



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 09:07 PM UTC

PDB ID : 8IJN / pdb_00008ijn
Title : Bovine Heart Cytochrome c Oxidase in the Nitric Oxide-Bound Fully Reduced State at 100 K
Authors : Tsukihara, T.; Shimada, A.; Muramoto, K.
Deposited on : 2023-02-27
Resolution : 1.80 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

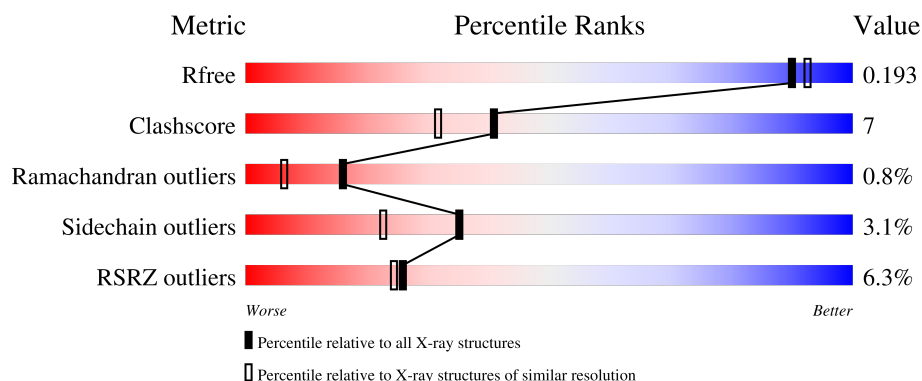
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	
1	N	514	
2	B	227	
2	O	227	
3	C	261	

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Mol	Chain	Length	Quality of chain
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
25	CDL	G	102	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32780 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	10	0
			4072	2716	631	687	38			
1	N	514	Total	C	N	O	S	0	9	0
			4072	2717	631	686	38			

- 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	2	0
			1831	1191	281	341	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	3	0
			2116	1415	336	351	14			
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, 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.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	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, 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 subunit 6C.

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

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

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, mitochondrial.

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

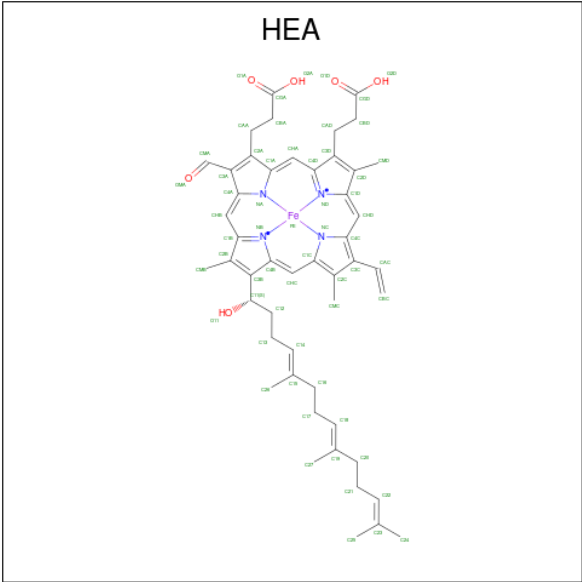
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

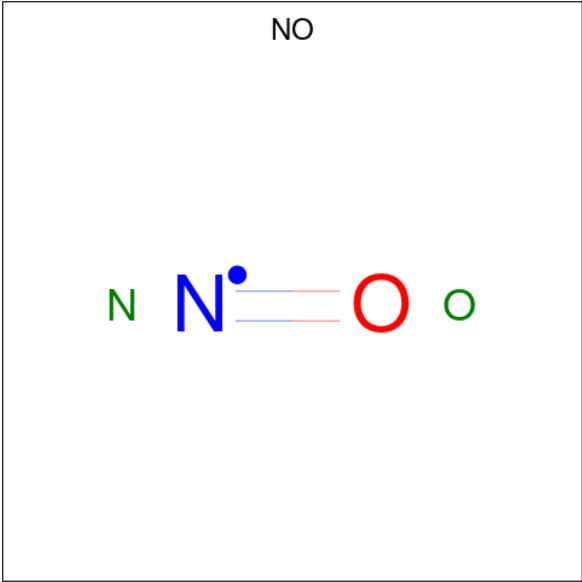
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (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 2 1 1	0	0
15	N	1	Total N O 2 1 1	0	0

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

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

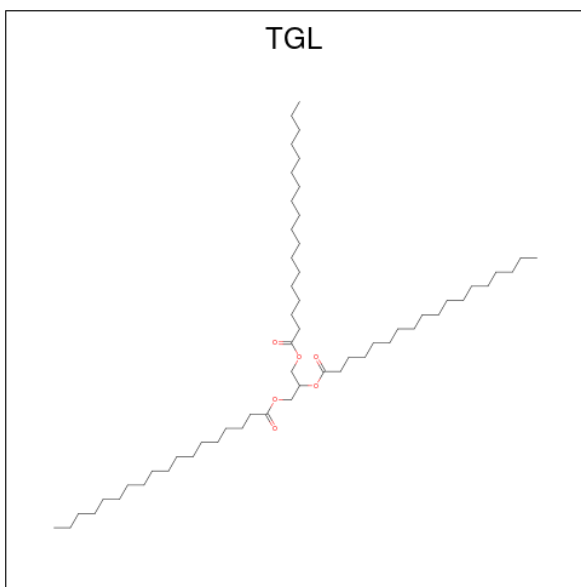
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

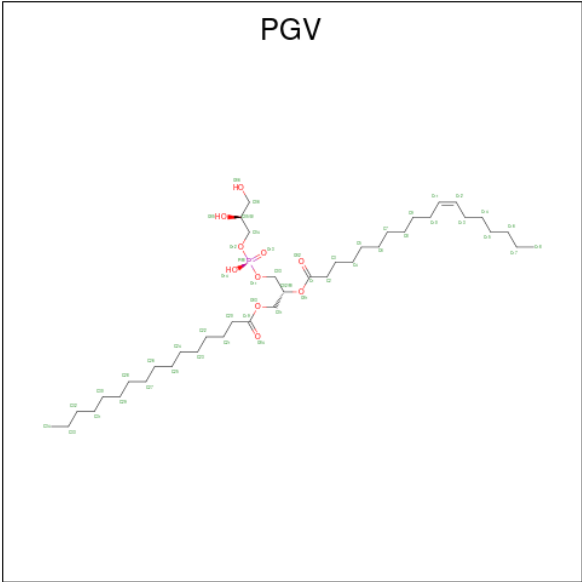
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

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



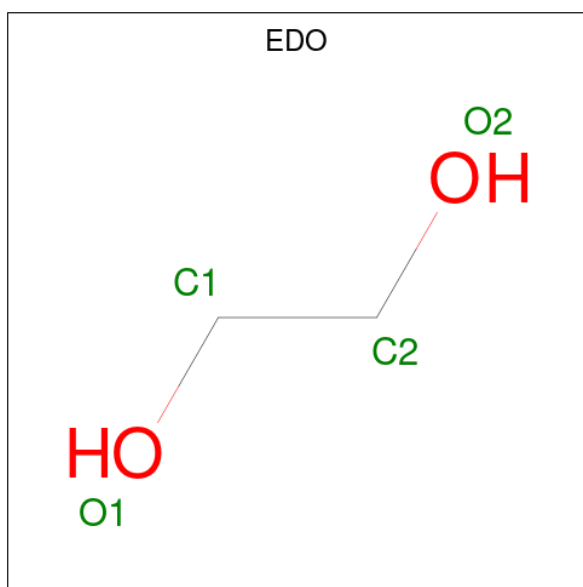
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- 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	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	N	1	Total	C	O	P	0	0
			46	37	8	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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



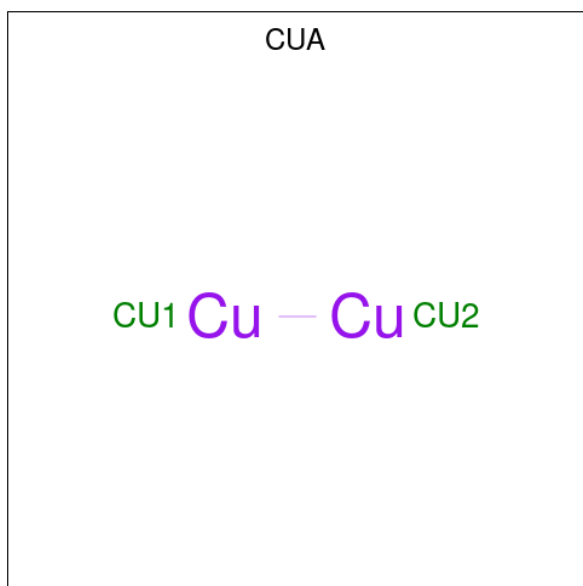
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	F	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21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

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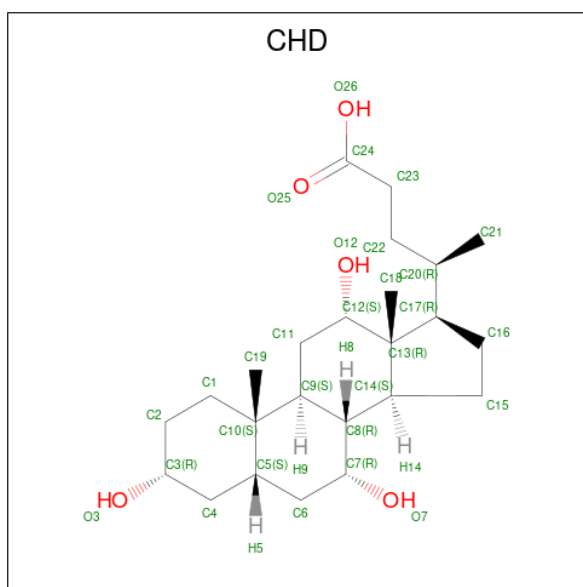
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	O	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	Q	1	Total C O 4 2 2	0	0
21	Q	1	Total C O 4 2 2	0	0
21	S	1	Total C O 4 2 2	0	0
21	S	1	Total C O 4 2 2	0	0
21	S	1	Total C O 4 2 2	0	0

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



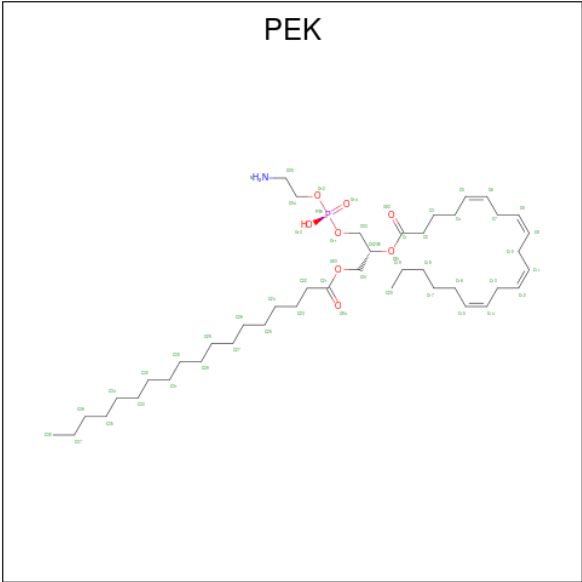
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

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



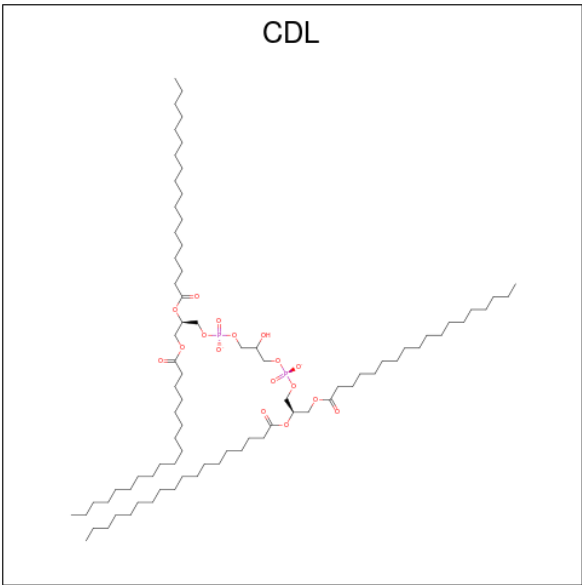
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	O	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0

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



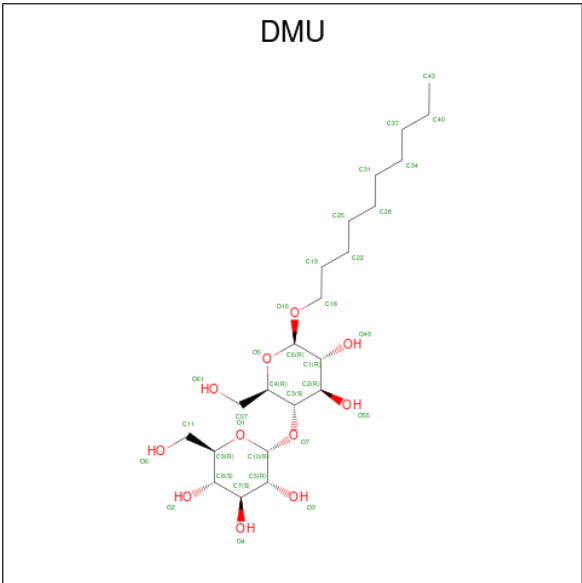
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	O	P		0	0
			50	41	8	1			
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



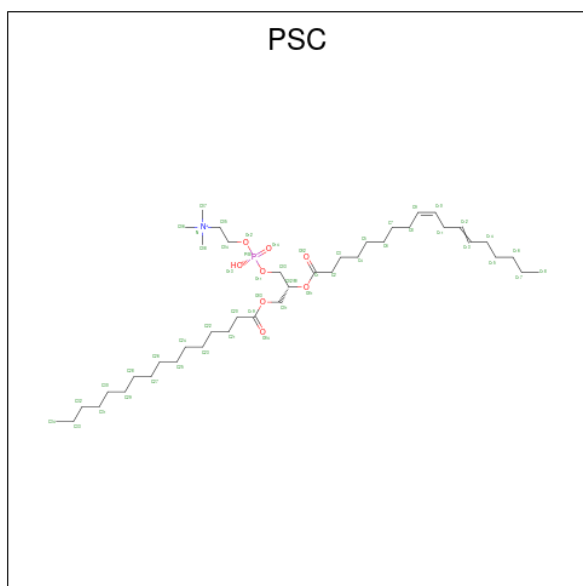
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	M	1	Total	C	O	0	0
			33	22	11		
26	O	1	Total	C	O	0	0
			22	16	6		
26	P	1	Total	C	O	0	0
			33	22	11		
26	W	1	Total	C	O	0	0
			32	21	11		
26	Z	1	Total	C	O	0	0
			33	22	11		

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



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

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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	229	Total 229	O 229	0	0
29	B	148	Total 149	O 149	0	1
29	C	120	Total 120	O 120	0	0
29	D	79	Total 79	O 79	0	0
29	E	48	Total 48	O 48	0	0
29	F	68	Total 68	O 68	0	0
29	G	48	Total 48	O 48	0	0
29	H	51	Total 51	O 51	0	0
29	I	39	Total 39	O 39	0	0
29	J	26	Total 26	O 26	0	0
29	K	30	Total 30	O 30	0	0
29	L	23	Total 23	O 23	0	0
29	M	24	Total 24	O 24	0	0
29	N	231	Total 231	O 231	0	0
29	O	146	Total 146	O 146	0	2
29	P	106	Total 106	O 106	0	0
29	Q	59	Total 59	O 59	0	0
29	R	55	Total 55	O 55	0	0

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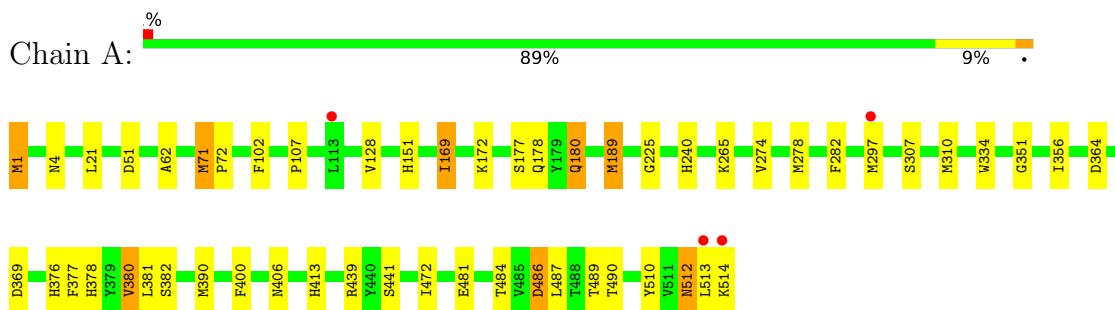
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	S	72	Total 72	O 72	0	0
29	T	51	Total 51	O 51	0	0
29	U	48	Total 48	O 48	0	0
29	V	29	Total 29	O 29	0	0
29	W	22	Total 22	O 22	0	0
29	X	22	Total 22	O 22	0	0
29	Y	17	Total 17	O 17	0	0
29	Z	17	Total 17	O 17	0	0

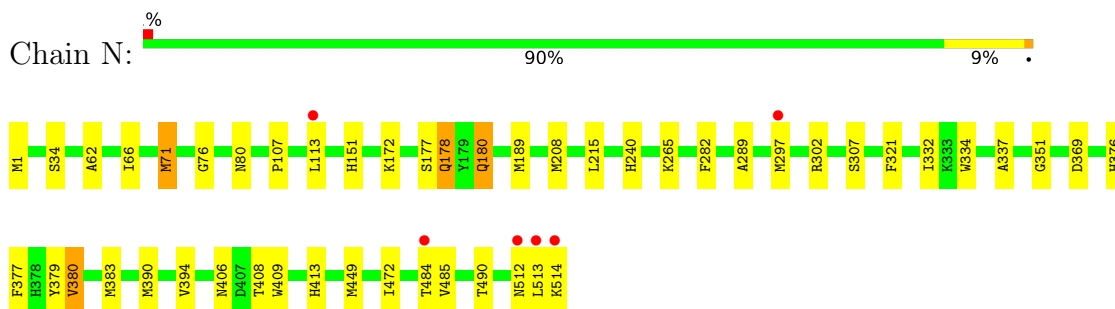
3 Residue-property plots [i](#)

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

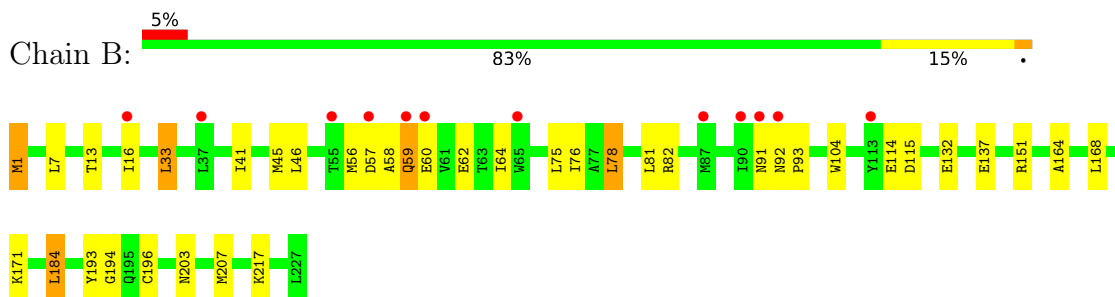
- Molecule 1: Cytochrome c oxidase subunit 1



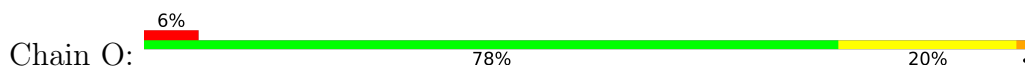
- Molecule 1: Cytochrome c oxidase subunit 1

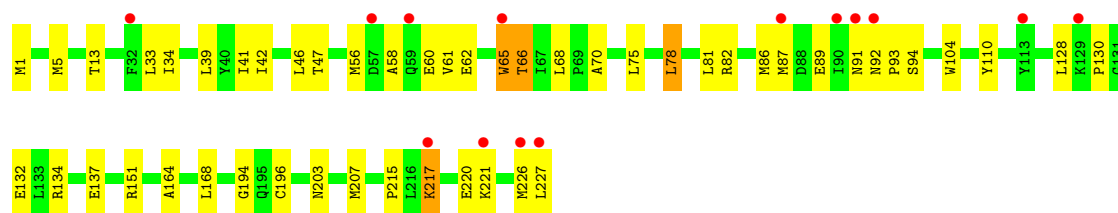


- Molecule 2: Cytochrome c oxidase subunit 2

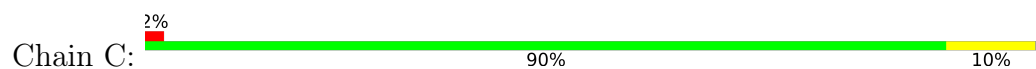


- Molecule 2: Cytochrome c oxidase subunit 2

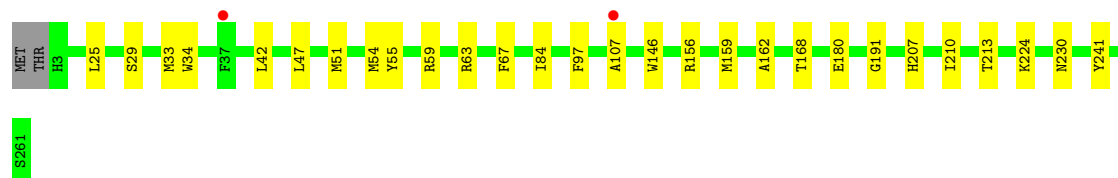
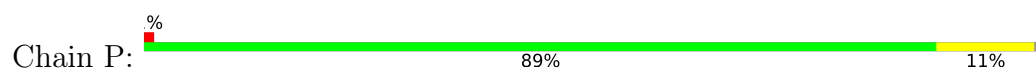




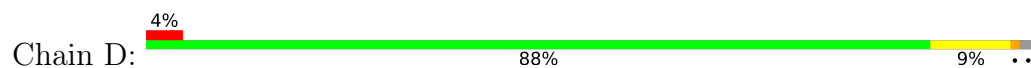
- Molecule 3: Cytochrome c oxidase subunit 3



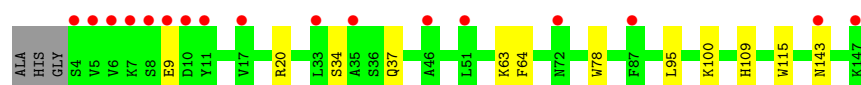
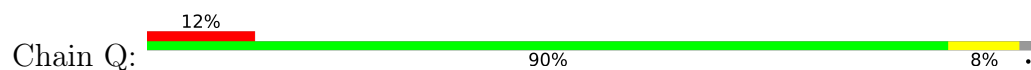
- Molecule 3: Cytochrome c oxidase subunit 3



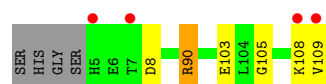
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



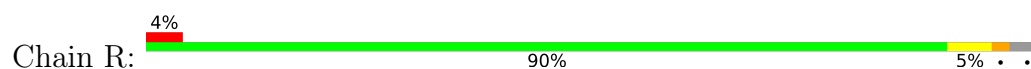
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

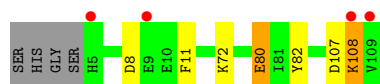


- Molecule 5: Cytochrome c oxidase subunit 5A

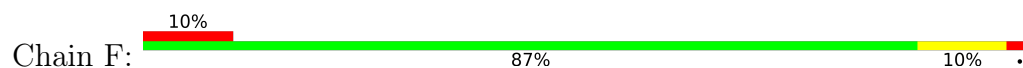


- Molecule 5: Cytochrome c oxidase subunit 5A





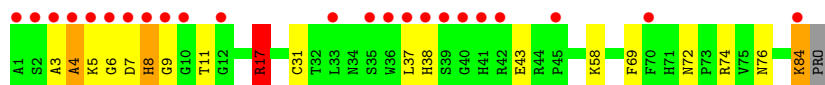
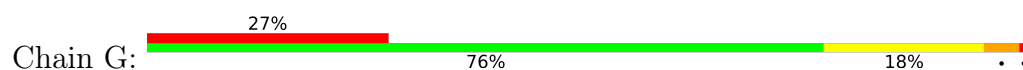
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



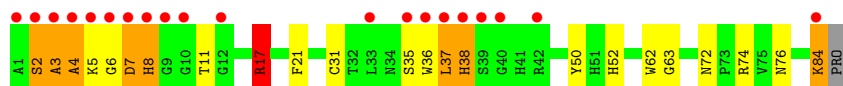
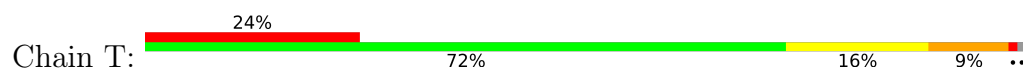
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



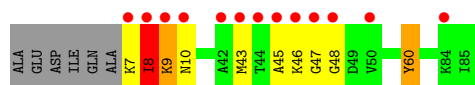
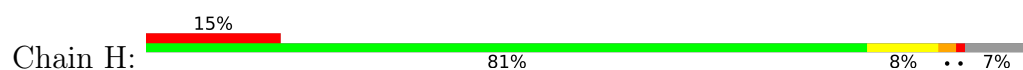
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



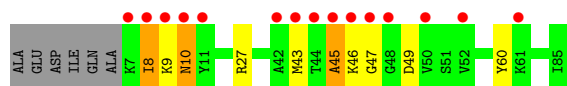
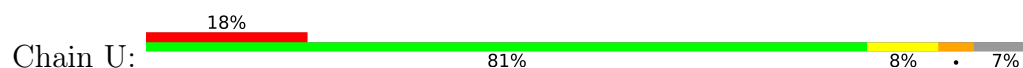
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



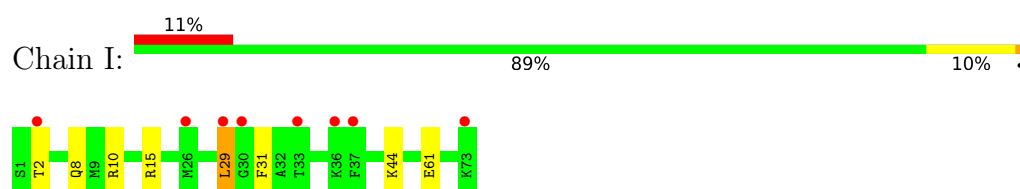
- Molecule 8: Cytochrome c oxidase subunit 6B1



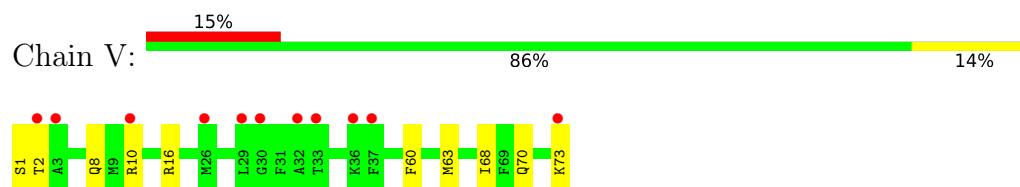
- Molecule 8: Cytochrome c oxidase subunit 6B1



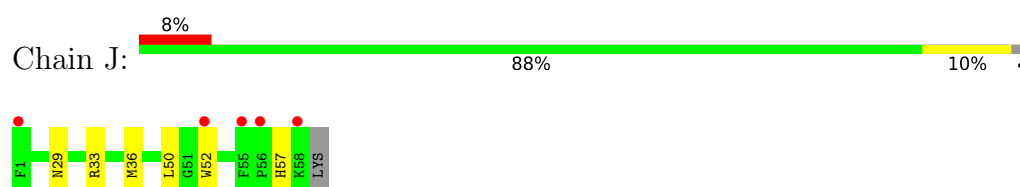
- Molecule 9: Cytochrome c oxidase subunit 6C



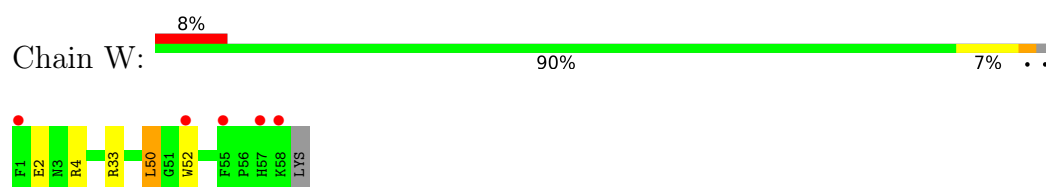
- Molecule 9: Cytochrome c oxidase subunit 6C



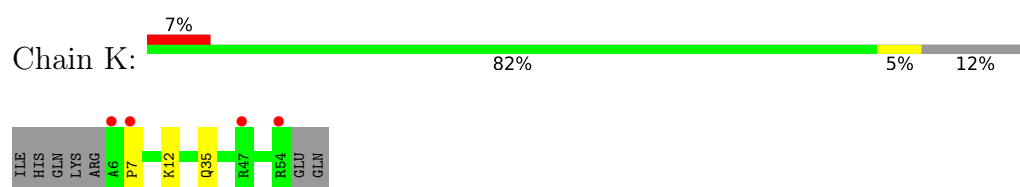
- Molecule 10: Cytochrome c oxidase subunit 7A1



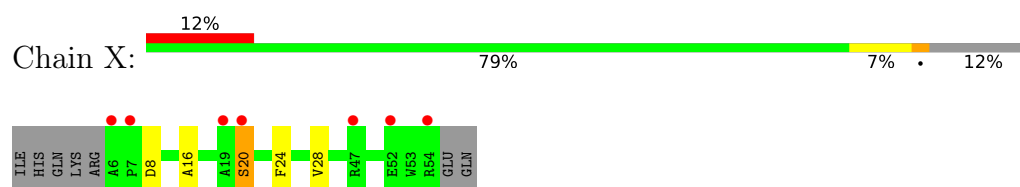
- Molecule 10: Cytochrome c oxidase subunit 7A1



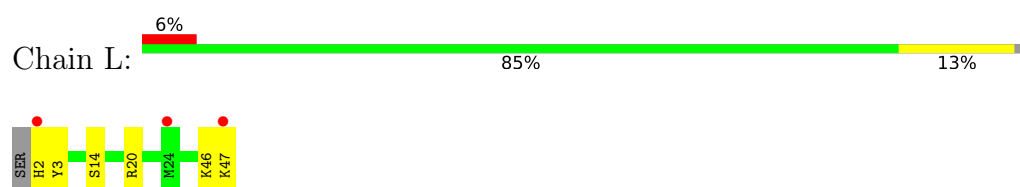
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



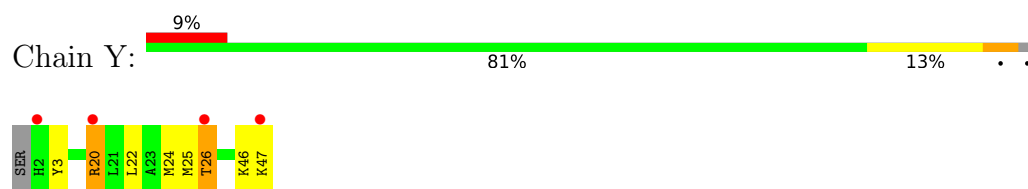
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



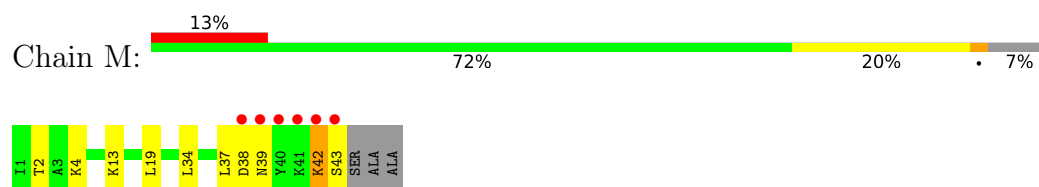
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



