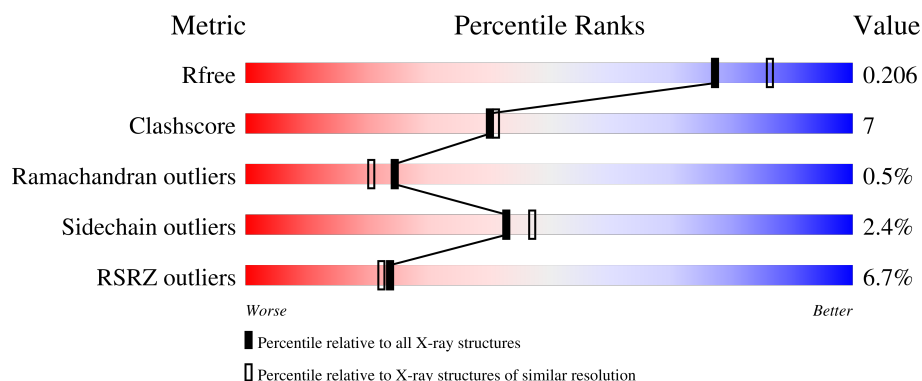
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	
1	N	514	
2	B	227	
2	O	227	

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Mol	Chain	Length	Quality of chain
3	C	260	
3	P	260	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	94	
6	S	94	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	N	613	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33247 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	20	0
			4128	2774	626	685	43			
1	N	514	Total	C	N	O	S	0	21	0
			4132	2773	627	687	45			

- 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	7	0
			1854	1209	281	343	21			
2	O	227	Total	C	N	O	S	0	6	0
			1849	1205	281	343	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	13	0
			2173	1461	338	358	16			
3	P	259	Total	C	N	O	S	0	12	0
			2168	1457	337	357	17			

- 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	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			857	548	144	162	3			
5	R	105	Total	C	N	O	S	0	1	0
			857	548	144	162	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	1	0
			721	448	127	140	6			
6	S	94	Total	C	N	O	S	0	1	0
			721	448	127	140	6			

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

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

- 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 polypeptide VIc.

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 VIIa-heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	2	0
			471	305	78	84	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	2	0
			471	305	78	84	4			

- Molecule 11 is a protein called Cytochrome c oxidase subunit VIIb.

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

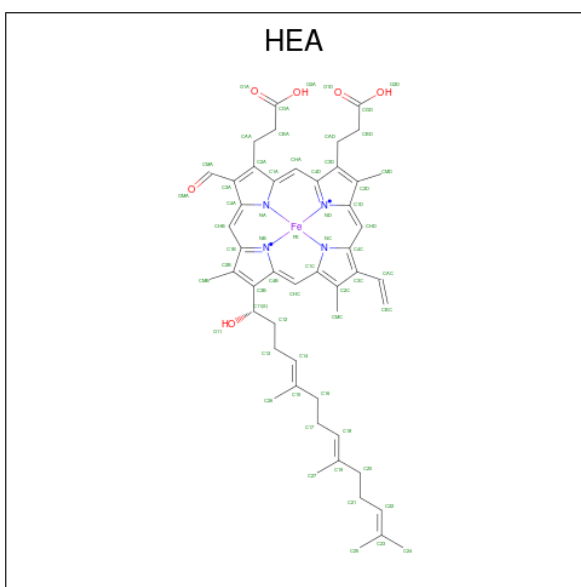
- Molecule 12 is a protein called Cytochrome c oxidase subunit VIIc.

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
			385	258	64	60	3			

- Molecule 13 is a protein called Cytochrome c oxidase subunit VIII-heart.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	1	0
			340	228	53	59			
13	Z	43	Total	C	N	O	0	1	0
			340	228	53	59			

- 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 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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

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

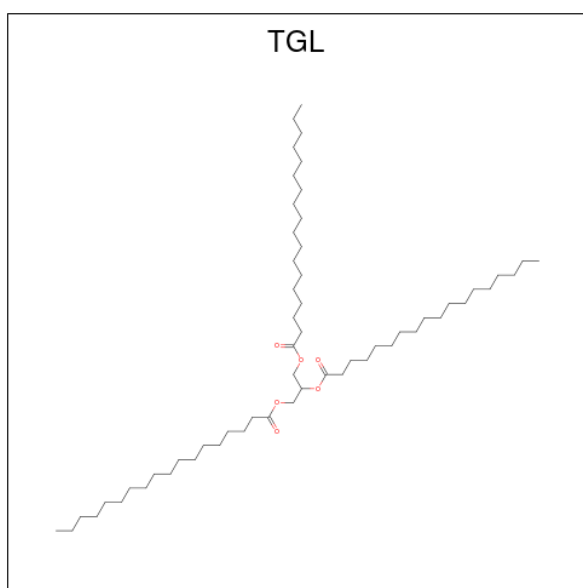
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

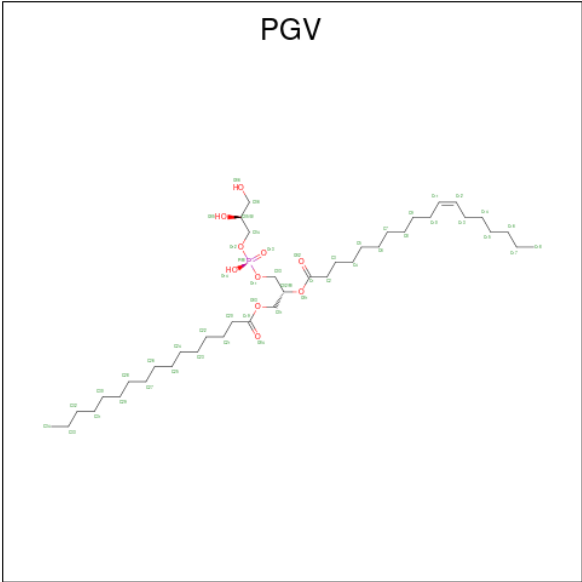
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		
17	P	1	Total	Na	0	0
			1	1		

- Molecule 18 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



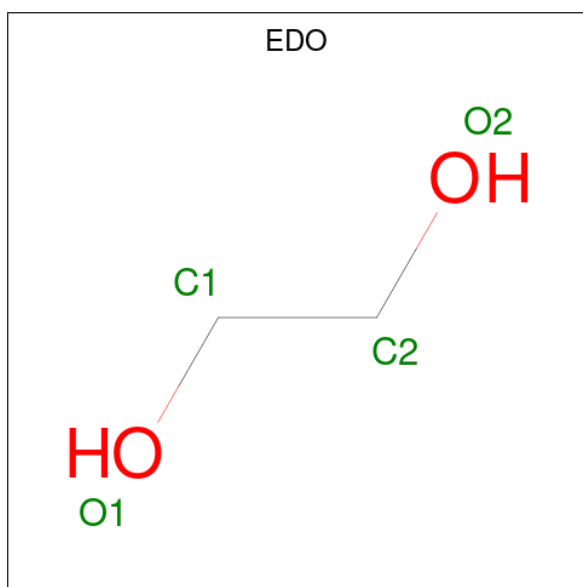
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	D	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	O	1	Total	C	O	0	0
			63	57	6		
18	Q	1	Total	C	O	0	0
			63	57	6		
18	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	M	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 20 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



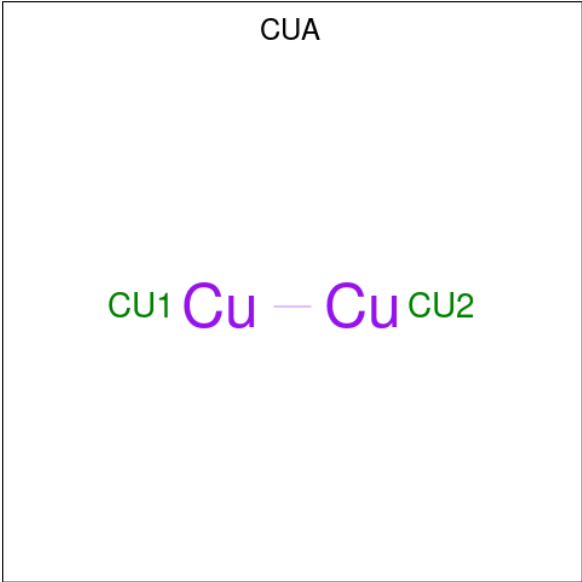
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	B	1	Total	C	O	0	0
			4	2	2		
20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

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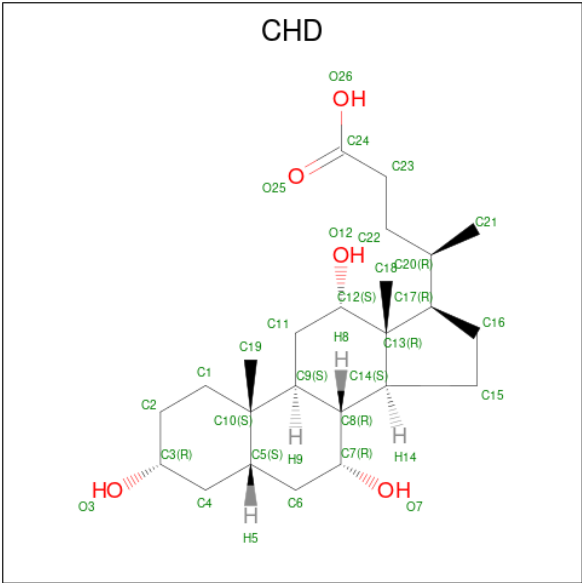
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	P	1	Total C O 4 2 2	0	0
20	R	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



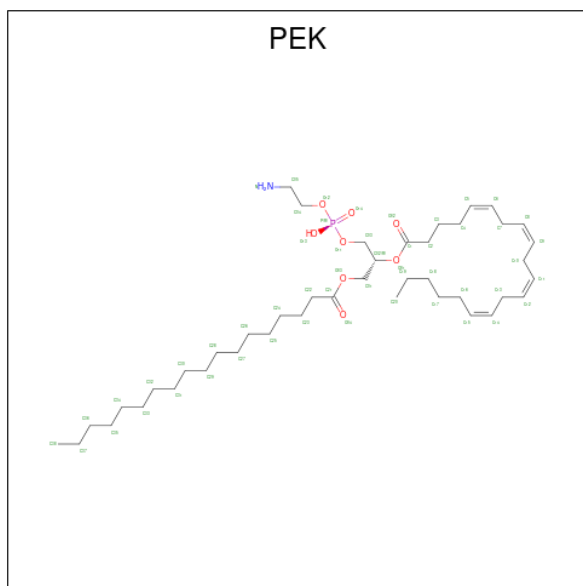
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	C	O	0
			29	24	5	
22	C	1	Total	C	O	0
			29	24	5	

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

- Molecule 23 is (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).



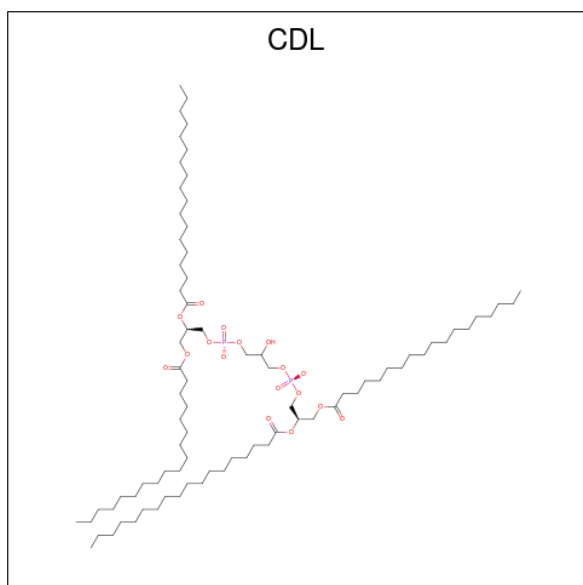
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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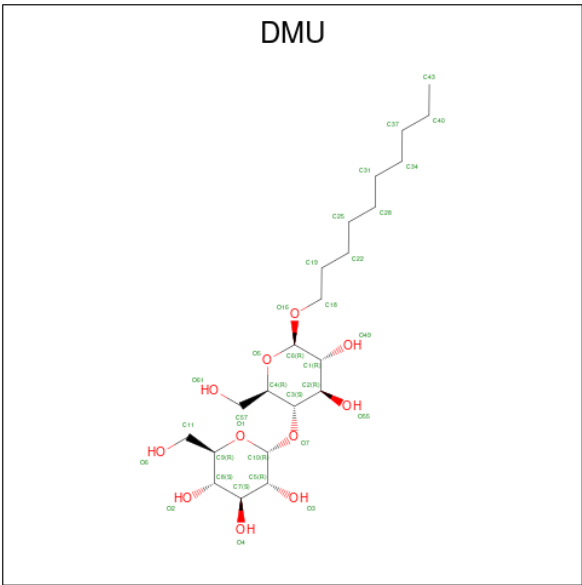
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



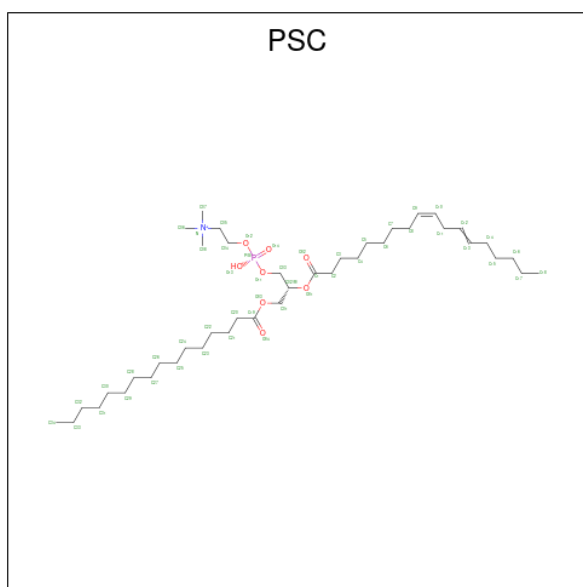
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	O	P		0	0
			100	81	17	2			
24	G	1	Total	C	O	P		0	0
			100	81	17	2			
24	P	1	Total	C	O	P		0	0
			100	81	17	2			
24	T	1	Total	C	O	P		0	0
			100	81	17	2			

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



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

- Molecule 26 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
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	245	Total	O	0	0
			245	245		
28	B	177	Total	O	0	1
			178	178		
28	C	103	Total	O	0	0
			103	103		
28	D	130	Total	O	0	0
			130	130		
28	E	92	Total	O	0	0
			92	92		

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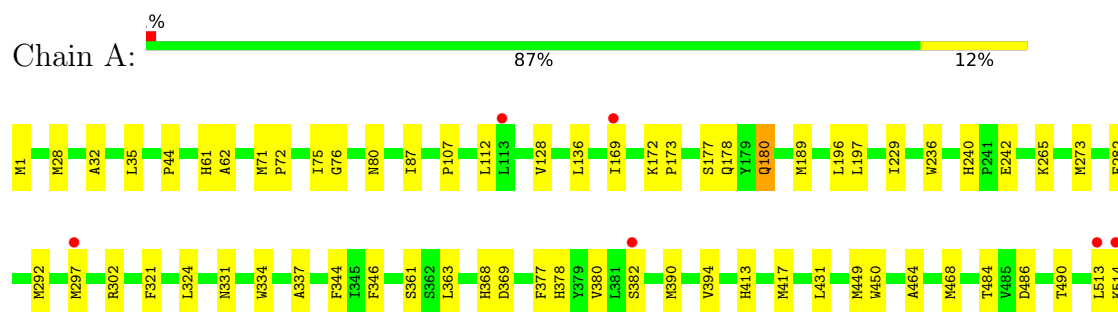
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	F	92	Total 92	O 92	0	0
28	G	58	Total 58	O 58	0	0
28	H	56	Total 56	O 56	0	0
28	I	48	Total 48	O 48	0	0
28	J	28	Total 28	O 28	0	0
28	K	42	Total 42	O 42	0	0
28	L	26	Total 26	O 26	0	0
28	M	27	Total 27	O 27	0	0
28	N	214	Total 214	O 214	0	0
28	O	128	Total 128	O 128	0	0
28	P	99	Total 99	O 99	0	0
28	Q	58	Total 58	O 58	0	0
28	R	62	Total 62	O 62	0	0
28	S	64	Total 64	O 64	0	0
28	T	51	Total 51	O 51	0	0
28	U	45	Total 45	O 45	0	0
28	V	31	Total 31	O 31	0	0
28	W	19	Total 19	O 19	0	0
28	X	11	Total 11	O 11	0	0
28	Y	21	Total 21	O 21	0	0
28	Z	14	Total 14	O 14	0	0

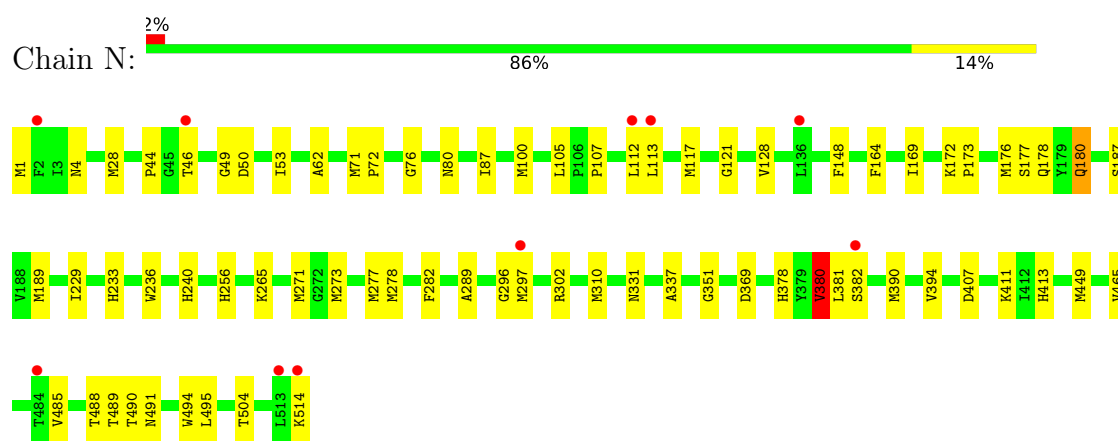
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

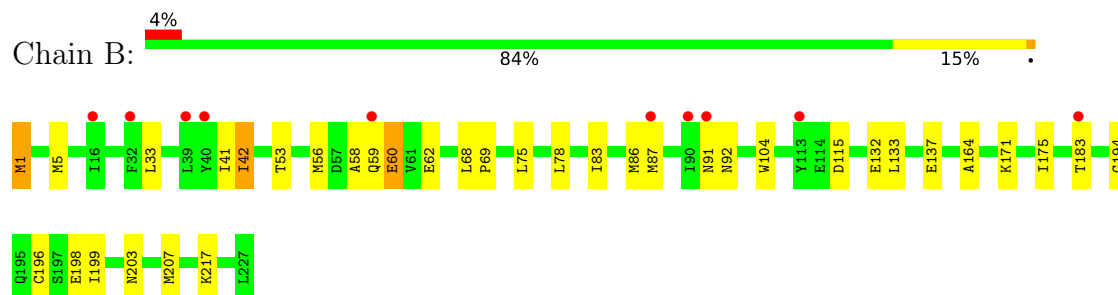
- Molecule 1: Cytochrome c oxidase subunit 1



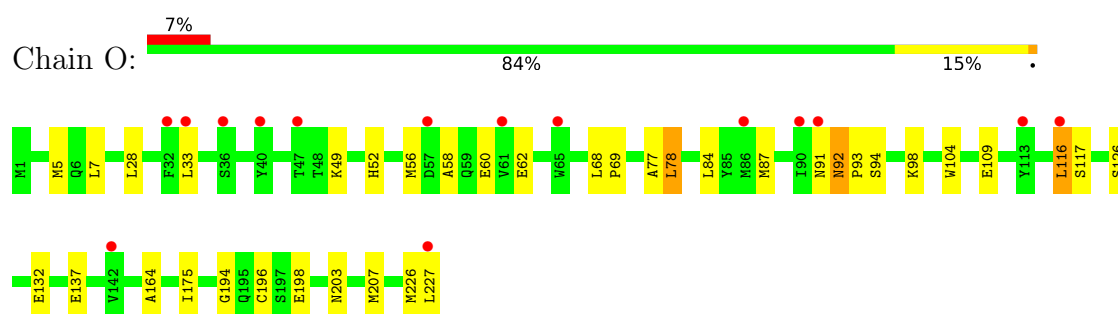
- Molecule 1: Cytochrome c oxidase subunit 1



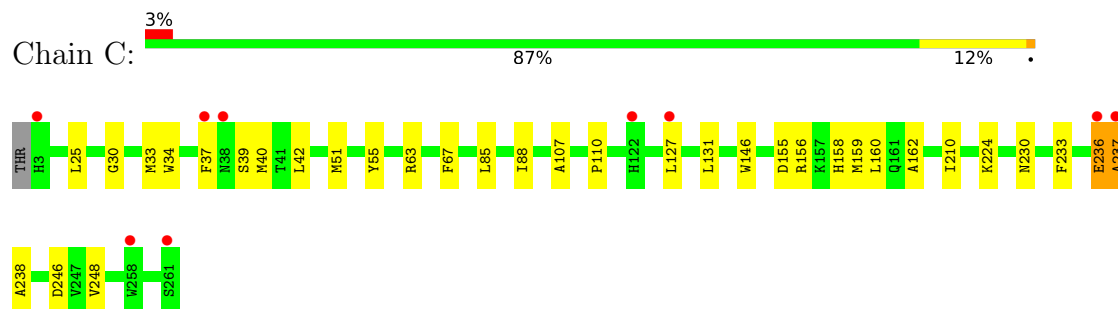
- Molecule 2: Cytochrome c oxidase subunit 2



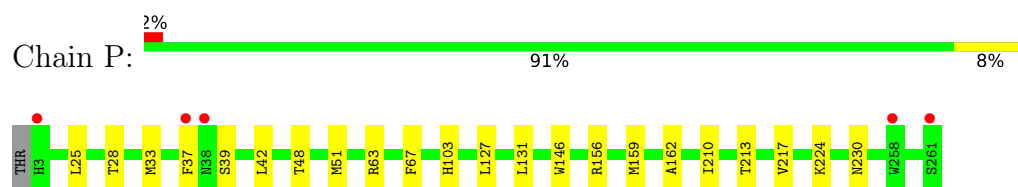
- Molecule 2: Cytochrome c oxidase subunit 2



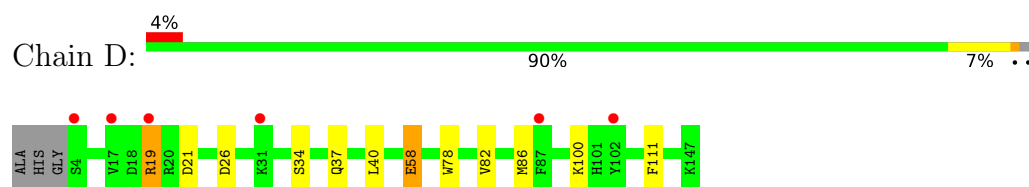
• Molecule 3: Cytochrome c oxidase subunit 3



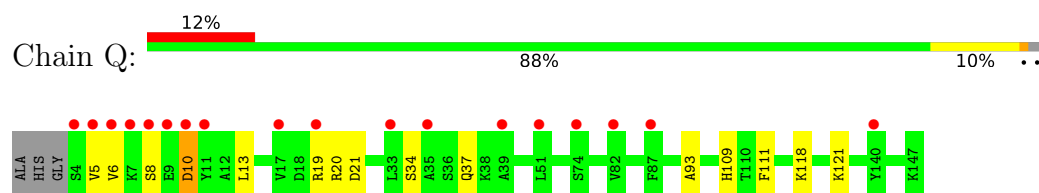
• Molecule 3: Cytochrome c oxidase subunit 3



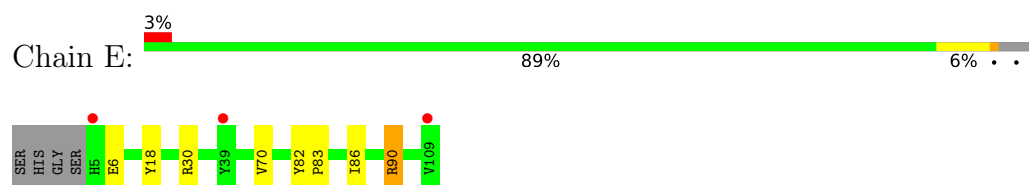
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



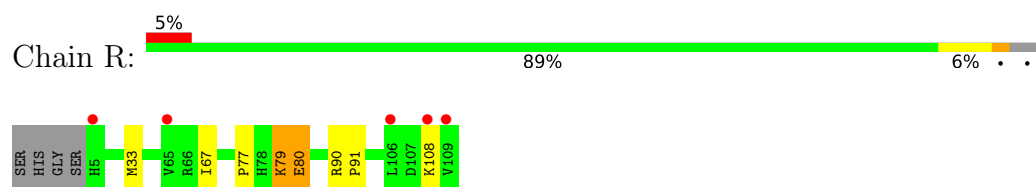
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



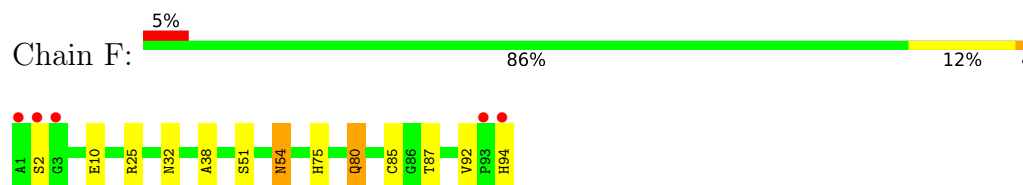
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



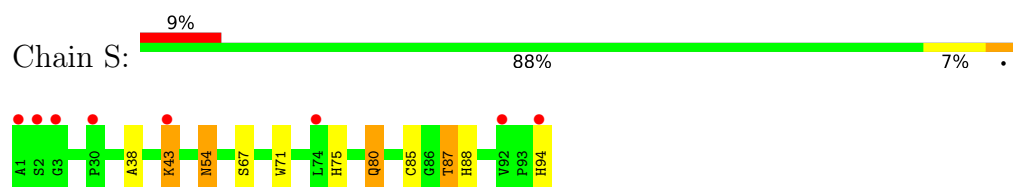
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



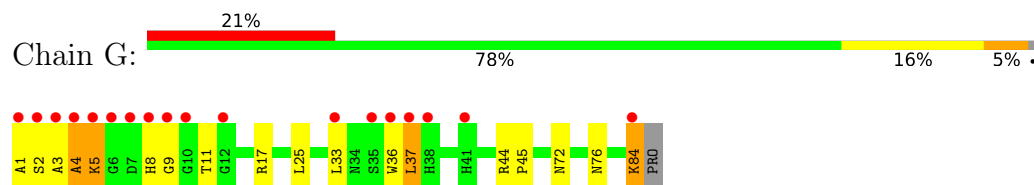
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



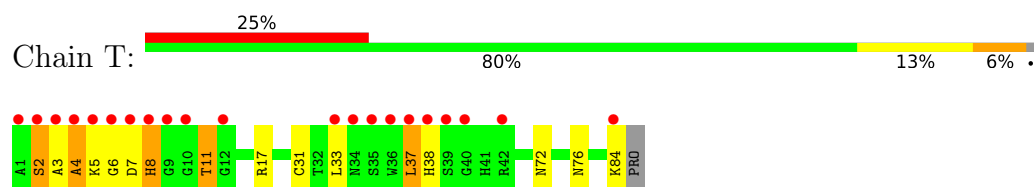
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



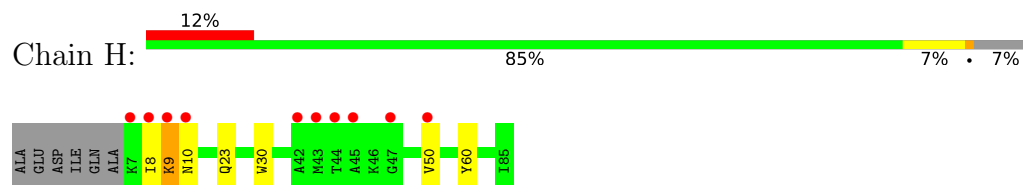
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



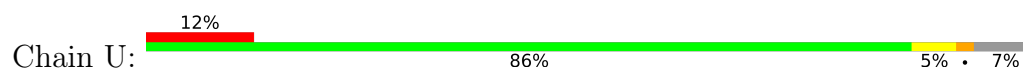
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1

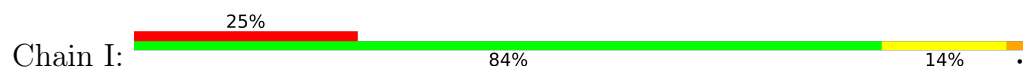


- Molecule 8: Cytochrome c oxidase subunit 6B1

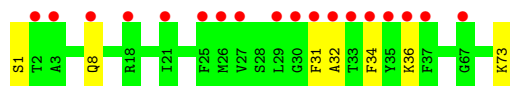
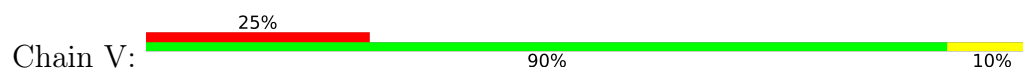




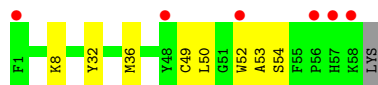
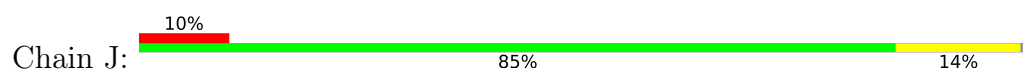
- Molecule 9: Cytochrome c oxidase polypeptide VIc



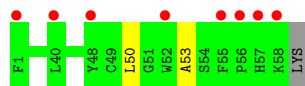
- Molecule 9: Cytochrome c oxidase polypeptide VIc



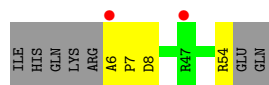
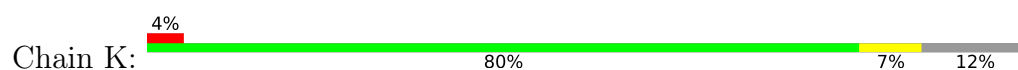
- Molecule 10: Cytochrome c oxidase subunit VIIa-heart



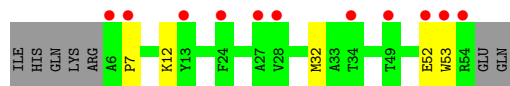
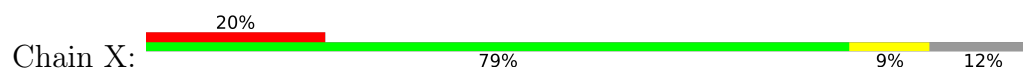
- Molecule 10: Cytochrome c oxidase subunit VIIa-heart



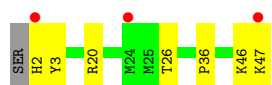
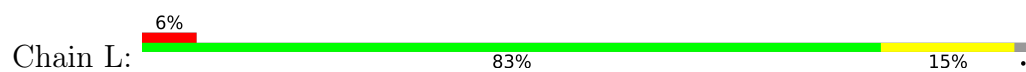
- Molecule 11: Cytochrome c oxidase subunit VIIb



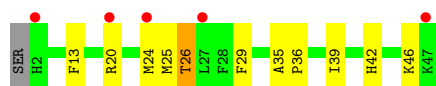
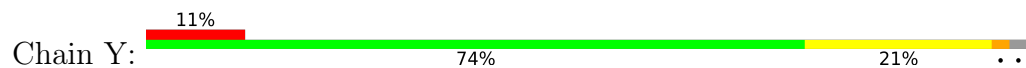
- Molecule 11: Cytochrome c oxidase subunit VIIb



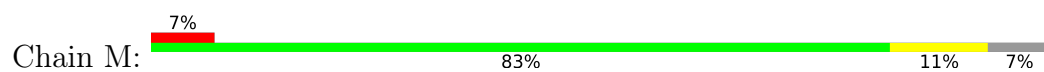
- Molecule 12: Cytochrome c oxidase subunit VIIc



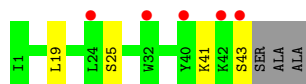
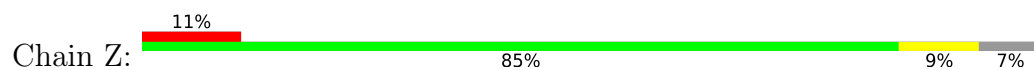
- Molecule 12: Cytochrome c oxidase subunit VIIc



- Molecule 13: Cytochrome c oxidase subunit VIII-heart



- Molecule 13: Cytochrome c oxidase subunit VIII-heart



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.04Å 205.69Å 177.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.99 40.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.99) 99.9 (40.00-1.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.182 , 0.203 0.184 , 0.206	Depositor DCC
R_{free} test set	23139 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33247	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: CUA, CDL, HEA, ZN, MG, CU, DMU, FME, SAC, TPO, NA, PEK, TGL, EDO, PGV, CHD, PSC

