



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:48 AM UTC

PDB ID : 3AG3 / pdb_00003ag3
Title : Bovine Heart Cytochrome c Oxidase in the Nitric Oxide-bound Fully Reduced State at 100 K
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-03-19
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

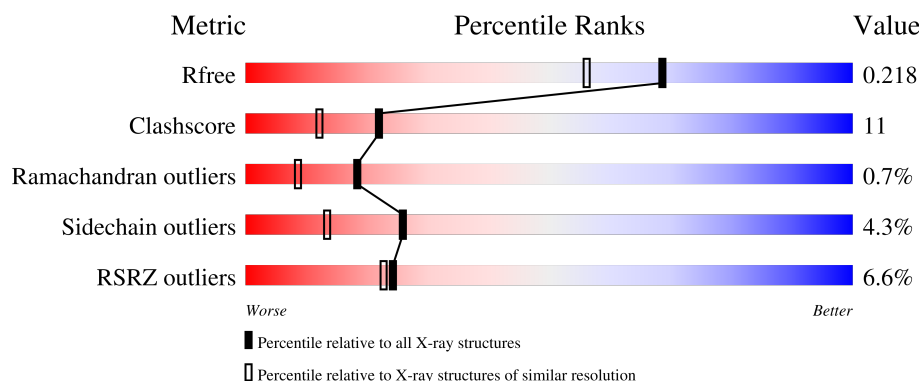
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



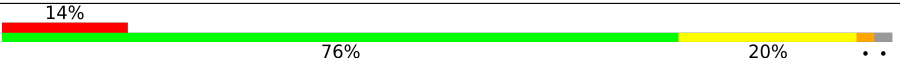
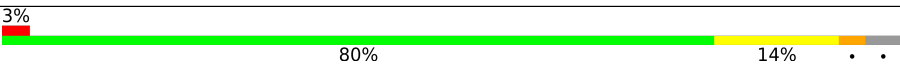
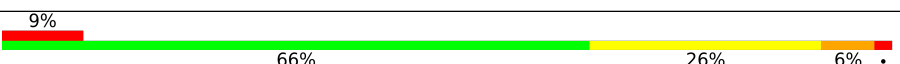
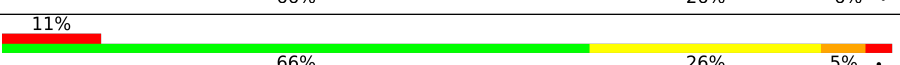
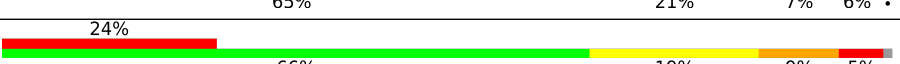
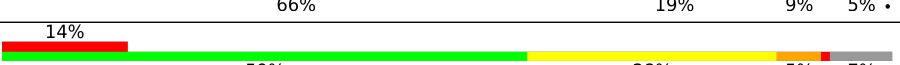
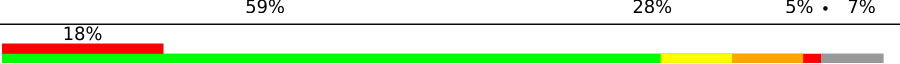
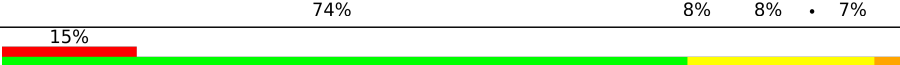
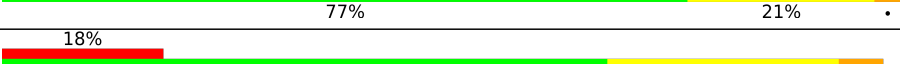
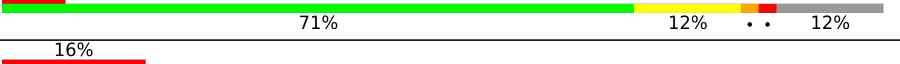
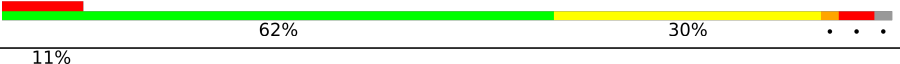
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	% 70% 25% ..
1	N	514	2% 68% 28% ..
2	B	227	6% 67% 24% 7% .
2	O	227	7% 69% 28% ..

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Mol	Chain	Length	Quality of chain
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	FME	N	1	-	X	-	-
2	FME	B	1	-	X	-	-
22	PSC	B	229	-	-	X	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1059	X	-	-	-
24	UNX	C	262	-	-	-	X
24	UNX	P	262	-	-	-	X
25	PEK	G	1263	-	-	X	-
25	PEK	T	263	-	-	X	-
26	CDL	C	270	-	-	X	-
26	CDL	G	269	-	-	X	-
26	CDL	P	1270	-	-	X	-
26	CDL	T	1269	-	-	X	-
28	DMU	G	272	X	-	-	-
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	-
28	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32545 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	5	0
			4060	2712	628	684	36			
1	N	514	Total	C	N	O	S	0	5	0
			4060	2712	628	684	36			

- 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	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- 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	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

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.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

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

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

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

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

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

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide 7A1.

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

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

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

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			

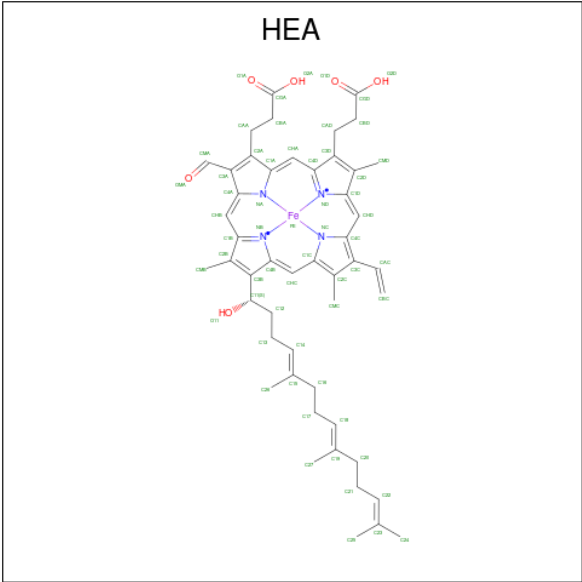
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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	0	0
			380	254	64	60	2			

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

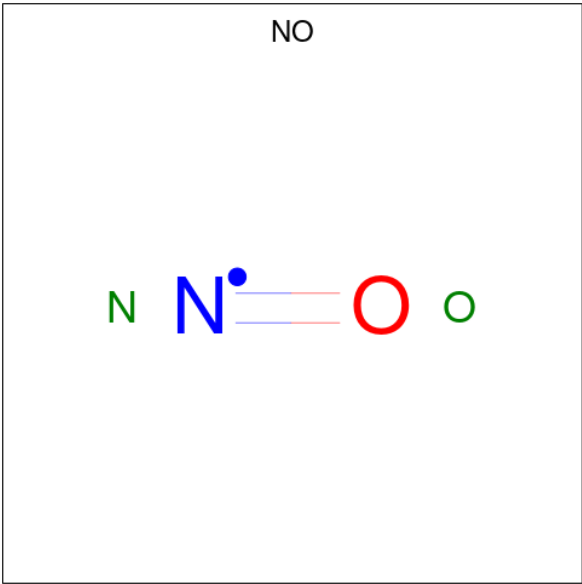
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is NITRIC OXIDE (CCD ID: NO) (formula: NO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	N	O	0	0
			2	1	1		
15	N	1	Total	N	O	0	0
			2	1	1		

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

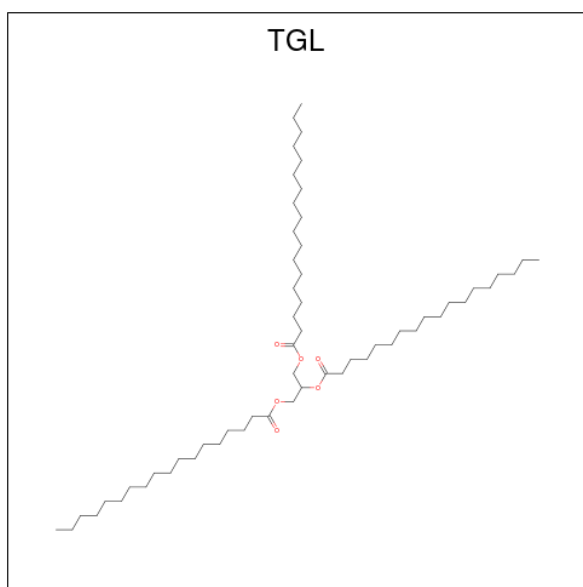
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (CCD ID: NA) (formula: Na).

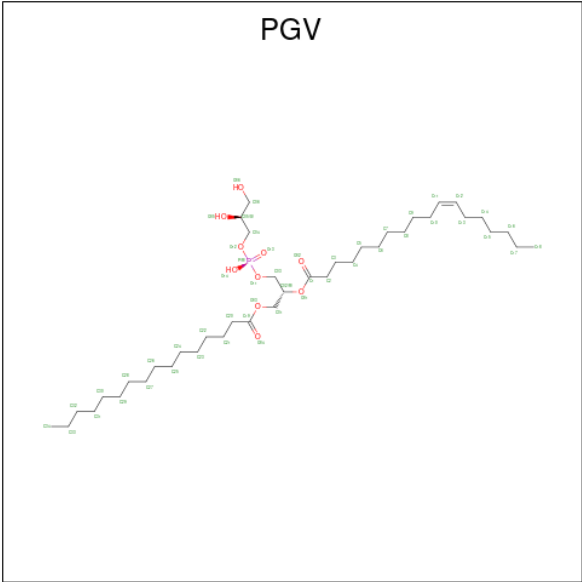
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		

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



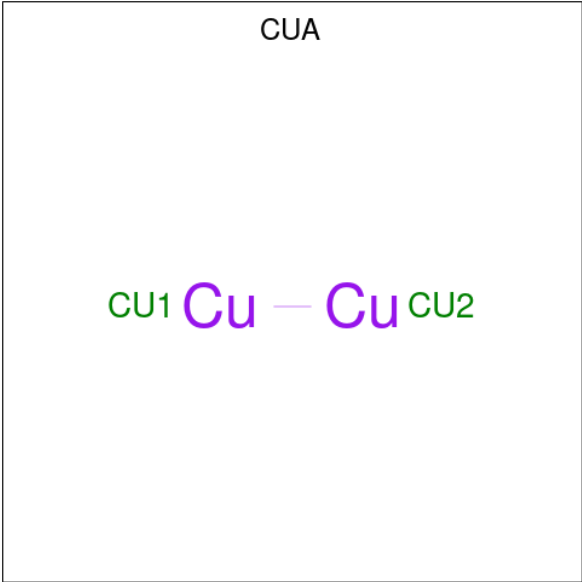
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

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



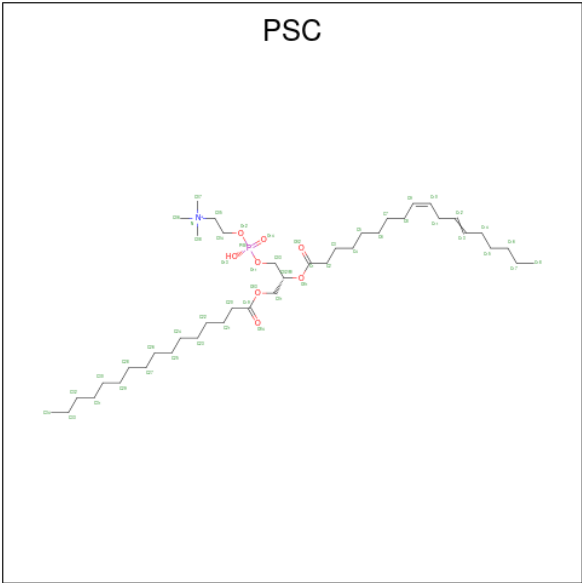
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	M	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

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



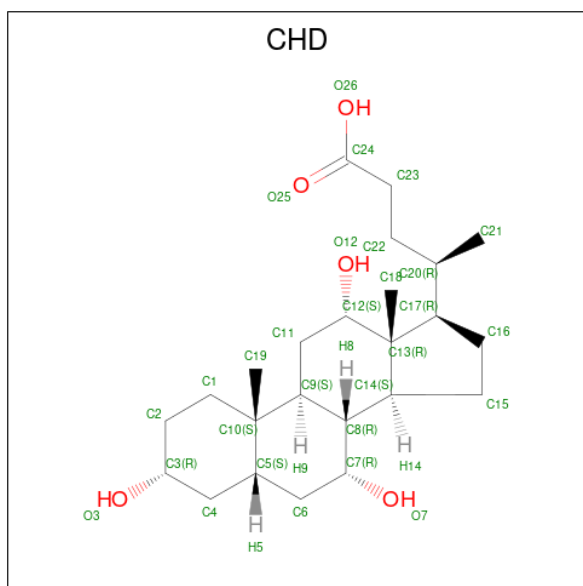
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).

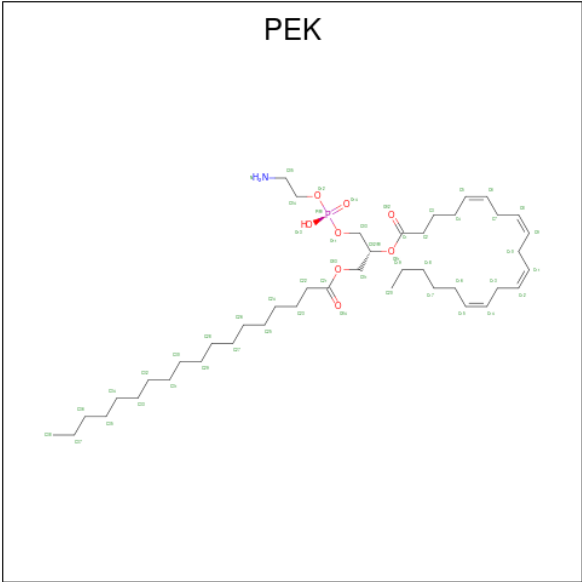


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	O	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0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

- Molecule 24 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

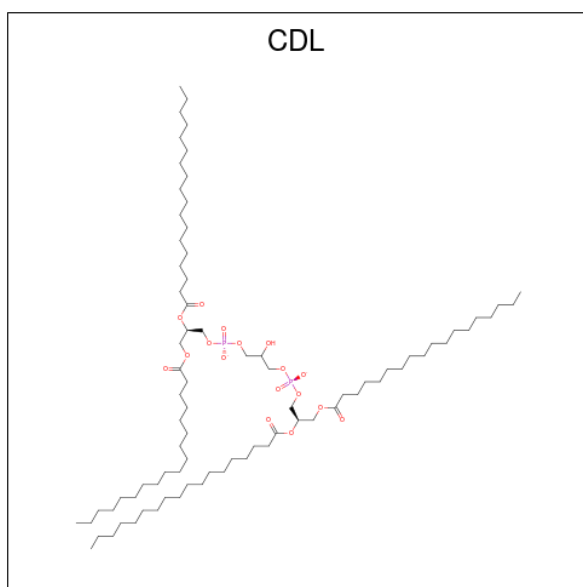
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	C	1	Total	X	0	0
			1	1		
24	P	1	Total	X	0	0
			1	1		

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYL)OXY]METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



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

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).

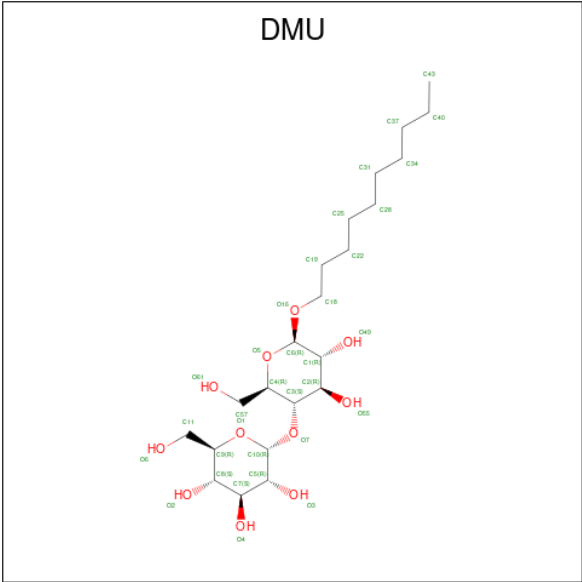


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- 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 DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	218	Total	O	0	0
			218	218		
29	B	143	Total	O	0	0
			143	143		
29	C	116	Total	O	0	0
			116	116		
29	D	80	Total	O	0	0
			80	80		
29	E	49	Total	O	0	0
			49	49		
29	F	61	Total	O	0	0
			61	61		
29	G	45	Total	O	0	0
			45	45		
29	H	51	Total	O	0	0
			51	51		

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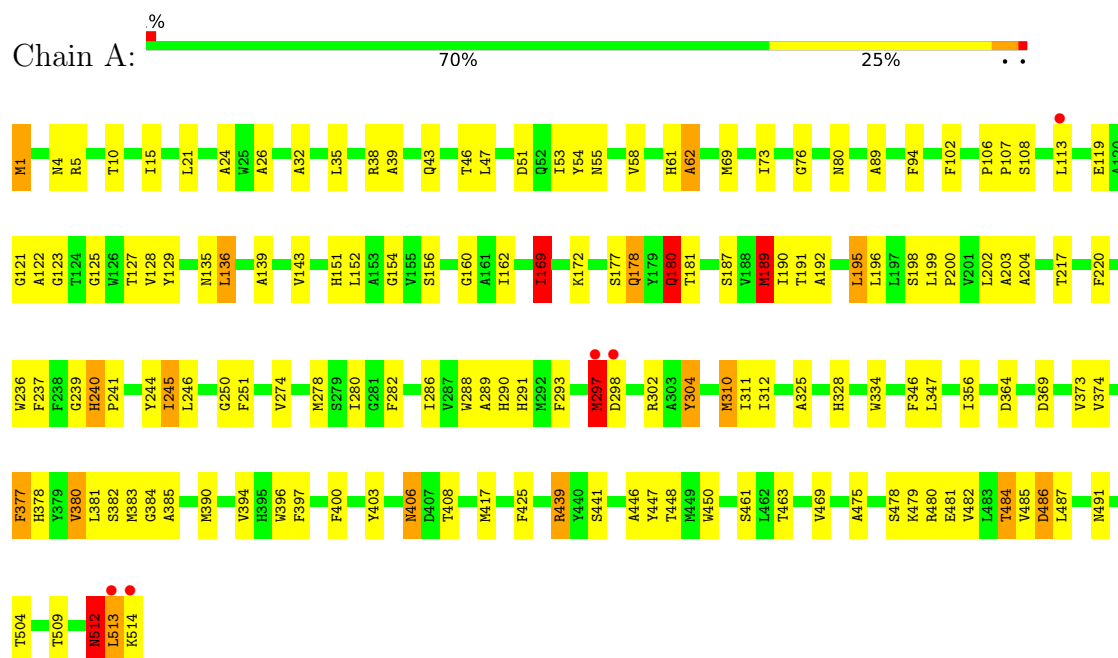
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	I	37	Total 37	O 37	0	0
29	J	24	Total 24	O 24	0	0
29	K	29	Total 29	O 29	0	0
29	L	23	Total 23	O 23	0	0
29	M	31	Total 31	O 31	0	0
29	N	222	Total 222	O 222	0	0
29	O	137	Total 137	O 137	0	0
29	P	102	Total 102	O 102	0	0
29	Q	65	Total 65	O 65	0	0
29	R	47	Total 47	O 47	0	0
29	S	64	Total 64	O 64	0	0
29	T	47	Total 47	O 47	0	0
29	U	49	Total 49	O 49	0	0
29	V	27	Total 27	O 27	0	0
29	W	19	Total 19	O 19	0	0
29	X	22	Total 22	O 22	0	0
29	Y	21	Total 21	O 21	0	0
29	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

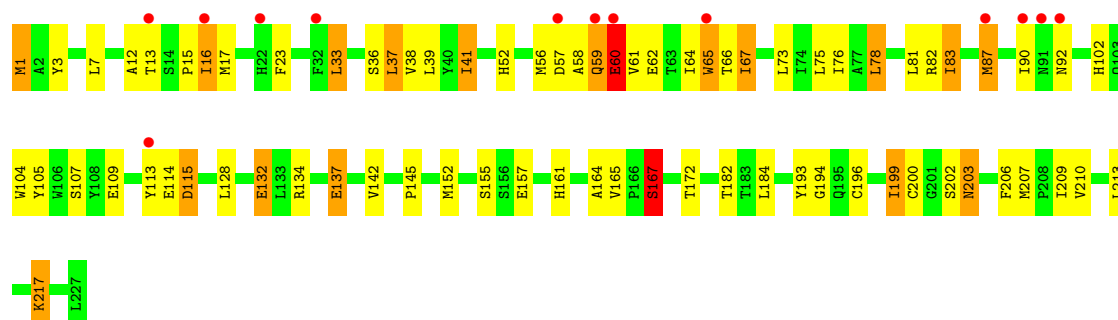


• Molecule 1: Cytochrome c oxidase subunit 1

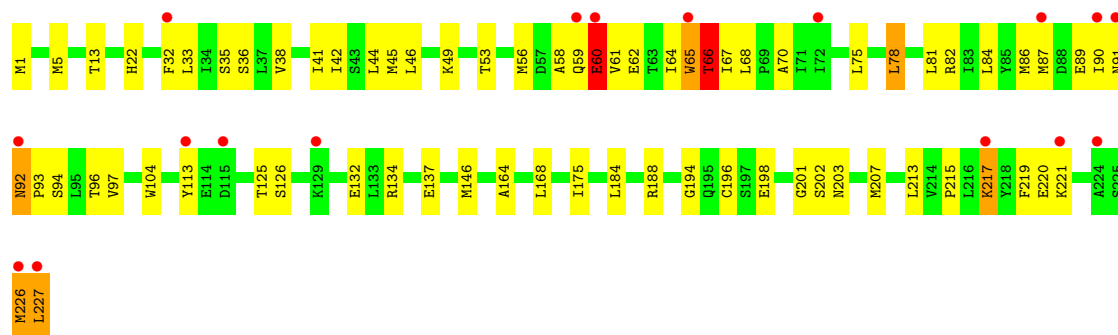




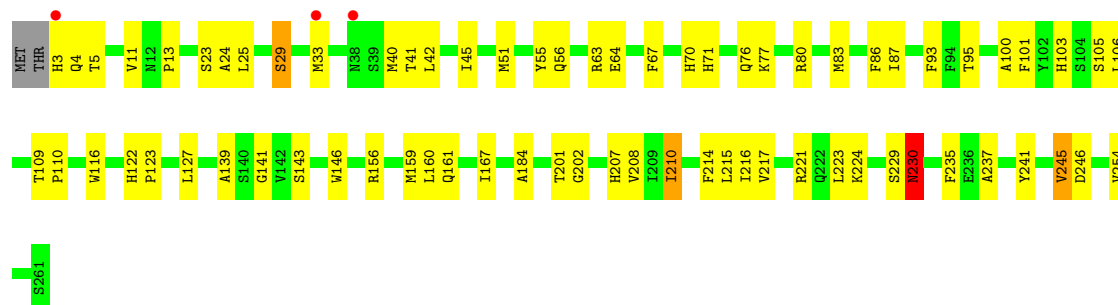
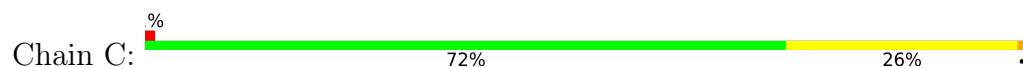
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

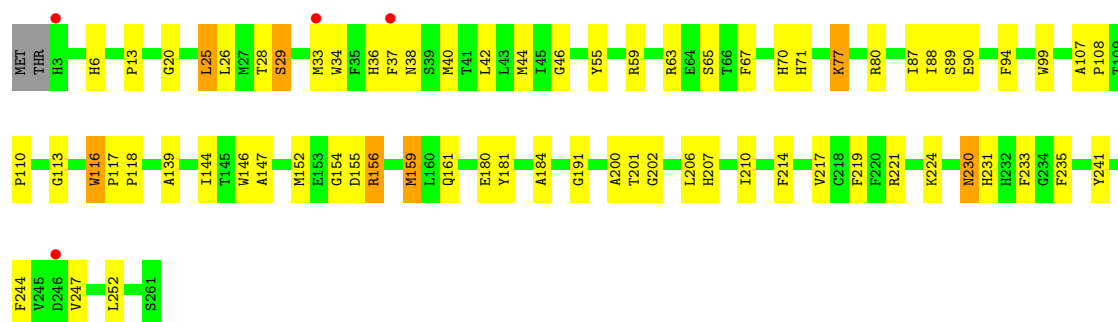


• Molecule 3: Cytochrome c oxidase subunit 3

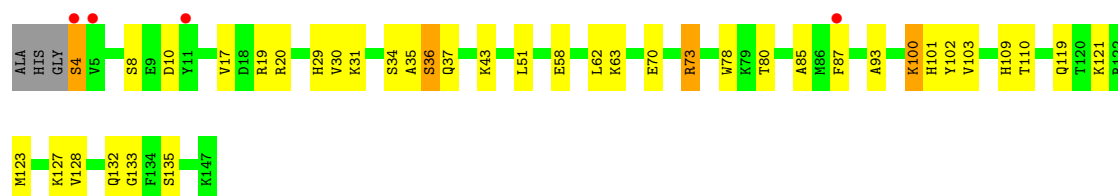


• Molecule 3: Cytochrome c oxidase subunit 3

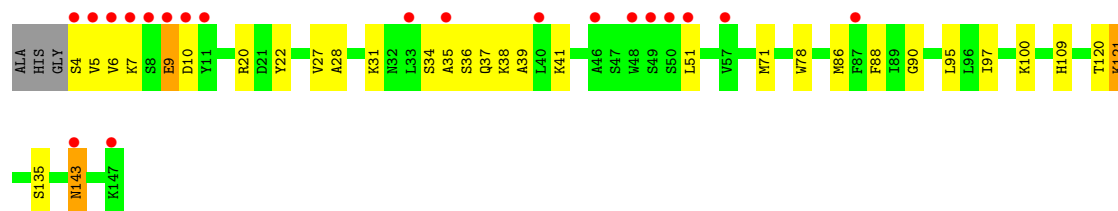
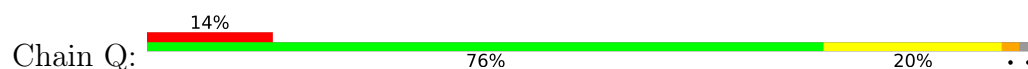




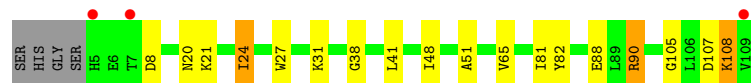
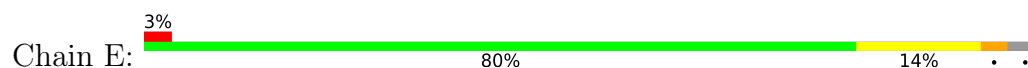
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



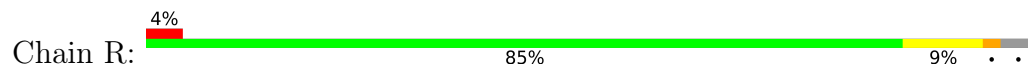
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



- Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 5: Cytochrome c oxidase subunit 5A

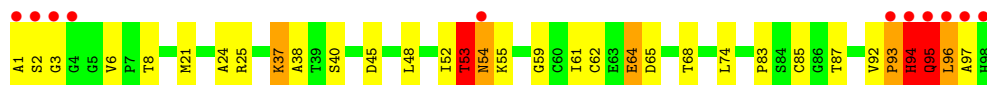


- Molecule 6: Cytochrome c oxidase subunit 5B





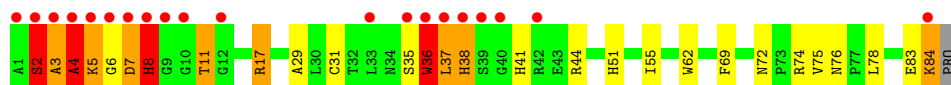
- Molecule 6: Cytochrome c oxidase subunit 5B



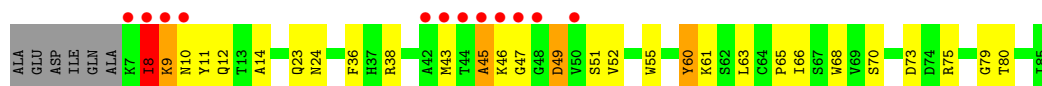
- Molecule 7: Cytochrome c oxidase subunit 6A2



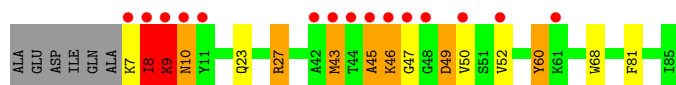
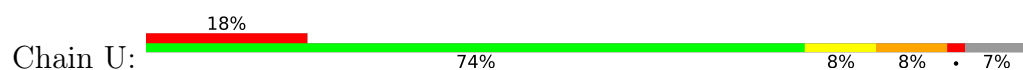
- Molecule 7: Cytochrome c oxidase subunit 6A2



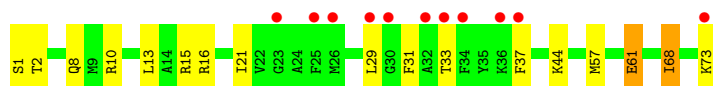
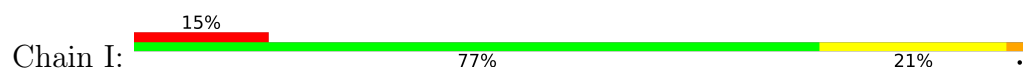
- Molecule 8: Cytochrome c oxidase subunit 6B1