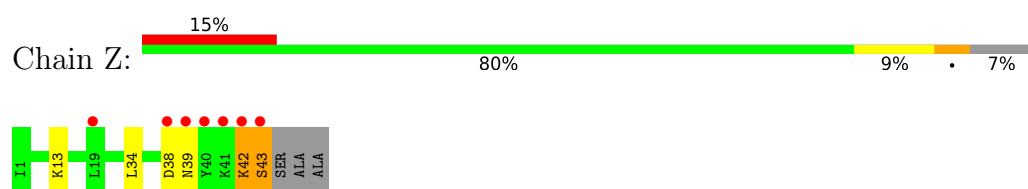
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.29Å 208.36Å 177.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.37 – 1.80 35.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.37-1.80) 99.6 (35.37-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.80Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.169 , 0.192 0.169 , 0.193	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)	0.38 , 62.2	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	0.97	EDS
Total number of atoms	32780	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: CHD, CUA, TPO, DMU, SAC, HEA, ZN, EDO, NO, TGL, PGV, PEK, NA, MG, PSC, FME, CDL, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.08	2/4230 (0.0%)	0.92	4/5775 (0.1%)
1	N	0.90	1/4224 (0.0%)	0.85	2/5767 (0.0%)
2	B	0.96	0/1878	0.96	5/2558 (0.2%)
2	O	0.74	0/1860	0.86	1/2534 (0.0%)
3	C	0.87	0/2219	0.79	0/3033
3	P	0.80	0/2197	0.75	0/3005
4	D	0.78	0/1229	0.77	0/1658
4	Q	0.56	0/1229	0.63	0/1658
5	E	0.74	0/871	0.72	0/1182
5	R	0.59	0/871	0.67	0/1182
6	F	0.84	1/765 (0.1%)	0.87	0/1038
6	S	0.69	0/765	0.83	2/1038 (0.2%)
7	G	0.81	0/690	0.87	2/937 (0.2%)
7	T	0.73	0/690	0.85	2/937 (0.2%)
8	H	0.73	0/682	0.77	0/921
8	U	0.60	0/682	0.76	0/921
9	I	0.62	0/605	0.69	0/802
9	V	0.56	0/605	0.70	0/802
10	J	0.68	0/471	0.66	0/636
10	W	0.53	0/471	0.62	0/636
11	K	0.72	0/398	0.77	0/546
11	X	0.46	0/398	0.54	0/546
12	L	0.83	0/393	0.86	0/526
12	Y	0.63	0/393	0.64	0/526
13	M	0.81	0/345	0.71	0/470
13	Z	0.54	0/345	0.57	0/470
All	All	0.83	4/29506 (0.0%)	0.81	18/40104 (0.0%)

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

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	189	MET	CB-CG	5.52	1.69	1.52
1	A	439	ARG	CD-NE	5.46	1.53	1.46
6	F	56	ARG	CZ-NH1	5.32	1.40	1.32
1	A	512	ASN	CB-CG	-5.02	1.39	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	-11.39	75.84	100.90
1	N	71	MET	CG-SD-CE	-9.19	80.68	100.90
1	A	189	MET	CG-SD-CE	-7.36	84.72	100.90
1	A	240	HIS	CA-CB-CG	-6.87	106.93	113.80
7	T	17	ARG	NE-CZ-NH1	6.56	128.06	121.50
6	S	94	HIS	CA-C-N	6.22	133.43	121.54
6	S	94	HIS	C-N-CA	6.22	133.43	121.54
1	N	240	HIS	CA-CB-CG	-6.15	107.65	113.80
2	B	64	ILE	CA-C-N	-6.05	112.61	122.65
2	B	64	ILE	C-N-CA	-6.05	112.61	122.65
7	G	17	ARG	NE-CZ-NH2	-5.96	113.84	119.20
7	T	17	ARG	NE-CZ-NH2	-5.77	114.01	119.20
1	A	102	PHE	CA-CB-CG	-5.63	108.17	113.80
2	B	114	GLU	CA-C-N	-5.60	114.48	122.77
2	B	114	GLU	C-N-CA	-5.60	114.48	122.77
2	O	65	TRP	CA-CB-CG	5.28	123.63	113.60
7	G	17	ARG	NE-CZ-NH1	5.18	126.68	121.50
2	B	82	ARG	CG-CD-NE	-5.14	100.69	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	4072	0	4041	45	0
1	N	4072	0	4044	47	0
2	B	1831	0	1839	25	0
2	O	1824	0	1833	34	0
3	C	2116	0	2034	26	0
3	P	2110	0	2027	33	0
4	D	1195	0	1183	11	0
4	Q	1195	0	1183	10	0
5	E	852	0	845	3	0
5	R	852	0	845	5	1
6	F	748	0	728	7	0
6	S	748	0	728	12	0
7	G	675	0	643	18	0
7	T	675	0	643	28	0
8	H	662	0	623	7	0
8	U	662	0	623	6	0
9	I	601	0	613	5	1
9	V	601	0	613	7	0
10	J	460	0	459	4	0
10	W	460	0	459	4	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	7	0
12	Y	380	0	380	8	0
13	M	335	0	352	6	0
13	Z	335	0	352	2	0
14	A	120	0	108	5	0
14	N	120	0	108	5	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	3	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	8	0
19	N	63	0	110	8	0
19	O	63	0	110	0	0
19	Q	63	0	110	9	0
20	A	102	0	152	4	0
20	C	102	0	152	9	0
20	N	97	0	145	5	0
20	P	102	0	152	6	0
21	A	16	0	24	1	0
21	B	4	0	6	0	0
21	C	4	0	6	0	0
21	F	4	0	6	0	0
21	N	24	0	36	2	0
21	O	8	0	12	0	0
21	P	8	0	12	1	0
21	Q	8	0	12	0	0
21	S	12	0	18	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	1	0
23	C	58	0	78	3	0
23	J	29	0	38	2	0
23	O	29	0	39	2	0
23	P	58	0	78	1	0
23	W	29	0	38	1	0
24	C	53	0	77	6	0
24	G	103	0	148	5	0
24	P	53	0	77	6	0
24	T	106	0	154	10	0
25	C	100	0	153	15	0
25	G	100	0	156	23	0
25	P	100	0	156	19	0
25	T	100	0	156	14	0
26	C	33	0	42	2	0
26	M	33	0	42	1	0
26	O	22	0	31	1	0
26	P	33	0	42	8	0
26	W	32	0	36	4	0
26	Z	33	0	42	1	0
27	E	52	0	80	12	0
27	R	52	0	80	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	229	0	0	2	0
29	B	149	0	0	3	0
29	C	120	0	0	1	0
29	D	79	0	0	1	0
29	E	48	0	0	0	0
29	F	68	0	0	1	0
29	G	48	0	0	1	0
29	H	51	0	0	0	0
29	I	39	0	0	2	0
29	J	26	0	0	0	0
29	K	30	0	0	1	0
29	L	23	0	0	0	0
29	M	24	0	0	0	0
29	N	231	0	0	4	0
29	O	146	0	0	1	0
29	P	106	0	0	2	0
29	Q	59	0	0	2	0
29	R	55	0	0	1	0
29	S	72	0	0	1	0
29	T	51	0	0	0	0
29	U	48	0	0	1	0
29	V	29	0	0	0	0
29	W	22	0	0	1	0
29	X	22	0	0	2	0
29	Y	17	0	0	1	0
29	Z	17	0	0	0	0
All	All	32780	0	31593	408	1

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 (408) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:94:HIS:CD2	6:S:95:GLN:H	1.72	1.05
21:N:614:EDO:O2	29:N:701:HOH:O	1.80	0.99
6:S:94:HIS:NE2	29:S:201:HOH:O	1.97	0.96
7:T:17:ARG:HH22	24:T:101:PEK:H041	1.27	0.96
6:S:94:HIS:HD2	6:S:95:GLN:H	1.09	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LEU:HD12	25:T:103:CDL:H351	1.53	0.88
7:G:72:ASN:H	7:G:76:ASN:HD22	1.20	0.88
7:T:72:ASN:H	7:T:76:ASN:HD22	1.22	0.87
25:G:102:CDL:H782	25:G:102:CDL:H561	1.58	0.86
1:N:406:ASN:HD21	20:N:608:PGV:H21	1.41	0.85
6:F:85:CYS:SG	6:F:87:THR:HG23	2.16	0.85
1:N:332:ILE:H	21:N:615:EDO:H12	1.41	0.84
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.59	0.82
12:L:20:ARG:HH22	19:L:101:TGL:HC32	1.44	0.82
12:L:20:ARG:NH2	19:L:101:TGL:HC32	1.96	0.80
24:P:302:PEK:H71	24:P:302:PEK:H32	1.64	0.80
25:C:305:CDL:H231	25:C:305:CDL:H661	1.64	0.80
3:P:67:PHE:HE1	25:P:305:CDL:H1	1.46	0.78
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.66	0.77
25:G:102:CDL:H511	25:G:102:CDL:H201	1.65	0.76
3:P:34:TRP:HE1	26:P:307:DMU:H29	1.51	0.75
3:C:210:ILE:HG12	20:C:303:PGV:H132	1.69	0.75
24:P:302:PEK:HN2	7:T:76:ASN:HD21	1.34	0.74
7:G:38:HIS:CE1	25:G:102:CDL:H111	2.23	0.73
29:N:867:HOH:O	2:O:87:MET:SD	2.47	0.73
25:G:102:CDL:H451	2:O:70:ALA:HB1	1.70	0.72
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.72	0.71
25:G:102:CDL:H351	2:O:81:LEU:HD12	1.72	0.71
7:G:84:LYS:H	7:G:84:LYS:HD2	1.54	0.71
6:S:52:ILE:O	6:S:94:HIS:CE1	2.43	0.71
7:G:17:ARG:HD2	29:O:429:HOH:O	1.91	0.70
19:N:607:TGL:HC32	12:Y:20:ARG:HH21	1.55	0.69
24:C:302:PEK:HN2	7:G:76:ASN:HD21	1.37	0.69
3:P:34:TRP:NE1	26:P:307:DMU:H29	2.07	0.69
6:S:94:HIS:HD2	6:S:95:GLN:N	1.89	0.68
29:B:413:HOH:O	7:T:17:ARG:HD2	1.95	0.67
25:G:102:CDL:H352	2:O:78:LEU:HD12	1.75	0.67
19:L:101:TGL:H231	19:L:101:TGL:HA92	1.75	0.67
7:T:17:ARG:NH2	24:T:101:PEK:H041	2.06	0.67
25:P:305:CDL:H341	25:P:305:CDL:H162	1.76	0.67
12:L:46:LYS:O	12:L:47:LYS:HB2	1.95	0.66
3:P:54:MET:HE3	25:P:305:CDL:H612	1.77	0.66
1:N:351:GLY:HA3	1:N:380[A]:VAL:HG13	1.77	0.66
3:C:51[B]:MET:HE2	25:C:305:CDL:H621	1.77	0.66
13:M:39:ASN:O	13:M:43:SER:OG	2.07	0.66
4:D:20:ARG:HG3	29:D:350:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:42:ILE:HG21	19:Q:201:TGL:H231	1.78	0.65
1:N:177:SER:H	1:N:180:GLN:NE2	1.96	0.64
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.80	0.63
7:G:37:LEU:HD11	25:G:102:CDL:H361	1.79	0.63
1:N:177:SER:H	1:N:180:GLN:HE21	1.46	0.63
3:P:63:ARG:HE	25:P:305:CDL:HA22	1.62	0.63
4:D:34:SER:H	4:D:37:GLN:NE2	1.96	0.63
20:A:609:PGV:H22	20:A:609:PGV:H011	1.80	0.63
7:T:5:LYS:HD2	24:T:102:PEK:H371	1.81	0.63
27:E:201:PSC:H072	9:I:10:ARG:HH21	1.64	0.62
6:F:51:SER:O	6:F:94:HIS:N	2.32	0.62
27:R:201:PSC:H071	9:V:10:ARG:HH21	1.64	0.62
27:R:201:PSC:C07	9:V:10:ARG:HH21	2.13	0.62
3:C:210:ILE:HD13	20:C:303:PGV:H301	1.81	0.62
2:O:13:THR:HB	2:O:168:LEU:HD23	1.81	0.62
3:C:224:LYS:CD	25:C:305:CDL:HB32	2.30	0.62
26:P:307:DMU:H30	7:T:62:TRP:HB3	1.80	0.62
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.96	0.62
20:A:609:PGV:H311	13:M:19:LEU:HD23	1.80	0.61
25:G:102:CDL:H531	25:G:102:CDL:H222	1.82	0.61
1:A:51:ASP:OD1	1:A:441:SER:OG	2.15	0.61
2:B:78:LEU:HD12	25:T:103:CDL:H352	1.81	0.61
1:N:472:ILE:HG21	19:N:607:TGL:HA91	1.83	0.61
19:N:607:TGL:HA62	12:Y:25:MET:HG2	1.82	0.60
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.67	0.60
1:A:472:ILE:HG21	19:L:101:TGL:HA91	1.84	0.60
1:A:377:PHE:HA	1:A:380[B]:VAL:HG22	1.84	0.60
20:C:303:PGV:H172	25:C:305:CDL:H662	1.84	0.59
4:D:78:TRP:CA	19:D:201:TGL:HB22	2.32	0.59
19:A:607:TGL:HA92	19:A:607:TGL:H252	1.84	0.59
26:W:102:DMU:O55	29:W:201:HOH:O	2.17	0.59
27:R:201:PSC:H142	27:R:201:PSC:H343	1.84	0.59
13:Z:39:ASN:O	13:Z:43:SER:OG	2.15	0.59
1:A:334:TRP:CZ3	19:D:201:TGL:HA52	2.38	0.58
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.39	0.58
1:N:151:HIS:CD2	24:P:302:PEK:H382	2.39	0.58
7:G:5:LYS:HD2	24:G:103:PEK:H371	1.84	0.58
10:W:50:LEU:HG	26:W:102:DMU:H18	1.86	0.58
2:O:66:THR:HG21	23:O:302:CHD:H3	1.86	0.58
6:S:85:CYS:SG	6:S:87:THR:HG23	2.44	0.58
12:L:2:HIS:CG	12:L:3:TYR:H	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:224:LYS:HD3	25:P:305:CDL:HB31	1.86	0.57
10:W:52:TRP:CD2	26:W:102:DMU:H1	2.29	0.57
4:D:34:SER:H	4:D:37:GLN:HE21	1.52	0.57
4:D:78:TRP:HA	19:D:201:TGL:HB22	1.86	0.57
1:A:334:TRP:CE3	19:D:201:TGL:HA31	2.40	0.57
25:G:102:CDL:H112	25:G:102:CDL:H1	1.87	0.57
20:N:608:PGV:H151	20:N:608:PGV:H321	1.85	0.56
2:B:56:MET:HA	27:E:201:PSC:H202	1.86	0.56
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.87	0.56
1:N:1:FME:HE2	12:Y:3:TYR:HE1	1.71	0.56
7:G:31:CYS:SG	25:G:102:CDL:H551	2.46	0.56
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.87	0.56
11:X:16:ALA:O	11:X:20:SER:OG	2.24	0.55
7:G:72:ASN:H	7:G:76:ASN:ND2	1.98	0.55
10:W:33:ARG:HG2	23:W:101:CHD:H151	1.88	0.55
2:B:41:ILE:HD13	27:E:201:PSC:C34	2.37	0.55
3:C:246:ASP:HB2	29:C:500:HOH:O	2.07	0.55
25:P:305:CDL:H242	25:P:305:CDL:H661	1.89	0.55
6:S:94:HIS:CD2	6:S:95:GLN:N	2.58	0.55
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.89	0.54
1:A:177:SER:H	1:A:180:GLN:NE2	2.05	0.54
7:T:2:SER:O	24:T:102:PEK:H331	2.08	0.54
10:J:33:ARG:HG2	23:J:101:CHD:H151	1.89	0.54
26:P:307:DMU:H40	7:T:63:GLY:H	1.71	0.54
3:P:34:TRP:CE2	26:P:307:DMU:H29	2.43	0.54
27:E:201:PSC:C07	9:I:10:ARG:HH21	2.21	0.53
3:P:34:TRP:CZ2	26:P:307:DMU:H29	2.44	0.53
3:P:63:ARG:HE	25:P:305:CDL:CA2	2.22	0.53
27:E:201:PSC:O14	27:E:201:PSC:H062	2.07	0.53
1:A:514:LYS:NZ	29:A:703:HOH:O	2.41	0.53
6:F:94:HIS:O	6:F:95:GLN:HB2	2.09	0.53
25:T:103:CDL:H1	25:T:103:CDL:H111	1.91	0.53
20:C:304:PGV:H62	20:C:304:PGV:H22	1.90	0.53
1:A:169:ILE:HD11	1:A:189:MET:HE1	1.90	0.53
12:L:20:ARG:HH22	19:L:101:TGL:HC61	1.74	0.53
7:T:31:CYS:SG	25:T:103:CDL:H551	2.49	0.53
19:A:607:TGL:H111	19:A:607:TGL:H283	1.91	0.52
3:C:224:LYS:HD3	25:C:305:CDL:HB32	1.90	0.52
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.90	0.52
3:P:67:PHE:CE1	25:P:305:CDL:H1	2.36	0.52
6:S:52:ILE:O	6:S:94:HIS:ND1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:21:PHE:CD2	24:T:101:PEK:H222	2.44	0.52
3:P:210:ILE:HG12	20:P:303:PGV:H132	1.90	0.52
20:A:609:PGV:H152	4:D:87:PHE:CZ	2.45	0.52
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.92	0.52
1:A:307:SER:HB3	25:T:103:CDL:H171	1.90	0.52
3:P:224:LYS:HD3	25:P:305:CDL:CB3	2.40	0.52
8:U:45:ALA:O	8:U:47:GLY:N	2.43	0.52
3:C:59:ARG:HA	25:C:305:CDL:H512	1.92	0.52
1:N:351:GLY:C	1:N:380[A]:VAL:HG13	2.35	0.52
3:P:33:MET:HE1	3:P:42:LEU:H	1.75	0.52
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.91	0.52
1:A:278:MET:SD	7:T:5:LYS:HB3	2.50	0.52
27:E:201:PSC:H142	27:E:201:PSC:H343	1.90	0.52
2:O:89:GLU:O	2:O:91:ASN:ND2	2.43	0.52
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.46	0.51
1:N:351:GLY:CA	1:N:380[A]:VAL:HG13	2.40	0.51
7:T:72:ASN:H	7:T:76:ASN:ND2	2.01	0.51
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.59	0.51
20:N:608:PGV:H011	20:N:608:PGV:H22	1.91	0.51
4:Q:78:TRP:HA	19:Q:201:TGL:HB22	1.93	0.51
3:P:59:ARG:HA	25:P:305:CDL:H512	1.92	0.51
3:P:67:PHE:HE1	25:P:305:CDL:C1	2.19	0.51
3:P:168:THR:HG22	24:T:101:PEK:H14	1.92	0.51
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.92	0.51
1:A:310:MET:HE3	1:A:356:ILE:HG23	1.92	0.51
7:G:9:GLY:HA3	1:N:178:GLN:HE21	1.75	0.51
7:T:8:HIS:ND1	24:T:102:PEK:H312	2.26	0.50
2:O:39:LEU:CD1	19:Q:201:TGL:H232	2.41	0.50
29:N:863:HOH:O	4:Q:20:ARG:HG3	2.11	0.50
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.94	0.50
2:O:62:GLU:O	2:O:66:THR:HB	2.12	0.50
1:A:484:THR:HB	13:M:2:THR:OG1	2.12	0.49
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.94	0.49
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.46	0.49
3:P:47:LEU:O	3:P:51:MET:HG2	2.12	0.49
9:I:44:LYS:HE2	29:I:135:HOH:O	2.13	0.49
25:G:102:CDL:H322	25:G:102:CDL:HA62	1.94	0.49
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.93	0.49
7:T:38:HIS:HE2	25:T:103:CDL:H111	1.77	0.49
19:A:607:TGL:HC81	2:B:7:LEU:HD11	1.94	0.49
4:D:127:LYS:HD2	29:I:131:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:210:ILE:HD13	20:P:303:PGV:H301	1.95	0.49
4:Q:109:HIS:HD2	29:Q:337:HOH:O	1.95	0.49
2:O:47:THR:HB	19:Q:201:TGL:H332	1.94	0.49
2:O:82:ARG:HH11	2:O:86:MET:HE1	1.78	0.49
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.48	0.49
4:Q:95:LEU:HD22	26:Z:101:DMU:H13	1.95	0.49
19:Q:201:TGL:HA91	19:Q:201:TGL:H242	1.94	0.49
2:B:78:LEU:CD1	25:T:103:CDL:H352	2.43	0.48
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.95	0.48
2:O:58:ALA:O	2:O:62:GLU:HG3	2.12	0.48
20:P:303:PGV:H172	25:P:305:CDL:H652	1.95	0.48
24:C:302:PEK:H221	7:G:69:PHE:CG	2.48	0.48
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.77	0.48
12:L:14:SER:H	19:L:101:TGL:HC31	1.79	0.48
2:B:58:ALA:O	2:B:62:GLU:HG3	2.12	0.48
8:H:45:ALA:O	8:H:47:GLY:N	2.45	0.48
6:S:94:HIS:O	6:S:95:GLN:HB2	2.12	0.48
3:C:213:THR:HG23	25:C:305:CDL:H771	1.95	0.48
25:G:102:CDL:C54	25:G:102:CDL:H241	2.43	0.48
1:N:1:FME:HE2	12:Y:3:TYR:CE1	2.48	0.48
25:T:103:CDL:H582	25:T:103:CDL:H552	1.53	0.48
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.12	0.48
2:O:56:MET:HA	27:R:201:PSC:H202	1.95	0.48
3:P:33:MET:HG3	26:W:102:DMU:H7	1.96	0.48
20:C:304:PGV:H161	25:T:103:CDL:H612	1.94	0.47
8:H:43:MET:HE3	8:H:48:GLY:HA3	1.95	0.47
8:H:45:ALA:C	8:H:47:GLY:H	2.21	0.47
10:J:29:ASN:HD22	10:J:29:ASN:H	1.60	0.47
11:K:7:PRO:O	11:K:12:LYS:HE3	2.13	0.47
19:Q:201:TGL:H361	9:V:16:ARG:HE	1.79	0.47
2:B:57:ASP:H	27:E:201:PSC:H202	1.78	0.47
8:H:43:MET:HE1	8:U:43:MET:HE1	1.96	0.47
21:P:308:EDO:H21	29:P:476:HOH:O	2.12	0.47
1:A:151:HIS:CD2	24:C:302:PEK:H382	2.49	0.47
19:N:607:TGL:HA92	19:N:607:TGL:H231	1.96	0.47
25:G:102:CDL:H182	1:N:307:SER:HB3	1.95	0.47
21:A:613:EDO:H21	2:B:59:GLN:HE21	1.78	0.47
19:D:201:TGL:H201	19:D:201:TGL:H231	1.60	0.47
19:N:607:TGL:H362	29:Y:117:HOH:O	2.15	0.47
2:O:164:ALA:O	2:O:194:GLY:HA3	2.13	0.47
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:103:CDL:H431	25:T:103:CDL:H402	1.80	0.47
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.29	0.47
1:A:274:VAL:HG12	1:A:278:MET:HE2	1.96	0.47
23:O:302:CHD:H12	23:O:302:CHD:H212	1.96	0.47
8:U:43:MET:HE3	8:U:49:ASP:N	2.29	0.47
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.96	0.47
1:N:302[B]:ARG:HH22	2:O:87:MET:HE1	1.80	0.47
7:T:7:ASP:OD1	7:T:8:HIS:N	2.48	0.47
3:C:67:PHE:HE1	25:C:305:CDL:C1	2.29	0.46
27:R:201:PSC:H063	27:R:201:PSC:H042	1.66	0.46
10:W:2:GLU:HB2	10:W:4:ARG:NH1	2.30	0.46
24:C:302:PEK:H221	7:G:69:PHE:CD2	2.51	0.46
3:P:156:ARG:HE	23:P:306:CHD:C24	2.26	0.46
19:Q:201:TGL:H351	9:V:16:ARG:HH21	1.81	0.46
3:C:95:THR:HG21	20:C:304:PGV:H302	1.98	0.46
24:C:302:PEK:H161	24:C:302:PEK:H102	1.97	0.46
1:N:513:LEU:O	1:N:514:LYS:HB2	2.16	0.46
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.98	0.46
7:G:8:HIS:CD2	24:G:103:PEK:H252	2.50	0.46
7:T:84:LYS:HD2	7:T:84:LYS:H	1.80	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.46
1:N:113:LEU:HD12	19:N:607:TGL:H141	1.98	0.46
2:O:217:LYS:HE2	2:O:220:GLU:OE2	2.16	0.46
24:P:302:PEK:H271	24:P:302:PEK:H6	1.98	0.46
12:L:2:HIS:CG	12:L:3:TYR:N	2.83	0.46
24:G:101:PEK:H383	25:G:102:CDL:H271	1.98	0.45
1:A:1:FME:HE2	1:A:4:ASN:HD22	1.80	0.45
1:A:382[B]:SER:OG	14:A:601:HEA:H121	2.15	0.45
25:C:305:CDL:H401	25:C:305:CDL:H371	1.53	0.45
1:N:377:PHE:HA	1:N:380[B]:VAL:HG22	1.98	0.45
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.51	0.45
3:P:213:THR:HG23	25:P:305:CDL:H762	1.98	0.45
3:P:224:LYS:CD	25:P:305:CDL:HB31	2.45	0.45
24:P:302:PEK:H12	24:P:302:PEK:H242	1.99	0.45
4:Q:100:LYS:HE2	29:Q:332:HOH:O	2.15	0.45
25:G:102:CDL:H241	25:G:102:CDL:H542	1.99	0.45
6:S:94:HIS:CG	6:S:95:GLN:H	2.22	0.45
3:C:156:ARG:HE	23:C:306:CHD:C24	2.28	0.45
4:Q:78:TRP:CA	19:Q:201:TGL:HB22	2.46	0.45
8:U:27:ARG:HG2	29:U:143:HOH:O	2.16	0.45
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PHE:HZ	25:T:103:CDL:H761	1.81	0.45
1:N:334:TRP:CZ3	19:Q:201:TGL:HA51	2.51	0.45
9:V:73:LYS:HD2	9:V:73:LYS:HA	1.87	0.45
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.16	0.45
3:C:67:PHE:HE1	25:C:305:CDL:H1	1.82	0.45
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.99	0.45
3:P:55:TYR:CE1	25:P:305:CDL:H161	2.52	0.45
1:A:21:LEU:HD23	19:L:101:TGL:H211	1.97	0.45
1:A:484:THR:HG22	29:A:909:HOH:O	2.17	0.45
5:E:8:ASP:HA	27:E:201:PSC:H071	1.99	0.45
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.99	0.45
25:G:102:CDL:H252	25:G:102:CDL:H221	1.87	0.45
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.98	0.45
26:P:307:DMU:H36	7:T:62:TRP:HB2	1.98	0.45
2:O:227:LEU:HD23	2:O:227:LEU:HA	1.70	0.45
5:R:108:LYS:O	5:R:108:LYS:HG2	2.17	0.45
7:T:35:SER:C	7:T:37:LEU:H	2.25	0.45
11:X:8:ASP:HB3	29:X:119:HOH:O	2.17	0.45
13:Z:42:LYS:HA	13:Z:42:LYS:HD2	1.67	0.44
8:H:9:LYS:O	8:H:10:ASN:HB2	2.17	0.44
2:O:34:ILE:HA	26:O:304:DMU:H25	1.99	0.44
2:O:41:ILE:HD13	27:R:201:PSC:H342	1.99	0.44
3:C:63:ARG:HH21	25:C:305:CDL:HA22	1.82	0.44
3:C:207:HIS:HD2	3:C:241:TYR:OH	2.00	0.44
11:K:35:GLN:NE2	29:K:101:HOH:O	2.49	0.44
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.17	0.44
1:A:169:ILE:CD1	1:A:189:MET:HE1	2.47	0.44
14:A:601:HEA:HMC3	14:A:601:HEA:HBC1	1.98	0.44
25:P:305:CDL:H532	25:P:305:CDL:H561	1.74	0.44
1:N:321:PHE:CD1	2:O:65:TRP:HB2	2.53	0.44
8:U:43:MET:HE3	8:U:49:ASP:H	1.81	0.44
10:J:52:TRP:O	10:J:57:HIS:HE1	2.00	0.44
3:C:250:LEU:HD22	25:G:102:CDL:H662	1.99	0.44
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.85	0.44
25:P:305:CDL:H412	25:P:305:CDL:H382	1.72	0.44
26:C:307:DMU:H1	7:G:69:PHE:HZ	1.83	0.44
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.53	0.44
8:U:9:LYS:O	8:U:10:ASN:HB2	2.18	0.44
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.99	0.44
6:F:94:HIS:HE1	29:F:229:HOH:O	2.01	0.44
1:N:321:PHE:CD2	27:R:201:PSC:H341	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:102:PEK:O04	24:T:102:PEK:H242	2.17	0.44
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.99	0.44
1:N:379:TYR:O	1:N:383[A]:MET:HB2	2.18	0.43
3:C:80:ARG:NH2	3:C:236:GLU:OE1	2.47	0.43
2:B:93:PRO:HG3	2:B:151:ARG:HB2	2.00	0.43
3:C:156:ARG:NE	23:C:306:CHD:O26	2.46	0.43
4:D:98:TRP:CE2	26:M:101:DMU:H11	2.53	0.43
5:E:105:GLY:O	5:E:108:LYS:HG2	2.18	0.43
26:C:307:DMU:O1	26:C:307:DMU:H29	2.18	0.43
8:H:7:LYS:O	8:H:8:ILE:HG22	2.19	0.43
3:P:207:HIS:HD2	3:P:241:TYR:OH	2.01	0.43
1:A:351:GLY:C	1:A:380[A]:VAL:HG13	2.44	0.43
24:C:302:PEK:H101	24:C:302:PEK:H71	1.82	0.43
3:C:47:LEU:O	3:C:51[B]:MET:HG3	2.18	0.43
13:M:42:LYS:HD2	13:M:42:LYS:HA	1.49	0.43
1:N:449:MET:SD	2:O:5:MET:HG2	2.59	0.43
19:N:607:TGL:HC51	19:N:607:TGL:OC1	2.18	0.43
20:P:304:PGV:H21	20:P:304:PGV:H51	1.75	0.43
26:P:307:DMU:H40	7:T:63:GLY:N	2.33	0.43
7:T:37:LEU:HD21	25:T:103:CDL:H361	1.99	0.43
2:B:56:MET:HG2	27:E:201:PSC:H211	2.01	0.43
11:X:8:ASP:HB2	29:X:107:HOH:O	2.17	0.43
1:A:278:MET:HB3	7:T:5:LYS:HD3	2.01	0.43
12:Y:20:ARG:HH11	12:Y:20:ARG:HB3	1.84	0.43
23:B:302:CHD:H212	23:B:302:CHD:H12	2.01	0.42
25:G:102:CDL:H552	25:G:102:CDL:H582	1.20	0.42
8:H:60:TYR:CD1	8:H:60:TYR:C	2.96	0.42
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.17	0.42
24:G:103:PEK:H21	3:P:84:ILE:HG12	2.01	0.42
1:N:66:ILE:O	1:N:71:MET:HG3	2.19	0.42
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.62	0.42
3:C:131:LEU:HD21	25:G:102:CDL:HB61	2.00	0.42
20:P:304:PGV:H272	20:P:304:PGV:H241	1.87	0.42
1:N:76:GLY:O	1:N:80:ASN:HB2	2.19	0.42
1:N:513:LEU:HA	1:N:513:LEU:HD23	1.68	0.42
1:A:378:HIS:HA	1:A:382[A]:SER:OG	2.19	0.42
3:C:107:ALA:HB2	20:C:304:PGV:H031	2.01	0.42
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	2.02	0.42
27:R:201:PSC:O14	29:R:301:HOH:O	2.22	0.42
11:X:24:PHE:O	11:X:28:VAL:HG12	2.20	0.42
12:Y:22:LEU:O	12:Y:26:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:MET:SD	27:E:201:PSC:H301	2.60	0.42
25:G:102:CDL:H201	25:G:102:CDL:C51	2.44	0.42
1:N:408:THR:CG2	20:N:608:PGV:H52	2.50	0.42
5:R:72:LYS:HB2	5:R:82:TYR:CD2	2.54	0.42
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.49	0.42
23:C:301:CHD:H3	25:T:103:CDL:OB3	2.20	0.42
25:C:305:CDL:H461	25:C:305:CDL:H421	2.02	0.42
1:N:380[B]:VAL:HG21	14:N:602:HEA:C3C	2.50	0.42
25:P:305:CDL:H161	25:P:305:CDL:H131	1.94	0.42
1:A:71:MET:HB3	1:A:71:MET:HE2	1.93	0.42
1:A:381[A]:LEU:HB2	14:A:602:HEA:CAC	2.50	0.42
2:B:1:FME:HCN	2:B:193:TYR:H	1.85	0.42
1:N:376:HIS:O	1:N:380[A]:VAL:HG22	2.20	0.42
25:C:305:CDL:H522	25:C:305:CDL:OB9	2.20	0.42
4:D:81:VAL:HG11	19:D:201:TGL:HB52	2.01	0.42
3:P:33:MET:CE	3:P:42:LEU:H	2.32	0.42
3:P:107:ALA:HB2	20:P:304:PGV:H031	2.02	0.42
25:C:305:CDL:H772	25:C:305:CDL:H651	2.01	0.41
25:G:102:CDL:H531	25:G:102:CDL:H241	2.02	0.41
3:P:29:SER:HB3	29:P:496:HOH:O	2.20	0.41
7:T:5:LYS:HG3	24:T:102:PEK:H383	2.01	0.41
1:A:486:ASP:HB3	1:A:487:LEU:HG	2.02	0.41
1:N:215:LEU:HD11	24:P:302:PEK:H272	2.01	0.41
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.51	0.41
3:C:98:PHE:CD2	24:T:102:PEK:H182	2.55	0.41
19:D:201:TGL:H331	19:D:201:TGL:H172	1.89	0.41
5:R:11:PHE:CG	27:R:201:PSC:H073	2.55	0.41
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.50	0.41
25:G:102:CDL:H782	25:G:102:CDL:C56	2.37	0.41
7:T:38:HIS:CE1	25:T:103:CDL:H122	2.56	0.41
5:E:90:ARG:NH2	5:E:103:GLU:OE2	2.54	0.41
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.55	0.41
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.55	0.41
5:R:8:ASP:OD1	27:R:201:PSC:H081	2.20	0.41
5:R:107:ASP:OD2	5:R:107:ASP:N	2.54	0.41
7:T:3:ALA:O	7:T:4:ALA:HB2	2.20	0.41
2:O:217:LYS:O	2:O:221:LYS:HG3	2.19	0.41
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.56	0.41
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.56	0.41
1:N:409:TRP:CZ2	20:N:608:PGV:H81	2.56	0.41
1:A:376:HIS:O	1:A:380[A]:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:102:CDL:H182	1:N:307:SER:CB	2.50	0.41
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.51	0.41
2:O:82:ARG:NH1	2:O:86:MET:HE1	2.36	0.41
25:P:305:CDL:H652	25:P:305:CDL:H621	1.72	0.41
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.03	0.41
20:C:303:PGV:H161	20:C:303:PGV:C12	2.51	0.41
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.03	0.41
2:B:41:ILE:HG21	27:E:201:PSC:H342	2.03	0.40
29:B:413:HOH:O	7:T:17:ARG:CD	2.63	0.40
7:G:58:LYS:NZ	29:G:202:HOH:O	2.53	0.40
10:J:36:MET:HG2	23:J:101:CHD:H221	2.03	0.40
1:A:364:ASP:OD2	14:A:602:HEA:O1A	2.39	0.40
3:C:51[A]:MET:HE1	20:C:303:PGV:H141	2.03	0.40
4:D:68:PHE:HA	4:D:71:MET:HE3	2.02	0.40
29:N:813:HOH:O	3:P:191:GLY:HA3	2.21	0.40
4:Q:63:LYS:HG2	4:Q:64:PHE:CE1	2.56	0.40
7:T:50:TYR:HB3	7:T:52:HIS:CE1	2.56	0.40
1:A:406:ASN:HD21	20:A:609:PGV:C2	2.35	0.40
2:B:41:ILE:HD13	27:E:201:PSC:H342	2.02	0.40
9:I:29:LEU:HA	9:I:29:LEU:HD12	1.79	0.40
1:N:71:MET:HB3	1:N:71:MET:HE2	1.77	0.40
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.51	0.40
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.56	0.40
1:A:400:PHE:HB3	19:L:101:TGL:H283	2.03	0.40
2:B:16:ILE:HG13	29:B:535:HOH:O	2.20	0.40
1:N:380[B]:VAL:HG21	14:N:602:HEA:C4C	2.51	0.40
19:N:607:TGL:H211	19:N:607:TGL:HA81	1.78	0.40
2:O:82:ARG:HG2	2:O:86:MET:HE3	2.03	0.40
1:A:489:THR:HA	6:F:71:TRP:O	2.22	0.40
2:B:13:THR:HB	2:B:168:LEU:HD23	2.03	0.40
6:F:96:LEU:HB3	6:F:97:ALA:H	1.64	0.40
7:G:8:HIS:ND1	24:G:103:PEK:H312	2.37	0.40