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	0.81	2/4315 (0.0%)	0.81	1/5889 (0.0%)
1	N	0.75	0/4322	0.84	4/5896 (0.1%)
2	B	0.78	1/1911 (0.1%)	0.83	1/2602 (0.0%)
2	O	0.68	1/1903 (0.1%)	0.80	0/2592
3	C	0.88	0/2299	0.78	4/3140 (0.1%)
3	P	0.85	0/2291	0.74	0/3128
4	D	0.69	0/1229	0.73	0/1658
4	Q	0.63	0/1229	0.77	0/1658
5	E	0.66	0/879	0.74	0/1192
5	R	0.62	0/879	0.76	0/1192
6	F	0.73	0/740	0.76	0/1003
6	S	0.72	0/740	0.77	0/1003
7	G	0.90	0/690	0.81	0/937
7	T	0.92	0/690	0.86	1/937 (0.1%)
8	H	0.65	0/682	0.76	0/921
8	U	0.64	0/682	0.80	0/921
9	I	0.58	0/605	0.85	0/802
9	V	0.49	0/605	0.84	0/802
10	J	0.67	0/488	0.76	0/658
10	W	0.68	0/488	0.75	0/658
11	K	0.76	0/398	0.84	0/546
11	X	0.71	0/398	0.82	0/546
12	L	0.72	0/393	0.78	0/526
12	Y	0.69	0/401	0.76	0/536
13	M	0.70	0/353	0.74	0/481
13	Z	0.64	0/353	0.83	0/481
All	All	0.75	4/29963 (0.0%)	0.80	11/40705 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	10.36	1.35	1.23
2	O	198	GLU	C-O	8.21	1.33	1.23
1	A	368	HIS	ND1-CE1	5.43	1.38	1.32
1	A	61	HIS	ND1-CE1	5.03	1.37	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	236	GLU	CA-C-N	-6.91	108.33	121.54
3	C	236	GLU	C-N-CA	-6.91	108.33	121.54
1	A	240	HIS	N-CA-CB	6.43	118.01	110.42
7	T	37	LEU	N-CA-C	-6.31	105.05	114.64
1	N	240	HIS	N-CA-CB	6.01	117.51	110.42
3	C	238	ALA	N-CA-C	-5.54	105.25	111.28
1	N	380	VAL	CB-CA-C	-5.49	104.65	112.22
1	N	105	LEU	CA-C-N	-5.20	115.02	120.38
1	N	105	LEU	C-N-CA	-5.20	115.02	120.38
2	B	199	ILE	N-CA-CB	5.18	116.45	110.49
3	C	236	GLU	N-CA-C	-5.15	102.23	109.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4128	0	4171	60	0
1	N	4132	0	4169	84	0
2	B	1854	0	1888	26	0
2	O	1849	0	1879	22	0
3	C	2173	0	2130	36	0
3	P	2168	0	2122	24	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	11	0
5	E	857	0	854	4	0
5	R	857	0	854	6	0
6	F	721	0	706	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	721	0	706	11	0
7	G	675	0	644	17	0
7	T	675	0	643	15	0
8	H	662	0	623	6	0
8	U	662	0	623	3	0
9	I	601	0	613	9	0
9	V	601	0	613	4	0
10	J	471	0	474	10	0
10	W	471	0	474	3	0
11	K	384	0	366	2	0
11	X	384	0	366	5	0
12	L	380	0	380	9	0
12	Y	385	0	389	12	0
13	M	340	0	363	5	0
13	Z	340	0	363	3	0
14	A	120	0	108	3	0
14	N	120	0	108	3	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	63	0	110	3	0
18	D	63	0	110	4	0
18	L	63	0	110	4	0
18	O	63	0	110	2	0
18	Q	63	0	110	0	0
18	Y	63	0	110	5	0
19	A	51	0	76	2	0
19	C	102	0	152	5	0
19	M	51	0	76	2	0
19	N	102	0	152	6	0
19	P	102	0	152	4	0
20	A	36	0	54	5	0
20	B	4	0	6	0	0
20	C	12	0	18	0	0
20	D	8	0	12	2	0
20	E	4	0	6	1	0
20	F	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	40	0	60	9	0
20	P	4	0	6	0	0
20	R	4	0	6	0	0
20	S	8	0	12	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	3	0
22	J	29	0	38	0	0
22	O	29	0	39	1	0
22	P	58	0	78	3	0
22	W	29	0	39	1	0
23	C	106	0	154	5	0
23	G	53	0	77	0	0
23	T	159	0	231	7	0
24	C	100	0	156	10	0
24	G	100	0	156	5	0
24	P	100	0	156	9	0
24	T	100	0	156	13	0
25	C	66	0	84	12	0
25	M	33	0	42	0	0
25	P	66	0	84	9	0
25	Z	33	0	42	0	0
26	E	52	0	80	10	0
26	O	52	0	80	6	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	245	0	0	11	0
28	B	178	0	0	5	0
28	C	103	0	0	2	0
28	D	130	0	0	2	0
28	E	92	0	0	0	0
28	F	92	0	0	1	0
28	G	58	0	0	0	0
28	H	56	0	0	2	0
28	I	48	0	0	0	0
28	J	28	0	0	2	0
28	K	42	0	0	1	0
28	L	26	0	0	0	0
28	M	27	0	0	0	0
28	N	214	0	0	7	0
28	O	128	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	P	99	0	0	1	0
28	Q	58	0	0	1	0
28	R	62	0	0	0	0
28	S	64	0	0	0	0
28	T	51	0	0	0	0
28	U	45	0	0	0	0
28	V	31	0	0	1	0
28	W	19	0	0	0	0
28	X	11	0	0	3	0
28	Y	21	0	0	0	0
28	Z	14	0	0	0	0
All	All	33247	0	32270	417	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (417) 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)
1:N:113[B]:LEU:CG	1:N:117[B]:MET:HE2	1.65	1.26
3:C:236:GLU:O	3:C:237:ALA:CB	1.79	1.26
1:N:113[B]:LEU:HG	1:N:117[B]:MET:CE	1.69	1.22
20:A:615:EDO:H22	28:A:920:HOH:O	1.42	1.19
3:C:33[B]:MET:SD	25:C:313:DMU:H11	1.83	1.18
1:N:28[B]:MET:HE2	1:N:28[B]:MET:HA	1.22	1.17
1:A:28[B]:MET:HA	1:A:28[B]:MET:CE	1.83	1.09
26:O:304:PSC:H02	26:O:304:PSC:H212	1.37	1.07
3:C:236:GLU:O	3:C:237:ALA:HB3	1.45	1.05
1:A:28[B]:MET:HE3	1:A:28[B]:MET:CA	1.88	1.03
6:S:85:CYS:SG	6:S:87:THR:HG23	1.99	1.02
25:C:313:DMU:H8	10:J:53:ALA:HB2	1.43	1.00
3:C:67:PHE:HE2	24:C:307:CDL:H1	1.24	0.99
7:G:84:LYS:H	7:G:84:LYS:HD2	1.27	0.99
1:N:113[B]:LEU:HG	1:N:117[B]:MET:HE2	1.03	0.99
1:N:113[B]:LEU:CD1	1:N:117[B]:MET:HE2	1.93	0.97
20:N:615:EDO:H22	28:N:884:HOH:O	1.64	0.96
3:P:33[B]:MET:SD	25:P:309:DMU:H11	2.06	0.95
1:A:28[B]:MET:HA	1:A:28[B]:MET:HE3	0.97	0.95
25:C:313:DMU:C19	10:J:53:ALA:HB2	1.97	0.94
11:X:32:MET:HB2	28:X:101:HOH:O	1.71	0.90
3:C:236:GLU:O	3:C:237:ALA:HB2	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:ARG:HE	24:C:307:CDL:HA21	1.37	0.88
1:N:491:ASN:HA	20:N:613:EDO:H12	1.56	0.87
3:P:67:PHE:HE2	24:P:305:CDL:H1	1.39	0.85
7:G:72:ASN:H	7:G:76:ASN:HD22	1.23	0.85
1:N:169:ILE:HG13	1:N:189[A]:MET:HE1	1.57	0.85
6:F:85:CYS:SG	6:F:87:THR:HG23	2.17	0.84
6:F:75:HIS:H	6:F:80:GLN:HE22	1.27	0.82
5:R:80:GLU:H	5:R:80:GLU:CD	1.88	0.82
3:C:33[B]:MET:SD	25:C:313:DMU:H6	2.20	0.82
1:N:28[B]:MET:HE2	1:N:28[B]:MET:CA	2.07	0.81
4:Q:93:ALA:HB1	28:X:101:HOH:O	1.80	0.81
9:I:31:PHE:O	9:I:34:PHE:N	2.14	0.81
26:O:304:PSC:H02	26:O:304:PSC:C21	2.11	0.80
1:N:28[B]:MET:HA	1:N:28[B]:MET:CE	2.08	0.80
6:S:43:LYS:HD2	6:S:43:LYS:H	1.47	0.80
1:N:117[A]:MET:HE3	12:Y:39:ILE:HG23	1.65	0.79
25:P:309:DMU:C19	10:W:53:ALA:HB2	2.12	0.79
8:H:23:GLN:NE2	28:H:101:HOH:O	2.16	0.79
23:C:303:PEK:HN2	7:G:76:ASN:HD21	1.32	0.78
1:N:297[B]:MET:HG3	1:N:302:ARG:HG3	1.64	0.78
4:D:34:SER:H	4:D:37:GLN:HE21	1.31	0.76
1:N:100[B]:MET:HE1	19:N:607:PGV:H82	1.68	0.76
3:P:63:ARG:HE	24:P:305:CDL:HA22	1.49	0.76
7:T:72:ASN:H	7:T:76:ASN:HD22	1.33	0.76
12:L:20:ARG:HH22	18:L:101:TGL:HC32	1.52	0.74
6:S:75:HIS:H	6:S:80:GLN:HE22	1.34	0.73
1:A:297[B]:MET:HG2	28:A:780:HOH:O	1.89	0.72
1:N:297[B]:MET:HG2	28:N:788:HOH:O	1.89	0.71
8:U:9:LYS:HD3	8:U:10:ASN:H	1.55	0.71
1:N:113[B]:LEU:CG	1:N:117[B]:MET:CE	2.43	0.70
20:N:612:EDO:H11	20:N:613:EDO:H11	1.72	0.70
6:S:43:LYS:H	6:S:43:LYS:CD	2.04	0.70
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.73	0.70
4:D:78:TRP:CA	18:D:201:TGL:HB22	2.21	0.69
4:D:78:TRP:HA	18:D:201:TGL:HB22	1.74	0.69
7:T:2:SER:OG	23:T:101:PEK:H311	1.94	0.68
24:T:104:CDL:H251	24:T:104:CDL:H542	1.75	0.68
3:C:67:PHE:CE2	24:C:307:CDL:H1	2.17	0.67
7:T:76:ASN:HD21	23:T:102:PEK:HN2	1.40	0.67
1:N:46:THR:HG22	1:N:49:GLY:H	1.58	0.67
6:S:85:CYS:SG	6:S:87:THR:CG2	2.81	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:ARG:HG2	4:D:19:ARG:HH21	1.59	0.67
25:P:309:DMU:H9	10:W:53:ALA:HB2	1.76	0.67
9:I:33:THR:HA	9:I:36:LYS:HB3	1.77	0.67
6:F:54:ASN:H	6:F:54:ASN:HD22	1.42	0.66
2:B:53:THR:HG21	28:D:305:HOH:O	1.94	0.66
1:A:28[B]:MET:CE	1:A:28[B]:MET:CA	2.59	0.66
19:N:606:PGV:H311	13:Z:19:LEU:HD23	1.76	0.66
23:T:103:PEK:H382	24:T:104:CDL:H273	1.77	0.65
1:A:112:LEU:C	1:A:112:LEU:HD23	2.21	0.65
1:A:417[B]:MET:HE2	1:A:464:ALA:HB3	1.79	0.65
7:G:84:LYS:H	7:G:84:LYS:CD	2.04	0.65
1:A:361[A]:SER:OG	28:A:701:HOH:O	2.15	0.64
1:N:117[A]:MET:HE2	1:N:117[A]:MET:HA	1.78	0.64
9:V:8:GLN:CD	28:V:103:HOH:O	2.40	0.64
25:C:313:DMU:H20	10:J:50:LEU:HB2	1.78	0.64
3:C:33[A]:MET:HE3	3:C:39:SER:OG	1.98	0.64
25:P:309:DMU:H8	10:W:53:ALA:HB2	1.79	0.64
1:A:394[A]:VAL:HG12	20:A:611:EDO:H22	1.80	0.63
6:S:43:LYS:HD2	6:S:43:LYS:N	2.13	0.63
4:D:26:ASP:HB3	20:D:202:EDO:H21	1.81	0.63
3:P:210:ILE:HD13	19:P:303:PGV:H301	1.80	0.63
7:T:31:CYS:SG	24:T:104:CDL:H552	2.38	0.62
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.79	0.62
25:C:313:DMU:H9	10:J:49:CYS:O	1.99	0.62
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.30	0.62
1:A:417[B]:MET:HE2	1:A:464:ALA:CB	2.30	0.61
25:C:313:DMU:H9	10:J:53:ALA:HB2	1.78	0.61
3:C:233:PHE:O	3:C:236:GLU:O	2.19	0.61
1:N:46:THR:CG2	1:N:49:GLY:H	2.13	0.61
9:I:31:PHE:O	9:I:32:ALA:C	2.42	0.60
1:A:71[B]:MET:HB3	1:A:72:PRO:HD3	1.83	0.60
2:O:28:LEU:HD21	18:O:302:TGL:HG12	1.83	0.60
3:P:63:ARG:HE	24:P:305:CDL:CA2	2.14	0.60
7:T:31:CYS:SG	24:T:104:CDL:H532	2.42	0.60
24:C:307:CDL:HB21	24:C:307:CDL:OB6	2.02	0.60
2:B:56:MET:HA	26:E:201:PSC:H201	1.84	0.60
24:C:307:CDL:HA22	28:J:201:HOH:O	2.02	0.59
4:D:34:SER:H	4:D:37:GLN:NE2	1.99	0.59
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.67	0.59
18:L:101:TGL:OC1	18:L:101:TGL:HC41	2.02	0.59
1:A:417[B]:MET:HE3	28:A:841:HOH:O	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:HG12	1:A:189[A]:MET:HE1	1.83	0.59
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.84	0.59
1:N:256:HIS:HE1	20:N:613:EDO:H22	1.67	0.59
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.38	0.58
1:N:187:SER:HB3	1:N:277[B]:MET:HE1	1.84	0.58
12:L:20:ARG:NH2	18:L:101:TGL:HC32	2.17	0.58
3:P:37:PHE:CE2	25:P:309:DMU:H13	2.38	0.58
1:A:297[B]:MET:HG3	1:A:302:ARG:HG3	1.84	0.58
4:Q:10:ASP:HB3	4:Q:13:LEU:HD12	1.86	0.58
1:A:297[B]:MET:CG	1:A:302:ARG:HG3	2.34	0.57
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.87	0.57
2:O:56:MET:HA	26:O:304:PSC:H201	1.85	0.57
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.44	0.57
3:P:33[B]:MET:SD	25:P:309:DMU:H6	2.45	0.56
4:D:82:VAL:HG12	4:D:86:MET:HE2	1.88	0.56
1:N:87:ILE:O	1:N:173:PRO:HD3	2.06	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.05	0.56
1:A:112:LEU:HG	28:A:932:HOH:O	2.05	0.56
3:C:30:GLY:HA2	3:C:42[B]:LEU:HB3	1.88	0.56
24:T:104:CDL:OA7	24:T:104:CDL:H331	2.05	0.56
1:A:282:PHE:HA	7:T:4:ALA:CB	2.35	0.56
1:N:113[B]:LEU:CD1	1:N:117[B]:MET:CE	2.78	0.55
1:N:28[B]:MET:CA	1:N:28[B]:MET:CE	2.79	0.55
3:P:33[B]:MET:SD	25:P:309:DMU:C22	2.90	0.55
12:Y:13:PHE:HB3	18:Y:101:TGL:HA21	1.89	0.55
2:B:183:THR:HG23	28:B:556:HOH:O	2.06	0.55
13:M:19:LEU:HD23	19:M:101:PGV:H311	1.87	0.55
3:C:156:ARG:HE	22:C:308:CHD:C24	2.20	0.55
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.89	0.55
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.54
26:E:201:PSC:H21	26:E:201:PSC:H231	1.88	0.54
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.88	0.54
9:I:33:THR:O	9:I:37:PHE:N	2.33	0.54
9:I:28:SER:O	9:I:32:ALA:N	2.31	0.54
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.89	0.54
1:N:100[B]:MET:HE1	19:N:607:PGV:C8	2.36	0.54
1:A:324:LEU:HD22	2:B:42:ILE:HG13	1.89	0.54
2:B:87:MET:HE2	28:B:413:HOH:O	2.08	0.54
1:N:273:MET:HE2	28:N:827:HOH:O	2.07	0.54
2:O:58:ALA:O	2:O:62:GLU:HG3	2.08	0.54
1:A:484:THR:HG22	28:A:933:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:303:PGV:H171	24:P:305:CDL:H651	1.89	0.54
3:C:85:LEU:HD23	3:C:88[B]:ILE:HD11	1.90	0.53
25:C:313:DMU:H10	10:J:49:CYS:HB3	1.90	0.53
4:D:78:TRP:N	18:D:201:TGL:HB22	2.23	0.53
6:S:43:LYS:HE2	6:S:88:HIS:CE1	2.43	0.53
1:A:331[B]:ASN:ND2	4:D:21:ASP:HB3	2.24	0.53
1:A:71[B]:MET:HG3	1:A:75:ILE:HD12	1.91	0.53
1:A:334:TRP:CZ3	18:D:201:TGL:HA52	2.44	0.53
1:A:321:PHE:CD1	26:E:201:PSC:H341	2.44	0.53
7:G:3:ALA:O	7:G:4:ALA:HB2	2.09	0.53
1:N:112:LEU:HD23	1:N:112:LEU:C	2.34	0.52
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.38	0.52
12:Y:20:ARG:HD3	12:Y:20:ARG:C	2.34	0.52
2:B:58:ALA:O	2:B:62:GLU:HG3	2.09	0.52
19:N:607:PGV:H322	23:T:102:PEK:H371	1.90	0.52
3:C:33[B]:MET:SD	25:C:313:DMU:C22	2.76	0.52
3:C:210:ILE:HG12	19:C:305:PGV:H132	1.90	0.52
6:F:54:ASN:HD22	6:F:54:ASN:N	2.04	0.52
1:N:173:PRO:HD2	1:N:176[B]:MET:HE2	1.90	0.52
6:S:67:SER:OG	20:S:103:EDO:H21	2.10	0.52
1:A:297[A]:MET:HB2	28:A:780:HOH:O	2.09	0.51
1:N:76:GLY:O	1:N:80:ASN:HB2	2.09	0.51
1:N:236:TRP:CH2	14:N:602:HEA:HBD1	2.45	0.51
1:N:28[B]:MET:HE1	1:N:465:VAL:CG1	2.40	0.51
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.93	0.51
11:X:7:PRO:HB2	11:X:12:LYS:HE3	1.91	0.51
12:Y:25:MET:HG2	18:Y:101:TGL:HA62	1.92	0.51
26:E:201:PSC:H41	26:E:201:PSC:H252	1.93	0.51
1:N:256:HIS:CE1	20:N:613:EDO:H22	2.43	0.51
1:N:351:GLY:C	1:N:380:VAL:HG13	2.35	0.51
9:I:31:PHE:CD1	9:I:31:PHE:C	2.88	0.51
12:L:2:HIS:CG	12:L:3:TYR:H	2.28	0.51
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.93	0.51
20:A:616:EDO:H22	28:A:715:HOH:O	2.10	0.51
7:G:3:ALA:O	7:G:4:ALA:CB	2.59	0.50
7:G:72:ASN:H	7:G:76:ASN:ND2	2.00	0.50
3:C:33[B]:MET:SD	25:C:313:DMU:C18	2.95	0.50
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.47	0.50
23:C:304:PEK:H132	7:G:25:LEU:HD22	1.92	0.50
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.50
3:P:51[B]:MET:HE3	24:P:305:CDL:H381	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:210:ILE:HG21	19:C:305:PGV:H282	1.92	0.50
1:A:449[A]:MET:SD	2:B:5[A]:MET:HG2	2.52	0.50
2:B:68[B]:LEU:HD23	26:E:201:PSC:H171	1.93	0.50
7:G:1:ALA:HB2	19:P:304:PGV:H321	1.92	0.50
7:T:38:HIS:NE2	24:T:104:CDL:H111	2.26	0.50
2:O:84:LEU:HA	2:O:87:MET:HE2	1.92	0.50
3:C:51[A]:MET:HE1	19:C:305:PGV:H161	1.92	0.49
6:F:51:SER:O	6:F:94:HIS:N	2.35	0.49
1:N:4[B]:ASN:ND2	28:N:702:HOH:O	2.44	0.49
25:P:308:DMU:H35	28:P:426:HOH:O	2.11	0.49
19:M:101:PGV:H32	19:M:101:PGV:H012	1.94	0.49
1:N:236:TRP:HH2	14:N:602:HEA:HBD1	1.77	0.49
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.95	0.49
25:P:309:DMU:H32	25:P:309:DMU:H29	1.94	0.49
1:A:76:GLY:O	1:A:80:ASN:HB2	2.13	0.49
1:N:117[A]:MET:HE2	12:Y:42:HIS:CD2	2.47	0.49
10:J:8:LYS:NZ	28:J:201:HOH:O	2.46	0.49
12:L:46:LYS:O	12:L:47:LYS:HB2	2.12	0.49
3:P:33[A]:MET:HE3	3:P:39:SER:OG	2.13	0.49
3:C:51[A]:MET:SD	24:C:307:CDL:H612	2.53	0.49
1:N:177:SER:H	1:N:180:GLN:NE2	2.11	0.49
7:T:72:ASN:H	7:T:76:ASN:ND2	2.08	0.49
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.93	0.49
3:C:155:ASP:OD2	6:F:2:SER:HA	2.13	0.49
4:D:19:ARG:NH2	28:D:302:HOH:O	2.45	0.49
5:R:33[A]:MET:HE2	5:R:67:ILE:HG12	1.95	0.49
24:T:104:CDL:H581	24:T:104:CDL:H762	1.95	0.49
1:A:71[B]:MET:HE1	1:A:242:GLU:OE1	2.13	0.48
7:T:37:LEU:HD23	24:T:104:CDL:H381	1.95	0.48
24:T:104:CDL:H542	24:T:104:CDL:C25	2.42	0.48
3:C:37:PHE:CE2	25:C:313:DMU:H13	2.48	0.48
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.13	0.48
5:R:80:GLU:CD	5:R:80:GLU:N	2.64	0.48
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.95	0.48
5:E:86:ILE:O	5:E:90:ARG:HG2	2.13	0.48
8:H:23:GLN:HG3	28:H:141:HOH:O	2.13	0.48
9:I:31:PHE:O	9:I:33:THR:N	2.46	0.48
3:C:248:VAL:HG22	23:T:101:PEK:H161	1.95	0.48
7:T:3:ALA:O	7:T:4:ALA:CB	2.61	0.48
1:A:177:SER:H	1:A:180:GLN:HE21	1.61	0.48
5:R:77:PRO:HA	5:R:79:LYS:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:GLU:H	2:B:60:GLU:CD	2.21	0.48
3:C:160:LEU:HD13	22:C:308:CHD:H181	1.95	0.48
1:N:28[B]:MET:HE1	1:N:465:VAL:HG11	1.96	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
10:J:54:SER:O	12:L:46:LYS:HE2	2.14	0.47
25:C:313:DMU:H7	10:J:52:TRP:CE3	2.49	0.47
1:N:71[A]:MET:HB2	1:N:72:PRO:HD3	1.94	0.47
6:F:54:ASN:H	6:F:54:ASN:ND2	2.09	0.47
6:S:54:ASN:HD22	6:S:54:ASN:C	2.22	0.47
7:T:17:ARG:HH22	23:T:103:PEK:H041	1.79	0.47
12:Y:13:PHE:HB3	18:Y:101:TGL:CA2	2.45	0.47
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.95	0.47
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.62	0.47
4:D:19:ARG:HH21	4:D:19:ARG:CG	2.25	0.47
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.96	0.47
3:P:127:LEU:HB3	24:T:104:CDL:OB3	2.15	0.47
1:N:46:THR:HG21	1:N:49:GLY:HA2	1.96	0.47
1:N:488:THR:HB	1:N:495:LEU:HD13	1.97	0.47
2:O:126:SER:OG	28:O:401:HOH:O	2.20	0.47
1:A:136[B]:LEU:HD11	28:A:937:HOH:O	2.13	0.47
18:A:606:TGL:HA41	18:A:606:TGL:HA92	1.97	0.46
2:B:41:ILE:HG21	26:E:201:PSC:H342	1.96	0.46
7:G:37:LEU:HD22	24:G:101:CDL:H381	1.96	0.46
2:B:41:ILE:HD13	26:E:201:PSC:H342	1.97	0.46
1:N:169:ILE:CG1	1:N:189[A]:MET:HE1	2.39	0.46
7:G:72:ASN:N	7:G:76:ASN:HD22	2.02	0.46
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.97	0.46
22:C:308:CHD:H42	28:C:499:HOH:O	2.14	0.46
1:N:28[A]:MET:HE3	12:Y:29:PHE:CD1	2.51	0.46
1:N:297[B]:MET:SD	1:N:302:ARG:CG	3.03	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.97	0.46
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.97	0.46
24:C:307:CDL:H191	24:C:307:CDL:H752	1.98	0.46
8:H:9:LYS:O	8:H:10:ASN:HB2	2.14	0.46
3:P:224:LYS:HE3	24:P:305:CDL:HB32	1.97	0.46
1:A:324:LEU:CD2	2:B:42:ILE:HG13	2.46	0.46
2:B:217:LYS:HG2	28:B:506:HOH:O	2.16	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.97	0.46
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.98	0.46
22:O:301:CHD:H212	22:O:301:CHD:H12	1.96	0.46
12:Y:24[B]:MET:HE3	12:Y:24[B]:MET:HB2	1.85	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:606:PGV:H221	19:N:606:PGV:H011	1.98	0.46
3:P:213:THR:HG23	24:P:305:CDL:H771	1.98	0.46
1:A:377:PHE:HA	1:A:380:VAL:HG12	1.97	0.45
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.97	0.45
3:C:107:ALA:HB2	19:C:306:PGV:H031	1.96	0.45
28:N:728:HOH:O	2:O:87:MET:SD	2.61	0.45
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.51	0.45
4:Q:109:HIS:HD2	28:Q:338:HOH:O	1.99	0.45
1:A:87:ILE:O	1:A:173:PRO:HD3	2.15	0.45
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.52	0.45
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.49	0.45
7:G:4:ALA:CB	1:N:282:PHE:HA	2.46	0.45
2:B:68[B]:LEU:HB3	2:B:69:PRO:HD3	1.99	0.45
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.14	0.45
26:E:201:PSC:H31	9:I:14:ALA:HB1	1.99	0.44
1:N:271:MET:HB2	20:N:617:EDO:H12	1.98	0.44
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.99	0.44
12:Y:20:ARG:NH2	18:Y:101:TGL:HC32	2.32	0.44
19:A:607:PGV:H262	19:C:305:PGV:H292	1.99	0.44
1:A:71[B]:MET:HE3	1:A:71[B]:MET:HB2	1.69	0.44
6:F:92:VAL:HG23	6:F:92:VAL:O	2.17	0.44
8:H:9:LYS:HD3	8:H:9:LYS:HA	1.63	0.44
3:P:210:ILE:HG21	19:P:303:PGV:H282	1.98	0.44
7:T:11:TPO:HA	7:T:11:TPO:O2P	2.16	0.44
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.16	0.44
23:T:102:PEK:H71	23:T:102:PEK:H32	1.98	0.44
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	2.00	0.44
1:A:292:MET:O	1:A:297[B]:MET:HE3	2.18	0.44
1:N:297[B]:MET:HG3	1:N:302:ARG:CG	2.43	0.44
1:A:486:ASP:OD2	4:D:19:ARG:HD2	2.18	0.44
3:P:48:THR:HA	3:P:51[B]:MET:HE2	2.00	0.44
2:O:52:HIS:HE1	26:O:304:PSC:H211	1.82	0.44
9:V:31:PHE:O	9:V:34:PHE:N	2.46	0.44
2:B:83:ILE:HA	2:B:86[B]:MET:HG2	2.00	0.43
12:L:46:LYS:O	12:L:47:LYS:CB	2.66	0.43
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.52	0.43
1:N:176[B]:MET:HE3	1:N:176[B]:MET:HB3	1.81	0.43
26:O:304:PSC:H222	26:O:304:PSC:H251	1.56	0.43
1:A:273:MET:HE2	28:A:725:HOH:O	2.18	0.43
2:B:56:MET:HB3	26:E:201:PSC:H222	2.00	0.43
7:G:84:LYS:HD2	7:G:84:LYS:N	2.10	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.92	0.43
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.43
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.01	0.43
1:A:196:LEU:HD21	3:C:88[B]:ILE:HG13	2.00	0.43
1:A:344:PHE:CD1	1:A:344:PHE:C	2.96	0.43
24:C:307:CDL:OA5	24:C:307:CDL:HB22	2.18	0.43
1:N:310:MET:HE1	2:O:77:ALA:HB2	2.00	0.43
23:C:303:PEK:H11	23:C:303:PEK:H172	2.00	0.43
3:P:217:VAL:HG22	24:P:305:CDL:H732	2.00	0.43
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.47	0.43
10:J:32:TYR:CZ	10:J:36[B]:MET:HG3	2.54	0.43
1:N:378:HIS:O	1:N:382:SER:HB2	2.19	0.43
8:U:60:TYR:CD1	8:U:60:TYR:C	2.97	0.43
9:V:31:PHE:CD1	9:V:31:PHE:C	2.97	0.43
1:N:331[B]:ASN:ND2	4:Q:21:ASP:HB3	2.33	0.43
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.81	0.43
2:B:60:GLU:CD	2:B:60:GLU:N	2.77	0.43
3:C:131:LEU:HD21	24:G:101:CDL:H521	2.00	0.43
1:N:164:PHE:HE2	20:N:615:EDO:H21	1.84	0.43
2:O:68[B]:LEU:HB3	2:O:69:PRO:HD3	2.00	0.43
1:N:100[B]:MET:CE	19:N:607:PGV:H82	2.44	0.43
1:N:233:HIS:CE1	1:N:297[A]:MET:HE1	2.53	0.43
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.43
2:O:116:LEU:HD12	2:O:117:SER:N	2.33	0.43
18:A:606:TGL:H142	18:A:606:TGL:HA82	2.00	0.43
2:B:183:THR:HG22	28:B:428:HOH:O	2.19	0.43
8:H:9:LYS:O	8:H:10:ASN:CB	2.67	0.43
3:C:224:LYS:CD	24:C:307:CDL:HB31	2.49	0.42
2:O:7:LEU:HD11	18:O:302:TGL:H191	2.01	0.42
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.42	0.42
19:A:607:PGV:H183	23:C:303:PEK:H322	2.01	0.42
3:C:158:HIS:CE1	6:F:2:SER:H	2.36	0.42
1:N:50:ASP:CG	1:N:53:ILE:HG12	2.44	0.42
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	2.01	0.42
3:C:158:HIS:HE1	6:F:2:SER:H	1.67	0.42
5:E:18:TYR:CE2	20:E:202:EDO:H22	2.54	0.42
24:G:101:CDL:H212	24:G:101:CDL:H511	2.01	0.42
24:G:101:CDL:H361	2:O:78:LEU:HD12	2.00	0.42
1:N:187:SER:HB3	1:N:277[B]:MET:CE	2.50	0.42
1:N:489:THR:HA	6:S:71:TRP:O	2.19	0.42
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:26:THR:HG23	13:M:25:SER:CB	2.49	0.42
22:W:101:CHD:H183	22:W:101:CHD:H222	2.02	0.42
13:M:34:LEU:HA	13:M:37[A]:LEU:HG	2.02	0.42
3:C:55:TYR:HA	24:C:307:CDL:H551	2.02	0.42
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.02	0.42
3:P:103:HIS:ND1	22:P:301:CHD:O25	2.53	0.42
3:C:246:ASP:HB2	28:C:481:HOH:O	2.19	0.42
23:C:304:PEK:H041	7:G:17:ARG:HH22	1.84	0.42
1:A:197:LEU:HD21	7:T:2:SER:HB2	2.02	0.42
26:E:201:PSC:H062	26:E:201:PSC:H042	1.80	0.42
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.55	0.42
18:L:101:TGL:H202	18:L:101:TGL:H231	1.84	0.42
1:N:180:GLN:HE21	1:N:180:GLN:HB2	1.69	0.42
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.20	0.42
1:A:28[B]:MET:CE	13:M:26:PHE:HE2	2.33	0.42
28:B:455:HOH:O	24:T:104:CDL:H332	2.20	0.42
1:A:236:TRP:HH2	14:A:602:HEA:HBD1	1.85	0.41
1:A:346[A]:PHE:HZ	18:A:606:TGL:H122	1.85	0.41
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.55	0.41
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.02	0.41
1:A:514:LYS:HE2	28:F:220:HOH:O	2.19	0.41
20:A:608:EDO:H22	6:F:32:ASN:HD21	1.84	0.41
1:N:113[B]:LEU:CD2	1:N:117[B]:MET:HE1	2.50	0.41
1:N:494:TRP:CH2	20:N:608:EDO:H12	2.55	0.41
20:D:202:EDO:C2	5:E:30:ARG:HH21	2.33	0.41
3:P:67:PHE:CE2	24:P:305:CDL:H1	2.32	0.41
3:C:85:LEU:HA	3:C:88[B]:ILE:HG12	2.01	0.41
5:R:108:LYS:HA	5:R:108:LYS:HD3	1.78	0.41
1:A:468:MET:HG3	20:A:611:EDO:O1	2.19	0.41
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.56	0.41
24:T:104:CDL:H541	24:T:104:CDL:H712	2.02	0.41
11:K:6:ALA:HA	11:K:7:PRO:HD3	1.96	0.41
1:N:113[B]:LEU:HG	1:N:117[B]:MET:HE1	1.86	0.41
11:X:52:GLU:HG2	28:X:103:HOH:O	2.20	0.41
13:Z:41:LYS:C	13:Z:43:SER:H	2.29	0.41
28:A:814:HOH:O	4:D:100:LYS:HD3	2.19	0.41
1:N:407:ASP:O	1:N:411:LYS:HG3	2.21	0.41
1:N:449:MET:SD	2:O:5:MET:HG2	2.60	0.41
26:O:304:PSC:H042	26:O:304:PSC:H063	1.85	0.41
3:P:156:ARG:HH21	22:P:306:CHD:C24	2.34	0.41
1:A:44:PRO:HG3	4:D:111:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:HIS:HA	1:A:382:SER:HB2	2.03	0.41
20:N:614:EDO:H11	28:N:884:HOH:O	2.21	0.41
7:G:44:ARG:HA	7:G:45:PRO:HD3	1.90	0.41
2:O:98:LYS:HB2	2:O:109:GLU:HB2	2.03	0.41
3:P:33[B]:MET:HG3	3:P:42:LEU:HD12	2.02	0.41
12:Y:26:THR:HG23	13:Z:25:SER:HB2	2.03	0.41
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.03	0.40
2:B:5[B]:MET:HE3	2:B:5[B]:MET:HB3	1.91	0.40
11:K:8:ASP:HB2	28:K:117:HOH:O	2.20	0.40
1:N:148:PHE:HB3	3:P:28:THR:HB	2.02	0.40
1:N:390:MET:O	1:N:394[A]:VAL:HG22	2.21	0.40
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.90	0.40
1:N:117[A]:MET:CE	12:Y:42:HIS:CD2	3.04	0.40
9:V:32:ALA:O	9:V:36:LYS:HB2	2.20	0.40
7:G:5:LYS:HB3	1:N:278[B]:MET:HE2	2.02	0.40
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.87	0.40
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.19	0.40
1:N:411:LYS:NZ	28:N:708:HOH:O	2.54	0.40
18:Y:101:TGL:H231	18:Y:101:TGL:H202	1.95	0.40
1:A:417[B]:MET:CE	1:A:464:ALA:HB3	2.50	0.40
24:G:101:CDL:H751	24:G:101:CDL:H561	2.03	0.40
12:L:26:THR:HG23	13:M:25:SER:HB3	2.04	0.40
1:N:113[B]:LEU:HD11	1:N:117[B]:MET:CE	2.50	0.40
3:P:131:LEU:HD11	24:T:104:CDL:H561	2.04	0.40
22:P:301:CHD:H12	22:P:301:CHD:H212	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	532/514 (104%)	520 (98%)	12 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	533/514 (104%)	520 (98%)	13 (2%)	0	100	100
2	B	232/227 (102%)	227 (98%)	4 (2%)	1 (0%)	30	27
2	O	231/227 (102%)	225 (97%)	5 (2%)	1 (0%)	30	27
3	C	270/260 (104%)	263 (97%)	6 (2%)	1 (0%)	30	27
3	P	269/260 (104%)	262 (97%)	7 (3%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	5 (4%)	1 (1%)	18	14
5	E	104/109 (95%)	103 (99%)	0	1 (1%)	12	8
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
6	S	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
7	G	81/85 (95%)	71 (88%)	6 (7%)	4 (5%)	1	0
7	T	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
8	H	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	9	5
8	U	77/85 (91%)	72 (94%)	5 (6%)	0	100	100
9	I	71/73 (97%)	68 (96%)	2 (3%)	1 (1%)	9	4
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	58/59 (98%)	57 (98%)	1 (2%)	0	100	100
10	W	58/59 (98%)	57 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	2
13	M	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
13	Z	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
All	All	3586/3604 (100%)	3478 (97%)	91 (2%)	17 (0%)	24	21

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	237	ALA
7	G	4	ALA
7	G	8	HIS

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Mol	Chain	Res	Type
4	Q	8	SER
7	T	4	ALA
7	G	5	LYS
7	T	8	HIS
5	E	6	GLU
7	T	5	LYS
7	T	7	ASP
9	I	32	ALA
12	Y	46	LYS
8	H	8	ILE
2	O	92	ASN
2	B	92	ASN
7	G	9	GLY
7	T	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	446/426 (105%)	440 (99%)	6 (1%)	61	68
1	N	447/426 (105%)	440 (98%)	7 (2%)	55	62
2	B	217/210 (103%)	208 (96%)	9 (4%)	27	26
2	O	216/210 (103%)	209 (97%)	7 (3%)	34	35
3	C	237/225 (105%)	234 (99%)	3 (1%)	61	68
3	P	236/225 (105%)	234 (99%)	2 (1%)	73	80
4	D	128/129 (99%)	126 (98%)	2 (2%)	55	62
4	Q	128/129 (99%)	125 (98%)	3 (2%)	44	49
5	E	93/95 (98%)	91 (98%)	2 (2%)	45	50
5	R	93/95 (98%)	91 (98%)	2 (2%)	45	50
6	F	79/78 (101%)	77 (98%)	2 (2%)	42	45
6	S	79/78 (101%)	74 (94%)	5 (6%)	16	13
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	14
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	25
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	16
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	18
9	V	57/57 (100%)	56 (98%)	1 (2%)	51	58
10	J	51/50 (102%)	51 (100%)	0	100	100
10	W	51/50 (102%)	50 (98%)	1 (2%)	48	54
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	44
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	40/40 (100%)	39 (98%)	1 (2%)	42	45
13	M	38/38 (100%)	38 (100%)	0	100	100
13	Z	38/38 (100%)	38 (100%)	0	100	100
All	All	3124/3074 (102%)	3051 (98%)	73 (2%)	43	49

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35[A]	LEU
1	A	35[B]	LEU
1	A	128	VAL
1	A	180	GLN
1	A	363	LEU
1	A	369	ASP
2	B	33	LEU
2	B	42	ILE
2	B	59	GLN
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	127	LEU
3	C	159	MET
3	C	230	ASN
4	D	19	ARG

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Mol	Chain	Res	Type
4	D	58	GLU
5	E	70	VAL
5	E	90	ARG
6	F	54	ASN
6	F	80	GLN
7	G	2	SER
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	84	LYS
8	H	9	LYS
8	H	50	VAL
8	H	60	TYR
9	I	15	ARG
9	I	25	PHE
9	I	33	THR
11	K	54	ARG
1	N	128	VAL
1	N	180	GLN
1	N	369	ASP
1	N	380	VAL
1	N	381	LEU
1	N	485	VAL
1	N	504	THR
2	O	33	LEU
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	116	LEU
2	O	227	LEU
3	P	159	MET
3	P	230	ASN
4	Q	5	VAL
4	Q	6	VAL
4	Q	10	ASP
5	R	79	LYS
5	R	80	GLU
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
6	S	87	THR

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Mol	Chain	Res	Type
6	S	94	HIS
7	T	2	SER
7	T	8	HIS
7	T	33	LEU
7	T	84	LYS
8	U	8	ILE
8	U	9	LYS
8	U	50	VAL
8	U	60	TYR
9	V	73	LYS
10	W	50	LEU
12	Y	26	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	55	ASN
1	A	180	GLN
1	A	422	ASN
2	B	59	GLN
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	29	HIS
4	D	37	GLN
4	D	119	GLN
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
8	H	28	ASN
8	H	31	GLN
8	H	32	ASN
9	I	20	HIS
11	K	35	GLN
1	N	180	GLN
2	O	52	HIS

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Mol	Chain	Res	Type
2	O	92	ASN
2	O	181	GLN
2	O	195	GLN
2	O	203	ASN
3	P	3	HIS
3	P	50	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	76	ASN
4	Q	101	HIS
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
7	T	76	ASN
8	U	31	GLN
8	U	37	HIS
10	W	29	ASN
13	Z	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	N	1	1	8,9,10	0.51	0	8,9,11	1.22	2 (25%)
7	TPO	T	11	7	8,10,11	1.45	1 (12%)	10,14,16	0.93	0
1	FME	A	1	1	8,9,10	0.56	0	8,9,11	1.52	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SAC	V	1	9	7,8,9	2.06	2 (28%)	7,9,11	0.99	0
9	SAC	I	1	9	7,8,9	1.99	2 (28%)	7,9,11	0.79	0
2	FME	O	1	2	8,9,10	0.58	0	8,9,11	1.01	0
7	TPO	G	11	7	8,10,11	1.44	1 (12%)	10,14,16	0.87	0
2	FME	B	1	2	8,9,10	0.75	0	8,9,11	1.16	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	2/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
1	FME	A	1	1	-	4/7/9/11	-
9	SAC	V	1	9	-	2/7/8/10	-
9	SAC	I	1	9	-	2/7/8/10	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	0/7/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	4.67	1.33	1.23
9	V	1	SAC	OAC-C1A	4.63	1.33	1.23
7	G	11	TPO	P-O1P	2.92	1.59	1.50
7	T	11	TPO	P-O1P	2.88	1.59	1.50
9	V	1	SAC	CA-N	2.69	1.50	1.46
9	I	1	SAC	CA-N	2.10	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	3.09	115.47	109.50
1	N	1	FME	C-CA-N	2.20	113.74	109.50
1	N	1	FME	O-C-CA	-2.12	119.32	124.77
2	B	1	FME	O-C-CA	-2.10	119.36	124.77
1	A	1	FME	O-C-CA	-2.07	119.45	124.77

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 89 ligands modelled in this entry, 10 are monoatomic - leaving 79 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
22	CHD	J	101	-	32,32,32	0.59	0	51,51,51	1.59	9 (17%)
19	PGV	P	304	-	50,50,50	0.98	2 (4%)	53,56,56	0.94	2 (3%)
20	EDO	A	613	-	3,3,3	0.47	0	2,2,2	0.50	0
20	EDO	A	614	-	3,3,3	0.33	0	2,2,2	0.44	0
22	CHD	O	301	-	32,32,32	0.69	1 (3%)	51,51,51	1.15	4 (7%)
20	EDO	A	612	-	3,3,3	0.50	0	2,2,2	0.45	0
19	PGV	C	305	-	50,50,50	0.86	2 (4%)	53,56,56	0.82	1 (1%)
20	EDO	S	102	-	3,3,3	0.43	0	2,2,2	0.43	0
25	DMU	C	312	-	34,34,34	0.57	1 (2%)	45,45,45	1.26	5 (11%)
18	TGL	Q	201	-	62,62,62	1.31	6 (9%)	65,65,65	1.12	6 (9%)
19	PGV	N	607	-	50,50,50	0.90	2 (4%)	53,56,56	0.87	2 (3%)
22	CHD	W	101	-	32,32,32	0.57	0	51,51,51	1.50	8 (15%)
22	CHD	P	306	-	32,32,32	0.58	0	51,51,51	1.64	11 (21%)
24	CDL	G	101	-	99,99,99	1.41	12 (12%)	105,111,111	1.08	5 (4%)
20	EDO	P	307	-	3,3,3	0.43	0	2,2,2	0.37	0
20	EDO	A	608	-	3,3,3	0.39	0	2,2,2	0.44	0
20	EDO	F	102	-	3,3,3	0.38	0	2,2,2	0.47	0
23	PEK	T	102	-	52,52,52	0.90	3 (5%)	55,57,57	0.87	3 (5%)
20	EDO	B	303	-	3,3,3	0.38	0	2,2,2	0.43	0
20	EDO	D	202	-	3,3,3	0.47	0	2,2,2	0.29	0
20	EDO	N	613	-	3,3,3	0.32	0	2,2,2	0.62	0
20	EDO	N	614	-	3,3,3	0.44	0	2,2,2	0.18	0
21	CUA	O	303	2	0,1,1	-	-	-	-	-
20	EDO	E	202	-	3,3,3	0.39	0	2,2,2	0.37	0
20	EDO	A	616	-	3,3,3	0.40	0	2,2,2	0.22	0
20	EDO	S	103	-	3,3,3	0.45	0	2,2,2	0.18	0
20	EDO	A	610	-	3,3,3	0.44	0	2,2,2	0.53	0
22	CHD	P	301	-	32,32,32	0.63	0	51,51,51	1.01	2 (3%)
18	TGL	O	302	-	62,62,62	1.31	6 (9%)	65,65,65	1.12	3 (4%)
25	DMU	Z	101	-	34,34,34	0.47	0	45,45,45	0.72	2 (4%)
20	EDO	R	201	-	3,3,3	0.49	0	2,2,2	0.45	0
14	HEA	A	602	1	67,67,67	2.07	27 (40%)	81,103,103	1.28	10 (12%)
20	EDO	F	103	-	3,3,3	0.58	0	2,2,2	0.46	0
19	PGV	P	303	-	50,50,50	0.90	2 (4%)	53,56,56	0.84	3 (5%)
23	PEK	T	101	-	52,52,52	0.95	2 (3%)	55,57,57	0.93	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PEK	T	103	-	52,52,52	0.97	2 (3%)	55,57,57	0.88	3 (5%)
24	CDL	T	104	-	99,99,99	1.41	12 (12%)	105,111,111	1.11	6 (5%)
20	EDO	C	309	-	3,3,3	0.43	0	2,2,2	0.36	0
25	DMU	M	102	-	34,34,34	0.47	0	45,45,45	0.70	0
20	EDO	D	203	-	3,3,3	0.46	0	2,2,2	0.43	0
25	DMU	P	309	-	34,34,34	0.59	1 (2%)	45,45,45	0.84	1 (2%)
14	HEA	N	602	1	67,67,67	2.09	24 (35%)	81,103,103	1.24	8 (9%)
19	PGV	N	606	-	50,50,50	0.97	2 (4%)	53,56,56	0.98	2 (3%)
23	PEK	G	102	-	52,52,52	0.94	2 (3%)	55,57,57	0.96	3 (5%)
25	DMU	C	313	-	34,34,34	0.60	1 (2%)	45,45,45	1.05	3 (6%)
20	EDO	N	610	-	3,3,3	0.44	0	2,2,2	0.42	0
20	EDO	N	609	-	3,3,3	0.37	0	2,2,2	0.46	0
20	EDO	F	104	-	3,3,3	0.45	0	2,2,2	0.51	0
14	HEA	N	601	1	67,67,67	2.18	28 (41%)	81,103,103	1.33	11 (13%)
18	TGL	A	606	-	62,62,62	1.31	6 (9%)	65,65,65	1.43	8 (12%)
19	PGV	C	306	-	50,50,50	0.96	2 (4%)	53,56,56	0.97	2 (3%)
19	PGV	M	101	-	50,50,50	0.98	2 (4%)	53,56,56	1.01	3 (5%)
20	EDO	N	617	-	3,3,3	0.38	0	2,2,2	0.46	0
26	PSC	E	201	-	51,51,51	1.11	3 (5%)	57,59,59	1.02	2 (3%)
23	PEK	C	304	-	52,52,52	0.96	2 (3%)	55,57,57	0.94	2 (3%)
22	CHD	C	301	-	32,32,32	0.65	0	51,51,51	1.00	3 (5%)
22	CHD	C	308	-	32,32,32	0.61	0	51,51,51	1.52	11 (21%)
20	EDO	N	611	-	3,3,3	0.39	0	2,2,2	0.30	0
26	PSC	O	304	-	51,51,51	1.12	3 (5%)	57,59,59	1.02	3 (5%)
24	CDL	P	305	-	99,99,99	1.41	12 (12%)	105,111,111	1.12	8 (7%)
24	CDL	C	307	-	99,99,99	1.42	12 (12%)	105,111,111	1.11	4 (3%)
18	TGL	Y	101	-	62,62,62	1.31	6 (9%)	65,65,65	1.03	3 (4%)
18	TGL	D	201	-	62,62,62	1.32	6 (9%)	65,65,65	0.98	3 (4%)
20	EDO	N	615	-	3,3,3	0.35	0	2,2,2	0.45	0
20	EDO	N	616	-	3,3,3	0.43	0	2,2,2	0.37	0
23	PEK	C	303	-	52,52,52	0.84	2 (3%)	55,57,57	0.86	1 (1%)
20	EDO	N	608	-	3,3,3	0.49	0	2,2,2	0.27	0
18	TGL	L	101	-	62,62,62	1.32	6 (9%)	65,65,65	1.07	4 (6%)
25	DMU	P	308	-	34,34,34	0.59	1 (2%)	45,45,45	1.02	2 (4%)
20	EDO	A	611	-	3,3,3	0.39	0	2,2,2	0.34	0
20	EDO	N	612	-	3,3,3	0.55	0	2,2,2	0.23	0
19	PGV	A	607	-	50,50,50	0.89	2 (4%)	53,56,56	0.93	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CUA	B	301	2	0,1,1	-	-	-		
22	CHD	B	302	-	32,32,32	0.71	0	51,51,51	1.08	2 (3%)
20	EDO	A	615	-	3,3,3	0.38	0	2,2,2	0.47	0
20	EDO	C	311	-	3,3,3	0.55	0	2,2,2	0.28	0
14	HEA	A	601	1	67,67,67	2.18	26 (38%)	81,103,103	1.31	13 (16%)
20	EDO	A	609	-	3,3,3	0.52	0	2,2,2	0.54	0
20	EDO	C	310	-	3,3,3	0.45	0	2,2,2	0.40	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
22	CHD	J	101	-	-	5/9/74/74	0/4/4/4
19	PGV	P	304	-	-	31/55/55/55	-
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	A	614	-	-	1/1/1/1	-
22	CHD	O	301	-	-	2/9/74/74	0/4/4/4
20	EDO	A	612	-	-	0/1/1/1	-
19	PGV	C	305	-	-	16/55/55/55	-
20	EDO	S	102	-	-	0/1/1/1	-
25	DMU	C	312	-	-	6/19/59/59	0/2/2/2
18	TGL	Q	201	-	-	35/65/65/65	-
19	PGV	N	607	-	-	11/55/55/55	-
22	CHD	W	101	-	-	5/9/74/74	0/4/4/4
22	CHD	P	306	-	-	8/9/74/74	0/4/4/4
24	CDL	G	101	-	-	61/110/110/110	-
20	EDO	P	307	-	-	0/1/1/1	-
20	EDO	A	608	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
23	PEK	T	102	-	-	20/56/56/56	-
20	EDO	B	303	-	-	1/1/1/1	-
20	EDO	D	202	-	-	1/1/1/1	-
20	EDO	N	613	-	-	1/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	E	202	-	-	0/1/1/1	-
20	EDO	A	616	-	-	1/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
20	EDO	A	610	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	P	301	-	-	2/9/74/74	0/4/4/4
18	TGL	O	302	-	-	33/65/65/65	-
25	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
20	EDO	R	201	-	-	0/1/1/1	-
14	HEA	A	602	1	-	9/36/76/76	-
20	EDO	F	103	-	-	0/1/1/1	-
19	PGV	P	303	-	-	16/55/55/55	-
23	PEK	T	101	-	-	32/56/56/56	-
23	PEK	T	103	-	-	26/56/56/56	-
24	CDL	T	104	-	-	61/110/110/110	-
20	EDO	C	309	-	-	0/1/1/1	-
25	DMU	M	102	-	-	4/19/59/59	0/2/2/2
20	EDO	D	203	-	-	0/1/1/1	-
25	DMU	P	309	-	-	7/19/59/59	0/2/2/2
14	HEA	N	602	1	-	9/36/76/76	-
19	PGV	N	606	-	-	30/55/55/55	-
23	PEK	G	102	-	-	32/56/56/56	-
25	DMU	C	313	-	-	8/19/59/59	0/2/2/2
20	EDO	N	610	-	-	0/1/1/1	-
20	EDO	N	609	-	-	1/1/1/1	-
20	EDO	F	104	-	-	1/1/1/1	-
14	HEA	N	601	1	-	4/36/76/76	-
18	TGL	A	606	-	-	36/65/65/65	-
19	PGV	C	306	-	-	24/55/55/55	-
19	PGV	M	101	-	-	31/55/55/55	-
20	EDO	N	617	-	-	0/1/1/1	-
26	PSC	E	201	-	-	31/55/55/55	-
23	PEK	C	304	-	-	30/56/56/56	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
22	CHD	C	308	-	-	9/9/74/74	0/4/4/4
26	PSC	O	304	-	-	34/55/55/55	-
20	EDO	N	611	-	-	0/1/1/1	-
24	CDL	P	305	-	-	63/110/110/110	-
24	CDL	C	307	-	-	57/110/110/110	-
18	TGL	Y	101	-	-	37/65/65/65	-
18	TGL	D	201	-	-	38/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	615	-	-	1/1/1/1	-
20	EDO	N	616	-	-	0/1/1/1	-
23	PEK	C	303	-	-	16/56/56/56	-
20	EDO	N	608	-	-	1/1/1/1	-
18	TGL	L	101	-	-	37/65/65/65	-
25	DMU	P	308	-	-	8/19/59/59	0/2/2/2
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	N	612	-	-	0/1/1/1	-
19	PGV	A	607	-	-	11/55/55/55	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	C	311	-	-	0/1/1/1	-
14	HEA	A	601	1	-	6/36/76/76	-
20	EDO	A	609	-	-	0/1/1/1	-
20	EDO	C	310	-	-	0/1/1/1	-