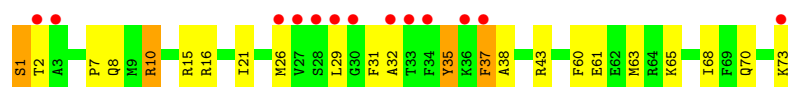
- Molecule 8: Cytochrome c oxidase subunit 6B1



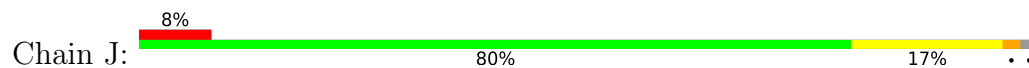
- Molecule 9: Cytochrome c oxidase subunit 6C



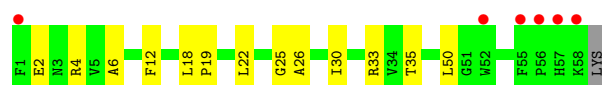
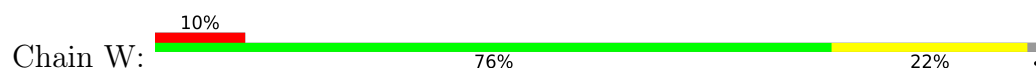
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase polypeptide 7A1



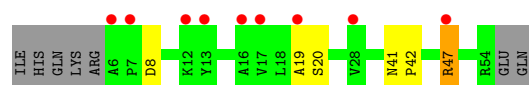
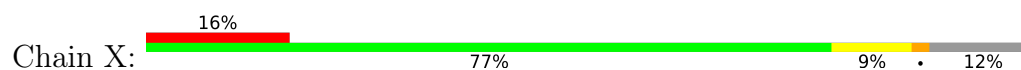
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



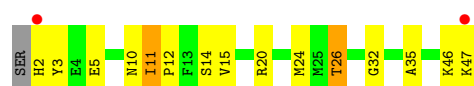
- Molecule 11: Cytochrome c oxidase subunit 7B



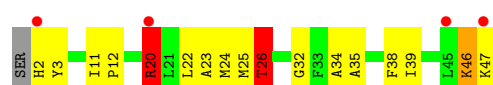
- Molecule 11: Cytochrome c oxidase subunit 7B



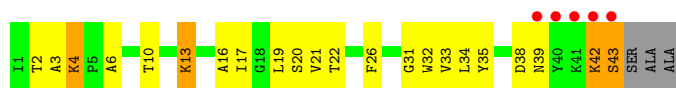
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 12: Cytochrome c oxidase subunit 7C



● Molecule 13: Cytochrome c oxidase subunit 8B



● Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.29Å 208.36Å 177.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 40.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 99.6 (40.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.175 , 0.203 0.192 , 0.218	Depositor DCC
R_{free} test set	30652 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32545	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: HEA, FME, DMU, CUA, TPO, TGL, MG, NO, PSC, PEK, ZN, NA, SAC, CU, UNX, CHD, CDL, PGV

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	2.11	101/4189 (2.4%)	1.68	50/5722 (0.9%)
1	N	2.11	94/4189 (2.2%)	1.64	55/5722 (1.0%)
2	B	2.10	46/1860 (2.5%)	1.70	20/2534 (0.8%)
2	O	1.85	24/1860 (1.3%)	1.57	16/2534 (0.6%)
3	C	1.88	36/2197 (1.6%)	1.55	20/3005 (0.7%)
3	P	1.93	38/2197 (1.7%)	1.54	21/3005 (0.7%)
4	D	1.90	19/1229 (1.5%)	1.52	22/1658 (1.3%)
4	Q	1.67	9/1229 (0.7%)	1.42	14/1658 (0.8%)
5	E	1.80	8/871 (0.9%)	1.48	6/1182 (0.5%)
5	R	1.59	5/871 (0.6%)	1.37	3/1182 (0.3%)
6	F	2.12	20/765 (2.6%)	1.67	10/1038 (1.0%)
6	S	1.97	15/765 (2.0%)	1.76	18/1038 (1.7%)
7	G	1.99	15/690 (2.2%)	1.67	10/937 (1.1%)
7	T	1.86	12/690 (1.7%)	1.64	12/937 (1.3%)
8	H	1.90	16/682 (2.3%)	1.48	4/921 (0.4%)
8	U	1.54	5/682 (0.7%)	1.44	5/921 (0.5%)
9	I	1.69	5/605 (0.8%)	1.38	2/802 (0.2%)
9	V	1.68	3/605 (0.5%)	1.45	4/802 (0.5%)
10	J	1.61	2/471 (0.4%)	1.48	3/636 (0.5%)
10	W	1.81	8/471 (1.7%)	1.46	2/636 (0.3%)
11	K	1.78	4/398 (1.0%)	1.59	7/546 (1.3%)
11	X	1.49	2/398 (0.5%)	1.39	2/546 (0.4%)
12	L	1.87	5/393 (1.3%)	1.56	4/526 (0.8%)
12	Y	1.92	8/393 (2.0%)	1.51	1/526 (0.2%)
13	M	2.02	10/345 (2.9%)	1.54	2/470 (0.4%)
13	Z	1.72	6/345 (1.7%)	1.48	1/470 (0.2%)
All	All	1.93	516/29390 (1.8%)	1.58	314/39954 (0.8%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	1	0
6	F	0	1
6	S	0	1
All	All	1	3

The worst 5 of 516 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	512	ASN	CA-CB	11.95	1.72	1.53
1	N	310	MET	SD-CE	-10.19	1.54	1.79
1	A	482	VAL	CA-CB	10.15	1.64	1.54
1	N	189	MET	CB-CG	10.09	1.82	1.52
6	S	54	ASN	CB-CG	-10.08	1.26	1.52

The worst 5 of 314 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	54	ASN	CB-CA-C	-11.26	88.11	109.72
7	G	17	ARG	NE-CZ-NH2	-11.19	109.13	119.20
7	T	17	ARG	NE-CZ-NH2	-10.77	109.50	119.20
4	D	20	ARG	NE-CZ-NH2	-10.56	109.69	119.20
1	N	250	GLY	N-CA-C	-10.31	99.57	112.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	66	THR	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	TYR	Sidechain
6	F	93	PRO	Peptide
6	S	93	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4060	0	4037	59	0
1	N	4060	0	4037	71	0
2	B	1824	0	1833	30	0
2	O	1824	0	1833	37	1
3	C	2110	0	2027	30	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	12	0
4	Q	1195	0	1183	11	0
5	E	852	0	845	8	0
5	R	852	0	845	8	1
6	F	748	0	728	17	0
6	S	748	0	728	19	1
7	G	675	0	643	43	0
7	T	675	0	643	51	0
8	H	662	0	623	13	0
8	U	662	0	623	12	0
9	I	601	0	613	6	1
9	V	601	0	613	16	0
10	J	460	0	459	4	0
10	W	460	0	459	6	0
11	K	384	0	366	1	0
11	X	384	0	366	4	0
12	L	380	0	380	10	0
12	Y	380	0	380	11	0
13	M	335	0	352	10	0
13	Z	335	0	352	3	0
14	A	120	0	107	6	0
14	N	120	0	108	3	0
15	A	2	0	0	0	0
15	N	2	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	8	0
19	L	63	0	110	15	0
19	N	63	0	110	15	0
19	O	63	0	110	10	0
19	Q	63	0	110	12	0
20	A	51	0	76	0	0
20	C	102	0	152	8	0
20	M	51	0	76	15	0
20	N	102	0	152	9	0
20	P	102	0	152	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	26	0
22	R	52	0	80	15	0
23	B	29	0	36	2	0
23	C	58	0	73	4	0
23	J	29	0	36	1	0
23	O	29	0	39	3	0
23	P	58	0	73	6	0
23	W	29	0	36	1	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	53	0	77	8	0
25	G	106	0	154	43	0
25	P	106	0	154	24	0
25	T	53	0	77	21	0
26	C	100	0	156	25	0
26	G	100	0	156	30	0
26	P	100	0	156	25	0
26	T	100	0	156	27	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	37	4	0
28	M	33	0	37	0	0
28	P	33	0	39	6	0
28	Z	33	0	38	2	0
29	A	218	0	0	6	0
29	B	143	0	0	7	0
29	C	116	0	0	3	0
29	D	80	0	0	3	0
29	E	49	0	0	0	0
29	F	61	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	G	45	0	0	2	0
29	H	51	0	0	1	0
29	I	37	0	0	2	0
29	J	24	0	0	0	0
29	K	29	0	0	0	0
29	L	23	0	0	1	0
29	M	31	0	0	2	0
29	N	222	0	0	7	0
29	O	137	0	0	5	0
29	P	102	0	0	0	0
29	Q	65	0	0	3	0
29	R	47	0	0	0	0
29	S	64	0	0	0	0
29	T	47	0	0	2	0
29	U	49	0	0	2	0
29	V	27	0	0	2	0
29	W	19	0	0	0	0
29	X	22	0	0	3	0
29	Y	21	0	0	1	0
29	Z	14	0	0	1	0
All	All	32545	0	31351	662	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 662 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)
25:P:1265:PEK:H383	26:T:1269:CDL:C27	1.21	1.67
1:N:484:THR:CB	1:N:484:THR:CG2	1.77	1.60
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.70	1.55
1:N:189:MET:CG	1:N:189:MET:CB	1.82	1.52
4:Q:121:LYS:NZ	4:Q:121:LYS:CE	1.74	1.50

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:OG1	5:R:80:GLU:OE1[3_647]	1.64	0.56
2:O:126:SER:O	6:S:94:HIS:CB[2_684]	2.11	0.09

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	517/514 (101%)	504 (98%)	13 (2%)	0	100	100
1	N	517/514 (101%)	501 (97%)	16 (3%)	0	100	100
2	B	225/227 (99%)	220 (98%)	4 (2%)	1 (0%)	30	19
2	O	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	30	19
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	135 (95%)	6 (4%)	1 (1%)	18	8
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	0
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	0
7	G	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	1	0
7	T	81/85 (95%)	69 (85%)	8 (10%)	4 (5%)	1	0
8	H	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	1	0
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	1	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3514/3614 (97%)	3380 (96%)	108 (3%)	26 (1%)	18	8

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS

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	430/426 (101%)	415 (96%)	15 (4%)	32	19
1	N	430/426 (101%)	420 (98%)	10 (2%)	44	33
2	B	210/210 (100%)	200 (95%)	10 (5%)	23	11
2	O	210/210 (100%)	199 (95%)	11 (5%)	21	9
3	C	224/226 (99%)	222 (99%)	2 (1%)	70	67
3	P	224/226 (99%)	219 (98%)	5 (2%)	45	34
4	D	128/129 (99%)	124 (97%)	4 (3%)	35	23
4	Q	128/129 (99%)	122 (95%)	6 (5%)	23	11
5	E	92/95 (97%)	91 (99%)	1 (1%)	65	60
5	R	92/95 (97%)	90 (98%)	2 (2%)	45	34
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	18
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	4
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	2
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	2
8	H	71/75 (95%)	67 (94%)	4 (6%)	19	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	8
9	I	57/57 (100%)	49 (86%)	8 (14%)	3	1
9	V	57/57 (100%)	50 (88%)	7 (12%)	4	1
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	38
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	38
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	9
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	9
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	28
12	Y	39/40 (98%)	35 (90%)	4 (10%)	7	2
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	1
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	1
All	All	3048/3082 (99%)	2917 (96%)	131 (4%)	26	13

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	V	29	LEU
10	W	50	LEU
13	Z	43	SER
9	I	33	THR
9	I	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	180	GLN
3	P	68	GLN
8	U	31	GLN
1	N	422	ASN
2	O	181	GLN

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$
9	SAC	I	1	9	7,8,9	2.78	2 (28%)	7,9,11	2.02	3 (42%)
7	TPO	T	11	7	8,10,11	3.30	5 (62%)	10,14,16	2.22	5 (50%)
1	FME	A	1	1	8,9,10	2.15	2 (25%)	8,9,11	8.37	5 (62%)
1	FME	N	1	1	8,9,10	1.15	1 (12%)	8,9,11	7.49	5 (62%)
7	TPO	G	11	7	8,10,11	3.05	6 (75%)	10,14,16	1.74	3 (30%)
9	SAC	V	1	9	7,8,9	3.10	2 (28%)	7,9,11	3.06	2 (28%)
2	FME	B	1	2	8,9,10	3.71	6 (75%)	8,9,11	7.39	6 (75%)
2	FME	O	1	2	8,9,10	1.79	3 (37%)	8,9,11	6.12	3 (37%)

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

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-OG1	7.13	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CN-N	6.83	1.55	1.33
9	V	1	SAC	CA-N	5.92	1.55	1.46
7	G	11	TPO	P-OG1	5.87	1.69	1.59
1	A	1	FME	CA-N	5.34	1.54	1.46

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CA-N-CN	-22.50	88.22	122.82
1	N	1	FME	CA-N-CN	-19.41	92.96	122.82
2	O	1	FME	CA-N-CN	-16.83	96.94	122.82
2	B	1	FME	CA-N-CN	-13.91	101.44	122.82
2	B	1	FME	O1-CN-N	-13.08	91.52	125.32

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	2	0
1	A	1	FME	3	0
1	N	1	FME	2	0
7	G	11	TPO	3	0
9	V	1	SAC	1	0
2	B	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 46 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
26	CDL	T	1269	-	99,99,99	1.47	12 (12%)	105,111,111	1.71	21 (20%)
23	CHD	C	271	-	32,32,32	1.10	2 (6%)	51,51,51	5.03	32 (62%)
23	CHD	C	525	-	32,32,32	1.79	8 (25%)	51,51,51	5.08	35 (68%)
23	CHD	P	1525	-	32,32,32	2.00	13 (40%)	51,51,51	5.47	37 (72%)
21	CUA	O	228	2	0,1,1	-	-	-	-	-
26	CDL	P	1270	-	99,99,99	1.59	15 (15%)	105,111,111	1.89	23 (21%)
23	CHD	P	1271	-	32,32,32	0.99	1 (3%)	51,51,51	5.17	35 (68%)
20	PGV	P	1267	-	50,50,50	1.04	2 (4%)	53,56,56	1.67	11 (20%)
21	CUA	B	228	2	0,1,1	-	-	-	-	-
20	PGV	A	522	-	50,50,50	1.20	4 (8%)	53,56,56	1.53	9 (16%)
26	CDL	C	270	-	99,99,99	1.58	15 (15%)	105,111,111	1.84	19 (18%)
26	CDL	G	269	-	99,99,99	1.56	13 (13%)	105,111,111	1.60	22 (20%)
25	PEK	C	264	-	52,52,52	1.16	5 (9%)	55,57,57	2.19	12 (21%)
15	NO	A	520	14,16	0,1,1	-	-	-	-	-
25	PEK	G	265	-	52,52,52	1.51	4 (7%)	55,57,57	1.66	9 (16%)
19	TGL	N	1522	-	62,62,62	1.72	10 (16%)	65,65,65	1.97	17 (26%)
25	PEK	P	1264	-	52,52,52	0.97	2 (3%)	55,57,57	2.26	12 (21%)
28	DMU	G	272	-	34,34,34	1.47	6 (17%)	45,45,45	3.58	24 (53%)
28	DMU	P	1272	-	34,34,34	1.71	6 (17%)	45,45,45	3.48	27 (60%)
19	TGL	A	521	-	62,62,62	1.42	6 (9%)	65,65,65	1.80	13 (20%)
14	HEA	A	516	15,1	67,67,67	1.74	14 (20%)	81,103,103	2.69	33 (40%)
23	CHD	O	229	-	32,32,32	2.00	12 (37%)	51,51,51	5.52	32 (62%)
20	PGV	N	1266	-	50,50,50	1.25	5 (10%)	53,56,56	1.57	9 (16%)
14	HEA	N	515	1	67,67,67	1.81	18 (26%)	81,103,103	2.10	32 (39%)
20	PGV	N	1524	-	50,50,50	1.32	3 (6%)	53,56,56	1.38	8 (15%)
28	DMU	M	526	-	34,34,34	1.23	4 (11%)	45,45,45	3.60	27 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	C	267	-	50,50,50	0.92	1 (2%)	53,56,56	1.40	11 (20%)
25	PEK	P	1265	-	52,52,52	1.49	6 (11%)	55,57,57	1.54	8 (14%)
23	CHD	W	1059	-	32,32,32	1.02	1 (3%)	51,51,51	5.12	36 (70%)
20	PGV	M	524	-	50,50,50	1.23	2 (4%)	53,56,56	1.50	9 (16%)
19	TGL	L	522	-	62,62,62	1.77	7 (11%)	65,65,65	2.17	16 (24%)
15	NO	N	520	14,16	0,1,1	-	-	-	-	-
23	CHD	J	60	-	32,32,32	1.18	2 (6%)	51,51,51	5.09	33 (64%)
20	PGV	P	1268	-	50,50,50	1.49	3 (6%)	53,56,56	1.74	9 (16%)
20	PGV	C	268	-	50,50,50	1.38	4 (8%)	53,56,56	1.70	6 (11%)
19	TGL	O	1521	-	62,62,62	1.48	6 (9%)	65,65,65	1.77	12 (18%)
22	PSC	B	229	-	51,51,51	1.28	3 (5%)	57,59,59	1.25	8 (14%)
23	CHD	B	1085	-	32,32,32	2.19	11 (34%)	51,51,51	5.33	35 (68%)
25	PEK	G	1263	-	52,52,52	1.46	4 (7%)	55,57,57	1.45	7 (12%)
19	TGL	D	523	-	62,62,62	1.64	7 (11%)	65,65,65	1.76	15 (23%)
14	HEA	A	515	1	67,67,67	2.14	19 (28%)	81,103,103	2.21	26 (32%)
22	PSC	R	1229	-	51,51,51	1.43	3 (5%)	57,59,59	1.31	6 (10%)
28	DMU	Z	1526	-	34,34,34	1.15	4 (11%)	45,45,45	3.44	25 (55%)
25	PEK	T	263	-	52,52,52	1.28	4 (7%)	55,57,57	1.41	7 (12%)
14	HEA	N	516	15,1	67,67,67	1.72	20 (29%)	81,103,103	2.30	37 (45%)
19	TGL	Q	1523	-	62,62,62	1.58	7 (11%)	65,65,65	1.49	8 (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
26	CDL	T	1269	-	-	59/110/110/110	-
23	CHD	C	271	-	1/1/12/12	5/9/74/74	0/4/4/4
23	CHD	C	525	-	-	1/9/74/74	0/4/4/4
23	CHD	P	1525	-	-	4/9/74/74	0/4/4/4
26	CDL	P	1270	-	-	68/110/110/110	-
23	CHD	P	1271	-	1/1/12/12	3/9/74/74	0/4/4/4
20	PGV	P	1267	-	-	13/55/55/55	-
20	PGV	A	522	-	-	8/55/55/55	-
26	CDL	C	270	-	-	69/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	G	269	-	-	58/110/110/110	-
25	PEK	C	264	-	-	21/56/56/56	-
25	PEK	G	265	-	-	28/56/56/56	-
19	TGL	N	1522	-	-	42/65/65/65	-
28	DMU	G	272	-	6/6/10/10	11/19/59/59	0/2/2/2
28	DMU	P	1272	-	6/6/10/10	13/19/59/59	0/2/2/2
25	PEK	P	1264	-	-	22/56/56/56	-
19	TGL	A	521	-	-	39/65/65/65	-
14	HEA	A	516	15,1	-	5/36/76/76	-
23	CHD	O	229	-	-	3/9/74/74	0/4/4/4
20	PGV	N	1266	-	-	17/55/55/55	-
14	HEA	N	515	1	-	5/36/76/76	-
20	PGV	N	1524	-	-	25/55/55/55	-
28	DMU	M	526	-	4/4/10/10	7/19/59/59	0/2/2/2
20	PGV	C	267	-	-	11/55/55/55	-
25	PEK	P	1265	-	-	30/56/56/56	-
23	CHD	W	1059	-	1/1/12/12	6/9/74/74	0/4/4/4
20	PGV	M	524	-	-	34/55/55/55	-
19	TGL	L	522	-	-	36/65/65/65	-
23	CHD	J	60	-	2/2/12/12	6/9/74/74	0/4/4/4
20	PGV	P	1268	-	-	26/55/55/55	-
20	PGV	C	268	-	-	35/55/55/55	-
19	TGL	O	1521	-	-	30/65/65/65	-
22	PSC	B	229	-	-	39/55/55/55	-
23	CHD	B	1085	-	-	2/9/74/74	0/4/4/4
25	PEK	G	1263	-	-	30/56/56/56	-
19	TGL	D	523	-	-	40/65/65/65	-
14	HEA	A	515	1	-	5/36/76/76	-
22	PSC	R	1229	-	-	30/55/55/55	-
28	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
25	PEK	T	263	-	-	31/56/56/56	-
14	HEA	N	516	15,1	-	6/36/76/76	-
19	TGL	Q	1523	-	-	37/65/65/65	-

The worst 5 of 294 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	515	HEA	C11-C3B	9.21	1.62	1.51
20	P	1268	PGV	O01-C1	7.63	1.55	1.34
19	L	522	TGL	OG2-CB1	7.53	1.55	1.34
19	N	1522	TGL	OG2-CB1	7.31	1.54	1.34
20	C	268	PGV	O01-C1	6.46	1.52	1.34

The worst 5 of 813 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C6-C5-C10	15.58	129.24	112.66
23	O	229	CHD	C6-C5-C10	15.40	129.05	112.66
23	O	229	CHD	C14-C13-C12	13.96	120.18	107.42
23	B	1085	CHD	C1-C10-C5	13.82	127.58	107.75
23	C	271	CHD	C10-C9-C8	13.42	126.80	111.84

5 of 26 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	C	271	CHD	C9
23	J	60	CHD	C17
23	J	60	CHD	C9
23	P	1271	CHD	C9
23	W	1059	CHD	C17

5 of 970 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	C	267	PGV	C10-C11-C12-C13
20	C	268	PGV	O03-C01-C02-O01
20	C	268	PGV	C04-C05-C06-O06
20	C	268	PGV	O02-C1-O01-C02
20	M	524	PGV	C03-O11-P-O12

There are no ring outliers.

38 monomers are involved in 361 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	T	1269	CDL	27	0
23	C	271	CHD	4	0
23	P	1525	CHD	1	0
26	P	1270	CDL	25	0
23	P	1271	CHD	5	0

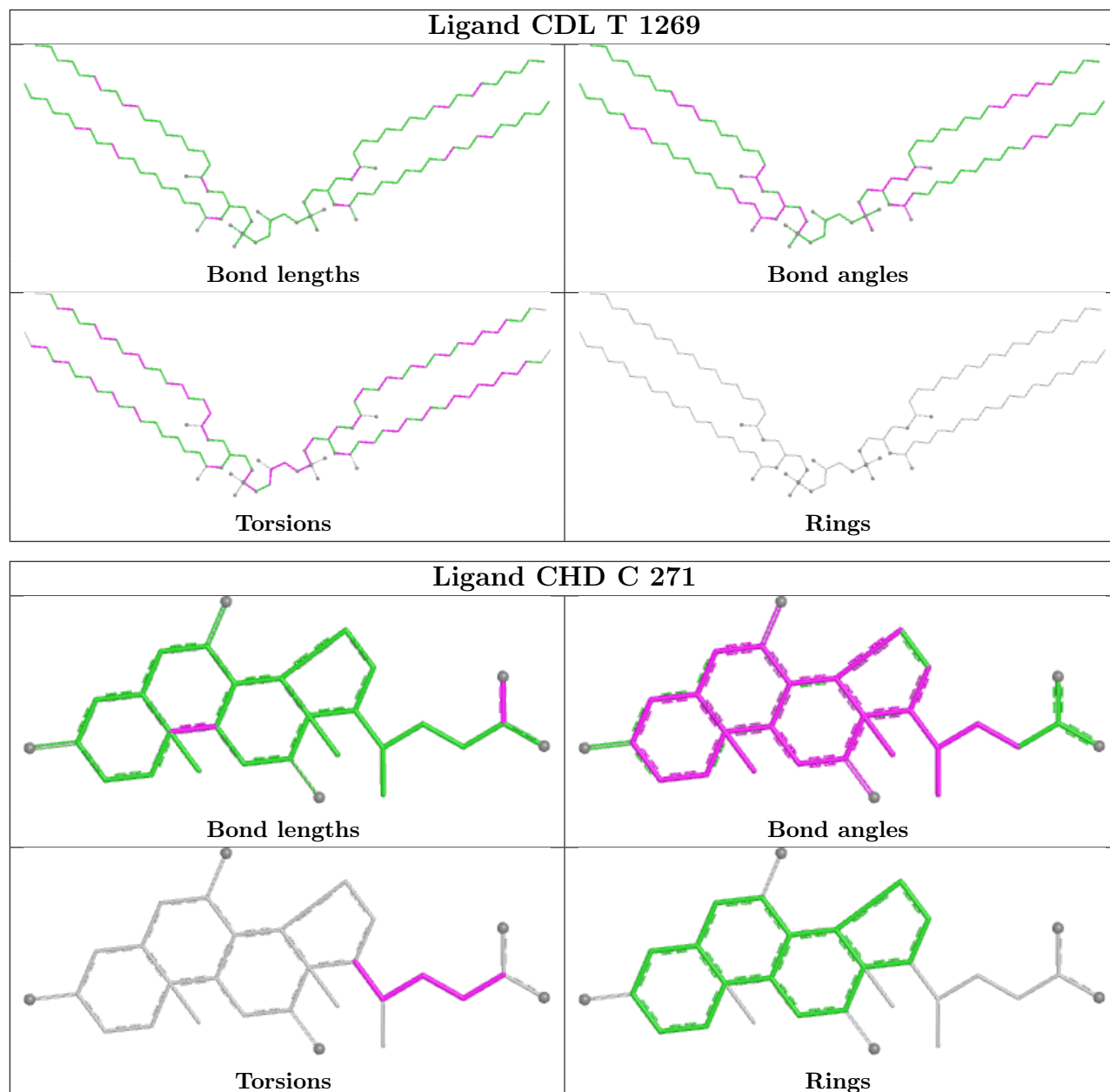
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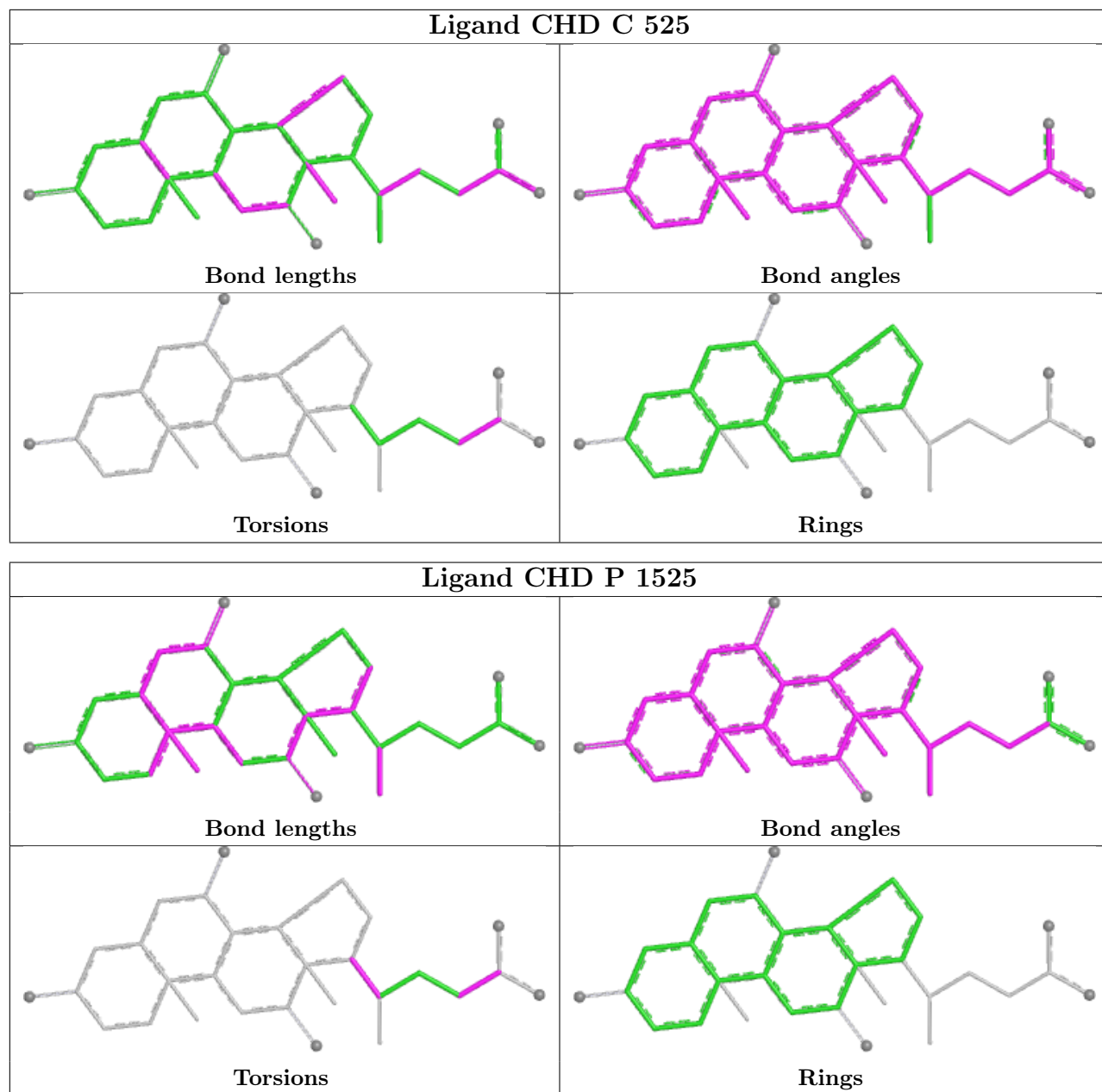
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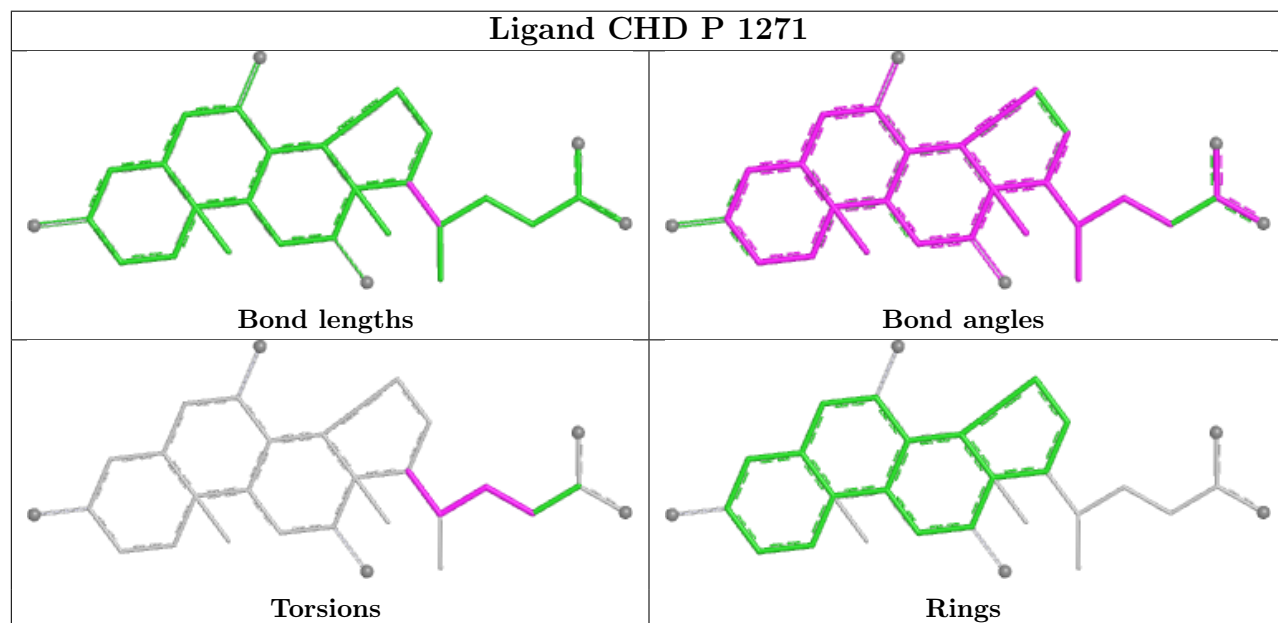
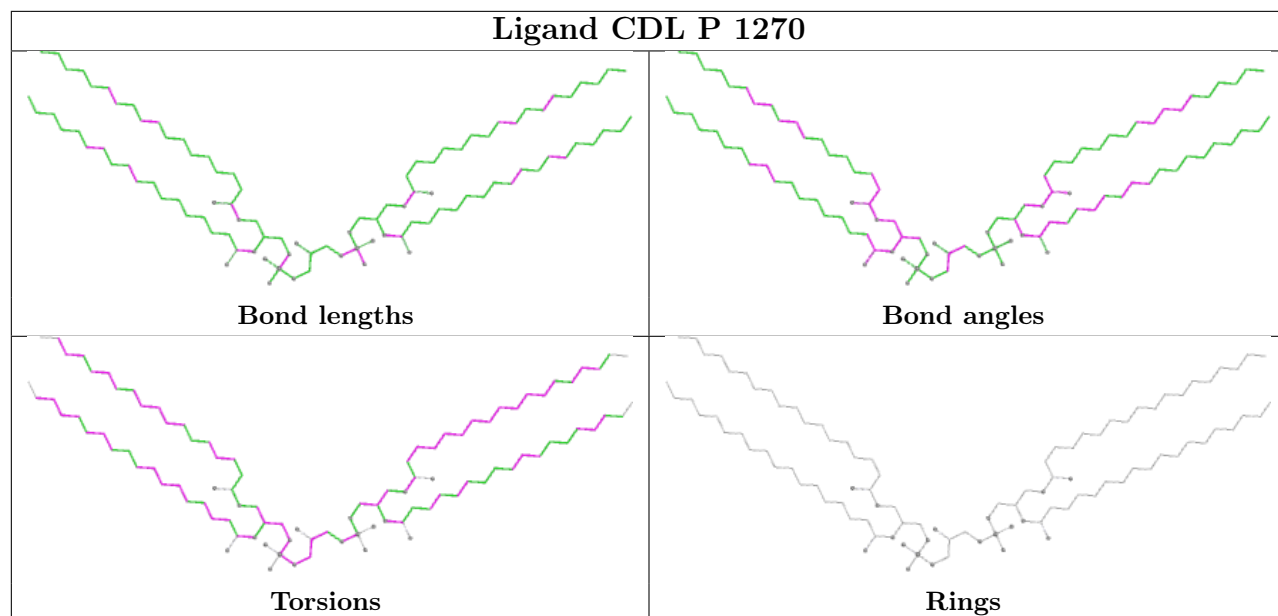
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	P	1267	PGV	5	0
26	C	270	CDL	25	0
26	G	269	CDL	30	0
25	C	264	PEK	8	0
25	G	265	PEK	19	0
19	N	1522	TGL	15	0
25	P	1264	PEK	7	0
28	G	272	DMU	4	0
28	P	1272	DMU	6	0
19	A	521	TGL	8	0
14	A	516	HEA	2	0
23	O	229	CHD	3	0
20	N	1266	PGV	1	0
14	N	515	HEA	3	0
20	N	1524	PGV	8	0
20	C	267	PGV	5	0
25	P	1265	PEK	17	0
23	W	1059	CHD	1	0
20	M	524	PGV	15	0
19	L	522	TGL	15	0
23	J	60	CHD	1	0
20	P	1268	PGV	1	0
20	C	268	PGV	3	0
19	O	1521	TGL	10	0
22	B	229	PSC	26	0
23	B	1085	CHD	2	0
25	G	1263	PEK	24	0
19	D	523	TGL	8	0
14	A	515	HEA	4	0
22	R	1229	PSC	15	0
28	Z	1526	DMU	2	0
25	T	263	PEK	21	0
19	Q	1523	TGL	12	0