All (1) 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]	2.17	0.03

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	522/514 (102%)	509 (98%)	13 (2%)	0	100	100
1	N	521/514 (101%)	509 (98%)	12 (2%)	0	100	100
2	B	227/227 (100%)	222 (98%)	4 (2%)	1 (0%)	30	19
2	O	225/227 (99%)	217 (96%)	6 (3%)	2 (1%)	14	5
3	C	260/261 (100%)	255 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	6 (4%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	90 (94%)	2 (2%)	4 (4%)	2	0
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	3	0
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
7	T	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	2	0
8	U	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	1	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	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%)	40 (98%)	1 (2%)	0	100	100
All	All	3528/3614 (98%)	3410 (97%)	91 (3%)	27 (1%)	16	6

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
6	F	94	HIS
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
2	O	60	GLU
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	H	8	ILE
8	H	46	LYS
8	U	10	ASN
8	U	46	LYS
6	F	96	LEU
7	G	6	GLY
7	G	8	HIS
8	U	8	ILE
8	U	45	ALA
2	B	92	ASN
7	G	3	ALA
6	S	96	LEU
7	T	3	ALA
8	H	9	LYS
7	T	6	GLY
2	O	92	ASN

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	435/426 (102%)	427 (98%)	8 (2%)	51	43
1	N	434/426 (102%)	426 (98%)	8 (2%)	51	43
2	B	212/210 (101%)	202 (95%)	10 (5%)	23	11
2	O	210/210 (100%)	200 (95%)	10 (5%)	23	11
3	C	227/226 (100%)	225 (99%)	2 (1%)	70	67
3	P	224/226 (99%)	221 (99%)	3 (1%)	61	54
4	D	128/129 (99%)	123 (96%)	5 (4%)	28	16
4	Q	128/129 (99%)	126 (98%)	2 (2%)	55	47
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	34
5	R	92/95 (97%)	90 (98%)	2 (2%)	45	34
6	F	81/81 (100%)	77 (95%)	4 (5%)	22	10
6	S	81/81 (100%)	78 (96%)	3 (4%)	30	18
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	7
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	2
8	H	71/75 (95%)	69 (97%)	2 (3%)	38	26
8	U	71/75 (95%)	69 (97%)	2 (3%)	38	26
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	4
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	9
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%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	40	28
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	9
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	1
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	1
All	All	3062/3082 (99%)	2967 (97%)	95 (3%)	35	23

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	A	169	ILE
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	297	MET
1	A	369	ASP
1	A	380[A]	VAL
1	A	380[B]	VAL
1	A	486	ASP
2	B	33	LEU
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
2	B	184	LEU
2	B	217	LYS
3	C	159	MET
3	C	230	ASN
4	D	4	SER
4	D	20	ARG
4	D	31	LYS
4	D	51	LEU
4	D	58	GLU
5	E	90	ARG
5	E	109	VAL
6	F	48	LEU
6	F	94	HIS
6	F	95	GLN
6	F	96	LEU
7	G	17	ARG
7	G	43	GLU
7	G	74	ARG
7	G	84	LYS
8	H	8	ILE
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	29	LEU
9	I	61	GLU
10	J	50	LEU
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP

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Mol	Chain	Res	Type
13	M	42	LYS
1	N	178	GLN
1	N	180	GLN
1	N	369	ASP
1	N	380[A]	VAL
1	N	380[B]	VAL
1	N	484	THR
1	N	485	VAL
1	N	512	ASN
2	O	33	LEU
2	O	61	VAL
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	110	TYR
2	O	217	LYS
2	O	226	MET
3	P	159	MET
3	P	180	GLU
3	P	230	ASN
4	Q	9	GLU
4	Q	143	ASN
5	R	80	GLU
5	R	108	LYS
6	S	37	LYS
6	S	80	GLN
6	S	96	LEU
7	T	2	SER
7	T	17	ARG
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
7	T	74	ARG
7	T	84	LYS
8	U	8	ILE
8	U	60	TYR
9	V	2	THR
9	V	8	GLN
9	V	70	GLN
10	W	50	LEU

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Mol	Chain	Res	Type
11	X	20	SER
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	512	ASN
2	B	181	GLN
3	C	3	HIS
3	C	68	GLN
3	C	161	GLN
4	D	29	HIS
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	119	GLN
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
7	G	34	ASN
7	G	76	ASN
8	H	31	GLN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	170	ASN
1	N	178	GLN
1	N	180	GLN
1	N	422	ASN
1	N	512	ASN
2	O	91	ASN
2	O	181	GLN

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Mol	Chain	Res	Type
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
3	P	161	GLN
4	Q	32	ASN
4	Q	37	GLN
4	Q	76	ASN
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	94	HIS
7	T	76	ASN
8	U	28	ASN
8	U	32	ASN
10	W	29	ASN
10	W	57	HIS
11	X	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	A	1	1	8,9,10	0.49	0	8,9,11	1.66	1 (12%)
1	FME	N	1	1	8,9,10	0.49	0	8,9,11	1.16	0
2	FME	B	1	2	8,9,10	2.09	3 (37%)	8,9,11	3.39	4 (50%)
9	SAC	V	1	9	7,8,9	0.60	0	7,9,11	2.03	3 (42%)
7	TPO	G	11	7	8,10,11	1.61	2 (25%)	10,14,16	1.39	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TPO	T	11	7	8,10,11	1.67	2 (25%)	10,14,16	1.38	1 (10%)
9	SAC	I	1	9	7,8,9	0.60	0	7,9,11	0.82	0
2	FME	O	1	2	8,9,10	1.08	1 (12%)	8,9,11	3.80	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	4/7/9/11	-
1	FME	N	1	1	-	5/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
9	SAC	V	1	9	-	6/7/8/10	-
7	TPO	G	11	7	-	3/9/11/13	-
7	TPO	T	11	7	-	4/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-
2	FME	O	1	2	-	2/7/9/11	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CN-N	3.74	1.45	1.33
2	B	1	FME	CA-N	3.74	1.52	1.46
7	T	11	TPO	P-O1P	3.08	1.60	1.50
7	G	11	TPO	P-O1P	3.07	1.60	1.50
7	T	11	TPO	P-OG1	2.47	1.63	1.59
7	G	11	TPO	P-OG1	2.12	1.63	1.59
2	B	1	FME	CG-SD	-2.12	1.70	1.81
2	O	1	FME	CG-SD	-2.09	1.70	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CA-N-CN	-10.11	107.27	122.82
2	B	1	FME	C-CA-N	7.29	123.58	109.50
2	B	1	FME	CA-N-CN	-3.91	116.80	122.82
7	G	11	TPO	CG2-CB-CA	3.73	120.52	113.26
7	T	11	TPO	CG2-CB-CA	3.45	119.98	113.26
9	V	1	SAC	C-CA-N	3.41	116.08	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.24	102.96	112.87
2	B	1	FME	O1-CN-N	-3.07	117.39	125.32
1	A	1	FME	CA-N-CN	-3.00	118.21	122.82
2	O	1	FME	CG-CB-CA	-2.95	103.86	112.87
9	V	1	SAC	O-C-CA	-2.85	117.43	124.77
9	V	1	SAC	CB-CA-C	-2.42	106.02	111.35

There are no chirality outliers.

All (29) 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
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	N-CA-CB-OG
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
2	O	1	FME	O1-CN-N-CA
2	O	1	FME	CB-CA-N-CN
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	C-CA-N-C1A
9	V	1	SAC	CB-CA-N-C1A
9	V	1	SAC	C-CA-CB-OG
9	I	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	N-CA-CB-OG
9	I	1	SAC	OAC-C1A-N-CA
1	N	1	FME	CA-CB-CG-SD
1	N	1	FME	CB-CG-SD-CE
1	A	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG
7	T	11	TPO	CB-OG1-P-O1P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
1	N	1	FME	2	0
2	B	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 78 ligands modelled in this entry, 8 are monoatomic - leaving 70 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	$\# Z > 2$
25	CDL	C	305	-	99,99,99	1.45	13 (13%)	105,111,111	1.59	14 (13%)
14	HEA	A	601	1	67,67,67	1.94	20 (29%)	81,103,103	1.94	21 (25%)
20	PGV	C	303	-	50,50,50	0.91	3 (6%)	53,56,56	1.10	5 (9%)
21	EDO	P	309	-	3,3,3	0.75	0	2,2,2	0.42	0
24	PEK	C	302	-	52,52,52	0.84	3 (5%)	55,57,57	1.47	10 (18%)
24	PEK	P	302	-	52,52,52	0.75	2 (3%)	55,57,57	1.51	5 (9%)
24	PEK	T	101	-	52,52,52	1.06	2 (3%)	55,57,57	1.32	5 (9%)
25	CDL	T	103	-	99,99,99	1.40	12 (12%)	105,111,111	1.50	12 (11%)
21	EDO	A	611	-	3,3,3	0.91	0	2,2,2	0.72	0
21	EDO	S	102	-	3,3,3	1.01	0	2,2,2	0.64	0
20	PGV	N	609	-	50,50,50	1.06	3 (6%)	53,56,56	1.14	4 (7%)
26	DMU	W	102	-	33,33,34	0.86	1 (3%)	44,44,45	2.39	20 (45%)
22	CUA	B	301	2	0,1,1	-	-	-	-	-
22	CUA	O	301	2	0,1,1	-	-	-	-	-
27	PSC	E	201	-	51,51,51	1.09	3 (5%)	57,59,59	1.21	4 (7%)
21	EDO	A	613	-	3,3,3	0.46	0	2,2,2	0.33	0
23	CHD	C	301	-	32,32,32	0.98	3 (9%)	51,51,51	1.61	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	TGL	Q	201	-	62,62,62	1.03	3 (4%)	65,65,65	1.00	3 (4%)
23	CHD	J	101	-	32,32,32	0.72	0	51,51,51	1.83	13 (25%)
21	EDO	A	612	-	3,3,3	0.60	0	2,2,2	0.30	0
26	DMU	M	101	-	34,34,34	0.60	1 (2%)	45,45,45	0.96	2 (4%)
27	PSC	R	201	-	51,51,51	1.15	3 (5%)	57,59,59	1.21	5 (8%)
15	NO	N	603	16,14	0,1,1	-	-	-	-	-
14	HEA	N	602	1,15	67,67,67	1.77	21 (31%)	81,103,103	1.71	24 (29%)
21	EDO	N	612	-	3,3,3	0.45	0	2,2,2	0.31	0
20	PGV	A	609	-	50,50,50	1.01	2 (4%)	53,56,56	1.23	7 (13%)
23	CHD	P	306	-	32,32,32	0.66	0	51,51,51	1.26	3 (5%)
21	EDO	N	613	-	3,3,3	0.42	0	2,2,2	0.62	0
21	EDO	N	614	-	3,3,3	0.68	0	2,2,2	0.51	0
20	PGV	A	608	-	50,50,50	1.04	6 (12%)	53,56,56	1.25	5 (9%)
25	CDL	G	102	-	99,99,99	1.44	12 (12%)	105,111,111	1.51	13 (12%)
21	EDO	N	611	-	3,3,3	0.71	0	2,2,2	0.84	0
23	CHD	C	306	-	32,32,32	0.65	0	51,51,51	1.18	5 (9%)
21	EDO	F	102	-	3,3,3	0.92	0	2,2,2	0.68	0
21	EDO	O	306	-	3,3,3	0.50	0	2,2,2	0.17	0
26	DMU	C	307	-	34,34,34	0.78	1 (2%)	45,45,45	1.67	10 (22%)
26	DMU	Z	101	-	34,34,34	0.43	0	45,45,45	0.84	0
20	PGV	C	304	-	50,50,50	1.00	2 (4%)	53,56,56	1.48	7 (13%)
21	EDO	Q	203	-	3,3,3	0.16	0	2,2,2	0.83	0
23	CHD	P	301	-	32,32,32	1.03	2 (6%)	51,51,51	1.37	7 (13%)
24	PEK	G	101	-	49,49,52	1.10	3 (6%)	52,54,57	1.28	3 (5%)
14	HEA	N	601	1	67,67,67	1.77	18 (26%)	81,103,103	1.88	25 (30%)
23	CHD	O	302	-	32,32,32	1.02	1 (3%)	51,51,51	1.49	7 (13%)
26	DMU	O	304	-	22,22,34	0.74	0	27,27,45	1.73	6 (22%)
21	EDO	B	303	-	3,3,3	0.69	0	2,2,2	0.59	0
26	DMU	P	307	-	34,34,34	0.88	1 (2%)	45,45,45	2.03	11 (24%)
21	EDO	N	615	-	3,3,3	0.62	0	2,2,2	0.30	0
19	TGL	A	607	-	62,62,62	1.07	3 (4%)	65,65,65	1.15	6 (9%)
21	EDO	Q	202	-	3,3,3	0.36	0	2,2,2	0.46	0
25	CDL	P	305	-	99,99,99	1.46	13 (13%)	105,111,111	1.63	14 (13%)
14	HEA	A	602	1,15	67,67,67	1.96	20 (29%)	81,103,103	2.08	32 (39%)
15	NO	A	603	16,14	0,1,1	-	-	-	-	-
19	TGL	O	303	-	62,62,62	1.06	3 (4%)	65,65,65	1.18	5 (7%)
21	EDO	S	103	-	3,3,3	0.54	0	2,2,2	0.56	0
21	EDO	P	308	-	3,3,3	0.44	0	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	TGL	L	101	-	62,62,62	1.16	3 (4%)	65,65,65	1.68	10 (15%)
20	PGV	N	608	-	45,45,50	1.06	2 (4%)	48,50,56	1.56	9 (18%)
20	PGV	P	303	-	50,50,50	0.72	1 (2%)	53,56,56	1.14	7 (13%)
21	EDO	A	610	-	3,3,3	1.09	0	2,2,2	0.89	0
20	PGV	P	304	-	50,50,50	1.04	2 (4%)	53,56,56	1.46	6 (11%)
21	EDO	N	610	-	3,3,3	0.79	0	2,2,2	0.52	0
21	EDO	O	305	-	3,3,3	0.86	0	2,2,2	0.28	0
23	CHD	W	101	-	32,32,32	0.70	0	51,51,51	1.98	15 (29%)
24	PEK	G	103	-	52,52,52	1.04	2 (3%)	55,57,57	1.49	4 (7%)
19	TGL	D	201	-	62,62,62	1.12	4 (6%)	65,65,65	1.04	4 (6%)
21	EDO	S	104	-	3,3,3	0.63	0	2,2,2	0.40	0
23	CHD	B	302	-	32,32,32	0.95	1 (3%)	51,51,51	1.52	11 (21%)
21	EDO	C	308	-	3,3,3	0.32	0	2,2,2	0.93	0
19	TGL	N	607	-	62,62,62	1.14	3 (4%)	65,65,65	1.34	11 (16%)
24	PEK	T	102	-	52,52,52	1.02	2 (3%)	55,57,57	1.69	6 (10%)

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
25	CDL	C	305	-	-	47/110/110/110	-
14	HEA	A	601	1	-	7/36/76/76	-
20	PGV	C	303	-	-	6/55/55/55	-
21	EDO	P	309	-	-	0/1/1/1	-
24	PEK	C	302	-	-	13/56/56/56	-
24	PEK	P	302	-	-	19/56/56/56	-
24	PEK	T	101	-	-	35/56/56/56	-
25	CDL	T	103	-	-	47/110/110/110	-
21	EDO	A	611	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
20	PGV	N	609	-	-	8/55/55/55	-
26	DMU	W	102	-	-	5/18/58/59	0/2/2/2
27	PSC	E	201	-	-	32/55/55/55	-
21	EDO	A	613	-	-	0/1/1/1	-
23	CHD	C	301	-	-	1/9/74/74	0/4/4/4
19	TGL	Q	201	-	-	25/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	J	101	-	-	5/9/74/74	0/4/4/4
21	EDO	A	612	-	-	0/1/1/1	-
26	DMU	M	101	-	-	6/19/59/59	0/2/2/2
27	PSC	R	201	-	-	23/55/55/55	-
21	EDO	N	612	-	-	0/1/1/1	-
14	HEA	N	602	1,15	-	4/36/76/76	-
20	PGV	A	609	-	-	19/55/55/55	-
23	CHD	P	306	-	-	2/9/74/74	0/4/4/4
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	N	614	-	-	1/1/1/1	-
20	PGV	A	608	-	-	8/55/55/55	-
25	CDL	G	102	-	-	50/110/110/110	-
21	EDO	N	611	-	-	0/1/1/1	-
23	CHD	C	306	-	-	4/9/74/74	0/4/4/4
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	O	306	-	-	0/1/1/1	-
26	DMU	C	307	-	-	6/19/59/59	0/2/2/2
26	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
20	PGV	C	304	-	-	15/55/55/55	-
21	EDO	Q	203	-	-	1/1/1/1	-
23	CHD	P	301	-	-	2/9/74/74	0/4/4/4
24	PEK	G	101	-	-	25/51/51/56	-
14	HEA	N	601	1	-	7/36/76/76	-
23	CHD	O	302	-	-	2/9/74/74	0/4/4/4
26	DMU	O	304	-	-	6/13/33/59	0/1/1/2
21	EDO	B	303	-	-	0/1/1/1	-
26	DMU	P	307	-	-	10/19/59/59	0/2/2/2
21	EDO	N	615	-	-	0/1/1/1	-
19	TGL	A	607	-	-	33/65/65/65	-
21	EDO	Q	202	-	-	1/1/1/1	-
25	CDL	P	305	-	-	57/110/110/110	-
14	HEA	A	602	1,15	-	5/36/76/76	-
21	EDO	S	103	-	-	0/1/1/1	-
19	TGL	O	303	-	-	33/65/65/65	-
21	EDO	P	308	-	-	1/1/1/1	-
19	TGL	L	101	-	-	29/65/65/65	-
20	PGV	N	608	-	-	20/47/47/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	P	303	-	-	9/55/55/55	-
21	EDO	A	610	-	-	0/1/1/1	-
20	PGV	P	304	-	-	18/55/55/55	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	O	305	-	-	0/1/1/1	-
23	CHD	W	101	-	-	6/9/74/74	0/4/4/4
24	PEK	G	103	-	-	22/56/56/56	-
19	TGL	D	201	-	-	30/65/65/65	-
21	EDO	S	104	-	-	0/1/1/1	-
23	CHD	B	302	-	-	2/9/74/74	0/4/4/4
21	EDO	C	308	-	-	1/1/1/1	-
19	TGL	N	607	-	-	32/65/65/65	-
24	PEK	T	102	-	-	25/56/56/56	-

All (200) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C11-C3B	5.79	1.58	1.51
19	N	607	TGL	OG2-CB1	5.33	1.49	1.34
19	L	101	TGL	OG2-CB1	5.21	1.49	1.34
24	T	101	PEK	O03-C21	5.17	1.48	1.33
20	P	304	PGV	O01-C1	5.11	1.48	1.34
14	N	601	HEA	CHA-C1A	5.03	1.48	1.38
24	G	101	PEK	O03-C21	4.83	1.47	1.33
25	C	305	CDL	OB8-CB7	4.81	1.47	1.33
24	G	103	PEK	O03-C21	4.81	1.47	1.33
19	L	101	TGL	OG3-CC1	4.81	1.47	1.33
20	A	609	PGV	O03-C19	4.79	1.47	1.33
25	G	102	CDL	OA8-CA7	4.77	1.47	1.33
24	G	103	PEK	O01-C1	4.76	1.47	1.34
24	T	102	PEK	O03-C21	4.73	1.47	1.33
25	G	102	CDL	OA6-CA5	4.65	1.47	1.34
19	N	607	TGL	OG1-CA1	4.62	1.46	1.33
25	G	102	CDL	OB6-CB5	4.60	1.47	1.34
19	O	303	TGL	OG3-CC1	4.58	1.46	1.33
19	A	607	TGL	OG2-CB1	4.58	1.47	1.34
20	N	608	PGV	O03-C19	4.57	1.46	1.33
19	A	607	TGL	OG1-CA1	4.55	1.46	1.33
20	C	304	PGV	O01-C1	4.54	1.47	1.34
25	P	305	CDL	OB8-CB7	4.54	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	305	CDL	OA8-CA7	4.54	1.46	1.33
19	Q	201	TGL	OG1-CA1	4.54	1.46	1.33
19	A	607	TGL	OG3-CC1	4.51	1.46	1.33
24	G	101	PEK	O01-C1	4.51	1.47	1.34
27	R	201	PSC	O01-C1	4.50	1.47	1.34
25	P	305	CDL	OA6-CA5	4.49	1.47	1.34
25	G	102	CDL	OB8-CB7	4.48	1.46	1.33
19	O	303	TGL	OG2-CB1	4.46	1.46	1.34
25	T	103	CDL	OA6-CA5	4.43	1.46	1.34
19	O	303	TGL	OG1-CA1	4.41	1.46	1.33
19	N	607	TGL	OG3-CC1	4.40	1.46	1.33
24	T	102	PEK	O01-C1	4.39	1.46	1.34
25	T	103	CDL	OB8-CB7	4.38	1.46	1.33
25	C	305	CDL	OA8-CA7	4.38	1.46	1.33
25	T	103	CDL	OA8-CA7	4.30	1.45	1.33
25	T	103	CDL	OB6-CB5	4.23	1.46	1.34
27	E	201	PSC	O01-C1	4.22	1.46	1.34
19	D	201	TGL	OG1-CA1	4.21	1.45	1.33
19	Q	201	TGL	OG2-CB1	4.20	1.46	1.34
20	C	304	PGV	O03-C19	4.18	1.45	1.33
19	L	101	TGL	OG1-CA1	4.17	1.45	1.33
20	N	608	PGV	O01-C1	4.15	1.46	1.34
24	T	101	PEK	O01-C1	4.14	1.46	1.34
20	A	609	PGV	O01-C1	4.13	1.45	1.34
14	N	601	HEA	C1A-C2A	-4.10	1.38	1.45
14	N	602	HEA	CHD-C1D	4.08	1.46	1.38
19	D	201	TGL	OG2-CB1	4.03	1.45	1.34
25	P	305	CDL	C59-C58	-4.03	1.31	1.51
20	P	304	PGV	O03-C19	4.01	1.45	1.33
14	A	601	HEA	C1A-C2A	-4.00	1.38	1.45
25	C	305	CDL	C59-C58	-3.98	1.32	1.51
25	C	305	CDL	C79-C78	-3.97	1.32	1.51
27	R	201	PSC	C13-C12	3.96	1.54	1.31
25	G	102	CDL	C59-C58	-3.96	1.32	1.51
25	P	305	CDL	C82-C81	-3.92	1.32	1.51
25	P	305	CDL	C79-C78	-3.91	1.32	1.51
25	C	305	CDL	C82-C81	-3.88	1.32	1.51
25	P	305	CDL	C19-C18	-3.88	1.32	1.51
14	A	602	HEA	C4A-NA	-3.88	1.32	1.39
14	A	602	HEA	CHA-C4D	3.88	1.48	1.39
25	G	102	CDL	C62-C61	-3.83	1.32	1.51
19	Q	201	TGL	OG3-CC1	3.81	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	305	CDL	OA6-CA5	3.81	1.45	1.34
27	R	201	PSC	O03-C19	3.80	1.44	1.33
25	T	103	CDL	C59-C58	-3.80	1.32	1.51
25	P	305	CDL	C22-C21	-3.78	1.33	1.51
25	P	305	CDL	C62-C61	-3.75	1.33	1.51
27	E	201	PSC	O03-C19	3.75	1.44	1.33
27	E	201	PSC	C13-C12	3.74	1.53	1.31
14	A	601	HEA	C4A-NA	-3.74	1.32	1.39
25	T	103	CDL	C82-C81	-3.74	1.33	1.51
26	P	307	DMU	O16-C6	3.73	1.46	1.40
25	T	103	CDL	C62-C61	-3.72	1.33	1.51
24	P	302	PEK	O03-C21	3.69	1.44	1.33
19	D	201	TGL	OB1-CB1	3.68	1.33	1.22
20	N	609	PGV	O03-C19	3.67	1.44	1.33
25	G	102	CDL	C19-C18	-3.67	1.33	1.51
25	C	305	CDL	C62-C61	-3.66	1.33	1.51
14	N	602	HEA	CHC-C4B	3.64	1.45	1.38
14	A	602	HEA	C4C-NC	-3.64	1.32	1.39
14	A	601	HEA	C1D-ND	-3.64	1.33	1.40
25	G	102	CDL	C82-C81	-3.64	1.33	1.51
14	A	601	HEA	CHD-C1D	3.63	1.45	1.38
14	A	602	HEA	CHD-C1D	3.63	1.45	1.38
25	T	103	CDL	C39-C38	-3.60	1.33	1.51
14	A	602	HEA	O11-C11	3.59	1.50	1.42
14	A	602	HEA	CMC-C2C	3.58	1.58	1.50
25	T	103	CDL	C79-C78	-3.57	1.34	1.51
20	N	609	PGV	O01-C1	3.57	1.44	1.34
25	G	102	CDL	C22-C21	-3.57	1.34	1.51
25	C	305	CDL	C22-C21	-3.56	1.34	1.51
14	A	602	HEA	C1A-C2A	-3.56	1.38	1.45
19	D	201	TGL	OG3-CC1	3.55	1.43	1.33
14	A	602	HEA	CHB-C4A	3.54	1.45	1.38
14	A	601	HEA	C4C-NC	-3.54	1.33	1.39
25	C	305	CDL	C42-C41	-3.53	1.34	1.51
14	A	602	HEA	C11-C3B	3.52	1.55	1.51
25	C	305	CDL	C19-C18	-3.52	1.34	1.51
25	T	103	CDL	C22-C21	-3.51	1.34	1.51
25	G	102	CDL	C79-C78	-3.51	1.34	1.51
25	C	305	CDL	OB6-CB5	3.48	1.44	1.34
25	P	305	CDL	C39-C38	-3.46	1.34	1.51
25	G	102	CDL	C42-C41	-3.46	1.34	1.51
25	T	103	CDL	C19-C18	-3.45	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	103	CDL	C42-C41	-3.45	1.34	1.51
25	P	305	CDL	C42-C41	-3.42	1.34	1.51
25	G	102	CDL	C39-C38	-3.40	1.34	1.51
25	C	305	CDL	C39-C38	-3.36	1.35	1.51
14	N	601	HEA	C4B-NB	-3.35	1.34	1.40
14	A	601	HEA	CHC-C4B	3.29	1.45	1.38
14	N	601	HEA	C3A-C4A	-3.26	1.40	1.46
14	A	602	HEA	C4D-C3D	-3.24	1.39	1.45
25	P	305	CDL	OB6-CB5	3.22	1.43	1.34
14	A	601	HEA	CHA-C1A	3.15	1.44	1.38
14	N	601	HEA	CHC-C4B	3.14	1.44	1.38
14	N	602	HEA	CHA-C1A	3.10	1.44	1.38
26	W	102	DMU	O16-C6	3.08	1.45	1.40
14	N	602	HEA	C4D-C3D	-3.05	1.39	1.45
26	C	307	DMU	O16-C6	2.99	1.45	1.40
14	N	601	HEA	C4B-C3B	-2.99	1.39	1.44
14	N	602	HEA	C1A-C2A	-2.97	1.40	1.45
14	A	601	HEA	CHB-C1B	2.97	1.45	1.39
14	N	602	HEA	CHB-C4A	2.96	1.44	1.38
20	N	609	PGV	O01-C02	-2.94	1.39	1.46
20	A	608	PGV	O03-C19	2.84	1.41	1.33
25	C	305	CDL	PB2-OB3	2.84	1.60	1.50
14	A	602	HEA	CHA-C1A	2.82	1.43	1.38
20	C	303	PGV	O01-C1	2.80	1.42	1.34
14	A	602	HEA	C1D-ND	-2.79	1.35	1.40
24	C	302	PEK	O03-C01	-2.79	1.38	1.45
14	A	601	HEA	CBD-CGD	2.78	1.57	1.50
14	A	602	HEA	CHB-C1B	2.74	1.45	1.39
23	P	301	CHD	C11-C9	2.72	1.58	1.53
14	A	601	HEA	FE-NB	2.71	2.03	1.94
14	N	601	HEA	C4D-ND	-2.71	1.33	1.38
14	A	601	HEA	FE-NC	2.71	2.04	1.95
14	N	602	HEA	CHD-C4C	2.68	1.45	1.39
14	N	601	HEA	FE-ND	2.67	2.03	1.94
14	N	602	HEA	C4B-C3B	-2.67	1.40	1.44
14	N	601	HEA	C1D-ND	-2.67	1.35	1.40
14	N	602	HEA	CHC-C1C	2.63	1.45	1.39
23	O	302	CHD	O7-C7	2.63	1.48	1.43
14	A	602	HEA	C1B-NB	-2.61	1.33	1.38
14	N	602	HEA	C3A-C4A	-2.60	1.41	1.46
14	A	601	HEA	C12-C13	2.60	1.61	1.53
14	A	601	HEA	FE-NA	2.59	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	CHC-C1C	2.57	1.45	1.39
14	A	602	HEA	CHC-C4B	2.55	1.43	1.38
14	A	601	HEA	CHA-C4D	2.54	1.45	1.39
14	N	601	HEA	CHD-C4C	2.54	1.45	1.39
14	N	601	HEA	CHC-C1C	2.53	1.45	1.39
20	A	608	PGV	O01-C02	-2.51	1.40	1.46
24	C	302	PEK	O01-C1	2.51	1.41	1.34
14	A	602	HEA	CBA-CGA	2.47	1.56	1.50
14	N	602	HEA	C4A-NA	-2.46	1.35	1.39
14	N	601	HEA	C1B-C2B	-2.46	1.39	1.44
23	P	301	CHD	C18-C13	-2.46	1.50	1.54
14	A	601	HEA	C12-C11	-2.43	1.48	1.53
14	N	602	HEA	FE-NB	2.39	2.02	1.94
14	N	602	HEA	C4C-NC	-2.39	1.35	1.39
20	P	303	PGV	O01-C1	2.39	1.41	1.34
14	N	601	HEA	CHB-C4A	2.38	1.43	1.38
14	N	601	HEA	O11-C11	2.38	1.48	1.42
20	A	608	PGV	O01-C1	2.37	1.41	1.34
26	M	101	DMU	O16-C6	2.36	1.44	1.40
14	N	602	HEA	CHA-C4D	2.36	1.44	1.39
23	C	301	CHD	C23-C24	2.34	1.56	1.50
14	N	602	HEA	C4B-NB	-2.33	1.36	1.40
24	G	101	PEK	P-O12	2.33	1.63	1.54
14	N	602	HEA	O11-C11	2.29	1.47	1.42
23	C	301	CHD	C11-C9	2.28	1.57	1.53
25	P	305	CDL	PB2-OB3	2.27	1.58	1.50
20	A	608	PGV	C01-C02	2.27	1.57	1.50
14	A	601	HEA	CAA-C2A	2.26	1.57	1.51
14	N	602	HEA	C1D-C2D	-2.26	1.39	1.44
14	A	602	HEA	C1C-C2C	-2.25	1.37	1.43
14	N	602	HEA	FE-ND	2.23	2.01	1.94
14	A	601	HEA	CBA-CGA	2.22	1.55	1.50
14	A	602	HEA	C4B-C3B	-2.20	1.40	1.44
14	A	602	HEA	C14-C15	2.19	1.38	1.33
20	C	303	PGV	C03-C02	2.19	1.57	1.50
23	B	302	CHD	C11-C12	2.18	1.56	1.53
14	N	602	HEA	C1D-ND	-2.15	1.36	1.40
14	A	602	HEA	CAD-C3D	2.14	1.56	1.51
14	N	602	HEA	C16-C15	2.14	1.55	1.51
14	N	602	HEA	C1A-NA	-2.13	1.35	1.39
14	N	601	HEA	CMA-C3A	2.11	1.50	1.45
14	A	601	HEA	C4D-C3D	-2.10	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	608	PGV	O03-C01	2.10	1.49	1.45
14	N	601	HEA	CHD-C1D	2.08	1.42	1.38
20	A	608	PGV	C03-C02	2.07	1.57	1.50
14	N	601	HEA	CHA-C4D	2.06	1.43	1.39
24	C	302	PEK	C2-C1	2.06	1.56	1.50
20	C	303	PGV	O01-C02	-2.06	1.41	1.46
14	N	601	HEA	FE-NB	2.05	2.01	1.94
23	C	301	CHD	O26-C24	-2.04	1.24	1.30
24	P	302	PEK	C05-C04	2.03	1.58	1.49