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	FE-ND	5.52	2.11	1.94
14	N	602	HEA	FE-ND	5.18	2.10	1.94
14	A	602	HEA	FE-ND	5.15	2.10	1.94
14	N	602	HEA	FE-NB	5.13	2.10	1.94
14	N	601	HEA	FE-NA	5.02	2.11	1.95
14	A	601	HEA	FE-NC	4.84	2.11	1.95
14	N	601	HEA	FE-ND	4.77	2.09	1.94
18	D	201	TGL	OG1-CA1	4.74	1.47	1.33
18	A	606	TGL	OG2-CB1	4.65	1.47	1.34
24	C	307	CDL	OA8-CA7	4.64	1.46	1.33
14	A	602	HEA	FE-NC	4.63	2.10	1.95
24	C	307	CDL	OB8-CB7	4.61	1.46	1.33
14	N	601	HEA	FE-NC	4.60	2.10	1.95
18	L	101	TGL	OG2-CB1	4.60	1.47	1.34
24	P	305	CDL	OA8-CA7	4.57	1.46	1.33
18	Q	201	TGL	OG2-CB1	4.57	1.47	1.34
18	O	302	TGL	OG2-CB1	4.56	1.47	1.34
18	L	101	TGL	OG1-CA1	4.56	1.46	1.33
18	Y	101	TGL	OG2-CB1	4.55	1.47	1.34
19	N	606	PGV	O03-C19	4.55	1.46	1.33
24	T	104	CDL	OB8-CB7	4.55	1.46	1.33
24	G	101	CDL	OB8-CB7	4.53	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	101	PGV	O03-C19	4.51	1.46	1.33
18	Y	101	TGL	OG3-CC1	4.51	1.46	1.33
24	P	305	CDL	OB8-CB7	4.51	1.46	1.33
24	G	101	CDL	OB6-CB5	4.50	1.47	1.34
23	C	304	PEK	O03-C21	4.50	1.46	1.33
18	D	201	TGL	OG3-CC1	4.49	1.46	1.33
23	C	304	PEK	O01-C1	4.49	1.47	1.34
18	O	302	TGL	OG1-CA1	4.49	1.46	1.33
19	P	304	PGV	O03-C19	4.48	1.46	1.33
18	Q	201	TGL	OG3-CC1	4.48	1.46	1.33
24	T	104	CDL	OB6-CB5	4.48	1.46	1.34
26	O	304	PSC	O03-C19	4.48	1.46	1.33
23	T	103	PEK	O03-C21	4.46	1.46	1.33
23	T	103	PEK	O01-C1	4.45	1.46	1.34
26	E	201	PSC	O01-C1	4.45	1.46	1.34
18	A	606	TGL	OG1-CA1	4.45	1.46	1.33
14	A	601	HEA	FE-NA	4.43	2.09	1.95
23	T	101	PEK	O03-C21	4.43	1.46	1.33
19	C	306	PGV	O01-C1	4.43	1.46	1.34
18	A	606	TGL	OG3-CC1	4.42	1.46	1.33
18	Q	201	TGL	OG1-CA1	4.40	1.46	1.33
24	G	101	CDL	OA8-CA7	4.40	1.46	1.33
18	O	302	TGL	OG3-CC1	4.39	1.46	1.33
19	P	304	PGV	O01-C1	4.38	1.46	1.34
23	G	102	PEK	O03-C21	4.38	1.46	1.33
26	E	201	PSC	O03-C19	4.37	1.46	1.33
23	T	101	PEK	O01-C1	4.37	1.46	1.34
14	N	602	HEA	FE-NA	4.36	2.09	1.95
14	A	602	HEA	FE-NA	4.36	2.09	1.95
19	N	606	PGV	O01-C1	4.35	1.46	1.34
24	C	307	CDL	OB6-CB5	4.35	1.46	1.34
23	G	102	PEK	O01-C1	4.34	1.46	1.34
26	O	304	PSC	O01-C1	4.33	1.46	1.34
24	T	104	CDL	OA8-CA7	4.33	1.46	1.33
19	N	607	PGV	O03-C19	4.32	1.45	1.33
19	M	101	PGV	O01-C1	4.32	1.46	1.34
18	L	101	TGL	OG3-CC1	4.31	1.45	1.33
24	C	307	CDL	OA6-CA5	4.31	1.46	1.34
24	T	104	CDL	OA6-CA5	4.29	1.46	1.34
19	C	306	PGV	O03-C19	4.28	1.45	1.33
14	N	601	HEA	C3A-C4A	-4.28	1.38	1.46
19	A	607	PGV	O03-C19	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	101	CDL	OA6-CA5	4.26	1.46	1.34
24	P	305	CDL	OA6-CA5	4.26	1.46	1.34
14	N	601	HEA	FE-NB	4.23	2.07	1.94
24	P	305	CDL	OB6-CB5	4.22	1.46	1.34
14	A	601	HEA	C3A-C4A	-4.15	1.38	1.46
18	Y	101	TGL	OG1-CA1	4.14	1.45	1.33
14	A	601	HEA	FE-NB	4.13	2.07	1.94
23	T	102	PEK	O03-C21	4.06	1.45	1.33
18	D	201	TGL	OG2-CB1	4.05	1.45	1.34
14	N	602	HEA	CHB-C4A	4.04	1.46	1.38
14	A	602	HEA	FE-NB	3.99	2.07	1.94
14	N	602	HEA	FE-NC	3.94	2.08	1.95
14	A	602	HEA	CHB-C4A	3.91	1.46	1.38
19	P	303	PGV	O03-C19	3.88	1.44	1.33
19	C	305	PGV	O03-C19	3.83	1.44	1.33
19	P	303	PGV	O01-C1	3.79	1.45	1.34
23	C	303	PEK	O01-C1	3.78	1.44	1.34
18	Y	101	TGL	C20-CA9	-3.77	1.33	1.51
26	O	304	PSC	C13-C12	3.77	1.53	1.31
26	E	201	PSC	C13-C12	3.74	1.52	1.31
18	L	101	TGL	C20-CA9	-3.73	1.33	1.51
23	T	102	PEK	O01-C1	3.73	1.44	1.34
24	T	104	CDL	C62-C61	-3.69	1.33	1.51
24	C	307	CDL	C59-C58	-3.69	1.33	1.51
18	L	101	TGL	C10-CB9	-3.68	1.33	1.51
24	G	101	CDL	C22-C21	-3.68	1.33	1.51
24	G	101	CDL	C19-C18	-3.68	1.33	1.51
24	P	305	CDL	C22-C21	-3.66	1.33	1.51
24	T	104	CDL	C19-C18	-3.66	1.33	1.51
18	O	302	TGL	C20-CA9	-3.66	1.33	1.51
24	P	305	CDL	C59-C58	-3.66	1.33	1.51
24	T	104	CDL	C22-C21	-3.66	1.33	1.51
24	C	307	CDL	C62-C61	-3.65	1.33	1.51
24	T	104	CDL	C59-C58	-3.65	1.33	1.51
24	C	307	CDL	C82-C81	-3.65	1.33	1.51
24	P	305	CDL	C19-C18	-3.64	1.33	1.51
14	N	601	HEA	C4B-C3B	-3.64	1.38	1.44
18	O	302	TGL	C15-CC9	-3.64	1.33	1.51
18	Y	101	TGL	C15-CC9	-3.64	1.33	1.51
24	C	307	CDL	C79-C78	-3.64	1.33	1.51
24	P	305	CDL	C42-C41	-3.63	1.33	1.51
24	G	101	CDL	C39-C38	-3.63	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	303	PEK	O03-C21	3.63	1.43	1.33
18	Y	101	TGL	C10-CB9	-3.63	1.33	1.51
14	N	601	HEA	CHA-C1A	3.63	1.45	1.38
24	T	104	CDL	C42-C41	-3.63	1.33	1.51
24	T	104	CDL	C39-C38	-3.63	1.33	1.51
14	A	602	HEA	CHA-C1A	3.63	1.45	1.38
24	C	307	CDL	C22-C21	-3.62	1.33	1.51
18	A	606	TGL	C20-CA9	-3.61	1.33	1.51
24	T	104	CDL	C79-C78	-3.61	1.33	1.51
14	A	601	HEA	C1D-ND	-3.61	1.34	1.40
18	Q	201	TGL	C10-CB9	-3.61	1.33	1.51
24	C	307	CDL	C19-C18	-3.61	1.33	1.51
24	P	305	CDL	C62-C61	-3.60	1.33	1.51
24	G	101	CDL	C62-C61	-3.60	1.33	1.51
18	A	606	TGL	C10-CB9	-3.60	1.33	1.51
24	G	101	CDL	C59-C58	-3.60	1.33	1.51
24	G	101	CDL	C42-C41	-3.59	1.33	1.51
24	P	305	CDL	C79-C78	-3.59	1.33	1.51
14	A	601	HEA	CHB-C4A	3.59	1.45	1.38
18	O	302	TGL	C10-CB9	-3.59	1.33	1.51
24	C	307	CDL	C42-C41	-3.59	1.33	1.51
14	A	602	HEA	CHD-C1D	3.59	1.45	1.38
14	A	601	HEA	C4B-C3B	-3.59	1.38	1.44
18	A	606	TGL	C15-CC9	-3.58	1.33	1.51
18	D	201	TGL	C10-CB9	-3.58	1.34	1.51
18	D	201	TGL	C15-CC9	-3.58	1.34	1.51
14	A	601	HEA	CHA-C1A	3.58	1.45	1.38
18	L	101	TGL	C15-CC9	-3.58	1.34	1.51
24	P	305	CDL	C82-C81	-3.58	1.34	1.51
24	P	305	CDL	C39-C38	-3.57	1.34	1.51
24	G	101	CDL	C79-C78	-3.55	1.34	1.51
18	Q	201	TGL	C20-CA9	-3.55	1.34	1.51
24	G	101	CDL	C82-C81	-3.55	1.34	1.51
24	T	104	CDL	C82-C81	-3.54	1.34	1.51
19	C	305	PGV	O01-C1	3.54	1.44	1.34
18	D	201	TGL	C20-CA9	-3.54	1.34	1.51
18	Q	201	TGL	C15-CC9	-3.53	1.34	1.51
14	N	602	HEA	CHD-C1D	3.51	1.45	1.38
24	C	307	CDL	C39-C38	-3.50	1.34	1.51
14	A	601	HEA	CHD-C1D	3.42	1.45	1.38
14	N	602	HEA	CHA-C1A	3.40	1.45	1.38
14	N	602	HEA	C4B-NB	-3.40	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C4D-C3D	-3.40	1.39	1.45
19	N	607	PGV	O01-C1	3.39	1.43	1.34
19	A	607	PGV	O01-C1	3.38	1.43	1.34
14	A	601	HEA	C4D-C3D	-3.34	1.39	1.45
14	N	601	HEA	CHD-C1D	3.33	1.45	1.38
14	N	601	HEA	C4B-NB	-3.33	1.34	1.40
14	A	602	HEA	C1A-C2A	-3.33	1.39	1.45
14	A	601	HEA	CHC-C4B	3.32	1.45	1.38
14	N	601	HEA	C1A-C2A	-3.23	1.39	1.45
14	N	602	HEA	C1A-C2A	-3.21	1.39	1.45
14	N	601	HEA	CHB-C4A	3.21	1.44	1.38
14	N	601	HEA	CHC-C4B	3.19	1.44	1.38
14	A	602	HEA	C4D-C3D	-3.18	1.39	1.45
14	N	602	HEA	C1D-ND	-3.17	1.34	1.40
14	A	602	HEA	C3A-C4A	-3.17	1.40	1.46
14	N	602	HEA	C1C-NC	-3.16	1.33	1.39
14	A	602	HEA	C4A-NA	-3.16	1.33	1.39
14	A	601	HEA	C1A-C2A	-3.08	1.39	1.45
14	N	601	HEA	C1D-ND	-3.07	1.34	1.40
14	A	601	HEA	C4B-NB	-3.05	1.35	1.40
14	N	601	HEA	C1C-NC	-3.04	1.33	1.39
14	N	602	HEA	C3A-C4A	-3.03	1.40	1.46
14	N	601	HEA	C4D-C3D	-3.03	1.39	1.45
14	A	602	HEA	CHC-C4B	3.02	1.44	1.38
14	N	601	HEA	C1A-NA	-2.98	1.34	1.39
14	A	601	HEA	C4A-NA	-2.91	1.34	1.39
14	N	602	HEA	CHD-C4C	2.90	1.45	1.39
14	A	601	HEA	C1A-NA	-2.82	1.34	1.39
14	N	601	HEA	C4A-NA	-2.78	1.34	1.39
14	A	602	HEA	C4B-C3B	-2.78	1.39	1.44
14	N	602	HEA	C4A-NA	-2.77	1.34	1.39
14	N	601	HEA	C1D-C2D	-2.76	1.38	1.44
14	N	602	HEA	CHC-C4B	2.75	1.44	1.38
14	A	602	HEA	CHD-C4C	2.75	1.45	1.39
14	A	602	HEA	C1B-NB	-2.73	1.33	1.38
14	N	601	HEA	CHB-C1B	2.68	1.45	1.39
14	A	601	HEA	CHC-C1C	2.67	1.45	1.39
14	A	602	HEA	C4B-NB	-2.67	1.35	1.40
14	N	601	HEA	CHC-C1C	2.67	1.45	1.39
14	A	601	HEA	C4C-NC	-2.64	1.34	1.39
14	N	601	HEA	C4C-NC	-2.63	1.34	1.39
14	A	601	HEA	C1D-C2D	-2.60	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C4D-ND	-2.59	1.33	1.38
25	C	313	DMU	O16-C6	2.57	1.44	1.40
14	N	602	HEA	CHB-C1B	2.57	1.45	1.39
14	A	601	HEA	C1B-NB	-2.56	1.33	1.38
14	N	602	HEA	C4B-C3B	-2.50	1.40	1.44
14	N	601	HEA	CHA-C4D	2.49	1.44	1.39
14	A	602	HEA	C1D-ND	-2.48	1.35	1.40
14	A	602	HEA	CHB-C1B	2.48	1.44	1.39
14	A	601	HEA	C1C-NC	-2.47	1.35	1.39
14	N	602	HEA	C4D-ND	-2.47	1.34	1.38
25	P	308	DMU	O16-C6	2.46	1.44	1.40
14	A	601	HEA	CHB-C1B	2.45	1.44	1.39
14	N	601	HEA	C1B-C2B	-2.43	1.39	1.44
14	A	602	HEA	C1A-NA	-2.37	1.35	1.39
25	C	312	DMU	O16-C6	2.37	1.44	1.40
14	N	601	HEA	CHD-C4C	2.36	1.44	1.39
14	A	601	HEA	C4D-ND	-2.35	1.34	1.38
14	A	602	HEA	C1C-NC	-2.34	1.35	1.39
14	N	602	HEA	CHC-C1C	2.33	1.44	1.39
14	A	601	HEA	O11-C11	2.31	1.48	1.42
14	N	601	HEA	C1B-NB	-2.31	1.34	1.38
25	P	309	DMU	O16-C6	2.30	1.44	1.40
14	N	602	HEA	C4C-NC	-2.25	1.35	1.39
14	A	601	HEA	CHD-C4C	2.23	1.44	1.39
14	N	601	HEA	C4D-ND	-2.22	1.34	1.38
14	A	602	HEA	CHA-C4D	2.19	1.44	1.39
14	A	602	HEA	C1B-C2B	-2.17	1.40	1.44
14	A	602	HEA	CHC-C1C	2.16	1.44	1.39
14	A	602	HEA	O11-C11	2.16	1.47	1.42
23	T	102	PEK	O01-C02	-2.14	1.41	1.46
14	N	602	HEA	C1B-NB	-2.12	1.34	1.38
14	N	601	HEA	O11-C11	2.11	1.47	1.42
14	N	602	HEA	C1D-C2D	-2.11	1.40	1.44
14	A	602	HEA	C1D-C2D	-2.10	1.40	1.44
14	N	601	HEA	C3B-C2B	2.08	1.39	1.34
22	O	301	CHD	O26-C24	-2.06	1.24	1.30
14	N	602	HEA	CHA-C4D	2.04	1.43	1.39
14	A	602	HEA	C4C-NC	-2.02	1.35	1.39
14	A	601	HEA	C1B-C2B	-2.01	1.40	1.44

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C17-C13-C14	-5.02	95.08	100.11
18	A	606	TGL	OG2-CB1-CB2	4.59	121.41	111.48
24	T	104	CDL	OB6-CB5-C51	4.41	121.02	111.48
24	C	307	CDL	OA6-CA5-C11	4.26	120.69	111.48
24	G	101	CDL	OB6-CB5-C51	4.23	120.64	111.48
19	N	606	PGV	O01-C1-C2	4.19	120.56	111.48
26	O	304	PSC	O01-C1-C2	4.19	120.55	111.48
26	E	201	PSC	O01-C1-C2	4.18	120.53	111.48
18	Y	101	TGL	OG2-CB1-CB2	4.13	120.41	111.48
22	J	101	CHD	C14-C13-C12	4.09	111.15	107.42
18	A	606	TGL	OG3-CC1-CC2	4.06	124.22	111.83
22	P	306	CHD	C10-C9-C8	4.04	116.34	111.84
22	W	101	CHD	C17-C13-C14	-4.04	96.06	100.11
23	G	102	PEK	O01-C1-C2	4.03	120.21	111.48
22	J	101	CHD	C16-C17-C20	4.03	118.28	112.18
18	O	302	TGL	OG2-CB1-CB2	4.01	120.17	111.48
18	A	606	TGL	CG2-OG2-CB1	4.00	127.38	117.80
19	M	101	PGV	O01-C1-C2	3.98	120.08	111.48
24	G	101	CDL	OA6-CA5-C11	3.97	120.06	111.48
14	N	601	HEA	C12-C11-C3B	3.93	118.27	112.12
23	C	304	PEK	O01-C1-C2	3.92	119.96	111.48
19	C	306	PGV	O01-C1-C2	3.90	119.92	111.48
24	C	307	CDL	OB6-CB5-C51	3.86	119.83	111.48
24	T	104	CDL	OA6-CA5-C11	3.85	119.80	111.48
25	C	312	DMU	O16-C6-C1	3.83	114.09	108.27
24	P	305	CDL	OA6-CA5-C11	3.76	119.61	111.48
23	T	101	PEK	O01-C1-C2	3.73	119.55	111.48
24	P	305	CDL	OB6-CB5-C51	3.73	119.54	111.48
22	W	101	CHD	C16-C17-C20	3.65	117.71	112.18
19	A	607	PGV	O03-C19-C20	3.62	122.87	111.83
14	N	602	HEA	OMA-CMA-C3A	-3.62	117.46	125.62
25	C	312	DMU	C1-C2-C3	3.62	117.89	109.68
18	L	101	TGL	OG2-CB1-CB2	3.59	119.25	111.48
22	B	302	CHD	C15-C14-C13	3.54	106.97	103.54
22	W	101	CHD	C14-C13-C12	3.52	110.63	107.42
23	T	103	PEK	O01-C1-C2	3.47	118.99	111.48
14	A	601	HEA	C12-C11-C3B	3.42	117.47	112.12
22	P	306	CHD	C1-C2-C3	3.42	115.01	110.48
22	C	308	CHD	C10-C9-C8	3.39	115.62	111.84
19	P	304	PGV	O01-C1-C2	3.39	118.81	111.48
19	P	304	PGV	O03-C19-C20	3.38	122.15	111.83
19	N	607	PGV	O03-C19-C20	3.38	122.14	111.83
22	P	306	CHD	C9-C10-C5	3.33	113.14	108.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	101	PGV	O03-C19-C20	3.24	121.70	111.83
24	P	305	CDL	OB8-CB7-C71	3.24	121.70	111.83
14	N	601	HEA	C3C-C4C-NC	3.23	112.52	109.80
23	T	102	PEK	O03-C21-C22	3.21	121.61	111.83
18	Q	201	TGL	OG1-CA1-CA2	3.17	121.50	111.83
18	L	101	TGL	OG1-CA1-CA2	3.17	121.49	111.83
18	A	606	TGL	OG3-CC1-OC1	-3.14	115.77	123.63
18	Q	201	TGL	OG3-CC1-CC2	3.14	121.41	111.83
14	A	601	HEA	C13-C12-C11	-3.13	109.39	114.39
22	P	306	CHD	C6-C5-C10	3.11	115.97	112.66
14	A	601	HEA	C26-C15-C16	3.09	120.59	115.23
25	C	312	DMU	C6-O5-C4	-3.06	107.75	113.72
18	Q	201	TGL	OG2-CB1-CB2	3.05	118.07	111.48
22	O	301	CHD	C6-C5-C4	-3.03	107.77	111.23
18	D	201	TGL	OG3-CC1-CC2	3.02	121.06	111.83
14	A	602	HEA	CAD-C3D-C2D	3.02	133.53	127.87
24	T	104	CDL	OA8-CA7-C31	3.02	121.04	111.83
19	C	306	PGV	O03-C19-C20	3.01	121.02	111.83
18	A	606	TGL	OG2-CG2-CG1	3.00	119.09	108.34
24	C	307	CDL	OB8-CB7-C71	2.97	120.90	111.83
22	C	308	CHD	C15-C14-C13	2.94	106.39	103.54
23	T	103	PEK	O03-C21-C22	2.89	120.65	111.83
22	C	308	CHD	C15-C14-C8	2.88	122.31	118.36
14	A	602	HEA	CAD-C3D-C4D	-2.87	119.69	124.70
23	C	304	PEK	O03-C21-C22	2.86	120.57	111.83
22	J	101	CHD	C22-C20-C17	2.86	116.26	110.33
23	C	303	PEK	O01-C1-C2	2.85	117.66	111.48
23	T	101	PEK	O03-C21-C22	2.84	120.50	111.83
22	P	306	CHD	C15-C14-C8	2.83	122.24	118.36
22	C	308	CHD	C9-C10-C5	2.83	112.44	108.51
14	A	601	HEA	OMA-CMA-C3A	-2.82	119.25	125.62
25	C	313	DMU	C2-C3-C4	2.81	117.17	110.93
24	G	101	CDL	OA8-CA7-C31	2.78	120.33	111.83
22	C	308	CHD	C14-C8-C9	-2.77	105.88	109.75
25	C	313	DMU	C1-C2-C3	2.77	115.97	109.68
18	O	302	TGL	OG3-CC1-CC2	2.77	120.27	111.83
22	C	308	CHD	C17-C13-C12	-2.76	115.18	117.67
22	W	101	CHD	C22-C20-C17	2.74	116.01	110.33
19	A	607	PGV	O03-C19-O04	-2.74	116.77	123.63
14	N	601	HEA	CAA-CBA-CGA	-2.73	106.43	113.67
25	P	309	DMU	O7-C3-C4	2.73	116.63	109.48
24	P	305	CDL	OA8-CA7-C31	2.72	120.13	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	O2A-CGA-CBA	2.72	122.58	114.00
22	C	308	CHD	C1-C2-C3	2.72	114.08	110.48
18	L	101	TGL	OG3-CC1-CC2	2.71	120.10	111.83
23	G	102	PEK	O03-C21-C22	2.70	120.07	111.83
24	P	305	CDL	CB4-OB6-CB5	-2.70	111.34	117.80
14	N	602	HEA	CAD-CBD-CGD	-2.69	106.52	113.67
25	C	312	DMU	C6-C1-C2	2.69	115.67	110.01
14	N	601	HEA	C26-C15-C16	2.68	119.88	115.23
26	O	304	PSC	O03-C19-C20	2.68	120.00	111.83
14	N	601	HEA	C13-C12-C11	-2.68	110.12	114.39
22	P	306	CHD	C14-C8-C9	-2.67	106.02	109.75
14	A	602	HEA	O1A-CGA-CBA	-2.67	114.63	123.09
22	W	101	CHD	C6-C5-C10	2.67	115.50	112.66
22	C	301	CHD	C15-C14-C13	2.66	106.12	103.54
22	P	306	CHD	C15-C14-C13	2.66	106.12	103.54
18	A	606	TGL	CG3-OG3-CC1	2.66	126.83	117.12
18	O	302	TGL	OG1-CA1-CA2	2.65	119.93	111.83
14	N	601	HEA	CHC-C4B-NB	2.65	127.64	124.37
14	N	602	HEA	C27-C19-C20	2.65	119.82	115.23
19	N	606	PGV	O03-C19-C20	2.64	119.88	111.83
26	E	201	PSC	O03-C19-C20	2.63	119.86	111.83
14	A	602	HEA	C20-C19-C18	-2.60	115.33	121.17
18	A	606	TGL	OG1-CA1-CA2	2.60	119.77	111.83
22	P	306	CHD	C1-C10-C9	-2.60	107.31	111.34
14	N	602	HEA	CMB-C2B-C3B	-2.60	125.25	130.28
25	C	313	DMU	O5-C4-C3	2.59	115.08	109.72
23	T	102	PEK	O01-C1-C2	2.59	117.08	111.48
22	C	308	CHD	C23-C22-C20	-2.59	109.63	114.46
22	P	301	CHD	C6-C7-C8	2.59	114.32	111.50
22	O	301	CHD	C15-C14-C13	2.58	106.05	103.54
14	N	601	HEA	O1A-CGA-CBA	-2.57	114.94	123.09
18	D	201	TGL	OG1-CA1-CA2	2.56	119.64	111.83
14	A	602	HEA	C27-C19-C20	2.54	119.63	115.23
18	A	606	TGL	CG3-CG2-CG1	-2.53	105.88	111.78
24	G	101	CDL	OB8-CB7-C71	2.53	119.55	111.83
24	P	305	CDL	OB8-CB7-OB9	-2.53	117.31	123.63
14	A	601	HEA	C13-C14-C15	-2.52	121.86	127.62
22	J	101	CHD	C6-C5-C4	-2.52	108.35	111.23
22	C	308	CHD	C16-C17-C13	2.50	105.97	103.54
24	C	307	CDL	OA8-CA7-C31	2.49	119.43	111.83
18	Q	201	TGL	OG3-CC1-OC1	-2.47	117.46	123.63
18	Y	101	TGL	OG3-CC1-CC2	2.46	119.33	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	101	TGL	OG1-CA1-CA2	2.44	119.28	111.83
24	T	104	CDL	OB8-CB7-C71	2.44	119.27	111.83
14	A	601	HEA	C17-C18-C19	-2.43	122.05	127.62
14	N	602	HEA	CMB-C2B-C1B	2.41	128.81	125.03
14	A	601	HEA	O11-C11-C3B	-2.41	106.84	111.26
22	C	308	CHD	C13-C17-C20	-2.41	116.57	119.48
14	N	601	HEA	O2A-CGA-CBA	2.39	121.54	114.00
19	C	305	PGV	O01-C1-C2	2.39	116.64	111.48
25	C	312	DMU	C18-O16-C6	2.39	117.75	113.68
22	P	306	CHD	C6-C7-C8	2.38	114.10	111.50
14	A	602	HEA	CMB-C2B-C3B	-2.38	125.67	130.28
14	A	601	HEA	O1A-CGA-CBA	-2.37	115.57	123.09
14	A	602	HEA	C13-C12-C11	-2.36	110.62	114.39
22	O	301	CHD	C13-C17-C20	-2.35	116.64	119.48
14	A	601	HEA	CHC-C4B-NB	2.34	127.26	124.37
22	O	301	CHD	C11-C9-C8	2.33	114.34	110.89
18	Q	201	TGL	OG1-CG1-CG2	2.31	115.06	108.40
22	W	101	CHD	C9-C10-C5	2.29	111.70	108.51
14	A	602	HEA	C1D-C2D-C3D	-2.29	104.57	106.98
14	A	601	HEA	C26-C15-C14	-2.29	117.75	123.63
14	A	601	HEA	CAA-CBA-CGA	-2.26	107.66	113.67
19	N	607	PGV	O03-C19-O04	-2.26	117.97	123.63
25	P	308	DMU	O16-C6-C1	2.26	111.70	108.27
14	N	602	HEA	C3A-C2A-C1A	-2.25	104.92	107.05
23	T	103	PEK	O03-C21-O04	-2.23	118.04	123.63
22	B	302	CHD	C14-C8-C7	2.23	114.82	111.85
24	G	101	CDL	OA6-CA5-OA7	-2.23	118.50	123.70
22	P	306	CHD	C2-C1-C10	2.21	116.47	112.74
18	D	201	TGL	OG3-CC1-OC1	-2.21	118.11	123.63
22	C	301	CHD	O25-C24-C23	-2.20	116.12	123.09
14	A	602	HEA	C3A-C2A-C1A	-2.19	104.97	107.05
18	Q	201	TGL	OG1-CA1-OA1	-2.18	118.16	123.63
22	P	301	CHD	C19-C10-C1	-2.18	104.84	108.31
14	N	602	HEA	CBD-CAD-C3D	2.17	118.53	112.53
22	J	101	CHD	C21-C20-C17	-2.17	109.63	112.88
25	Z	101	DMU	C10-O7-C3	-2.15	112.88	117.98
18	L	101	TGL	OG3-CC1-OC1	-2.15	118.26	123.63
14	A	601	HEA	O2A-CGA-CBA	2.14	120.77	114.00
14	N	602	HEA	O2A-CGA-CBA	2.14	120.76	114.00
25	Z	101	DMU	C1-C2-C3	2.13	114.52	109.68
19	P	303	PGV	O14-P-O13	2.13	122.35	112.44
14	N	601	HEA	CBA-CAA-C2A	2.13	118.41	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	C4B-NB-C1B	2.12	107.72	105.21
22	J	101	CHD	C1-C10-C5	2.12	110.79	107.75
14	N	601	HEA	C13-C14-C15	-2.11	122.80	127.62
22	W	101	CHD	C1-C10-C5	2.10	110.77	107.75
24	P	305	CDL	OA6-CA5-OA7	-2.10	118.79	123.70
25	P	308	DMU	C18-O16-C6	2.10	117.26	113.68
22	J	101	CHD	C15-C14-C13	2.09	105.57	103.54
19	P	303	PGV	O01-C1-C2	2.08	115.99	111.48
22	P	306	CHD	C5-C4-C3	-2.07	109.58	112.71
22	C	308	CHD	C22-C23-C24	-2.07	106.97	112.49
23	G	102	PEK	O01-C1-O02	-2.06	118.88	123.70
24	T	104	CDL	OA8-CA7-OA9	-2.06	118.48	123.63
19	A	607	PGV	O01-C1-C2	2.05	115.92	111.48
22	W	101	CHD	C6-C5-C4	-2.05	108.88	111.23
26	O	304	PSC	O01-C1-O02	-2.05	118.91	123.70
14	A	601	HEA	C3C-C4C-NC	2.04	111.51	109.80
24	T	104	CDL	OA6-CA5-OA7	-2.04	118.95	123.70
19	P	303	PGV	O03-C19-O04	-2.03	118.56	123.63
23	T	102	PEK	O03-C21-O04	-2.02	118.58	123.63
19	M	101	PGV	O03-C19-O04	-2.02	118.58	123.63
22	J	101	CHD	C9-C10-C5	2.01	111.30	108.51
24	P	305	CDL	CB6-OB8-CB7	2.00	124.44	117.12
22	C	301	CHD	C19-C10-C1	-2.00	105.12	108.31

There are no chirality outliers.

All (961) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C2A-C3A-CMA-OMA
14	A	602	HEA	C2A-C3A-CMA-OMA
14	A	602	HEA	C2D-C3D-CAD-CBD
14	A	602	HEA	C4D-C3D-CAD-CBD
14	N	601	HEA	C2A-C3A-CMA-OMA
14	N	602	HEA	C2A-C3A-CMA-OMA
18	A	606	TGL	CB2-CB1-OG2-CG2
18	A	606	TGL	CC2-CC1-OG3-CG3
18	A	606	TGL	OC1-CC1-OG3-CG3
18	D	201	TGL	OB1-CB1-OG2-CG2
18	D	201	TGL	OG1-CG1-CG2-OG2
18	L	101	TGL	CB2-CB1-OG2-CG2
18	O	302	TGL	OB1-CB1-OG2-CG2
18	Y	101	TGL	CB2-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
19	M	101	PGV	C03-O11-P-O13
19	M	101	PGV	C04-O12-P-O11
19	M	101	PGV	C04-C05-C06-O06
19	N	606	PGV	C03-O11-P-O12
19	N	606	PGV	C03-O11-P-O13
19	N	606	PGV	C03-O11-P-O14
19	N	606	PGV	C04-O12-P-O11
19	N	606	PGV	C04-O12-P-O13
19	N	606	PGV	C04-O12-P-O14
19	N	606	PGV	O01-C02-C03-O11
19	N	606	PGV	C04-C05-C06-O06
19	N	606	PGV	O02-C1-O01-C02
19	N	606	PGV	C2-C1-O01-C02
19	P	304	PGV	C03-O11-P-O12
19	P	304	PGV	C02-C03-O11-P
23	C	304	PEK	C03-O11-P-O12
23	C	304	PEK	C04-O12-P-O14
23	C	304	PEK	O12-C04-C05-N
23	G	102	PEK	C03-O11-P-O12
23	G	102	PEK	C03-O11-P-O13
23	G	102	PEK	O12-C04-C05-N
23	G	102	PEK	C2-C1-O01-C02
23	T	101	PEK	O12-C04-C05-N
23	T	101	PEK	C2-C1-O01-C02
23	T	101	PEK	C12-C13-C14-C15
24	C	307	CDL	CA3-OA5-PA1-OA3
24	C	307	CDL	C11-CA5-OA6-CA4
24	C	307	CDL	CB2-OB2-PB2-OB5
24	C	307	CDL	C51-CB5-OB6-CB4
24	G	101	CDL	CA2-C1-CB2-OB2
24	G	101	CDL	CA2-OA2-PA1-OA3
24	G	101	CDL	CA2-OA2-PA1-OA4
24	G	101	CDL	CA2-OA2-PA1-OA5
24	G	101	CDL	C11-CA5-OA6-CA4
24	G	101	CDL	CB2-OB2-PB2-OB3
24	G	101	CDL	CB3-OB5-PB2-OB2
24	G	101	CDL	OB6-CB4-CB6-OB8
24	P	305	CDL	CA2-C1-CB2-OB2
24	P	305	CDL	CA2-OA2-PA1-OA4
24	P	305	CDL	CA2-OA2-PA1-OA5
24	P	305	CDL	CA3-OA5-PA1-OA2
24	P	305	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
24	P	305	CDL	CB2-OB2-PB2-OB5
24	P	305	CDL	CB3-OB5-PB2-OB2
24	P	305	CDL	CB3-OB5-PB2-OB3
24	P	305	CDL	CB3-OB5-PB2-OB4
24	P	305	CDL	C51-CB5-OB6-CB4
24	P	305	CDL	CB4-CB6-OB8-CB7
24	T	104	CDL	CA2-OA2-PA1-OA3
24	T	104	CDL	CA2-OA2-PA1-OA5
24	T	104	CDL	CA3-OA5-PA1-OA2
24	T	104	CDL	CA3-OA5-PA1-OA3
24	T	104	CDL	CA3-OA5-PA1-OA4
24	T	104	CDL	C11-CA5-OA6-CA4
24	T	104	CDL	OA9-CA7-OA8-CA6
24	T	104	CDL	C1-CB2-OB2-PB2
24	T	104	CDL	CB2-OB2-PB2-OB4
24	T	104	CDL	CB2-OB2-PB2-OB5
24	T	104	CDL	OB6-CB4-CB6-OB8
25	C	313	DMU	O5-C6-O16-C18
25	P	308	DMU	C1-C6-O16-C18
25	P	308	DMU	O5-C6-O16-C18
25	P	309	DMU	O5-C6-O16-C18
26	E	201	PSC	C03-O11-P-O12
26	E	201	PSC	C03-O11-P-O13
26	E	201	PSC	C04-O12-P-O13
26	E	201	PSC	O12-C04-C05-N
26	E	201	PSC	C2-C1-O01-C02
26	O	304	PSC	C03-O11-P-O12
26	O	304	PSC	C03-O11-P-O13
26	O	304	PSC	C04-O12-P-O11
26	O	304	PSC	C04-O12-P-O13
26	O	304	PSC	O12-C04-C05-N
26	O	304	PSC	C2-C1-O01-C02
18	D	201	TGL	OC1-CC1-OG3-CG3
18	Q	201	TGL	OC1-CC1-OG3-CG3
19	N	606	PGV	O04-C19-O03-C01
18	D	201	TGL	CC2-CC1-OG3-CG3
24	T	104	CDL	C31-CA7-OA8-CA6
18	Q	201	TGL	OA1-CA1-OG1-CG1
18	Y	101	TGL	OA1-CA1-OG1-CG1
25	P	308	DMU	O1-C10-O7-C3
25	P	309	DMU	C4-C3-O7-C10
24	P	305	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
18	A	606	TGL	OB1-CB1-OG2-CG2
18	L	101	TGL	OB1-CB1-OG2-CG2
18	Y	101	TGL	OB1-CB1-OG2-CG2
19	M	101	PGV	O02-C1-O01-C02
23	G	102	PEK	O02-C1-O01-C02
23	T	101	PEK	O02-C1-O01-C02
24	C	307	CDL	OB7-CB5-OB6-CB4
24	G	101	CDL	OA7-CA5-OA6-CA4
24	P	305	CDL	OA7-CA5-OA6-CA4
24	P	305	CDL	OB7-CB5-OB6-CB4
24	T	104	CDL	OA7-CA5-OA6-CA4
26	O	304	PSC	O02-C1-O01-C02
18	Q	201	TGL	CC2-CC1-OG3-CG3
19	N	606	PGV	C20-C19-O03-C01
23	T	101	PEK	C22-C21-O03-C01
24	G	101	CDL	C31-CA7-OA8-CA6
26	O	304	PSC	C20-C19-O03-C01
18	D	201	TGL	CB2-CB1-OG2-CG2
18	O	302	TGL	CB2-CB1-OG2-CG2
19	M	101	PGV	C2-C1-O01-C02
18	O	302	TGL	CC2-CC1-OG3-CG3
18	Q	201	TGL	CA2-CA1-OG1-CG1
18	Y	101	TGL	CA2-CA1-OG1-CG1
23	C	304	PEK	C22-C21-O03-C01
25	P	308	DMU	O6-C11-C9-O1
19	N	606	PGV	C10-C11-C12-C13
19	P	304	PGV	C10-C11-C12-C13
23	C	304	PEK	C13-C14-C15-C16
23	G	102	PEK	C4-C5-C6-C7
23	T	101	PEK	C7-C8-C9-C10
23	T	102	PEK	C4-C5-C6-C7
23	T	102	PEK	C13-C14-C15-C16
18	O	302	TGL	OC1-CC1-OG3-CG3
23	T	101	PEK	O04-C21-O03-C01
26	E	201	PSC	O04-C19-O03-C01
26	O	304	PSC	O04-C19-O03-C01
24	C	307	CDL	OA7-CA5-OA6-CA4
26	E	201	PSC	O02-C1-O01-C02
24	G	101	CDL	O1-C1-CA2-OA2
24	P	305	CDL	O1-C1-CB2-OB2
19	M	101	PGV	C20-C19-O03-C01
24	P	305	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
26	E	201	PSC	C20-C19-O03-C01
25	C	313	DMU	O5-C4-C57-O61
24	G	101	CDL	OA9-CA7-OA8-CA6
19	M	101	PGV	O04-C19-O03-C01
25	Z	101	DMU	O6-C11-C9-O1
23	C	304	PEK	O04-C21-O03-C01
19	M	101	PGV	C02-C03-O11-P
18	L	101	TGL	CA2-CA1-OG1-CG1
19	C	305	PGV	C10-C11-C12-C13
23	C	303	PEK	C13-C14-C15-C16
23	C	304	PEK	C7-C8-C9-C10
23	T	103	PEK	C4-C5-C6-C7
23	T	103	PEK	C13-C14-C15-C16
24	P	305	CDL	CB2-C1-CA2-OA2
23	G	102	PEK	C22-C21-O03-C01
24	T	104	CDL	C79-C80-C81-C82
25	Z	101	DMU	O6-C11-C9-C8
25	C	313	DMU	C3-C4-C57-O61
25	P	308	DMU	O6-C11-C9-C8
24	G	101	CDL	O1-C1-CB2-OB2
24	P	305	CDL	O1-C1-CA2-OA2
22	J	101	CHD	C13-C17-C20-C22
22	C	308	CHD	C17-C20-C22-C23
22	P	306	CHD	C17-C20-C22-C23
19	C	306	PGV	C10-C11-C12-C13
26	O	304	PSC	C11-C12-C13-C14
22	J	101	CHD	C13-C17-C20-C21
19	C	305	PGV	C28-C29-C30-C31
26	O	304	PSC	C19-C20-C21-C22
18	A	606	TGL	CB1-CB2-CB3-CB4
18	D	201	TGL	CA1-CA2-CA3-CA4
24	P	305	CDL	CA7-C31-C32-C33
23	G	102	PEK	O04-C21-O03-C01
24	G	101	CDL	C51-CB5-OB6-CB4
22	C	308	CHD	C20-C22-C23-C24
22	P	306	CHD	C21-C20-C22-C23
18	O	302	TGL	CB1-CB2-CB3-CB4
23	T	101	PEK	C21-C22-C23-C24
24	G	101	CDL	CB7-C71-C72-C73
24	C	307	CDL	O1-C1-CB2-OB2
24	T	104	CDL	O1-C1-CB2-OB2
24	C	307	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
18	L	101	TGL	OA1-CA1-OG1-CG1
18	A	606	TGL	CA1-CA2-CA3-CA4
24	C	307	CDL	CB7-C71-C72-C73
22	C	308	CHD	C21-C20-C22-C23
23	C	303	PEK	C10-C11-C12-C13
23	T	102	PEK	C10-C11-C12-C13
26	E	201	PSC	C11-C12-C13-C14
24	T	104	CDL	CA7-C31-C32-C33
26	O	304	PSC	C1-C2-C3-C4
22	J	101	CHD	C16-C17-C20-C21
18	L	101	TGL	C20-C21-C22-C23
18	Q	201	TGL	CC1-CC2-CC3-CC4
18	Q	201	TGL	OB1-CB1-OG2-CG2
23	C	304	PEK	O02-C1-O01-C02
24	G	101	CDL	OB7-CB5-OB6-CB4
24	C	307	CDL	CA2-C1-CB2-OB2
24	G	101	CDL	CB2-C1-CA2-OA2
24	T	104	CDL	CA2-C1-CB2-OB2
25	Z	101	DMU	O16-C18-C19-C22
22	W	101	CHD	C13-C17-C20-C21
24	C	307	CDL	CA5-C11-C12-C13
18	Q	201	TGL	CB2-CB1-OG2-CG2
23	C	304	PEK	C2-C1-O01-C02
19	M	101	PGV	C10-C11-C12-C13
23	T	101	PEK	C13-C14-C15-C16
24	C	307	CDL	OB9-CB7-OB8-CB6
19	P	304	PGV	C04-C05-C06-O06
18	O	302	TGL	CG1-CG2-OG2-CB1
22	W	101	CHD	C13-C17-C20-C22
25	P	309	DMU	C18-C19-C22-C25
25	P	308	DMU	O16-C18-C19-C22
18	L	101	TGL	C12-C13-C14-C29
18	A	606	TGL	C21-C20-CA9-CA8
19	P	304	PGV	C14-C15-C16-C17
24	C	307	CDL	C31-C32-C33-C34
24	C	307	CDL	C71-C72-C73-C74
24	G	101	CDL	C52-C53-C54-C55
18	D	201	TGL	C10-C11-C12-C13
18	O	302	TGL	CA5-CA6-CA7-CA8
19	C	305	PGV	C13-C14-C15-C16
19	P	303	PGV	C14-C15-C16-C17
23	C	304	PEK	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
23	G	102	PEK	C32-C33-C34-C35
19	P	303	PGV	C10-C11-C12-C13
23	C	303	PEK	C7-C8-C9-C10
23	T	102	PEK	C7-C8-C9-C10
23	T	103	PEK	C7-C8-C9-C10
18	L	101	TGL	CB5-CB6-CB7-CB8
18	O	302	TGL	C20-C21-C22-C23
19	C	306	PGV	C23-C24-C25-C26
19	P	304	PGV	C2-C3-C4-C5
25	C	313	DMU	C28-C31-C34-C37
18	A	606	TGL	C22-C23-C24-C25
18	D	201	TGL	C18-C19-C33-C34
18	O	302	TGL	C11-C10-CB9-CB8
18	Q	201	TGL	CB9-C10-C11-C12
18	Y	101	TGL	CA7-CA8-CA9-C20
23	C	304	PEK	C24-C25-C26-C27
26	O	304	PSC	C24-C25-C26-C27
26	O	304	PSC	C27-C28-C29-C30
26	O	304	PSC	C28-C29-C30-C31
19	N	606	PGV	O05-C05-C06-O06
18	O	302	TGL	CC9-C15-C16-C17
19	M	101	PGV	C22-C23-C24-C25
23	C	303	PEK	C34-C35-C36-C37
23	G	102	PEK	C26-C27-C28-C29
23	G	102	PEK	C33-C34-C35-C36
24	C	307	CDL	C63-C64-C65-C66
24	C	307	CDL	C83-C84-C85-C86
24	P	305	CDL	C82-C83-C84-C85
26	E	201	PSC	C5-C6-C7-C8
18	A	606	TGL	CB5-CB6-CB7-CB8
18	A	606	TGL	C16-C17-C18-C19
18	D	201	TGL	C11-C10-CB9-CB8
18	O	302	TGL	CC4-CC5-CC6-CC7
24	P	305	CDL	C15-C16-C17-C18
18	Y	101	TGL	CC2-CC3-CC4-CC5
19	P	303	PGV	C7-C8-C9-C10
24	G	101	CDL	C32-C33-C34-C35
24	P	305	CDL	C73-C74-C75-C76
19	C	306	PGV	C6-C7-C8-C9
26	O	304	PSC	C26-C27-C28-C29
18	Y	101	TGL	CA1-CA2-CA3-CA4
18	Q	201	TGL	CA2-CA3-CA4-CA5

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Mol	Chain	Res	Type	Atoms
18	Q	201	TGL	CC4-CC5-CC6-CC7
18	Y	101	TGL	CC3-CC4-CC5-CC6
24	G	101	CDL	C59-C60-C61-C62
24	P	305	CDL	C40-C41-C42-C43
18	A	606	TGL	CC4-CC5-CC6-CC7
18	L	101	TGL	CC3-CC4-CC5-CC6
18	O	302	TGL	C10-C11-C12-C13
19	N	607	PGV	C26-C27-C28-C29
23	G	102	PEK	C30-C31-C32-C33
23	T	101	PEK	C32-C33-C34-C35
24	C	307	CDL	C82-C83-C84-C85
24	G	101	CDL	C12-C13-C14-C15
24	G	101	CDL	C79-C80-C81-C82
25	C	313	DMU	C18-C19-C22-C25
19	C	305	PGV	C7-C8-C9-C10
23	T	101	PEK	C25-C26-C27-C28
24	C	307	CDL	C79-C80-C81-C82
14	N	602	HEA	C4D-C3D-CAD-CBD
18	Y	101	TGL	CB5-CB6-CB7-CB8
19	P	303	PGV	C24-C25-C26-C27
23	T	103	PEK	C29-C30-C31-C32
24	C	307	CDL	C21-C22-C23-C24
26	E	201	PSC	C25-C26-C27-C28
18	L	101	TGL	C21-C20-CA9-CA8
18	O	302	TGL	CA9-C20-C21-C22
18	Q	201	TGL	C23-C24-C25-C26
23	C	304	PEK	C23-C24-C25-C26
23	G	102	PEK	C28-C29-C30-C31
24	G	101	CDL	C36-C37-C38-C39
24	T	104	CDL	C71-C72-C73-C74
23	C	304	PEK	C21-C22-C23-C24
23	G	102	PEK	C1-C2-C3-C4
18	A	606	TGL	C13-C14-C29-C30
18	D	201	TGL	C21-C20-CA9-CA8
18	D	201	TGL	CC4-CC5-CC6-CC7
24	C	307	CDL	C23-C24-C25-C26
24	G	101	CDL	C54-C55-C56-C57
24	T	104	CDL	C73-C74-C75-C76
19	C	305	PGV	C14-C15-C16-C17
19	P	304	PGV	C4-C5-C6-C7
19	P	304	PGV	C5-C6-C7-C8
24	P	305	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
24	T	104	CDL	C23-C24-C25-C26
20	D	202	EDO	O1-C1-C2-O2
18	Q	201	TGL	CA6-CA7-CA8-CA9
18	Q	201	TGL	C21-C22-C23-C24
23	C	303	PEK	C26-C27-C28-C29
24	P	305	CDL	C41-C42-C43-C44
24	P	305	CDL	C81-C82-C83-C84
18	O	302	TGL	CA7-CA8-CA9-C20
19	N	606	PGV	C22-C23-C24-C25
23	G	102	PEK	C23-C24-C25-C26
24	T	104	CDL	C62-C63-C64-C65
24	T	104	CDL	C63-C64-C65-C66
18	Y	101	TGL	CB6-CB7-CB8-CB9
24	P	305	CDL	C13-C14-C15-C16
26	O	304	PSC	C6-C7-C8-C9
23	G	102	PEK	C13-C14-C15-C16
18	A	606	TGL	C16-C15-CC9-CC8
24	G	101	CDL	C77-C78-C79-C80
18	Y	101	TGL	C12-C13-C14-C29
24	P	305	CDL	C12-C13-C14-C15
25	P	308	DMU	C18-C19-C22-C25
18	A	606	TGL	CA3-CA4-CA5-CA6
18	D	201	TGL	C23-C24-C25-C26
18	Q	201	TGL	CC7-CC8-CC9-C15
23	G	102	PEK	C22-C23-C24-C25
23	T	102	PEK	C34-C35-C36-C37
18	A	606	TGL	C23-C24-C25-C26
23	C	303	PEK	C16-C17-C18-C19
23	C	304	PEK	C29-C30-C31-C32
18	O	302	TGL	CB7-CB8-CB9-C10
23	C	303	PEK	C28-C29-C30-C31
23	T	101	PEK	C34-C35-C36-C37
24	T	104	CDL	C34-C35-C36-C37
18	O	302	TGL	CA4-CA5-CA6-CA7
18	Y	101	TGL	CA6-CA7-CA8-CA9
18	Y	101	TGL	CB3-CB4-CB5-CB6
24	P	305	CDL	C42-C43-C44-C45
24	T	104	CDL	C33-C34-C35-C36
25	Z	101	DMU	C25-C28-C31-C34
26	E	201	PSC	C20-C21-C22-C23
23	T	103	PEK	C22-C21-O03-C01
24	G	101	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
18	A	606	TGL	C12-C13-C14-C29
18	A	606	TGL	CC9-C15-C16-C17
18	L	101	TGL	CC6-CC7-CC8-CC9
19	C	306	PGV	C21-C22-C23-C24
19	N	606	PGV	C7-C8-C9-C10
24	P	305	CDL	C43-C44-C45-C46
25	C	313	DMU	C19-C22-C25-C28
23	G	102	PEK	C29-C30-C31-C32
24	T	104	CDL	C11-C12-C13-C14
18	O	302	TGL	C16-C15-CC9-CC8
19	M	101	PGV	C24-C25-C26-C27
26	E	201	PSC	C21-C22-C23-C24
18	A	606	TGL	CA2-CA3-CA4-CA5
23	C	304	PEK	C31-C32-C33-C34
24	P	305	CDL	C52-C53-C54-C55
26	O	304	PSC	C29-C30-C31-C32
18	Y	101	TGL	C10-C11-C12-C13
23	T	101	PEK	C28-C29-C30-C31
25	P	309	DMU	C19-C22-C25-C28
24	C	307	CDL	C55-C56-C57-C58
24	G	101	CDL	C37-C38-C39-C40
26	O	304	PSC	C2-C3-C4-C5
18	L	101	TGL	C19-C33-C34-C35
23	T	103	PEK	C26-C27-C28-C29
19	C	306	PGV	C2-C1-O01-C02
24	T	104	CDL	C51-CB5-OB6-CB4
18	Y	101	TGL	C18-C19-C33-C34
19	P	303	PGV	C30-C31-C32-C33
24	T	104	CDL	OB7-CB5-OB6-CB4
18	A	606	TGL	CB4-CB5-CB6-CB7
18	Q	201	TGL	C13-C14-C29-C30
23	T	103	PEK	C24-C25-C26-C27
24	C	307	CDL	C80-C81-C82-C83
24	T	104	CDL	C52-C53-C54-C55
19	C	305	PGV	C24-C25-C26-C27
24	G	101	CDL	C73-C74-C75-C76
18	A	606	TGL	C15-C16-C17-C18
18	L	101	TGL	CB3-CB4-CB5-CB6
19	C	306	PGV	C7-C8-C9-C10
22	W	101	CHD	C16-C17-C20-C21
18	Y	101	TGL	C16-C15-CC9-CC8
18	D	201	TGL	CC7-CC8-CC9-C15

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Mol	Chain	Res	Type	Atoms
18	L	101	TGL	CA3-CA4-CA5-CA6
18	Q	201	TGL	C16-C17-C18-C19
18	D	201	TGL	CC6-CC7-CC8-CC9
26	E	201	PSC	C24-C25-C26-C27
24	P	305	CDL	CB7-C71-C72-C73
18	O	302	TGL	CA2-CA3-CA4-CA5
24	P	305	CDL	C18-C19-C20-C21
26	O	304	PSC	C20-C21-C22-C23
18	Q	201	TGL	CB4-CB5-CB6-CB7
19	C	306	PGV	C2-C3-C4-C5
24	P	305	CDL	C34-C35-C36-C37
18	L	101	TGL	C10-C11-C12-C13
19	C	306	PGV	C3-C4-C5-C6
19	C	306	PGV	C28-C29-C30-C31
19	C	306	PGV	C30-C31-C32-C33
19	P	303	PGV	C22-C23-C24-C25
23	C	303	PEK	C25-C26-C27-C28
24	C	307	CDL	C41-C42-C43-C44
24	T	104	CDL	C39-C40-C41-C42
19	C	306	PGV	C12-C13-C14-C15
19	P	304	PGV	C11-C10-C9-C8
19	N	606	PGV	C24-C25-C26-C27
18	Y	101	TGL	CA4-CA5-CA6-CA7
19	N	606	PGV	C23-C24-C25-C26
23	C	304	PEK	C25-C26-C27-C28
24	T	104	CDL	C32-C33-C34-C35
19	N	607	PGV	C23-C24-C25-C26
19	P	304	PGV	C20-C21-C22-C23
24	P	305	CDL	C23-C24-C25-C26
23	T	102	PEK	C3-C4-C5-C6
18	A	606	TGL	C11-C10-CB9-CB8
18	D	201	TGL	CC9-C15-C16-C17
19	C	305	PGV	C22-C23-C24-C25
19	P	304	PGV	C13-C14-C15-C16
19	P	304	PGV	C24-C25-C26-C27
26	E	201	PSC	C23-C24-C25-C26
18	O	302	TGL	C12-C13-C14-C29
18	Y	101	TGL	C11-C12-C13-C14
18	Y	101	TGL	C17-C18-C19-C33
24	G	101	CDL	C15-C16-C17-C18
24	T	104	CDL	C53-C54-C55-C56
23	C	304	PEK	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
19	P	304	PGV	O12-C04-C05-C06
18	A	606	TGL	C11-C12-C13-C14
18	D	201	TGL	C13-C14-C29-C30
18	L	101	TGL	C21-C22-C23-C24
18	Y	101	TGL	CB2-CB3-CB4-CB5
24	G	101	CDL	C57-C58-C59-C60
22	P	306	CHD	C20-C22-C23-C24
18	O	302	TGL	CA6-CA7-CA8-CA9
18	Q	201	TGL	C10-C11-C12-C13
18	Y	101	TGL	CA2-CA3-CA4-CA5
19	N	606	PGV	C2-C3-C4-C5
26	E	201	PSC	C2-C3-C4-C5
19	P	304	PGV	C29-C30-C31-C32
18	O	302	TGL	CA1-CA2-CA3-CA4
18	Q	201	TGL	C21-C20-CA9-CA8
24	G	101	CDL	C34-C35-C36-C37
19	M	101	PGV	O05-C05-C06-O06
23	T	103	PEK	O04-C21-O03-C01
18	Y	101	TGL	CA9-C20-C21-C22
18	A	606	TGL	CA5-CA6-CA7-CA8
18	L	101	TGL	C17-C18-C19-C33
24	P	305	CDL	C62-C63-C64-C65
19	C	305	PGV	C12-C13-C14-C15
19	M	101	PGV	C12-C13-C14-C15
19	N	607	PGV	C11-C10-C9-C8
23	G	102	PEK	C2-C3-C4-C5
23	T	101	PEK	C15-C16-C17-C18
23	T	102	PEK	C15-C16-C17-C18
24	C	307	CDL	C54-C55-C56-C57
24	G	101	CDL	C42-C43-C44-C45
24	P	305	CDL	C56-C57-C58-C59
19	N	606	PGV	C01-C02-C03-O11
24	C	307	CDL	OA5-CA3-CA4-CA6
19	C	306	PGV	O02-C1-O01-C02
19	P	304	PGV	C6-C7-C8-C9
24	C	307	CDL	C14-C15-C16-C17
24	C	307	CDL	C76-C77-C78-C79
24	T	104	CDL	C80-C81-C82-C83
18	Q	201	TGL	C19-C33-C34-C35
24	T	104	CDL	C56-C57-C58-C59
24	G	101	CDL	OB9-CB7-OB8-CB6
18	D	201	TGL	CB1-CB2-CB3-CB4