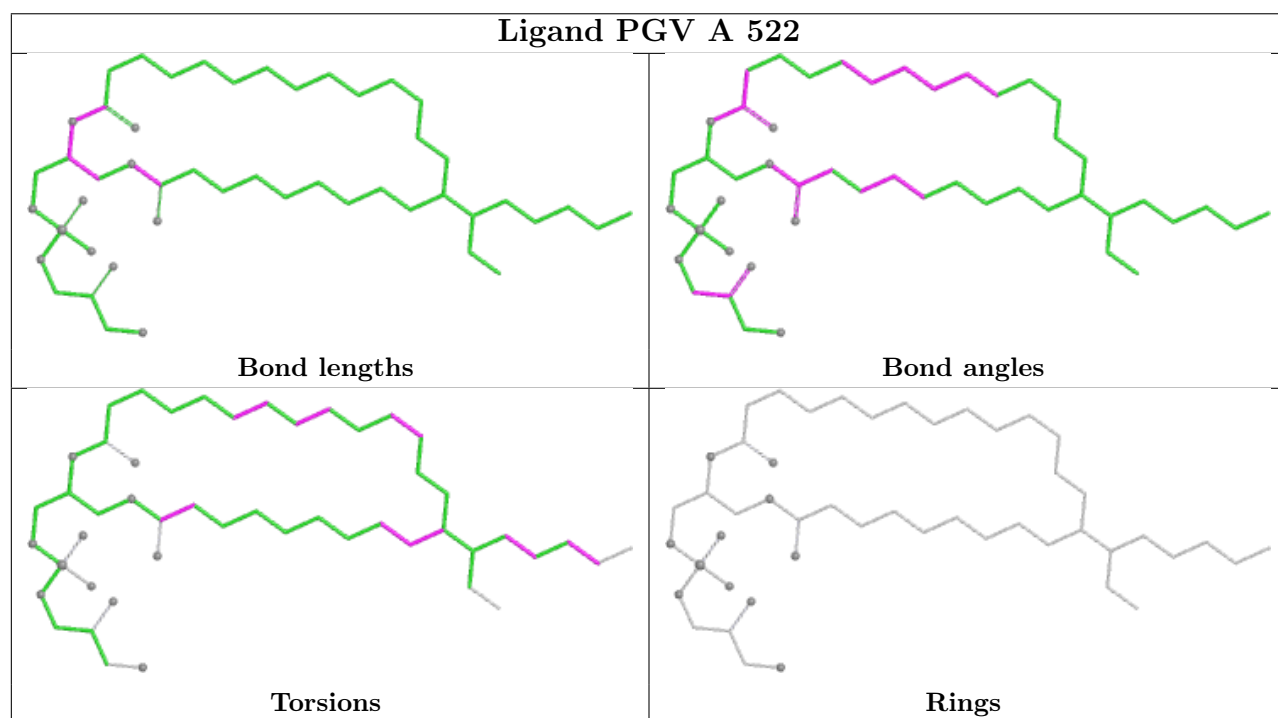
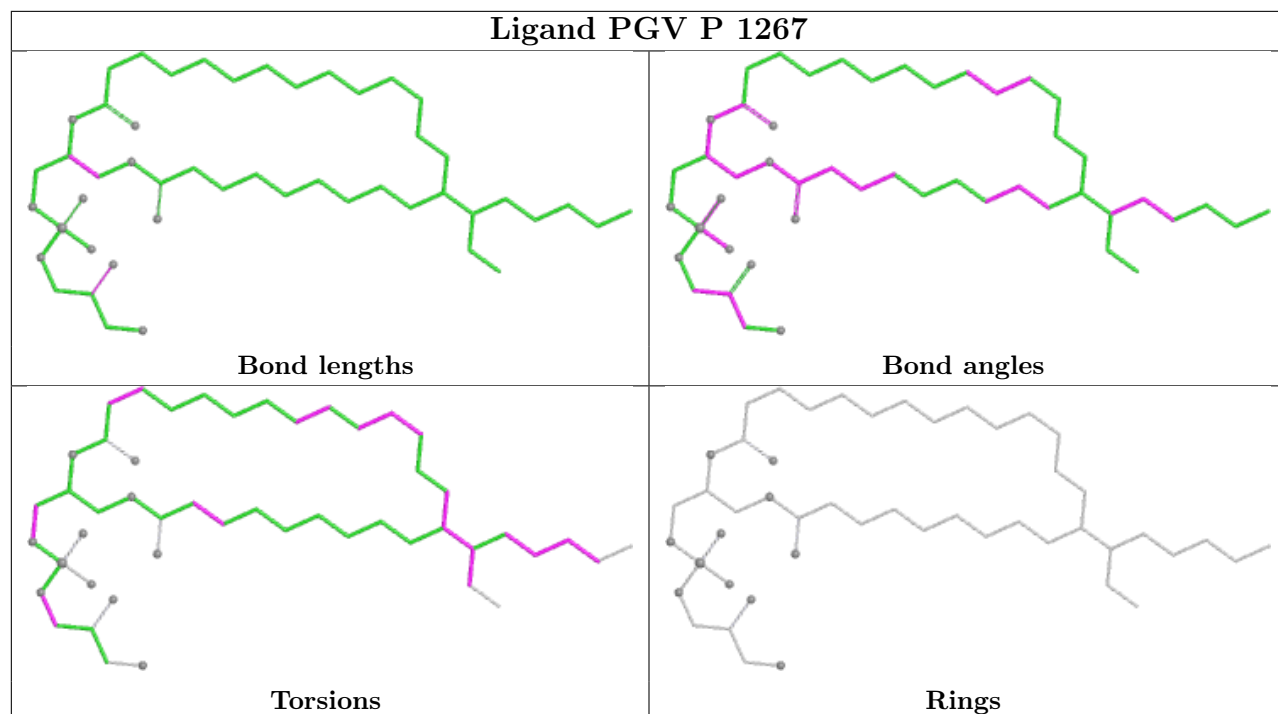
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

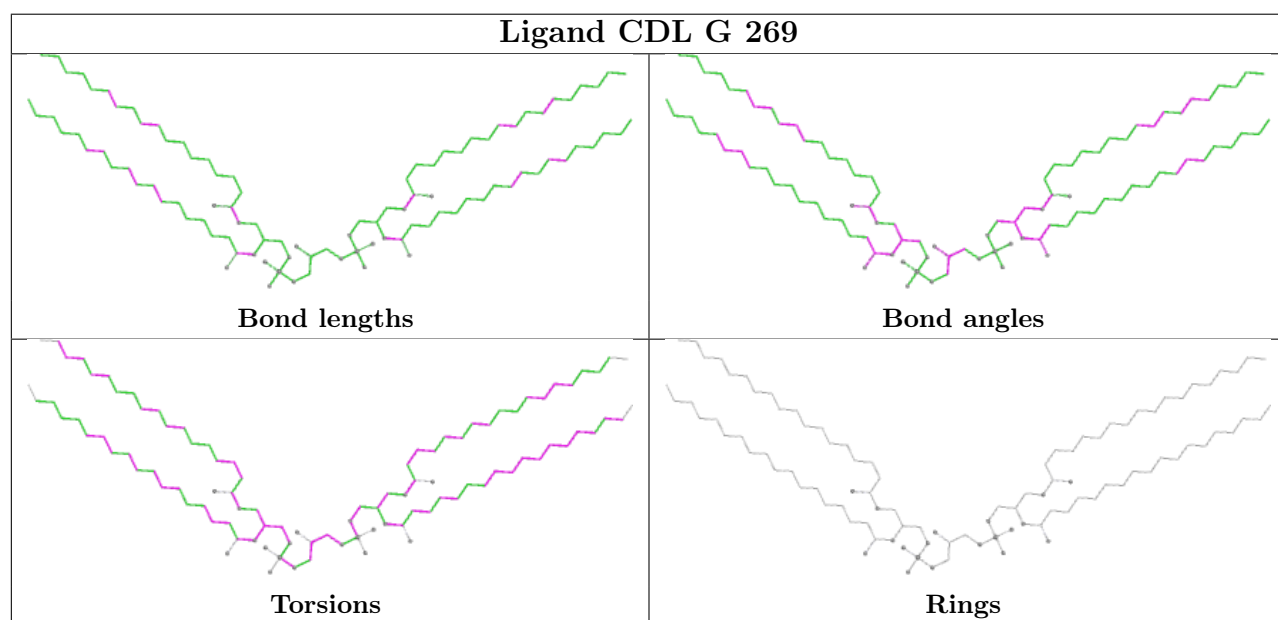
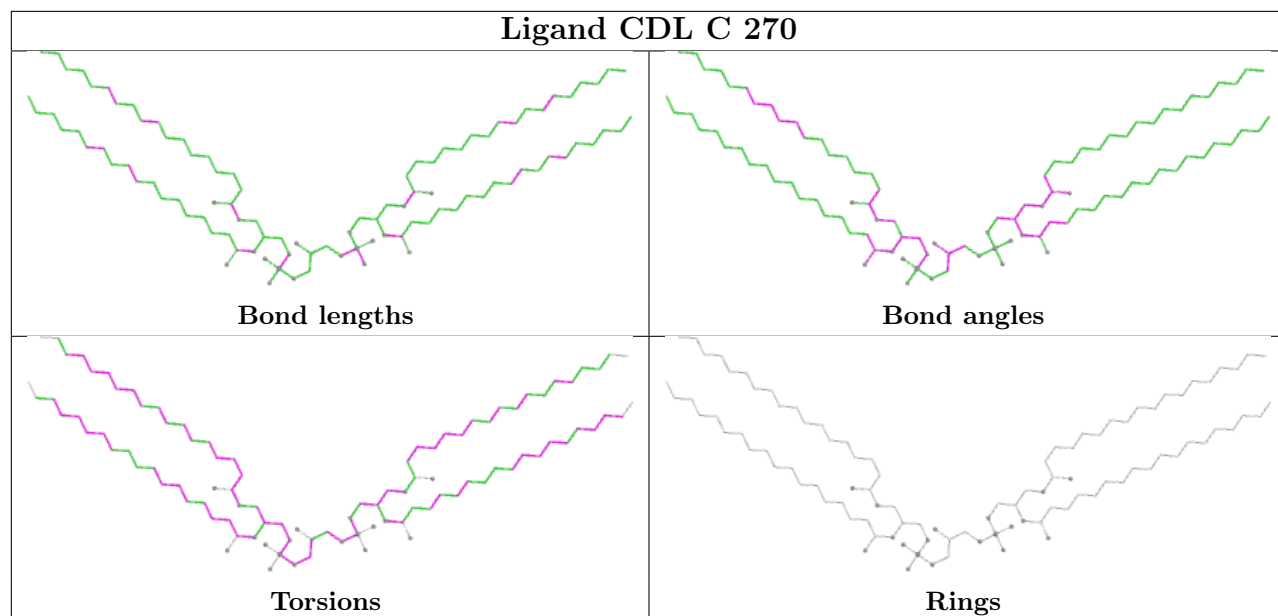
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



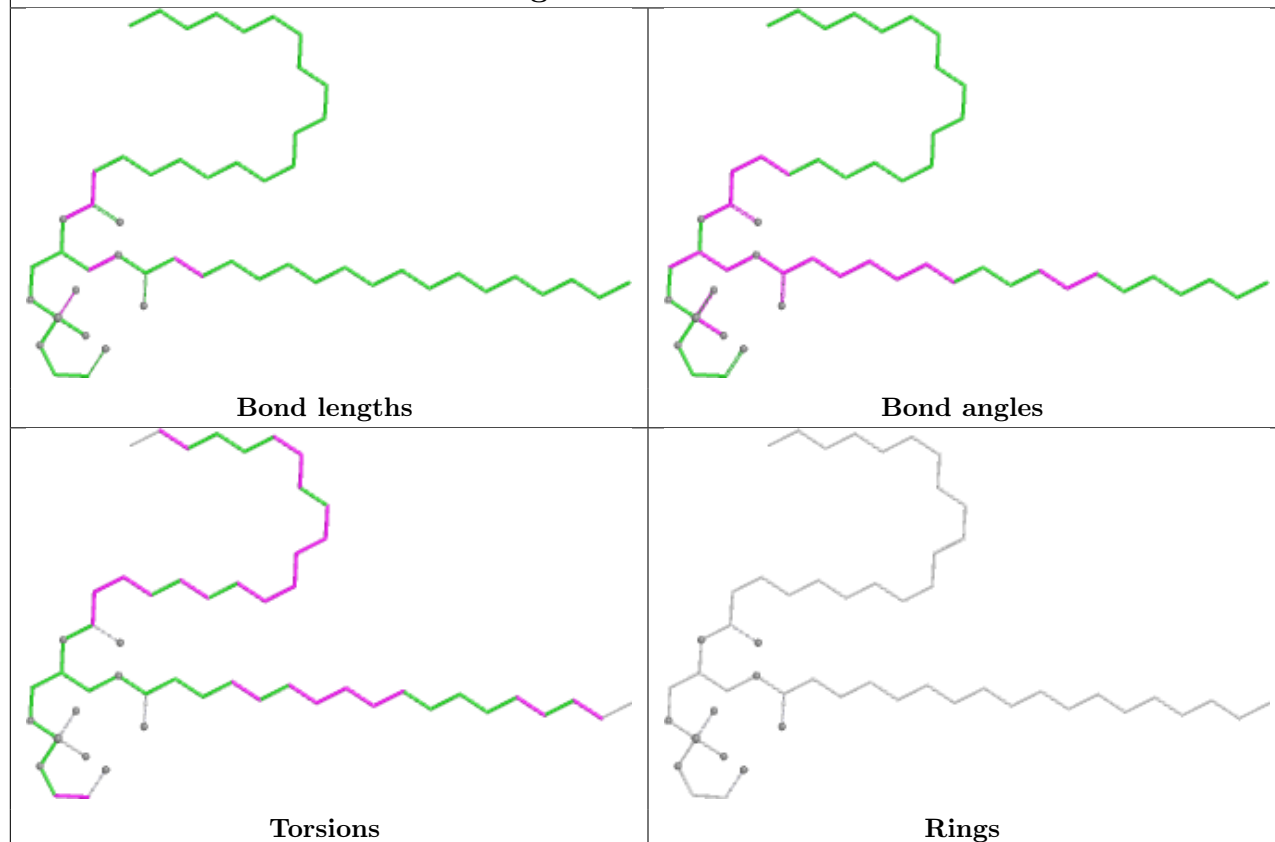




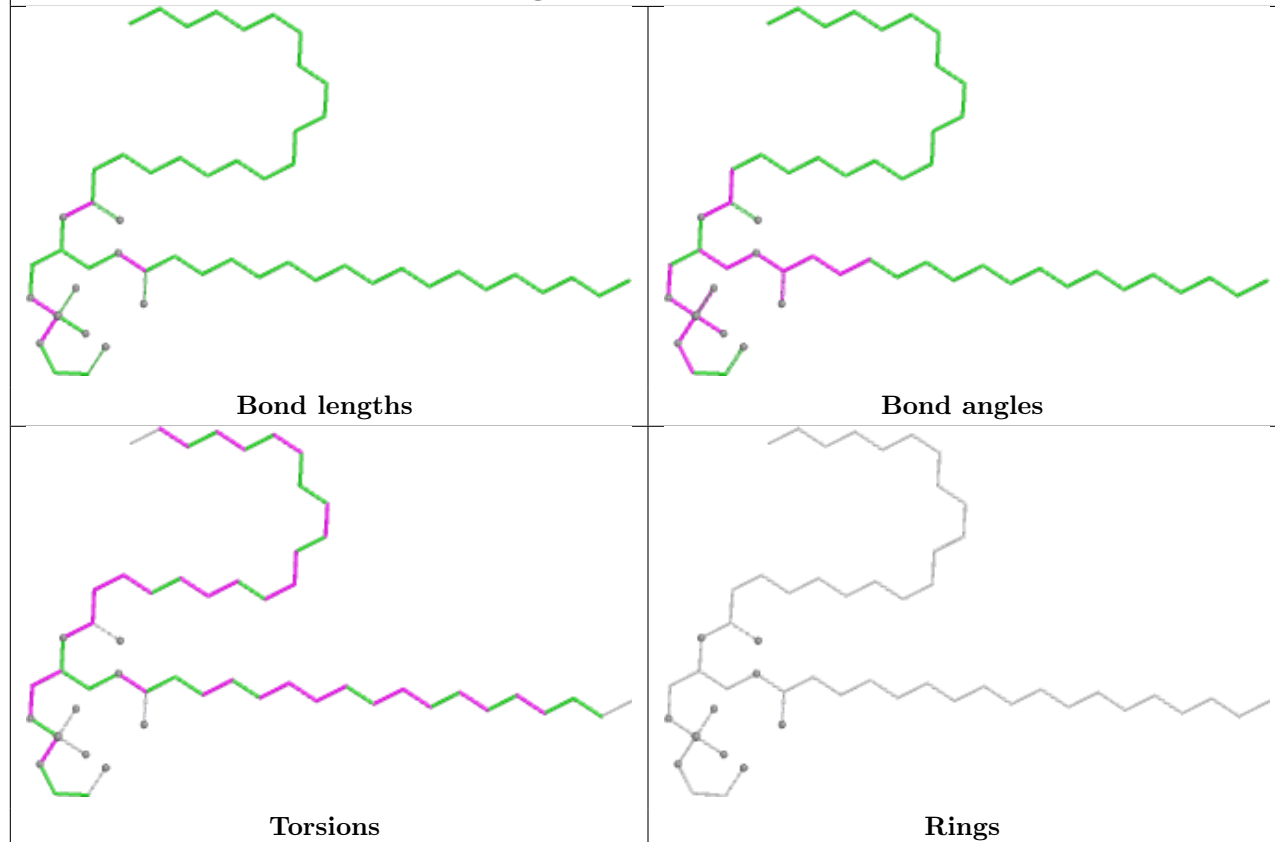


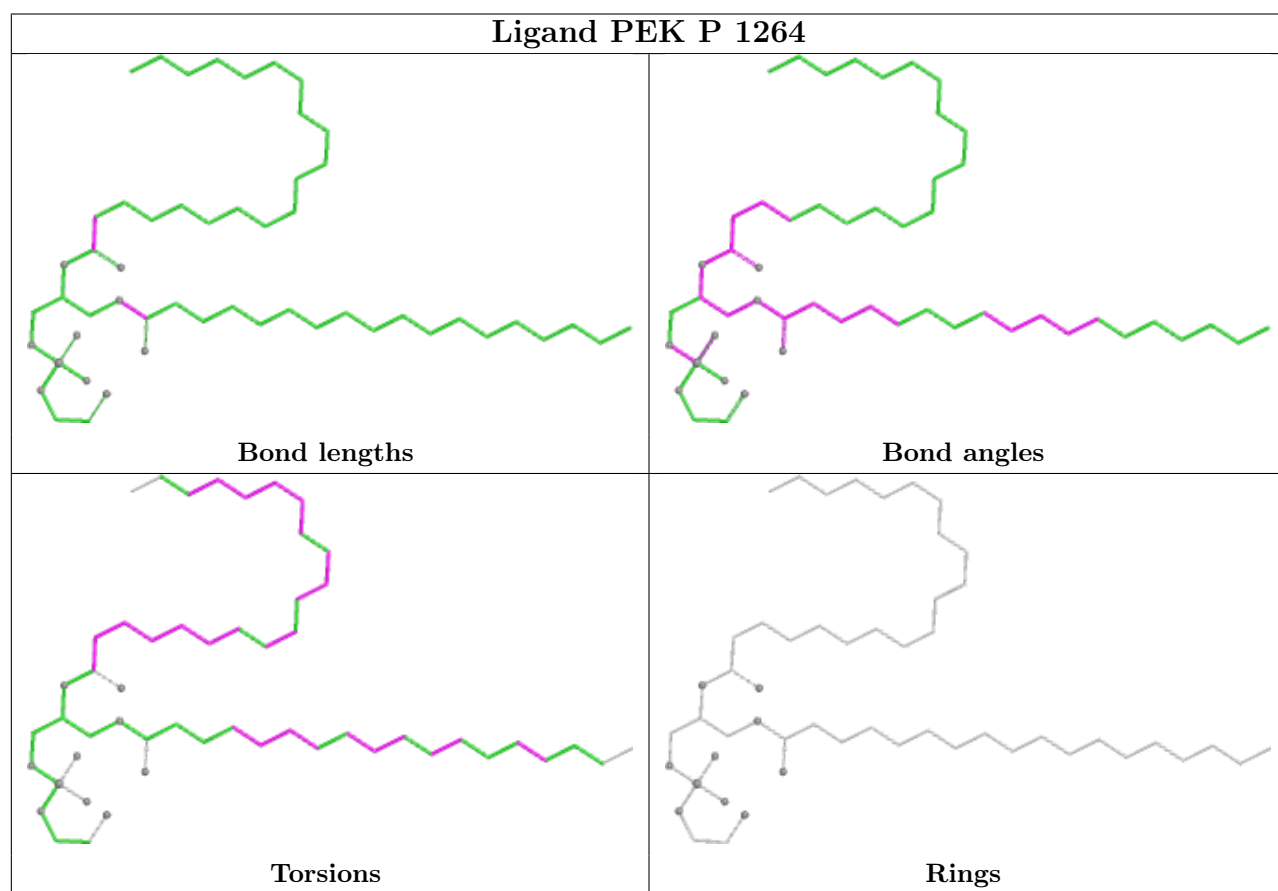
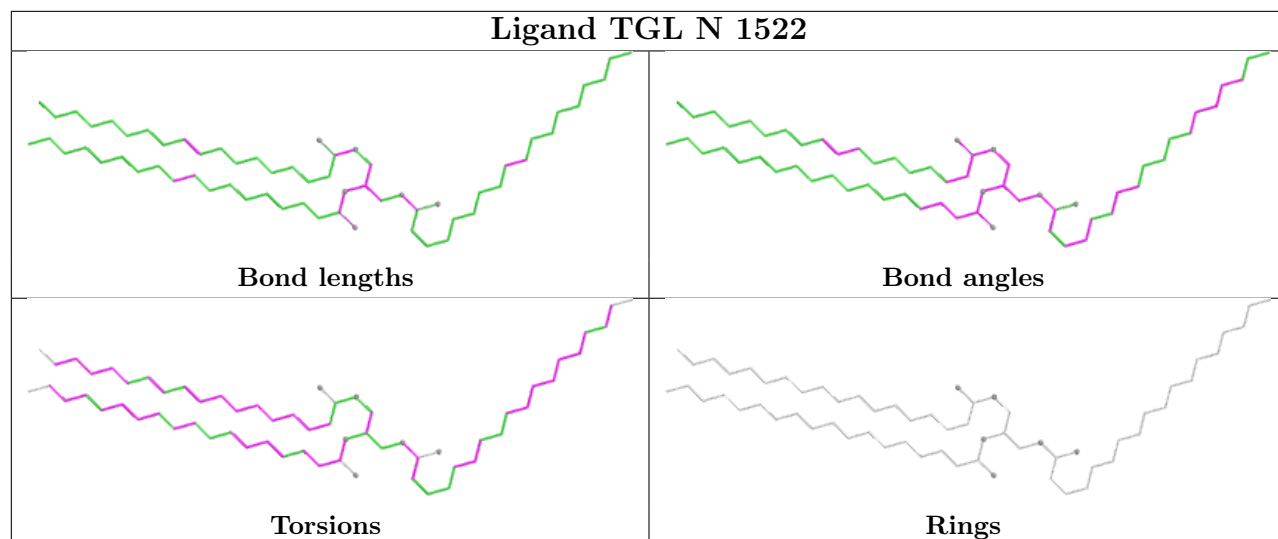