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	307	DMU	C18-O16-C6	7.87	127.12	113.68
24	P	302	PEK	C2-C3-C4	7.52	129.78	113.35
25	C	305	CDL	CB4-OB6-CB5	-7.02	100.98	117.80
14	A	601	HEA	C13-C12-C11	-6.98	103.24	114.39
25	P	305	CDL	CB4-OB6-CB5	-6.90	101.29	117.80
24	G	103	PEK	C03-C02-C01	-6.78	95.98	111.78
19	L	101	TGL	CG2-OG2-CB1	6.61	133.62	117.80
25	T	103	CDL	OA6-CA5-C11	6.40	125.33	111.48
24	T	102	PEK	O01-C1-C2	5.76	123.95	111.48
24	T	102	PEK	O03-C21-C22	5.75	129.37	111.83
19	O	303	TGL	OG2-CB1-CB2	5.43	123.23	111.48
25	T	103	CDL	OB6-CB5-C51	5.41	123.18	111.48
20	C	304	PGV	O03-C19-C20	5.37	128.20	111.83
26	P	307	DMU	O5-C6-O16	5.35	122.69	110.04
23	O	302	CHD	C18-C13-C12	-5.21	103.84	109.06
20	P	304	PGV	O03-C19-C20	5.19	127.66	111.83
26	W	102	DMU	O49-C1-C6	5.16	122.37	110.08
26	W	102	DMU	C10-O1-C9	5.14	123.75	113.72
25	G	102	CDL	OA8-CA7-C31	5.13	127.48	111.83
20	P	304	PGV	O01-C1-C2	5.13	122.58	111.48
25	G	102	CDL	OB6-CB5-C51	5.06	122.43	111.48
14	N	601	HEA	C13-C12-C11	-5.02	106.37	114.39
25	G	102	CDL	OA6-CA5-C11	4.94	122.16	111.48
19	L	101	TGL	OG2-CG2-CG3	4.92	126.00	108.34
24	T	102	PEK	O03-C21-O04	-4.90	111.37	123.63
26	P	307	DMU	C10-O1-C9	4.86	123.21	113.72
23	P	301	CHD	C1-C2-C3	-4.83	104.08	110.48
24	C	302	PEK	C03-C02-C01	-4.83	100.53	111.78
24	T	101	PEK	O03-C21-C22	4.81	126.50	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	E	201	PSC	O01-C1-C2	4.73	121.71	111.48
25	T	103	CDL	OA8-CA7-C31	4.71	126.19	111.83
24	G	101	PEK	O03-C21-C22	4.62	125.93	111.83
19	A	607	TGL	OG2-CB1-CB2	4.57	121.37	111.48
20	C	304	PGV	O01-C1-C2	4.57	121.37	111.48
14	A	602	HEA	CHB-C4A-NA	4.52	129.37	124.45
25	C	305	CDL	OB8-CB7-C71	4.51	125.58	111.83
26	W	102	DMU	O1-C10-C5	4.50	119.61	110.37
19	D	201	TGL	CG2-OG2-CB1	-4.50	107.04	117.80
25	P	305	CDL	OA8-CA7-C31	4.49	125.54	111.83
25	P	305	CDL	C52-C51-CB5	-4.45	97.37	113.69
25	C	305	CDL	OB6-CB5-C51	4.43	121.06	111.48
20	N	608	PGV	O03-C19-C20	4.38	125.20	111.83
25	C	305	CDL	C52-C51-CB5	-4.35	97.76	113.69
14	A	602	HEA	C4A-CHB-C1B	-4.34	116.80	126.02
14	A	602	HEA	C4C-CHD-C1D	-4.32	116.09	126.25
23	C	306	CHD	C15-C14-C13	4.30	107.71	103.54
23	J	101	CHD	C17-C13-C14	-4.28	95.82	100.11
26	C	307	DMU	C10-O1-C9	4.26	122.04	113.72
26	W	102	DMU	O1-C9-C8	4.26	117.37	109.70
24	G	103	PEK	O01-C1-C2	4.26	120.69	111.48
24	G	101	PEK	O01-C1-C2	4.25	120.68	111.48
19	N	607	TGL	CG2-OG2-CB1	4.23	127.93	117.80
23	W	101	CHD	C22-C20-C17	4.23	119.09	110.33
23	W	101	CHD	C17-C13-C14	-4.21	95.89	100.11
26	O	304	DMU	O5-C4-C57	4.21	116.88	106.44
26	C	307	DMU	O7-C10-C5	4.21	118.45	108.09
23	W	101	CHD	C14-C13-C12	4.16	111.22	107.42
23	J	101	CHD	C22-C20-C17	4.15	118.93	110.33
19	L	101	TGL	OG3-CC1-OC1	-4.12	113.33	123.63
26	W	102	DMU	C10-O7-C3	-4.07	108.32	117.98
23	P	306	CHD	C21-C20-C22	-4.07	104.05	110.34
24	T	102	PEK	C03-C02-C01	-4.06	102.33	111.78
27	R	201	PSC	O01-C1-C2	4.05	120.24	111.48
14	N	602	HEA	C4C-CHD-C1D	-4.05	116.73	126.25
14	A	601	HEA	CAA-CBA-CGA	-4.04	102.95	113.67
14	A	601	HEA	O11-C11-C12	4.00	119.75	109.14
23	W	101	CHD	C9-C10-C5	3.98	114.05	108.51
23	J	101	CHD	C13-C17-C20	3.97	124.29	119.48
24	T	101	PEK	O01-C1-C2	3.95	120.02	111.48
26	W	102	DMU	O16-C6-C1	3.93	114.24	108.27
19	Q	201	TGL	CG2-OG2-CB1	-3.92	108.42	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	CHA-C4D-C3D	-3.89	119.10	124.77
26	W	102	DMU	C1-C2-C3	-3.89	100.86	109.68
14	A	602	HEA	C2B-C1B-NB	3.88	114.39	109.90
25	P	305	CDL	CA6-CA4-CA3	-3.87	102.76	111.78
26	W	102	DMU	C7-C8-C9	3.86	117.22	110.23
26	C	307	DMU	C2-C3-C4	-3.85	102.40	110.93
25	P	305	CDL	OA6-CA5-C11	3.84	119.79	111.48
23	J	101	CHD	C14-C13-C12	3.84	110.92	107.42
24	P	302	PEK	O01-C1-O02	-3.84	114.73	123.70
23	O	302	CHD	C13-C17-C20	-3.84	114.84	119.48
14	N	601	HEA	O2A-CGA-CBA	3.82	126.07	114.00
14	A	602	HEA	O11-C11-C3B	-3.82	104.26	111.26
20	A	608	PGV	O03-C19-C20	3.76	123.29	111.83
24	G	103	PEK	O03-C01-C02	3.75	119.22	108.40
25	P	305	CDL	OB8-CB7-C71	3.75	123.27	111.83
14	A	601	HEA	C3C-C4C-NC	3.72	112.94	109.80
14	A	602	HEA	CHD-C4C-NC	3.68	130.53	123.86
14	A	602	HEA	CHA-C1A-NA	3.66	128.44	124.45
19	L	101	TGL	CC3-CC2-CC1	3.65	127.06	113.69
19	N	607	TGL	OG2-CB1-CB2	3.64	119.35	111.48
26	O	304	DMU	C2-C3-C4	3.64	116.83	110.23
14	N	601	HEA	CHA-C4D-ND	3.61	128.31	124.42
23	W	101	CHD	C13-C17-C20	3.59	123.83	119.48
25	G	102	CDL	CA6-OA8-CA7	3.57	130.18	117.12
23	C	301	CHD	C21-C20-C22	-3.57	104.82	110.34
23	W	101	CHD	C4-C3-C2	-3.56	106.28	110.62
25	G	102	CDL	OA8-CA7-OA9	-3.54	114.76	123.63
20	N	608	PGV	C01-O03-C19	3.53	130.01	117.12
20	N	608	PGV	C03-C02-C01	3.51	119.96	111.78
23	W	101	CHD	C16-C17-C20	3.50	117.48	112.18
23	W	101	CHD	C23-C22-C20	-3.50	107.93	114.46
14	N	601	HEA	C2D-C1D-ND	3.49	113.85	109.84
26	P	307	DMU	O1-C10-C5	3.49	117.53	110.37
24	G	101	PEK	O03-C21-O04	-3.48	114.93	123.63
23	B	302	CHD	C21-C20-C22	-3.47	104.96	110.34
25	C	305	CDL	OA6-CA5-C11	3.47	118.99	111.48
25	P	305	CDL	OA8-CA7-OA9	-3.46	114.97	123.63
14	A	602	HEA	CHB-C1B-C2B	-3.46	119.56	125.03
14	A	601	HEA	O1A-CGA-CBA	-3.45	112.14	123.09
23	J	101	CHD	C9-C10-C5	3.45	113.30	108.51
25	P	305	CDL	OB6-CB5-C51	3.44	118.93	111.48
24	T	102	PEK	O01-C1-O02	-3.44	115.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	305	CDL	OA6-CA4-CA3	3.44	120.67	108.34
20	N	609	PGV	O01-C1-O02	-3.43	115.69	123.70
14	A	601	HEA	C17-C18-C19	-3.41	119.83	127.62
14	N	601	HEA	O11-C11-C3B	-3.40	105.03	111.26
14	N	602	HEA	CHD-C1D-ND	3.40	128.57	124.37
19	L	101	TGL	OG3-CC1-CC2	3.40	122.19	111.83
14	N	601	HEA	C1A-CHA-C4D	-3.39	118.82	126.02
25	T	103	CDL	OA6-CA5-OA7	-3.38	115.80	123.70
14	A	601	HEA	O11-C11-C3B	-3.38	105.06	111.26
23	O	302	CHD	C14-C13-C12	3.38	110.50	107.42
24	C	302	PEK	O03-C01-C02	-3.37	98.68	108.40
20	N	608	PGV	O01-C1-C2	3.37	118.77	111.48
14	N	602	HEA	CHC-C1C-C2C	-3.36	117.67	127.43
20	C	303	PGV	C22-C21-C20	-3.35	100.80	113.13
23	B	302	CHD	C13-C14-C8	-3.35	110.48	114.72
23	C	301	CHD	C18-C13-C12	3.34	112.40	109.06
14	A	601	HEA	CAD-CBD-CGD	-3.34	104.82	113.67
14	N	602	HEA	C1C-CHC-C4B	-3.33	118.42	126.25
20	P	304	PGV	C21-C20-C19	-3.33	101.50	113.69
19	D	201	TGL	OG1-CA1-CA2	3.33	121.98	111.83
23	P	301	CHD	C22-C20-C17	-3.32	103.45	110.33
20	A	609	PGV	C4-C3-C2	-3.32	100.94	113.13
14	N	602	HEA	C13-C12-C11	-3.31	109.10	114.39
20	N	608	PGV	O03-C19-O04	-3.30	115.36	123.63
19	A	607	TGL	OG1-CA1-CA2	3.26	121.77	111.83
23	B	302	CHD	C11-C9-C10	-3.24	110.42	113.70
19	Q	201	TGL	OG2-CB1-CB2	3.23	118.46	111.48
14	A	601	HEA	C2D-C1D-ND	3.22	113.54	109.84
25	T	103	CDL	OA8-CA7-OA9	-3.22	115.58	123.63
25	T	103	CDL	CB4-OB6-CB5	-3.22	110.10	117.80
23	O	302	CHD	C16-C17-C20	-3.21	107.32	112.18
23	B	302	CHD	C6-C5-C4	-3.21	107.56	111.23
24	T	101	PEK	O03-C21-O04	-3.19	115.66	123.63
20	N	609	PGV	O03-C19-C20	3.19	121.55	111.83
20	A	609	PGV	O03-C19-C20	3.18	121.53	111.83
24	C	302	PEK	O01-C1-O02	-3.15	116.33	123.70
26	C	307	DMU	O1-C10-C5	3.15	116.85	110.37
14	N	601	HEA	C3C-C4C-NC	3.15	112.45	109.80
14	A	602	HEA	CHA-C4D-C3D	-3.14	120.20	124.77
23	J	101	CHD	C11-C9-C10	-3.13	110.52	113.70
14	A	601	HEA	O2A-CGA-CBA	3.13	123.88	114.00
14	A	602	HEA	O1D-CGD-CBD	-3.12	113.18	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	301	CHD	C23-C22-C20	-3.12	108.63	114.46
19	O	303	TGL	OG1-CA1-CA2	3.12	121.34	111.83
23	C	301	CHD	C15-C14-C13	-3.11	100.53	103.54
20	A	608	PGV	C23-C22-C21	-3.10	98.71	114.37
14	A	601	HEA	CAD-C3D-C4D	3.09	130.09	124.70
20	N	608	PGV	O01-C02-C01	3.08	119.41	108.34
23	W	101	CHD	C11-C9-C10	-3.08	110.58	113.70
14	A	602	HEA	C3B-C4B-NB	3.06	113.36	109.84
14	N	601	HEA	O2D-CGD-CBD	3.05	123.62	114.00
19	O	303	TGL	OG3-CC1-CC2	3.03	121.08	111.83
23	C	306	CHD	C11-C9-C10	-3.01	110.65	113.70
26	O	304	DMU	C3-C2-C1	3.01	116.11	110.83
26	W	102	DMU	C6-C1-C2	-3.01	103.69	110.01
26	W	102	DMU	C6-O5-C4	3.00	119.59	113.72
14	A	601	HEA	C13-C14-C15	-3.00	120.75	127.62
23	C	301	CHD	C22-C20-C17	-2.98	104.14	110.33
23	C	301	CHD	C18-C13-C17	-2.98	106.53	111.20
14	N	602	HEA	CMC-C2C-C1C	2.96	129.93	125.42
20	N	608	PGV	C4-C3-C2	-2.96	102.25	113.13
14	N	602	HEA	C21-C20-C19	2.95	122.95	113.19
14	A	602	HEA	C3D-C4D-ND	2.95	113.20	110.35
14	A	601	HEA	C2B-C1B-NB	2.95	113.31	109.90
19	A	607	TGL	OG3-CC1-CC2	2.94	120.79	111.83
20	P	304	PGV	O03-C19-O04	-2.93	116.29	123.63
23	C	301	CHD	C22-C23-C24	-2.93	104.68	112.49
20	A	609	PGV	C28-C27-C26	-2.92	99.59	114.37
26	W	102	DMU	O61-C57-C4	-2.91	101.42	111.33
20	A	608	PGV	O03-C19-O04	-2.90	116.37	123.63
20	C	304	PGV	C01-O03-C19	2.90	127.72	117.12
25	C	305	CDL	OB8-CB7-OB9	-2.90	116.38	123.63
24	T	102	PEK	C01-O03-C21	2.90	127.70	117.12
20	C	304	PGV	O03-C19-O04	-2.89	116.39	123.63
14	A	602	HEA	CHA-C1A-C2A	-2.89	120.30	124.86
26	O	304	DMU	C6-O5-C4	-2.88	108.09	113.72
14	A	602	HEA	C4B-NB-C1B	-2.88	101.79	105.21
23	W	101	CHD	C1-C10-C5	2.88	111.88	107.75
26	C	307	DMU	O1-C9-C8	2.88	114.89	109.70
14	N	602	HEA	CAD-CBD-CGD	-2.87	106.06	113.67
25	G	102	CDL	CB4-OB6-CB5	-2.86	110.94	117.80
27	R	201	PSC	C03-C02-C01	-2.86	105.12	111.78
25	P	305	CDL	OA8-CA6-CA4	2.86	116.63	108.40
19	N	607	TGL	OG2-CG2-CG1	2.86	118.59	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	304	PGV	C21-C20-C19	-2.84	103.27	113.69
23	J	101	CHD	C4-C3-C2	-2.83	107.16	110.62
24	C	302	PEK	C30-C29-C28	-2.82	100.12	114.37
14	A	602	HEA	C4C-C3C-C2C	-2.80	103.82	107.30
23	W	101	CHD	C6-C5-C4	-2.80	108.03	111.23
14	A	601	HEA	C3D-C4D-ND	2.80	113.06	110.35
20	P	303	PGV	O03-C19-O04	-2.79	116.64	123.63
14	A	602	HEA	C1A-CHA-C4D	-2.78	120.11	126.02
27	E	201	PSC	O01-C1-O02	-2.78	117.20	123.70
26	O	304	DMU	O61-C57-C4	2.78	120.78	111.33
26	P	307	DMU	O16-C6-C1	-2.77	104.06	108.27
23	J	101	CHD	C16-C17-C20	2.77	116.37	112.18
20	P	303	PGV	O01-C1-O02	-2.77	117.23	123.70
27	E	201	PSC	O01-C02-C03	2.75	118.19	108.34
26	M	101	DMU	C18-O16-C6	-2.74	109.00	113.68
19	D	201	TGL	OG1-CA1-OA1	-2.73	116.80	123.63
19	L	101	TGL	CA4-CA3-CA2	-2.73	103.11	113.13
14	N	601	HEA	C1C-CHC-C4B	-2.72	119.84	126.25
24	P	302	PEK	C03-C02-C01	-2.72	105.44	111.78
14	A	602	HEA	C2D-C1D-ND	2.72	112.97	109.84
26	C	307	DMU	O5-C4-C57	2.71	113.17	106.44
20	N	609	PGV	O03-C19-O04	-2.71	116.86	123.63
14	N	602	HEA	C3B-C4B-NB	2.69	112.94	109.84
20	A	608	PGV	O01-C1-O02	-2.68	117.44	123.70
14	N	601	HEA	CAA-C2A-C1A	2.66	130.26	124.85
23	W	101	CHD	C18-C13-C14	-2.66	107.04	111.20
23	P	301	CHD	C16-C17-C20	-2.66	108.16	112.18
25	C	305	CDL	OA8-CA6-CA4	2.65	116.05	108.40
25	P	305	CDL	OA6-CA4-CA3	2.64	117.82	108.34
14	N	602	HEA	C3C-C2C-C1C	-2.64	104.06	107.17
14	A	602	HEA	C3C-C4C-NC	2.64	112.02	109.80
14	N	602	HEA	CHD-C1D-C2D	-2.63	119.47	126.95
25	C	305	CDL	OA8-CA7-C31	2.63	119.84	111.83
14	A	602	HEA	CAD-C3D-C4D	2.63	129.28	124.70
14	N	601	HEA	C12-C11-C3B	2.62	116.22	112.12
20	N	608	PGV	O14-P-O13	2.62	121.03	110.83
14	N	601	HEA	CAA-CBA-CGA	-2.61	106.73	113.67
14	N	601	HEA	C17-C18-C19	-2.61	121.65	127.62
19	L	101	TGL	CG3-OG3-CC1	2.61	126.66	117.12
14	N	601	HEA	C13-C14-C15	-2.60	121.66	127.62
14	N	602	HEA	C27-C19-C20	2.60	119.75	115.23
23	P	301	CHD	C22-C23-C24	-2.59	105.59	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	307	DMU	O7-C3-C4	2.59	116.26	109.48
25	G	102	CDL	C39-C38-C37	2.59	127.44	114.37
26	W	102	DMU	O5-C4-C3	2.58	115.05	109.72
14	N	602	HEA	CHC-C1C-NC	2.57	128.51	123.86
14	N	602	HEA	C3C-C4C-NC	2.57	111.96	109.80
20	N	609	PGV	O01-C1-C2	2.57	117.03	111.48
19	Q	201	TGL	OG1-CA1-CA2	2.56	119.64	111.83
14	N	601	HEA	C26-C15-C16	2.56	119.67	115.23
26	W	102	DMU	O55-C2-C1	2.56	116.41	110.38
14	N	601	HEA	O1A-CGA-CBA	-2.55	115.02	123.09
19	N	607	TGL	OG3-CC1-CC2	2.54	119.59	111.83
25	T	103	CDL	OB6-CB5-OB7	-2.54	117.76	123.70
24	C	302	PEK	C25-C24-C23	-2.54	101.55	114.37
25	C	305	CDL	OA6-CA4-CA6	-2.54	99.25	108.34
26	P	307	DMU	O1-C9-C8	2.52	114.25	109.70
19	N	607	TGL	OG3-CC1-OC1	-2.51	117.35	123.63
19	A	607	TGL	OG1-CA1-OA1	-2.51	117.36	123.63
14	A	601	HEA	C4C-C3C-C2C	-2.51	104.19	107.30
26	P	307	DMU	O5-C6-C1	-2.49	105.24	110.37
14	A	602	HEA	O2D-CGD-O1D	2.48	129.71	123.33
14	A	602	HEA	C1D-ND-C4D	-2.48	102.27	105.21
14	N	602	HEA	C2B-C1B-NB	2.47	112.76	109.90
23	C	306	CHD	C1-C10-C5	2.47	111.30	107.75
23	C	306	CHD	C16-C17-C13	2.47	105.94	103.54
14	A	602	HEA	C13-C14-C15	-2.47	121.97	127.62
14	N	602	HEA	CMD-C2D-C1D	2.47	128.89	125.03
25	C	305	CDL	C74-C73-C72	-2.46	101.93	114.37
24	G	103	PEK	O03-C21-C22	2.46	119.33	111.83
24	C	302	PEK	C01-O03-C21	2.46	126.10	117.12
27	R	201	PSC	C21-C20-C19	-2.45	104.70	113.69
19	N	607	TGL	OG2-CG2-CG3	2.45	117.12	108.34
14	A	601	HEA	CHA-C1A-C2A	-2.45	121.00	124.86
14	A	601	HEA	C1B-C2B-C3B	-2.44	103.97	106.80
23	J	101	CHD	C1-C10-C5	2.44	111.25	107.75
25	C	305	CDL	OB4-PB2-OB3	2.44	123.79	112.44
23	P	306	CHD	C6-C5-C4	-2.43	108.44	111.23
26	W	102	DMU	C10-C5-C7	2.42	115.11	110.01
19	L	101	TGL	CG3-CG2-CG1	-2.42	106.14	111.78
23	O	302	CHD	C11-C9-C10	-2.41	111.26	113.70
25	P	305	CDL	OB4-PB2-OB3	2.39	123.58	112.44
14	A	602	HEA	C21-C20-C19	2.39	121.11	113.19
14	A	602	HEA	C16-C15-C14	-2.39	115.80	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	307	DMU	O16-C6-C1	2.39	111.90	108.27
25	G	102	CDL	C40-C39-C38	2.38	126.42	114.37
23	B	302	CHD	C22-C20-C17	2.38	115.27	110.33
23	B	302	CHD	C19-C10-C5	-2.38	106.45	110.44
25	P	305	CDL	C81-C80-C79	-2.38	102.33	114.37
25	T	103	CDL	C58-C57-C56	-2.38	102.36	114.37
25	G	102	CDL	CB6-CB4-CB3	-2.38	106.25	111.78
24	C	302	PEK	C23-C22-C21	-2.37	104.99	113.69
26	O	304	DMU	C18-O16-C6	2.37	117.73	113.68
14	A	601	HEA	CHA-C4D-C3D	-2.36	121.33	124.77
14	N	602	HEA	O1A-CGA-CBA	-2.36	115.61	123.09
20	C	303	PGV	C21-C20-C19	-2.35	105.09	113.69
20	C	303	PGV	O03-C01-C02	-2.33	101.67	108.40
25	G	102	CDL	C58-C57-C56	-2.32	102.62	114.37
23	B	302	CHD	O26-C24-C23	2.32	121.34	114.00
23	B	302	CHD	C9-C11-C12	-2.31	111.27	114.29
26	M	101	DMU	C10-O7-C3	-2.30	112.52	117.98
14	A	602	HEA	CAD-CBD-CGD	-2.30	107.58	113.67
20	P	303	PGV	C21-C20-C19	-2.29	105.28	113.69
23	O	302	CHD	C5-C4-C3	-2.29	109.25	112.71
14	N	601	HEA	C2B-C1B-NB	2.29	112.56	109.90
14	N	602	HEA	C2C-C1C-NC	2.29	113.82	110.14
23	P	301	CHD	C10-C9-C8	-2.29	109.28	111.84
25	P	305	CDL	C42-C41-C40	2.29	125.95	114.37
14	A	602	HEA	CHD-C4C-C3C	-2.29	117.43	127.37
26	C	307	DMU	O61-C57-C4	2.29	119.13	111.33
26	P	307	DMU	O5-C4-C57	2.29	112.11	106.44
20	P	303	PGV	C22-C21-C20	-2.29	104.72	113.13
14	A	602	HEA	CBD-CAD-C3D	2.28	118.85	112.53
19	A	607	TGL	CG3-CG2-CG1	-2.27	106.49	111.78
23	C	301	CHD	O12-C12-C13	-2.27	107.18	111.02
23	W	101	CHD	C4-C5-C10	2.27	115.08	112.66
19	L	101	TGL	CA3-CA2-CA1	-2.27	105.37	113.69
14	N	602	HEA	CHC-C4B-C3B	-2.27	120.08	125.80
26	W	102	DMU	O5-C6-C1	-2.27	105.71	110.37
23	P	301	CHD	C21-C20-C22	-2.26	106.83	110.34
24	T	101	PEK	C01-O03-C21	2.26	125.39	117.12
14	N	601	HEA	C3D-C4D-ND	2.26	112.54	110.35
14	A	602	HEA	CHD-C1D-C2D	-2.26	120.52	126.95
20	C	304	PGV	O04-C19-C20	-2.26	114.95	123.78
24	C	302	PEK	C3-C2-C1	-2.25	105.43	113.69
26	W	102	DMU	C8-C7-C5	2.25	114.78	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	301	CHD	C19-C10-C1	-2.25	104.73	108.31
25	C	305	CDL	C81-C80-C79	-2.24	103.03	114.37
20	P	303	PGV	O14-P-O13	2.24	122.87	112.44
23	J	101	CHD	C18-C13-C14	-2.24	107.69	111.20
14	A	601	HEA	CBD-CAD-C3D	-2.24	106.34	112.53
23	J	101	CHD	C23-C22-C20	-2.23	110.29	114.46
24	C	302	PEK	C32-C31-C30	-2.23	103.10	114.37
19	N	607	TGL	OG1-CA1-CA2	2.22	118.61	111.83
14	N	602	HEA	C4C-NC-C1C	-2.22	102.20	105.82
23	J	101	CHD	C21-C20-C17	-2.21	109.56	112.88
24	C	302	PEK	O02-C1-C2	2.21	132.42	123.78
23	J	101	CHD	C6-C5-C4	-2.21	108.70	111.23
26	P	307	DMU	O7-C10-C5	2.20	113.51	108.09
14	N	601	HEA	C3B-C4B-NB	2.19	112.36	109.84
19	N	607	TGL	CA3-CA2-CA1	-2.18	105.69	113.69
19	N	607	TGL	CG3-OG3-CC1	2.18	125.08	117.12
14	N	601	HEA	CHC-C4B-NB	2.18	127.06	124.37
20	A	609	PGV	C8-C9-C10	-2.18	103.40	113.86
14	N	602	HEA	CAA-C2A-C1A	2.18	129.28	124.85
23	P	301	CHD	C23-C22-C20	-2.17	110.40	114.46
14	A	602	HEA	C2C-C1C-NC	2.17	113.62	110.14
23	B	302	CHD	C5-C4-C3	-2.16	109.45	112.71
19	D	201	TGL	CB3-CB2-CB1	2.16	121.61	113.69
25	G	102	CDL	OA6-CA5-OA7	-2.15	118.68	123.70
27	E	201	PSC	C14-C13-C12	-2.15	108.76	124.83
14	N	601	HEA	CHC-C1C-C2C	-2.14	121.21	127.43
20	A	609	PGV	C01-O03-C19	2.14	124.93	117.12
14	N	601	HEA	CHD-C1D-C2D	-2.14	120.87	126.95
14	A	602	HEA	CMB-C2B-C3B	-2.14	126.14	130.28
25	G	102	CDL	O1-C1-CA2	-2.14	102.32	109.70
26	W	102	DMU	C2-C3-C4	-2.13	106.21	110.93
23	C	306	CHD	C19-C10-C1	-2.13	104.92	108.31
14	N	601	HEA	CAD-C3D-C2D	2.13	131.85	127.87
25	T	103	CDL	OA8-CA6-CA4	-2.13	102.26	108.40
25	T	103	CDL	CB6-CB4-CB3	-2.13	106.83	111.78
23	C	301	CHD	C17-C13-C14	2.12	102.24	100.11
14	A	602	HEA	O1A-CGA-CBA	-2.12	116.38	123.09
27	R	201	PSC	O13-P-O14	2.11	122.27	112.44
19	N	607	TGL	CG1-OG1-CA1	2.11	124.84	117.12
20	A	608	PGV	C7-C6-C5	-2.11	103.72	114.37
26	C	307	DMU	C18-O16-C6	2.11	117.28	113.68
27	R	201	PSC	O01-C1-O02	-2.10	118.80	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	304	PGV	O14-P-O13	2.10	122.21	112.44
20	C	303	PGV	O03-C19-O04	-2.10	118.38	123.63
26	W	102	DMU	O7-C3-C2	2.09	112.54	107.23
23	W	101	CHD	C19-C10-C5	-2.09	106.95	110.44
26	P	307	DMU	C8-C7-C5	-2.09	107.17	110.83
19	A	607	TGL	OG3-CC1-OC1	-2.08	118.42	123.63
14	A	602	HEA	CMB-C2B-C1B	2.08	128.29	125.03
20	A	609	PGV	O14-P-O13	2.08	122.13	112.44
20	A	609	PGV	O03-C19-O04	-2.08	118.42	123.63
20	N	608	PGV	O03-C01-C02	-2.08	102.40	108.40
23	B	302	CHD	C2-C1-C10	-2.07	109.24	112.74
25	T	103	CDL	PA1-OA5-CA3	2.07	133.22	121.35
23	B	302	CHD	C18-C13-C17	-2.07	107.96	111.20
14	N	601	HEA	CHC-C4B-C3B	-2.07	120.58	125.80
26	W	102	DMU	O7-C10-C5	2.06	113.17	108.09
20	C	304	PGV	O14-P-O13	2.06	122.04	112.44
25	G	102	CDL	PA1-OA5-CA3	2.06	133.16	121.35
14	N	602	HEA	CHC-C4B-NB	2.06	126.92	124.37
20	P	303	PGV	O03-C01-C02	-2.06	102.46	108.40
19	L	101	TGL	OG3-CG3-CG2	-2.06	102.47	108.40
25	T	103	CDL	O1-C1-CA2	-2.05	102.59	109.70
14	A	601	HEA	CHA-C1A-NA	2.05	126.69	124.45
19	O	303	TGL	OG2-CB1-OB1	-2.05	118.91	123.70
14	N	602	HEA	CHD-C4C-NC	2.05	127.58	123.86
23	P	306	CHD	C11-C9-C10	-2.04	111.63	113.70
20	P	304	PGV	O04-C19-C20	-2.04	115.80	123.78
19	O	303	TGL	CG3-CG2-CG1	-2.04	107.03	111.78
14	N	602	HEA	CBD-CAD-C3D	2.04	118.17	112.53
25	P	305	CDL	C55-C54-C53	-2.04	104.06	114.37
20	C	303	PGV	O01-C1-C2	2.04	115.89	111.48
23	O	302	CHD	C19-C10-C1	-2.04	105.07	108.31
24	T	101	PEK	C3-C2-C1	-2.03	106.24	113.69
25	C	305	CDL	OB6-CB5-OB7	-2.03	118.96	123.70
14	A	601	HEA	O2D-CGD-CBD	2.03	120.40	114.00
20	P	303	PGV	C27-C26-C25	-2.02	104.16	114.37
26	W	102	DMU	O55-C2-C3	2.02	115.11	109.94
24	P	302	PEK	O11-P-O14	-2.02	100.95	108.94
24	P	302	PEK	O03-C01-C02	-2.01	102.59	108.40
23	W	101	CHD	C1-C10-C9	-2.01	108.21	111.34
19	N	607	TGL	CC3-CC2-CC1	2.01	121.07	113.69
26	P	307	DMU	O1-C9-C11	2.01	111.41	106.44

There are no chirality outliers.