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Mol	Chain	Res	Type	Atoms
23	G	102	PEK	C21-C22-C23-C24
19	P	304	PGV	C26-C27-C28-C29
14	N	602	HEA	C2D-C3D-CAD-CBD
18	O	302	TGL	C16-C17-C18-C19
18	O	302	TGL	C23-C24-C25-C26
23	T	102	PEK	C26-C27-C28-C29
23	T	102	PEK	C33-C34-C35-C36
25	C	312	DMU	C1-C6-O16-C18
19	A	607	PGV	C10-C11-C12-C13
23	C	303	PEK	C4-C5-C6-C7
23	C	304	PEK	O03-C01-C02-C03
24	C	307	CDL	CA3-CA4-CA6-OA8
24	C	307	CDL	CB3-CB4-CB6-OB8
24	P	305	CDL	CA3-CA4-CA6-OA8
24	T	104	CDL	CB3-CB4-CB6-OB8
18	L	101	TGL	C24-C25-C26-C27
19	N	606	PGV	C11-C10-C9-C8
23	C	304	PEK	C2-C3-C4-C5
23	T	102	PEK	C2-C3-C4-C5
19	P	304	PGV	C23-C24-C25-C26
26	O	304	PSC	C22-C23-C24-C25
24	C	307	CDL	C52-C53-C54-C55
24	C	307	CDL	C81-C82-C83-C84
20	A	614	EDO	O1-C1-C2-O2
18	O	302	TGL	C13-C14-C29-C30
24	T	104	CDL	C60-C61-C62-C63
22	C	308	CHD	C16-C17-C20-C21
24	T	104	CDL	C81-C82-C83-C84
19	P	303	PGV	C1-C2-C3-C4
24	T	104	CDL	C58-C59-C60-C61
25	C	312	DMU	O6-C11-C9-C8
24	G	101	CDL	C17-C18-C19-C20
18	Y	101	TGL	C19-C33-C34-C35
24	T	104	CDL	C15-C16-C17-C18
25	Z	101	DMU	C28-C31-C34-C37
24	G	101	CDL	C72-C73-C74-C75
19	P	304	PGV	C1-C2-C3-C4
19	P	304	PGV	C22-C23-C24-C25
19	N	606	PGV	C21-C22-C23-C24
24	G	101	CDL	C55-C56-C57-C58
18	Y	101	TGL	C23-C24-C25-C26
19	C	306	PGV	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
24	G	101	CDL	OA5-CA3-CA4-OA6
24	G	101	CDL	OB5-CB3-CB4-OB6
24	T	104	CDL	C24-C25-C26-C27
23	T	103	PEK	C16-C17-C18-C19
24	C	307	CDL	C60-C61-C62-C63
24	P	305	CDL	C31-C32-C33-C34
26	O	304	PSC	C5-C6-C7-C8
18	Y	101	TGL	C14-C29-C30-C31
23	C	304	PEK	C30-C31-C32-C33
24	P	305	CDL	C76-C77-C78-C79
19	C	306	PGV	C15-C16-C17-C18
19	M	101	PGV	C15-C16-C17-C18
24	C	307	CDL	C77-C78-C79-C80
24	G	101	CDL	C18-C19-C20-C21
24	T	104	CDL	C12-C13-C14-C15
23	T	101	PEK	O03-C01-C02-O01
24	P	305	CDL	C44-C45-C46-C47
19	A	607	PGV	C27-C28-C29-C30
23	T	101	PEK	C30-C31-C32-C33
18	L	101	TGL	C29-C30-C31-C32
18	A	606	TGL	C25-C26-C27-C28
23	G	102	PEK	C35-C36-C37-C38
23	T	102	PEK	C17-C18-C19-C20
18	D	201	TGL	CA6-CA7-CA8-CA9
19	P	304	PGV	C31-C32-C33-C34
19	M	101	PGV	C11-C10-C9-C8
18	O	302	TGL	C25-C26-C27-C28
18	Y	101	TGL	C29-C30-C31-C32
23	C	303	PEK	C17-C18-C19-C20
24	C	307	CDL	C37-C38-C39-C40
18	Q	201	TGL	CA9-C20-C21-C22
23	T	101	PEK	C16-C17-C18-C19
23	T	103	PEK	C17-C18-C19-C20
19	A	607	PGV	C31-C32-C33-C34
18	Y	101	TGL	C33-C34-C35-C36
18	L	101	TGL	C18-C19-C33-C34
18	Q	201	TGL	C12-C13-C14-C29
26	O	304	PSC	C23-C24-C25-C26
19	P	304	PGV	O05-C05-C06-O06
18	L	101	TGL	C11-C10-CB9-CB8
19	A	607	PGV	C30-C31-C32-C33
19	N	606	PGV	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
25	C	312	DMU	C34-C37-C40-C43
26	E	201	PSC	C30-C31-C32-C33
19	N	607	PGV	C31-C32-C33-C34
23	C	304	PEK	C35-C36-C37-C38
24	P	305	CDL	C14-C15-C16-C17
19	M	101	PGV	C31-C32-C33-C34
18	L	101	TGL	C11-C12-C13-C14
24	P	305	CDL	C19-C20-C21-C22
18	D	201	TGL	CA4-CA5-CA6-CA7
19	A	607	PGV	C23-C24-C25-C26
24	G	101	CDL	C76-C77-C78-C79
19	P	303	PGV	C31-C32-C33-C34
25	C	313	DMU	O6-C11-C9-C8
24	C	307	CDL	C40-C41-C42-C43
23	T	103	PEK	C35-C36-C37-C38
19	C	306	PGV	C20-C21-C22-C23
24	G	101	CDL	C75-C76-C77-C78
24	G	101	CDL	C21-C22-C23-C24
24	C	307	CDL	C13-C14-C15-C16
24	C	307	CDL	C44-C45-C46-C47
18	D	201	TGL	C21-C22-C23-C24
19	M	101	PGV	C28-C29-C30-C31
19	C	306	PGV	C19-C20-C21-C22
18	D	201	TGL	C33-C34-C35-C36
23	T	101	PEK	C26-C27-C28-C29
23	T	103	PEK	C28-C29-C30-C31
18	A	606	TGL	CG1-CG2-CG3-OG3
24	G	101	CDL	CB3-CB4-CB6-OB8
24	T	104	CDL	CA3-CA4-CA6-OA8
24	P	305	CDL	C74-C75-C76-C77
18	L	101	TGL	CA6-CA7-CA8-CA9
18	Q	201	TGL	CA4-CA5-CA6-CA7
23	T	103	PEK	C22-C23-C24-C25
24	G	101	CDL	C60-C61-C62-C63
26	O	304	PSC	O01-C02-C03-O11
23	T	102	PEK	C28-C29-C30-C31
24	G	101	CDL	C82-C83-C84-C85
18	A	606	TGL	C17-C18-C19-C33
23	C	303	PEK	C15-C16-C17-C18
19	C	305	PGV	C02-C03-O11-P
19	P	303	PGV	C02-C03-O11-P
24	C	307	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
24	P	305	CDL	C57-C58-C59-C60
18	D	201	TGL	CA9-C20-C21-C22
18	O	302	TGL	C14-C29-C30-C31
19	M	101	PGV	C23-C24-C25-C26
18	A	606	TGL	OG1-CG1-CG2-OG2
18	Y	101	TGL	OG2-CG2-CG3-OG3
19	P	304	PGV	O03-C01-C02-O01
23	C	304	PEK	O03-C01-C02-O01
24	C	307	CDL	OB6-CB4-CB6-OB8
24	T	104	CDL	OA6-CA4-CA6-OA8
23	C	304	PEK	C6-C7-C8-C9
23	G	102	PEK	C9-C10-C11-C12
23	G	102	PEK	C12-C13-C14-C15
23	T	101	PEK	C11-C10-C9-C8
23	T	102	PEK	C9-C10-C11-C12
23	T	103	PEK	C11-C10-C9-C8
23	T	103	PEK	C9-C10-C11-C12
26	E	201	PSC	C9-C10-C11-C12
26	O	304	PSC	C9-C10-C11-C12
26	O	304	PSC	C10-C11-C12-C13
18	D	201	TGL	C16-C17-C18-C19
24	P	305	CDL	C53-C54-C55-C56
18	Q	201	TGL	CC6-CC7-CC8-CC9
18	D	201	TGL	CC5-CC6-CC7-CC8
25	M	102	DMU	O6-C11-C9-C8
22	C	308	CHD	C16-C17-C20-C22
19	M	101	PGV	C21-C22-C23-C24
23	G	102	PEK	C34-C35-C36-C37
22	C	308	CHD	C13-C17-C20-C21
23	T	102	PEK	C23-C24-C25-C26
19	P	304	PGV	C30-C31-C32-C33
25	M	102	DMU	O16-C18-C19-C22
18	Q	201	TGL	CA5-CA6-CA7-CA8
24	G	101	CDL	C64-C65-C66-C67
24	P	305	CDL	C16-C17-C18-C19
19	C	305	PGV	C15-C16-C17-C18
24	T	104	CDL	C16-C17-C18-C19
19	P	304	PGV	C12-C13-C14-C15
19	N	607	PGV	C27-C28-C29-C30
19	P	304	PGV	C01-C02-C03-O11
23	T	103	PEK	C01-C02-C03-O11
24	P	305	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
18	A	606	TGL	CB2-CB3-CB4-CB5
24	T	104	CDL	C82-C83-C84-C85
19	C	305	PGV	C1-C2-C3-C4
19	N	607	PGV	C10-C11-C12-C13
24	T	104	CDL	C64-C65-C66-C67
18	A	606	TGL	CG1-CG2-OG2-CB1
18	Q	201	TGL	CG3-CG2-OG2-CB1
18	A	606	TGL	CC7-CC8-CC9-C15
24	T	104	CDL	C57-C58-C59-C60
18	O	302	TGL	CA3-CA4-CA5-CA6
19	P	304	PGV	O12-C04-C05-O05
18	A	606	TGL	C29-C30-C31-C32
26	E	201	PSC	C31-C32-C33-C34
19	P	304	PGV	O01-C02-C03-O11
26	E	201	PSC	O01-C02-C03-O11
24	G	101	CDL	C23-C24-C25-C26
24	G	101	CDL	C56-C57-C58-C59
22	C	308	CHD	C13-C17-C20-C22
18	D	201	TGL	OG1-CG1-CG2-CG3
18	Q	201	TGL	CG1-CG2-CG3-OG3
19	M	101	PGV	O03-C01-C02-C03
25	Z	101	DMU	C19-C22-C25-C28
24	T	104	CDL	C20-C21-C22-C23
19	C	306	PGV	C13-C14-C15-C16
19	C	305	PGV	C29-C30-C31-C32
23	G	102	PEK	C25-C26-C27-C28
26	O	304	PSC	C05-C04-O12-P
18	A	606	TGL	C20-C21-C22-C23
23	C	303	PEK	C29-C30-C31-C32
18	A	606	TGL	OG2-CG2-CG3-OG3
18	Q	201	TGL	OG2-CG2-CG3-OG3
19	M	101	PGV	O03-C01-C02-O01
24	C	307	CDL	OA6-CA4-CA6-OA8
18	D	201	TGL	C11-C12-C13-C14
19	C	306	PGV	C29-C30-C31-C32
24	G	101	CDL	C22-C23-C24-C25
24	P	305	CDL	C38-C39-C40-C41
24	T	104	CDL	C38-C39-C40-C41
18	Y	101	TGL	C16-C17-C18-C19
24	C	307	CDL	C15-C16-C17-C18
19	M	101	PGV	C19-C20-C21-C22
23	T	101	PEK	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
24	C	307	CDL	C56-C57-C58-C59
19	P	303	PGV	C21-C22-C23-C24
24	C	307	CDL	C17-C18-C19-C20
23	T	101	PEK	C23-C24-C25-C26
18	Q	201	TGL	CB5-CB6-CB7-CB8
24	C	307	CDL	C39-C40-C41-C42
25	P	309	DMU	C28-C31-C34-C37
18	O	302	TGL	CC5-CC6-CC7-CC8
23	G	102	PEK	C10-C11-C12-C13
19	P	303	PGV	C12-C13-C14-C15
24	T	104	CDL	C55-C56-C57-C58
26	E	201	PSC	C01-C02-C03-O11
26	O	304	PSC	C01-C02-C03-O11
24	P	305	CDL	CA5-C11-C12-C13
23	T	103	PEK	C31-C32-C33-C34
24	C	307	CDL	C12-C13-C14-C15
19	N	606	PGV	C02-C03-O11-P
24	T	104	CDL	C61-C62-C63-C64
18	Q	201	TGL	C29-C30-C31-C32
23	T	103	PEK	O01-C02-C03-O11
24	C	307	CDL	OA5-CA3-CA4-OA6
19	C	305	PGV	C30-C31-C32-C33
23	T	102	PEK	C31-C32-C33-C34
14	A	601	HEA	C4A-C3A-CMA-OMA
14	A	602	HEA	C4A-C3A-CMA-OMA
14	N	601	HEA	C4A-C3A-CMA-OMA
14	N	602	HEA	C4A-C3A-CMA-OMA
18	L	101	TGL	OG2-CG2-CG3-OG3
24	P	305	CDL	OA6-CA4-CA6-OA8
19	M	101	PGV	O12-C04-C05-C06
18	L	101	TGL	CG1-CG2-CG3-OG3
18	Y	101	TGL	CG1-CG2-CG3-OG3
19	P	304	PGV	O03-C01-C02-C03
25	C	312	DMU	O6-C11-C9-O1
24	T	104	CDL	C54-C55-C56-C57
19	C	305	PGV	C9-C10-C11-C12
19	P	303	PGV	C11-C12-C13-C14
24	T	104	CDL	C31-C32-C33-C34
20	B	303	EDO	O1-C1-C2-O2
18	D	201	TGL	CB2-CB3-CB4-CB5
19	M	101	PGV	C03-O11-P-O12
19	M	101	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
19	P	304	PGV	C03-O11-P-O13
19	P	304	PGV	C04-O12-P-O13
23	C	304	PEK	C03-O11-P-O14
23	G	102	PEK	C04-O12-P-O14
23	T	101	PEK	C03-O11-P-O14
23	T	102	PEK	O12-C04-C05-N
23	T	103	PEK	C04-O12-P-O14
24	C	307	CDL	CB2-OB2-PB2-OB3
24	G	101	CDL	CB3-OB5-PB2-OB3
24	P	305	CDL	CA3-OA5-PA1-OA3
24	P	305	CDL	CB2-OB2-PB2-OB3
24	T	104	CDL	CA2-OA2-PA1-OA4
26	E	201	PSC	C04-O12-P-O11
19	M	101	PGV	C2-C3-C4-C5
19	N	607	PGV	C30-C31-C32-C33
23	C	303	PEK	C23-C24-C25-C26
19	M	101	PGV	C05-C04-O12-P
24	G	101	CDL	C1-CA2-OA2-PA1
24	G	101	CDL	C1-CB2-OB2-PB2
24	P	305	CDL	C1-CA2-OA2-PA1
23	T	101	PEK	C10-C11-C12-C13
24	G	101	CDL	C33-C34-C35-C36
19	N	606	PGV	C15-C16-C17-C18
25	C	313	DMU	O6-C11-C9-O1
18	L	101	TGL	C14-C29-C30-C31
19	A	607	PGV	C14-C15-C16-C17
23	T	101	PEK	C29-C30-C31-C32
19	N	606	PGV	C31-C32-C33-C34
26	O	304	PSC	C15-C16-C17-C18
18	D	201	TGL	CB7-CB8-CB9-C10
19	C	306	PGV	C01-C02-C03-O11
24	G	101	CDL	OA5-CA3-CA4-CA6
24	G	101	CDL	OB5-CB3-CB4-CB6
24	T	104	CDL	C59-C60-C61-C62
19	M	101	PGV	C14-C15-C16-C17
24	C	307	CDL	C22-C23-C24-C25
24	C	307	CDL	C57-C58-C59-C60
18	O	302	TGL	CB3-CB4-CB5-CB6
23	T	102	PEK	C25-C26-C27-C28
25	M	102	DMU	C34-C37-C40-C43
19	P	303	PGV	C28-C29-C30-C31
23	T	101	PEK	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
25	C	312	DMU	C18-C19-C22-C25
18	D	201	TGL	OG2-CB1-CB2-CB3
19	C	305	PGV	C11-C12-C13-C14
20	N	613	EDO	O1-C1-C2-O2
24	C	307	CDL	C61-C62-C63-C64
24	P	305	CDL	C79-C80-C81-C82
23	T	101	PEK	C2-C3-C4-C5
18	Y	101	TGL	C20-C21-C22-C23
19	C	305	PGV	C23-C24-C25-C26
19	C	306	PGV	C14-C15-C16-C17
24	C	307	CDL	C59-C60-C61-C62
24	T	104	CDL	C13-C14-C15-C16
23	T	103	PEK	C27-C28-C29-C30
24	T	104	CDL	C35-C36-C37-C38
18	D	201	TGL	CA2-CA1-OG1-CG1
26	E	201	PSC	C3-C4-C5-C6
18	L	101	TGL	OG1-CG1-CG2-OG2
19	N	607	PGV	C20-C21-C22-C23
25	Z	101	DMU	C22-C25-C28-C31
25	C	312	DMU	O16-C18-C19-C22
18	D	201	TGL	C12-C13-C14-C29
24	T	104	CDL	CB4-CB3-OB5-PB2
26	E	201	PSC	C6-C7-C8-C9
19	M	101	PGV	O01-C1-C2-C3
18	Q	201	TGL	C24-C25-C26-C27
22	P	306	CHD	C16-C17-C20-C22
24	C	307	CDL	C16-C17-C18-C19
23	G	102	PEK	C7-C8-C9-C10
26	E	201	PSC	C01-C02-O01-C1
26	E	201	PSC	C03-C02-O01-C1
20	A	616	EDO	O1-C1-C2-O2
20	F	104	EDO	O1-C1-C2-O2
22	C	308	CHD	C22-C23-C24-O26
22	J	101	CHD	C22-C23-C24-O25
22	C	308	CHD	C22-C23-C24-O25
19	N	607	PGV	C24-C25-C26-C27
19	M	101	PGV	O12-C04-C05-O05
19	P	303	PGV	C05-C04-O12-P
24	P	305	CDL	CA4-CA3-OA5-PA1
19	M	101	PGV	C13-C14-C15-C16
14	A	602	HEA	CAA-CBA-CGA-O1A
24	C	307	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
19	N	606	PGV	C30-C31-C32-C33
22	P	306	CHD	C22-C23-C24-O25
22	W	101	CHD	C22-C23-C24-O25
23	T	103	PEK	C3-C4-C5-C6
23	T	103	PEK	C14-C15-C16-C17
14	N	602	HEA	CAA-CBA-CGA-O1A
22	P	306	CHD	C22-C23-C24-O26
23	G	102	PEK	C5-C6-C7-C8
23	G	102	PEK	C6-C7-C8-C9
23	T	103	PEK	C12-C13-C14-C15
18	A	606	TGL	CC5-CC6-CC7-CC8
19	N	606	PGV	C19-C20-C21-C22
14	N	601	HEA	CAD-CBD-CGD-O1D
14	A	602	HEA	C26-C15-C16-C17
14	N	602	HEA	CAD-CBD-CGD-O2D
26	O	304	PSC	C02-C01-O03-C19
24	P	305	CDL	C72-C73-C74-C75
18	L	101	TGL	C33-C34-C35-C36
14	N	601	HEA	CAD-CBD-CGD-O2D
22	W	101	CHD	C22-C23-C24-O26
19	N	606	PGV	C20-C21-C22-C23
14	A	602	HEA	CAA-CBA-CGA-O2A
26	O	304	PSC	C02-C03-O11-P
22	C	301	CHD	C22-C23-C24-O26
22	P	301	CHD	C22-C23-C24-O26
19	P	304	PGV	C3-C4-C5-C6
23	T	103	PEK	C23-C24-C25-C26
22	O	301	CHD	C22-C23-C24-O26
18	D	201	TGL	OA1-CA1-OG1-CG1
19	P	303	PGV	C19-C20-C21-C22
18	Y	101	TGL	CA3-CA4-CA5-CA6
14	N	602	HEA	CAA-CBA-CGA-O2A
22	B	302	CHD	C22-C23-C24-O26
14	N	602	HEA	C26-C15-C16-C17
18	D	201	TGL	CA5-CA6-CA7-CA8
20	N	609	EDO	O1-C1-C2-O2
20	N	615	EDO	O1-C1-C2-O2
19	A	607	PGV	O03-C19-C20-C21
22	J	101	CHD	C22-C23-C24-O26
24	G	101	CDL	CA4-CA3-OA5-PA1
24	C	307	CDL	C58-C59-C60-C61
24	P	305	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
23	T	103	PEK	C32-C33-C34-C35
24	P	305	CDL	C37-C38-C39-C40
26	E	201	PSC	C4-C5-C6-C7
23	C	304	PEK	C10-C11-C12-C13
14	N	602	HEA	CAD-CBD-CGD-O1D
26	E	201	PSC	C12-C13-C14-C15
14	A	602	HEA	CAD-CBD-CGD-O2D
19	A	607	PGV	C11-C10-C9-C8
18	Q	201	TGL	C11-C10-CB9-CB8
23	C	304	PEK	C17-C18-C19-C20
22	O	301	CHD	C22-C23-C24-O25
19	C	306	PGV	C02-C03-O11-P
24	C	307	CDL	C33-C34-C35-C36
22	P	306	CHD	C16-C17-C20-C21
14	A	602	HEA	CAD-CBD-CGD-O1D
18	O	302	TGL	C15-C16-C17-C18
19	N	606	PGV	C9-C10-C11-C12
22	B	302	CHD	C22-C23-C24-O25
25	M	102	DMU	O6-C11-C9-O1
24	P	305	CDL	C36-C37-C38-C39
24	P	305	CDL	OB6-CB4-CB6-OB8
26	O	304	PSC	O03-C01-C02-O01
19	C	306	PGV	O04-C19-O03-C01
23	T	101	PEK	C01-C02-C03-O11
24	G	101	CDL	C35-C36-C37-C38
18	A	606	TGL	CB3-CB4-CB5-CB6
18	L	101	TGL	CC1-CC2-CC3-CC4
19	A	607	PGV	C15-C16-C17-C18
23	G	102	PEK	C3-C4-C5-C6
23	T	102	PEK	C14-C15-C16-C17
26	O	304	PSC	C12-C13-C14-C15
19	C	306	PGV	C24-C25-C26-C27
24	T	104	CDL	C52-C51-CB5-OB6
14	A	601	HEA	CAD-CBD-CGD-O1D
19	N	607	PGV	C11-C12-C13-C14
23	T	101	PEK	C14-C15-C16-C17
19	A	607	PGV	C13-C14-C15-C16
19	C	306	PGV	C20-C19-O03-C01
24	C	307	CDL	C12-C11-CA5-OA6
23	C	304	PEK	O01-C1-C2-C3
23	T	101	PEK	O01-C1-C2-C3
24	P	305	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
22	P	301	CHD	C22-C23-C24-O25
19	P	303	PGV	C29-C30-C31-C32
18	D	201	TGL	OG1-CA1-CA2-CA3
18	D	201	TGL	OG3-CC1-CC2-CC3
23	C	304	PEK	C15-C16-C17-C18
25	P	309	DMU	C19-C18-O16-C6
22	C	301	CHD	C22-C23-C24-O25
18	L	101	TGL	OG1-CG1-CG2-CG3
14	A	601	HEA	C26-C15-C16-C17
18	L	101	TGL	OG2-CB1-CB2-CB3
18	Y	101	TGL	OG1-CA1-CA2-CA3
18	L	101	TGL	C23-C24-C25-C26
18	L	101	TGL	C16-C17-C18-C19
18	Q	201	TGL	C15-C16-C17-C18
18	O	302	TGL	OG3-CC1-CC2-CC3
23	T	102	PEK	O01-C1-C2-C3
24	T	104	CDL	C32-C31-CA7-OA8
26	E	201	PSC	O03-C19-C20-C21
26	O	304	PSC	C13-C14-C15-C16
20	N	608	EDO	O1-C1-C2-O2
24	G	101	CDL	C74-C75-C76-C77
18	L	101	TGL	CA9-C20-C21-C22
25	P	308	DMU	O5-C4-C57-O61
18	Q	201	TGL	C20-C21-C22-C23
23	C	303	PEK	C21-C22-C23-C24
18	D	201	TGL	CG1-CG2-OG2-CB1
18	D	201	TGL	CG3-CG2-OG2-CB1
18	Q	201	TGL	C18-C19-C33-C34
18	O	302	TGL	C11-C12-C13-C14
19	A	607	PGV	C26-C27-C28-C29
18	L	101	TGL	CA7-CA8-CA9-C20
23	T	101	PEK	O01-C02-C03-O11
14	A	601	HEA	CAD-CBD-CGD-O2D
24	G	101	CDL	C80-C81-C82-C83
18	A	606	TGL	OG1-CA1-CA2-CA3
23	C	304	PEK	O02-C1-C2-C3
23	C	303	PEK	C30-C31-C32-C33
24	C	307	CDL	C12-C11-CA5-OA7
18	D	201	TGL	OC1-CC1-CC2-CC3
18	Y	101	TGL	OA1-CA1-CA2-CA3
24	T	104	CDL	C32-C31-CA7-OA9
24	T	104	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
25	P	309	DMU	C22-C25-C28-C31
23	C	303	PEK	C24-C25-C26-C27
18	Y	101	TGL	C21-C22-C23-C24
23	G	102	PEK	C02-C03-O11-P
14	A	601	HEA	C14-C15-C16-C17
23	T	101	PEK	O02-C1-C2-C3
26	E	201	PSC	O04-C19-C20-C21
18	L	101	TGL	OG1-CA1-CA2-CA3
23	T	101	PEK	O03-C21-C22-C23
26	E	201	PSC	C19-C20-C21-C22
22	P	306	CHD	C13-C17-C20-C21
23	T	102	PEK	O02-C1-C2-C3
18	L	101	TGL	C16-C15-CC9-CC8
18	Y	101	TGL	OG2-CB1-CB2-CB3
19	N	607	PGV	O03-C19-C20-C21
24	G	101	CDL	C52-C51-CB5-OB6
24	P	305	CDL	C52-C51-CB5-OB6
18	Y	101	TGL	OB1-CB1-CB2-CB3
23	C	304	PEK	C14-C15-C16-C17
23	T	103	PEK	O01-C1-C2-C3
24	G	101	CDL	C32-C31-CA7-OA8
18	L	101	TGL	OB1-CB1-CB2-CB3
18	O	302	TGL	OC1-CC1-CC2-CC3

There are no ring outliers.

49 monomers are involved in 150 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	P	304	PGV	1	0
22	O	301	CHD	1	0
19	C	305	PGV	4	0
19	N	607	PGV	4	0
22	W	101	CHD	1	0
22	P	306	CHD	1	0
24	G	101	CDL	5	0
20	A	608	EDO	1	0
23	T	102	PEK	3	0
20	D	202	EDO	2	0
20	N	613	EDO	4	0
20	N	614	EDO	1	0
20	E	202	EDO	1	0
20	A	616	EDO	1	0

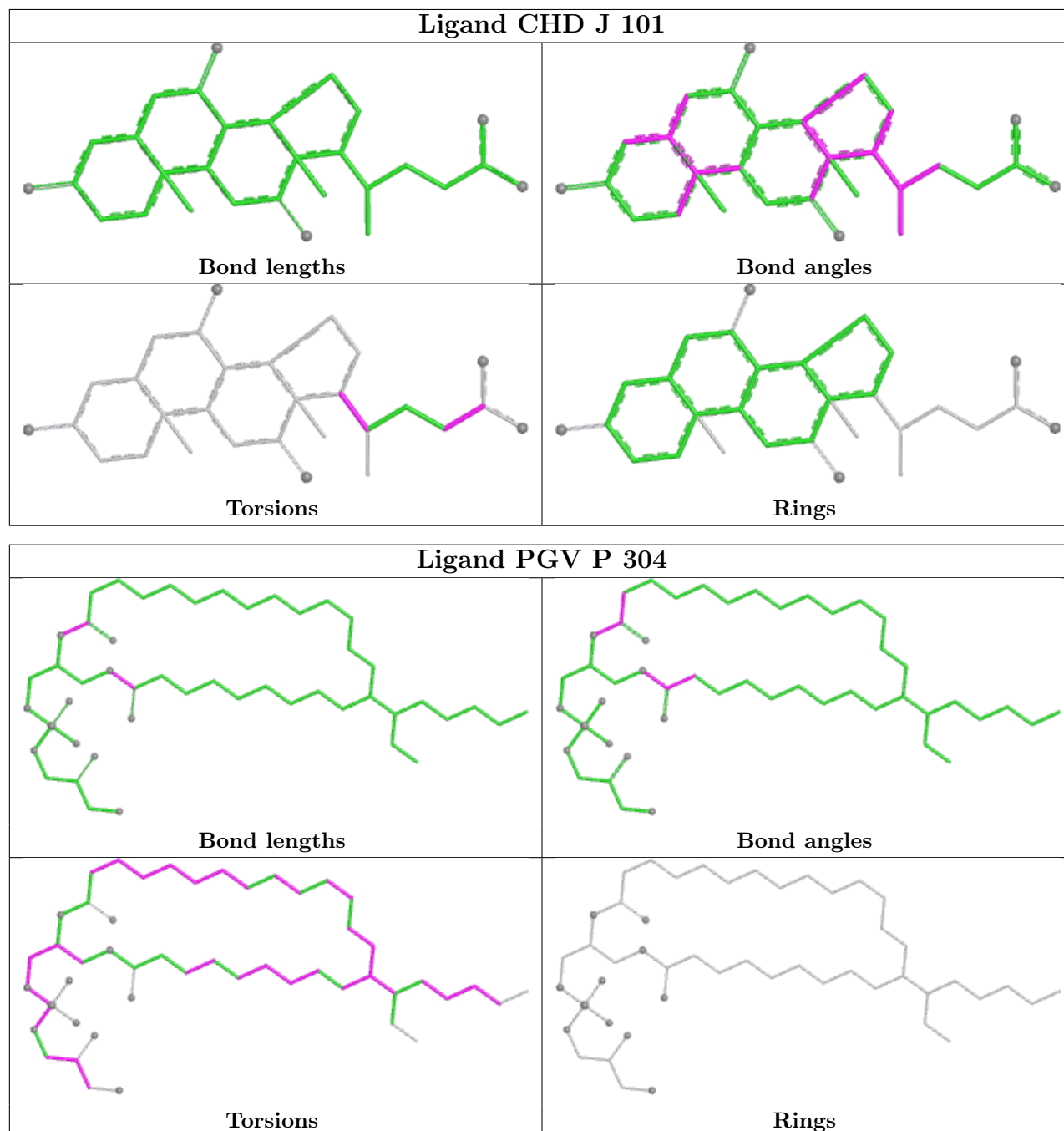
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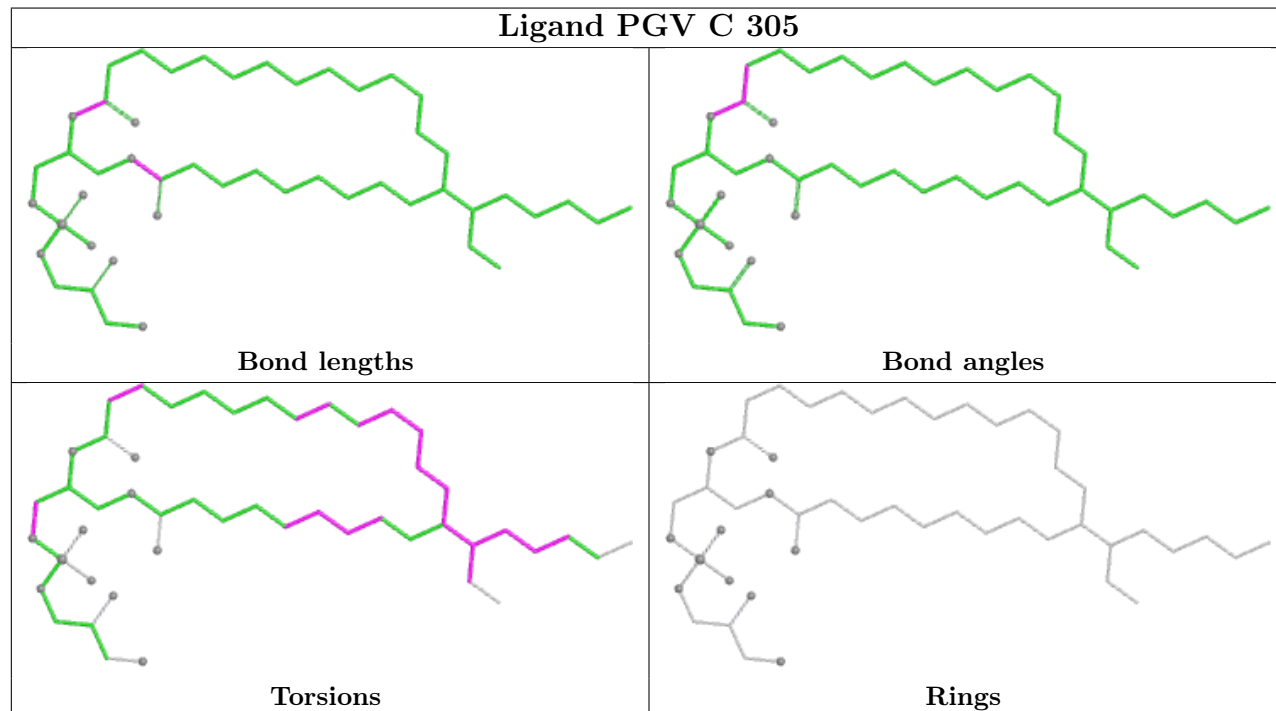
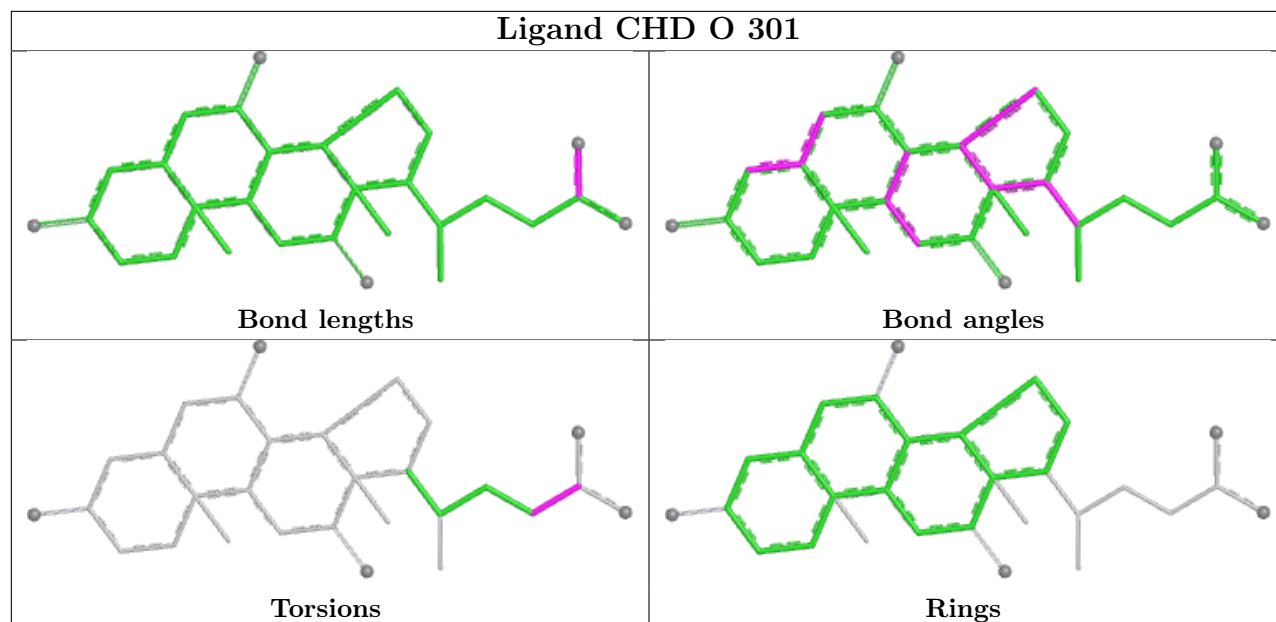
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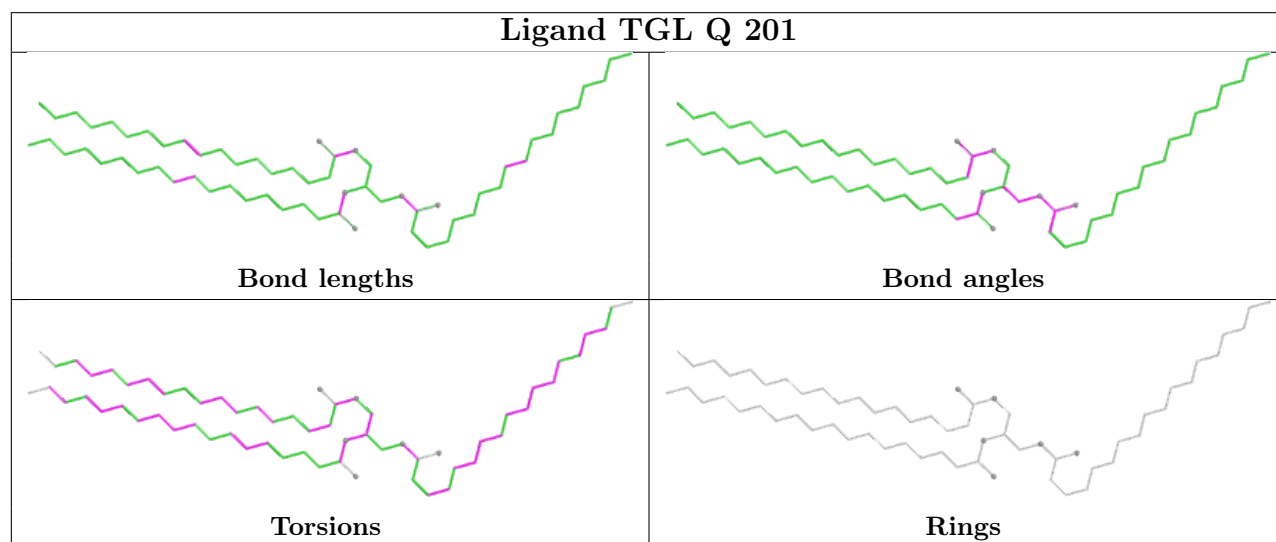
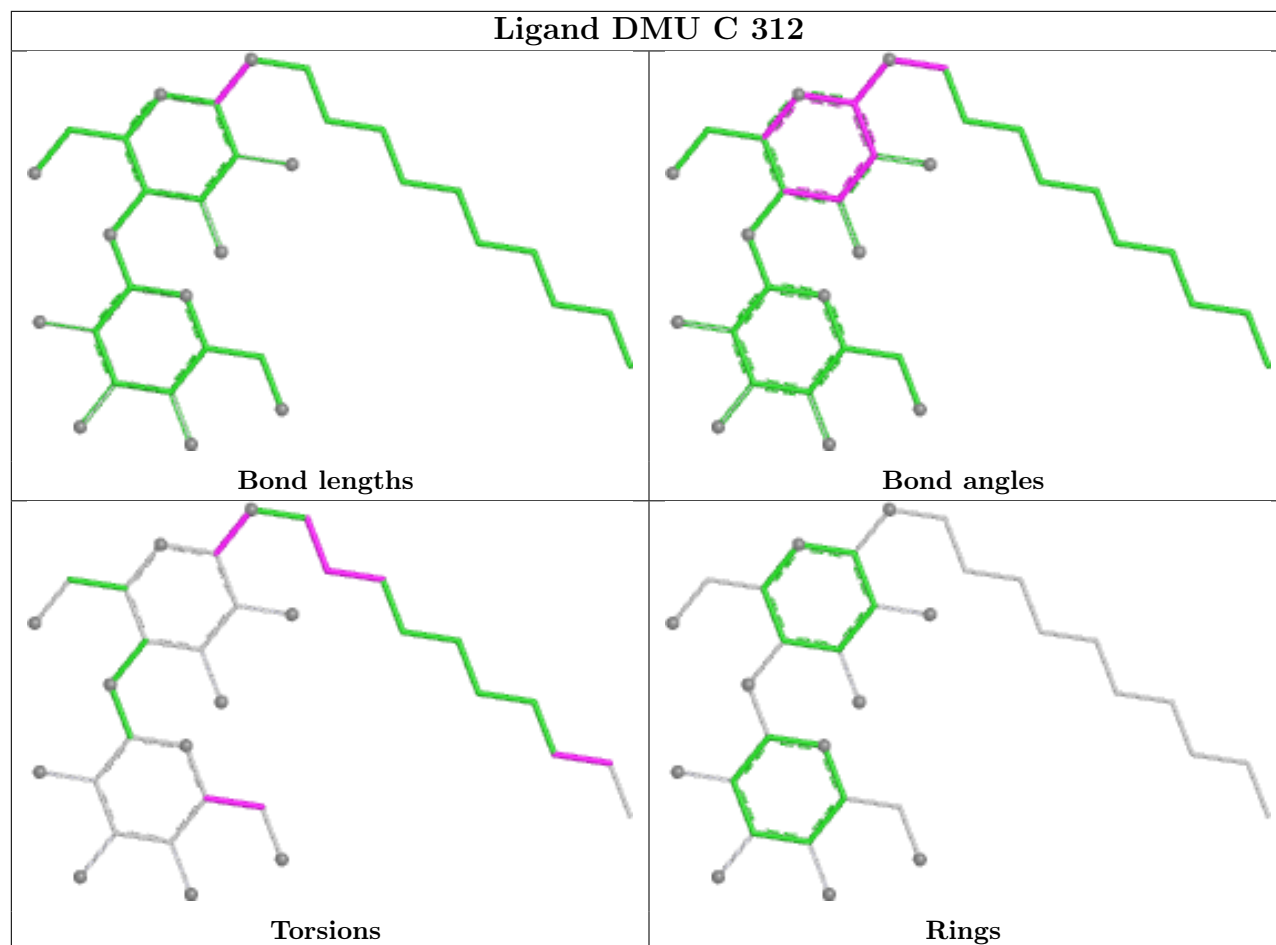
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	S	103	EDO	1	0
22	P	301	CHD	2	0
18	O	302	TGL	2	0
14	A	602	HEA	1	0
19	P	303	PGV	3	0
23	T	101	PEK	2	0
23	T	103	PEK	2	0
24	T	104	CDL	13	0
25	P	309	DMU	8	0
14	N	602	HEA	2	0
19	N	606	PGV	2	0
25	C	313	DMU	12	0
14	N	601	HEA	1	0
18	A	606	TGL	3	0
19	C	306	PGV	1	0
19	M	101	PGV	2	0
20	N	617	EDO	1	0
26	E	201	PSC	10	0
23	C	304	PEK	2	0
22	C	308	CHD	3	0
26	O	304	PSC	6	0
24	P	305	CDL	9	0
24	C	307	CDL	10	0
18	Y	101	TGL	5	0
18	D	201	TGL	4	0
20	N	615	EDO	2	0
23	C	303	PEK	3	0
20	N	608	EDO	1	0
18	L	101	TGL	4	0
25	P	308	DMU	1	0
20	A	611	EDO	2	0
20	N	612	EDO	1	0
19	A	607	PGV	2	0
20	A	615	EDO	1	0
14	A	601	HEA	2	0