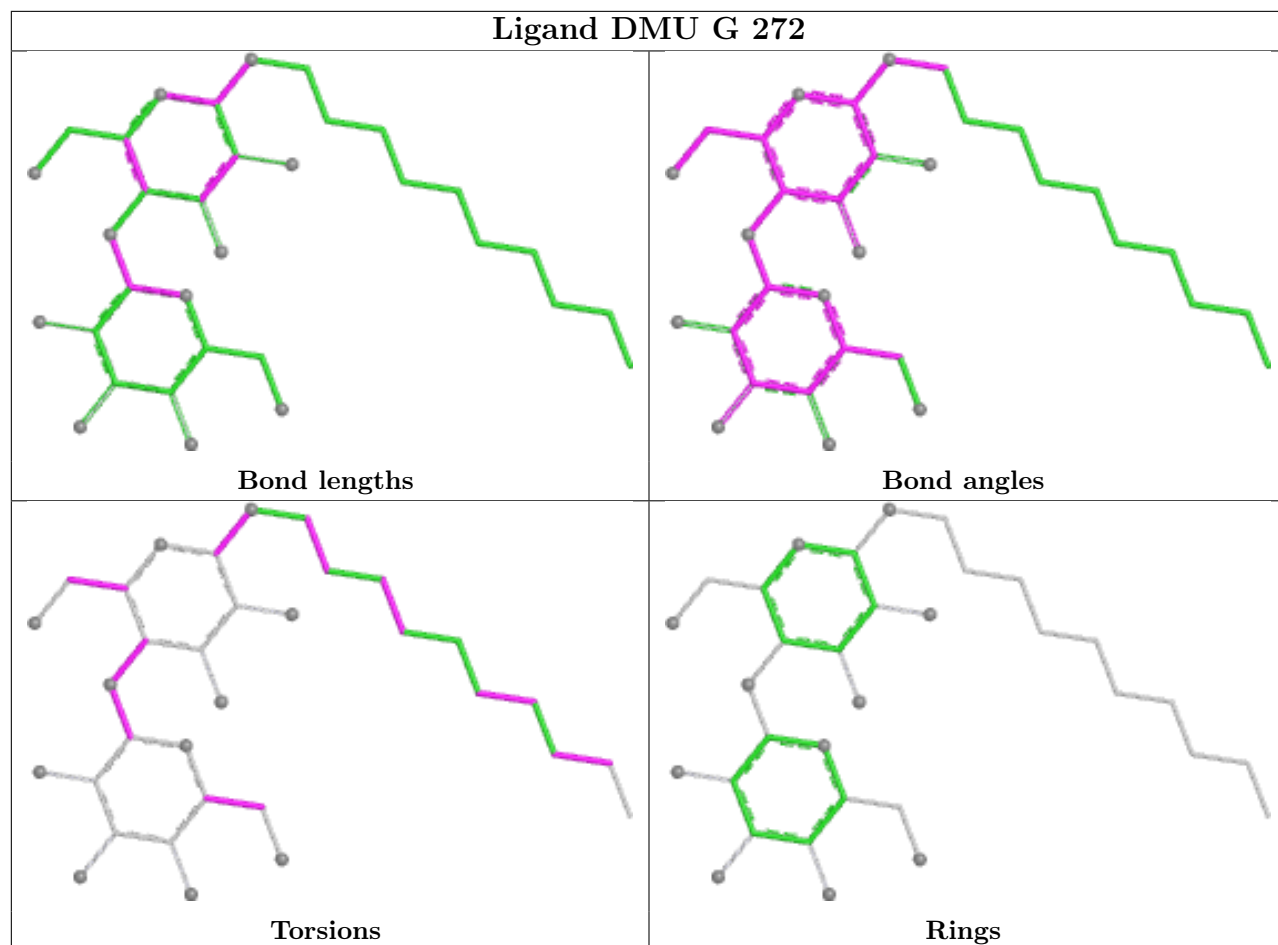
Ligand PEK C 264

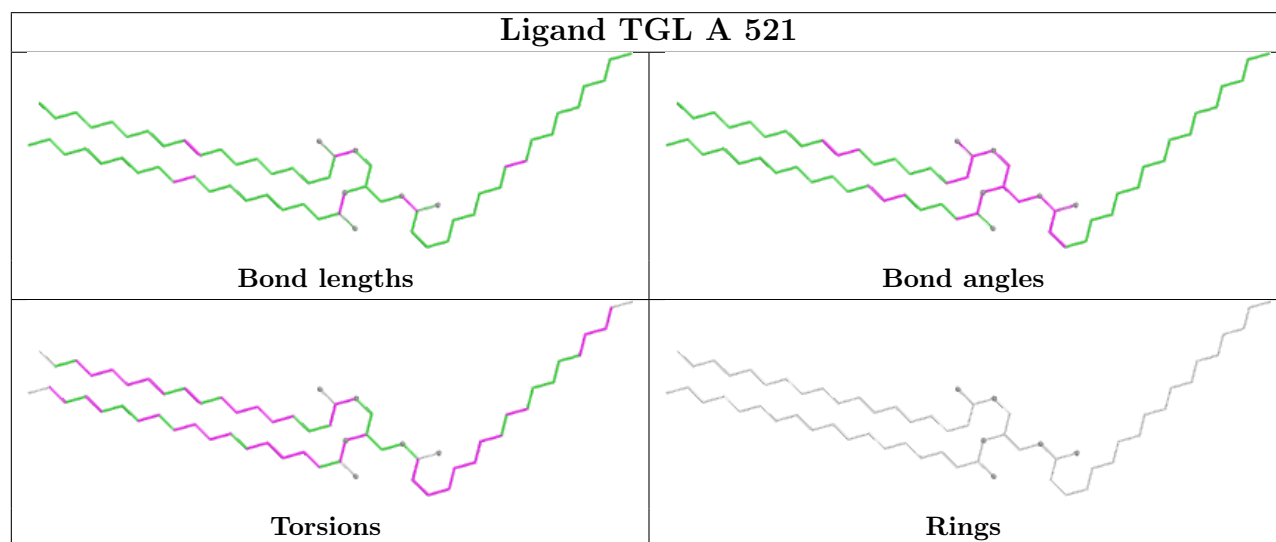
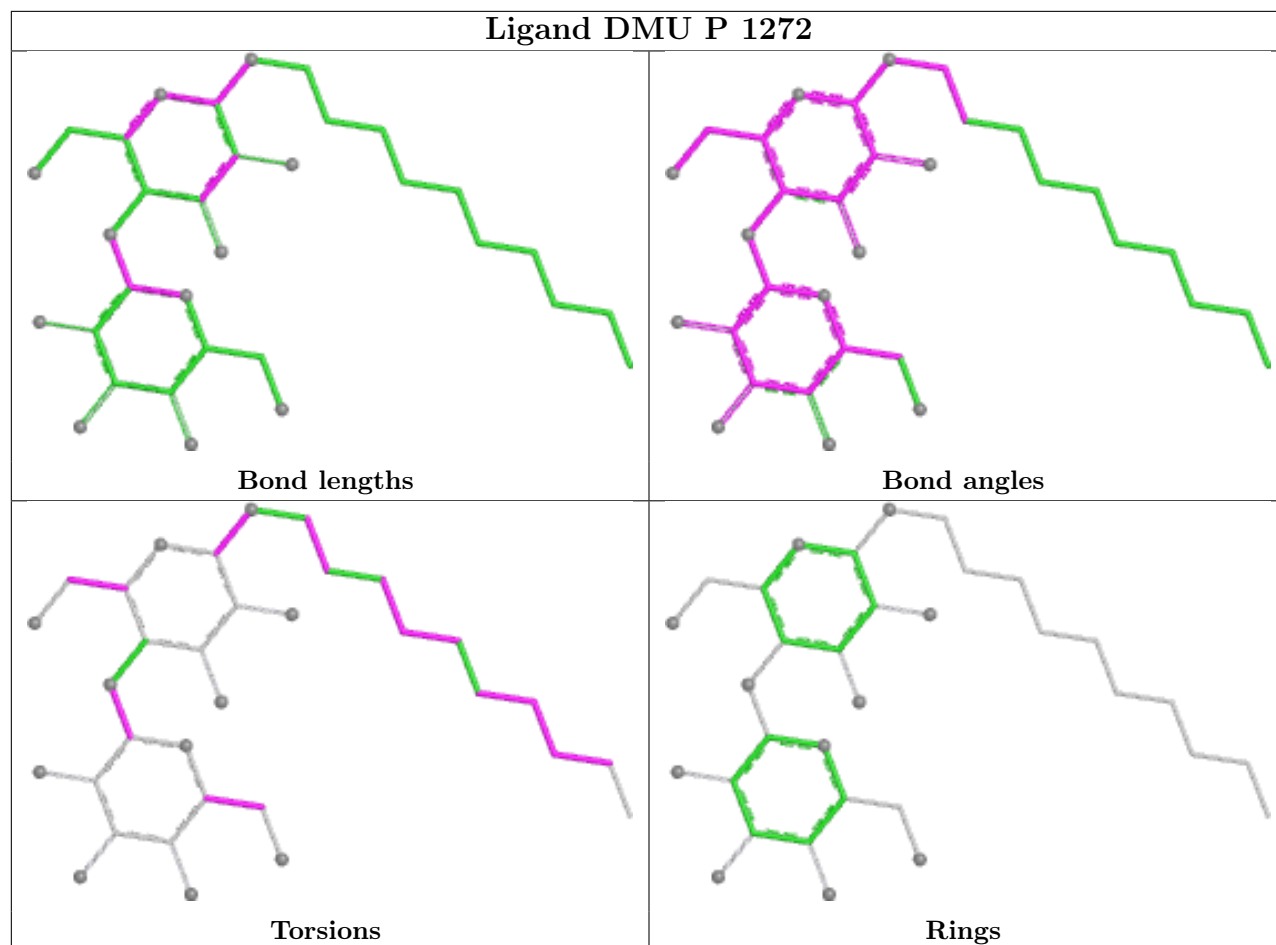


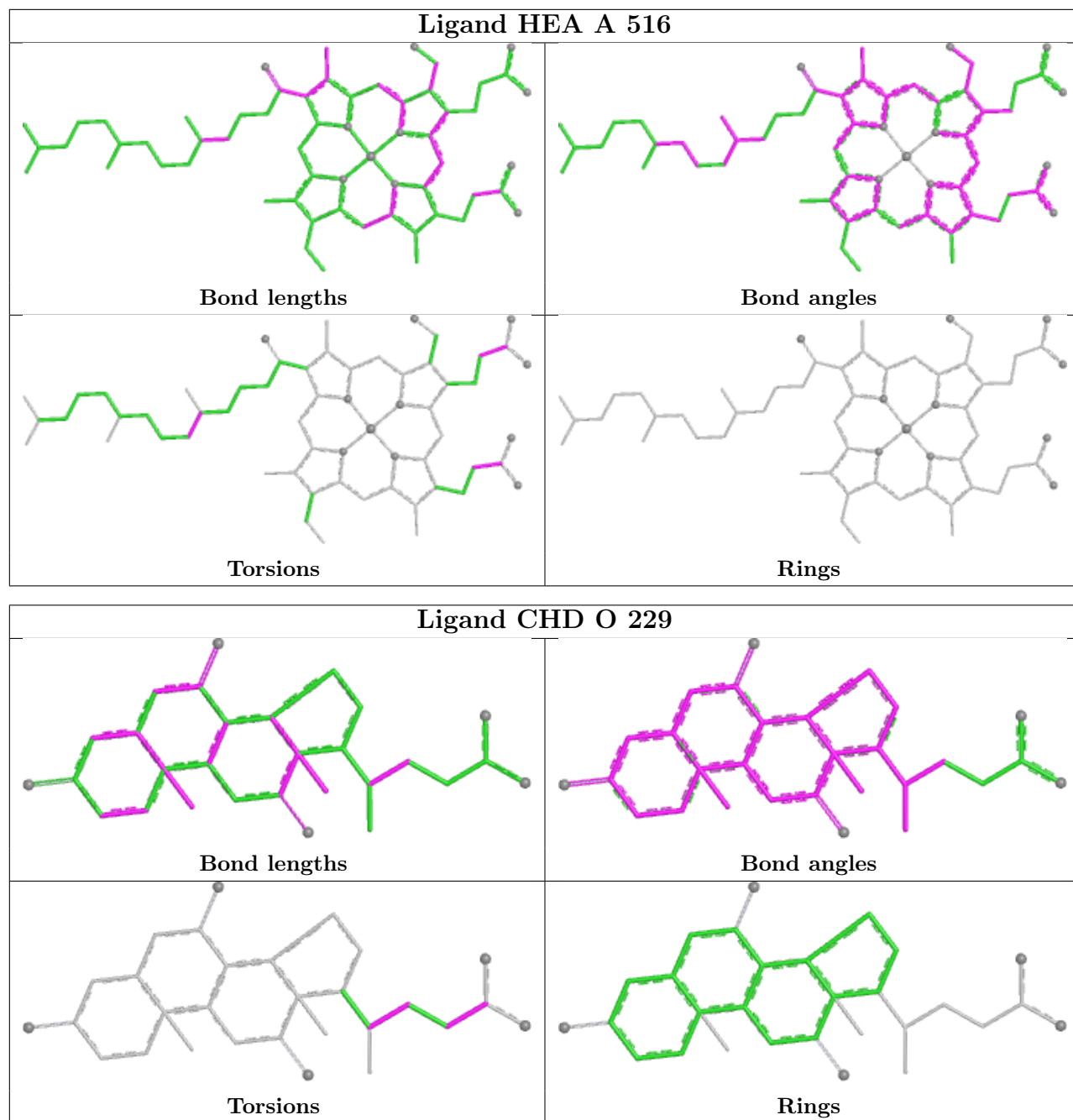
Ligand PEK G 265

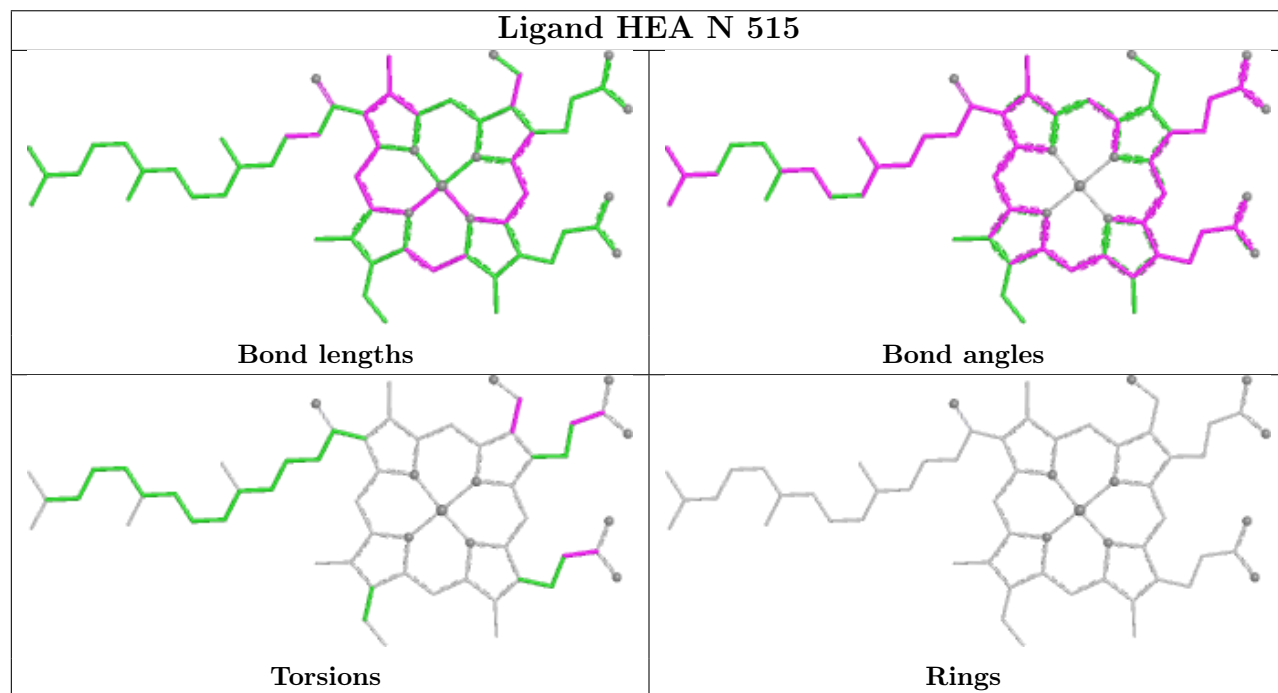
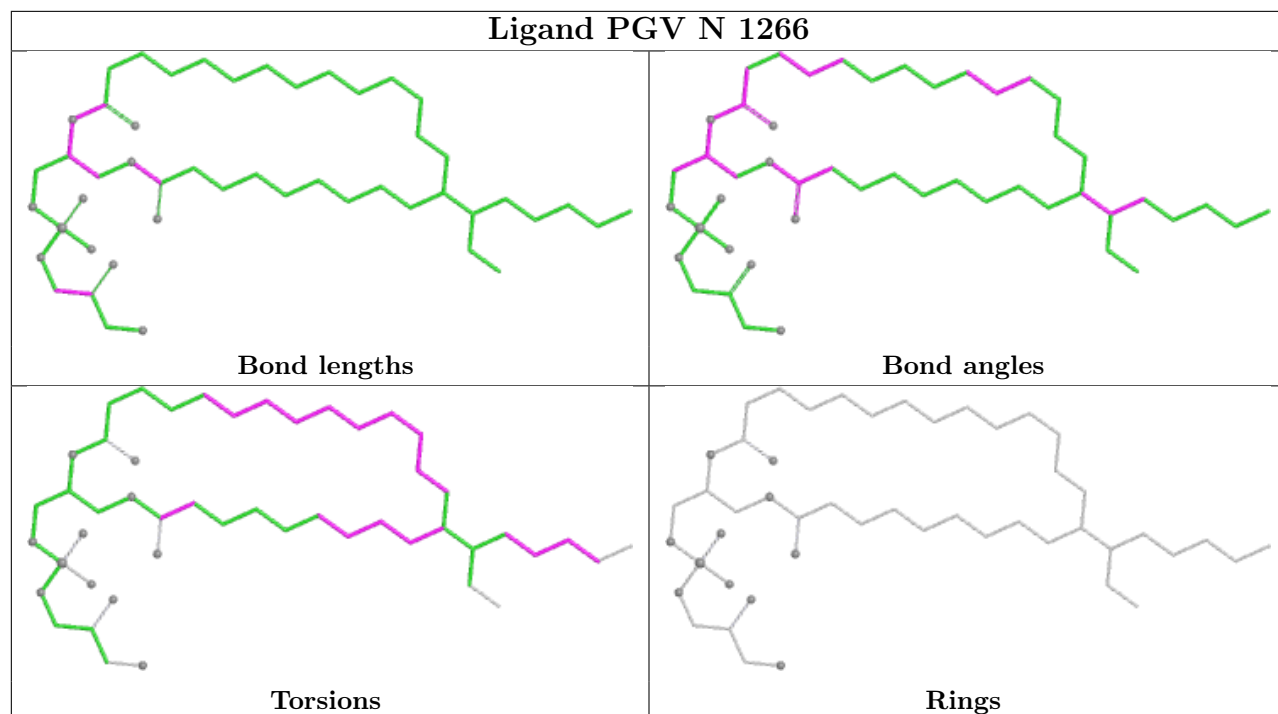


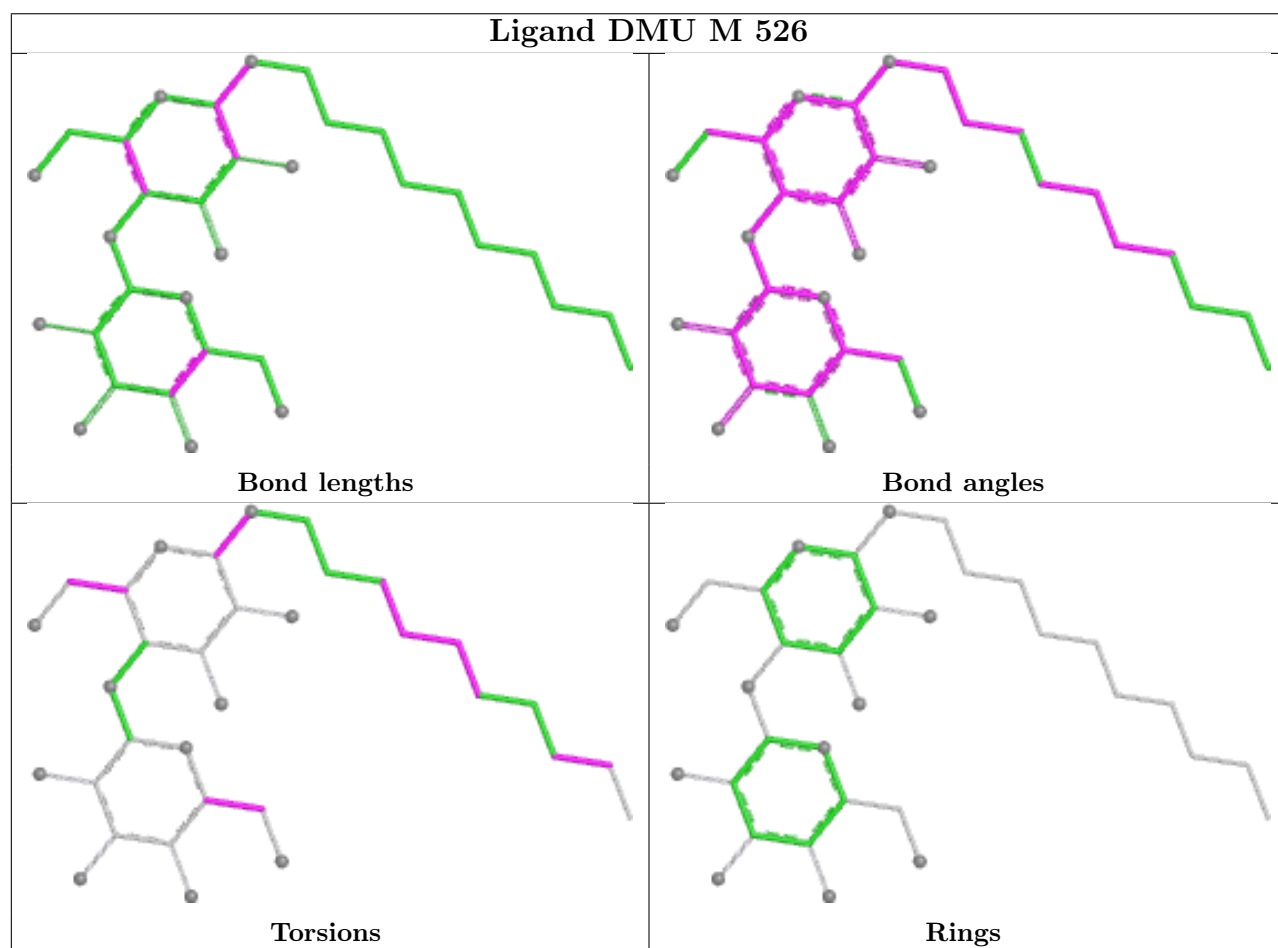
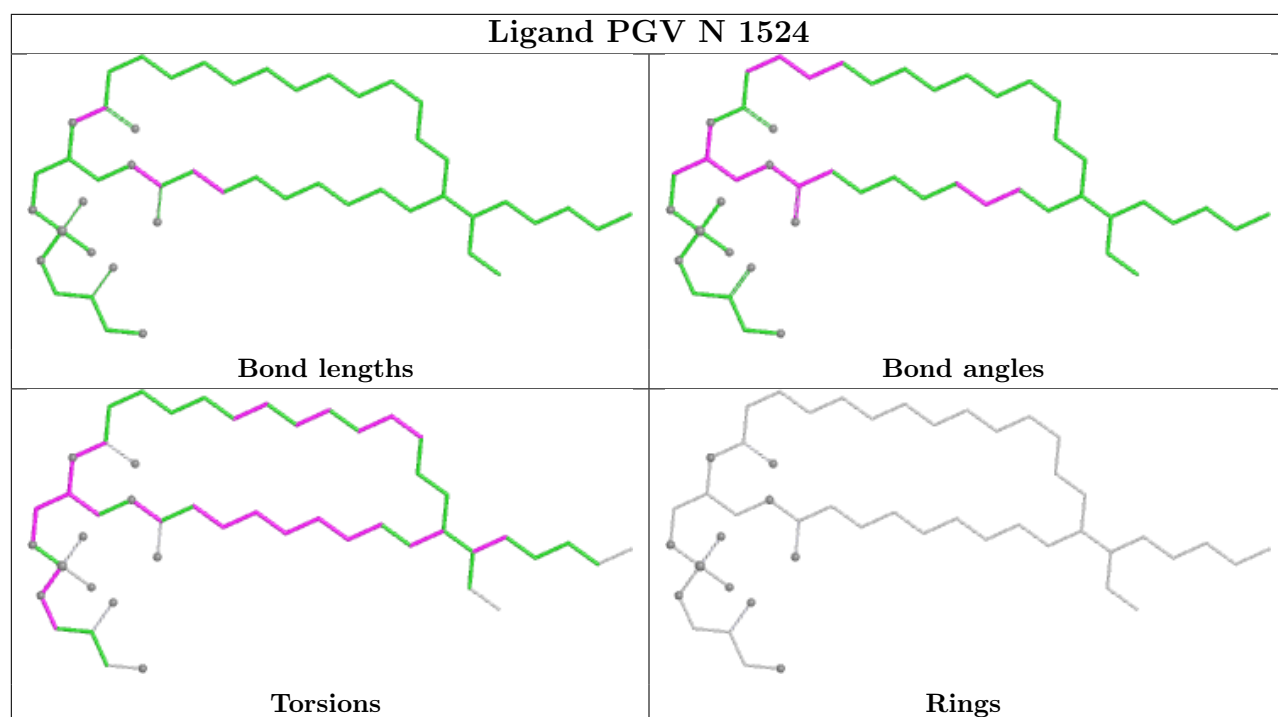


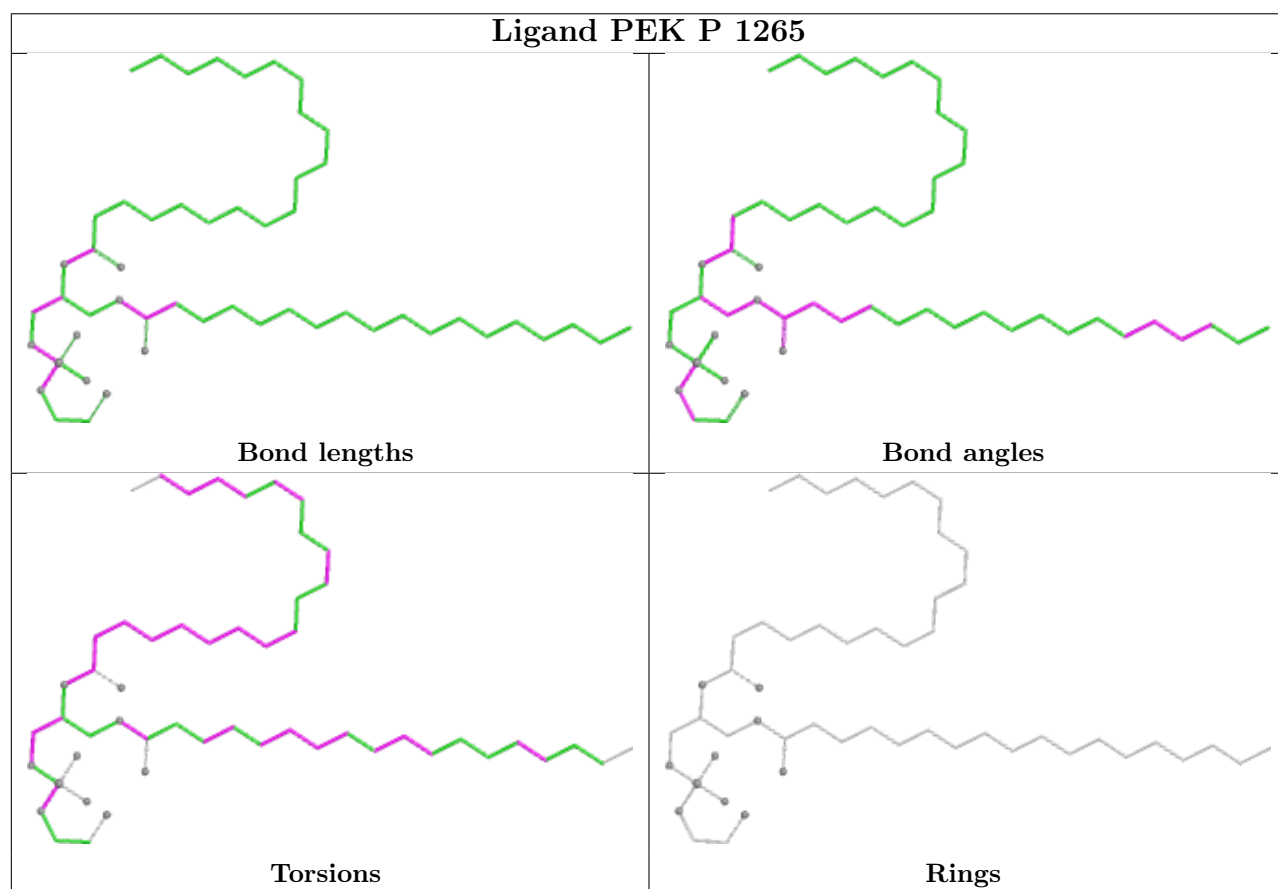
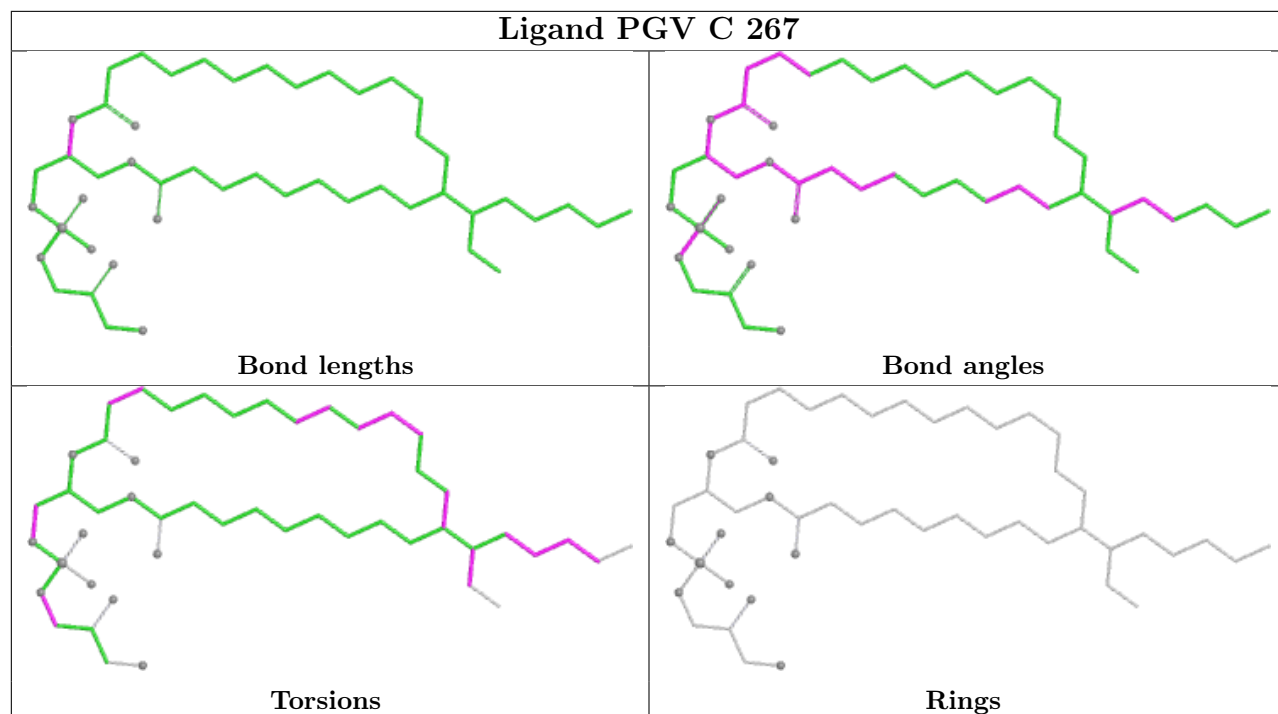