All (770) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	601	HEA	C2A-C3A-CMA-OMA
19	A	607	TGL	OG1-CG1-CG2-OG2
19	N	607	TGL	CB2-CB1-OG2-CG2
20	A	609	PGV	C03-O11-P-O12
20	A	609	PGV	C03-O11-P-O13
20	A	609	PGV	C04-O12-P-O11
20	A	609	PGV	C2-C1-O01-C02
20	A	609	PGV	O04-C19-O03-C01
20	A	609	PGV	C20-C19-O03-C01
20	C	304	PGV	C04-O12-P-O11
20	C	304	PGV	C04-O12-P-O13
20	N	608	PGV	C03-O11-P-O12
20	N	608	PGV	C03-O11-P-O13
20	N	608	PGV	C03-O11-P-O14
20	N	608	PGV	O02-C1-O01-C02
20	N	608	PGV	C2-C1-O01-C02
20	N	608	PGV	O04-C19-O03-C01
20	N	608	PGV	C20-C19-O03-C01
20	P	304	PGV	C04-O12-P-O11
20	P	304	PGV	C04-O12-P-O13
20	P	304	PGV	C2-C1-O01-C02
24	G	103	PEK	C11-C12-C13-C14
24	G	103	PEK	C12-C13-C14-C15
24	T	101	PEK	C04-O12-P-O11
24	T	101	PEK	C04-O12-P-O13
24	T	101	PEK	C5-C6-C7-C8
24	T	102	PEK	C03-O11-P-O12
24	T	102	PEK	C03-O11-P-O13
24	T	102	PEK	O03-C01-C02-O01
24	T	102	PEK	O12-C04-C05-N
24	T	102	PEK	O04-C21-O03-C01
24	T	102	PEK	C11-C10-C9-C8
25	C	305	CDL	CA3-OA5-PA1-OA2
25	C	305	CDL	C11-CA5-OA6-CA4
25	C	305	CDL	CB2-OB2-PB2-OB4
25	C	305	CDL	CB2-OB2-PB2-OB5
25	C	305	CDL	CB3-OB5-PB2-OB2
25	C	305	CDL	OB5-CB3-CB4-OB6
25	G	102	CDL	CA2-OA2-PA1-OA3
25	G	102	CDL	CA2-OA2-PA1-OA5
25	G	102	CDL	CA3-OA5-PA1-OA2
25	G	102	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
25	G	102	CDL	CB2-OB2-PB2-OB5
25	G	102	CDL	CB3-OB5-PB2-OB2
25	G	102	CDL	CB3-OB5-PB2-OB4
25	P	305	CDL	CA2-C1-CB2-OB2
25	P	305	CDL	CA2-OA2-PA1-OA4
25	P	305	CDL	CA2-OA2-PA1-OA5
25	P	305	CDL	CA3-OA5-PA1-OA2
25	P	305	CDL	C11-CA5-OA6-CA4
25	P	305	CDL	CB2-OB2-PB2-OB5
25	P	305	CDL	CB3-OB5-PB2-OB2
25	P	305	CDL	CB3-OB5-PB2-OB4
25	T	103	CDL	CA2-OA2-PA1-OA3
25	T	103	CDL	CA2-OA2-PA1-OA5
25	T	103	CDL	OA7-CA5-OA6-CA4
25	T	103	CDL	CB2-OB2-PB2-OB4
25	T	103	CDL	CB2-OB2-PB2-OB5
25	T	103	CDL	CB3-OB5-PB2-OB2
25	T	103	CDL	CB3-OB5-PB2-OB4
26	C	307	DMU	O5-C6-O16-C18
26	P	307	DMU	O5-C6-O16-C18
27	E	201	PSC	C03-O11-P-O12
27	E	201	PSC	C03-O11-P-O13
27	E	201	PSC	C04-O12-P-O11
27	E	201	PSC	C04-O12-P-O13
27	E	201	PSC	C04-O12-P-O14
27	E	201	PSC	O12-C04-C05-N
27	R	201	PSC	C04-O12-P-O11
27	R	201	PSC	C04-O12-P-O13
27	R	201	PSC	O12-C04-C05-N
25	C	305	CDL	OA9-CA7-OA8-CA6
25	G	102	CDL	OA9-CA7-OA8-CA6
20	C	304	PGV	C20-C19-O03-C01
25	C	305	CDL	C31-CA7-OA8-CA6
25	G	102	CDL	C31-CA7-OA8-CA6
20	C	304	PGV	O04-C19-O03-C01
20	A	609	PGV	O02-C1-O01-C02
20	P	304	PGV	O02-C1-O01-C02
25	C	305	CDL	OA7-CA5-OA6-CA4
25	P	305	CDL	OA7-CA5-OA6-CA4
27	E	201	PSC	O02-C1-O01-C02
19	Q	201	TGL	CC2-CC1-OG3-CG3
24	T	101	PEK	C22-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
26	O	304	DMU	O5-C4-C57-O61
25	T	103	CDL	C11-CA5-OA6-CA4
20	P	304	PGV	C20-C19-O03-C01
24	T	102	PEK	C22-C21-O03-C01
25	T	103	CDL	C31-CA7-OA8-CA6
20	C	303	PGV	C10-C11-C12-C13
20	C	304	PGV	C10-C11-C12-C13
24	T	101	PEK	C7-C8-C9-C10
24	T	101	PEK	C10-C11-C12-C13
24	T	102	PEK	C4-C5-C6-C7
20	P	304	PGV	O04-C19-O03-C01
24	T	101	PEK	O04-C21-O03-C01
25	T	103	CDL	OA9-CA7-OA8-CA6
19	N	607	TGL	OB1-CB1-OG2-CG2
20	A	609	PGV	O12-C04-C05-O05
25	C	305	CDL	O1-C1-CA2-OA2
25	C	305	CDL	O1-C1-CB2-OB2
25	P	305	CDL	O1-C1-CB2-OB2
24	G	103	PEK	C22-C21-O03-C01
19	Q	201	TGL	OC1-CC1-OG3-CG3
24	G	103	PEK	O04-C21-O03-C01
26	O	304	DMU	C3-C4-C57-O61
26	W	102	DMU	O5-C4-C57-O61
25	P	305	CDL	C51-CB5-OB6-CB4
27	E	201	PSC	C2-C1-O01-C02
25	C	305	CDL	C80-C81-C82-C83
19	L	101	TGL	CC1-CC2-CC3-CC4
26	P	307	DMU	O6-C11-C9-O1
23	P	306	CHD	C17-C20-C22-C23
19	D	201	TGL	CC2-CC1-OG3-CG3
25	P	305	CDL	C31-CA7-OA8-CA6
25	P	305	CDL	OA9-CA7-OA8-CA6
19	Q	201	TGL	CB9-C10-C11-C12
25	P	305	CDL	C20-C21-C22-C23
25	T	103	CDL	C60-C61-C62-C63
26	P	307	DMU	O5-C4-C57-O61
20	P	303	PGV	C10-C11-C12-C13
24	G	101	PEK	C13-C14-C15-C16
24	G	103	PEK	C4-C5-C6-C7
24	P	302	PEK	C4-C5-C6-C7
24	P	302	PEK	C10-C11-C12-C13
27	R	201	PSC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	OC1-CC1-OG3-CG3
23	P	306	CHD	C21-C20-C22-C23
24	G	101	PEK	O04-C21-O03-C01
20	A	609	PGV	O12-C04-C05-C06
25	C	305	CDL	CB2-C1-CA2-OA2
25	C	305	CDL	CA2-C1-CB2-OB2
25	P	305	CDL	CB2-C1-CA2-OA2
19	L	101	TGL	CA2-CA1-OG1-CG1
24	G	101	PEK	C22-C21-O03-C01
19	D	201	TGL	C13-C14-C29-C30
25	C	305	CDL	C37-C38-C39-C40
26	W	102	DMU	C3-C4-C57-O61
26	C	307	DMU	C3-C4-C57-O61
26	C	307	DMU	C1-C6-O16-C18
19	A	607	TGL	CA1-CA2-CA3-CA4
24	T	101	PEK	C1-C2-C3-C4
19	L	101	TGL	OA1-CA1-OG1-CG1
20	A	609	PGV	C4-C5-C6-C7
19	O	303	TGL	CB1-CB2-CB3-CB4
25	G	102	CDL	C37-C38-C39-C40
24	G	101	PEK	C10-C11-C12-C13
24	T	101	PEK	C13-C14-C15-C16
24	T	102	PEK	C13-C14-C15-C16
23	W	101	CHD	C13-C17-C20-C22
23	C	306	CHD	C17-C20-C22-C23
26	C	307	DMU	O5-C4-C57-O61
25	G	102	CDL	C55-C56-C57-C58
26	P	307	DMU	C3-C4-C57-O61
26	Z	101	DMU	C19-C22-C25-C28
19	D	201	TGL	CB1-CB2-CB3-CB4
19	O	303	TGL	CA1-CA2-CA3-CA4
20	A	609	PGV	C19-C20-C21-C22
24	G	101	PEK	C1-C2-C3-C4
23	C	306	CHD	C21-C20-C22-C23
19	N	607	TGL	CB1-CB2-CB3-CB4
19	Q	201	TGL	CB1-CB2-CB3-CB4
25	P	305	CDL	CB7-C71-C72-C73
27	R	201	PSC	C1-C2-C3-C4
19	Q	201	TGL	C13-C14-C29-C30
25	T	103	CDL	C40-C41-C42-C43
25	P	305	CDL	O1-C1-CA2-OA2
19	N	607	TGL	CA2-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
25	P	305	CDL	OB7-CB5-OB6-CB4
19	N	607	TGL	CC2-CC3-CC4-CC5
20	P	304	PGV	C10-C11-C12-C13
24	C	302	PEK	C13-C14-C15-C16
24	G	101	PEK	C4-C5-C6-C7
27	E	201	PSC	C11-C10-C9-C8
25	C	305	CDL	C51-CB5-OB6-CB4
19	N	607	TGL	OA1-CA1-OG1-CG1
26	C	307	DMU	O16-C18-C19-C22
19	A	607	TGL	CA9-C20-C21-C22
25	C	305	CDL	OB7-CB5-OB6-CB4
25	P	305	CDL	C38-C39-C40-C41
19	L	101	TGL	CC3-CC4-CC5-CC6
27	E	201	PSC	C04-C05-N-C06
27	E	201	PSC	C04-C05-N-C08
25	P	305	CDL	C60-C61-C62-C63
26	W	102	DMU	C1-C6-O16-C18
25	T	103	CDL	O1-C1-CB2-OB2
27	E	201	PSC	C03-C02-O01-C1
25	G	102	CDL	C15-C16-C17-C18
27	R	201	PSC	C22-C23-C24-C25
23	W	101	CHD	C16-C17-C20-C22
26	W	102	DMU	O5-C6-O16-C18
24	T	101	PEK	C34-C35-C36-C37
27	E	201	PSC	C04-C05-N-C07
23	J	101	CHD	C13-C17-C20-C22
19	D	201	TGL	C11-C10-CB9-CB8
20	C	304	PGV	C30-C31-C32-C33
19	O	303	TGL	C11-C12-C13-C14
25	P	305	CDL	C57-C58-C59-C60
24	T	102	PEK	C10-C11-C12-C13
19	L	101	TGL	CA3-CA4-CA5-CA6
19	Q	201	TGL	CA9-C20-C21-C22
25	G	102	CDL	C79-C80-C81-C82
26	O	304	DMU	O16-C18-C19-C22
20	C	304	PGV	O02-C1-O01-C02
19	Q	201	TGL	C16-C17-C18-C19
24	C	302	PEK	C26-C27-C28-C29
23	W	101	CHD	C13-C17-C20-C21
20	P	304	PGV	C1-C2-C3-C4
25	P	305	CDL	C73-C74-C75-C76
25	C	305	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
20	C	304	PGV	C2-C1-O01-C02
19	O	303	TGL	CA5-CA6-CA7-CA8
19	O	303	TGL	CA2-CA3-CA4-CA5
23	W	101	CHD	C16-C17-C20-C21
19	L	101	TGL	C23-C24-C25-C26
23	J	101	CHD	C13-C17-C20-C21
27	R	201	PSC	C29-C30-C31-C32
19	N	607	TGL	C12-C13-C14-C29
20	N	609	PGV	C30-C31-C32-C33
25	P	305	CDL	C82-C83-C84-C85
19	O	303	TGL	C12-C13-C14-C29
20	C	303	PGV	C7-C8-C9-C10
25	G	102	CDL	C20-C21-C22-C23
25	P	305	CDL	C41-C42-C43-C44
19	N	607	TGL	C22-C23-C24-C25
25	G	102	CDL	C77-C78-C79-C80
19	A	607	TGL	CB1-CB2-CB3-CB4
25	G	102	CDL	CB7-C71-C72-C73
20	N	608	PGV	C23-C24-C25-C26
25	C	305	CDL	C36-C37-C38-C39
26	M	101	DMU	C19-C22-C25-C28
25	P	305	CDL	C74-C75-C76-C77
19	A	607	TGL	CA5-CA6-CA7-CA8
25	T	103	CDL	C17-C18-C19-C20
19	L	101	TGL	CB2-CB3-CB4-CB5
19	L	101	TGL	CC2-CC3-CC4-CC5
19	N	607	TGL	CC5-CC6-CC7-CC8
19	N	607	TGL	CA9-C20-C21-C22
25	T	103	CDL	C57-C58-C59-C60
19	O	303	TGL	CB2-CB1-OG2-CG2
24	P	302	PEK	C7-C8-C9-C10
19	A	607	TGL	CB4-CB5-CB6-CB7
25	T	103	CDL	C82-C83-C84-C85
19	Q	201	TGL	C20-C21-C22-C23
19	Q	201	TGL	C21-C20-CA9-CA8
19	D	201	TGL	C23-C24-C25-C26
20	P	303	PGV	C13-C14-C15-C16
24	G	103	PEK	C25-C26-C27-C28
19	L	101	TGL	CA9-C20-C21-C22
20	N	608	PGV	C22-C23-C24-C25
20	P	303	PGV	C7-C8-C9-C10
19	Q	201	TGL	C17-C18-C19-C33

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Mol	Chain	Res	Type	Atoms
25	P	305	CDL	C71-C72-C73-C74
19	D	201	TGL	CC6-CC7-CC8-CC9
24	G	101	PEK	C25-C26-C27-C28
19	D	201	TGL	CA3-CA4-CA5-CA6
19	A	607	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	CB2-CB1-OG2-CG2
24	G	101	PEK	C2-C1-O01-C02
24	T	101	PEK	C2-C1-O01-C02
25	G	102	CDL	C51-CB5-OB6-CB4
25	T	103	CDL	C51-CB5-OB6-CB4
19	A	607	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	OB1-CB1-OG2-CG2
24	G	101	PEK	O02-C1-O01-C02
25	G	102	CDL	OB7-CB5-OB6-CB4
25	T	103	CDL	C55-C56-C57-C58
24	G	103	PEK	C15-C16-C17-C18
19	L	101	TGL	C25-C26-C27-C28
19	L	101	TGL	C19-C33-C34-C35
19	D	201	TGL	CC1-CC2-CC3-CC4
19	Q	201	TGL	CC1-CC2-CC3-CC4
19	Q	201	TGL	CC2-CC3-CC4-CC5
25	P	305	CDL	C76-C77-C78-C79
25	G	102	CDL	C56-C57-C58-C59
25	T	103	CDL	C79-C80-C81-C82
14	N	601	HEA	C26-C15-C16-C17
26	Z	101	DMU	C25-C28-C31-C34
19	O	303	TGL	CA9-C20-C21-C22
25	T	103	CDL	OB7-CB5-OB6-CB4
20	C	304	PGV	O01-C02-C03-O11
19	A	607	TGL	CA4-CA5-CA6-CA7
19	O	303	TGL	CB4-CB5-CB6-CB7
25	G	102	CDL	C11-CA5-OA6-CA4
19	A	607	TGL	C20-C21-C22-C23
19	L	101	TGL	C11-C12-C13-C14
26	P	307	DMU	O6-C11-C9-C8
25	P	305	CDL	C19-C20-C21-C22
19	O	303	TGL	OG1-CG1-CG2-OG2
19	Q	201	TGL	C11-C10-CB9-CB8
25	C	305	CDL	C61-C62-C63-C64
19	O	303	TGL	CA3-CA4-CA5-CA6
19	L	101	TGL	C11-C10-CB9-CB8
19	L	101	TGL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	N	607	TGL	CB5-CB6-CB7-CB8
19	O	303	TGL	C13-C14-C29-C30
25	C	305	CDL	C38-C39-C40-C41
26	W	102	DMU	C22-C25-C28-C31
19	O	303	TGL	OB1-CB1-OG2-CG2
24	T	101	PEK	O02-C1-O01-C02
20	P	303	PGV	C14-C15-C16-C17
25	G	102	CDL	C17-C18-C19-C20
25	T	103	CDL	C77-C78-C79-C80
27	E	201	PSC	C20-C21-C22-C23
24	T	101	PEK	C33-C34-C35-C36
25	T	103	CDL	C20-C21-C22-C23
25	T	103	CDL	C62-C63-C64-C65
27	R	201	PSC	C20-C19-O03-C01
24	P	302	PEK	C24-C25-C26-C27
24	T	101	PEK	C24-C25-C26-C27
24	P	302	PEK	C2-C3-C4-C5
24	T	102	PEK	C15-C16-C17-C18
20	N	608	PGV	C01-C02-C03-O11
19	Q	201	TGL	C18-C19-C33-C34
24	G	101	PEK	C22-C23-C24-C25
25	G	102	CDL	C43-C44-C45-C46
24	C	302	PEK	O04-C21-O03-C01
19	D	201	TGL	CA2-CA3-CA4-CA5
23	J	101	CHD	C16-C17-C20-C21
25	C	305	CDL	C41-C42-C43-C44
25	T	103	CDL	C56-C57-C58-C59
25	G	102	CDL	C13-C14-C15-C16
25	G	102	CDL	OA7-CA5-OA6-CA4
24	C	302	PEK	C10-C11-C12-C13
24	P	302	PEK	C13-C14-C15-C16
19	A	607	TGL	OG1-CG1-CG2-CG3
19	D	201	TGL	CG1-CG2-CG3-OG3
19	N	607	TGL	OG1-CG1-CG2-CG3
24	G	103	PEK	O03-C01-C02-C03
24	T	102	PEK	O03-C01-C02-C03
25	T	103	CDL	CA3-CA4-CA6-OA8
24	P	302	PEK	C15-C16-C17-C18
19	A	607	TGL	CB3-CB4-CB5-CB6
19	L	101	TGL	C12-C13-C14-C29
24	T	102	PEK	C30-C31-C32-C33
25	G	102	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	CA6-CA7-CA8-CA9
19	O	303	TGL	C15-C16-C17-C18
21	C	308	EDO	O1-C1-C2-O2
19	L	101	TGL	C18-C19-C33-C34
19	D	201	TGL	C21-C20-CA9-CA8
25	P	305	CDL	C59-C60-C61-C62
19	L	101	TGL	C22-C23-C24-C25
19	L	101	TGL	CC4-CC5-CC6-CC7
19	Q	201	TGL	CA6-CA7-CA8-CA9
26	Z	101	DMU	C18-C19-C22-C25
24	C	302	PEK	C22-C21-O03-C01
19	L	101	TGL	CG3-CG2-OG2-CB1
20	C	304	PGV	C11-C10-C9-C8
20	A	608	PGV	C29-C30-C31-C32
20	N	609	PGV	C29-C30-C31-C32
14	A	601	HEA	C2A-C3A-CMA-OMA
24	P	302	PEK	C27-C28-C29-C30
27	E	201	PSC	C1-C2-C3-C4
24	C	302	PEK	C4-C5-C6-C7
24	G	103	PEK	C13-C14-C15-C16
19	L	101	TGL	CA2-CA3-CA4-CA5
19	N	607	TGL	CA5-CA6-CA7-CA8
19	N	607	TGL	C11-C12-C13-C14
19	A	607	TGL	CA6-CA7-CA8-CA9
19	O	303	TGL	CC7-CC8-CC9-C15
20	A	608	PGV	C7-C8-C9-C10
25	T	103	CDL	C39-C40-C41-C42
26	O	304	DMU	C34-C37-C40-C43
19	O	303	TGL	CB3-CB4-CB5-CB6
19	N	607	TGL	C29-C30-C31-C32
20	P	303	PGV	C15-C16-C17-C18
25	P	305	CDL	C37-C38-C39-C40
19	L	101	TGL	OG1-CA1-CA2-CA3
25	T	103	CDL	C32-C31-CA7-OA8
25	P	305	CDL	C39-C40-C41-C42
25	T	103	CDL	C32-C33-C34-C35
25	T	103	CDL	C58-C59-C60-C61
19	D	201	TGL	C17-C18-C19-C33
19	O	303	TGL	C16-C17-C18-C19
25	T	103	CDL	C24-C25-C26-C27
19	A	607	TGL	CC2-CC1-OG3-CG3
19	O	303	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
25	G	102	CDL	C19-C20-C21-C22
25	G	102	CDL	C82-C83-C84-C85
27	E	201	PSC	C28-C29-C30-C31
24	T	101	PEK	C4-C5-C6-C7
25	T	103	CDL	C80-C81-C82-C83
24	C	302	PEK	C25-C26-C27-C28
24	G	103	PEK	C16-C17-C18-C19
24	P	302	PEK	C3-C4-C5-C6
25	C	305	CDL	C57-C58-C59-C60
25	G	102	CDL	C53-C54-C55-C56
20	A	609	PGV	C02-C03-O11-P
27	E	201	PSC	O01-C1-C2-C3
19	D	201	TGL	CB2-CB3-CB4-CB5
23	C	306	CHD	C20-C22-C23-C24
26	O	304	DMU	C1-C6-O16-C18
25	G	102	CDL	C58-C59-C60-C61
25	P	305	CDL	C58-C59-C60-C61
20	C	304	PGV	C01-C02-C03-O11
24	T	101	PEK	C01-C02-C03-O11
25	C	305	CDL	OA5-CA3-CA4-CA6
19	N	607	TGL	OG1-CA1-CA2-CA3
25	C	305	CDL	CA5-C11-C12-C13
27	R	201	PSC	C11-C10-C9-C8
19	N	607	TGL	C11-C10-CB9-CB8
27	R	201	PSC	O04-C19-O03-C01
20	A	608	PGV	C26-C27-C28-C29
19	Q	201	TGL	CB5-CB6-CB7-CB8
19	O	303	TGL	OG1-CG1-CG2-CG3
20	A	609	PGV	O03-C01-C02-C03
25	G	102	CDL	CA3-CA4-CA6-OA8
25	P	305	CDL	C75-C76-C77-C78
20	A	608	PGV	C31-C32-C33-C34
25	C	305	CDL	C63-C64-C65-C66
25	C	305	CDL	C58-C59-C60-C61
25	C	305	CDL	OA5-CA3-CA4-OA6
25	T	103	CDL	OA5-CA3-CA4-OA6
24	G	101	PEK	C31-C32-C33-C34
20	P	303	PGV	C02-C03-O11-P
25	P	305	CDL	CA4-CA3-OA5-PA1
24	P	302	PEK	C16-C17-C18-C19
24	T	101	PEK	C29-C30-C31-C32
19	A	607	TGL	C18-C19-C33-C34

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	OG2-CG2-CG3-OG3
20	A	609	PGV	O03-C01-C02-O01
24	G	103	PEK	O03-C01-C02-O01
25	G	102	CDL	OA6-CA4-CA6-OA8
25	P	305	CDL	OA6-CA4-CA6-OA8
25	T	103	CDL	OB6-CB4-CB6-OB8
24	C	302	PEK	C9-C10-C11-C12
24	G	101	PEK	C5-C6-C7-C8
24	G	101	PEK	C6-C7-C8-C9
24	G	101	PEK	C11-C10-C9-C8
24	G	101	PEK	C9-C10-C11-C12
24	G	101	PEK	C11-C12-C13-C14
24	G	101	PEK	C12-C13-C14-C15
24	G	103	PEK	C5-C6-C7-C8
24	G	103	PEK	C6-C7-C8-C9
24	G	103	PEK	C11-C10-C9-C8
24	G	103	PEK	C9-C10-C11-C12
24	P	302	PEK	C9-C10-C11-C12
24	T	101	PEK	C6-C7-C8-C9
24	T	101	PEK	C11-C10-C9-C8
24	T	101	PEK	C9-C10-C11-C12
24	T	101	PEK	C11-C12-C13-C14
24	T	102	PEK	C5-C6-C7-C8
24	T	102	PEK	C9-C10-C11-C12
24	T	102	PEK	C11-C12-C13-C14
24	T	102	PEK	C12-C13-C14-C15
27	E	201	PSC	C9-C10-C11-C12
27	E	201	PSC	C10-C11-C12-C13
27	R	201	PSC	C9-C10-C11-C12
27	R	201	PSC	C10-C11-C12-C13
24	G	103	PEK	C33-C34-C35-C36
20	P	304	PGV	C3-C4-C5-C6
19	Q	201	TGL	C12-C13-C14-C29
25	C	305	CDL	C59-C60-C61-C62
19	N	607	TGL	C19-C33-C34-C35
26	P	307	DMU	C22-C25-C28-C31
25	C	305	CDL	C60-C61-C62-C63
27	E	201	PSC	C21-C22-C23-C24
19	A	607	TGL	C16-C17-C18-C19
24	T	101	PEK	C22-C23-C24-C25
19	N	607	TGL	CC4-CC5-CC6-CC7
19	N	607	TGL	CB4-CB5-CB6-CB7