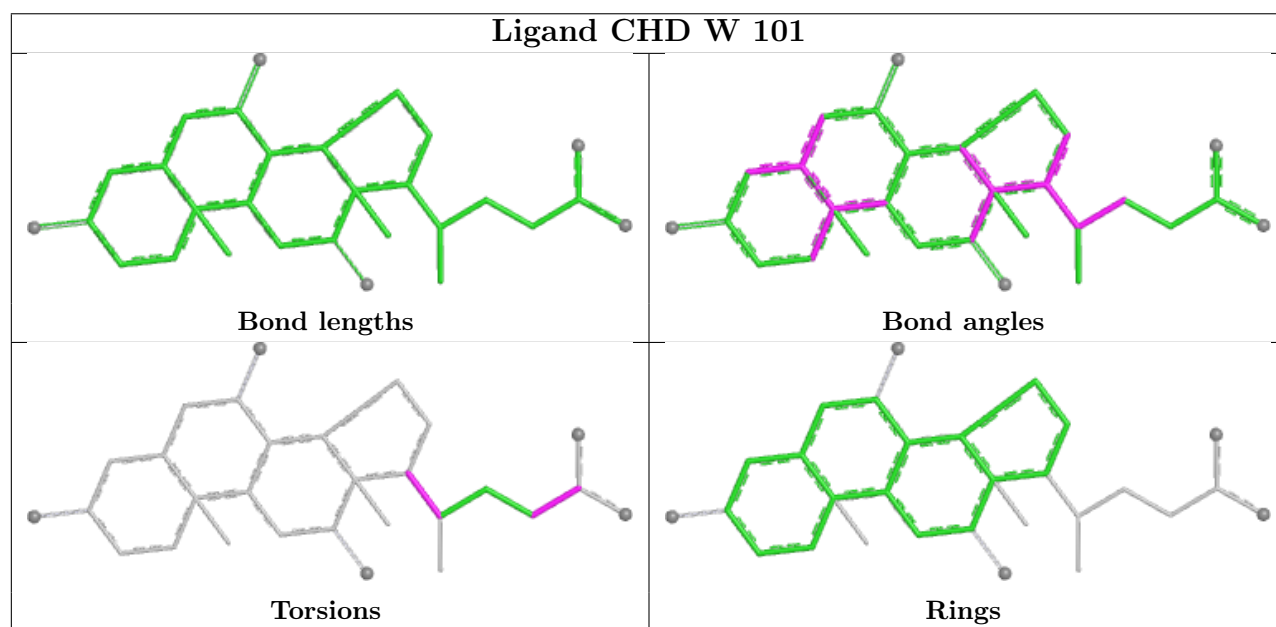
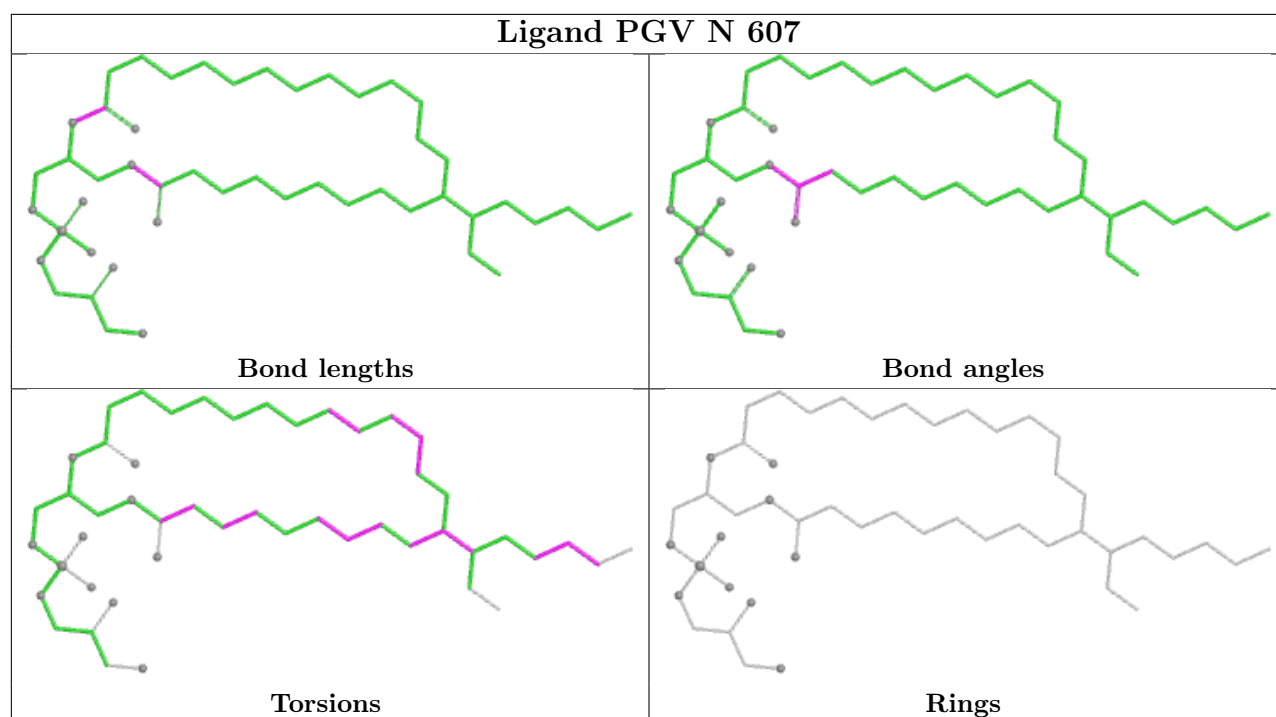
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

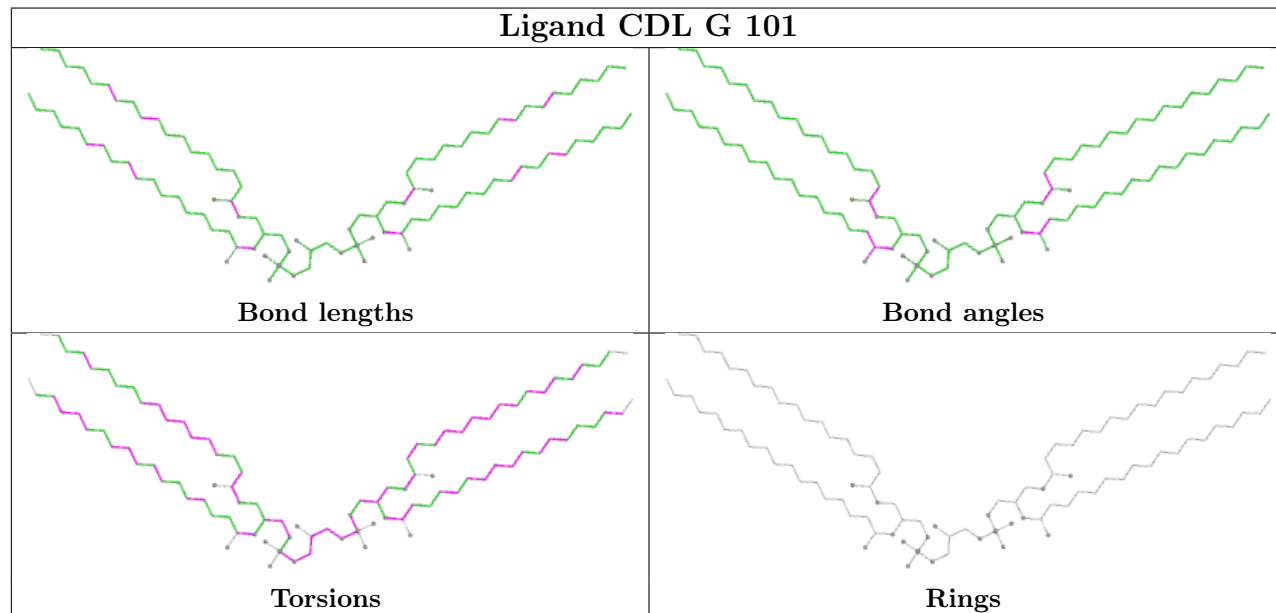
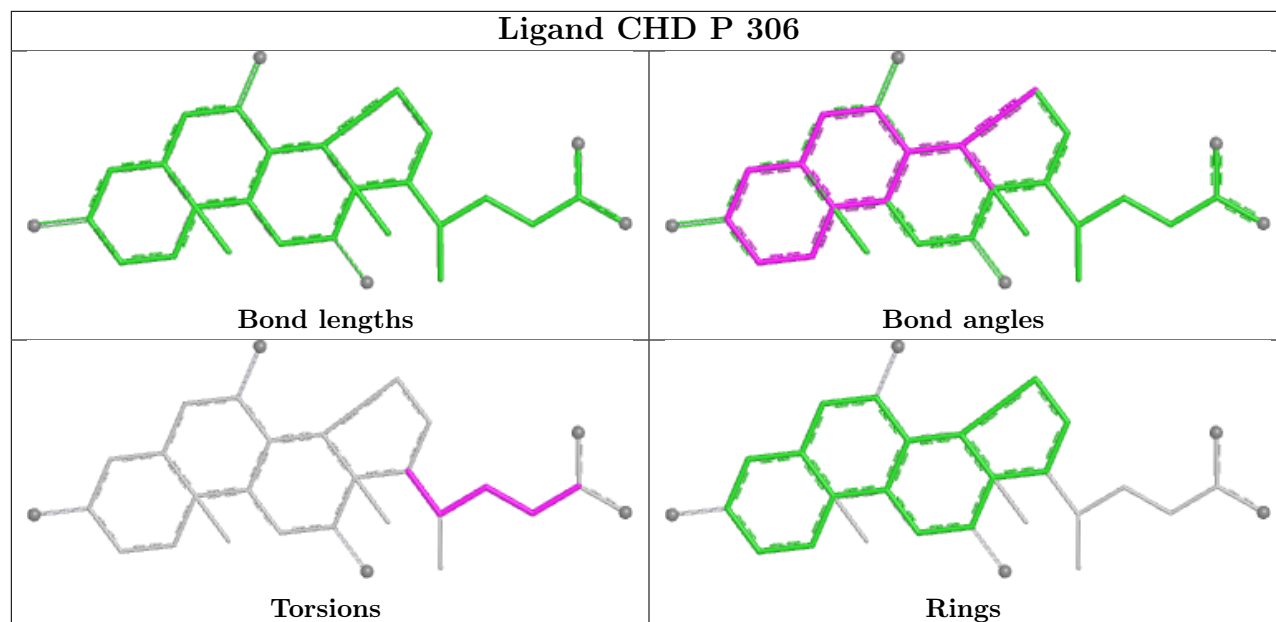
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



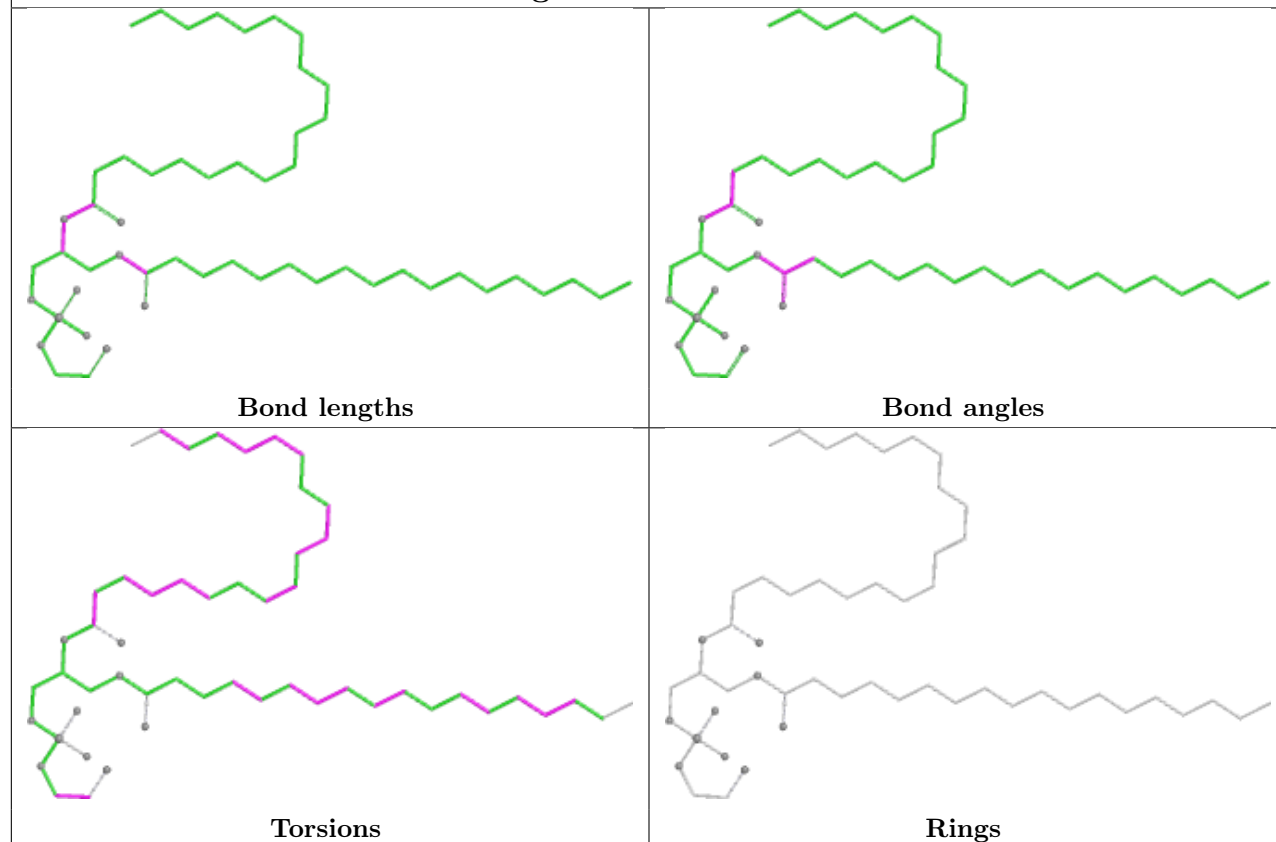




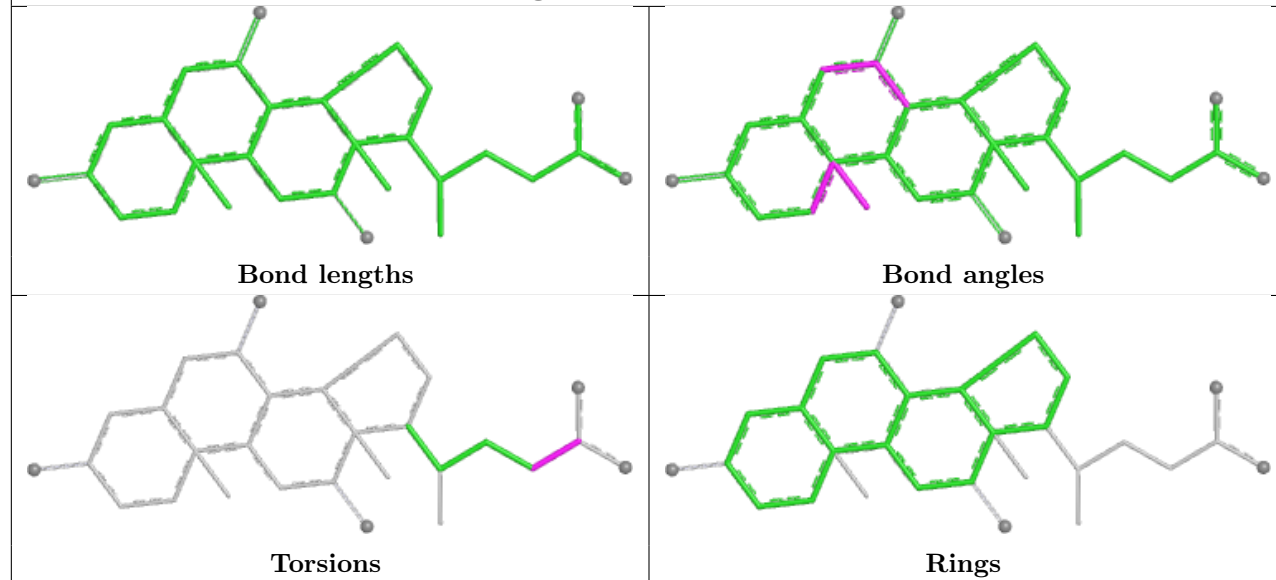


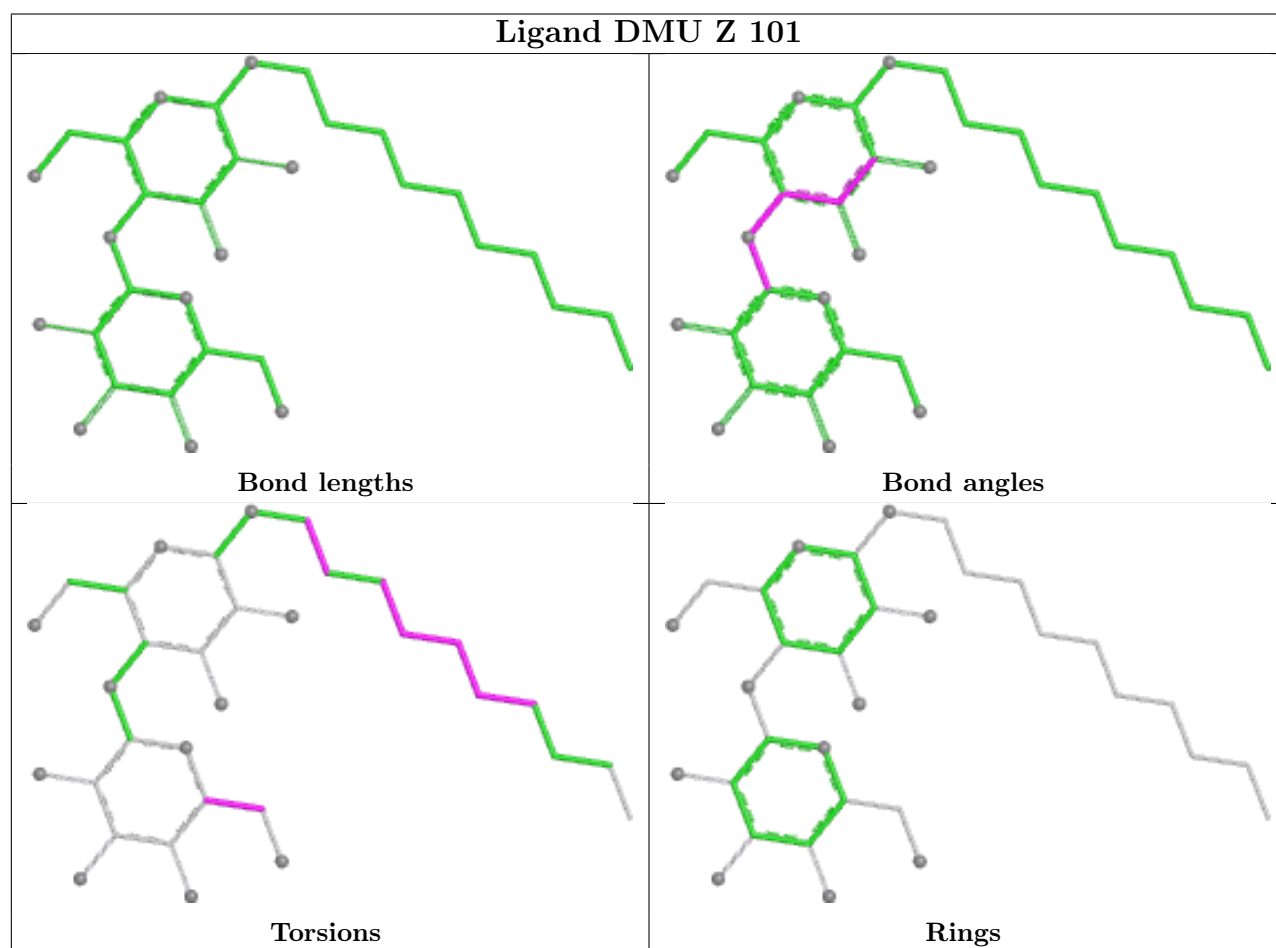
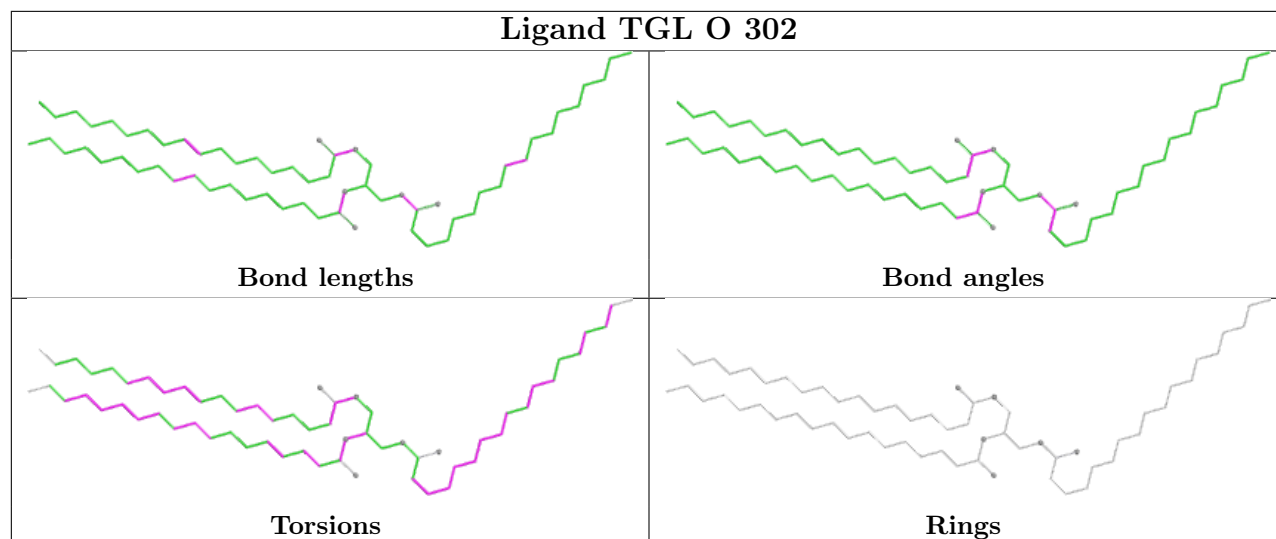


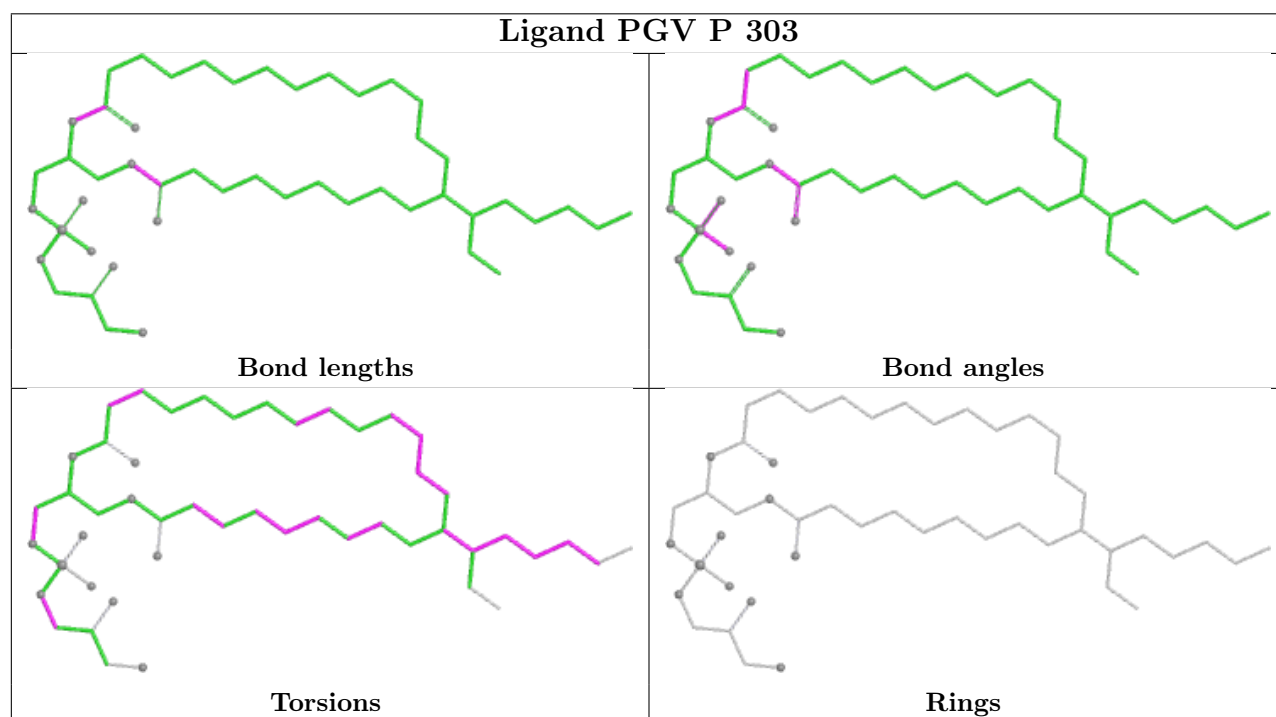
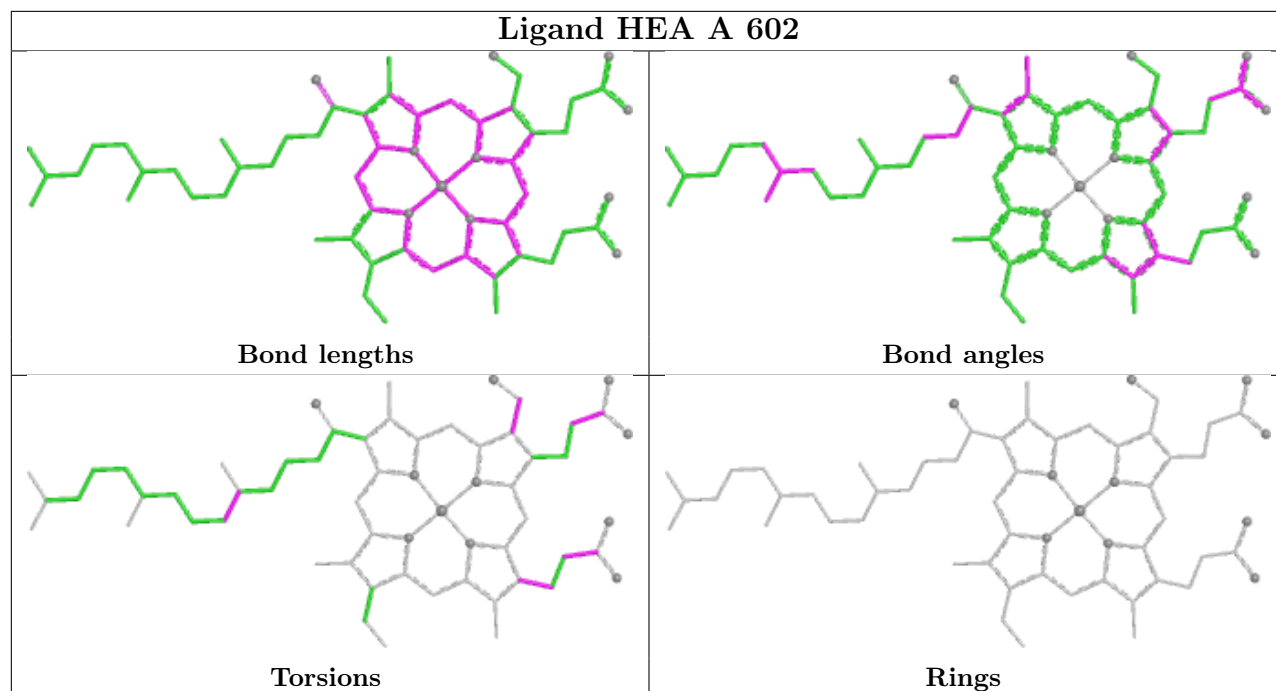
Ligand PEK T 102



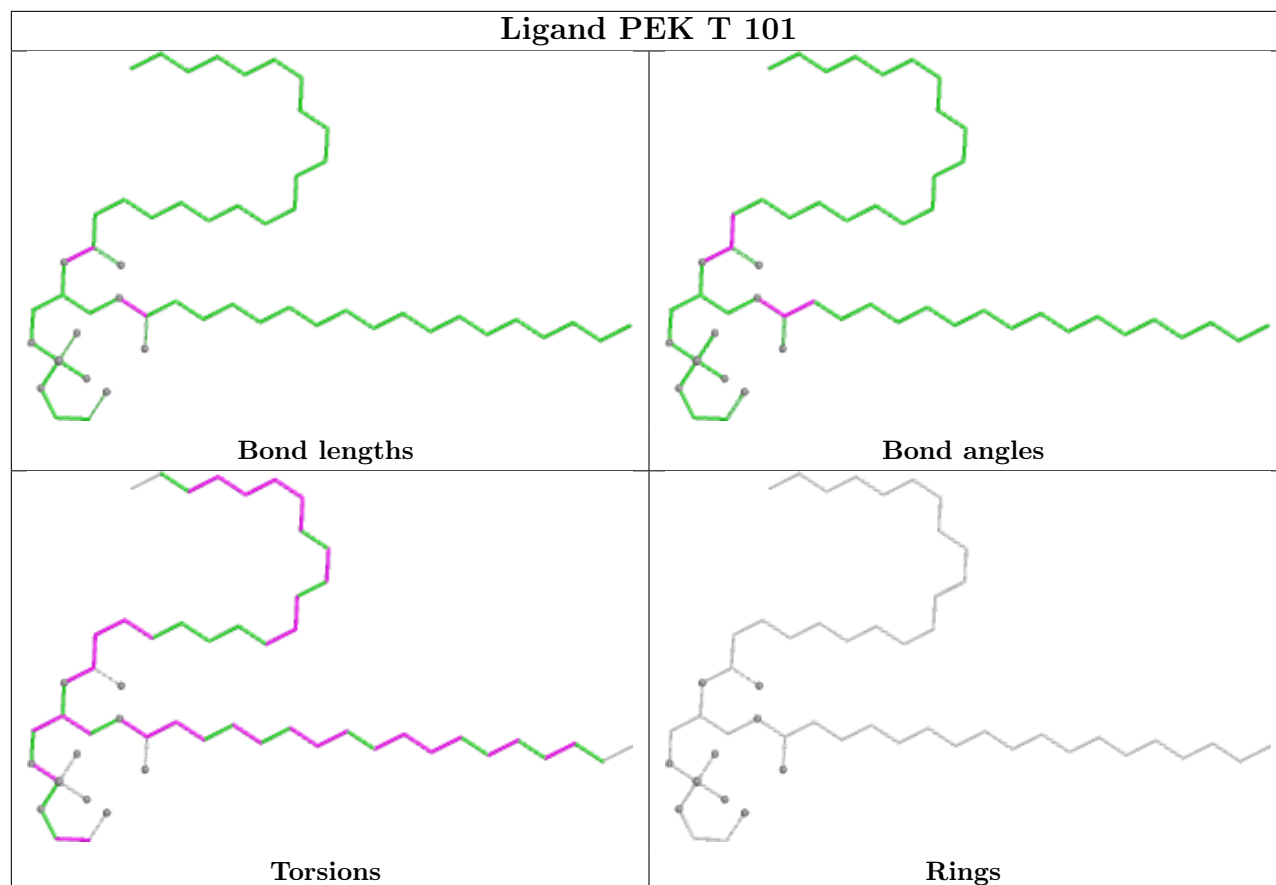
Ligand CHD P 301



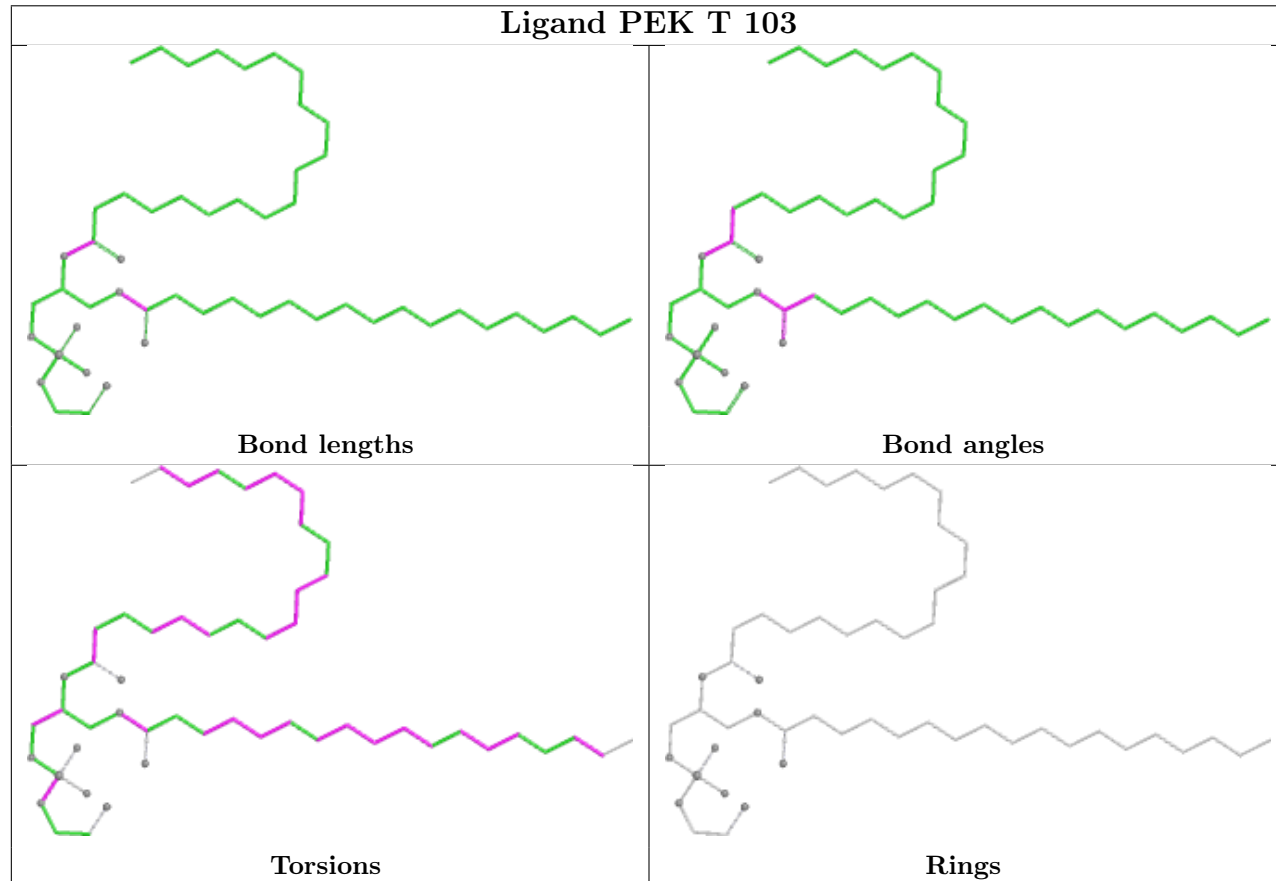


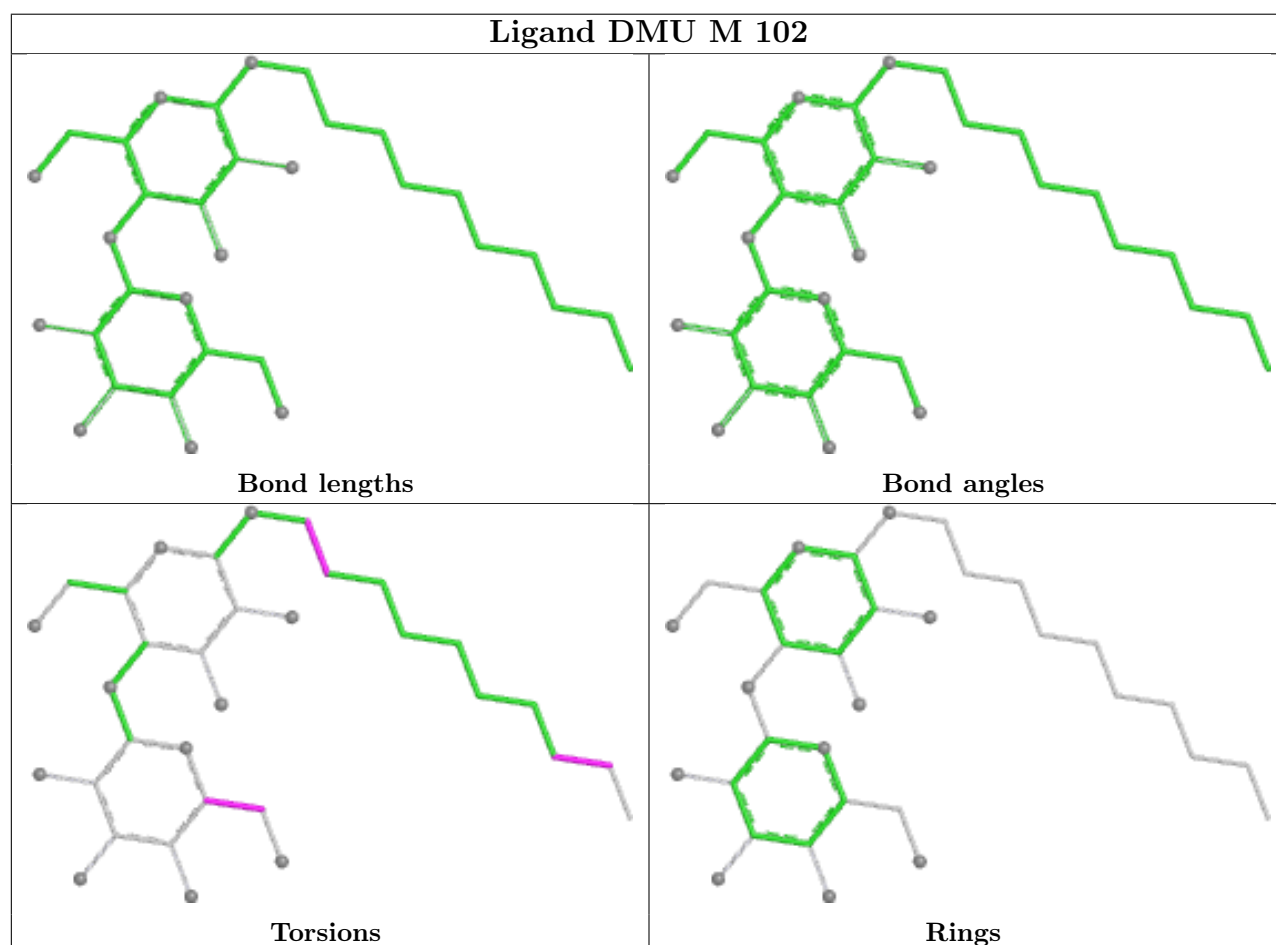
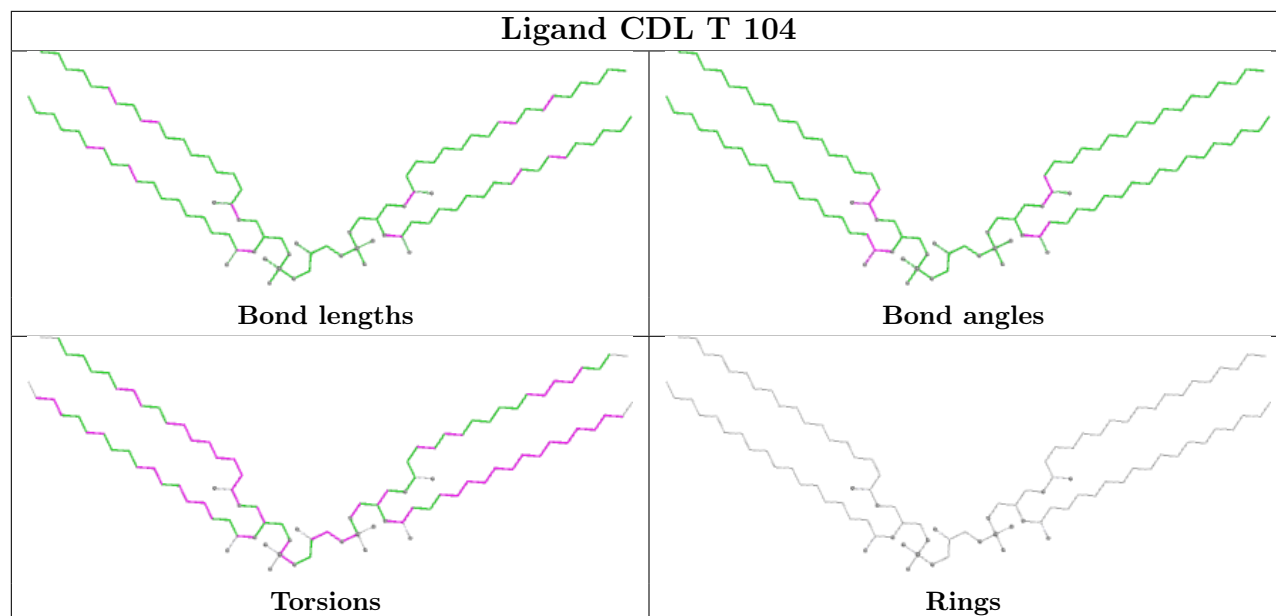


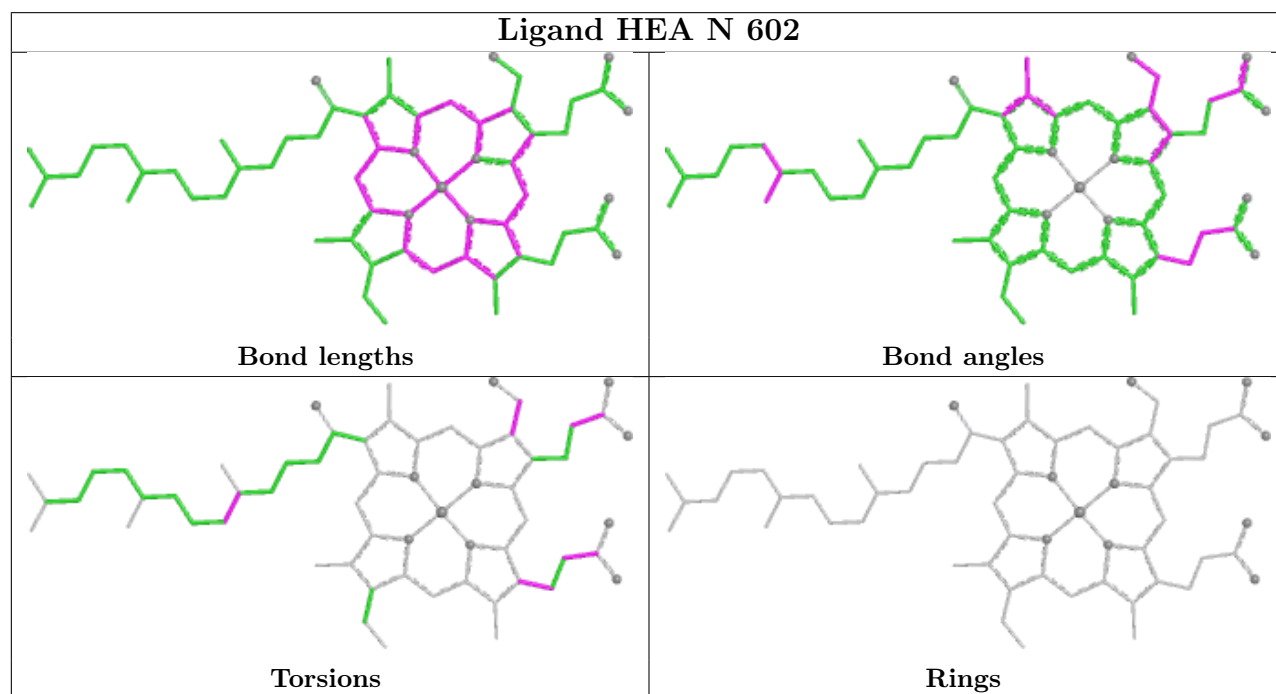
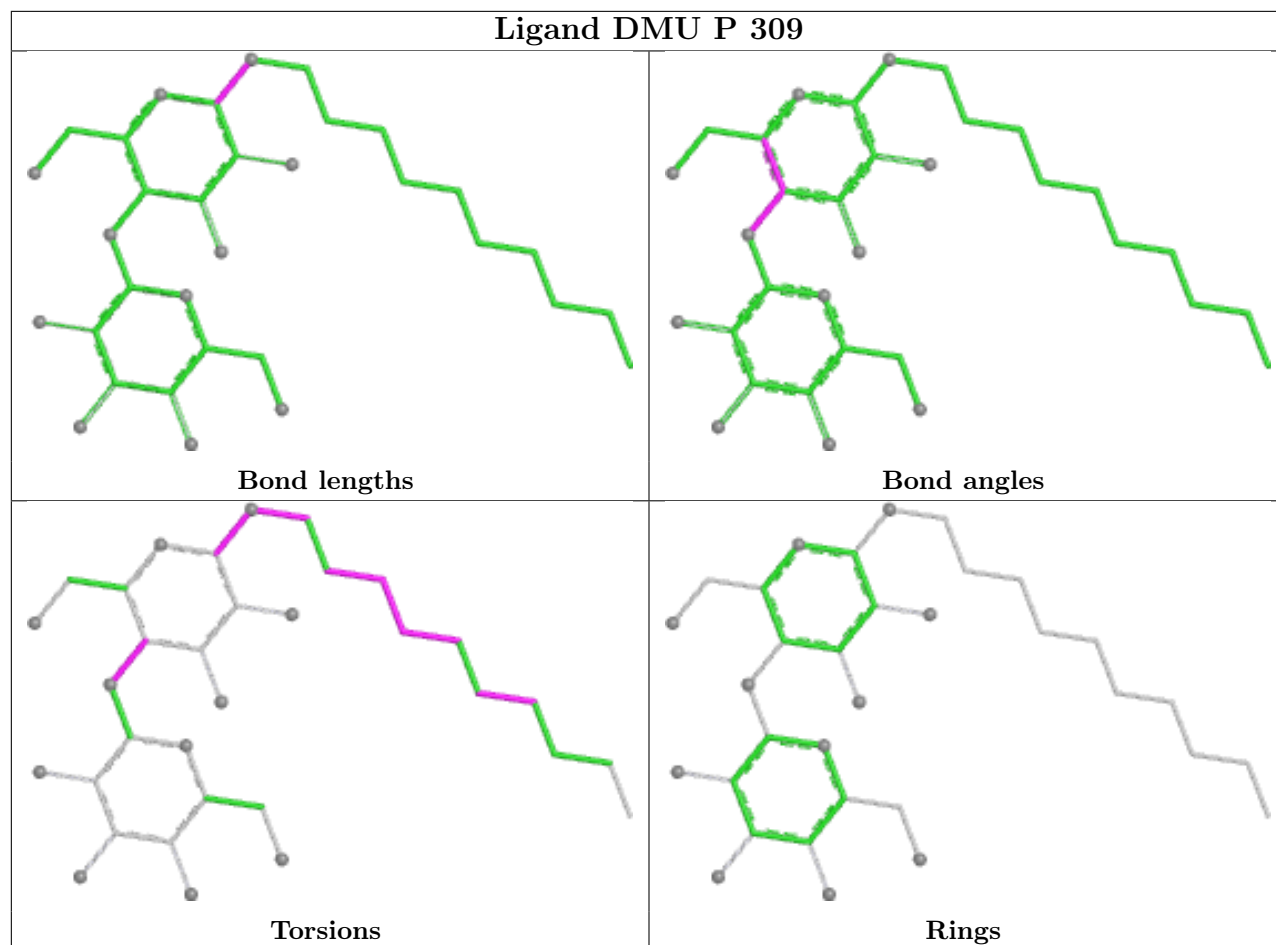
Ligand PEK T 101