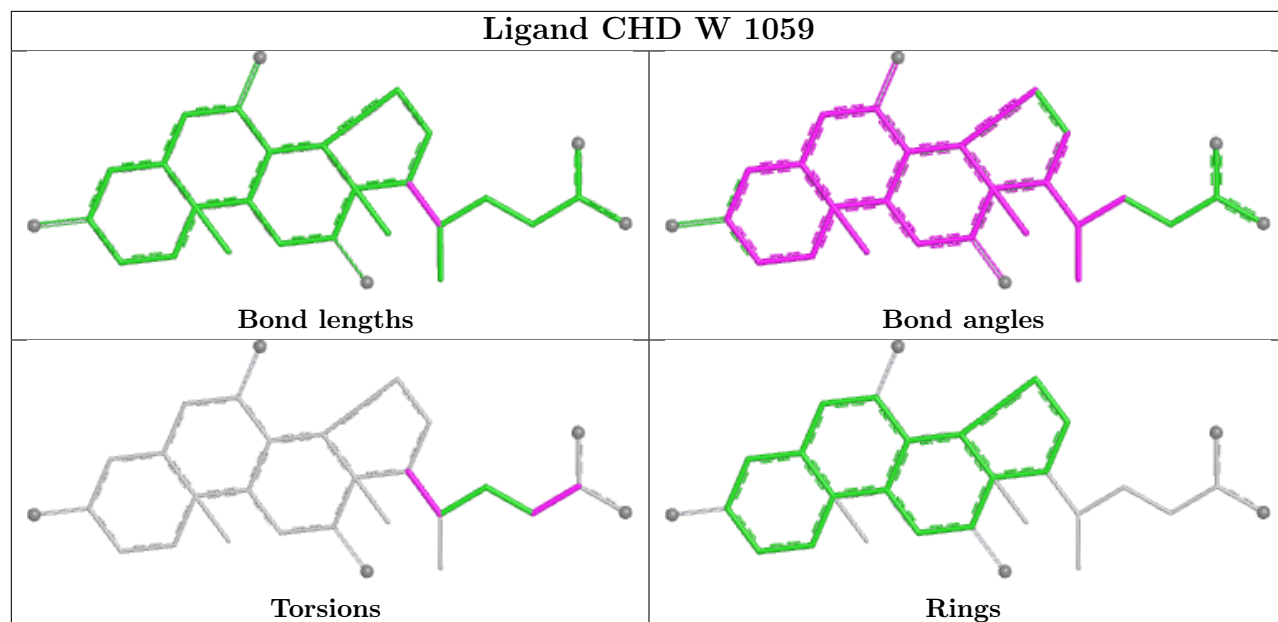




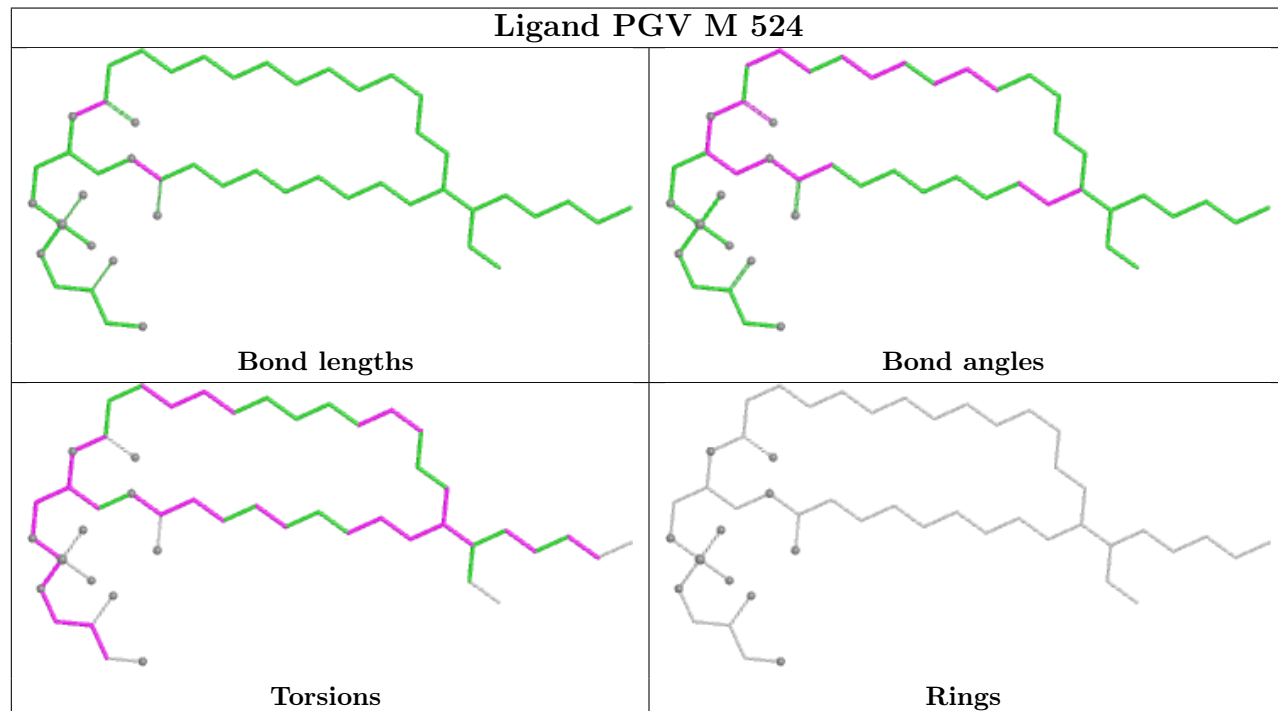


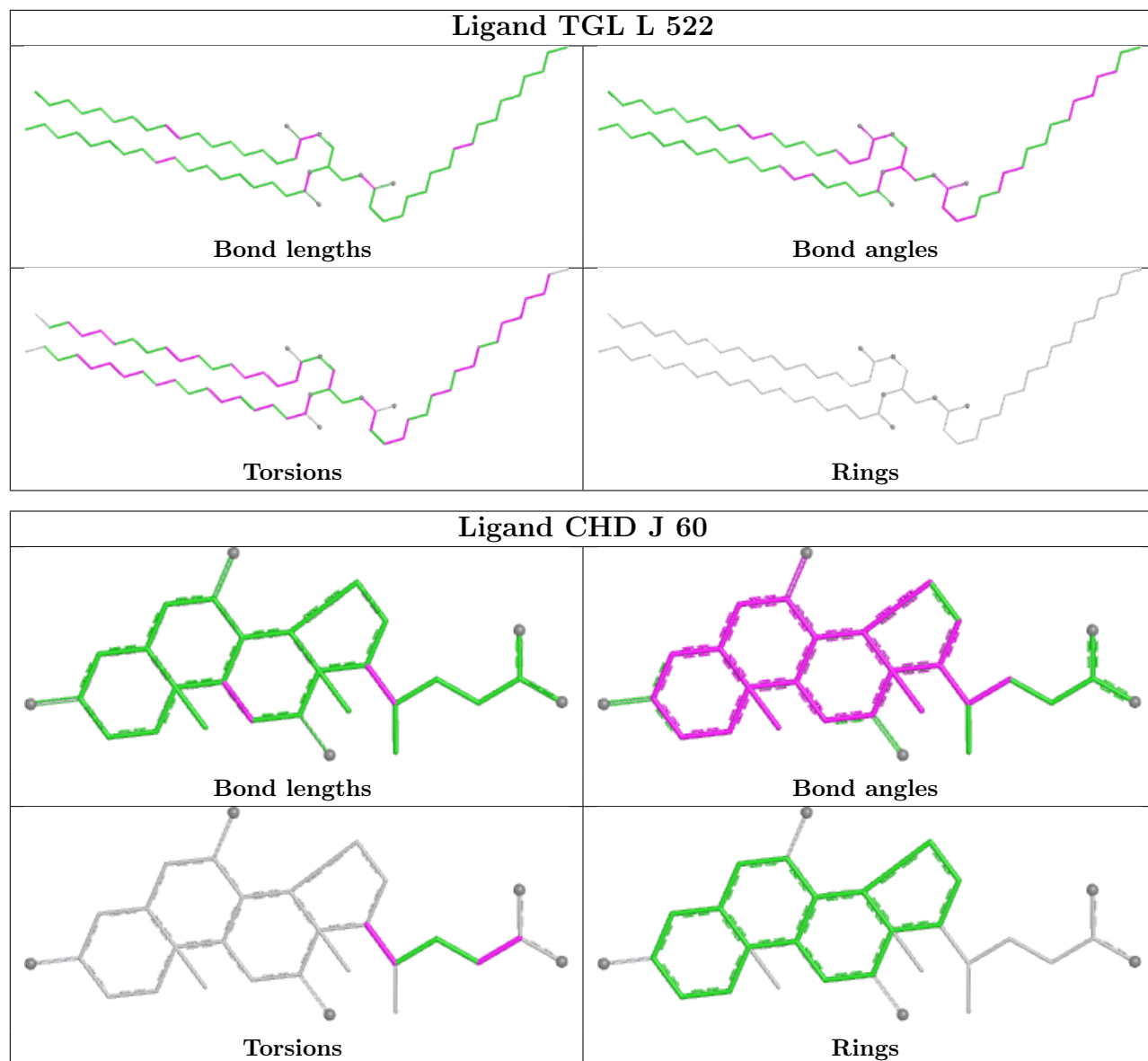


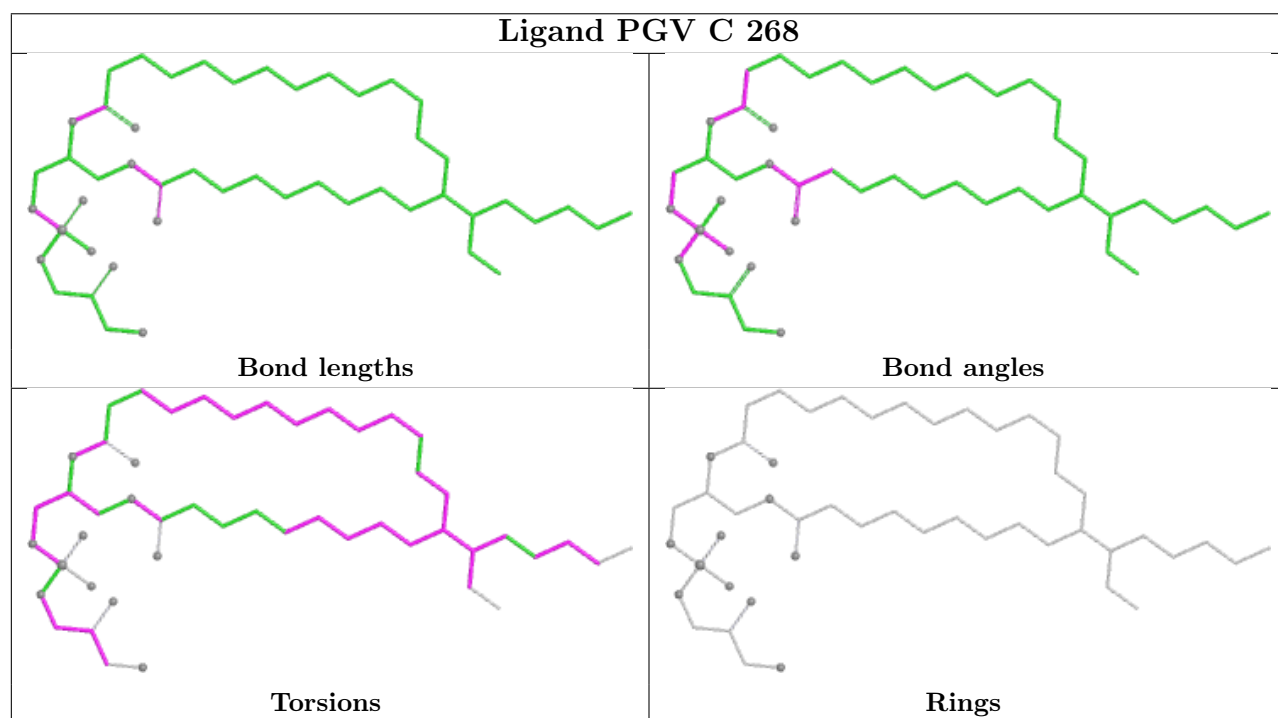
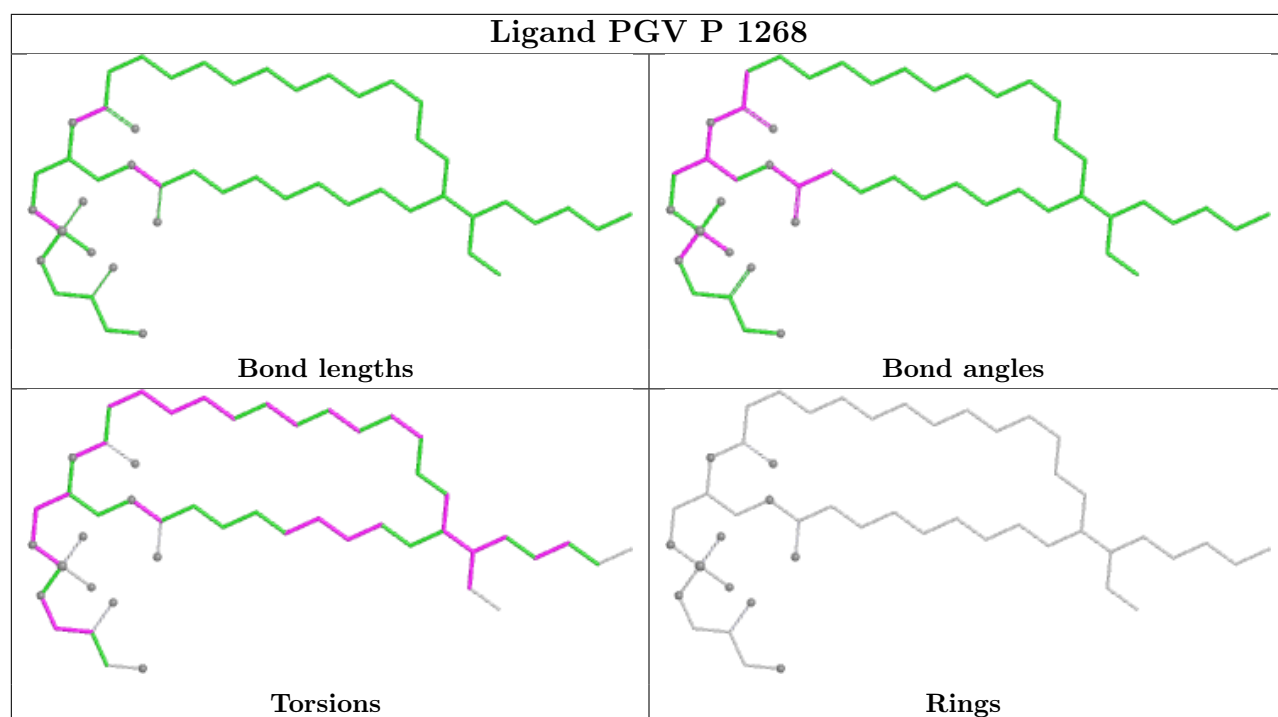
Ligand CHD W 1059

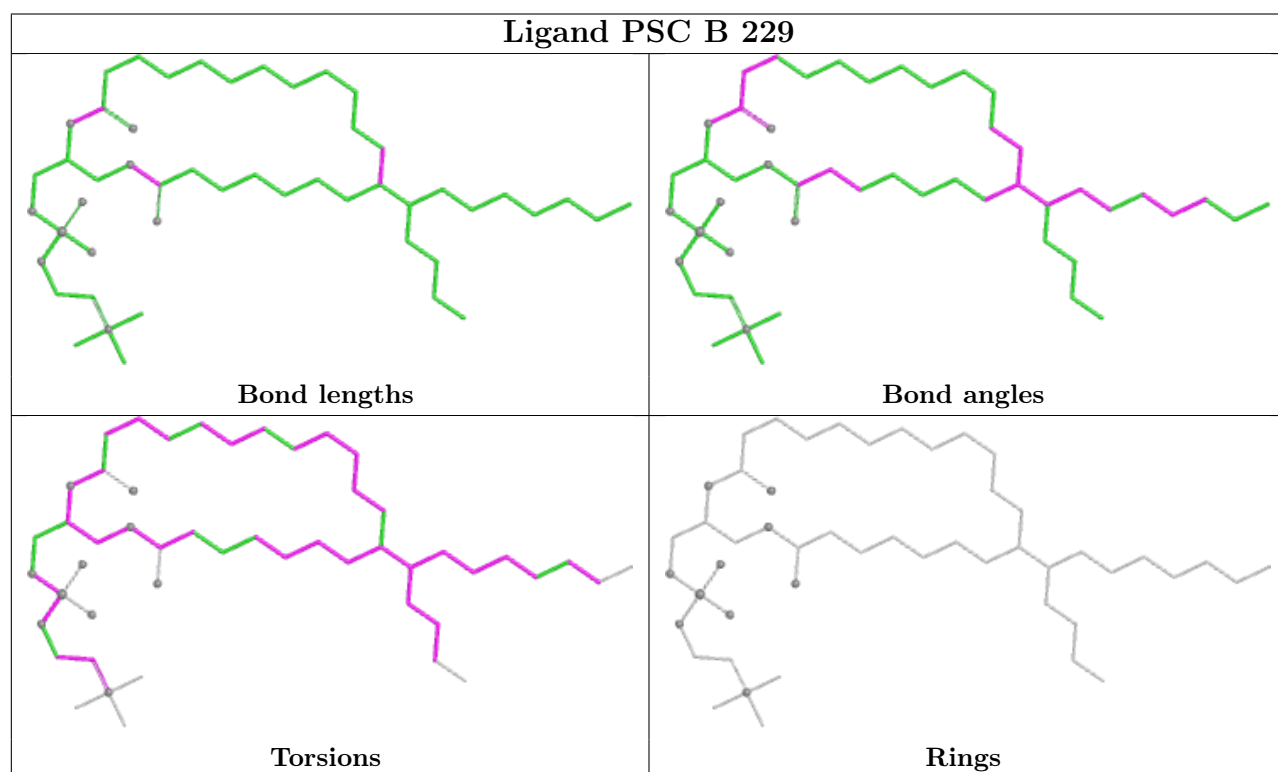
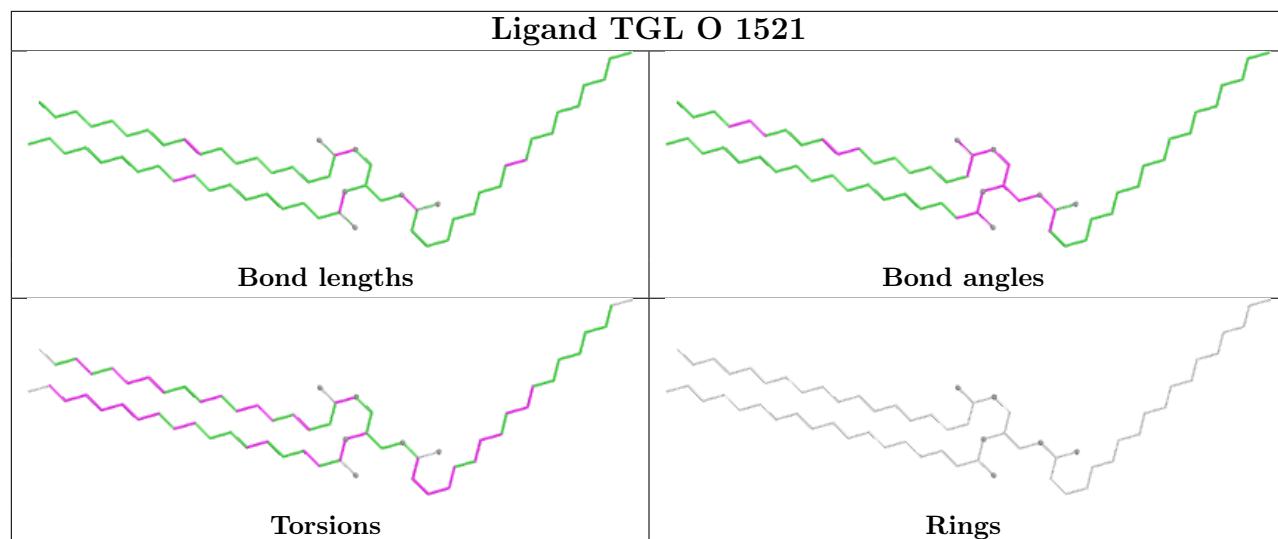


Ligand PGV M 524

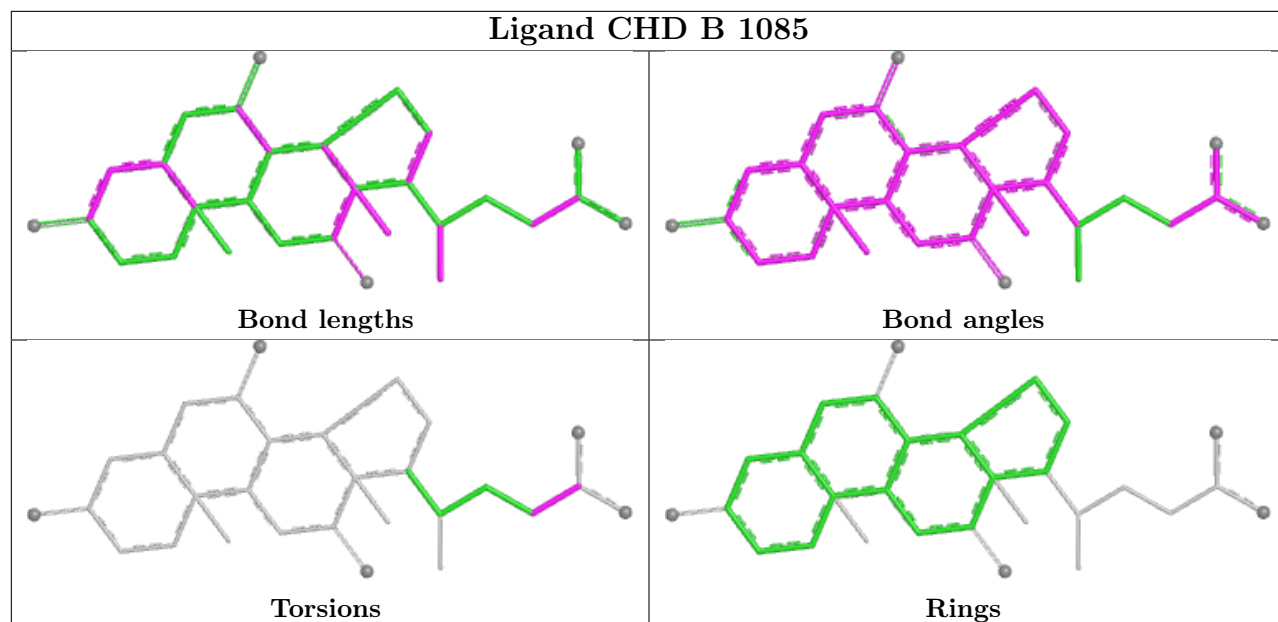




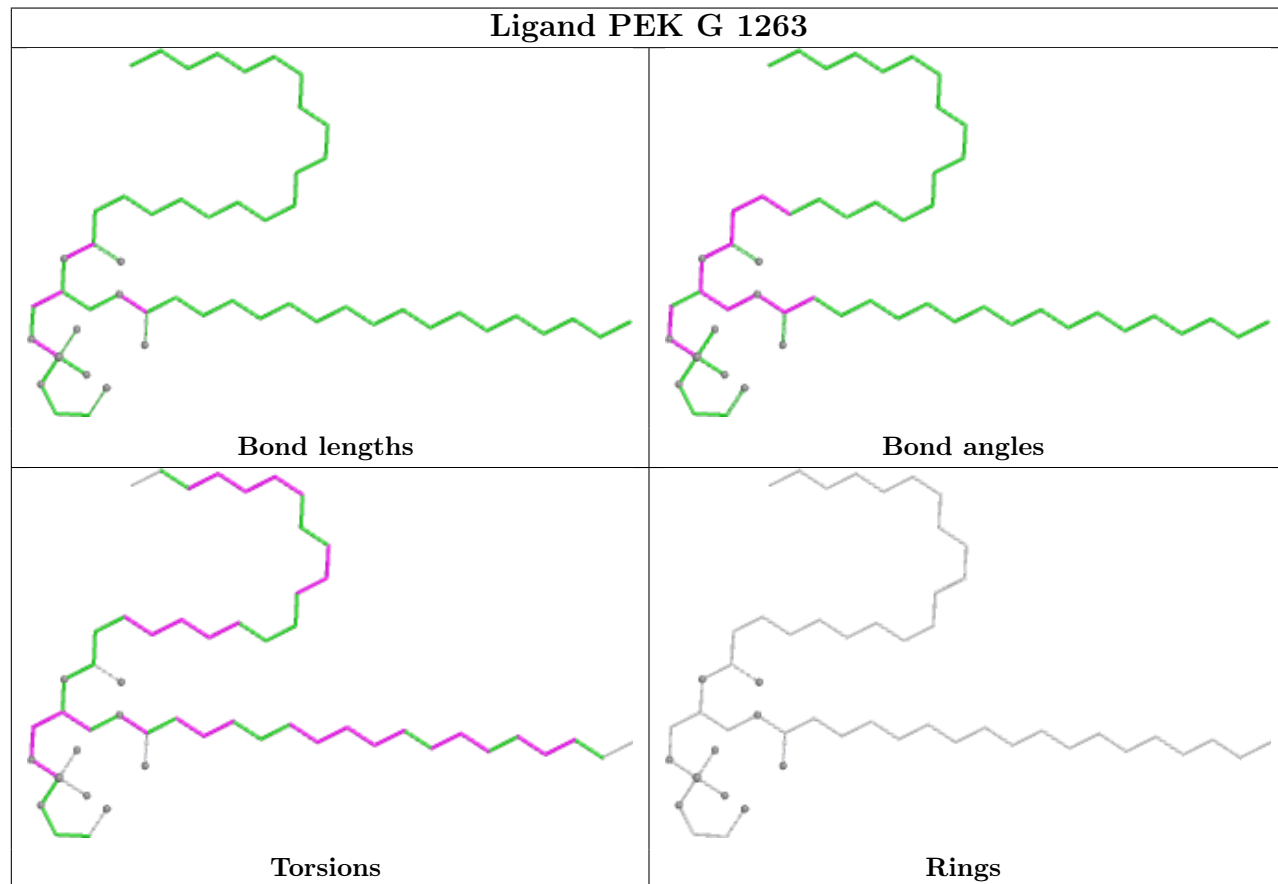


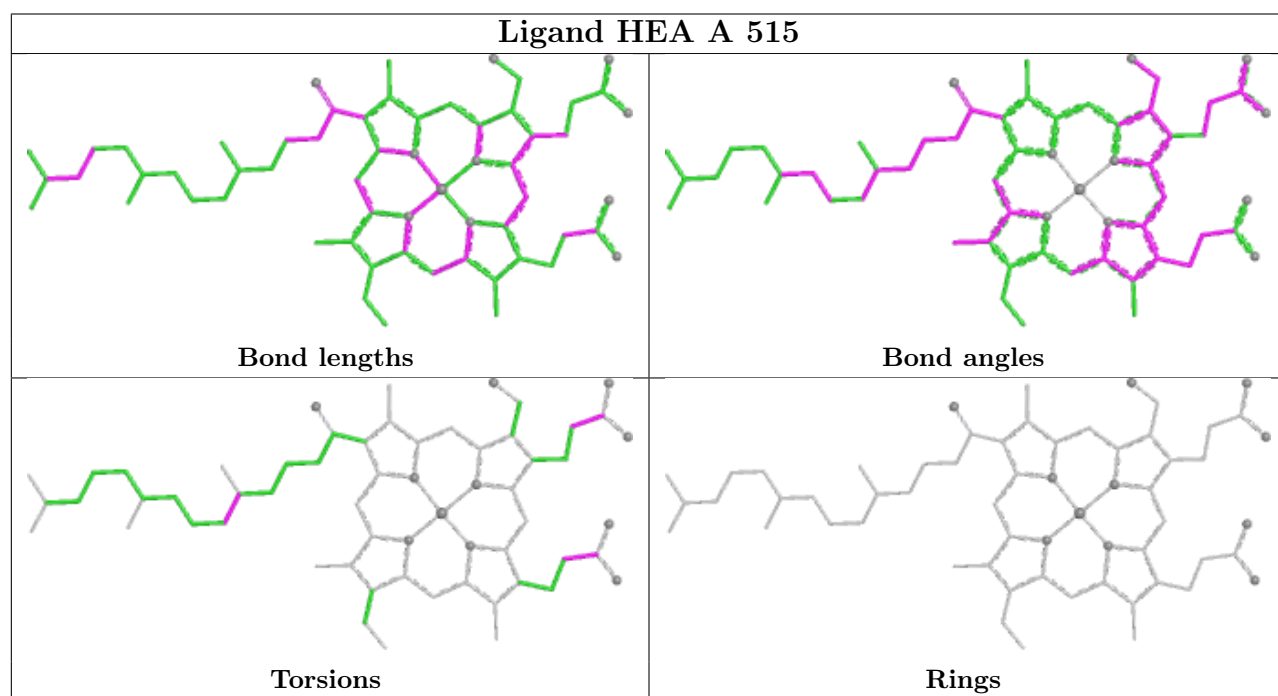
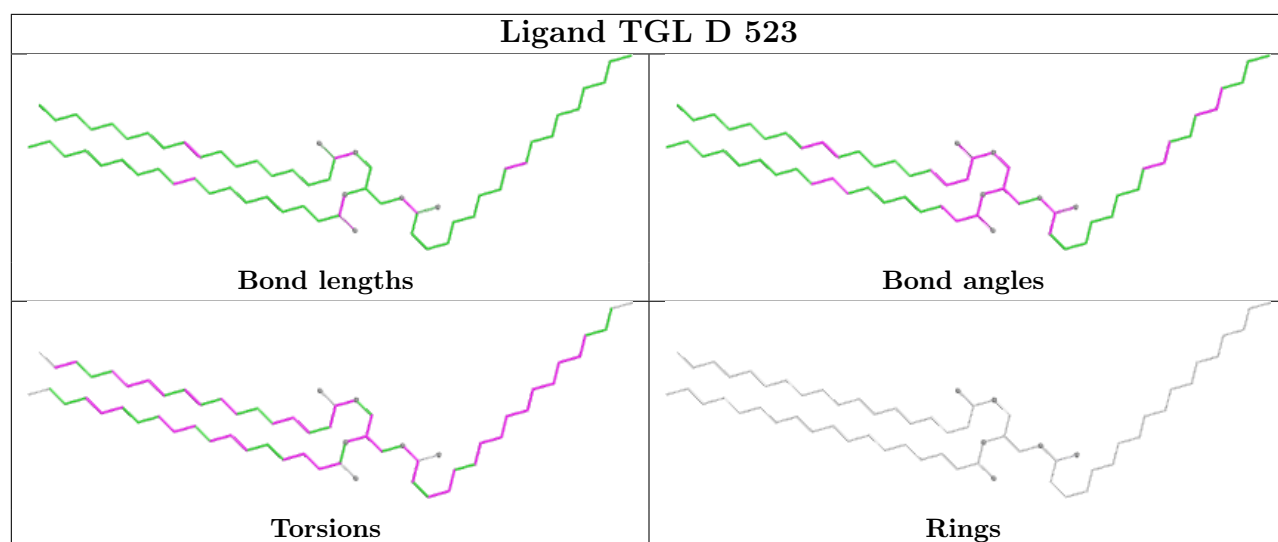