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Mol	Chain	Res	Type	Atoms
19	O	303	TGL	C11-C10-CB9-CB8
19	L	101	TGL	CB5-CB6-CB7-CB8
19	Q	201	TGL	C15-C16-C17-C18
27	E	201	PSC	C20-C19-O03-C01
19	D	201	TGL	CA5-CA6-CA7-CA8
19	O	303	TGL	CB6-CB7-CB8-CB9
19	A	607	TGL	CA2-CA3-CA4-CA5
20	N	609	PGV	C5-C6-C7-C8
26	M	101	DMU	C28-C31-C34-C37
27	E	201	PSC	C24-C25-C26-C27
20	A	609	PGV	C01-C02-C03-O11
24	G	101	PEK	C01-C02-C03-O11
25	C	305	CDL	OB5-CB3-CB4-CB6
25	P	305	CDL	OA5-CA3-CA4-CA6
27	E	201	PSC	C27-C28-C29-C30
24	G	103	PEK	C30-C31-C32-C33
24	C	302	PEK	C28-C29-C30-C31
25	G	102	CDL	C76-C77-C78-C79
19	A	607	TGL	C21-C20-CA9-CA8
19	A	607	TGL	OC1-CC1-OG3-CG3
20	P	304	PGV	C30-C31-C32-C33
19	O	303	TGL	OC1-CC1-OG3-CG3
19	O	303	TGL	C20-C21-C22-C23
26	M	101	DMU	O6-C11-C9-C8
20	N	608	PGV	O01-C02-C03-O11
24	G	101	PEK	O01-C02-C03-O11
24	T	101	PEK	O01-C02-C03-O11
25	C	305	CDL	C43-C44-C45-C46
19	Q	201	TGL	C23-C24-C25-C26
25	C	305	CDL	C14-C15-C16-C17
19	N	607	TGL	C17-C18-C19-C33
24	G	103	PEK	C7-C8-C9-C10
19	A	607	TGL	OG2-CG2-CG3-OG3
19	L	101	TGL	OG1-CG1-CG2-OG2
19	N	607	TGL	OG1-CG1-CG2-OG2
19	O	303	TGL	OG2-CG2-CG3-OG3
19	Q	201	TGL	OG2-CG2-CG3-OG3
25	G	102	CDL	OB6-CB4-CB6-OB8
25	T	103	CDL	OA6-CA4-CA6-OA8
26	Z	101	DMU	O6-C11-C9-O1
19	A	607	TGL	C11-C10-CB9-CB8
19	N	607	TGL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	O	303	TGL	CA6-CA7-CA8-CA9
26	Z	101	DMU	C34-C37-C40-C43
25	G	102	CDL	C39-C40-C41-C42
26	P	307	DMU	C25-C28-C31-C34
20	A	608	PGV	C5-C6-C7-C8
25	G	102	CDL	C74-C75-C76-C77
24	T	102	PEK	C31-C32-C33-C34
25	T	103	CDL	C22-C23-C24-C25
14	N	601	HEA	C14-C15-C16-C17
24	C	302	PEK	C2-C3-C4-C5
25	G	102	CDL	C40-C41-C42-C43
25	P	305	CDL	C63-C64-C65-C66
19	A	607	TGL	C13-C14-C29-C30
24	T	102	PEK	C22-C23-C24-C25
19	N	607	TGL	C18-C19-C33-C34
25	P	305	CDL	C36-C37-C38-C39
25	T	103	CDL	C1-CB2-OB2-PB2
20	P	304	PGV	C26-C27-C28-C29
26	M	101	DMU	C25-C28-C31-C34
25	P	305	CDL	OA5-CA3-CA4-OA6
27	R	201	PSC	C20-C21-C22-C23
27	R	201	PSC	C04-C05-N-C06
14	N	601	HEA	C4A-C3A-CMA-OMA
25	P	305	CDL	OB6-CB4-CB6-OB8
20	A	609	PGV	C10-C11-C12-C13
19	A	607	TGL	CG1-CG2-CG3-OG3
19	L	101	TGL	OG1-CG1-CG2-CG3
19	O	303	TGL	CG1-CG2-CG3-OG3
19	Q	201	TGL	CG1-CG2-CG3-OG3
24	T	101	PEK	O03-C01-C02-C03
25	G	102	CDL	C32-C31-CA7-OA8
19	D	201	TGL	CB9-C10-C11-C12
25	P	305	CDL	C78-C79-C80-C81
27	E	201	PSC	C26-C27-C28-C29
20	N	608	PGV	C19-C20-C21-C22
27	E	201	PSC	O04-C19-O03-C01
25	G	102	CDL	CA5-C11-C12-C13
24	G	103	PEK	C31-C32-C33-C34
20	A	609	PGV	C03-O11-P-O14
20	A	609	PGV	C04-O12-P-O13
20	C	304	PGV	C04-O12-P-O14
20	P	304	PGV	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
24	G	103	PEK	C03-O11-P-O12
24	T	101	PEK	C03-O11-P-O12
24	T	101	PEK	C03-O11-P-O13
24	T	101	PEK	C04-O12-P-O14
24	T	102	PEK	C03-O11-P-O14
25	C	305	CDL	CA3-OA5-PA1-OA3
25	C	305	CDL	CB2-OB2-PB2-OB3
25	C	305	CDL	CB3-OB5-PB2-OB3
25	G	102	CDL	CA2-OA2-PA1-OA4
25	G	102	CDL	CA3-OA5-PA1-OA3
25	P	305	CDL	CA3-OA5-PA1-OA3
25	P	305	CDL	CB2-OB2-PB2-OB3
25	T	103	CDL	CA2-OA2-PA1-OA4
25	T	103	CDL	CA3-OA5-PA1-OA3
25	P	305	CDL	C34-C35-C36-C37
20	N	608	PGV	C5-C6-C7-C8
20	C	303	PGV	C02-C03-O11-P
20	N	608	PGV	C02-C03-O11-P
25	C	305	CDL	CA4-CA3-OA5-PA1
25	C	305	CDL	CB7-C71-C72-C73
19	D	201	TGL	C20-C21-C22-C23
27	R	201	PSC	C12-C13-C14-C15
25	T	103	CDL	CB7-C71-C72-C73
25	C	305	CDL	C15-C16-C17-C18
19	N	607	TGL	CG1-CG2-OG2-CB1
25	G	102	CDL	C54-C55-C56-C57
19	N	607	TGL	C25-C26-C27-C28
19	A	607	TGL	CB7-CB8-CB9-C10
20	C	303	PGV	C9-C10-C11-C12
20	A	609	PGV	O01-C02-C03-O11
19	O	303	TGL	C21-C22-C23-C24
24	T	102	PEK	O02-C1-O01-C02
25	G	102	CDL	C1-CB2-OB2-PB2
25	P	305	CDL	C16-C17-C18-C19
25	P	305	CDL	C32-C31-CA7-OA8
27	R	201	PSC	O01-C1-C2-C3
20	N	608	PGV	C10-C11-C12-C13
20	N	609	PGV	C10-C11-C12-C13
19	L	101	TGL	CB4-CB5-CB6-CB7
25	G	102	CDL	C44-C45-C46-C47
25	G	102	CDL	CB3-CB4-CB6-OB8
24	G	101	PEK	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
25	G	102	CDL	C80-C81-C82-C83
20	P	303	PGV	C9-C10-C11-C12
19	N	607	TGL	CG2-CG1-OG1-CA1
21	P	308	EDO	O1-C1-C2-O2
19	L	101	TGL	OA1-CA1-CA2-CA3
25	T	103	CDL	CA2-C1-CB2-OB2
25	C	305	CDL	C56-C57-C58-C59
25	P	305	CDL	C17-C18-C19-C20
25	P	305	CDL	C80-C81-C82-C83
20	C	304	PGV	C3-C4-C5-C6
26	C	307	DMU	C2-C3-O7-C10
19	A	607	TGL	CC7-CC8-CC9-C15
19	D	201	TGL	CA7-CA8-CA9-C20
26	M	101	DMU	C22-C25-C28-C31
24	T	101	PEK	O03-C01-C02-O01
25	C	305	CDL	OB6-CB4-CB6-OB8
24	P	302	PEK	C22-C23-C24-C25
25	G	102	CDL	C57-C58-C59-C60
25	C	305	CDL	C23-C24-C25-C26
27	R	201	PSC	C2-C3-C4-C5
19	N	607	TGL	OA1-CA1-CA2-CA3
20	N	609	PGV	C7-C8-C9-C10
19	D	201	TGL	C15-C16-C17-C18
19	D	201	TGL	C12-C13-C14-C29
19	L	101	TGL	CA7-CA8-CA9-C20
14	A	601	HEA	C26-C15-C16-C17
25	C	305	CDL	C82-C83-C84-C85
23	O	302	CHD	C22-C23-C24-O25
23	W	101	CHD	C22-C23-C24-O26
20	C	303	PGV	C13-C14-C15-C16
23	B	302	CHD	C22-C23-C24-O25
25	C	305	CDL	C53-C54-C55-C56
14	A	602	HEA	CAD-CBD-CGD-O1D
14	A	602	HEA	CAA-CBA-CGA-O1A
20	P	304	PGV	C02-C03-O11-P
25	T	103	CDL	CB4-CB3-OB5-PB2
24	C	302	PEK	C7-C8-C9-C10
19	O	303	TGL	CC2-CC3-CC4-CC5
24	T	101	PEK	C27-C28-C29-C30
25	C	305	CDL	C72-C73-C74-C75
19	D	201	TGL	CA9-C20-C21-C22
23	J	101	CHD	C22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
25	T	103	CDL	OA5-CA3-CA4-CA6
23	O	302	CHD	C22-C23-C24-O26
20	C	303	PGV	C31-C32-C33-C34
23	W	101	CHD	C22-C23-C24-O25
24	C	302	PEK	C5-C6-C7-C8
24	P	302	PEK	C5-C6-C7-C8
24	T	101	PEK	C12-C13-C14-C15
25	T	103	CDL	C43-C44-C45-C46
14	N	602	HEA	CAA-CBA-CGA-O1A
19	N	607	TGL	CC6-CC7-CC8-CC9
14	N	602	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAD-CBD-CGD-O2D
19	O	303	TGL	CA4-CA5-CA6-CA7
14	A	601	HEA	CAD-CBD-CGD-O1D
19	O	303	TGL	C17-C18-C19-C33
27	E	201	PSC	C2-C3-C4-C5
14	N	601	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAA-CBA-CGA-O2A
14	A	602	HEA	C26-C15-C16-C17
14	N	601	HEA	CAD-CBD-CGD-O2D
24	G	101	PEK	C23-C24-C25-C26
14	A	601	HEA	CAD-CBD-CGD-O2D
19	A	607	TGL	C15-C16-C17-C18
25	P	305	CDL	CB3-CB4-CB6-OB8
14	A	602	HEA	CAA-CBA-CGA-O2A
23	B	302	CHD	C22-C23-C24-O26
19	A	607	TGL	C21-C22-C23-C24
25	C	305	CDL	C34-C35-C36-C37
26	P	307	DMU	O16-C18-C19-C22
21	Q	202	EDO	O1-C1-C2-O2
24	C	302	PEK	C14-C15-C16-C17
24	T	102	PEK	C3-C4-C5-C6
27	R	201	PSC	C7-C8-C9-C10
20	N	609	PGV	O03-C19-C20-C21
23	J	101	CHD	C22-C23-C24-O26
19	D	201	TGL	C33-C34-C35-C36
14	A	602	HEA	CAD-CBD-CGD-O2D
25	P	305	CDL	C43-C44-C45-C46
25	G	102	CDL	C32-C31-CA7-OA9
20	N	609	PGV	C9-C10-C11-C12
24	G	103	PEK	C3-C4-C5-C6
27	E	201	PSC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	C19-C33-C34-C35
19	L	101	TGL	OG2-CB1-CB2-CB3
19	Q	201	TGL	CC6-CC7-CC8-CC9
23	P	301	CHD	C22-C23-C24-O25
24	P	302	PEK	C22-C21-O03-C01
25	T	103	CDL	C54-C55-C56-C57
24	G	101	PEK	C03-O11-P-O13
19	N	607	TGL	OG2-CB1-CB2-CB3
20	A	608	PGV	C9-C10-C11-C12
25	P	305	CDL	C72-C73-C74-C75
26	P	307	DMU	C1-C6-O16-C18
20	N	608	PGV	C9-C10-C11-C12
23	C	301	CHD	C22-C23-C24-O25
19	A	607	TGL	CA3-CA4-CA5-CA6
24	G	101	PEK	C3-C4-C5-C6
24	T	101	PEK	C3-C4-C5-C6
27	R	201	PSC	C5-C6-C7-C8
25	T	103	CDL	C53-C54-C55-C56
25	C	305	CDL	CB3-CB4-CB6-OB8
25	T	103	CDL	CB3-CB4-CB6-OB8
19	A	607	TGL	CC5-CC6-CC7-CC8
19	A	607	TGL	CC3-CC4-CC5-CC6
26	O	304	DMU	C31-C34-C37-C40
14	A	601	HEA	C14-C15-C16-C17
27	E	201	PSC	C05-C04-O12-P
27	R	201	PSC	C05-C04-O12-P
26	P	307	DMU	C5-C10-O7-C3
21	N	614	EDO	O1-C1-C2-O2
20	N	609	PGV	C11-C12-C13-C14
24	G	103	PEK	C14-C15-C16-C17
19	D	201	TGL	OG2-CB1-CB2-CB3
27	E	201	PSC	O02-C1-C2-C3
24	T	102	PEK	C2-C1-O01-C02
20	C	304	PGV	C9-C10-C11-C12
20	N	608	PGV	C11-C12-C13-C14
25	P	305	CDL	C32-C31-CA7-OA9
25	G	102	CDL	CB4-CB3-OB5-PB2
19	D	201	TGL	C16-C17-C18-C19
27	E	201	PSC	C7-C8-C9-C10
24	P	302	PEK	O04-C21-O03-C01
25	P	305	CDL	C21-C22-C23-C24
19	D	201	TGL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
20	P	303	PGV	C24-C25-C26-C27
24	P	302	PEK	O03-C21-C22-C23
25	G	102	CDL	C62-C63-C64-C65
25	P	305	CDL	C23-C24-C25-C26
19	N	607	TGL	C10-C11-C12-C13
20	P	304	PGV	C14-C15-C16-C17
24	P	302	PEK	O01-C1-C2-C3
24	T	101	PEK	C26-C27-C28-C29
27	E	201	PSC	C23-C24-C25-C26
20	N	608	PGV	O03-C19-C20-C21
24	G	101	PEK	O01-C1-C2-C3
20	C	304	PGV	C31-C32-C33-C34
19	Q	201	TGL	C16-C15-CC9-CC8
25	P	305	CDL	C14-C15-C16-C17
24	T	102	PEK	C26-C27-C28-C29
19	O	303	TGL	C21-C20-CA9-CA8
24	T	101	PEK	O01-C1-C2-C3
20	N	608	PGV	C11-C10-C9-C8
24	T	102	PEK	C33-C34-C35-C36
19	N	607	TGL	CB3-CB4-CB5-CB6
25	T	103	CDL	C32-C31-CA7-OA9
25	G	102	CDL	C11-C12-C13-C14
25	P	305	CDL	CA3-CA4-OA6-CA5
27	R	201	PSC	C04-C05-N-C07
20	P	304	PGV	O12-C04-C05-O05
25	P	305	CDL	C61-C62-C63-C64
19	O	303	TGL	OG1-CA1-CA2-CA3
20	P	304	PGV	C15-C16-C17-C18
19	A	607	TGL	OG1-CA1-CA2-CA3
20	P	304	PGV	C28-C29-C30-C31
23	C	306	CHD	C22-C23-C24-O25
23	P	301	CHD	C22-C23-C24-O26
24	P	302	PEK	O04-C21-C22-C23
27	E	201	PSC	C19-C20-C21-C22
24	G	101	PEK	O02-C1-C2-C3
27	R	201	PSC	C04-C05-N-C08
20	P	303	PGV	C31-C32-C33-C34
19	L	101	TGL	C24-C25-C26-C27
19	O	303	TGL	C22-C23-C24-C25
20	N	608	PGV	O04-C19-C20-C21
26	M	101	DMU	O6-C11-C9-O1
14	N	601	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	R	201	PSC	O02-C1-C2-C3
20	A	608	PGV	O03-C19-C20-C21
20	A	608	PGV	C11-C12-C13-C14
24	T	101	PEK	C14-C15-C16-C17
24	T	101	PEK	O02-C1-C2-C3
19	Q	201	TGL	OG1-CA1-CA2-CA3
19	Q	201	TGL	OG2-CB1-CB2-CB3
14	A	601	HEA	CAA-CBA-CGA-O2A
21	Q	203	EDO	O1-C1-C2-O2
19	D	201	TGL	OG3-CC1-CC2-CC3
14	A	601	HEA	CAA-CBA-CGA-O1A
24	P	302	PEK	O02-C1-C2-C3
20	P	304	PGV	O01-C1-C2-C3
19	A	607	TGL	OA1-CA1-CA2-CA3

There are no ring outliers.

44 monomers are involved in 216 short contacts:

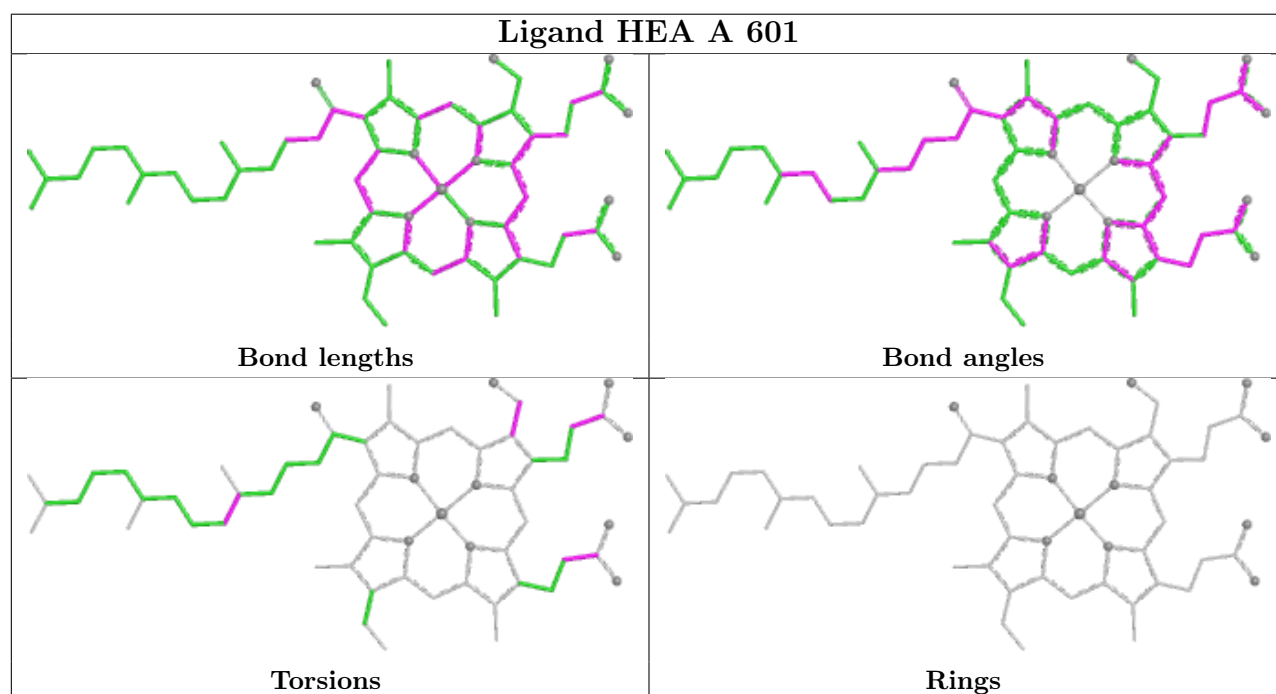
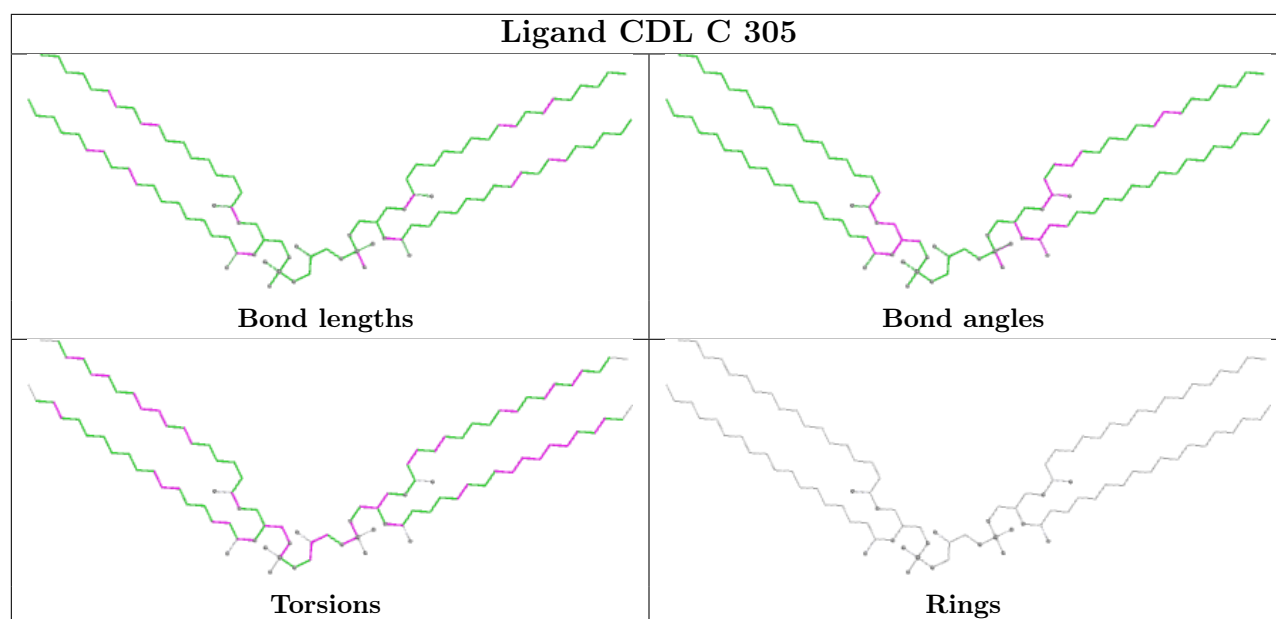
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	305	CDL	15	0
14	A	601	HEA	3	0
20	C	303	PGV	5	0
24	C	302	PEK	6	0
24	P	302	PEK	6	0
24	T	101	PEK	4	0
25	T	103	CDL	14	0
26	W	102	DMU	4	0
27	E	201	PSC	12	0
21	A	613	EDO	1	0
23	C	301	CHD	1	0
19	Q	201	TGL	9	0
23	J	101	CHD	2	0
26	M	101	DMU	1	0
27	R	201	PSC	10	0
14	N	602	HEA	2	0
20	A	609	PGV	4	0
23	P	306	CHD	1	0
21	N	614	EDO	1	0
25	G	102	CDL	23	0
23	C	306	CHD	2	0
26	C	307	DMU	2	0
26	Z	101	DMU	1	0

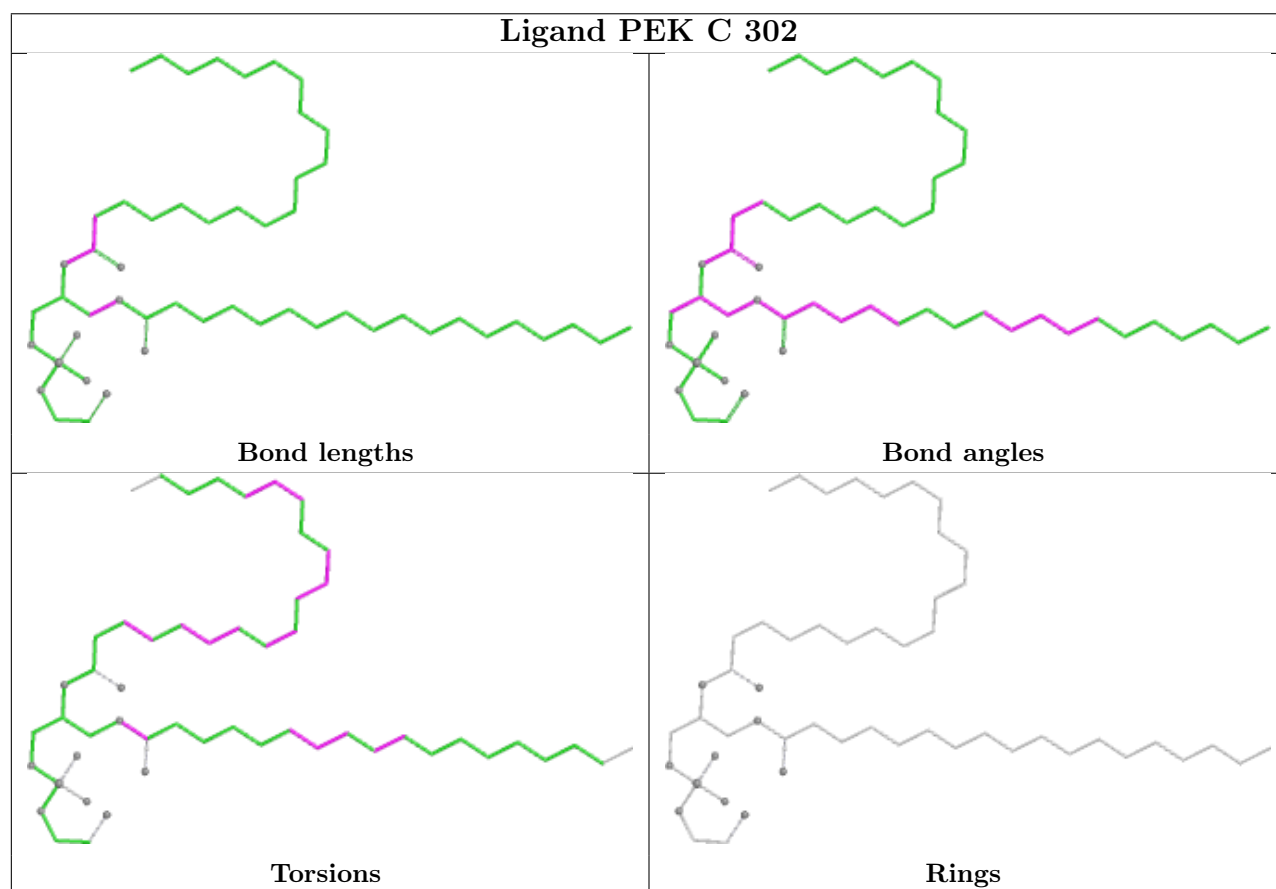
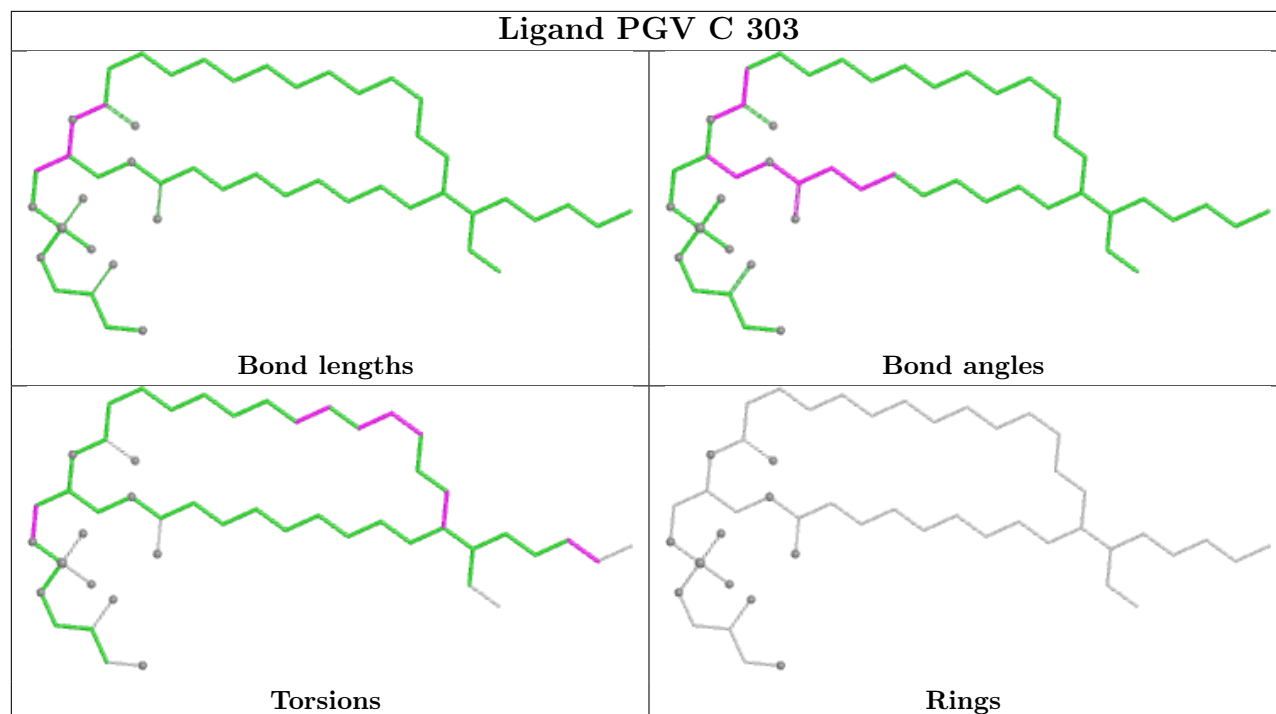
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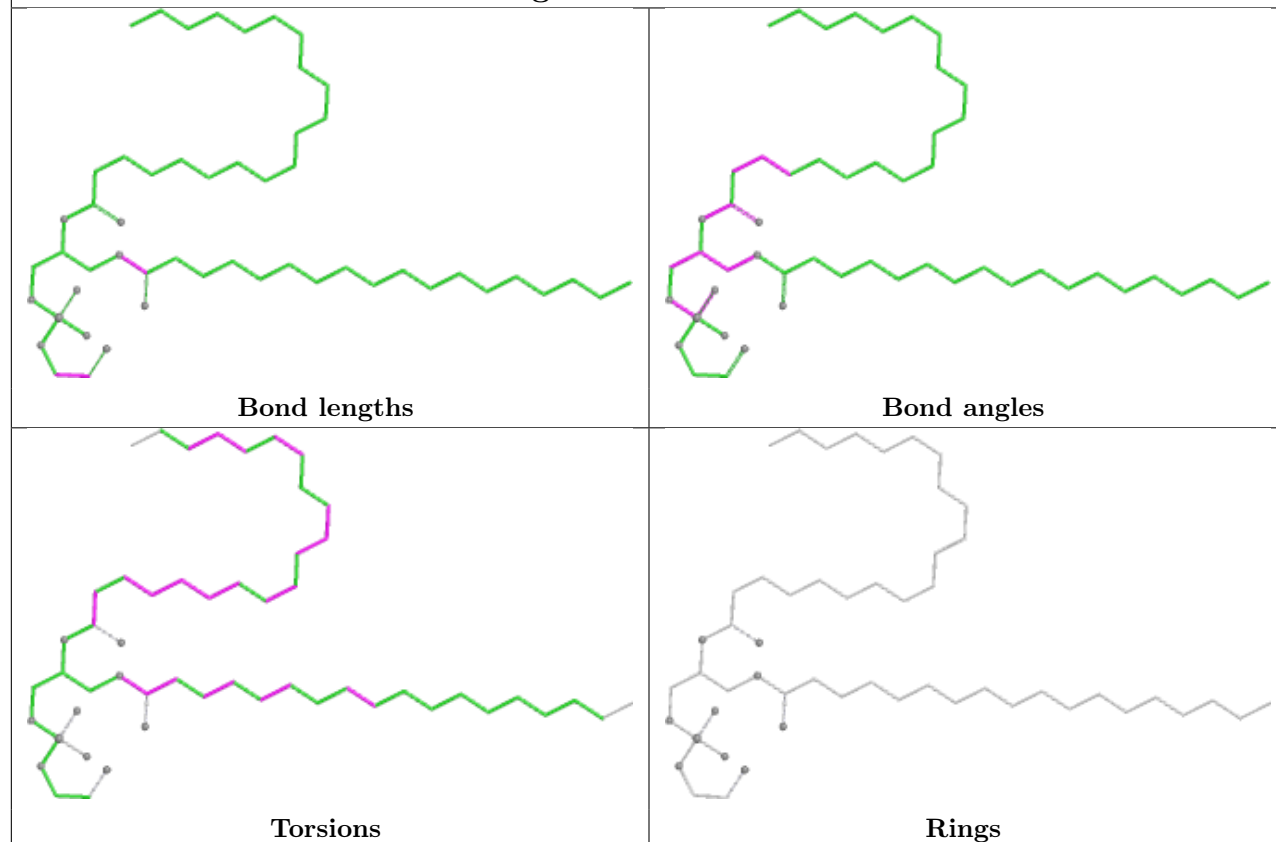
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	304	PGV	4	0
24	G	101	PEK	1	0
14	N	601	HEA	3	0
23	O	302	CHD	2	0
26	O	304	DMU	1	0
26	P	307	DMU	8	0
21	N	615	EDO	1	0
19	A	607	TGL	3	0
25	P	305	CDL	19	0
14	A	602	HEA	2	0
21	P	308	EDO	1	0
19	L	101	TGL	8	0
20	N	608	PGV	5	0
20	P	303	PGV	3	0
20	P	304	PGV	3	0
23	W	101	CHD	1	0
24	G	103	PEK	4	0
19	D	201	TGL	8	0
23	B	302	CHD	1	0
19	N	607	TGL	8	0
24	T	102	PEK	6	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.