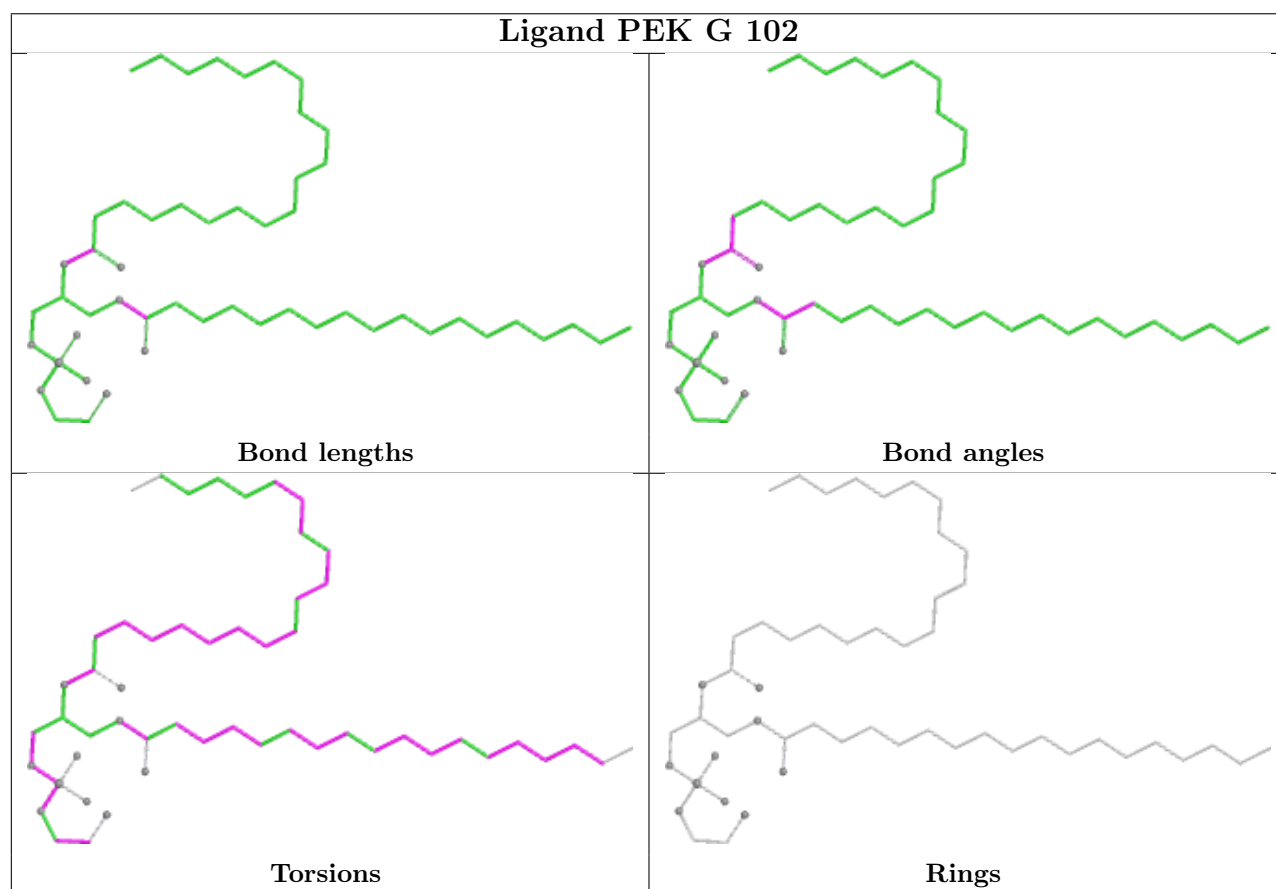
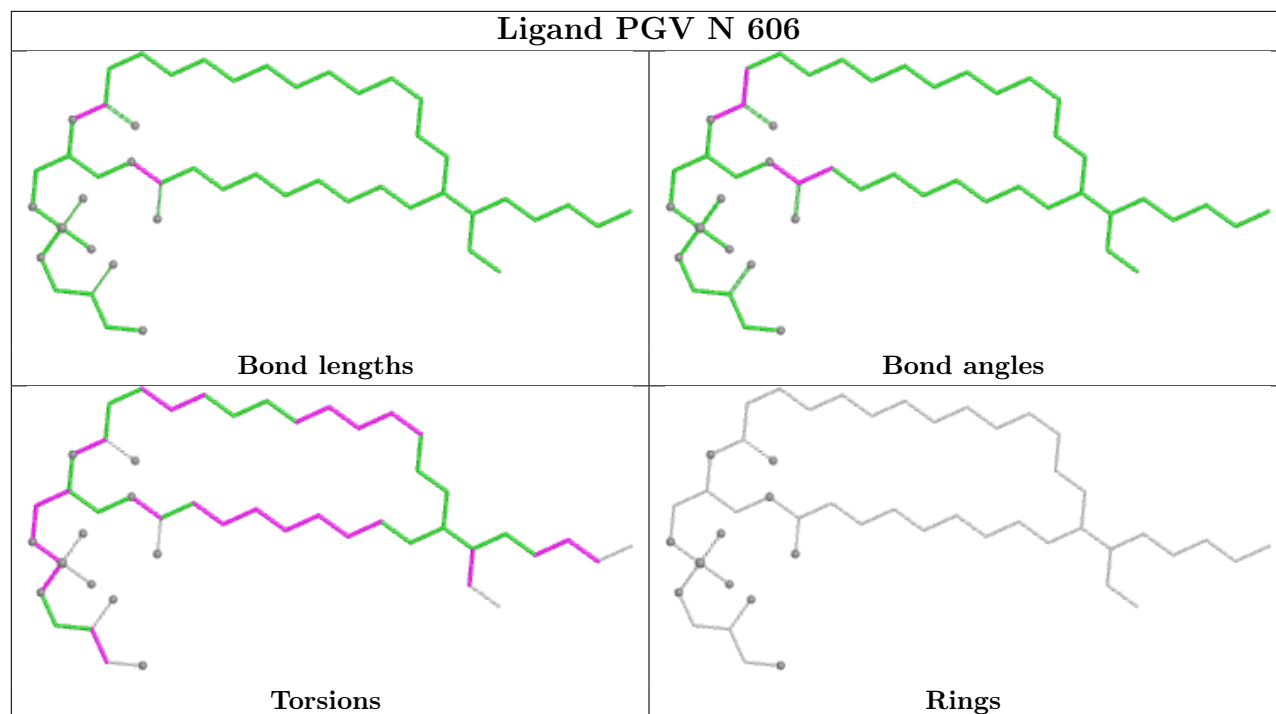


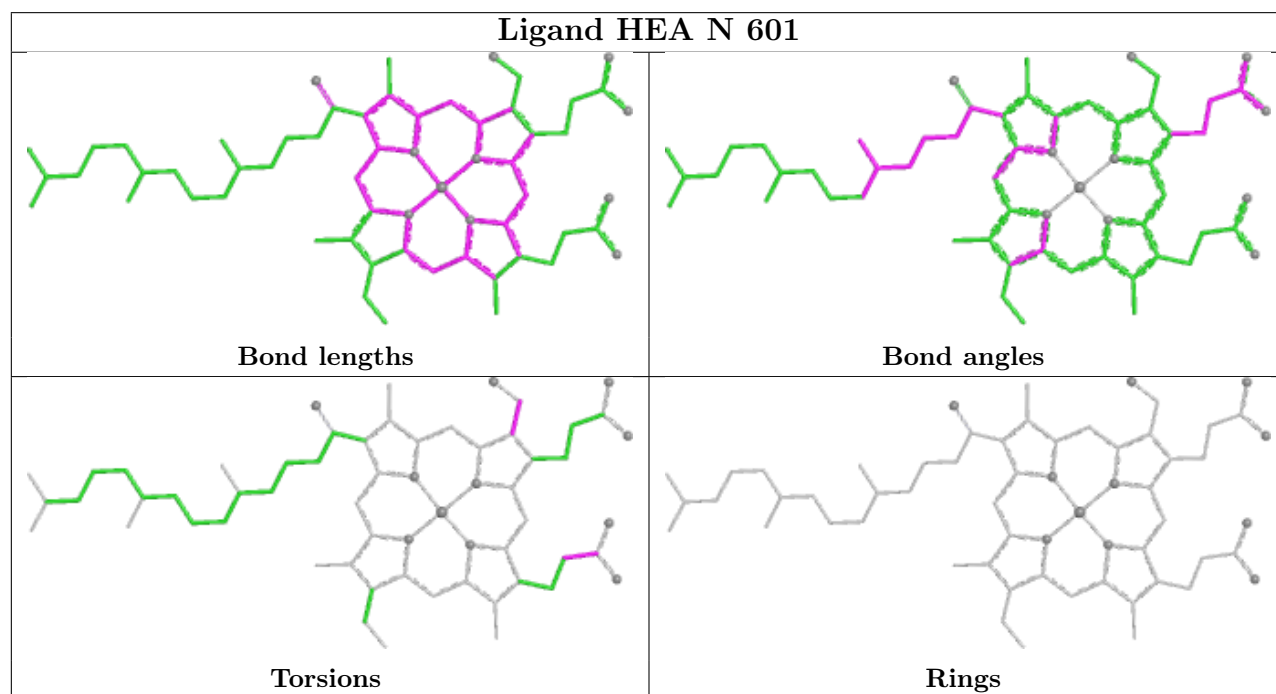
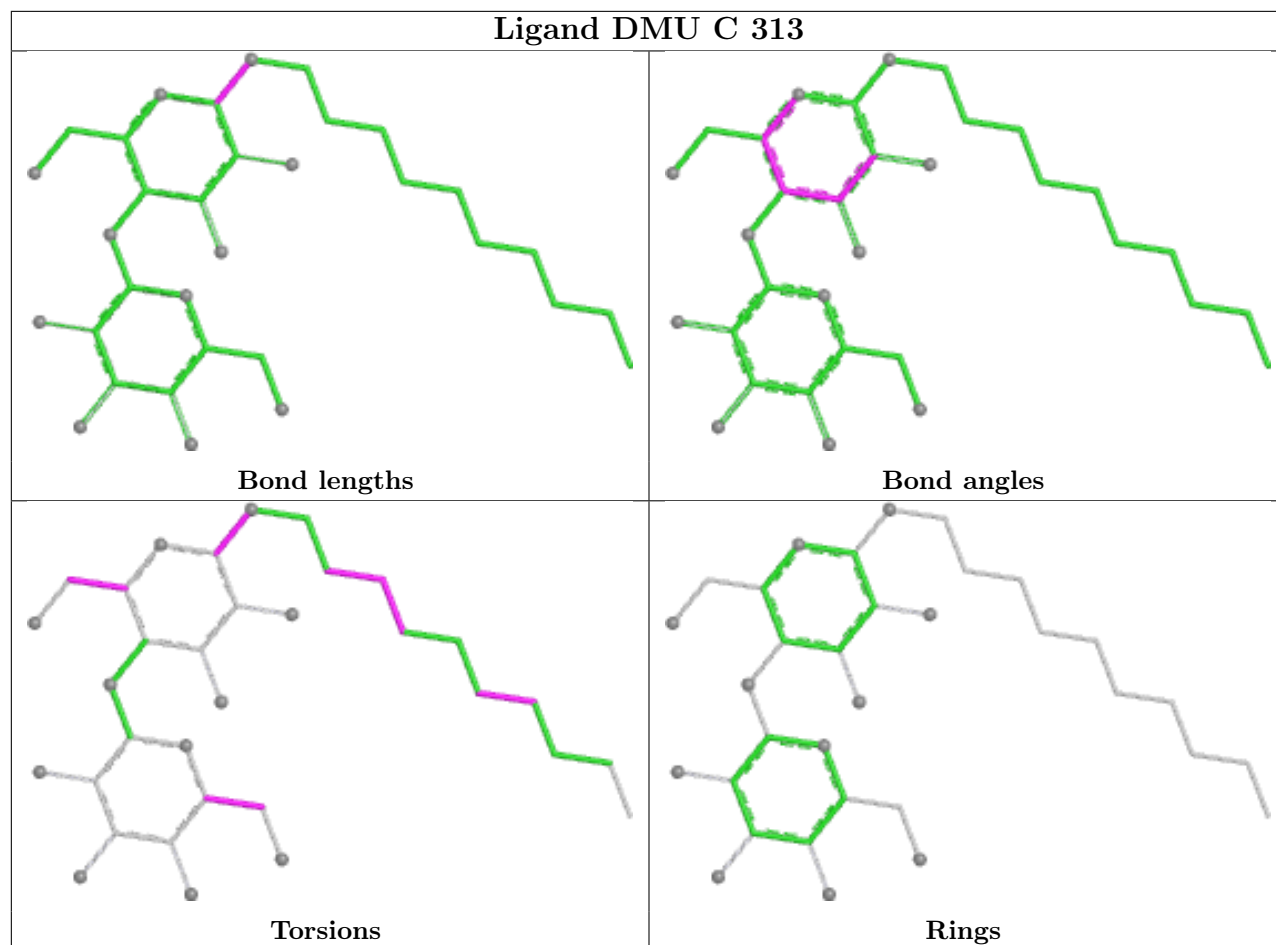
Ligand PEK T 103

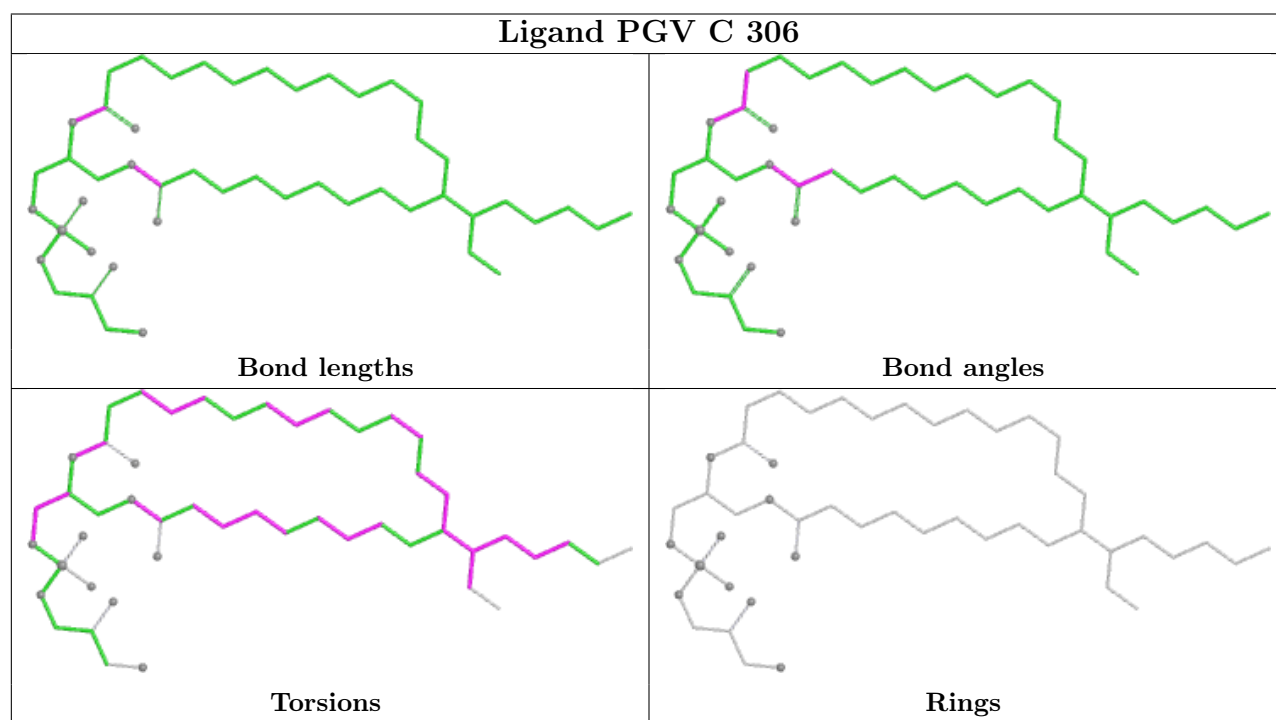
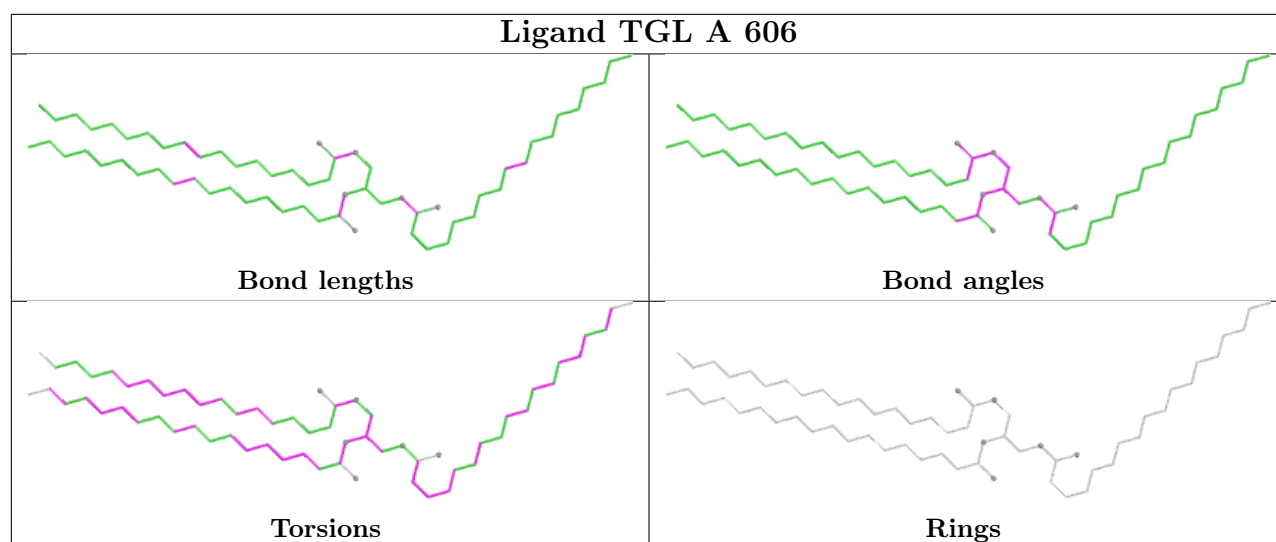


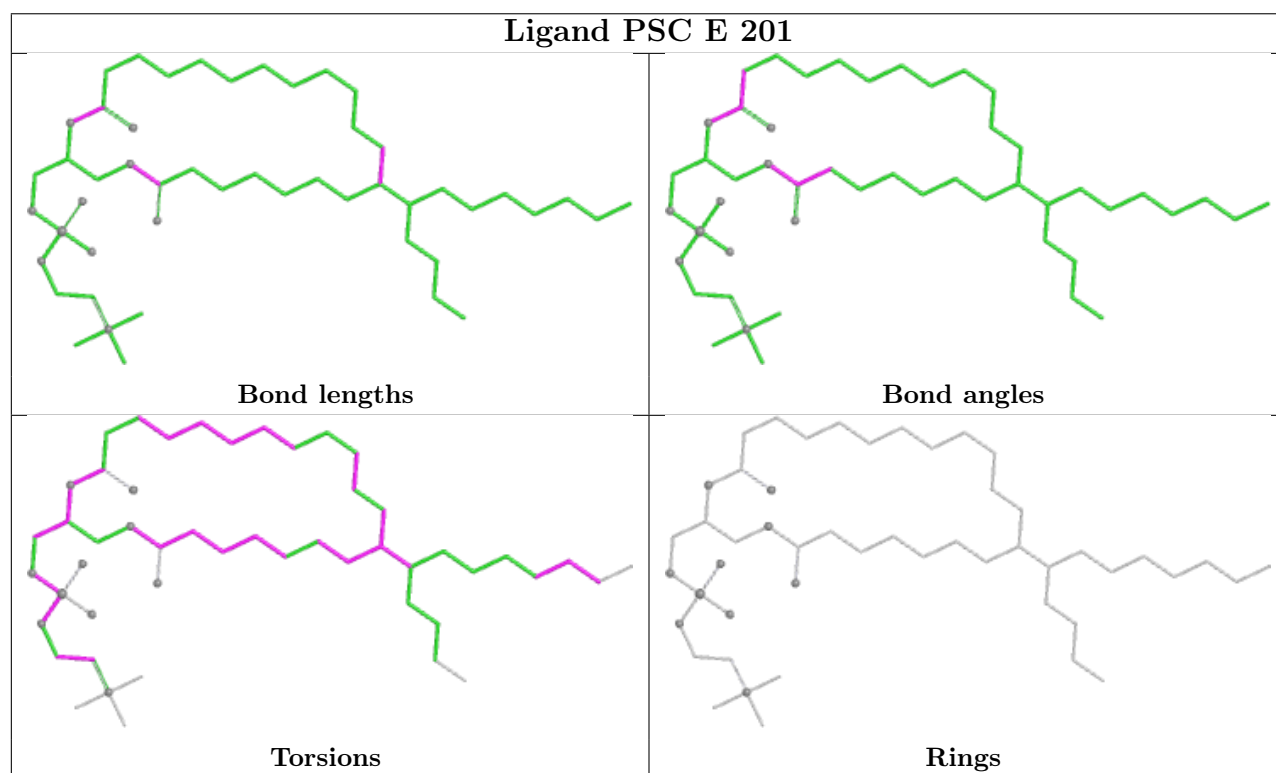
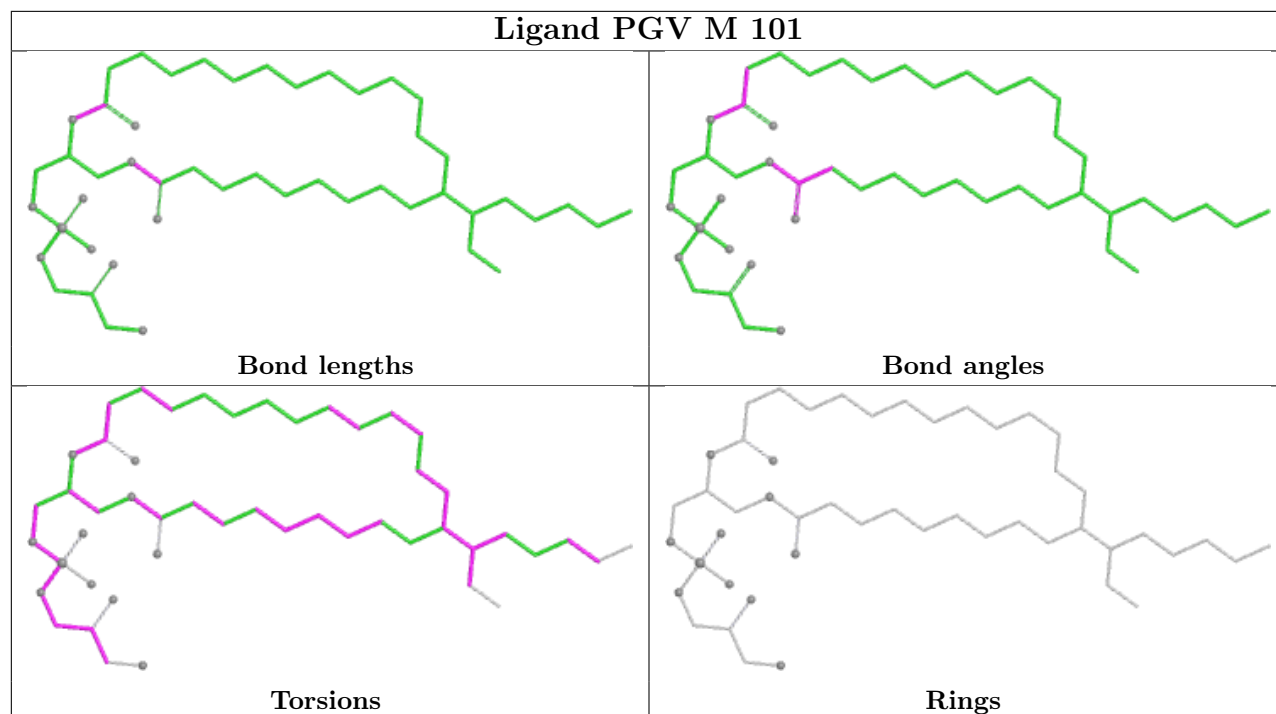




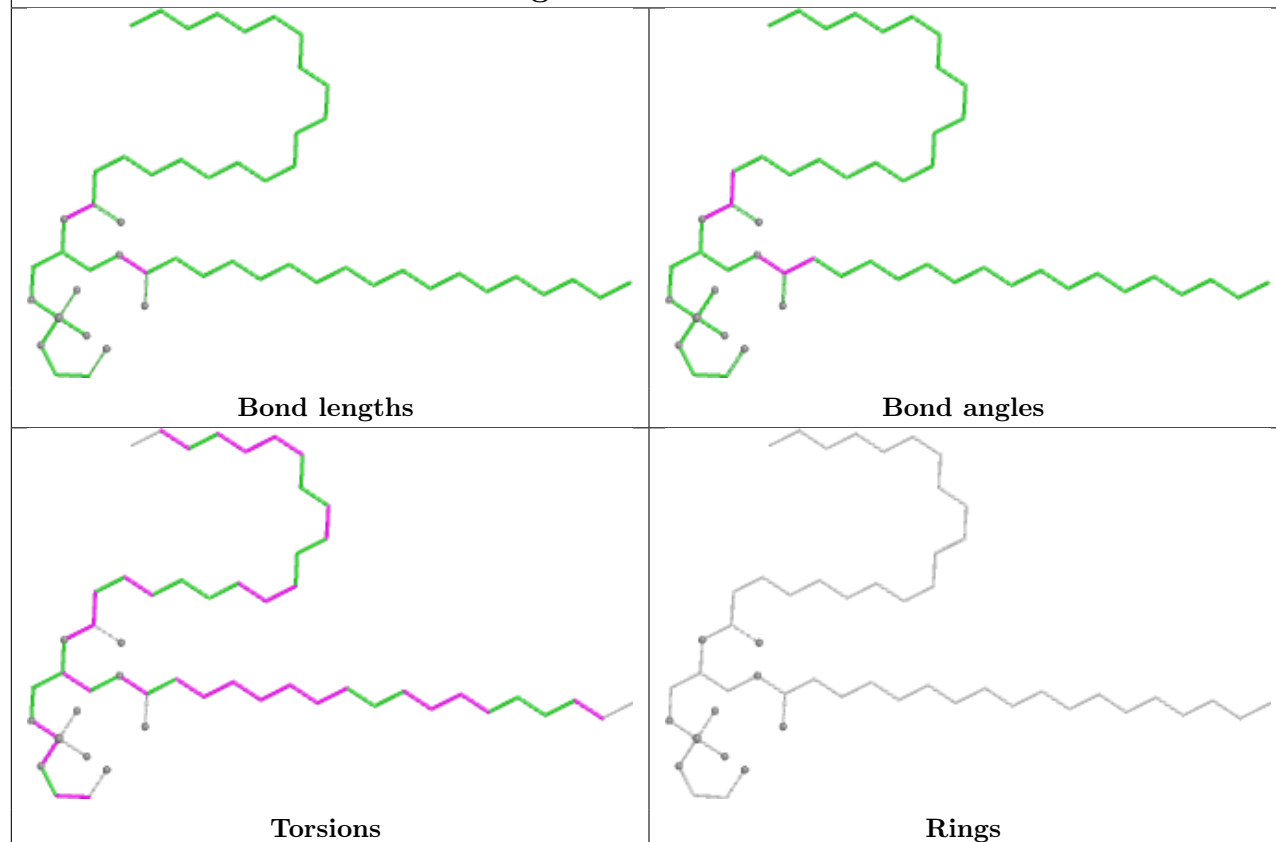




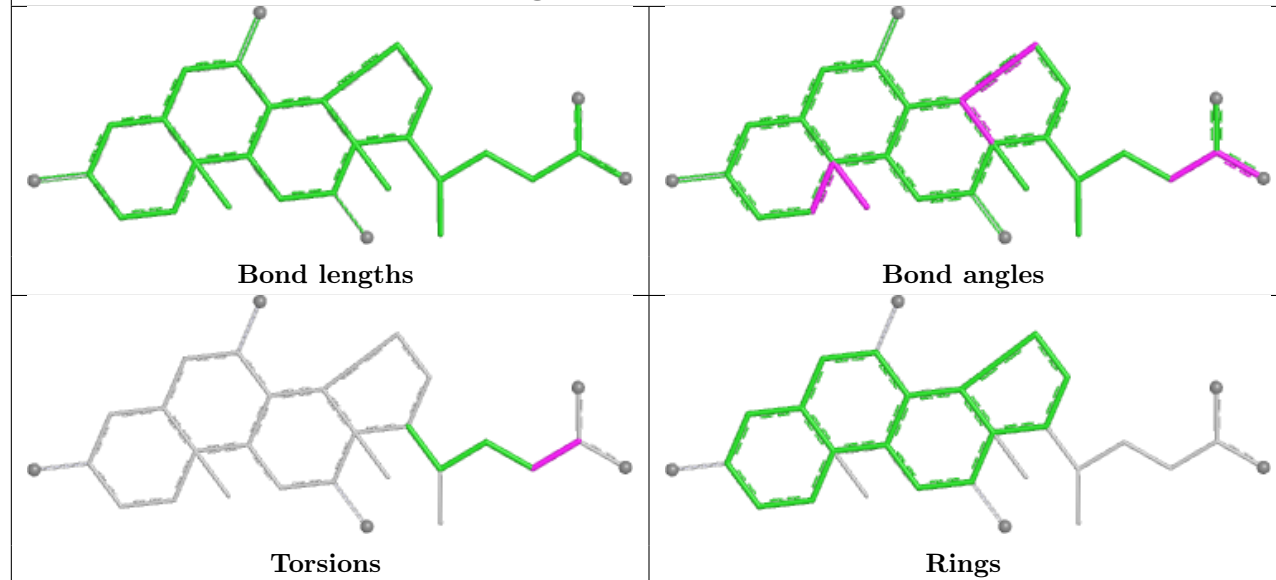


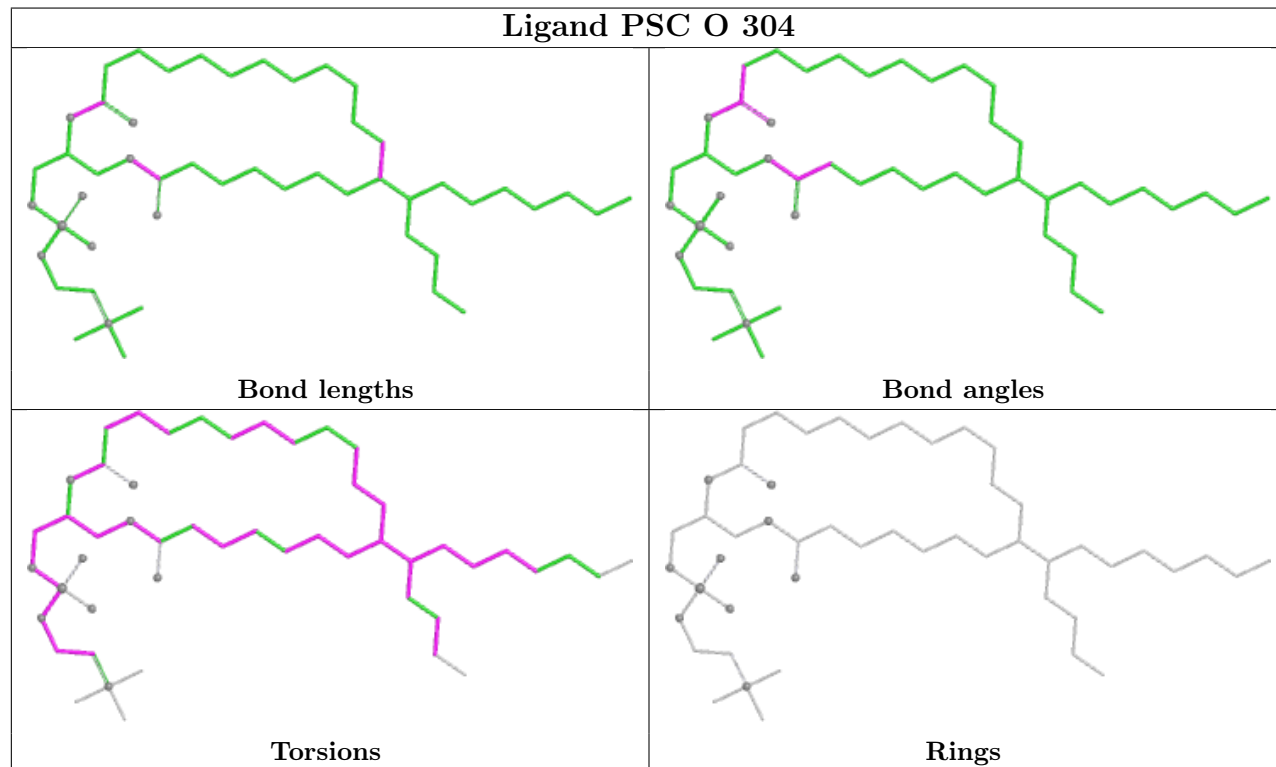
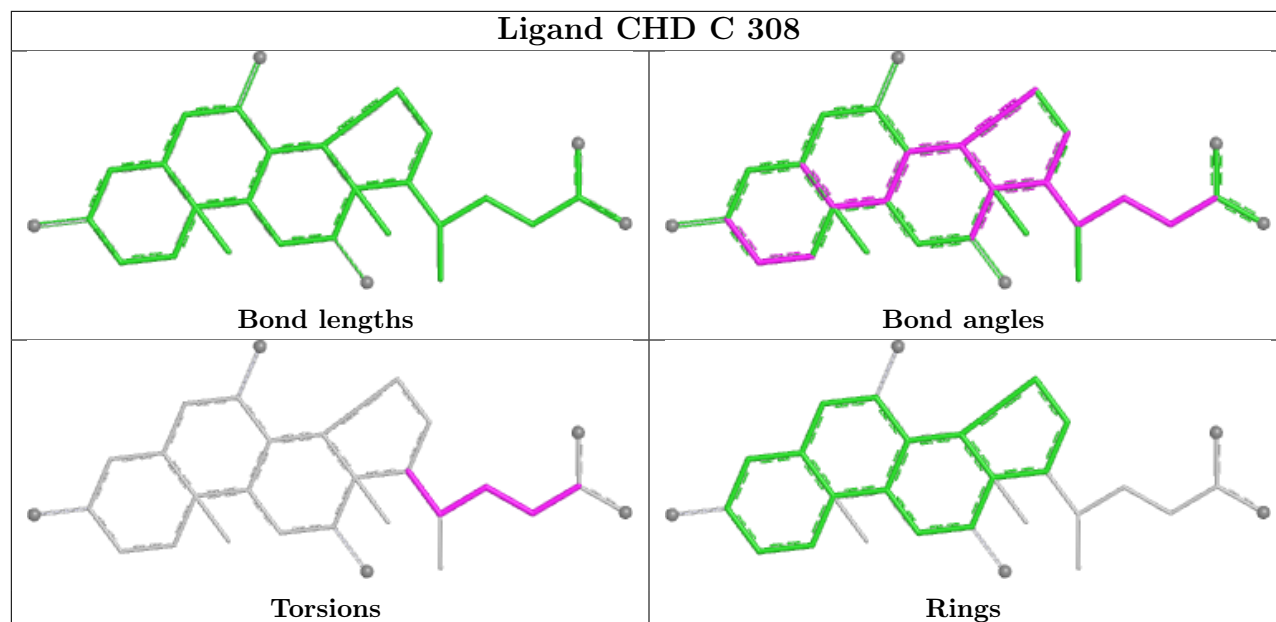


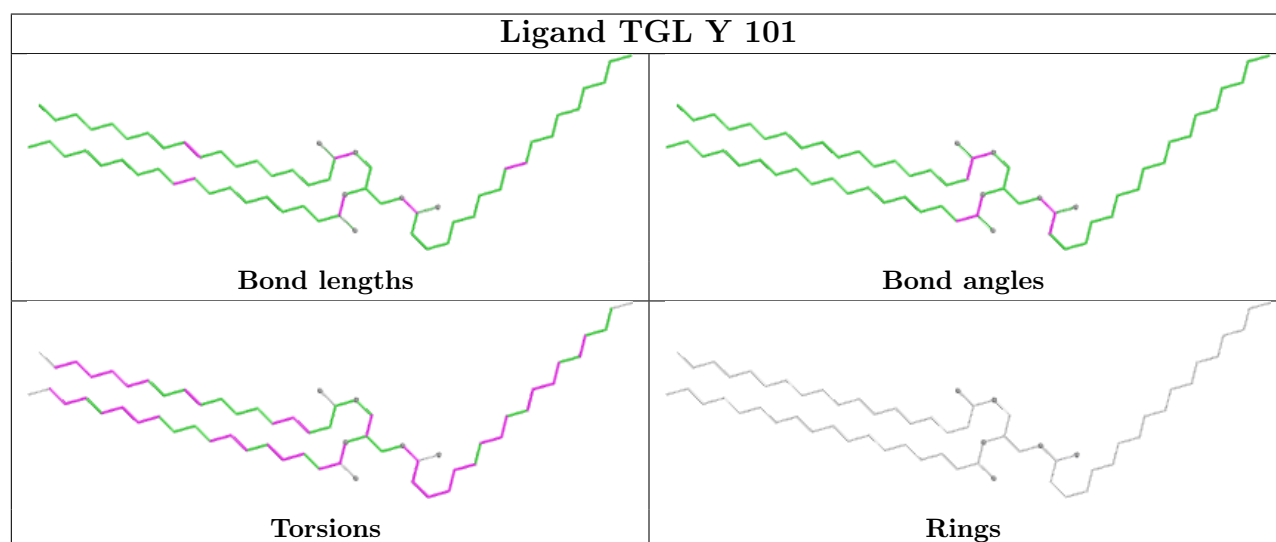
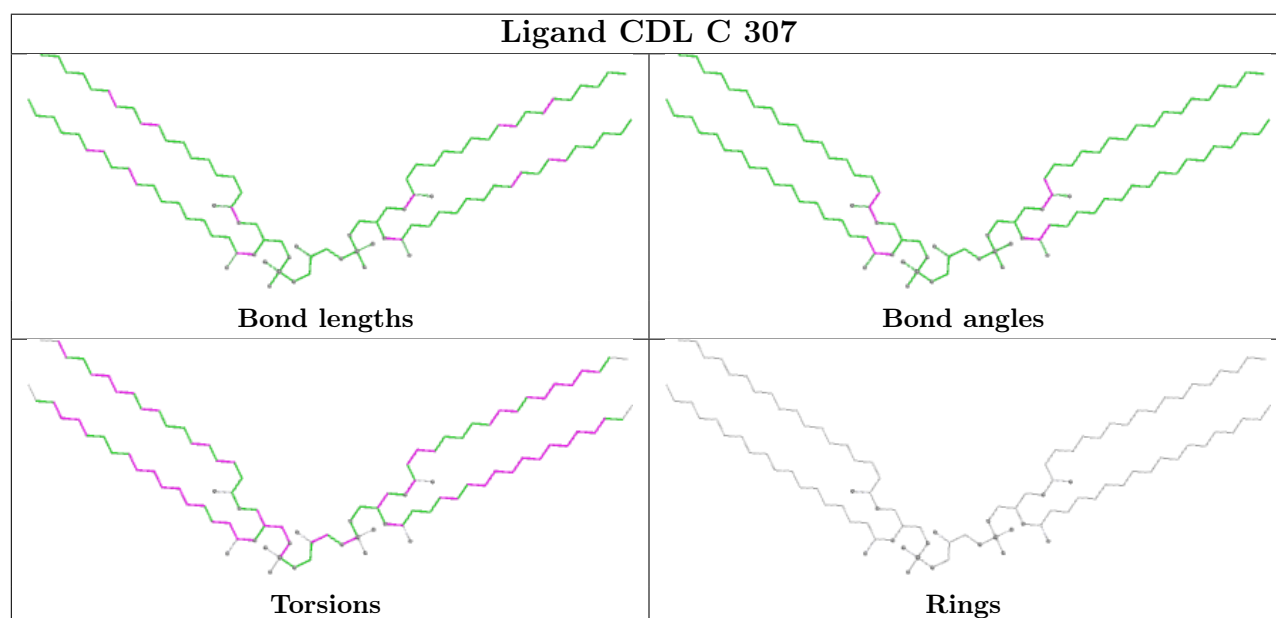
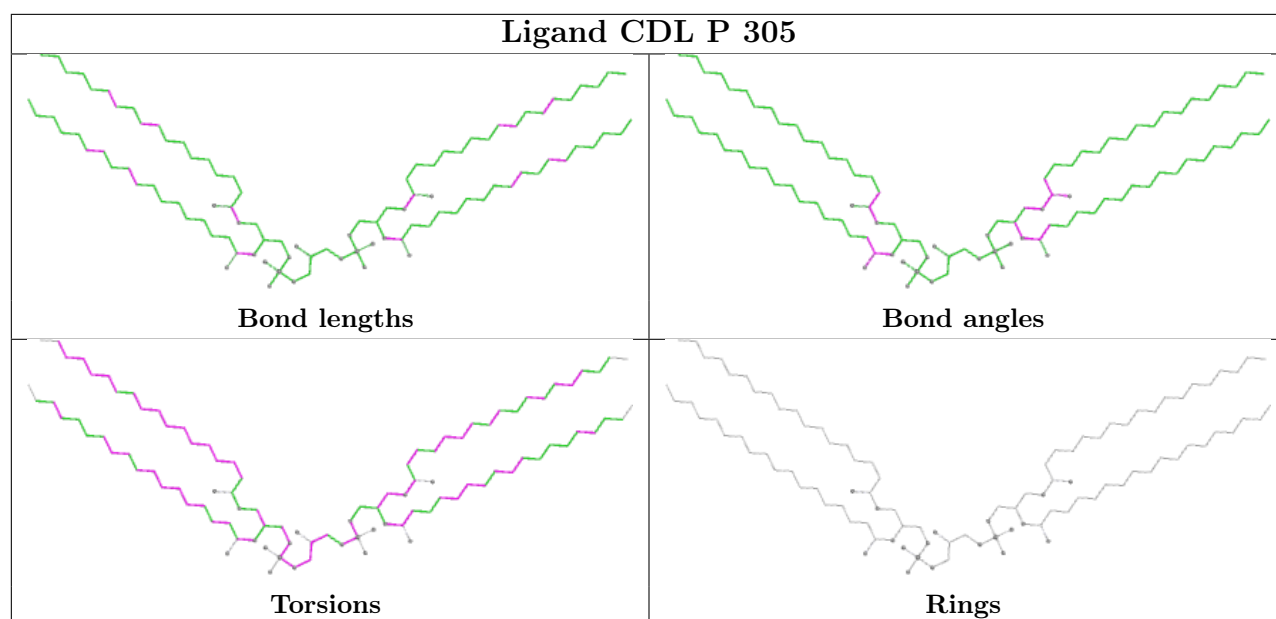
Ligand PEK C 304

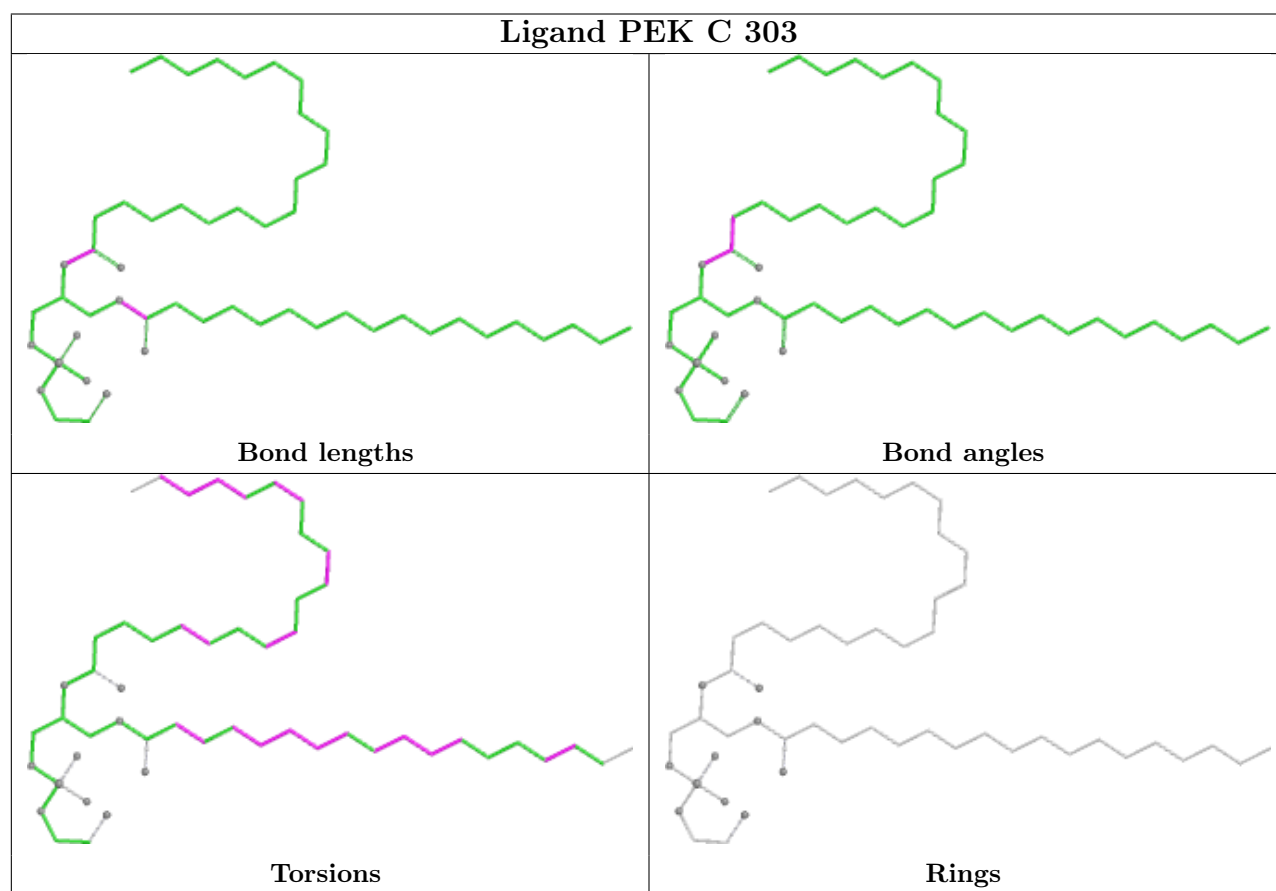
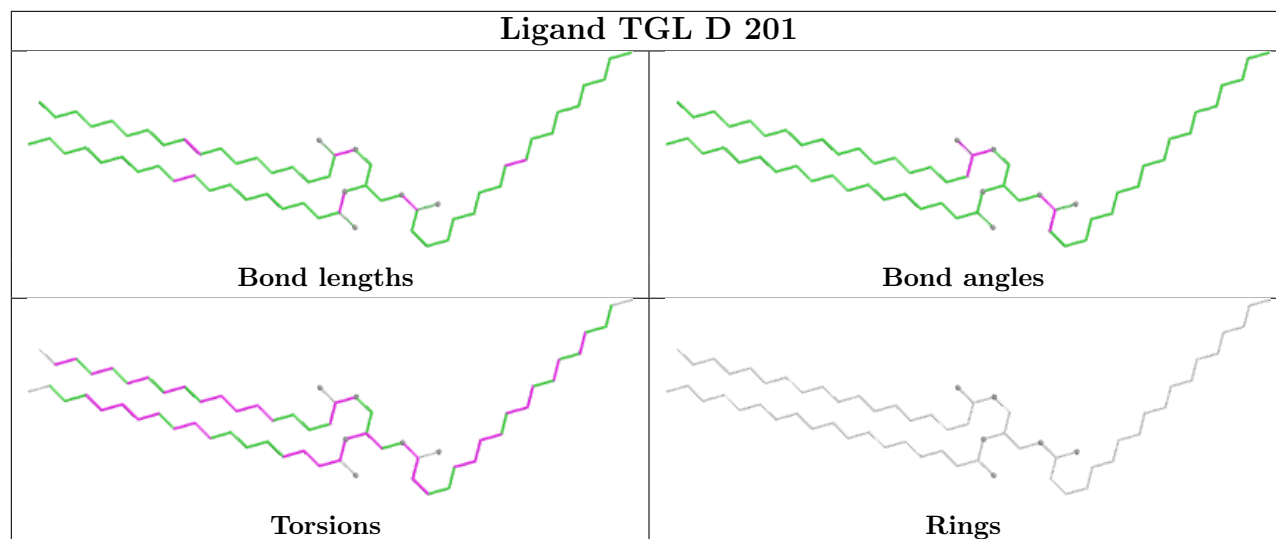