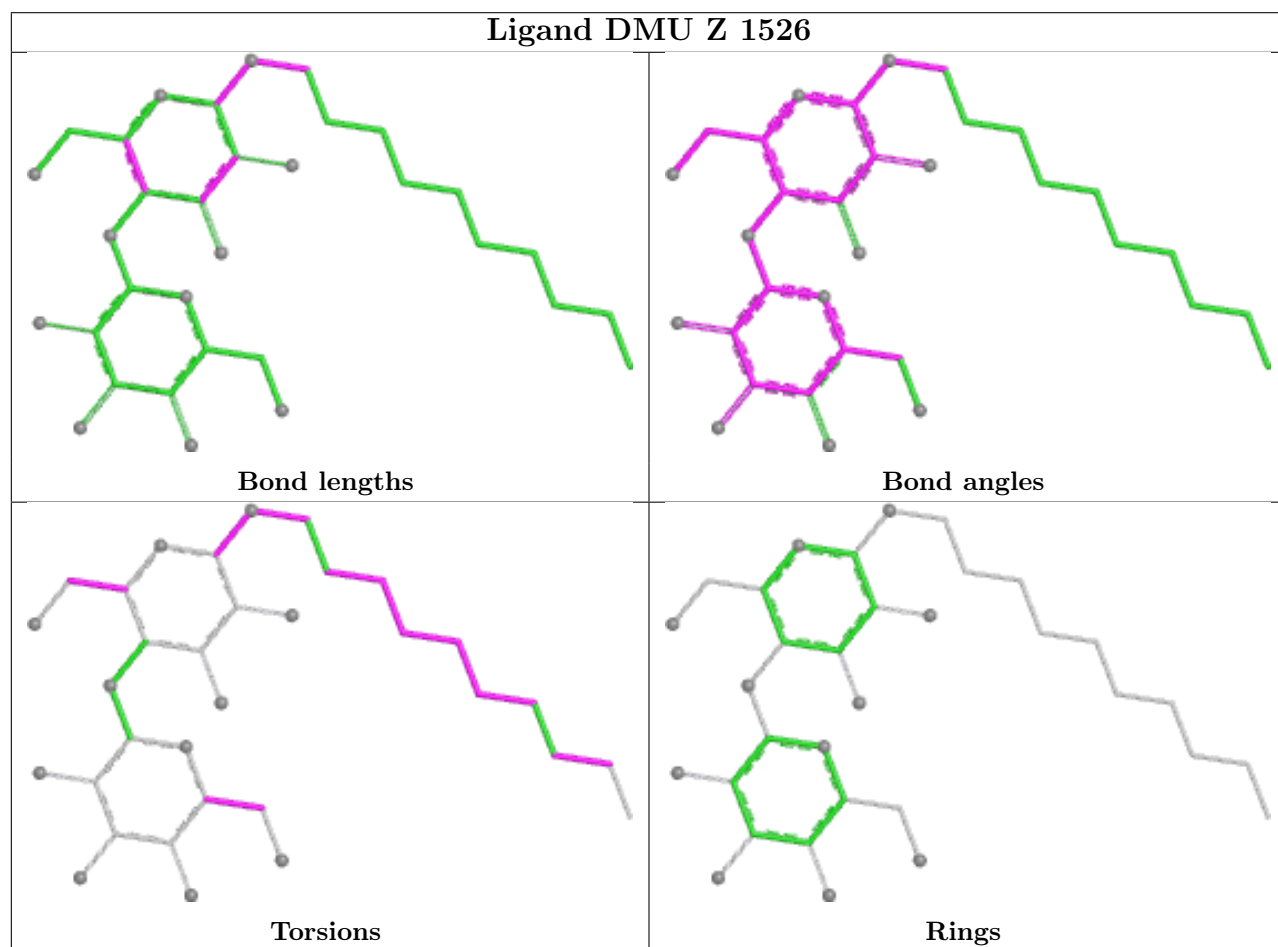
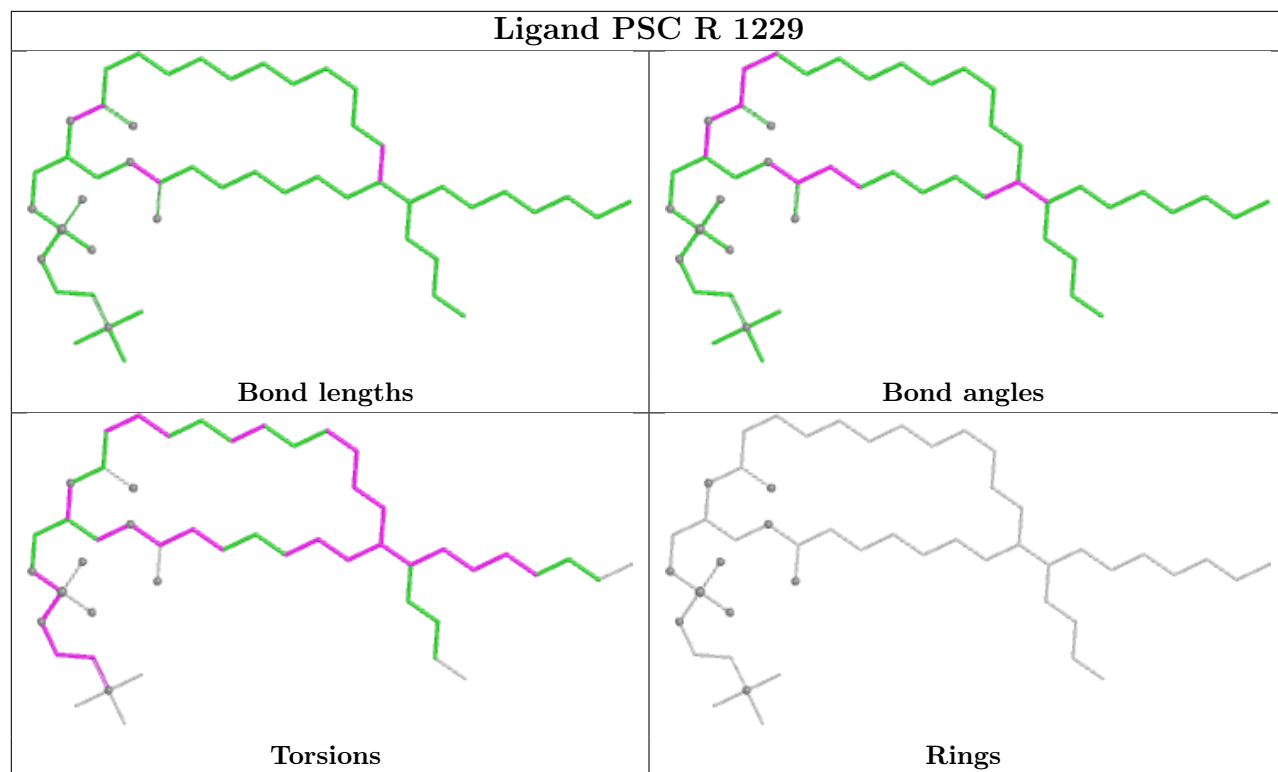
Ligand CHD B 1085

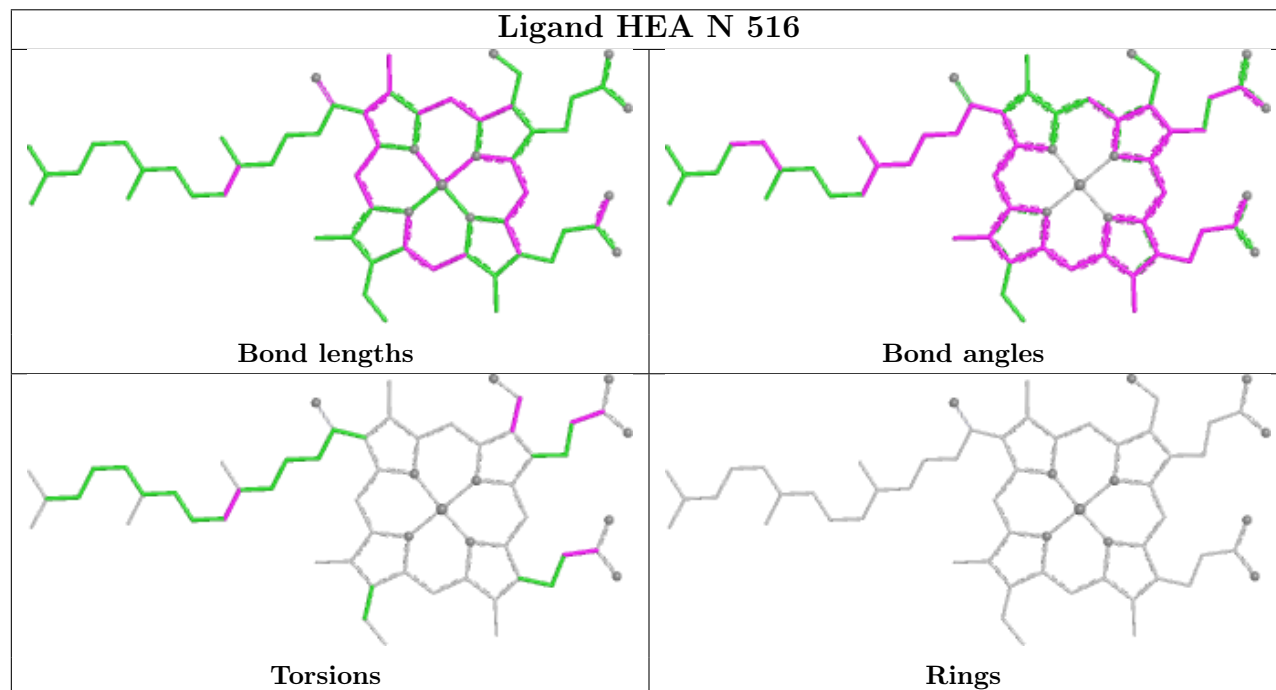
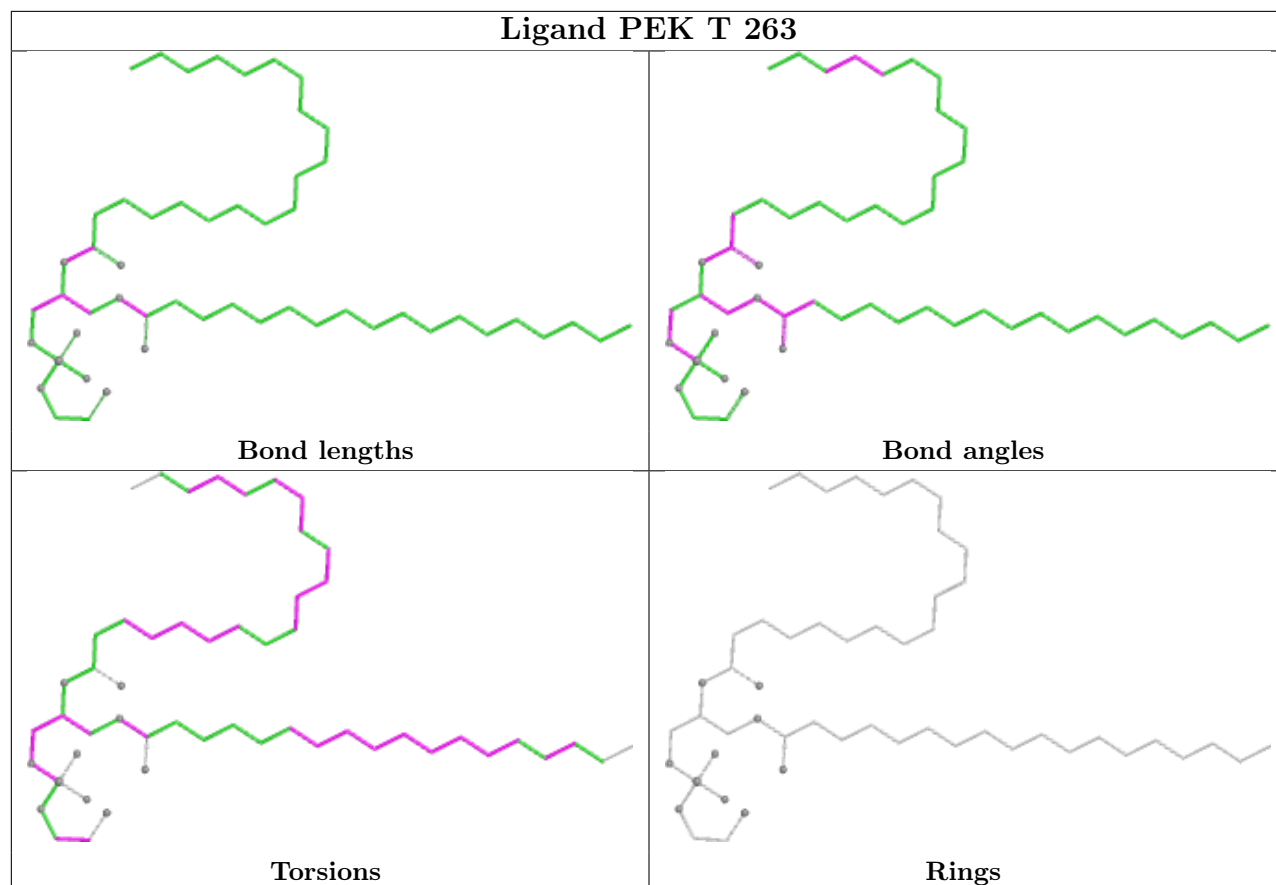


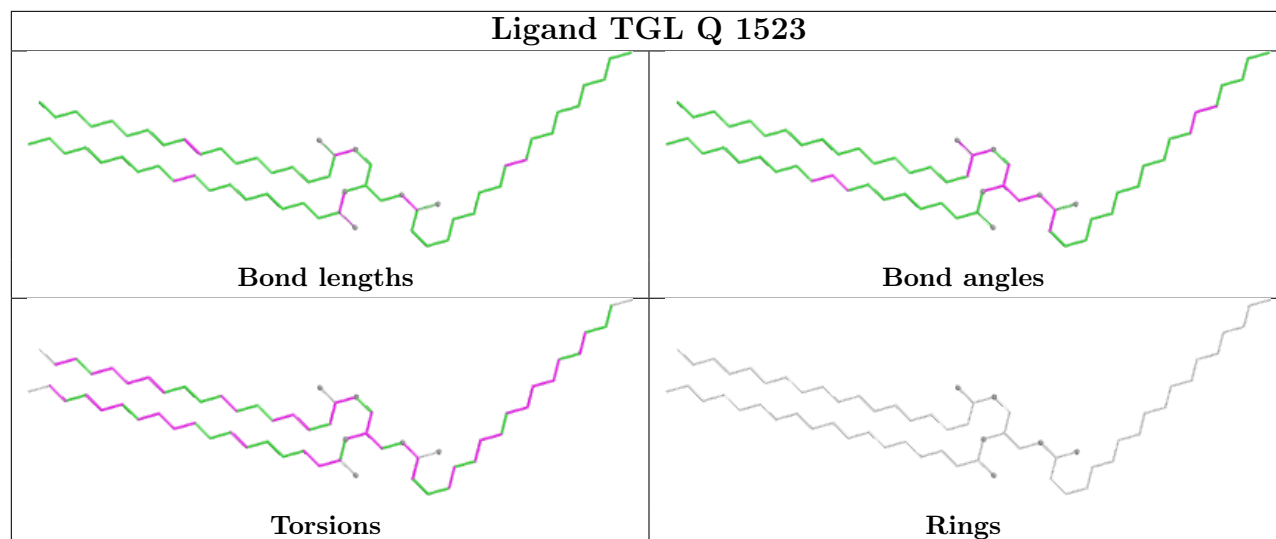
Ligand PEK G 1263











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%)	-0.43	5 (0%) 79 80	12, 25, 33, 64	5 (0%)
1	N	513/514 (99%)	-0.08	8 (1%) 70 71	14, 28, 36, 63	5 (0%)
2	B	226/227 (99%)	0.13	13 (5%) 29 27	20, 30, 48, 68	0
2	O	226/227 (99%)	0.53	17 (7%) 20 18	25, 34, 58, 80	0
3	C	259/261 (99%)	-0.22	3 (1%) 76 77	23, 27, 39, 61	0
3	P	259/261 (99%)	0.10	4 (1%) 72 72	25, 30, 41, 58	0
4	D	144/147 (97%)	0.33	4 (2%) 55 55	27, 34, 48, 64	0
4	Q	144/147 (97%)	1.16	20 (13%) 6 5	31, 40, 65, 115	0
5	E	105/109 (96%)	0.35	3 (2%) 53 53	28, 33, 58, 98	0
5	R	105/109 (96%)	0.76	4 (3%) 44 44	29, 37, 58, 101	0
6	F	98/98 (100%)	0.72	9 (9%) 14 12	26, 35, 79, 127	0
6	S	98/98 (100%)	1.00	11 (11%) 10 8	27, 37, 85, 121	0
7	G	83/85 (97%)	1.20	22 (26%) 1 1	25, 33, 90, 108	0
7	T	83/85 (97%)	1.35	20 (24%) 2 1	26, 34, 91, 107	0
8	H	79/85 (92%)	0.91	12 (15%) 5 4	27, 37, 83, 109	0
8	U	79/85 (92%)	1.10	15 (18%) 3 2	30, 41, 88, 109	0
9	I	72/73 (98%)	0.80	11 (15%) 5 4	28, 40, 57, 66	0
9	V	72/73 (98%)	1.19	13 (18%) 3 3	30, 44, 61, 77	0
10	J	58/59 (98%)	0.58	5 (8%) 16 14	27, 35, 56, 97	0
10	W	58/59 (98%)	0.99	6 (10%) 12 10	29, 37, 57, 102	0
11	K	49/56 (87%)	0.84	4 (8%) 17 15	30, 37, 52, 66	0
11	X	49/56 (87%)	1.27	9 (18%) 3 2	34, 42, 56, 72	0
12	L	46/47 (97%)	0.17	2 (4%) 40 39	25, 31, 48, 73	0
12	Y	46/47 (97%)	0.76	4 (8%) 16 14	29, 34, 51, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.68	5 (11%) 9 8	27, 31, 69, 98	0
13	Z	43/46 (93%)	1.17	7 (16%) 4 3	32, 37, 79, 106	0
All	All	3550/3614 (98%)	0.33	236 (6%) 24 23	12, 31, 58, 127	10 (0%)

The worst 5 of 236 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	19.4
6	F	1	ALA	14.0
4	Q	6	VAL	13.1
6	S	97	ALA	11.0
8	U	8	ILE	9.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	T	11	11/12	0.57	0.28	71,80,101,104	0
7	TPO	G	11	11/12	0.58	0.32	66,75,101,101	0
9	SAC	V	1	9/10	0.66	0.20	83,86,88,88	0
9	SAC	I	1	9/10	0.72	0.20	63,66,69,73	0
1	FME	N	1	10/11	0.86	0.17	42,48,77,80	0
1	FME	A	1	10/11	0.91	0.14	38,41,68,76	0
2	FME	B	1	10/11	0.95	0.09	20,30,40,52	0
2	FME	O	1	10/11	0.96	0.10	33,34,40,48	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	UNX	C	262	1/1	0.61	0.55	81,81,81,81	0
23	CHD	J	60	29/29	0.71	0.27	99,104,108,108	0
24	UNX	P	262	1/1	0.71	0.43	82,82,82,82	0
20	PGV	P	1268	51/51	0.73	0.26	57,77,111,112	0
28	DMU	P	1272	33/33	0.73	0.23	72,106,119,121	0
20	PGV	N	1524	51/51	0.74	0.26	41,76,121,123	0
23	CHD	W	1059	29/29	0.75	0.24	101,108,110,112	0
25	PEK	G	265	53/53	0.75	0.25	47,79,103,105	0
25	PEK	G	1263	53/53	0.75	0.28	51,96,123,124	0
25	PEK	P	1265	53/53	0.75	0.25	46,76,107,110	0
25	PEK	T	263	53/53	0.75	0.26	48,94,121,122	0
28	DMU	G	272	33/33	0.75	0.22	72,100,115,116	0
19	TGL	Q	1523	63/63	0.75	0.27	56,74,100,102	0
26	CDL	T	1269	100/100	0.77	0.24	59,86,115,118	0
19	TGL	N	1522	63/63	0.77	0.25	49,64,84,89	0
26	CDL	P	1270	100/100	0.77	0.26	36,86,117,120	0
20	PGV	C	268	51/51	0.78	0.26	51,79,108,111	0
26	CDL	G	269	100/100	0.78	0.23	58,86,116,120	0
19	TGL	D	523	63/63	0.78	0.25	53,67,97,99	0
20	PGV	M	524	51/51	0.79	0.24	40,70,127,129	0
19	TGL	A	521	63/63	0.79	0.24	53,72,88,92	0
26	CDL	C	270	100/100	0.80	0.23	42,84,109,110	0
19	TGL	L	522	63/63	0.80	0.23	36,62,78,81	0
22	PSC	R	1229	52/52	0.80	0.27	49,95,129,135	0
19	TGL	O	1521	63/63	0.81	0.21	53,75,88,92	0
22	PSC	B	229	52/52	0.82	0.25	45,95,136,139	0
23	CHD	C	271	29/29	0.87	0.13	54,61,65,73	0
28	DMU	Z	1526	33/33	0.87	0.14	40,50,71,75	0
23	CHD	P	1271	29/29	0.90	0.12	51,63,68,69	0
28	DMU	M	526	33/33	0.92	0.10	35,44,61,65	0
25	PEK	P	1264	53/53	0.94	0.14	25,49,81,82	0
20	PGV	N	1266	51/51	0.95	0.11	23,36,59,64	0
25	PEK	C	264	53/53	0.95	0.12	24,45,77,80	0
20	PGV	P	1267	51/51	0.95	0.12	23,37,80,82	0
23	CHD	O	229	29/29	0.96	0.07	21,25,31,33	0
23	CHD	P	1525	29/29	0.96	0.07	27,31,35,37	0
18	NA	N	519	1/1	0.96	0.09	31,31,31,31	0
23	CHD	C	525	29/29	0.96	0.07	21,30,35,38	0
20	PGV	C	267	51/51	0.97	0.10	22,33,73,74	0
23	CHD	B	1085	29/29	0.97	0.06	23,26,31,37	0
18	NA	A	519	1/1	0.97	0.09	28,28,28,28	0
17	MG	N	518	1/1	0.97	0.05	29,29,29,29	0

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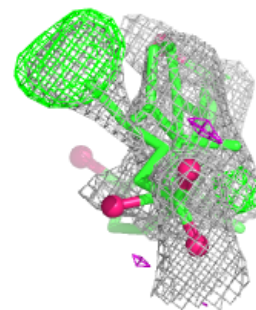
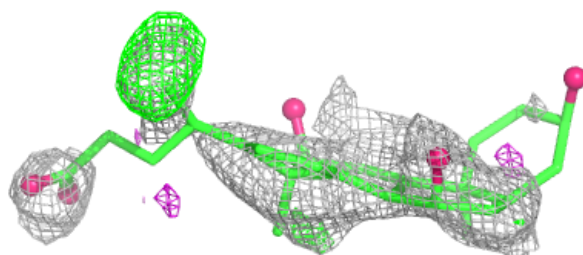
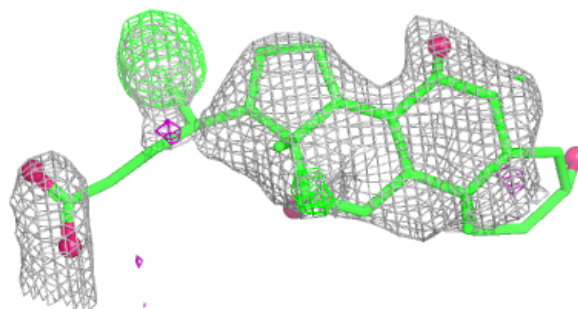
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	PGV	A	522	51/51	0.97	0.10	20,33,67,71	0
15	NO	A	520	2/2	0.98	0.06	24,24,24,25	0
17	MG	A	518	1/1	0.98	0.04	24,24,24,24	0
14	HEA	A	515	60/60	0.98	0.06	19,23,38,41	0
21	CUA	O	228	2/2	0.98	0.03	27,27,27,27	0
14	HEA	N	515	60/60	0.98	0.06	21,26,40,44	0
27	ZN	F	99	1/1	0.99	0.03	31,31,31,31	0
27	ZN	S	99	1/1	0.99	0.03	33,33,33,33	0
21	CUA	B	228	2/2	0.99	0.03	23,23,23,23	0
14	HEA	N	516	60/60	0.99	0.06	22,26,31,36	0
14	HEA	A	516	60/60	0.99	0.05	19,22,30,34	0
15	NO	N	520	2/2	0.99	0.05	26,26,26,31	0
16	CU	A	517	1/1	1.00	0.03	24,24,24,24	0
16	CU	N	517	1/1	1.00	0.04	26,26,26,26	0

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

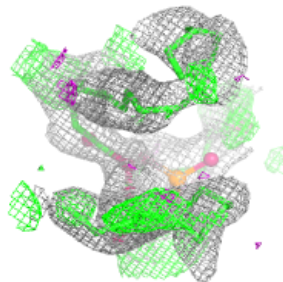
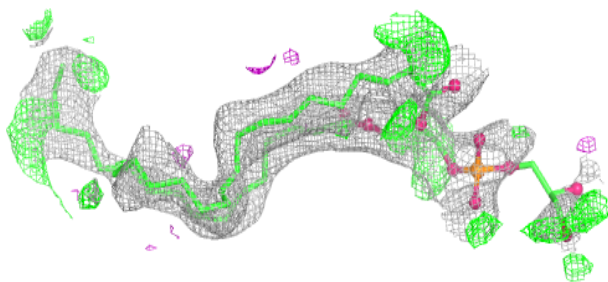
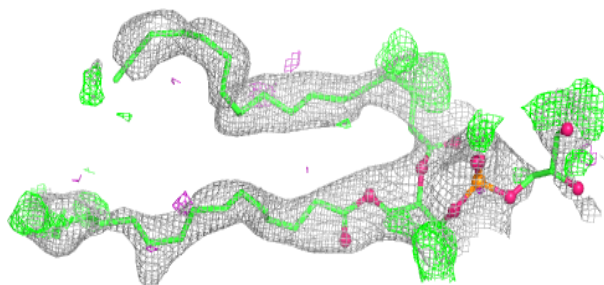
Electron density around CHD J 60:

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

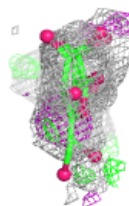
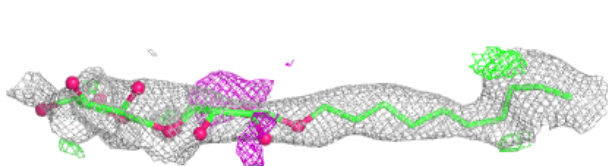
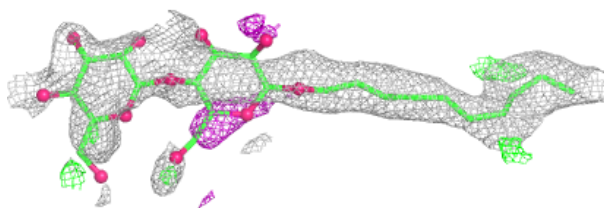


Electron density around PGV P 1268:

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

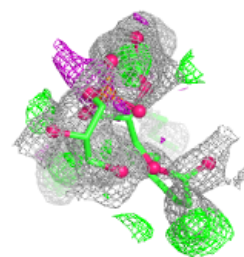
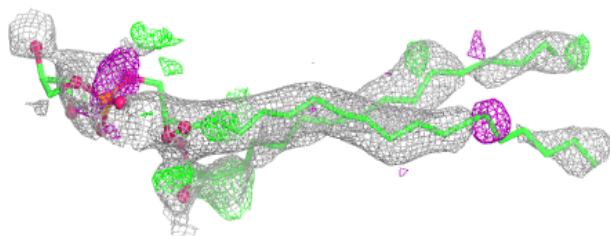
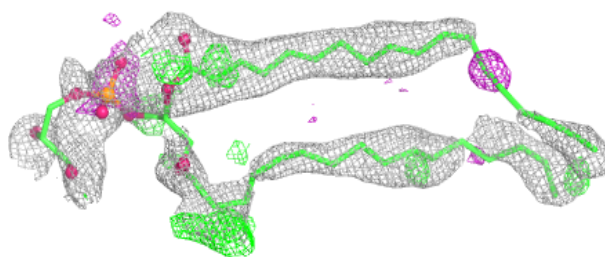
**Electron density around DMU P 1272:**

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

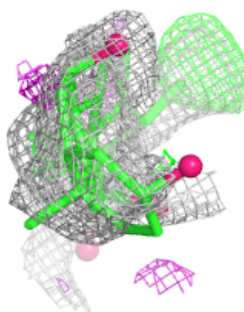
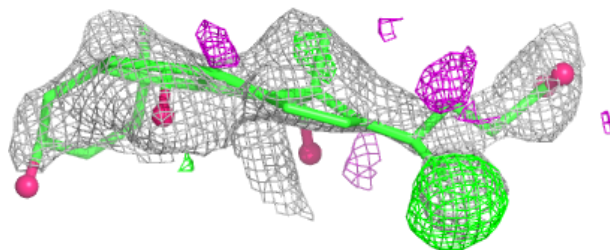
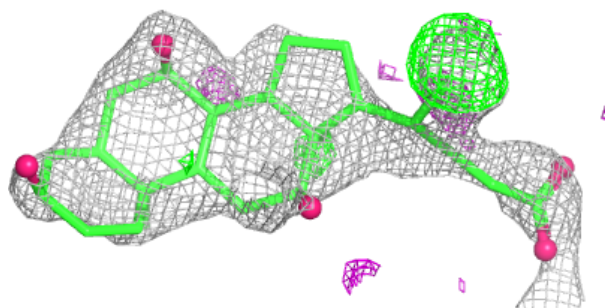


Electron density around PGV N 1524:

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

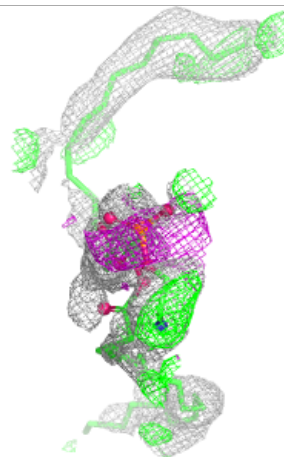
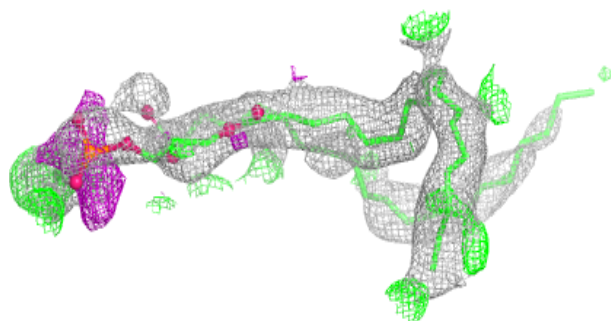
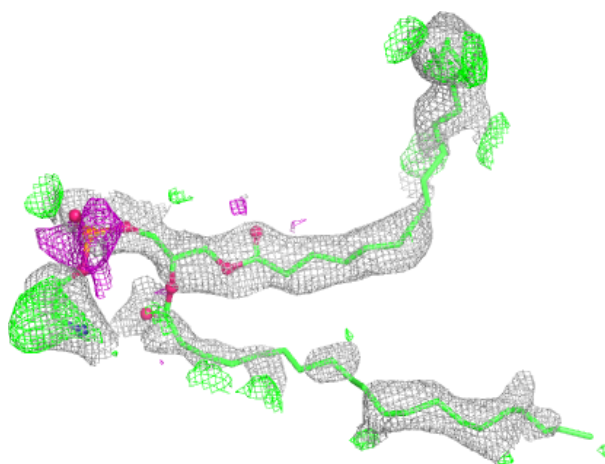
**Electron density around CHD W 1059:**

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



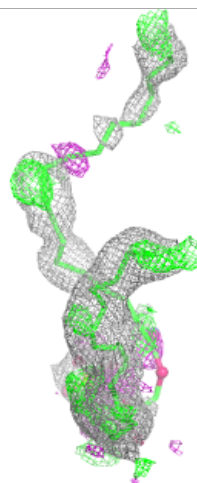
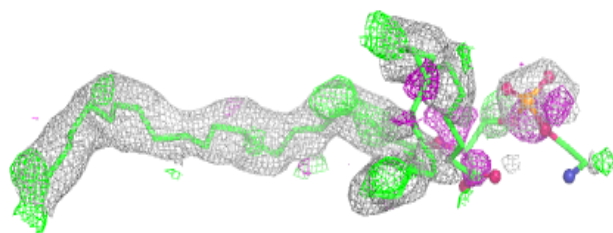
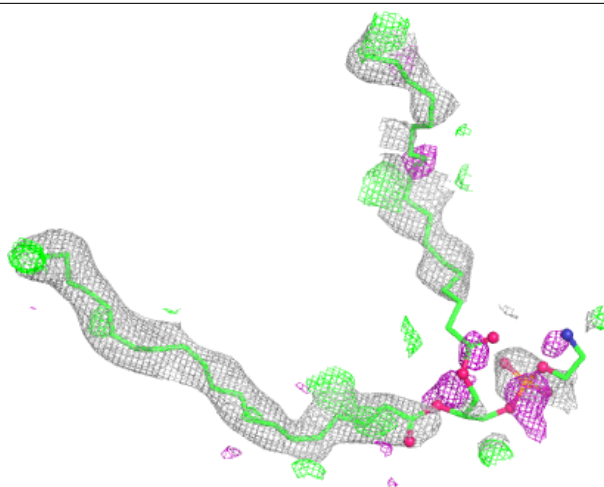
Electron density around PEK G 265:

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



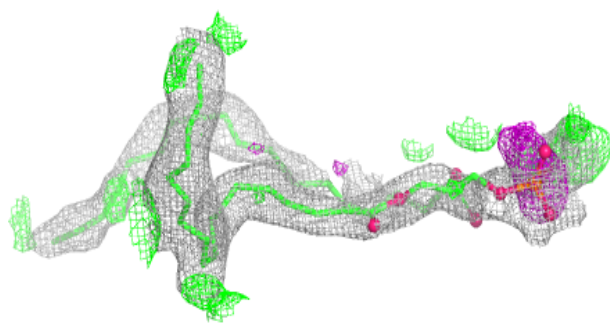
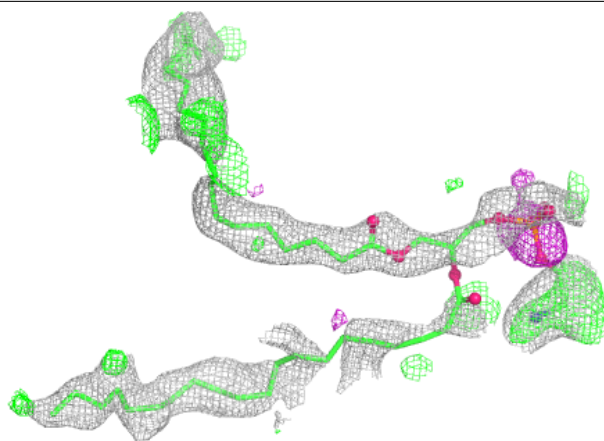
Electron density around PEK G 1263:

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



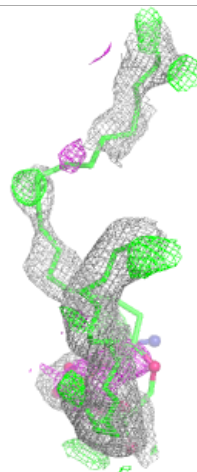
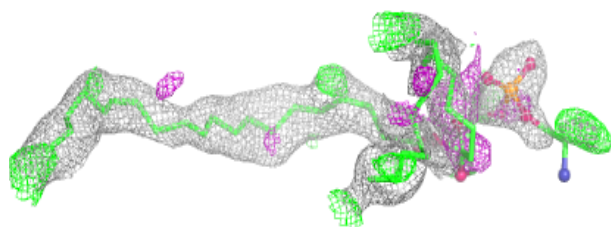
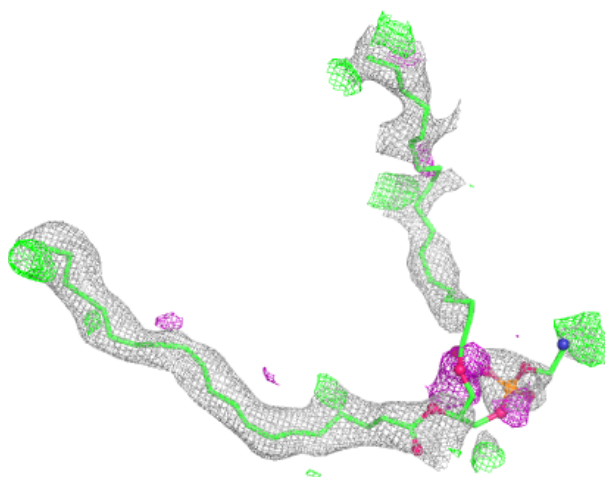
Electron density around PEK P 1265:

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



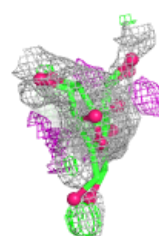
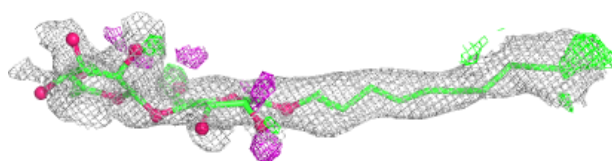
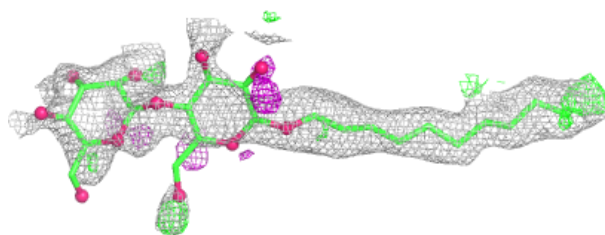
Electron density around PEK T 263:

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

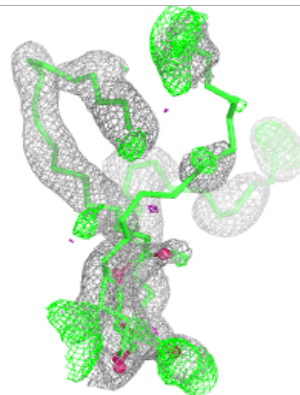
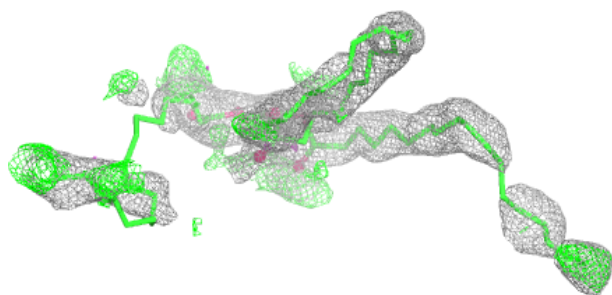
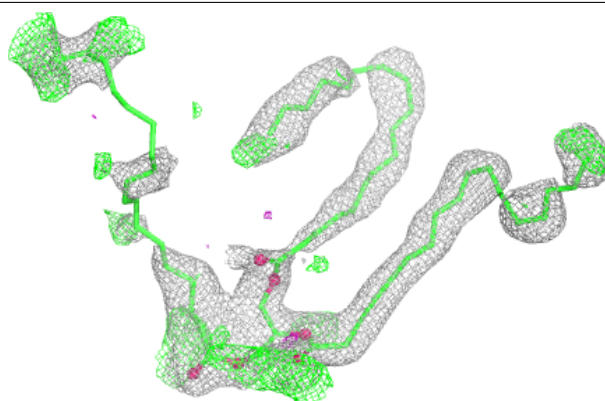


Electron density around DMU G 272:

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

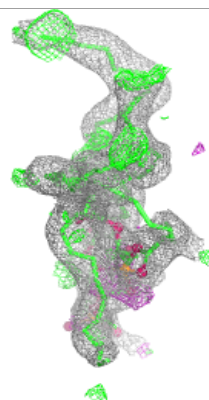
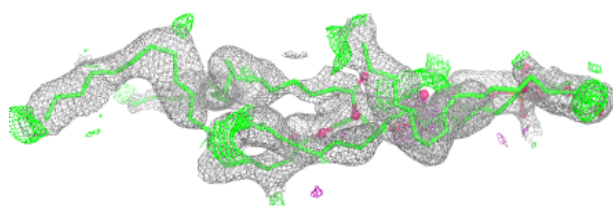
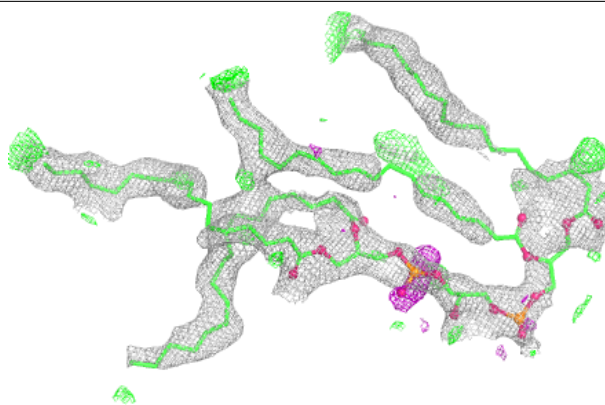
**Electron density around TGL Q 1523:**

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

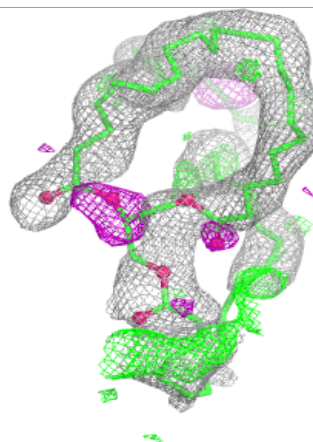
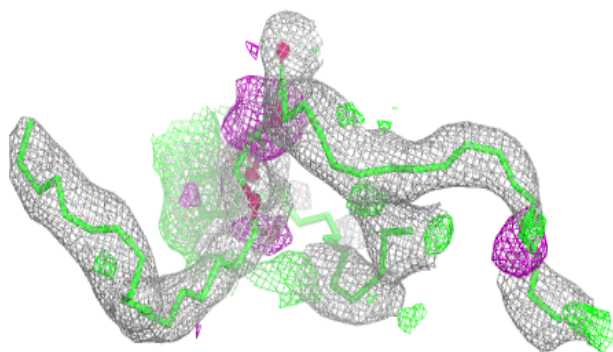
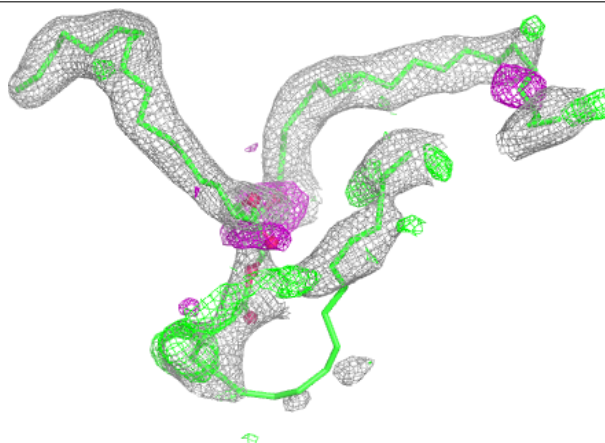


Electron density around CDL T 1269:

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

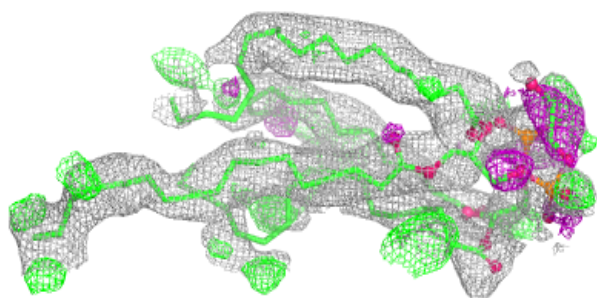
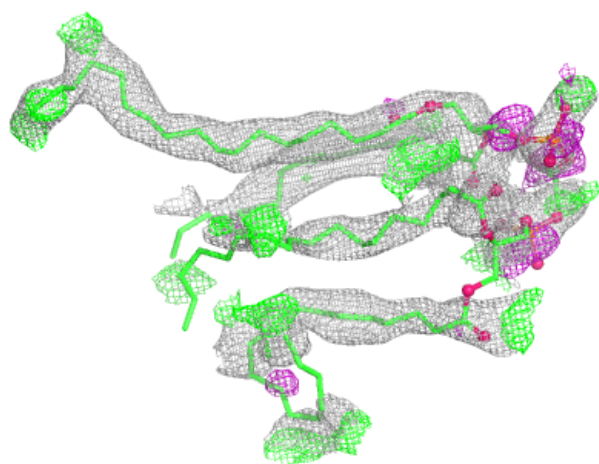
**Electron density around TGL N 1522:**

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



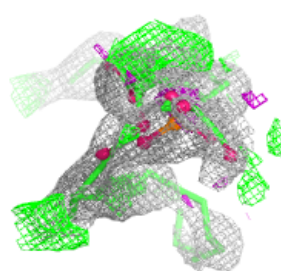
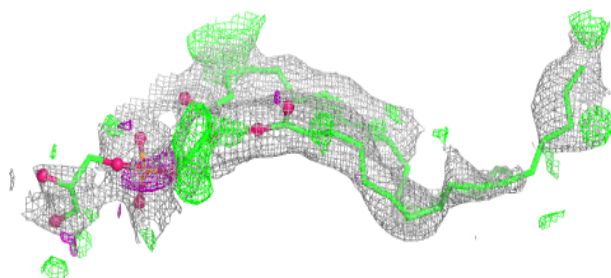
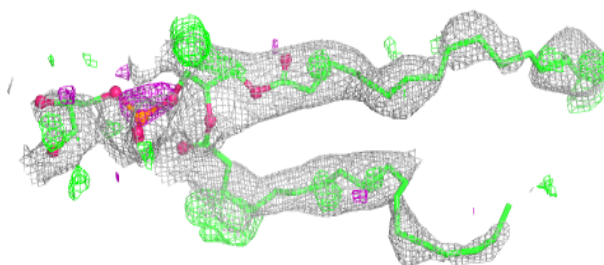
Electron density around CDL P 1270:

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

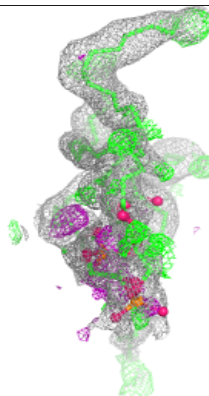
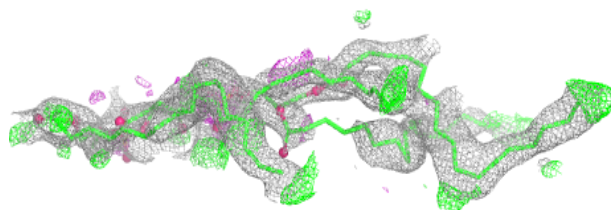
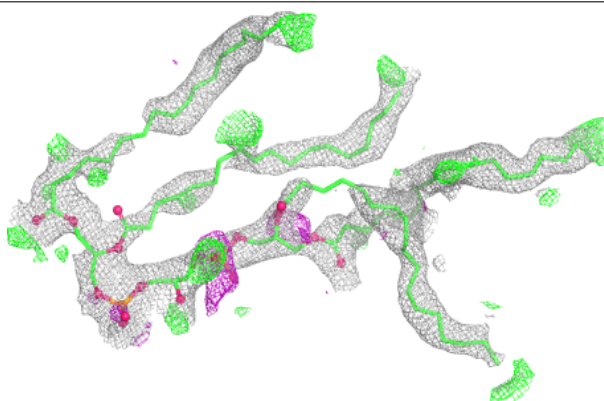


Electron density around PGV C 268:

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

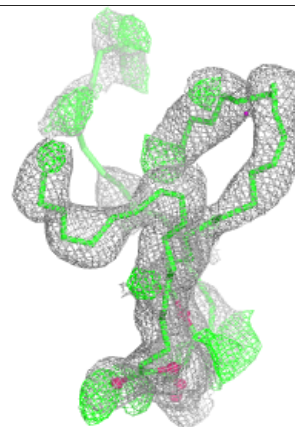
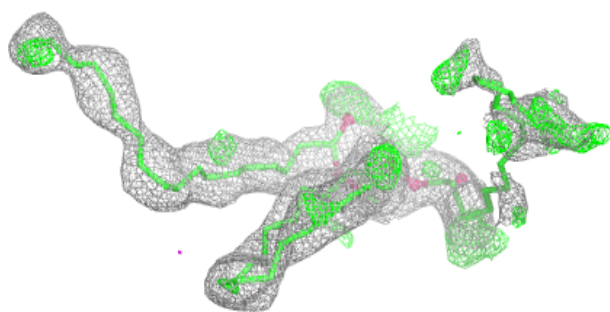
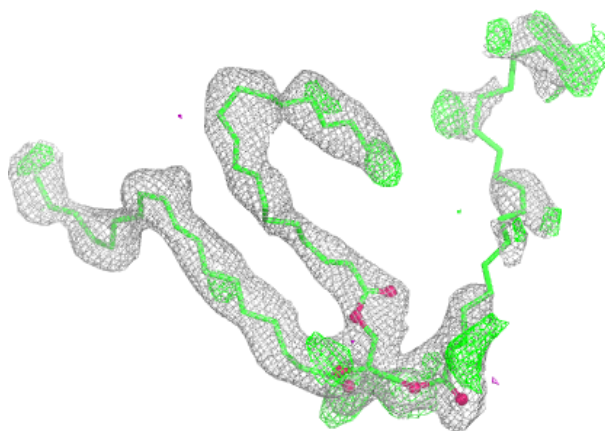
**Electron density around CDL G 269:**

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

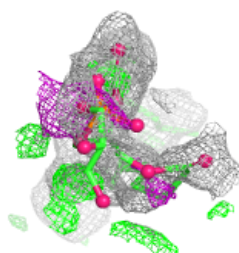
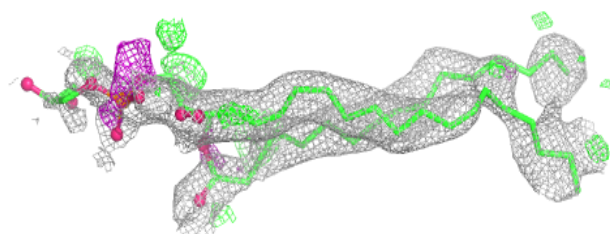
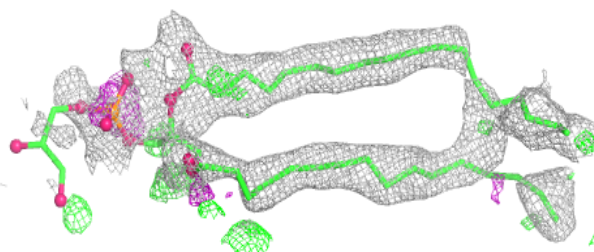


Electron density around TGL D 523:

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

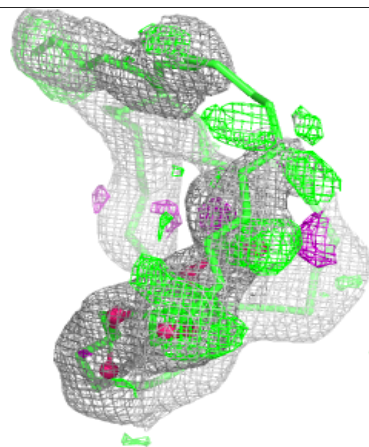
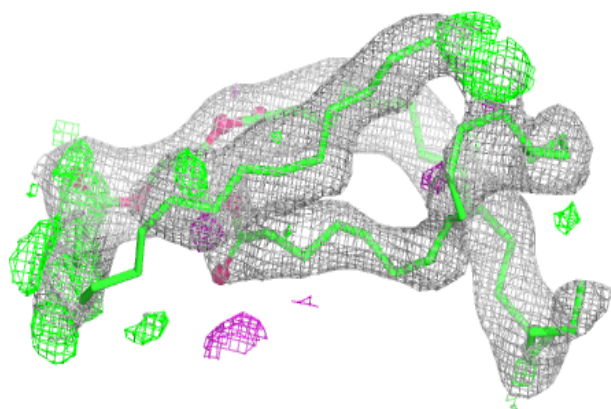
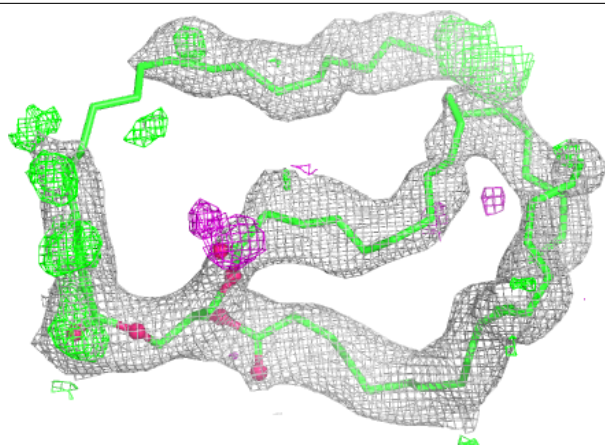
**Electron density around PGV M 524:**

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



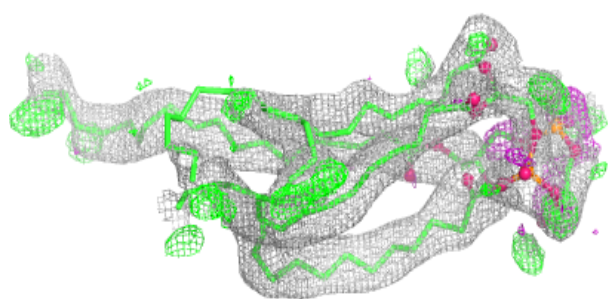
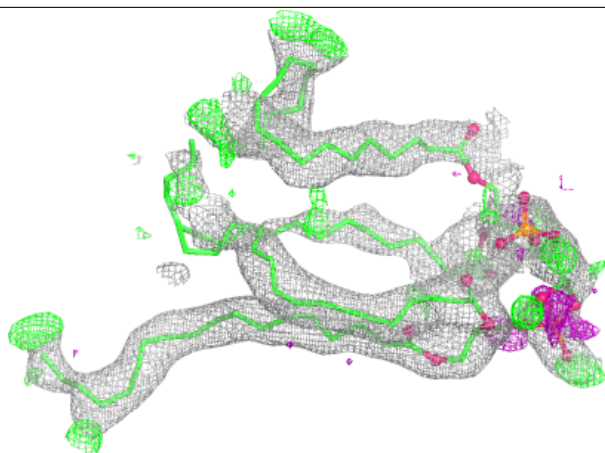
Electron density around TGL A 521:

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



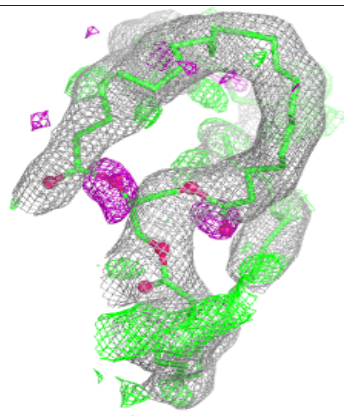
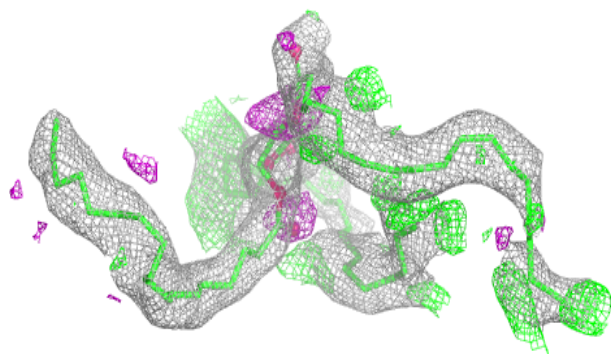
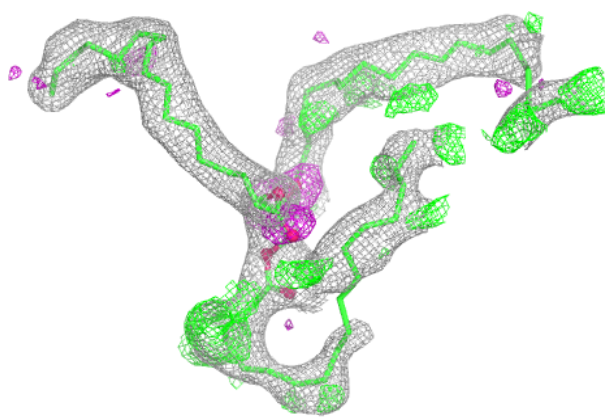
Electron density around CDL C 270:

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

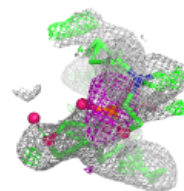
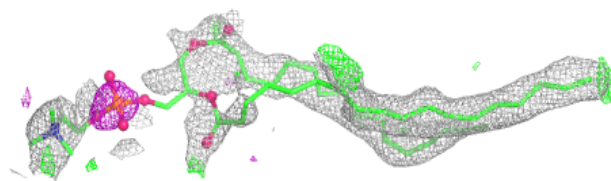
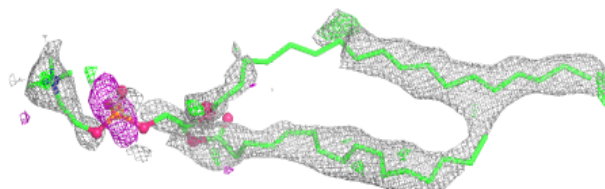


Electron density around TGL L 522:

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

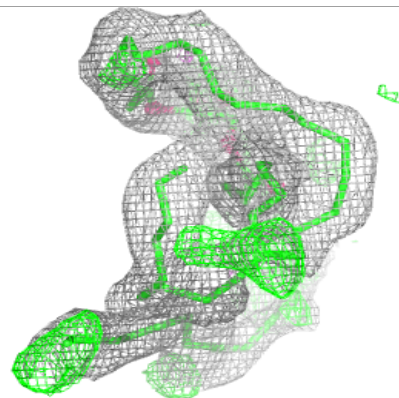
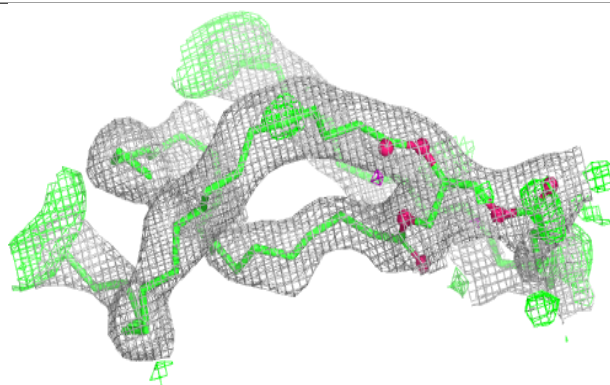
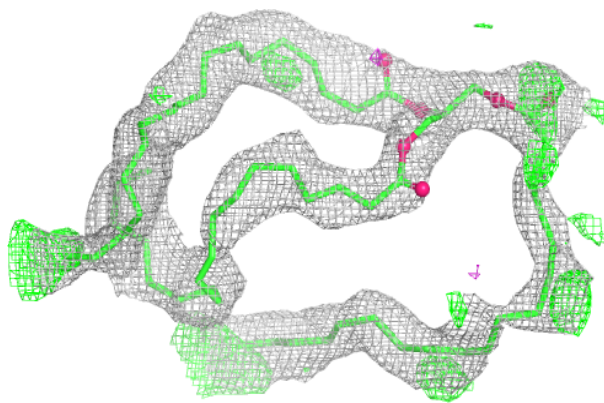
**Electron density around PSC R 1229:**

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

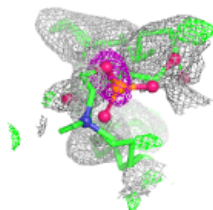
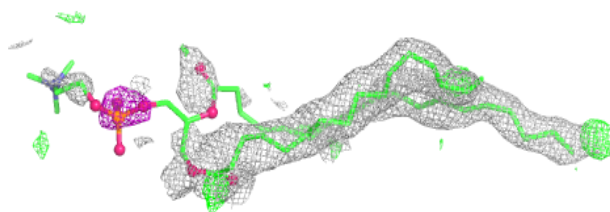
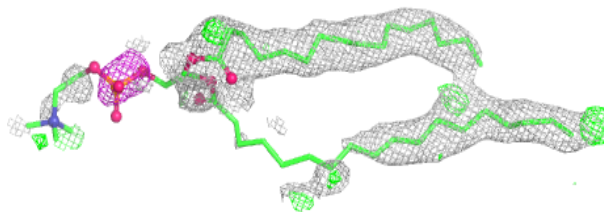


Electron density around TGL O 1521:

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

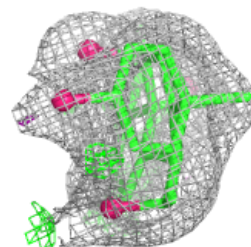
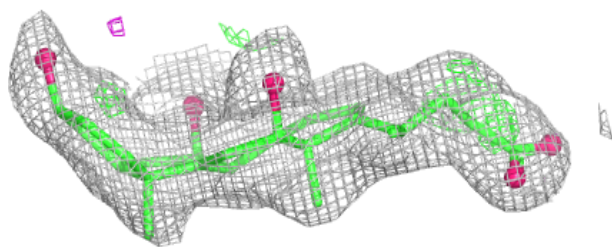
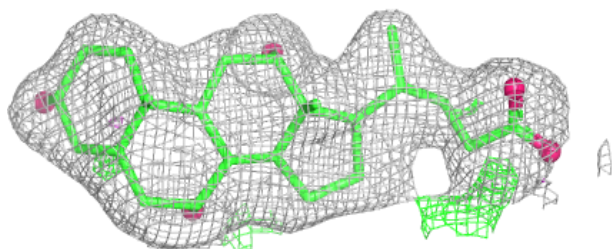
**Electron density around PSC B 229:**

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

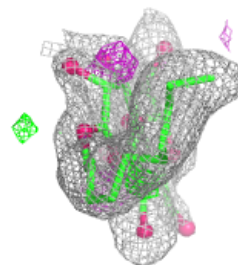
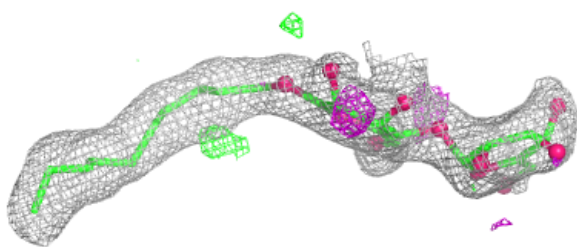
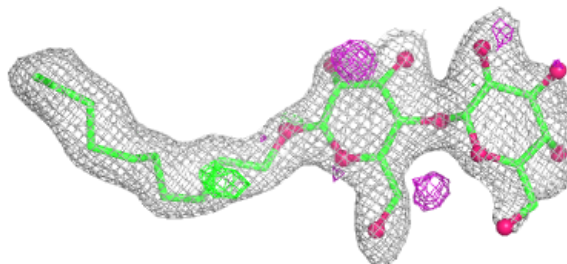


Electron density around CHD C 271:

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

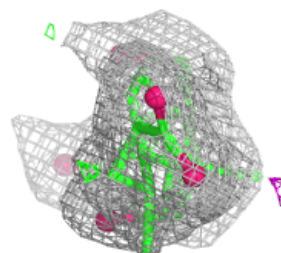
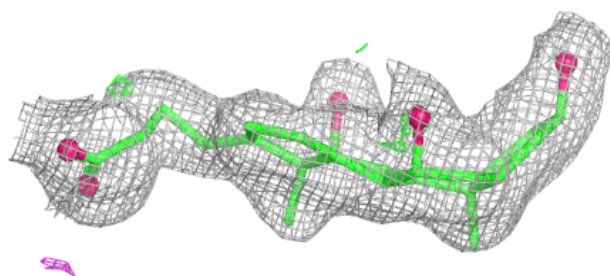
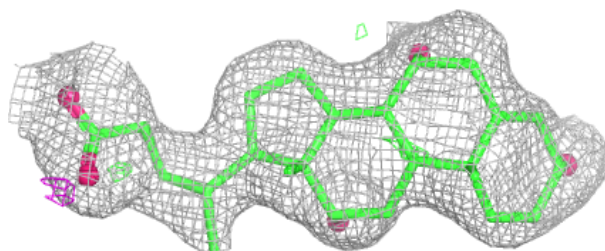
**Electron density around DMU Z 1526:**

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

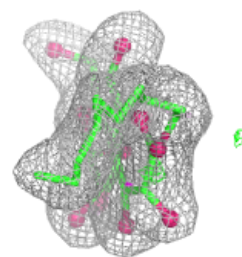
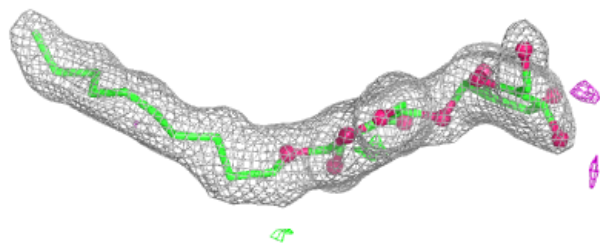
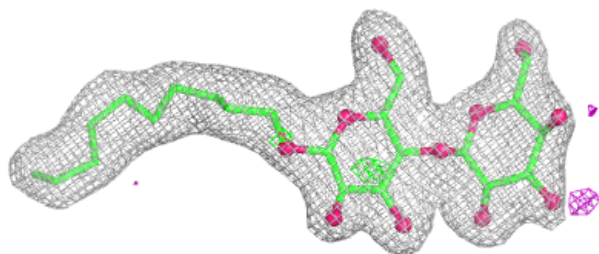


Electron density around CHD P 1271:

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

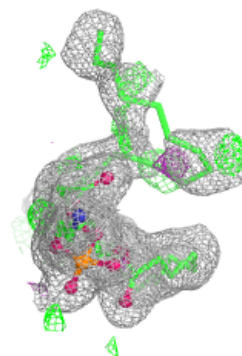
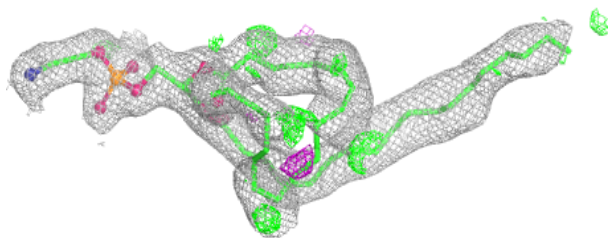
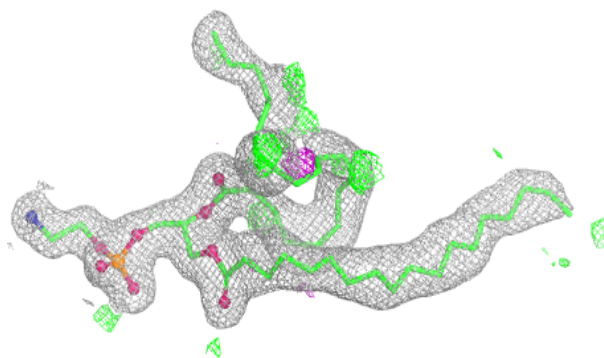
**Electron density around DMU M 526:**

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

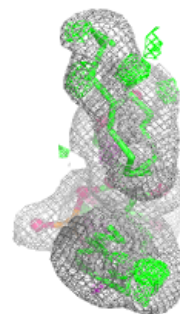
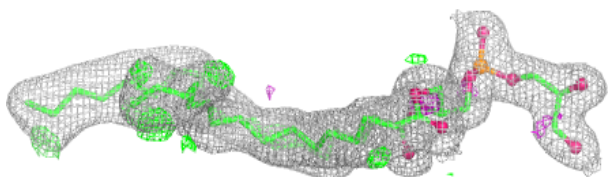
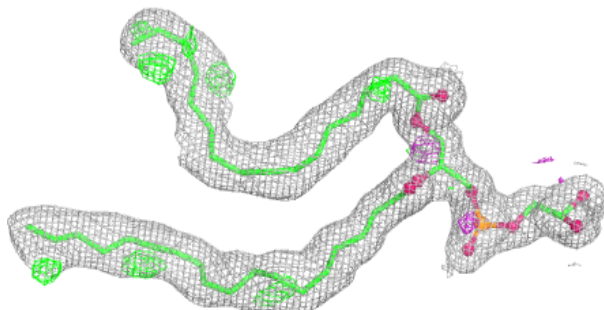


Electron density around PEK P 1264:

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

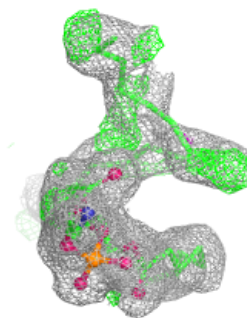
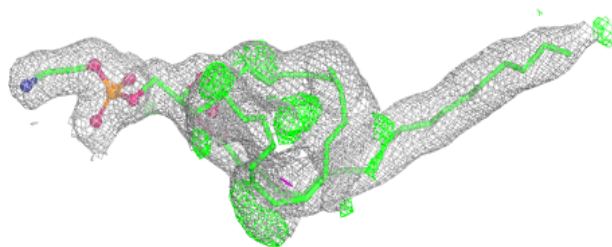
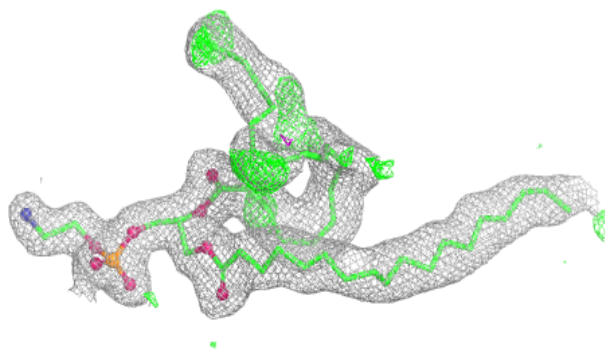
**Electron density around PGV N 1266:**

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

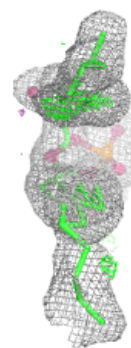
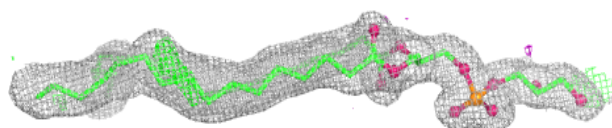
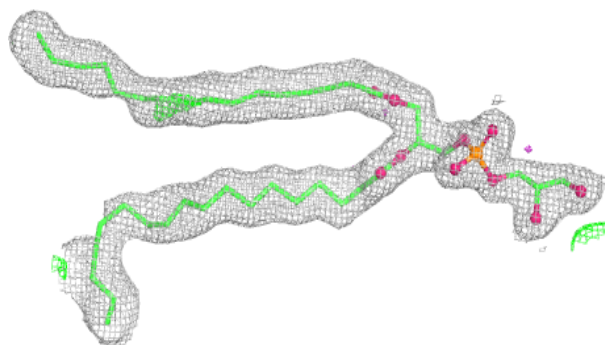


Electron density around PEK C 264:

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

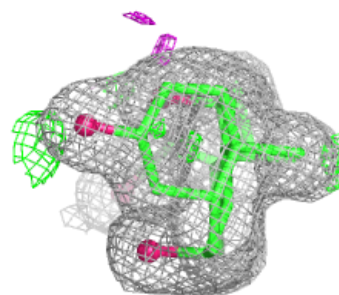
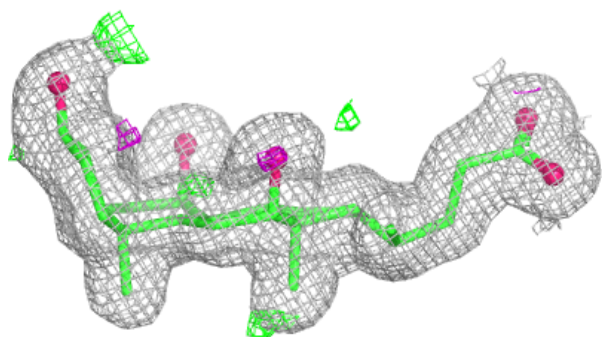
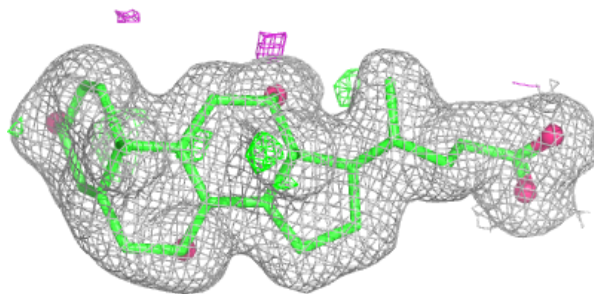
**Electron density around PGV P 1267:**

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

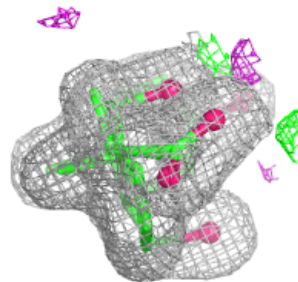
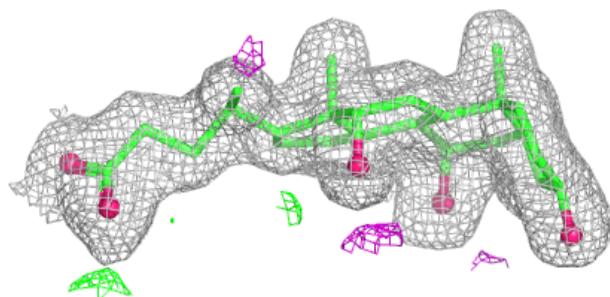
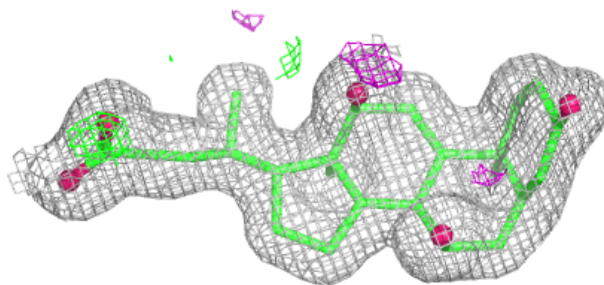


Electron density around CHD O 229:

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

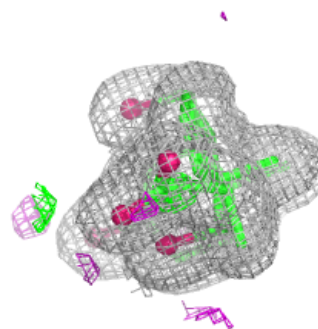
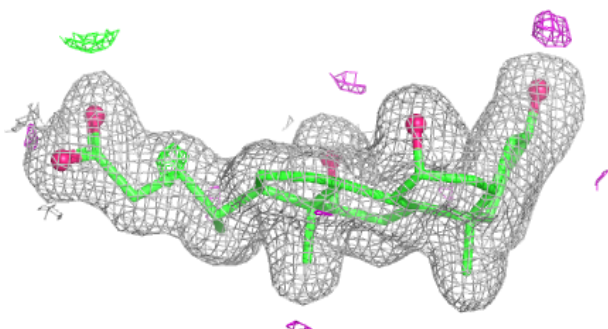
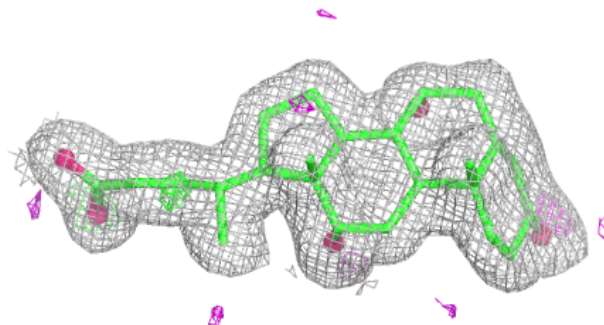
**Electron density around CHD P 1525:**

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

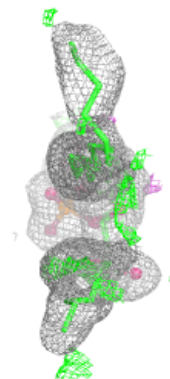
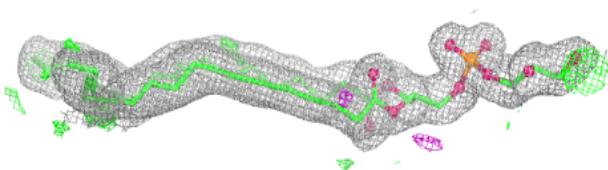
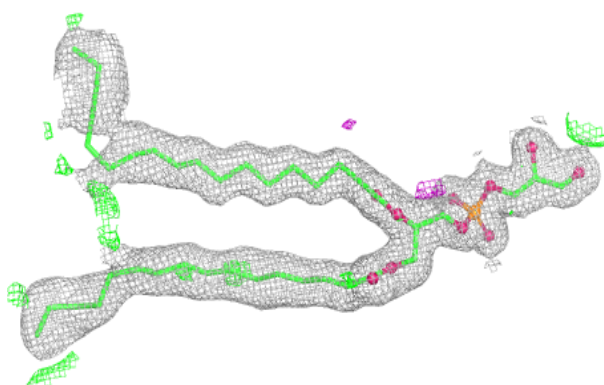


Electron density around CHD C 525:

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

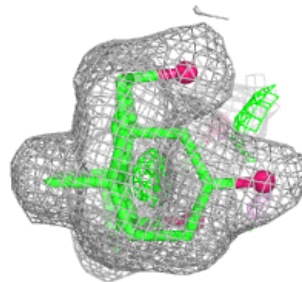
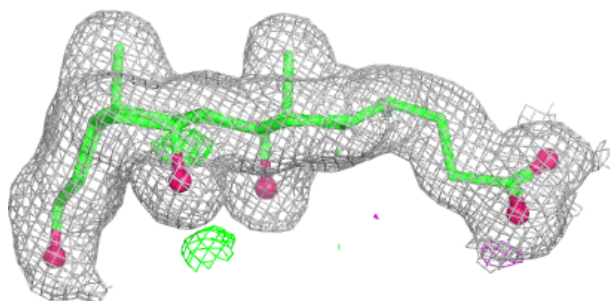
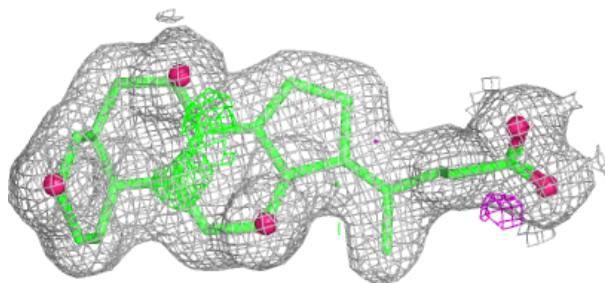
**Electron density around PGV C 267:**

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

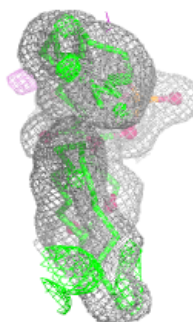
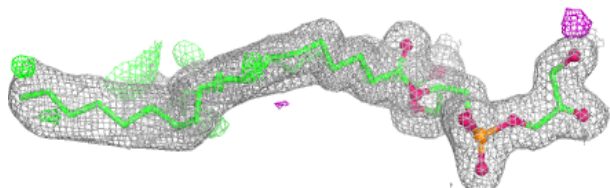
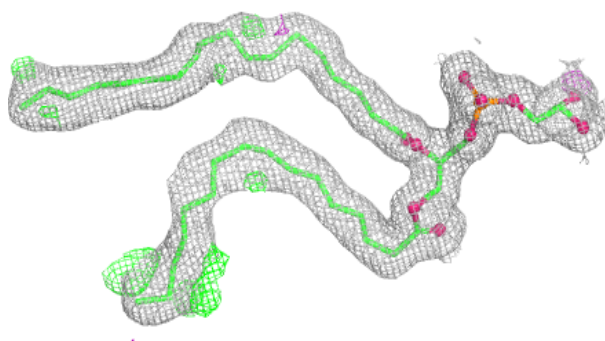


Electron density around CHD B 1085:

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

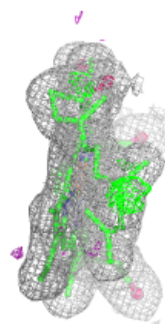
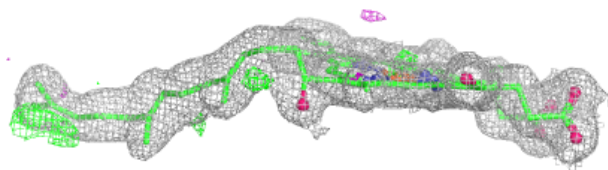
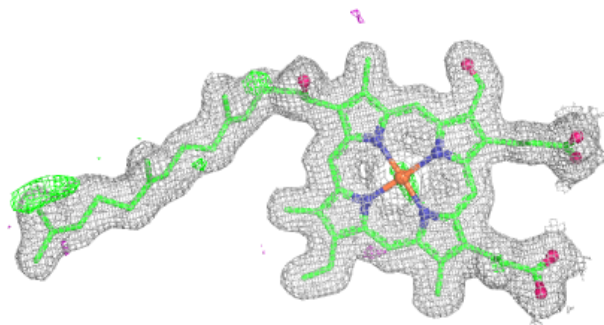
**Electron density around PGV A 522:**

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

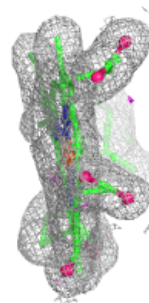
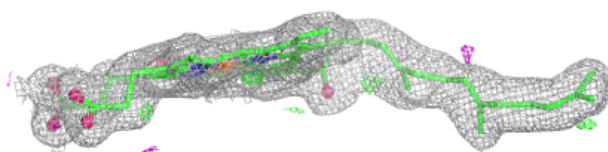
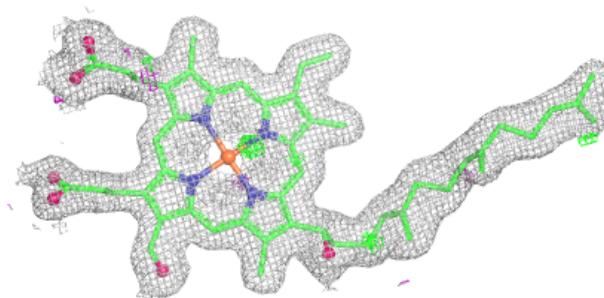


Electron density around HEA A 515:

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

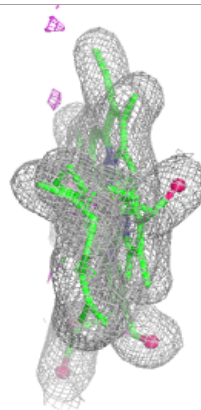
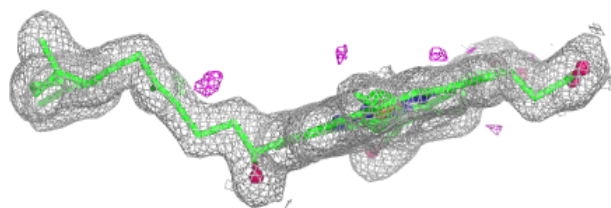
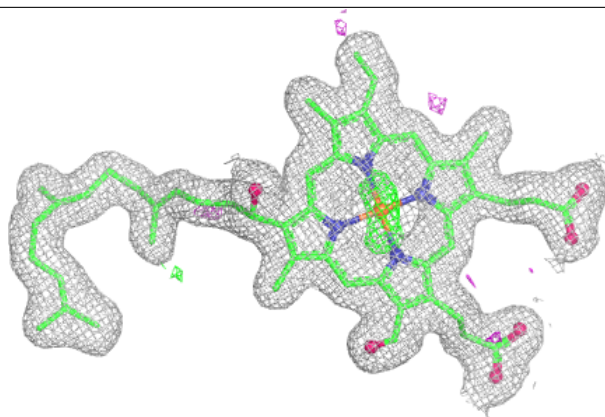
**Electron density around HEA N 515:**

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

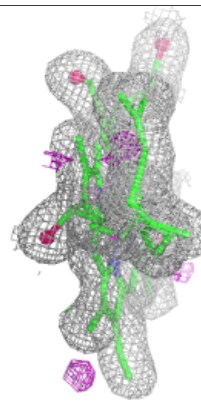
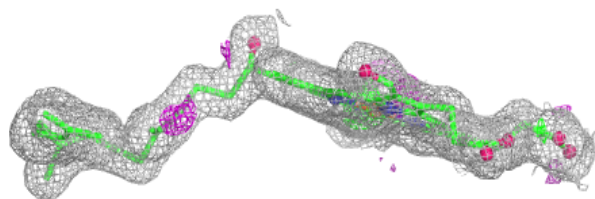
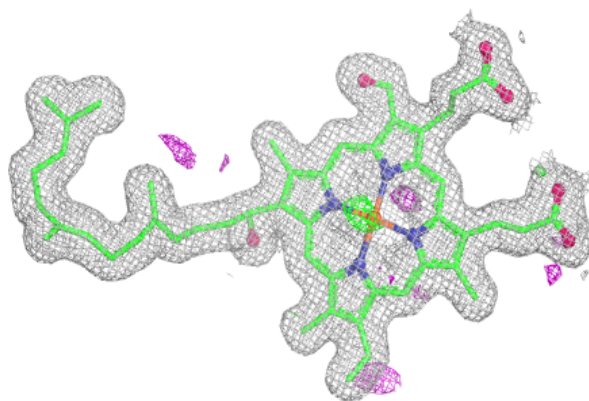


Electron density around HEA N 516:

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

**Electron density around HEA A 516:**

$2mF_o-DF_c$ (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.