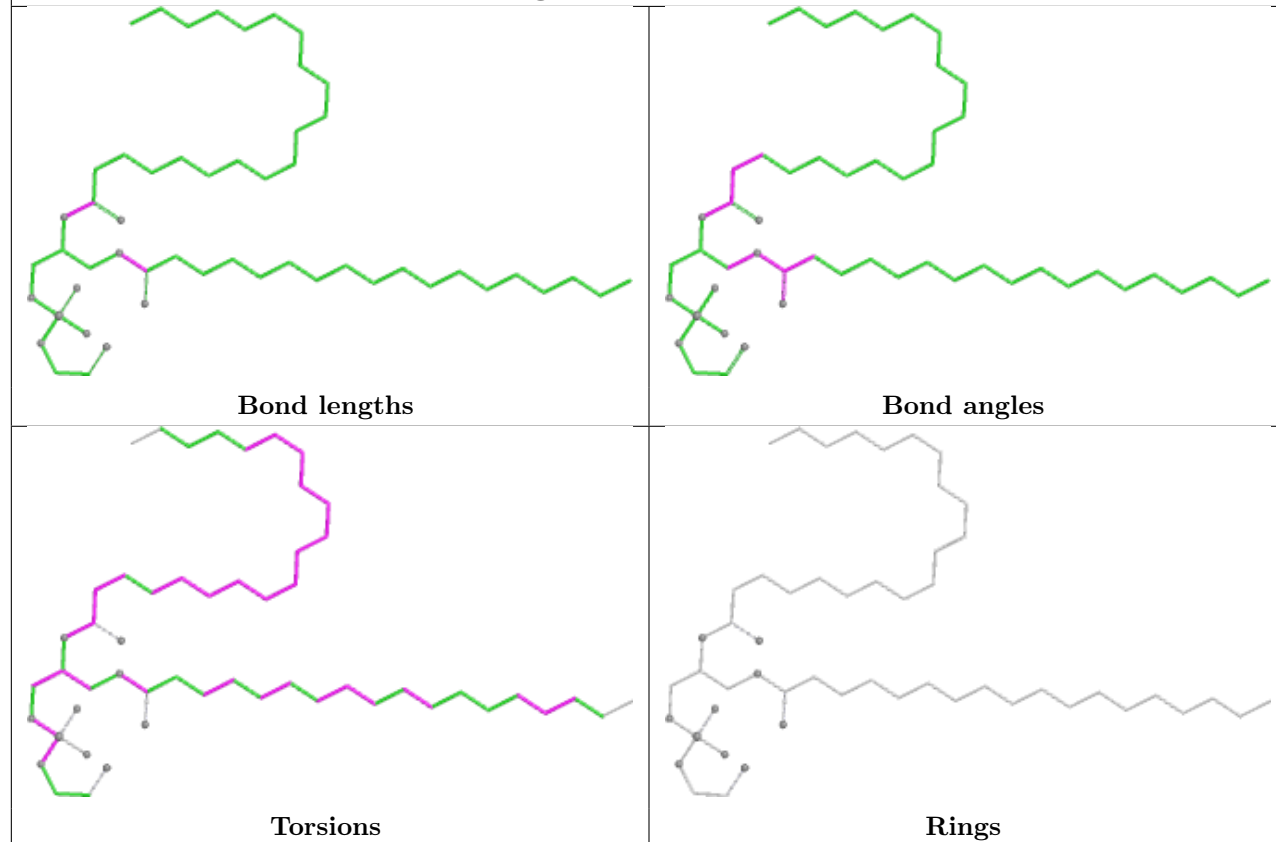


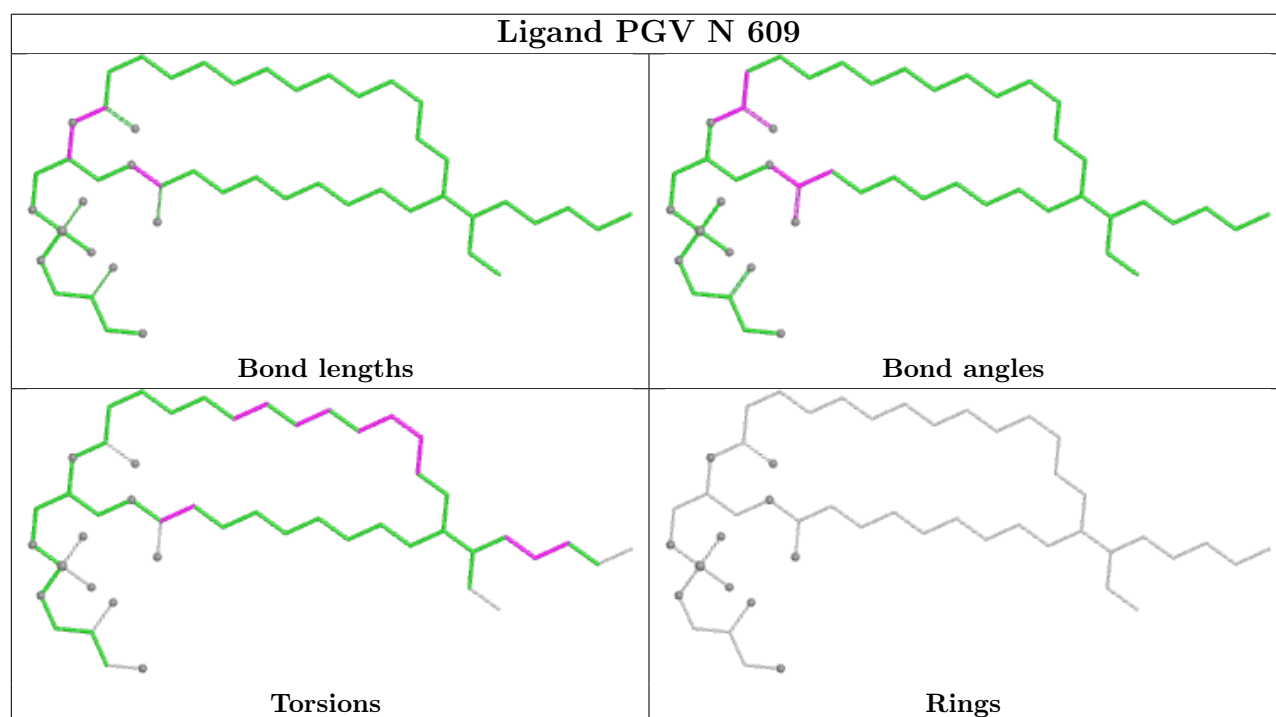
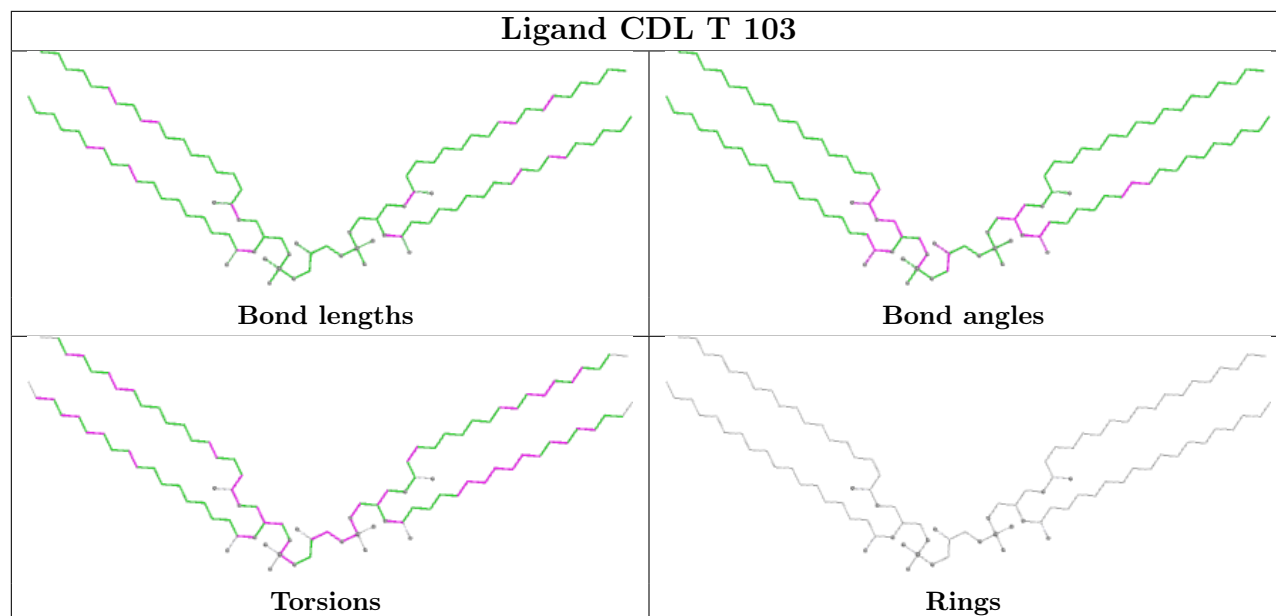


Ligand PEK P 302

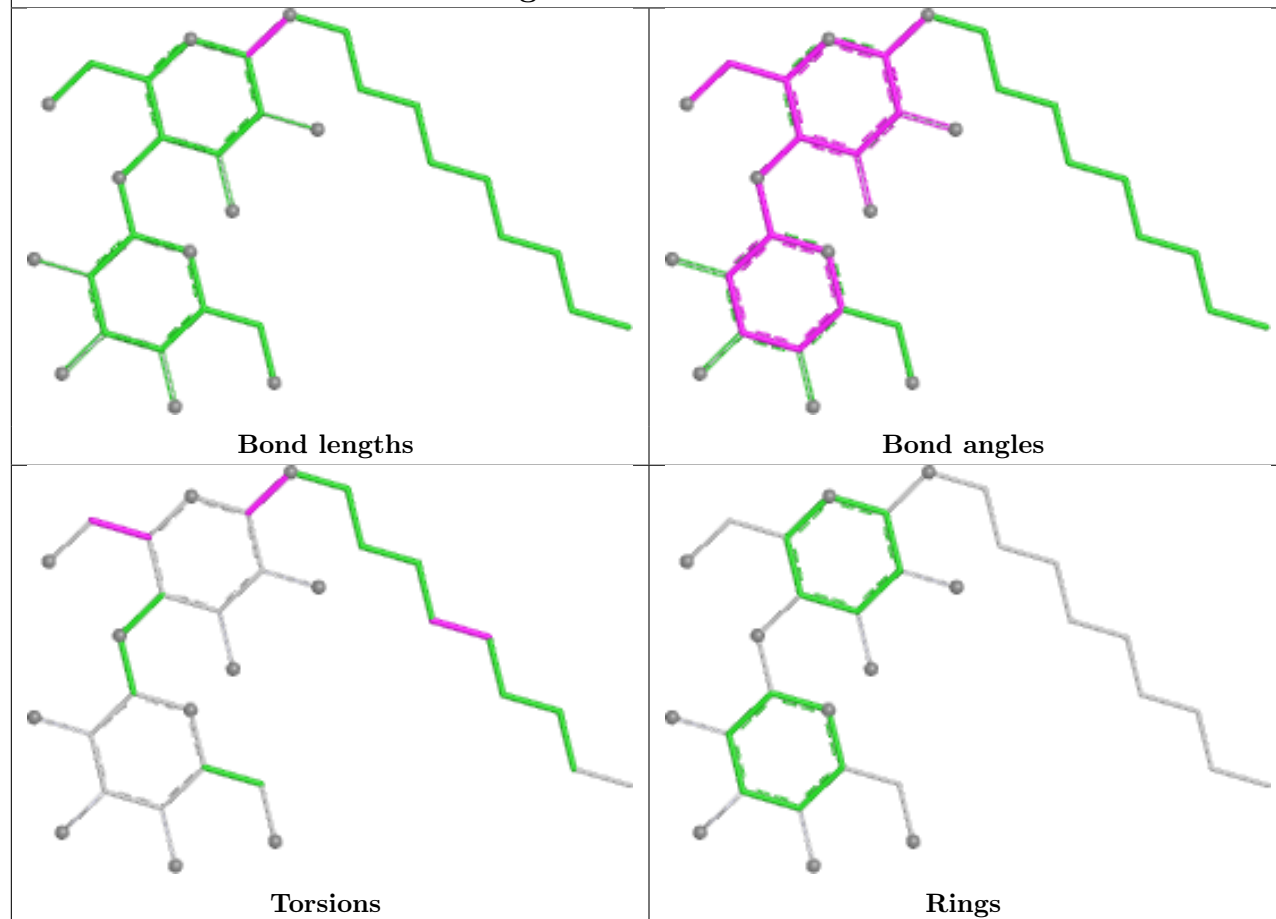


Ligand PEK T 101

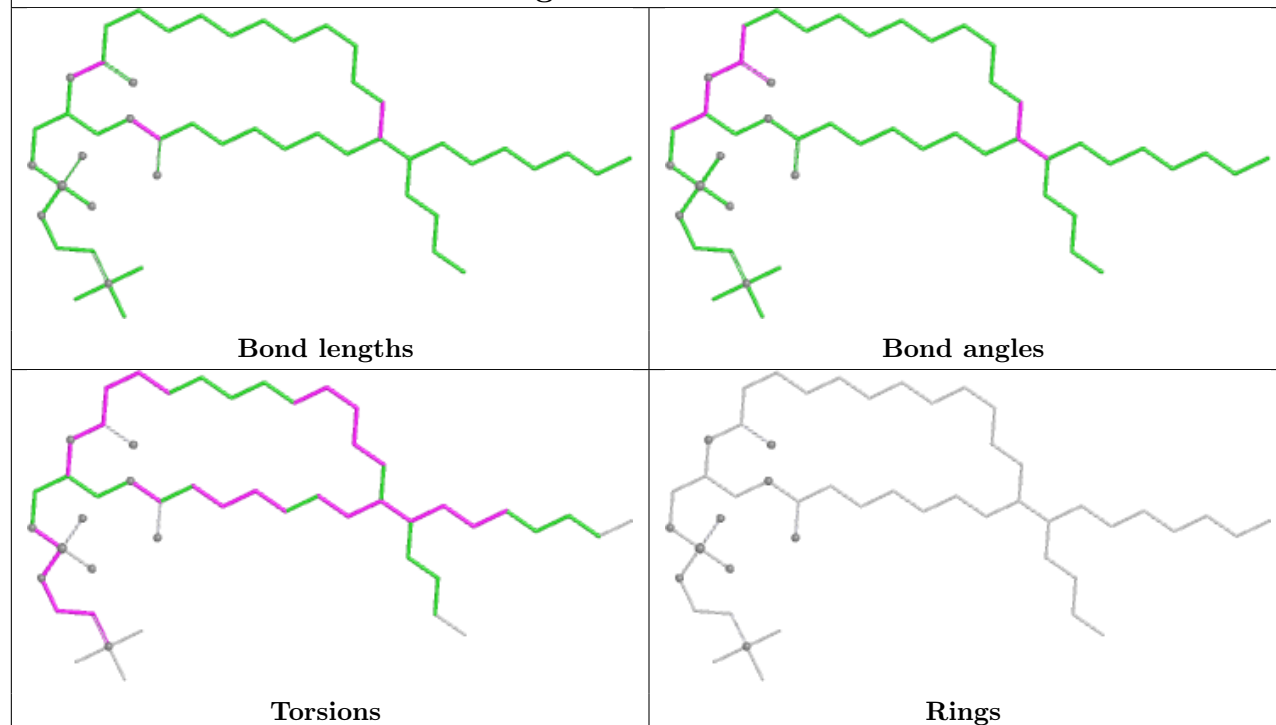


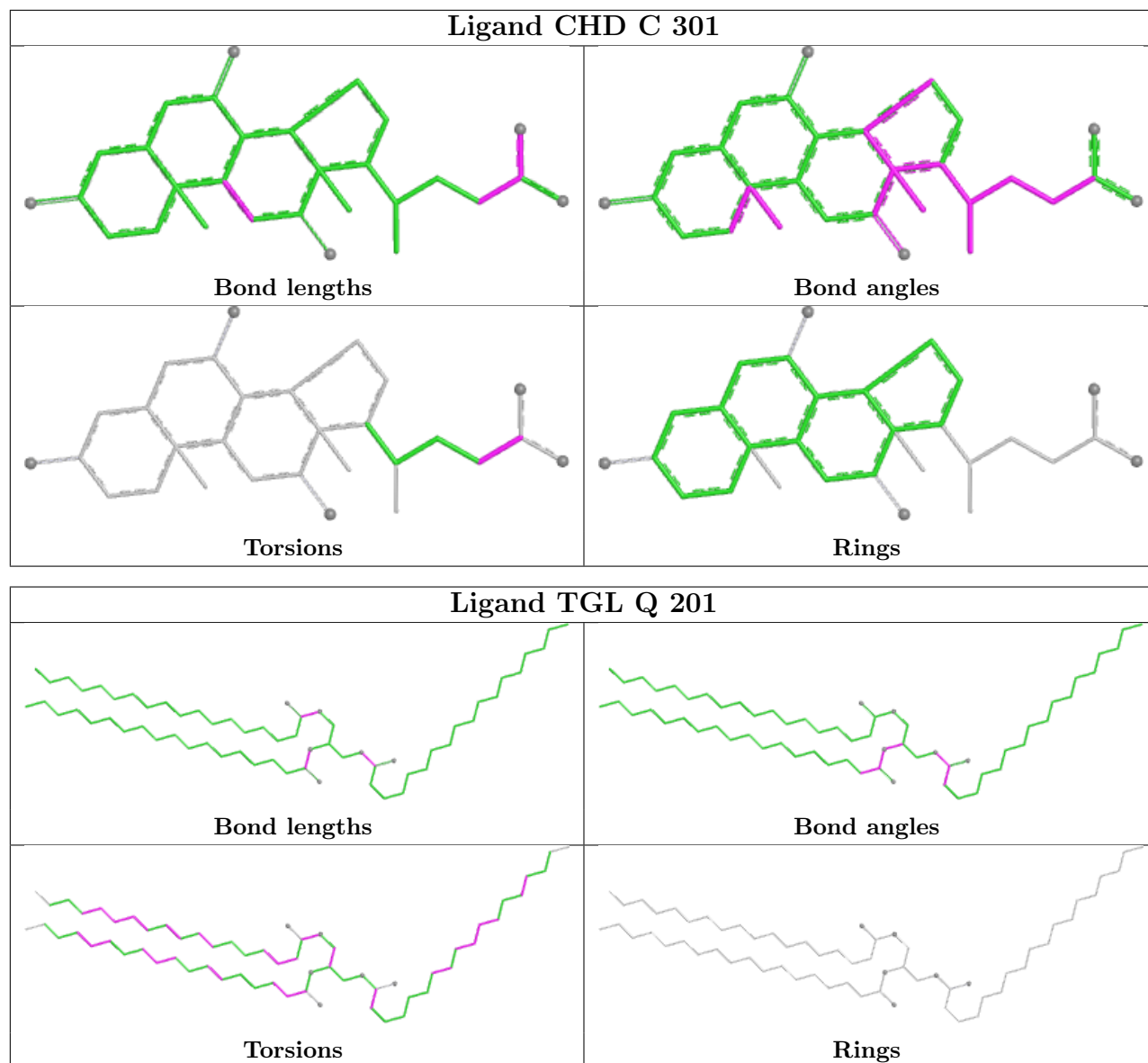


Ligand DMU W 102

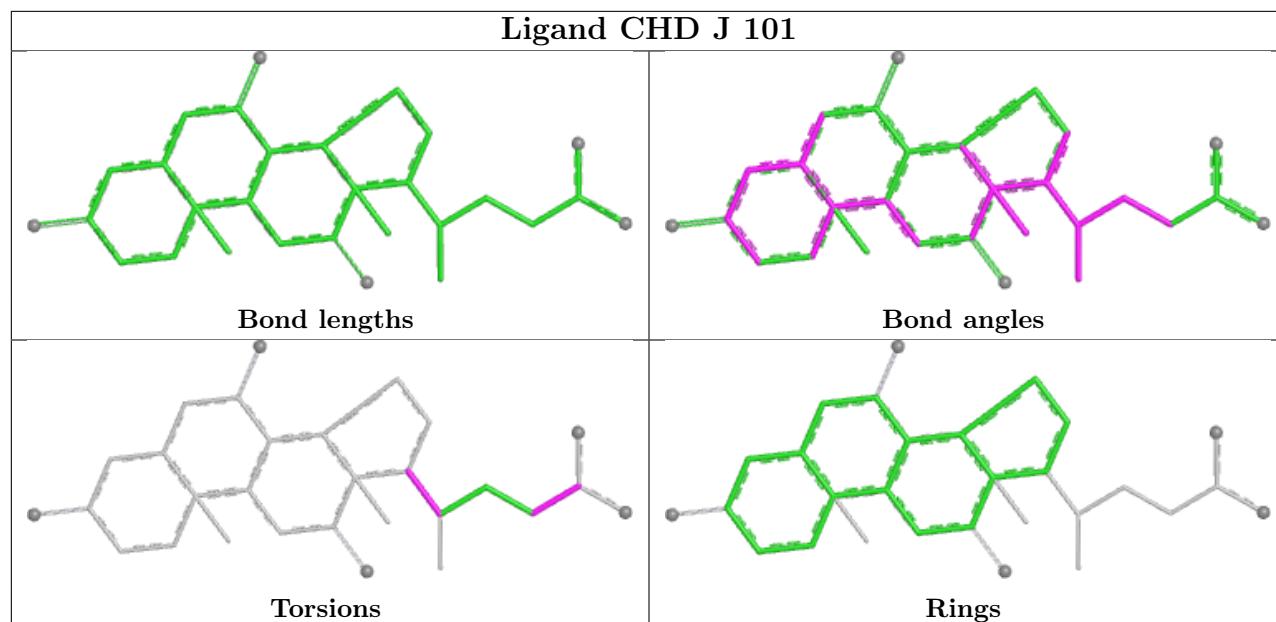


Ligand PSC E 201

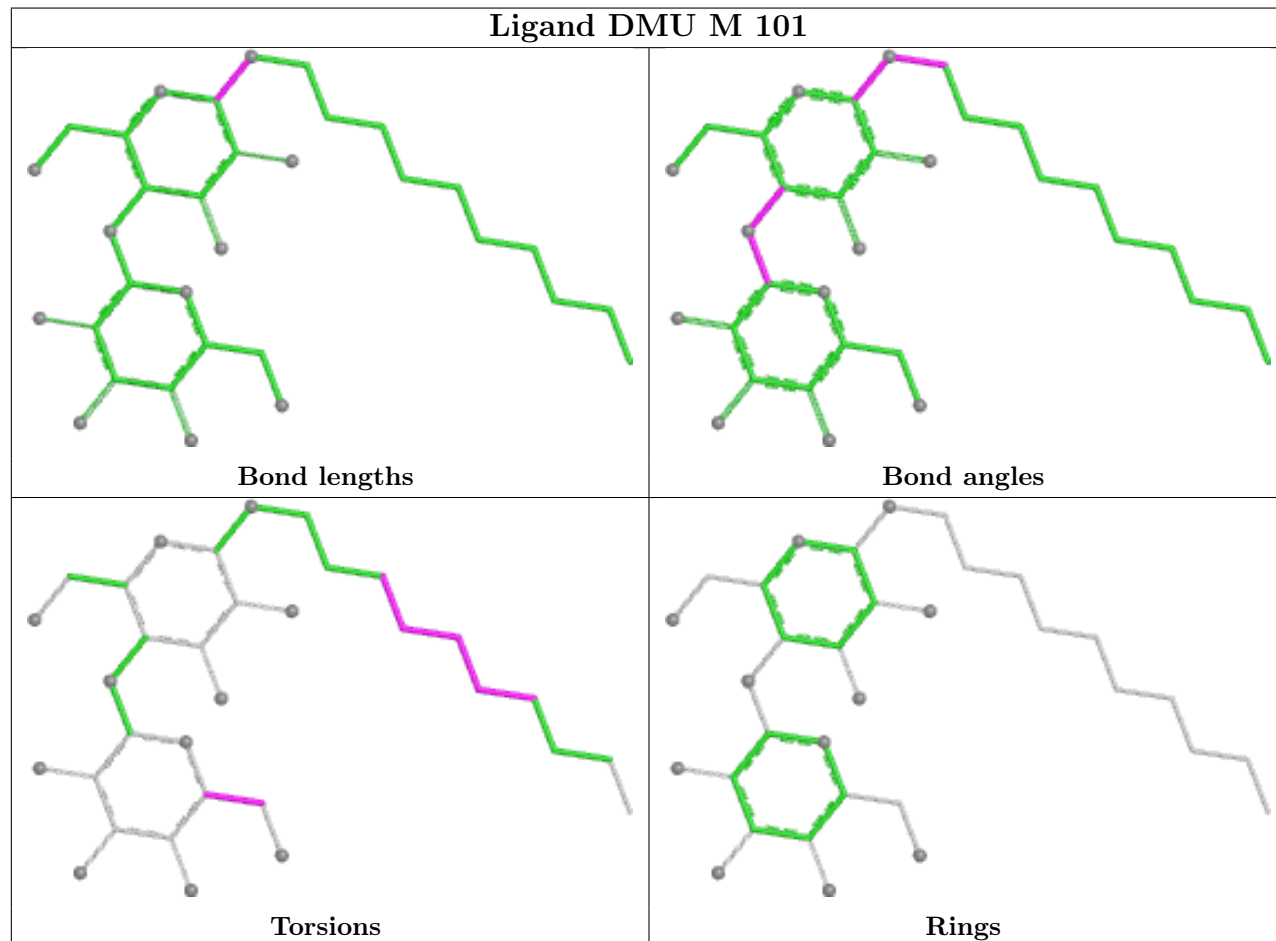




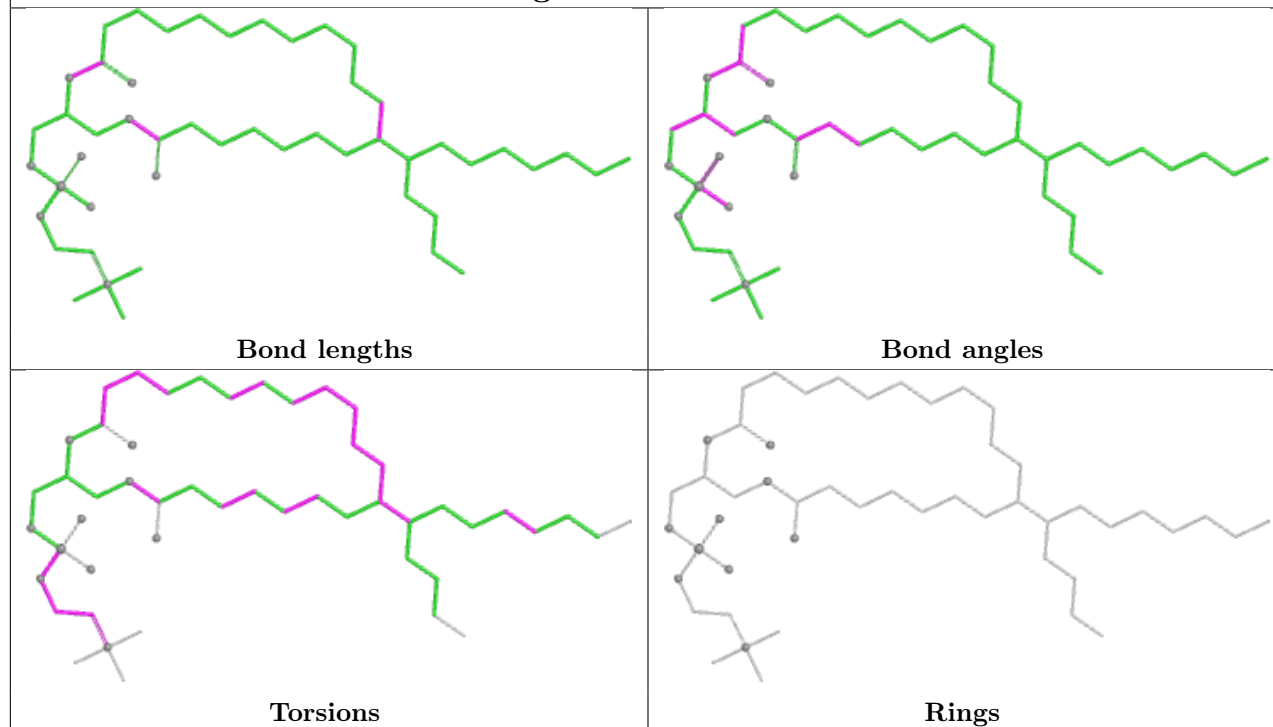
Ligand CHD J 101



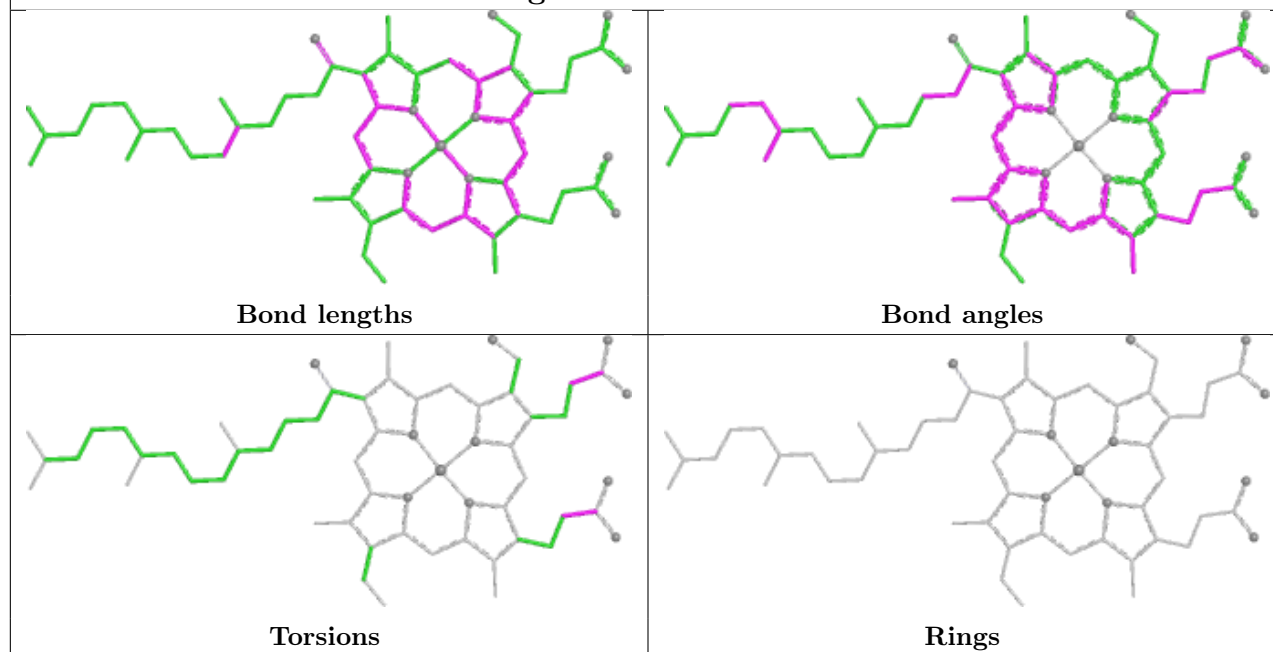
Ligand DMU M 101

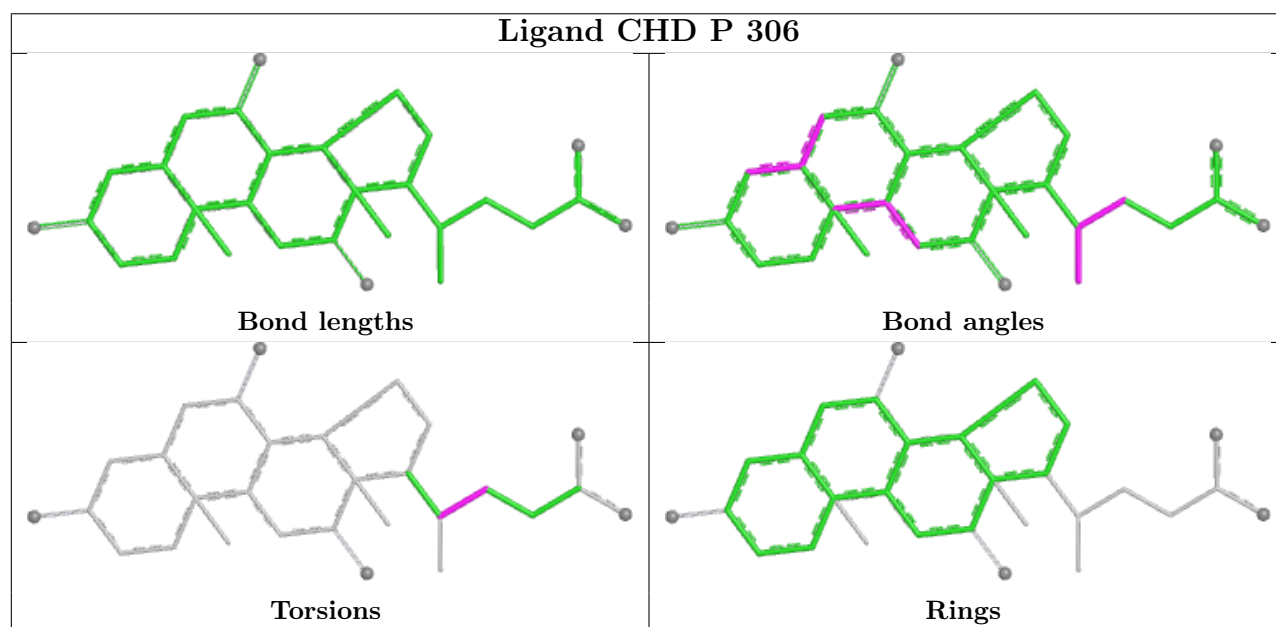
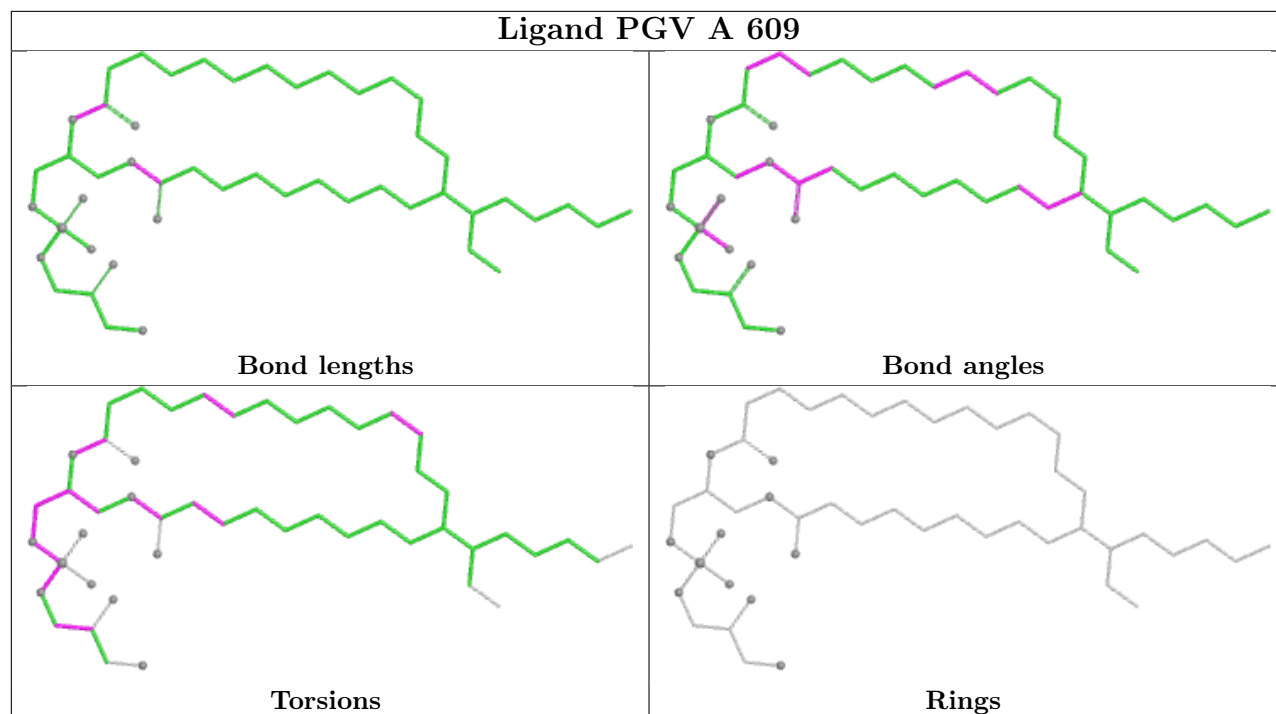