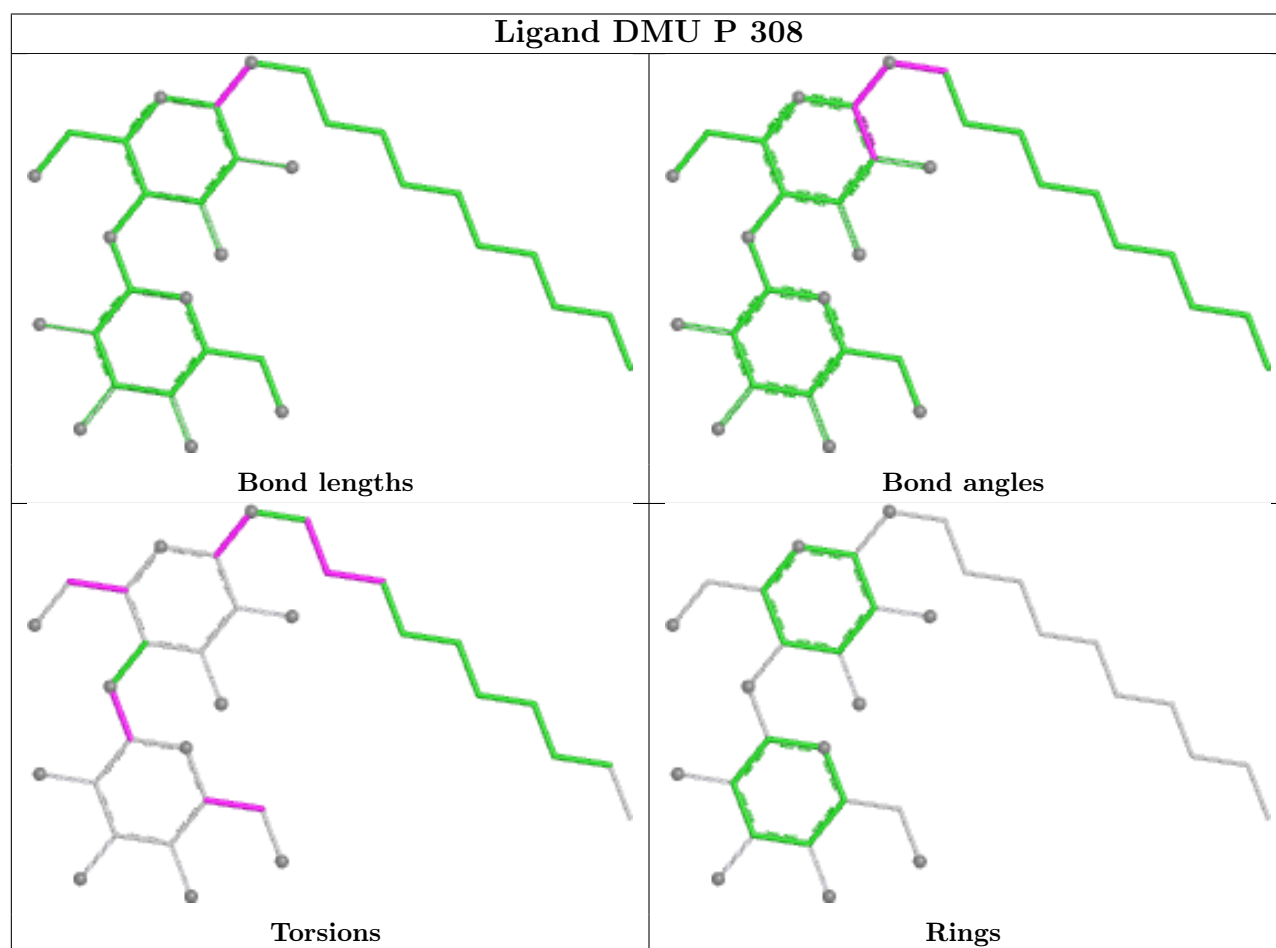
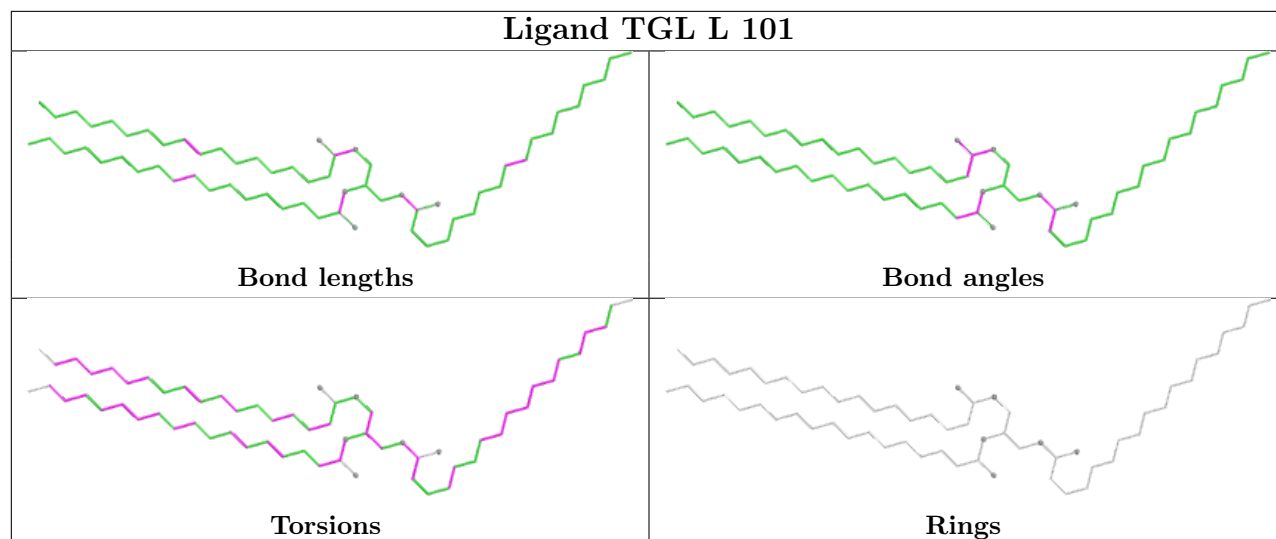
Ligand CHD C 301

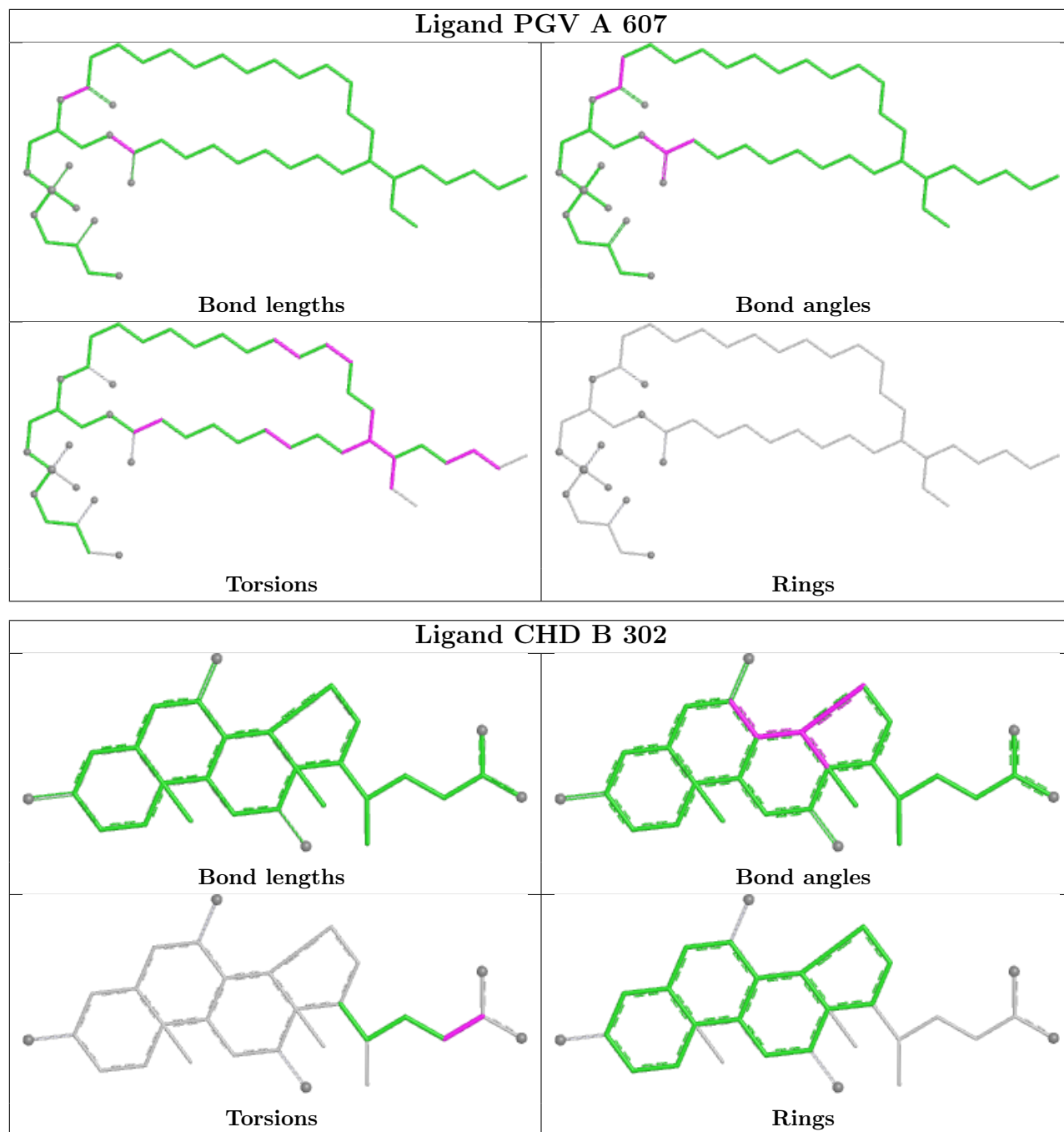


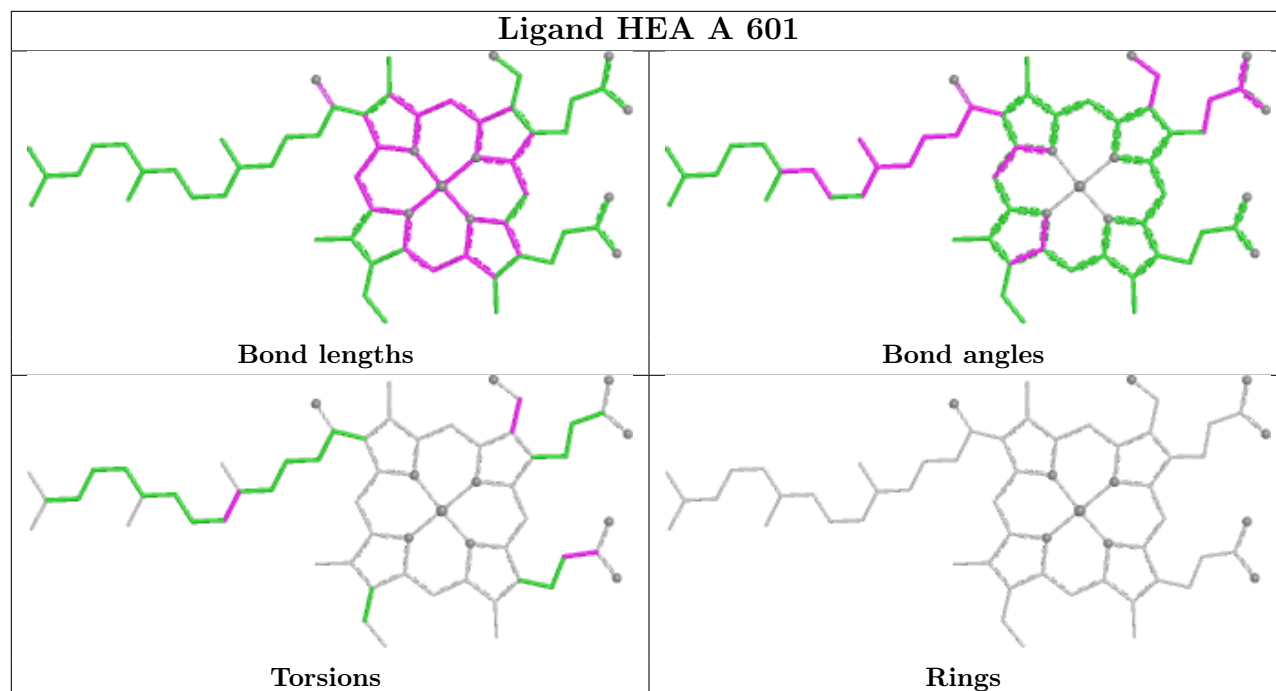












5.7 Other polymers [i](#)

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%)	-0.26	6 (1%) 76 76	19, 31, 39, 76	20 (3%)
1	N	513/514 (99%)	0.18	10 (1%) 66 66	20, 40, 53, 77	21 (4%)
2	B	226/227 (99%)	0.16	10 (4%) 39 38	22, 38, 57, 75	7 (3%)
2	O	226/227 (99%)	0.66	15 (6%) 24 23	29, 52, 72, 99	6 (2%)
3	C	259/260 (99%)	0.03	9 (3%) 47 46	17, 36, 48, 82	13 (5%)
3	P	259/260 (99%)	0.16	5 (1%) 66 66	20, 40, 50, 77	12 (4%)
4	D	144/147 (97%)	0.32	6 (4%) 40 39	34, 43, 55, 75	0
4	Q	144/147 (97%)	1.16	18 (12%) 8 7	48, 63, 88, 137	0
5	E	105/109 (96%)	0.20	3 (2%) 53 52	23, 44, 63, 109	1 (0%)
5	R	105/109 (96%)	0.58	5 (4%) 35 34	29, 55, 71, 115	1 (0%)
6	F	94/94 (100%)	0.62	5 (5%) 32 31	27, 46, 64, 119	1 (1%)
6	S	94/94 (100%)	0.88	8 (8%) 16 15	32, 51, 75, 117	1 (1%)
7	G	83/85 (97%)	1.51	18 (21%) 2 2	34, 44, 114, 145	0
7	T	83/85 (97%)	1.54	21 (25%) 1 1	35, 48, 108, 150	0
8	H	79/85 (92%)	0.72	10 (12%) 8 7	36, 47, 80, 99	0
8	U	79/85 (92%)	0.98	10 (12%) 8 7	43, 54, 93, 109	0
9	I	72/73 (98%)	1.26	18 (25%) 2 1	36, 50, 82, 91	0
9	V	72/73 (98%)	1.69	18 (25%) 2 1	42, 67, 95, 103	0
10	J	58/59 (98%)	0.71	6 (10%) 12 11	25, 47, 73, 117	2 (3%)
10	W	58/59 (98%)	1.00	8 (13%) 6 6	31, 54, 81, 128	2 (3%)
11	K	49/56 (87%)	0.46	2 (4%) 41 40	38, 45, 58, 66	0
11	X	49/56 (87%)	1.17	11 (22%) 2 2	56, 66, 83, 90	0
12	L	46/47 (97%)	0.21	3 (6%) 25 23	31, 38, 53, 84	0
12	Y	46/47 (97%)	1.08	5 (10%) 10 9	36, 54, 70, 108	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.29	3 (6%)	22 21	30, 38, 66, 104	1 (2%)
13	Z	43/46 (93%)	1.06	5 (11%)	9 8	43, 58, 85, 118	1 (2%)
All	All	3542/3604 (98%)	0.43	238 (6%)	24 22	17, 43, 75, 150	90 (2%)

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	12.8
6	S	1	ALA	12.2
4	Q	6	VAL	11.8
4	Q	5	VAL	9.8
7	G	3	ALA	9.6
7	T	5	LYS	9.4
9	I	29	LEU	9.4
7	G	5	LYS	9.1
7	T	7	ASP	9.0
7	T	3	ALA	9.0
7	G	2	SER	8.9
9	V	25	PHE	8.8
7	T	36	TRP	8.6
8	U	8	ILE	8.5
9	I	25	PHE	8.4
7	G	36	TRP	7.9
7	G	6	GLY	7.7
8	H	8	ILE	7.7
7	G	9	GLY	7.4
7	T	2	SER	7.0
9	I	30	GLY	6.9
7	G	10	GLY	6.8
7	G	1	ALA	6.5
7	G	8	HIS	6.3
7	G	4	ALA	6.3
10	J	58	LYS	6.2
7	T	4	ALA	6.1
6	F	94	HIS	6.0
6	S	3	GLY	6.0
9	V	30	GLY	5.9
7	G	7	ASP	5.9
7	T	6	GLY	5.7
7	T	9	GLY	5.7
8	H	45	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
6	F	2	SER	5.5
9	V	31	PHE	5.4
4	Q	7	LYS	5.3
7	T	1	ALA	5.2
9	V	29	LEU	5.2
9	I	37	PHE	5.1
1	N	113[A]	LEU	5.0
9	I	27	VAL	5.0
2	O	227	LEU	5.0
11	X	27	ALA	4.9
7	T	8	HIS	4.8
9	V	33	THR	4.8
6	F	3	GLY	4.8
7	T	33	LEU	4.7
7	T	37	LEU	4.7
4	Q	87	PHE	4.7
9	V	34	PHE	4.6
3	C	237	ALA	4.5
12	L	2	HIS	4.5
4	Q	8	SER	4.5
13	Z	43	SER	4.5
9	I	32	ALA	4.4
10	W	58	LYS	4.4
5	R	109	VAL	4.3
6	F	93	PRO	4.3
10	J	57	HIS	4.2
9	V	37	PHE	4.1
3	C	258	TRP	4.1
9	I	26	MET	4.1
9	V	27	VAL	4.1
3	C	37	PHE	4.0
10	J	1	PHE	4.0
12	Y	20	ARG	4.0
9	I	31	PHE	4.0
2	O	113	TYR	3.9
7	G	37	LEU	3.9
3	P	37	PHE	3.9
4	D	4	SER	3.9
6	S	2	SER	3.9
2	B	59	GLN	3.9
9	V	2	THR	3.9
9	I	19	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
4	Q	10	ASP	3.9
7	G	38	HIS	3.8
7	G	12	GLY	3.8
11	X	6	ALA	3.8
8	H	7	LYS	3.8
10	J	52	TRP	3.7
8	H	9	LYS	3.7
11	K	6	ALA	3.7
8	U	9	LYS	3.7
7	T	12	GLY	3.7
6	S	74	LEU	3.6
9	V	32	ALA	3.6
9	I	34	PHE	3.6
10	W	1	PHE	3.6
2	O	90	ILE	3.6
2	B	87	MET	3.6
7	T	84	LYS	3.6
7	T	35	SER	3.5
8	U	46	LYS	3.5
3	P	3	HIS	3.5
9	I	33	THR	3.5
11	X	52	GLU	3.5
3	C	3	HIS	3.5
6	S	94	HIS	3.5
7	G	84	LYS	3.5
4	D	31	LYS	3.4
2	B	113	TYR	3.4
12	L	24	MET	3.4
9	V	21	ILE	3.4
1	A	113[A]	LEU	3.4
1	N	513	LEU	3.4
9	I	28	SER	3.4
4	Q	4	SER	3.4
3	C	38[A]	ASN	3.3
3	P	38[A]	ASN	3.3
8	U	45	ALA	3.2
2	O	40	TYR	3.2
2	O	61	VAL	3.2
5	E	109	VAL	3.2
8	H	47	GLY	3.2
13	Z	32	TRP	3.2
10	W	57	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
12	Y	47	LYS	3.1
3	P	258	TRP	3.1
9	V	3	ALA	3.1
5	E	5	HIS	3.1
1	N	484	THR	3.1
5	R	65	VAL	3.0
7	T	38	HIS	3.0
4	Q	9	GLU	3.0
2	O	36[A]	SER	2.9
13	M	40	TYR	2.9
9	V	18	ARG	2.9
4	Q	33	LEU	2.9
7	T	10	GLY	2.9
10	W	56	PRO	2.8
7	G	41	HIS	2.8
13	M	42	LYS	2.8
2	B	90	ILE	2.8
2	B	91	ASN	2.8
11	K	47	ARG	2.8
10	J	48	TYR	2.8
12	Y	24[A]	MET	2.8
9	I	2	THR	2.8
4	D	19	ARG	2.8
12	Y	27	LEU	2.8
10	W	52	TRP	2.8
10	W	48	TYR	2.7
8	U	47	GLY	2.7
6	S	30	PRO	2.7
3	P	261	SER	2.7
11	X	54	ARG	2.7
12	Y	2	HIS	2.7
4	D	87	PHE	2.7
1	N	514	LYS	2.7
4	Q	35	ALA	2.6
1	N	297[A]	MET	2.6
8	U	7	LYS	2.6
9	V	36	LYS	2.6
1	A	513	LEU	2.6
4	Q	17	VAL	2.6
7	T	42	ARG	2.6
1	A	514	LYS	2.6
1	N	46	THR	2.6

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Mol	Chain	Res	Type	RSRZ
8	U	44	THR	2.6
3	C	261	SER	2.5
4	Q	11	TYR	2.5
13	Z	40	TYR	2.5
2	O	33	LEU	2.5
11	X	13	TYR	2.5
7	T	34	ASN	2.5
1	N	382	SER	2.5
9	I	21	ILE	2.5
9	V	8	GLN	2.5
2	O	86[A]	MET	2.5
9	V	26	MET	2.5
8	H	44	THR	2.5
7	T	40	GLY	2.4
9	V	67	GLY	2.4
8	H	43	MET	2.4
9	V	35	TYR	2.4
13	M	43	SER	2.4
10	W	55	PHE	2.4
10	J	56	PRO	2.4
6	S	92	VAL	2.4
7	T	39	SER	2.4
2	B	39	LEU	2.4
10	W	40	LEU	2.4
9	I	35	TYR	2.4
5	R	5	HIS	2.4
4	D	17	VAL	2.4
2	O	65	TRP	2.4
7	G	33	LEU	2.3
2	O	47	THR	2.3
11	X	34	THR	2.3
11	X	49	THR	2.3
4	Q	39	ALA	2.3
12	L	47	LYS	2.3
8	U	50	VAL	2.3
3	C	122	HIS	2.3
4	D	102	TYR	2.3
5	E	39	TYR	2.3
9	I	36	LYS	2.3
8	H	42	ALA	2.3
11	X	7	PRO	2.3
3	C	127	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
9	I	23	GLY	2.2
1	A	169	ILE	2.2
2	O	91	ASN	2.2
5	R	108	LYS	2.2
6	S	43	LYS	2.2
8	U	43	MET	2.2
4	Q	82	VAL	2.2
9	I	22	VAL	2.2
3	C	236	GLU	2.2
2	O	116	LEU	2.2
4	Q	51	LEU	2.2
1	A	382	SER	2.2
2	O	32	PHE	2.2
4	Q	140	TYR	2.2
8	H	50	VAL	2.2
2	O	57	ASP	2.2
4	Q	74	SER	2.2
5	R	106	LEU	2.2
2	B	40	TYR	2.1
11	X	28	VAL	2.1
7	G	35	SER	2.1
11	X	53	TRP	2.1
13	Z	42	LYS	2.1
1	N	112	LEU	2.1
1	N	136[A]	LEU	2.1
1	N	2	PHE	2.1
2	B	32	PHE	2.1
11	X	24	PHE	2.1
2	B	16	ILE	2.1
4	Q	19	ARG	2.1
2	O	142	VAL	2.1
8	H	10	ASN	2.1
1	A	297[A]	MET	2.0
13	Z	24	LEU	2.0
2	B	183	THR	2.0
8	U	27	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SAC	V	1	9/10	0.33	0.23	118,123,127,131	0
7	TPO	T	11	11/12	0.61	0.26	93,108,122,125	0
7	TPO	G	11	11/12	0.64	0.28	88,102,120,124	0
9	SAC	I	1	9/10	0.80	0.16	74,75,78,79	0
1	FME	N	1	10/11	0.88	0.15	58,63,83,86	0
1	FME	A	1	10/11	0.90	0.16	46,53,70,78	0
2	FME	O	1	10/11	0.95	0.12	52,53,59,60	0
2	FME	B	1	10/11	0.96	0.09	35,36,44,47	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($\text{\AA}^2$)	Q<0.9
25	DMU	P	308	33/33	0.61	0.25	71,126,142,143	0
22	CHD	W	101	29/29	0.72	0.21	89,96,106,107	0
22	CHD	J	101	29/29	0.73	0.20	73,78,100,104	0
24	CDL	P	305	100/100	0.74	0.30	65,90,111,114	0
25	DMU	C	312	33/33	0.75	0.20	65,100,138,139	0
19	PGV	P	304	51/51	0.75	0.27	66,92,122,129	0
23	PEK	G	102	53/53	0.76	0.24	55,101,139,150	0
24	CDL	G	101	100/100	0.77	0.29	65,97,136,145	0
23	PEK	C	304	53/53	0.77	0.28	60,91,135,141	0
19	PGV	C	306	51/51	0.77	0.24	62,82,121,124	0
23	PEK	T	101	53/53	0.77	0.27	56,94,139,144	0
18	TGL	Q	201	63/63	0.78	0.27	67,86,96,100	0
24	CDL	T	104	100/100	0.78	0.27	63,92,121,138	0
24	CDL	C	307	100/100	0.78	0.26	56,85,110,116	0
25	DMU	C	313	33/33	0.78	0.22	49,130,146,147	0
18	TGL	Y	101	63/63	0.78	0.28	63,83,104,107	0
18	TGL	D	201	63/63	0.79	0.27	56,71,89,92	0
18	TGL	L	101	63/63	0.79	0.28	46,71,85,86	0
20	EDO	S	103	4/4	0.79	0.24	57,66,69,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	PSC	E	201	52/52	0.79	0.26	56,87,141,150	0
23	PEK	T	103	53/53	0.80	0.25	59,85,124,134	0
19	PGV	N	606	51/51	0.80	0.26	70,87,126,128	0
18	TGL	A	606	63/63	0.80	0.28	53,78,95,98	0
26	PSC	O	304	52/52	0.80	0.25	60,92,142,154	0
22	CHD	P	306	29/29	0.81	0.18	71,76,81,81	0
20	EDO	B	303	4/4	0.81	0.25	62,72,75,79	0
20	EDO	P	307	4/4	0.81	0.30	82,88,90,97	0
18	TGL	O	302	63/63	0.81	0.30	64,87,99,105	0
19	PGV	M	101	51/51	0.81	0.23	49,77,115,124	0
25	DMU	P	309	33/33	0.82	0.20	64,128,146,149	0
17	NA	C	302	1/1	0.82	0.23	51,51,51,51	0
22	CHD	C	308	29/29	0.82	0.18	72,74,79,80	0
17	NA	P	302	1/1	0.83	0.19	51,51,51,51	0
25	DMU	Z	101	33/33	0.86	0.14	57,80,91,94	0
20	EDO	C	310	4/4	0.87	0.16	71,76,80,84	0
20	EDO	D	202	4/4	0.87	0.19	54,63,65,68	0
20	EDO	D	203	4/4	0.87	0.23	61,65,70,71	0
25	DMU	M	102	33/33	0.88	0.12	48,58,74,77	0
20	EDO	A	612	4/4	0.88	0.15	38,39,43,43	0
20	EDO	F	104	4/4	0.88	0.16	56,58,60,62	0
20	EDO	C	309	4/4	0.89	0.24	82,86,90,92	0
20	EDO	N	616	4/4	0.89	0.18	59,59,61,61	0
20	EDO	A	615	4/4	0.89	0.34	49,50,56,58	0
20	EDO	N	611	4/4	0.90	0.18	60,62,64,66	0
20	EDO	A	611	4/4	0.90	0.19	62,67,67,69	0
20	EDO	N	608	4/4	0.91	0.12	37,39,40,40	0
20	EDO	A	613	4/4	0.92	0.14	46,49,51,52	0
20	EDO	N	617	4/4	0.92	0.17	58,70,75,86	0
20	EDO	N	609	4/4	0.92	0.16	63,69,69,74	0
20	EDO	A	608	4/4	0.92	0.14	55,59,59,65	0
20	EDO	N	613	4/4	0.92	0.24	49,51,53,55	0
20	EDO	N	615	4/4	0.92	0.26	54,58,59,65	0
20	EDO	N	610	4/4	0.93	0.12	62,64,65,66	0
20	EDO	A	614	4/4	0.93	0.14	50,53,54,59	0
20	EDO	A	610	4/4	0.94	0.13	54,56,56,57	0
16	MG	N	604	1/1	0.94	0.12	44,44,44,44	0
23	PEK	T	102	53/53	0.94	0.15	40,58,95,98	0
16	MG	A	604	1/1	0.94	0.08	30,30,30,30	0
19	PGV	N	607	51/51	0.95	0.11	38,46,68,70	0
22	CHD	B	302	29/29	0.95	0.08	36,38,40,44	0
22	CHD	C	301	29/29	0.95	0.08	34,37,39,42	0

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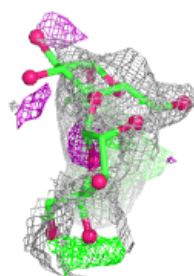
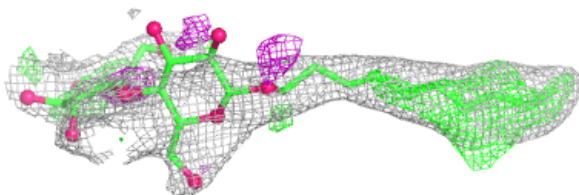
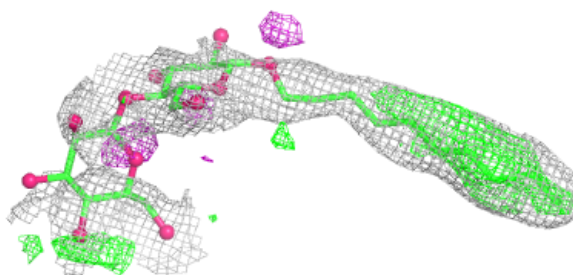
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	EDO	N	612	4/4	0.95	0.14	45,46,46,47	0
20	EDO	F	102	4/4	0.95	0.13	41,44,45,47	0
22	CHD	P	301	29/29	0.95	0.08	37,40,42,45	0
20	EDO	N	614	4/4	0.95	0.15	46,48,49,50	0
19	PGV	C	305	51/51	0.95	0.13	35,41,90,101	0
23	PEK	C	303	53/53	0.95	0.14	35,52,84,86	0
19	PGV	A	607	51/51	0.95	0.11	33,40,61,66	0
20	EDO	C	311	4/4	0.95	0.10	40,43,45,48	0
20	EDO	A	616	4/4	0.95	0.17	43,45,49,49	0
20	EDO	R	201	4/4	0.95	0.19	52,53,53,53	0
22	CHD	O	301	29/29	0.96	0.07	40,42,44,47	0
19	PGV	P	303	51/51	0.96	0.12	38,46,76,79	0
20	EDO	S	102	4/4	0.97	0.10	37,39,40,42	0
20	EDO	E	202	4/4	0.97	0.09	51,52,52,53	0
20	EDO	A	609	4/4	0.97	0.07	30,32,32,33	0
14	HEA	N	602	60/60	0.97	0.08	35,37,42,44	0
17	NA	A	605	1/1	0.98	0.05	30,30,30,30	0
14	HEA	A	601	60/60	0.98	0.07	25,28,38,40	0
20	EDO	F	103	4/4	0.98	0.06	31,33,33,33	0
21	CUA	B	301	2/2	0.98	0.03	30,30,30,30	0
14	HEA	A	602	60/60	0.98	0.06	26,28,34,38	0
14	HEA	N	601	60/60	0.98	0.08	36,42,49,51	0
17	NA	N	605	1/1	0.99	0.04	49,49,49,49	0
21	CUA	O	303	2/2	0.99	0.03	42,42,42,43	0
27	ZN	S	101	1/1	0.99	0.03	46,46,46,46	0
15	CU	A	603	1/1	1.00	0.01	28,28,28,28	0
27	ZN	F	101	1/1	1.00	0.02	39,39,39,39	0
15	CU	N	603	1/1	1.00	0.01	37,37,37,37	0

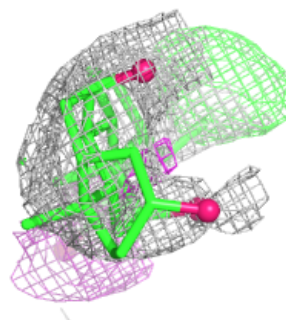
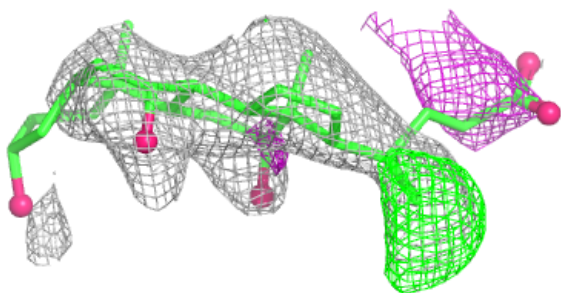
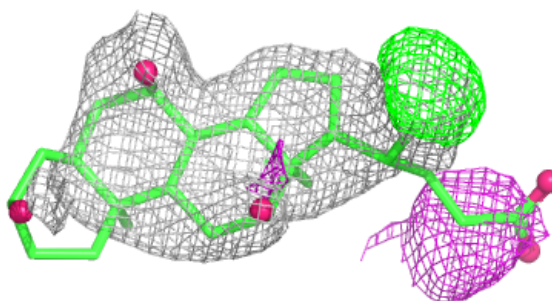
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU 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)

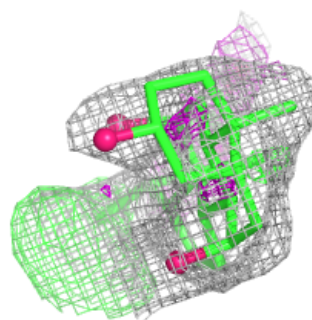
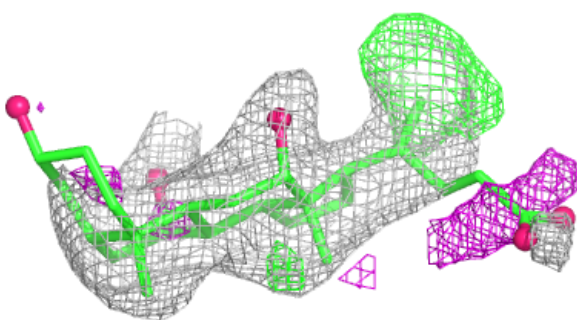
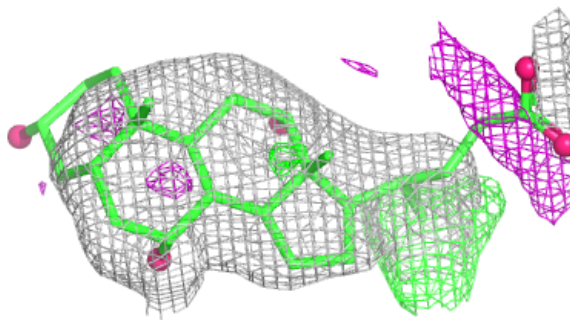
**Electron density around CHD W 101:**

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

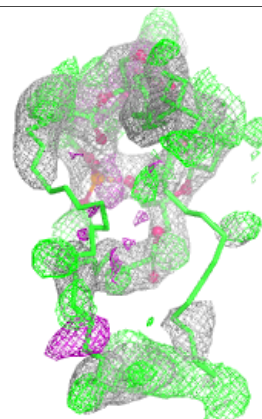
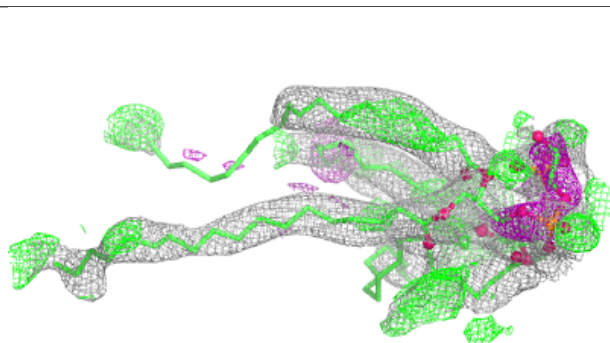
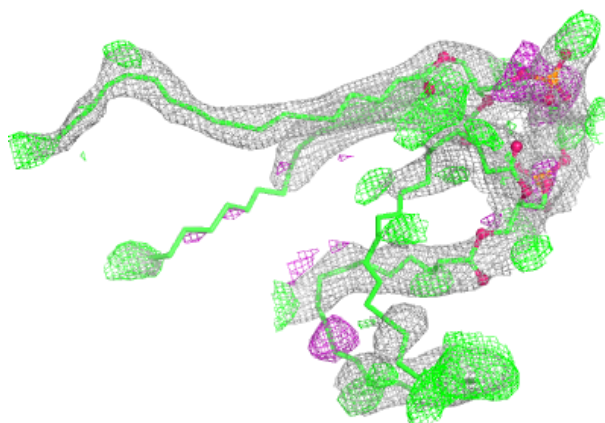


Electron density around CHD J 101:

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

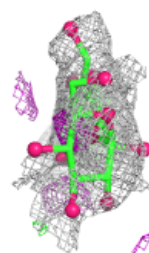
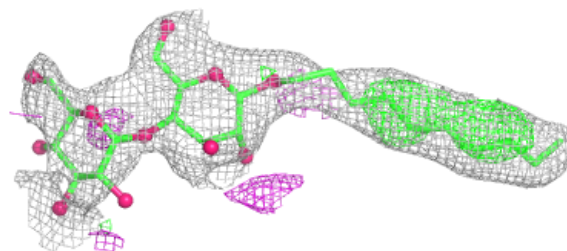
**Electron density around CDL P 305:**

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

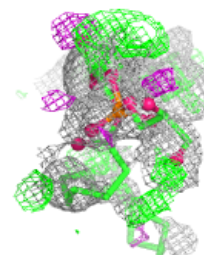
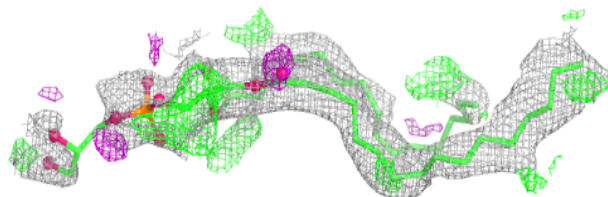
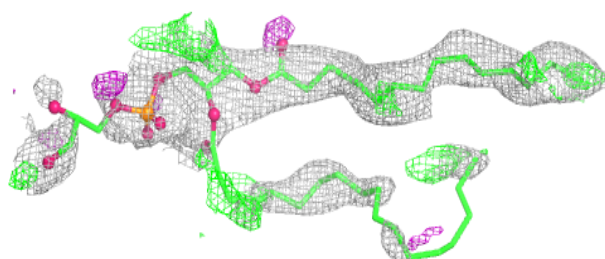


Electron density around DMU C 312:

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

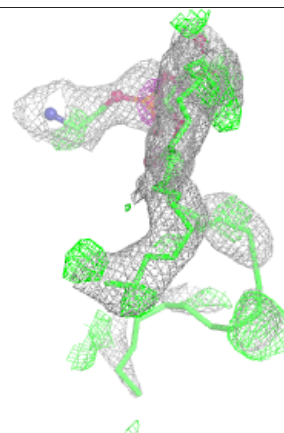
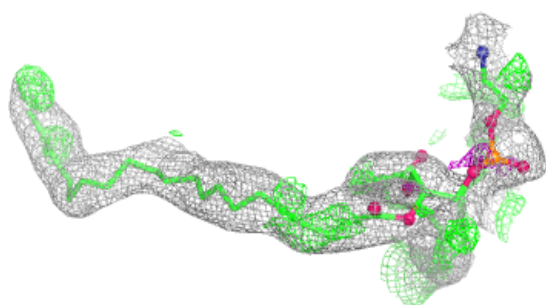
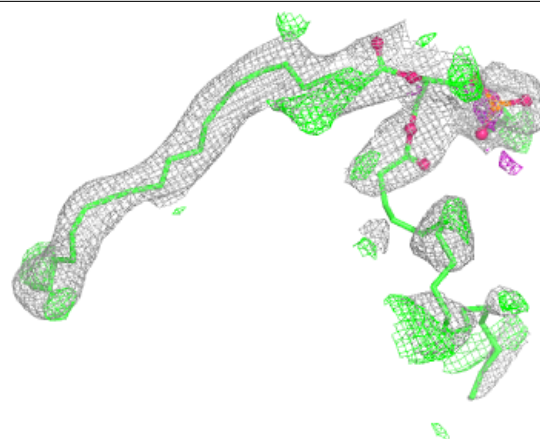
**Electron density around PGV P 304:**

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

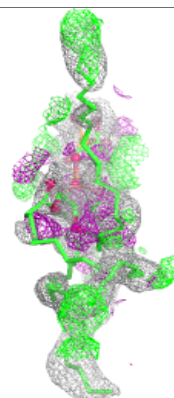
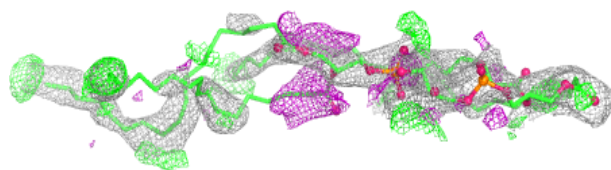
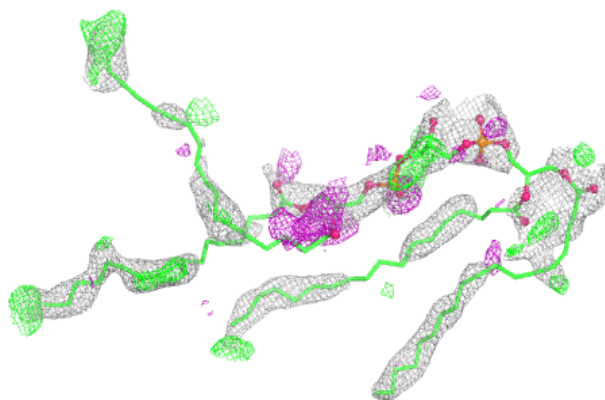


Electron density around PEK G 102:

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

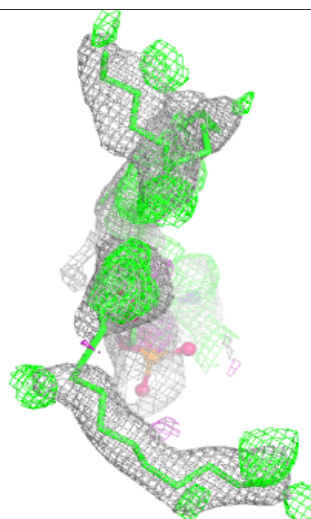
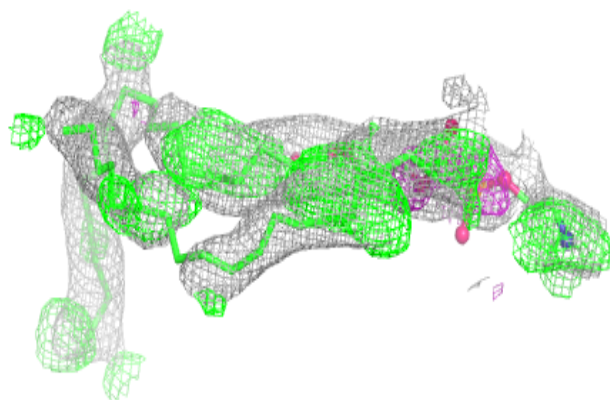
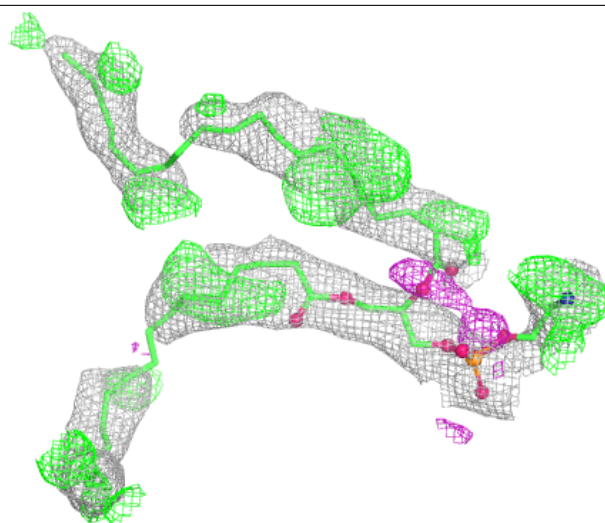
**Electron density around CDL G 101:**

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



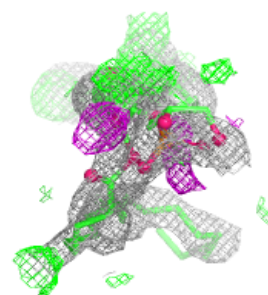
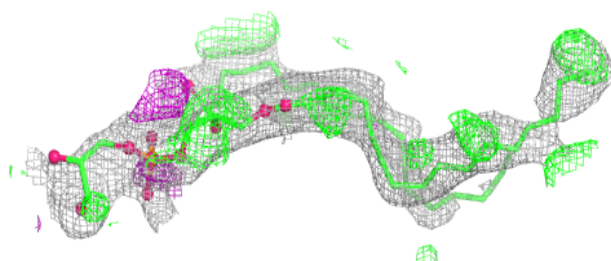
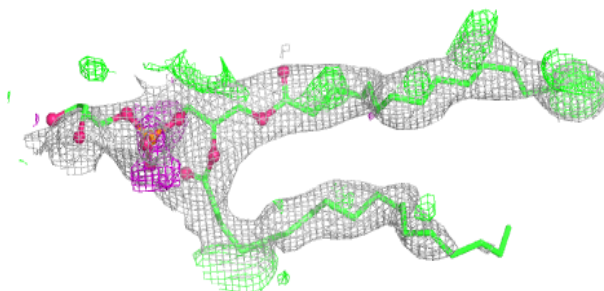
Electron density around PEK C 304:

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

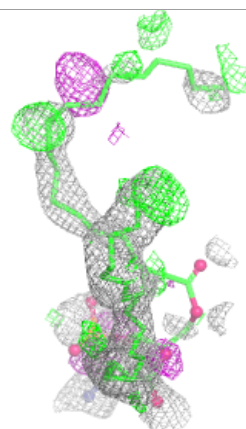
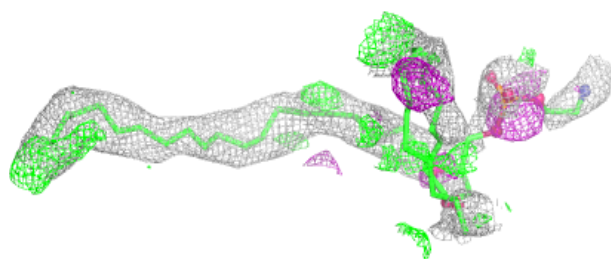
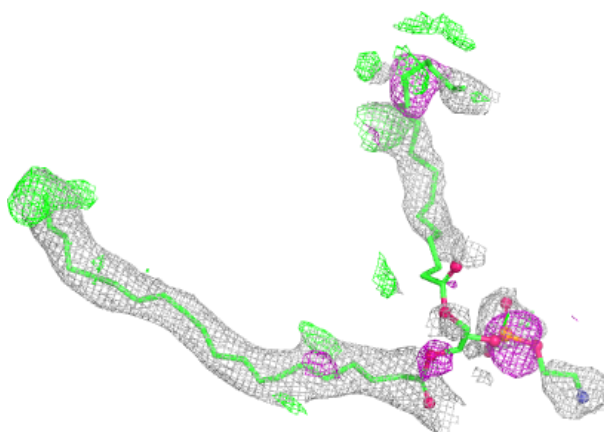


Electron density around PGV C 306:

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

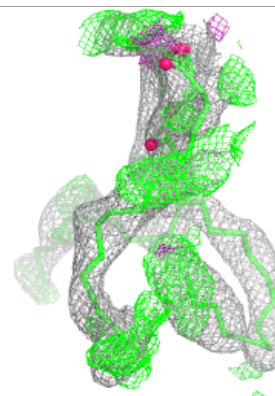
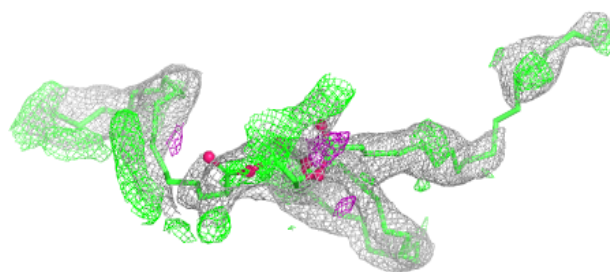
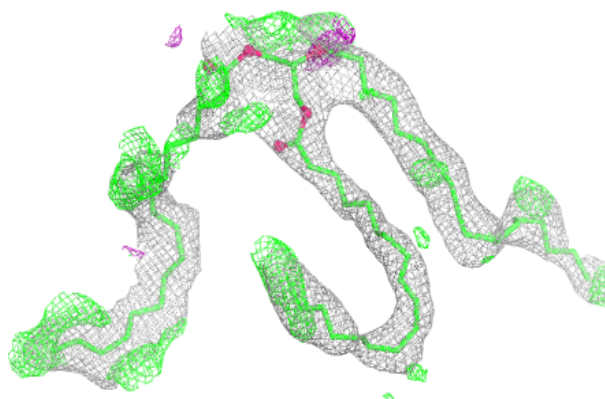
**Electron density around PEK T 101:**

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

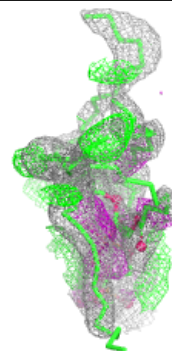
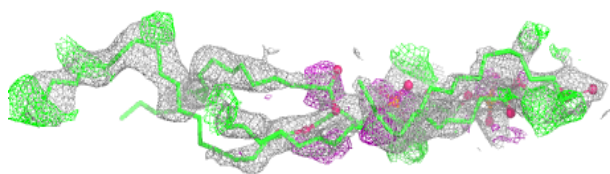
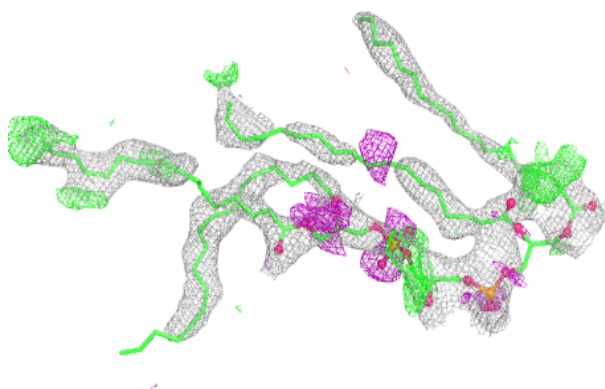


Electron density around TGL Q 201:

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

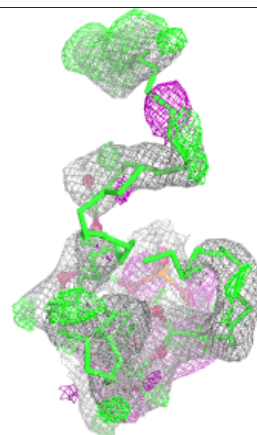
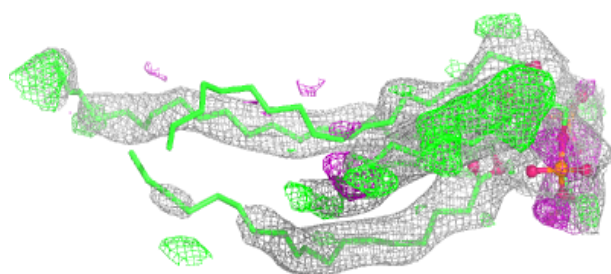
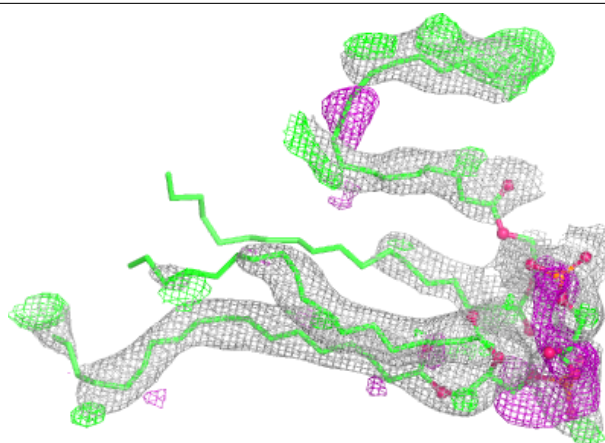
**Electron density around CDL T 104:**

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



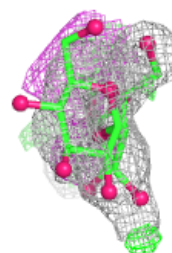
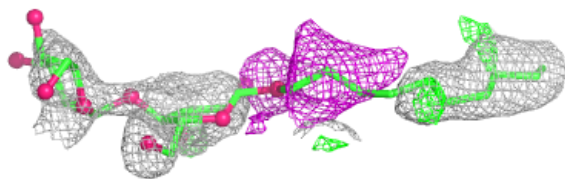
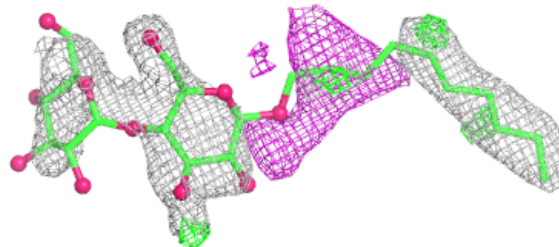
Electron density around CDL C 307:

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



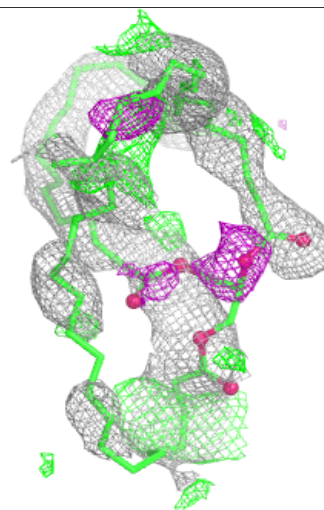
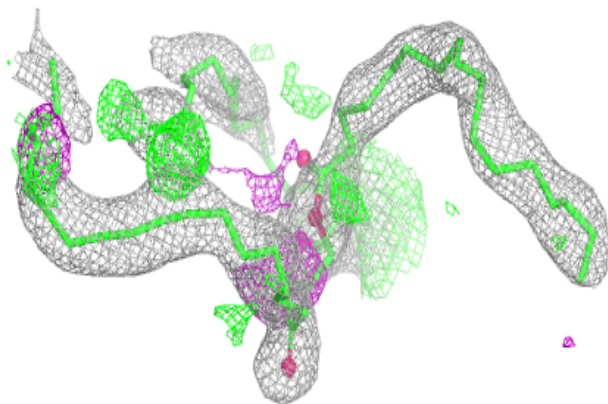
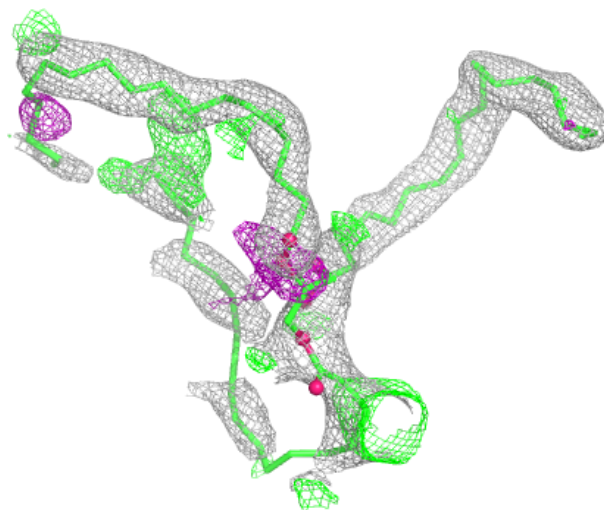
Electron density around DMU C 313:

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



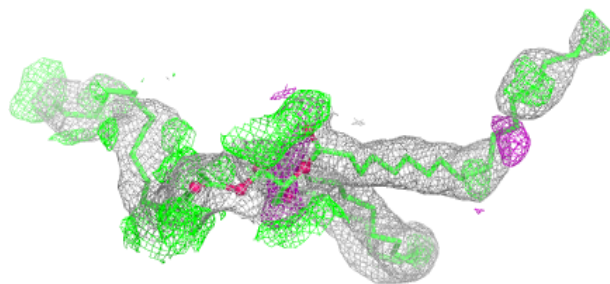
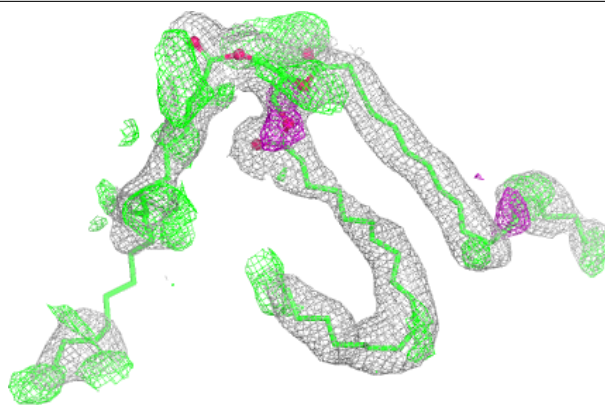
Electron density around TGL Y 101:

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



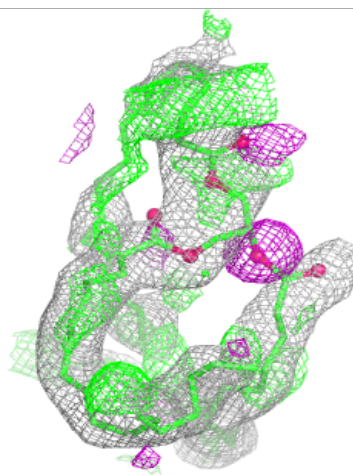
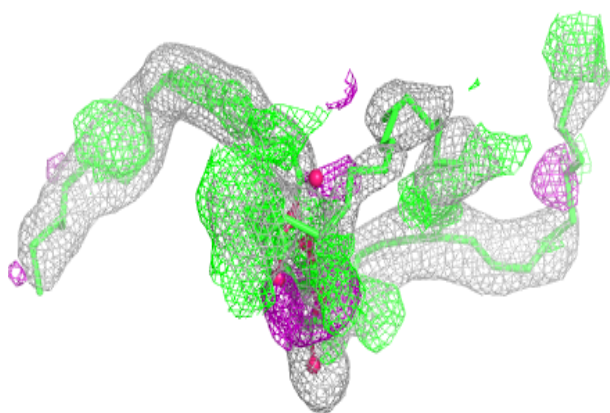
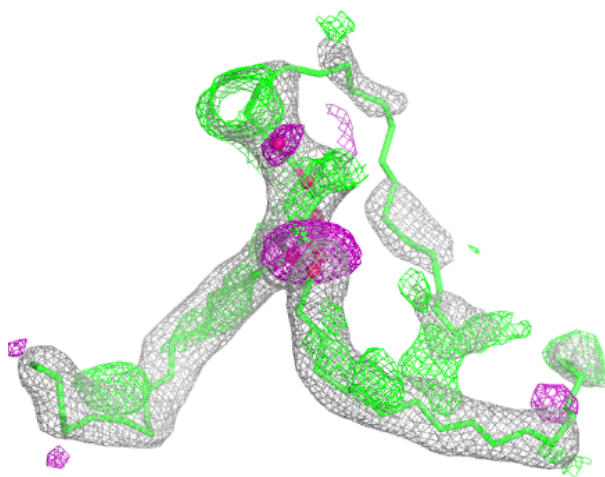
Electron density around TGL D 201:

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



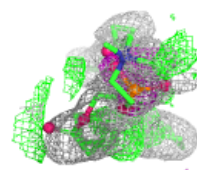
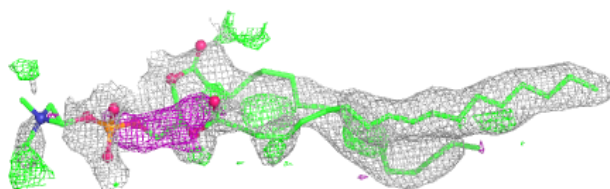
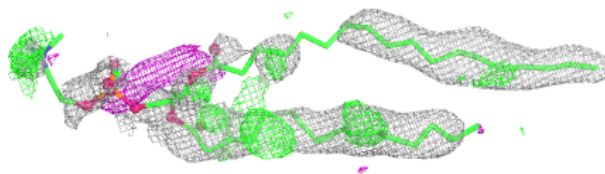
Electron density around TGL L 101:

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



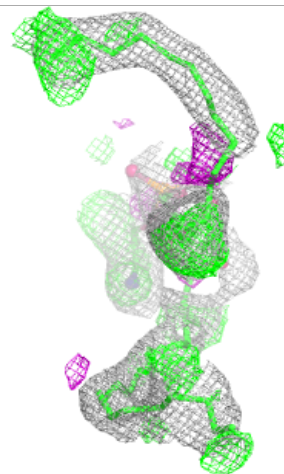
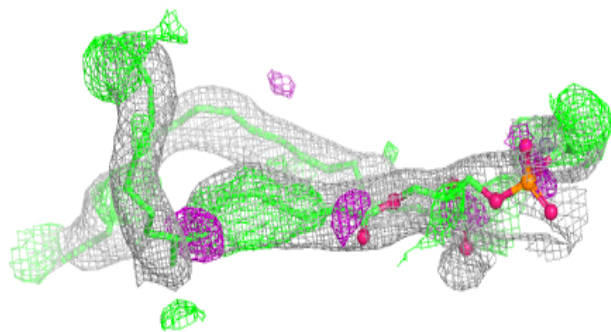
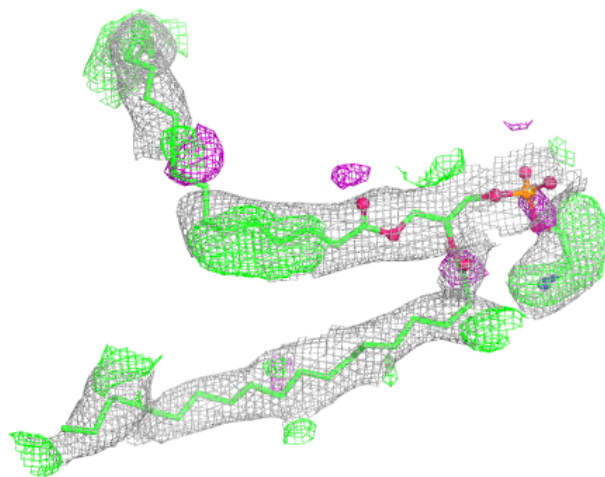
Electron density around PSC E 201:

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



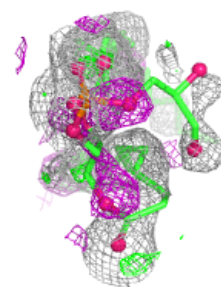
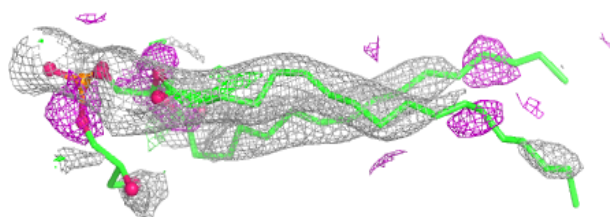
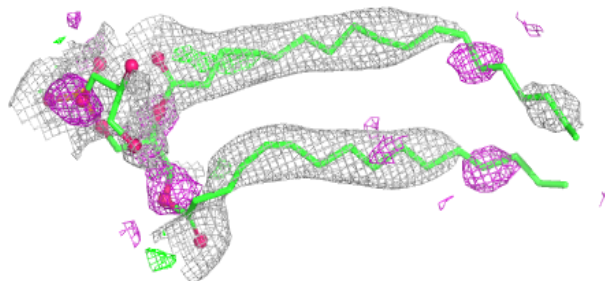
Electron density around PEK T 103:

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

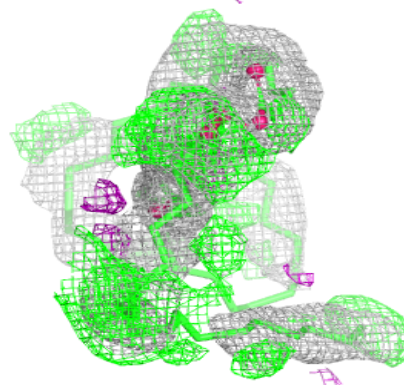
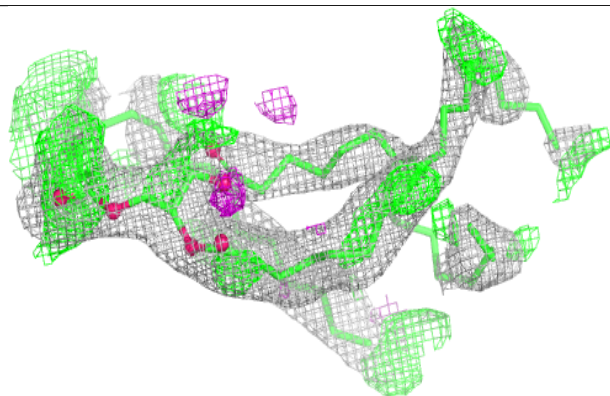
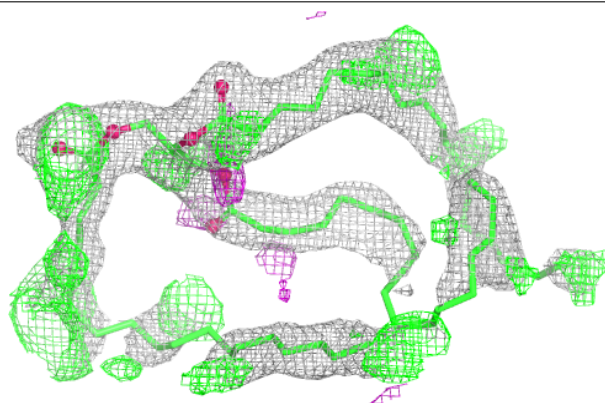


Electron density around PGV N 606:

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

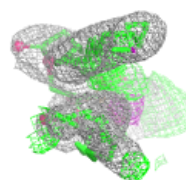
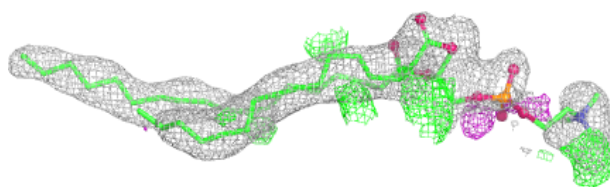
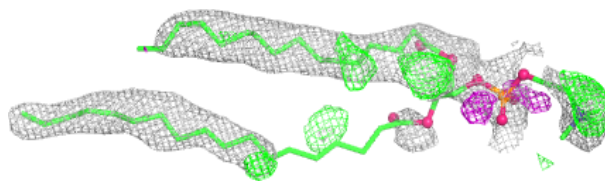
**Electron density around TGL A 606:**

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

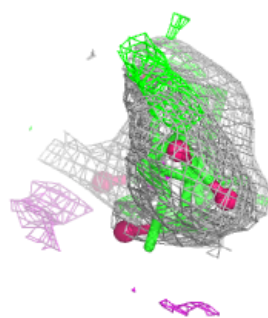
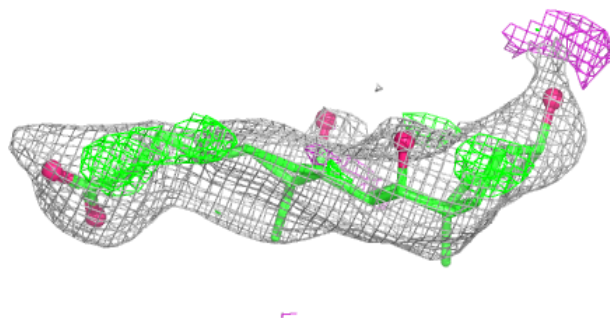
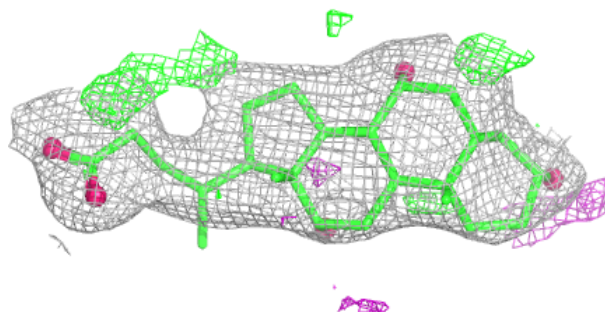


Electron density around PSC O 304:

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

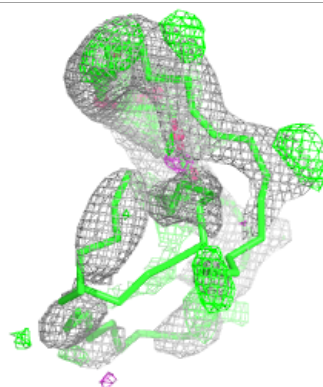
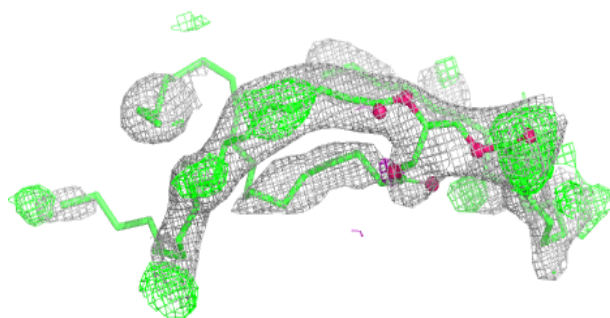
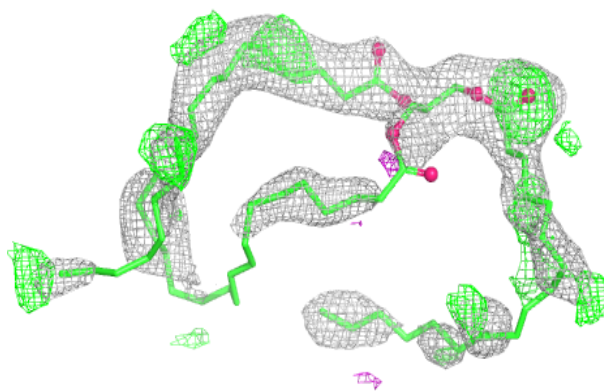
**Electron density around CHD P 306:**

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

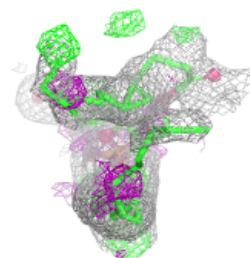
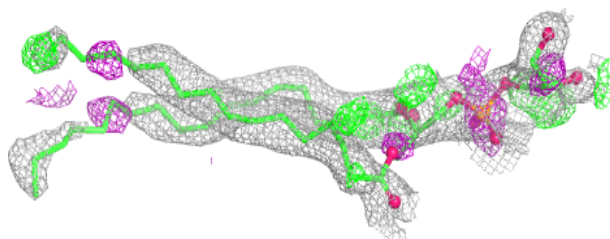
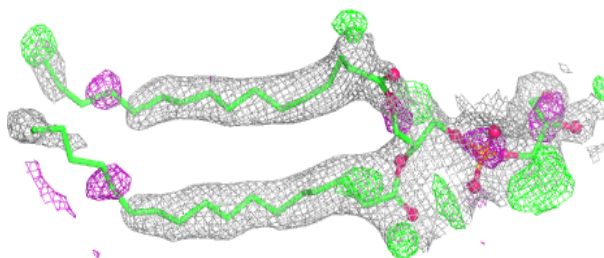


Electron density around TGL O 302:

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

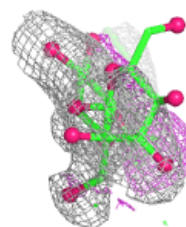
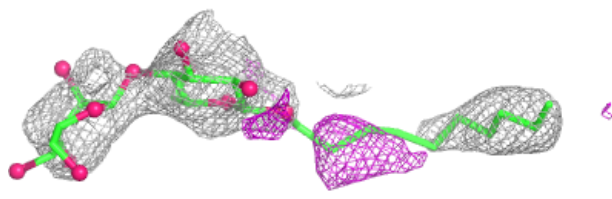
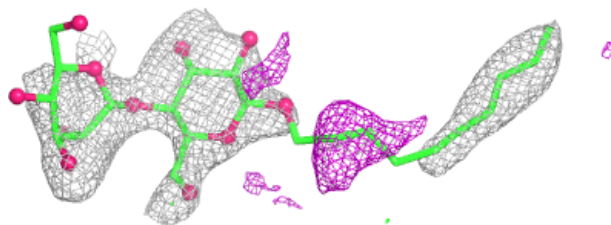
**Electron density around PGV M 101:**

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

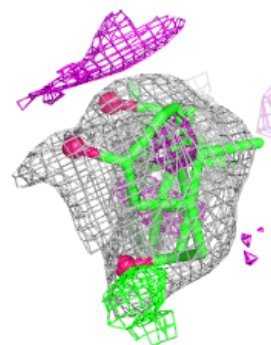
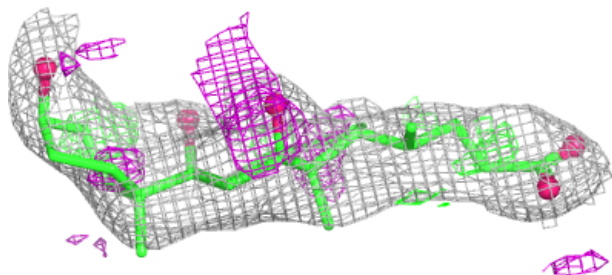
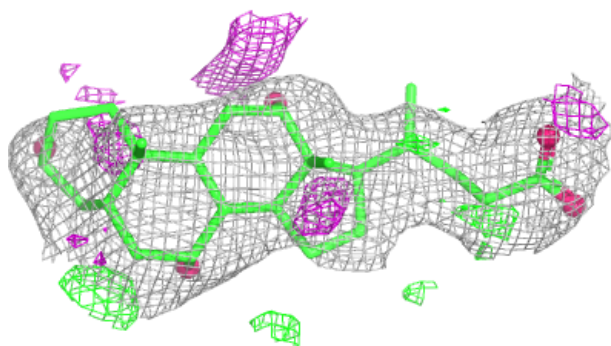


Electron density around DMU P 309:

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

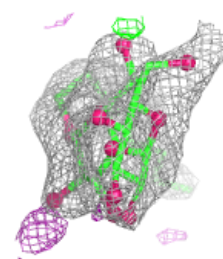
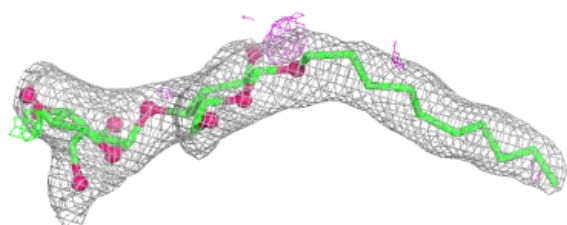
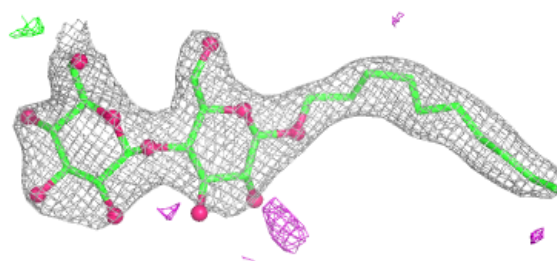
**Electron density around CHD C 308:**

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

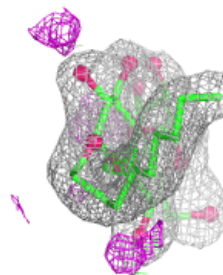
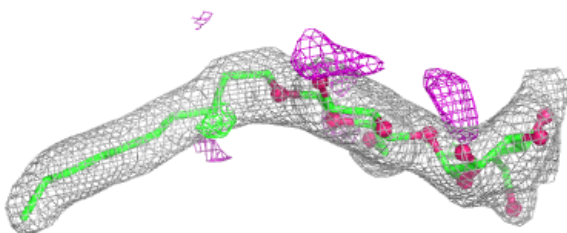
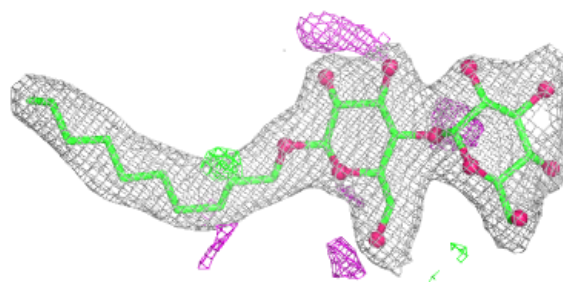


Electron density around DMU Z 101:

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

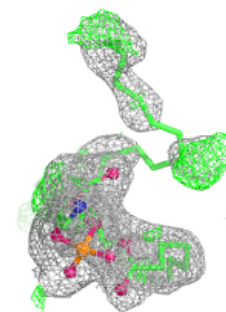
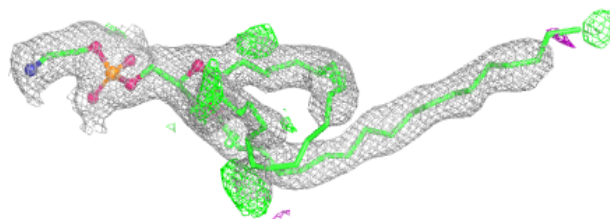
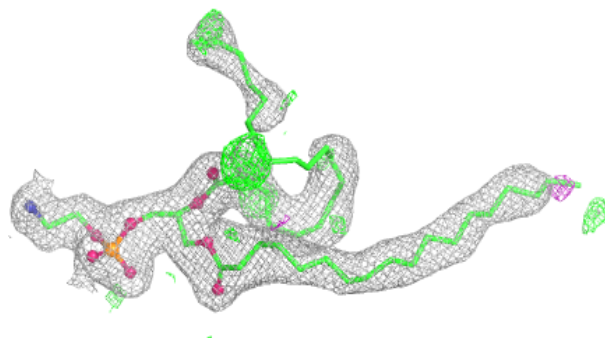
**Electron density around DMU M 102:**

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

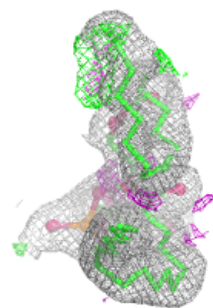
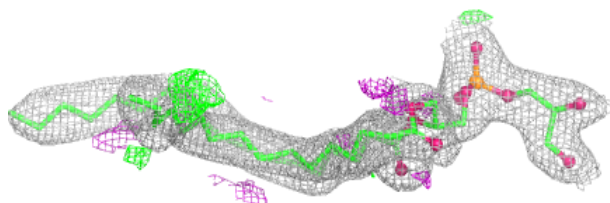
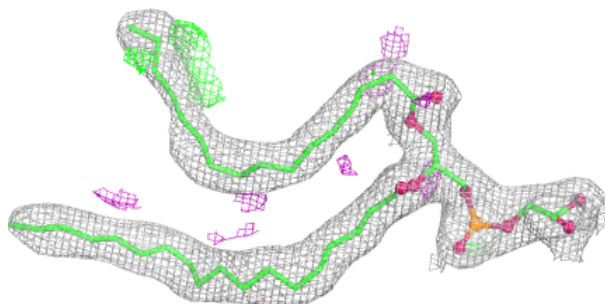


Electron density around PEK T 102:

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

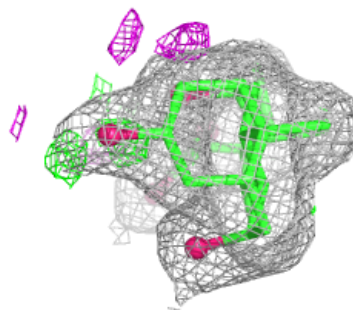
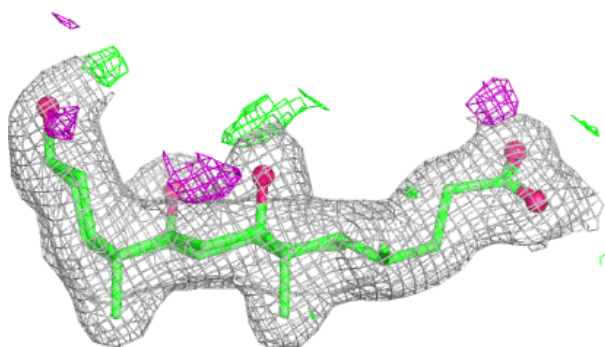
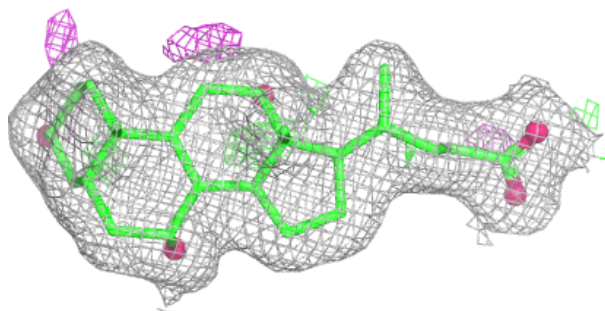
**Electron density around PGV N 607:**

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

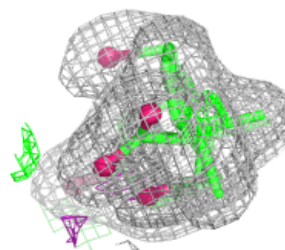
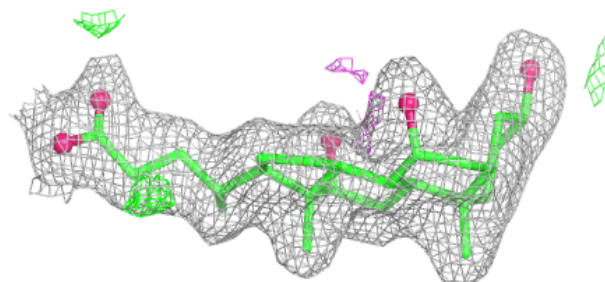
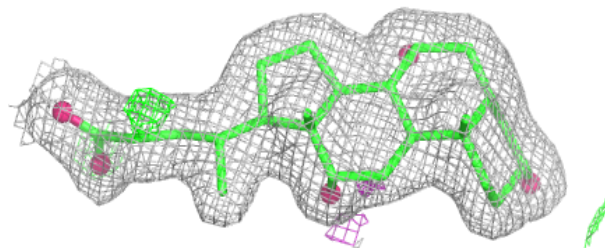


Electron density around CHD B 302:

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

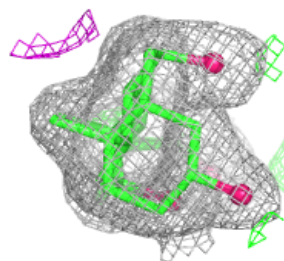
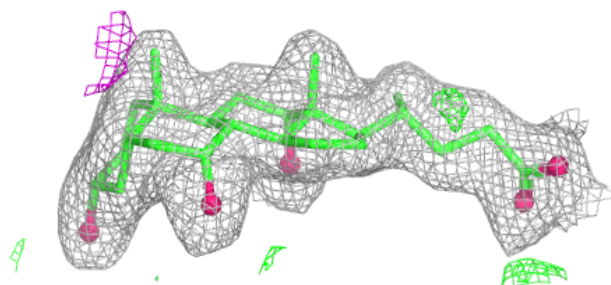
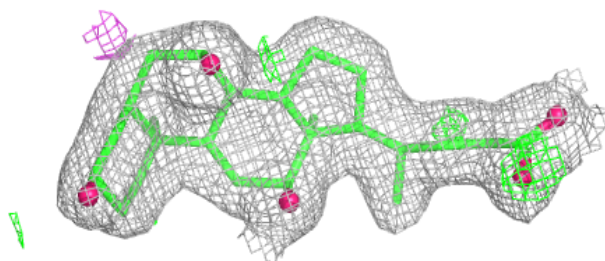
**Electron density around CHD C 301:**

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

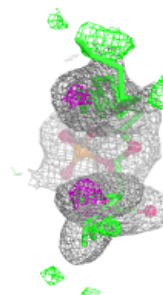
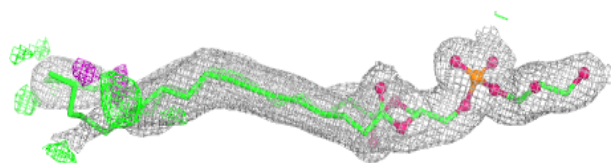
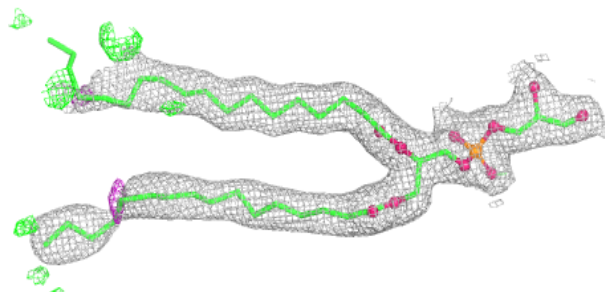


Electron density around CHD P 301:

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

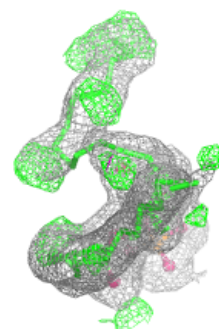
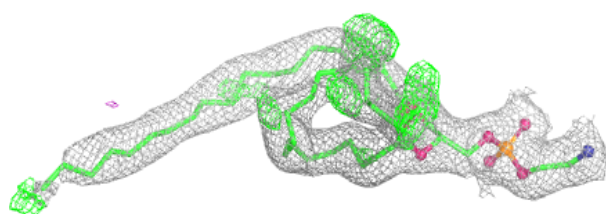
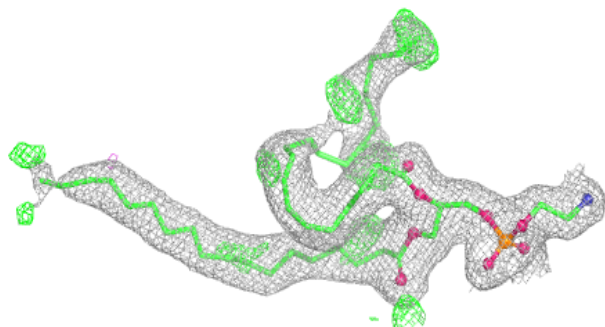
**Electron density around PGV C 305:**

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

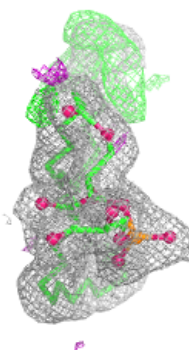
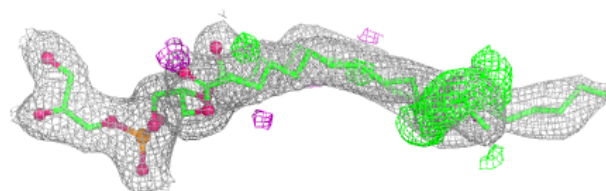
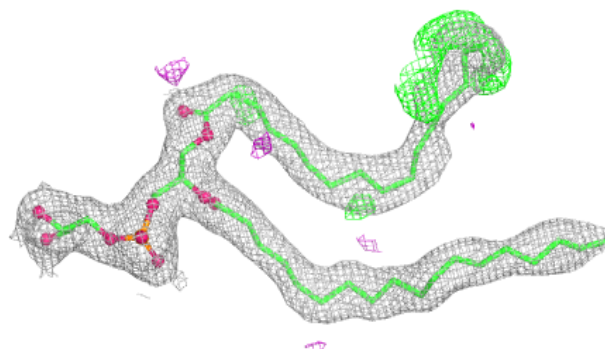


Electron density around PEK C 303:

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

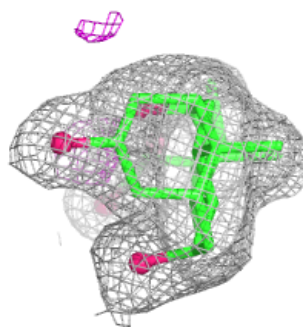
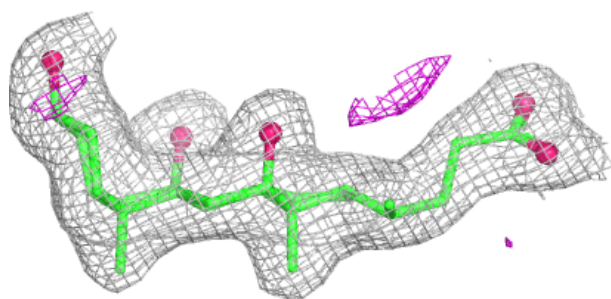
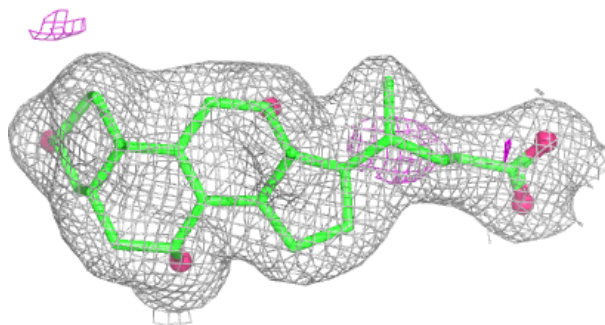
**Electron density around PGV A 607:**

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

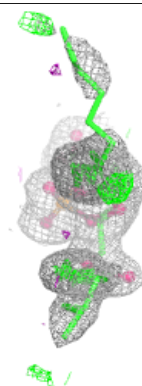
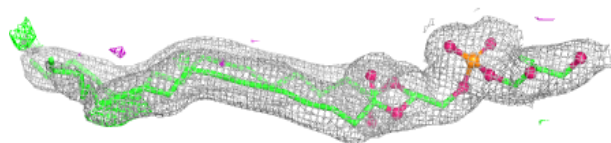
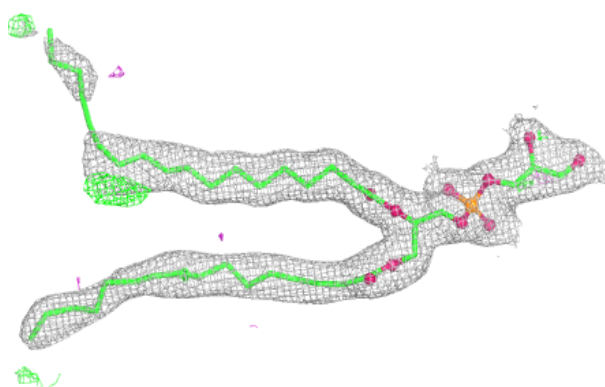


Electron density around CHD O 301:

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

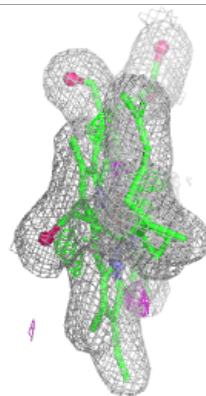
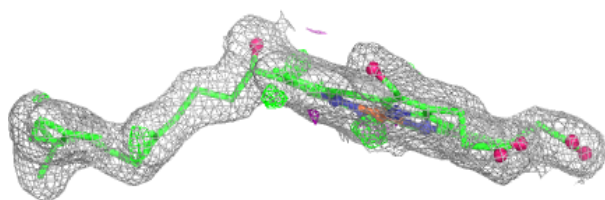
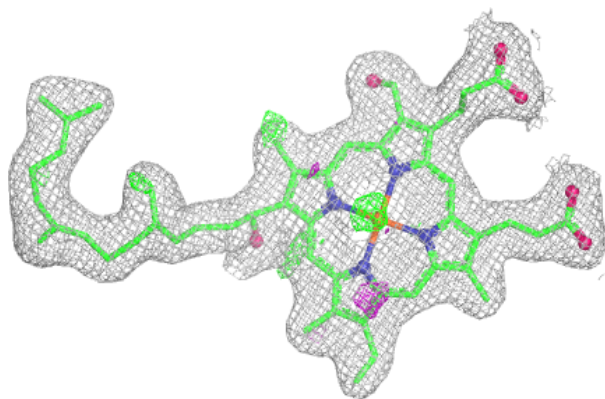
**Electron density around PGV P 303:**

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

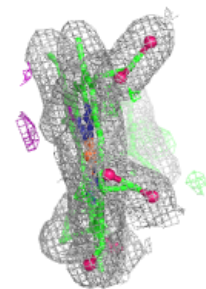
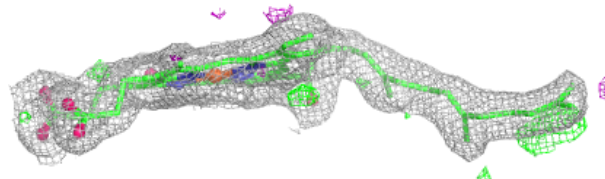
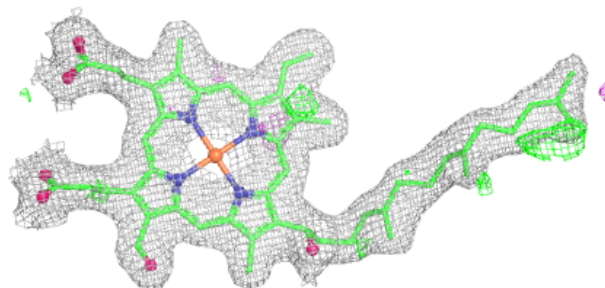


Electron density around HEA N 602:

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

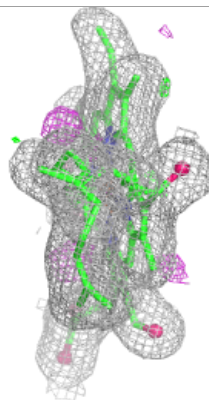
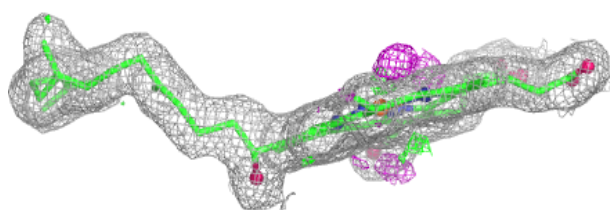
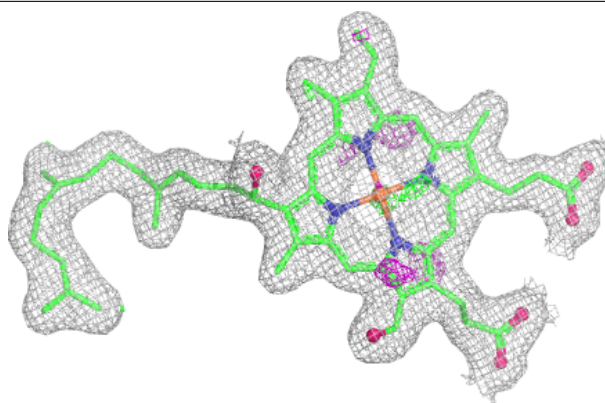
**Electron density around HEA A 601:**

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

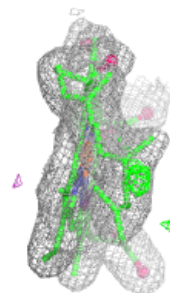
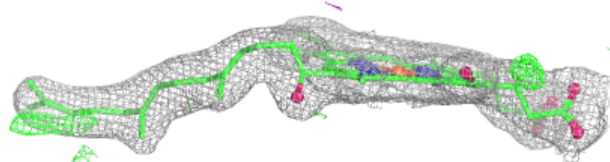
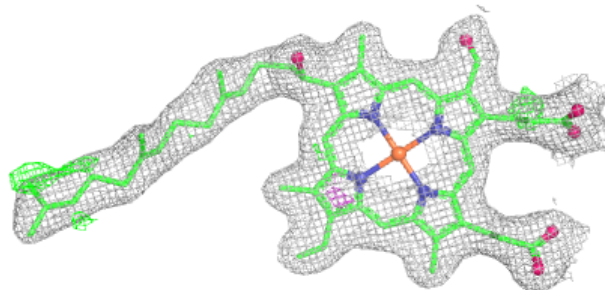


Electron density around HEA A 602:

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

**Electron density around HEA N 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.