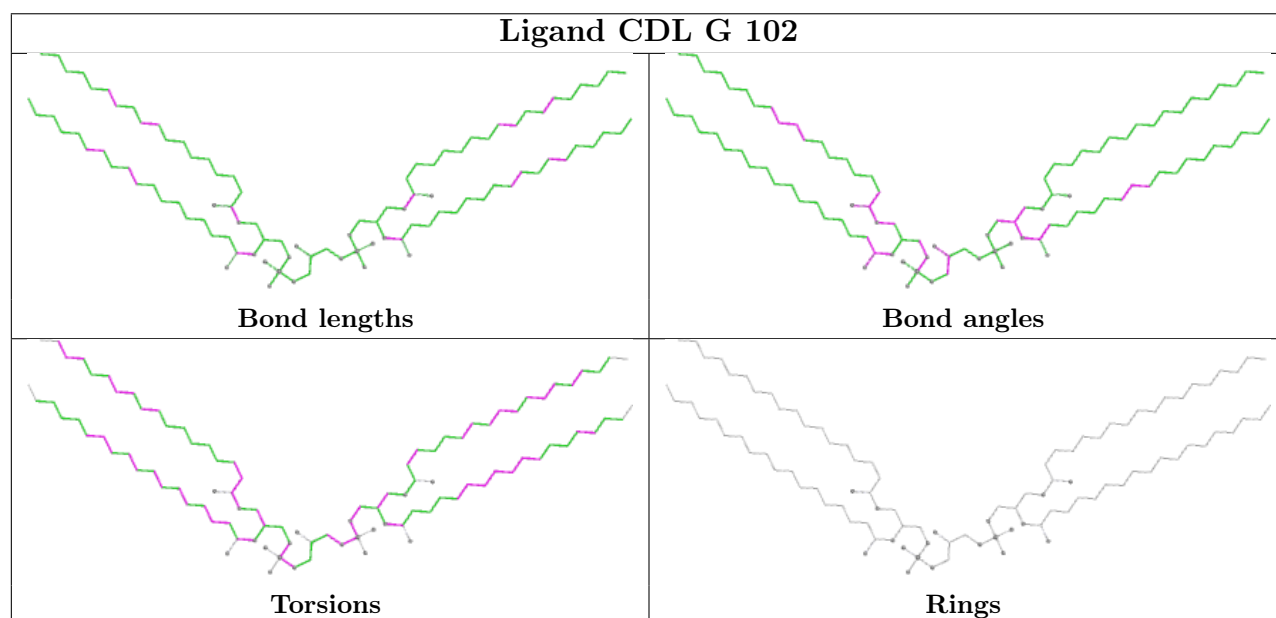
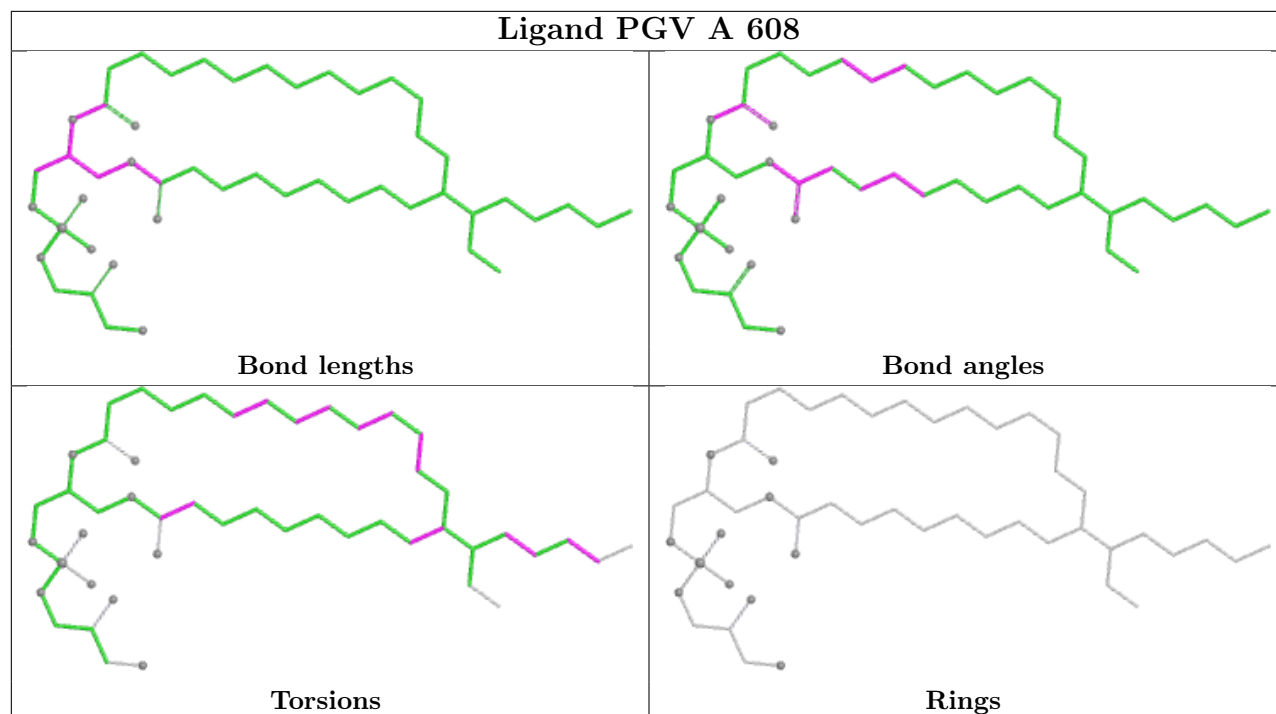
Ligand PSC R 201

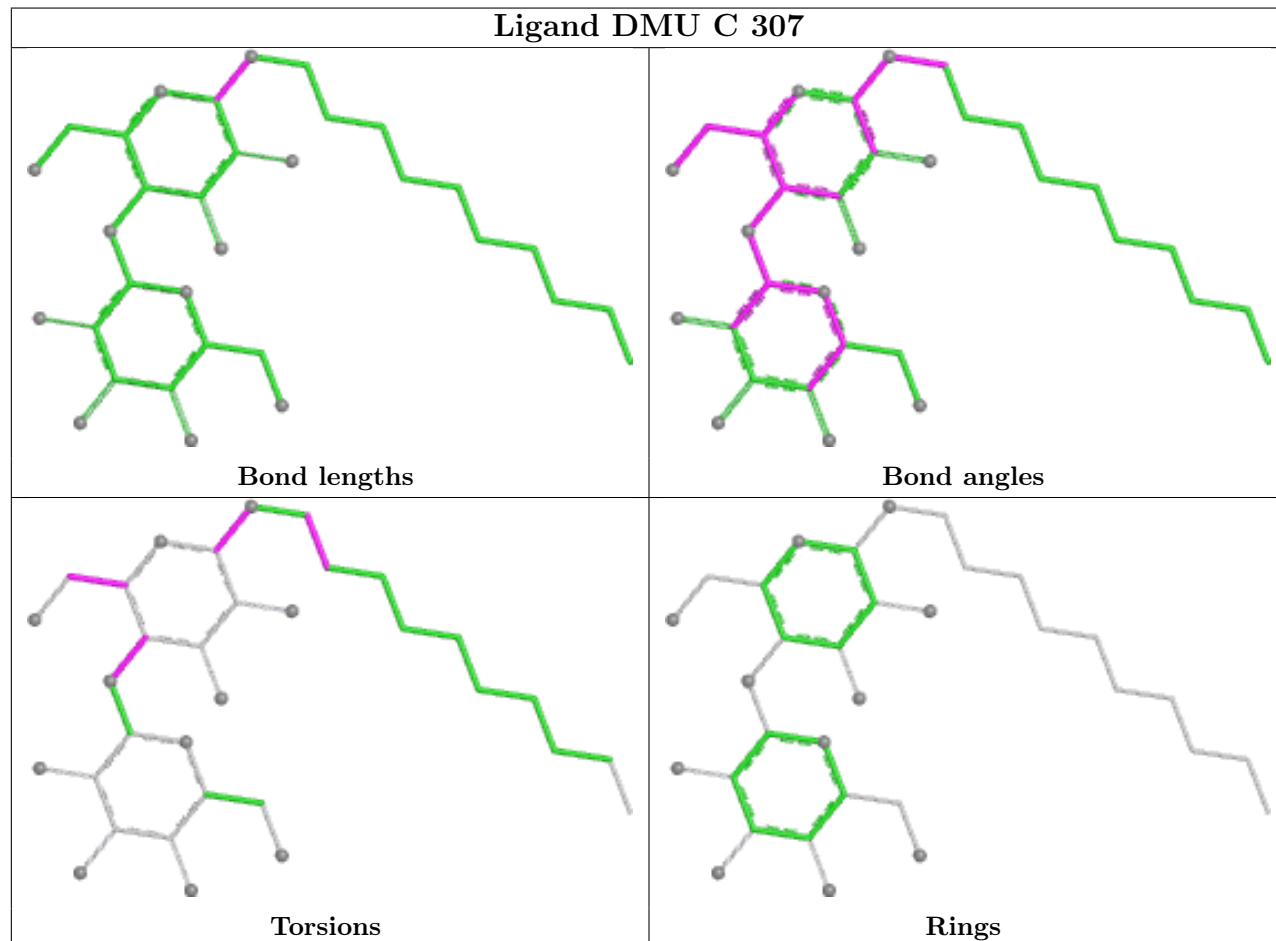
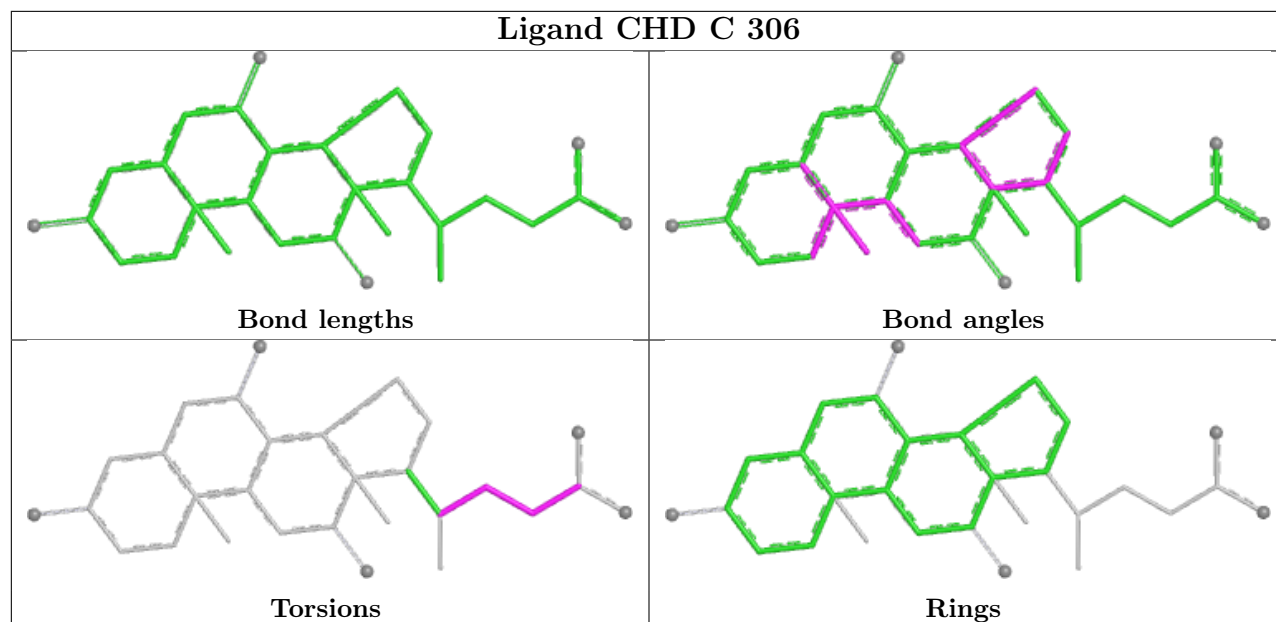


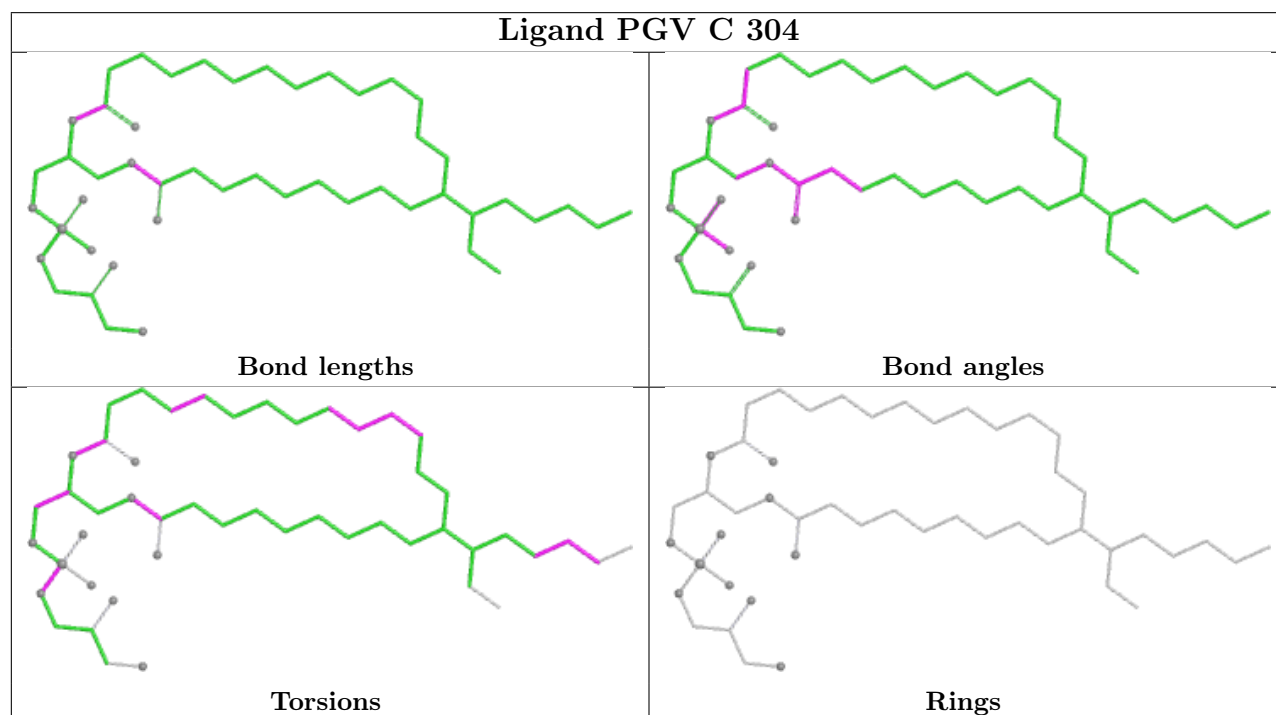
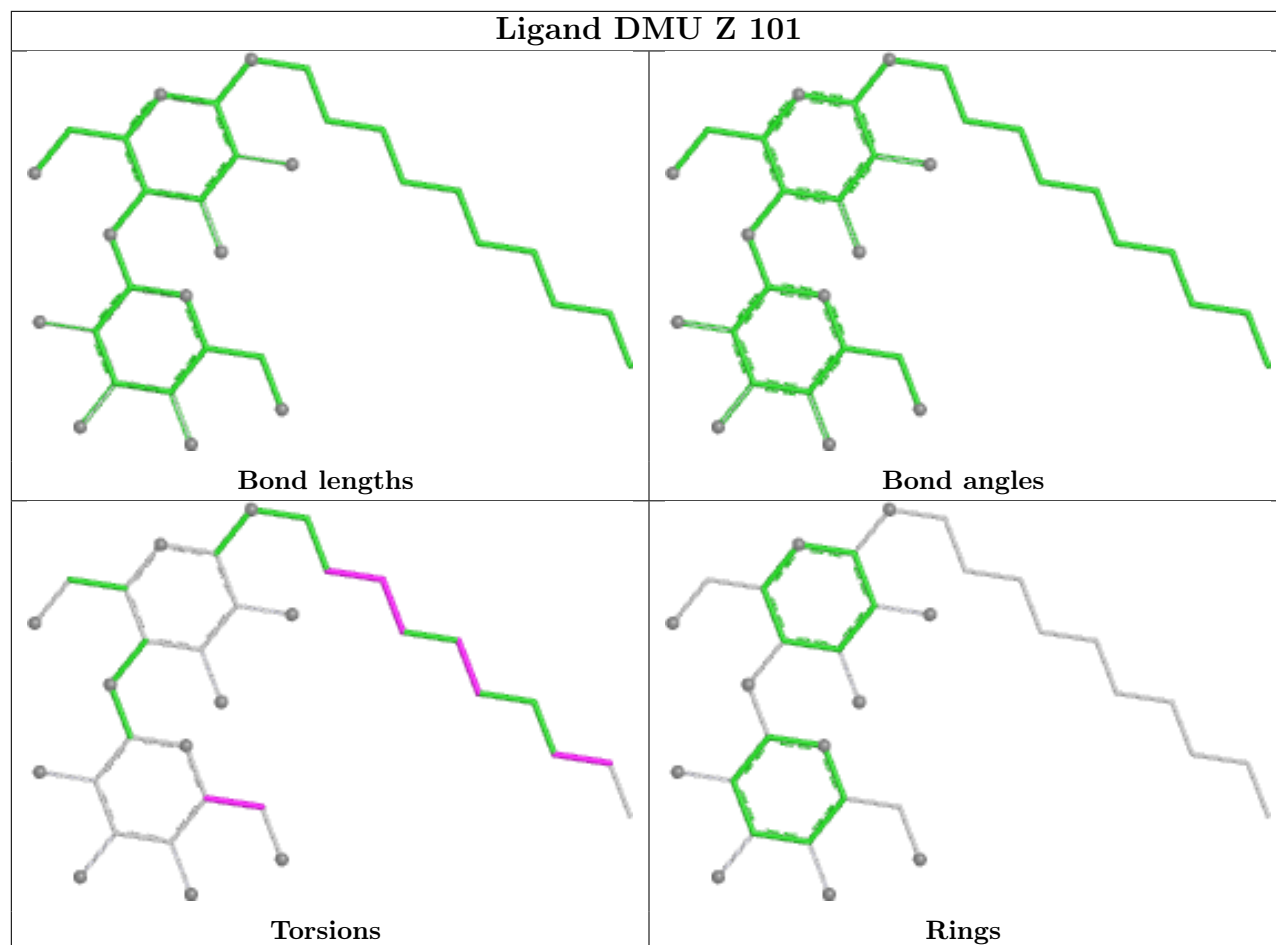
Ligand HEA N 602

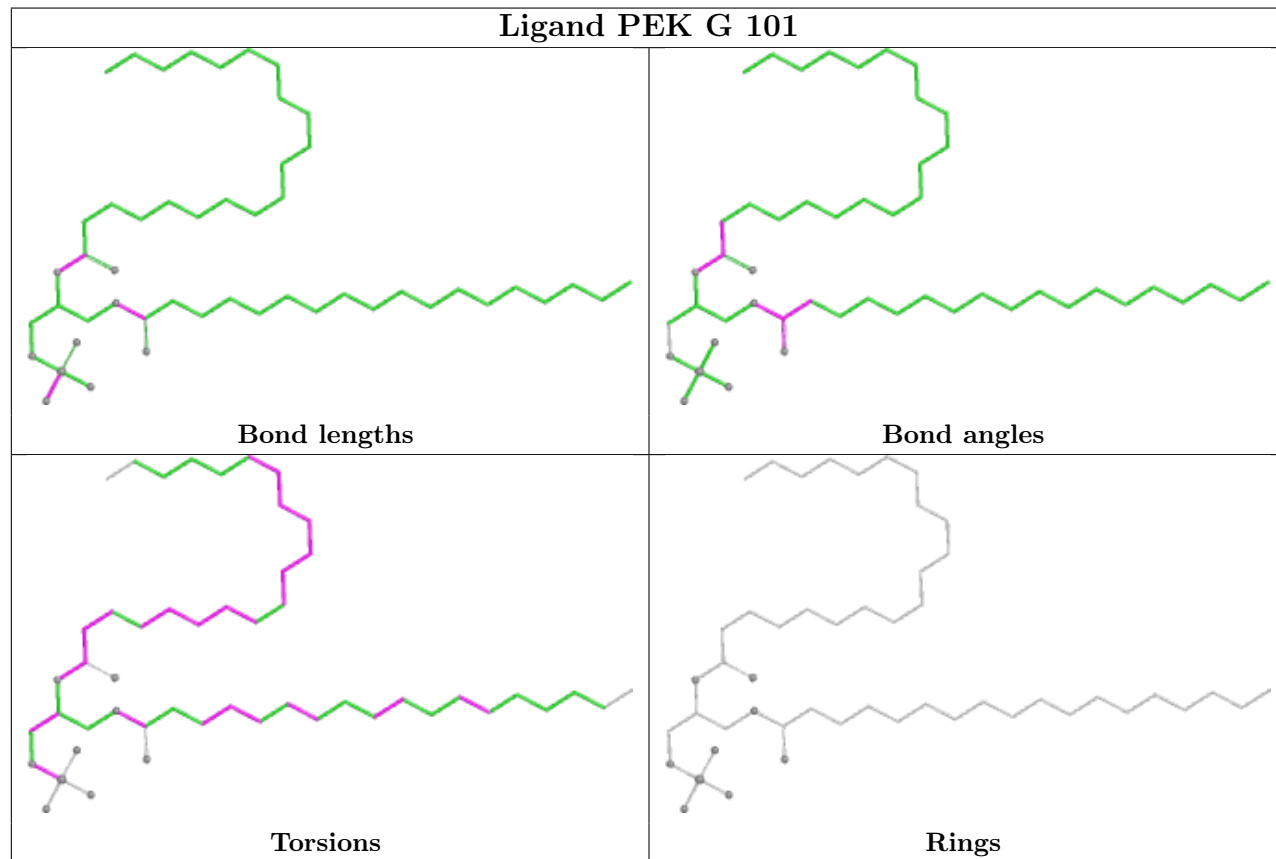
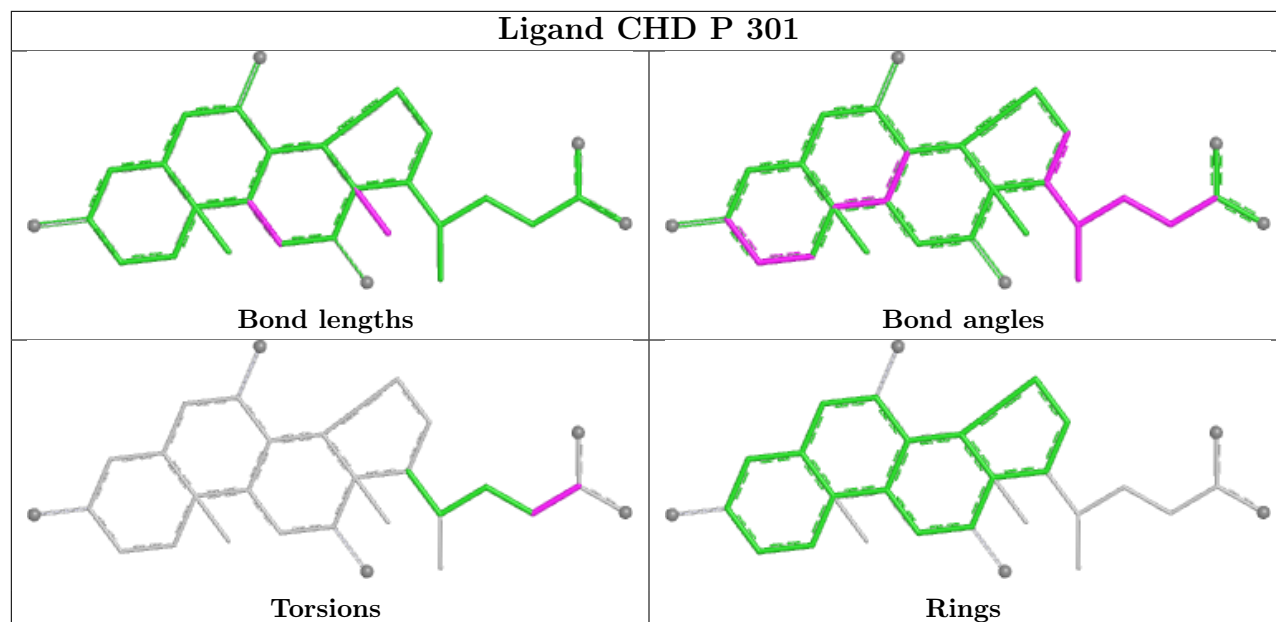


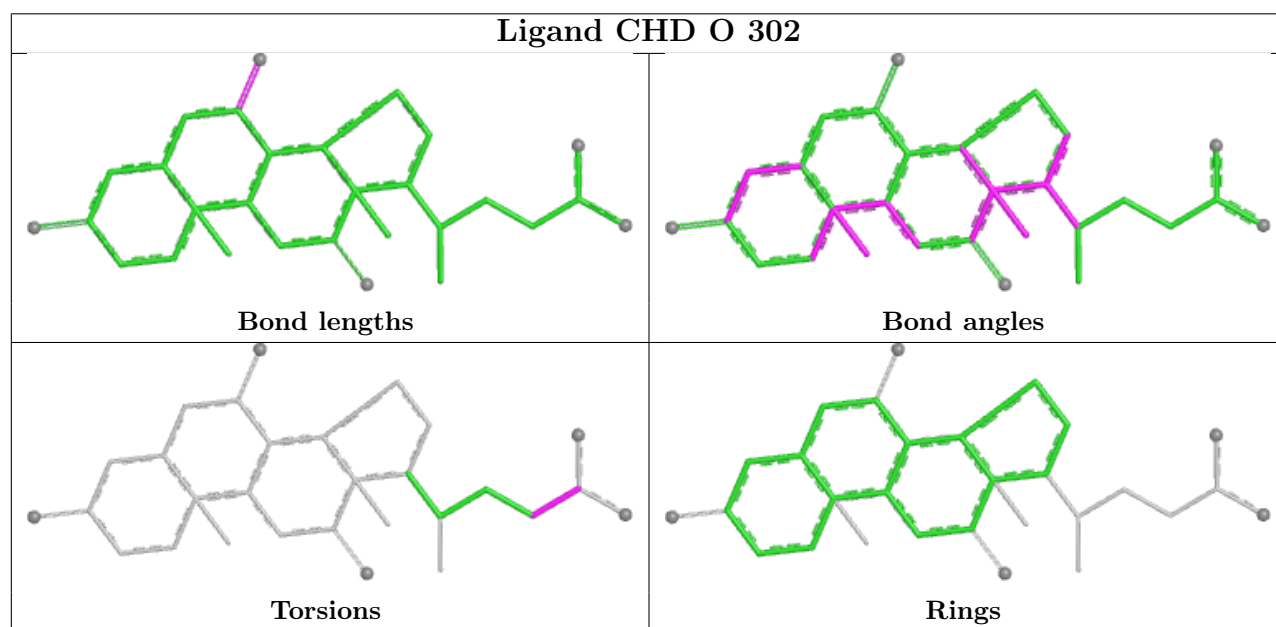
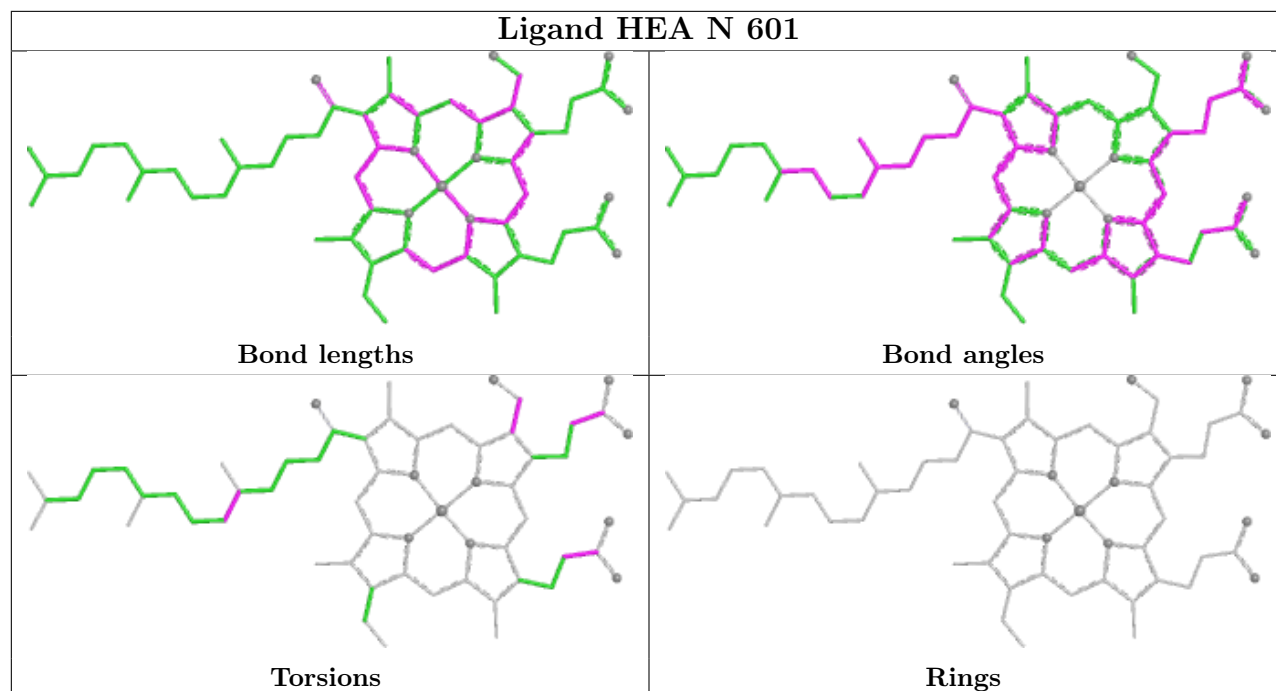


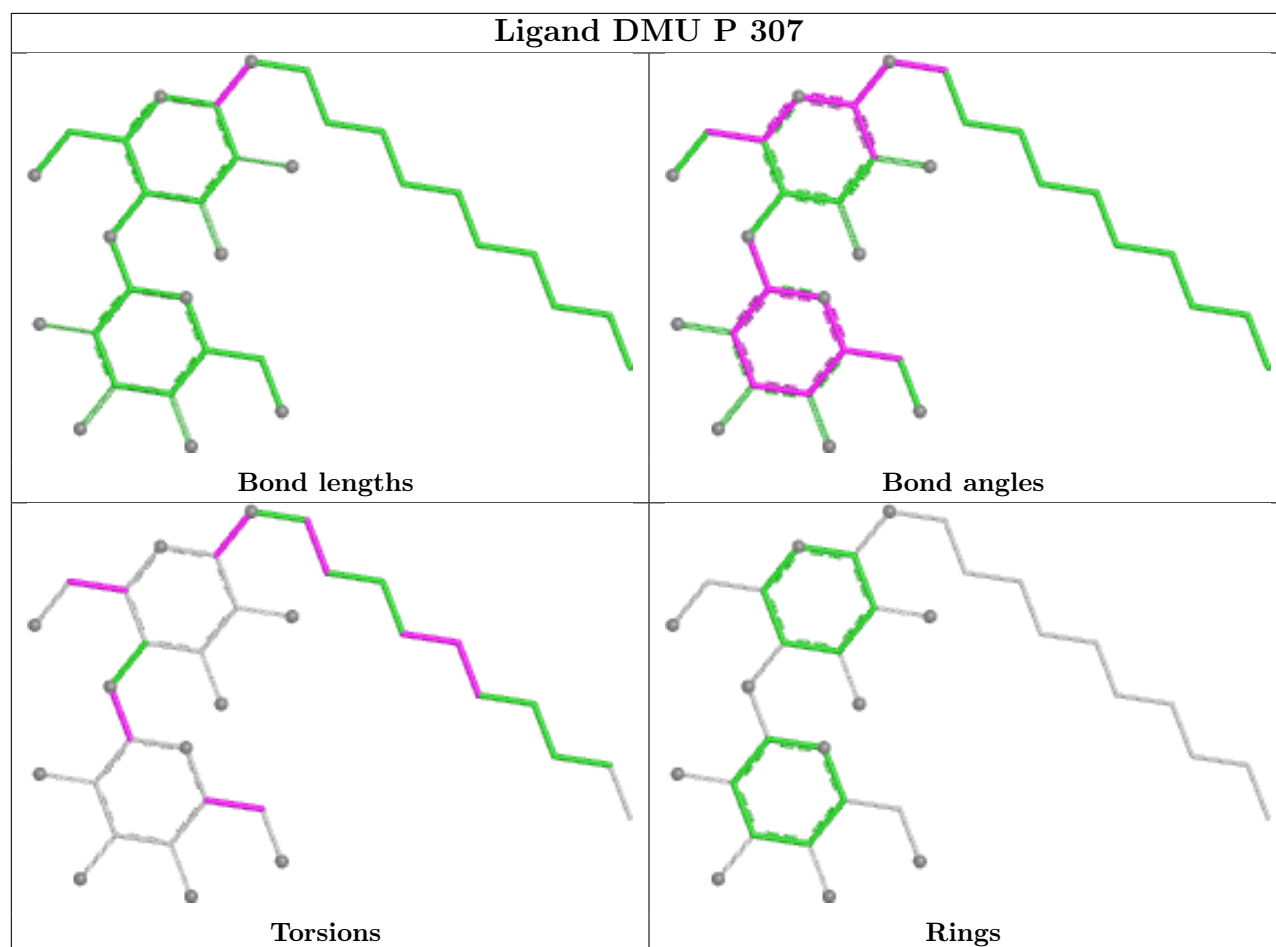
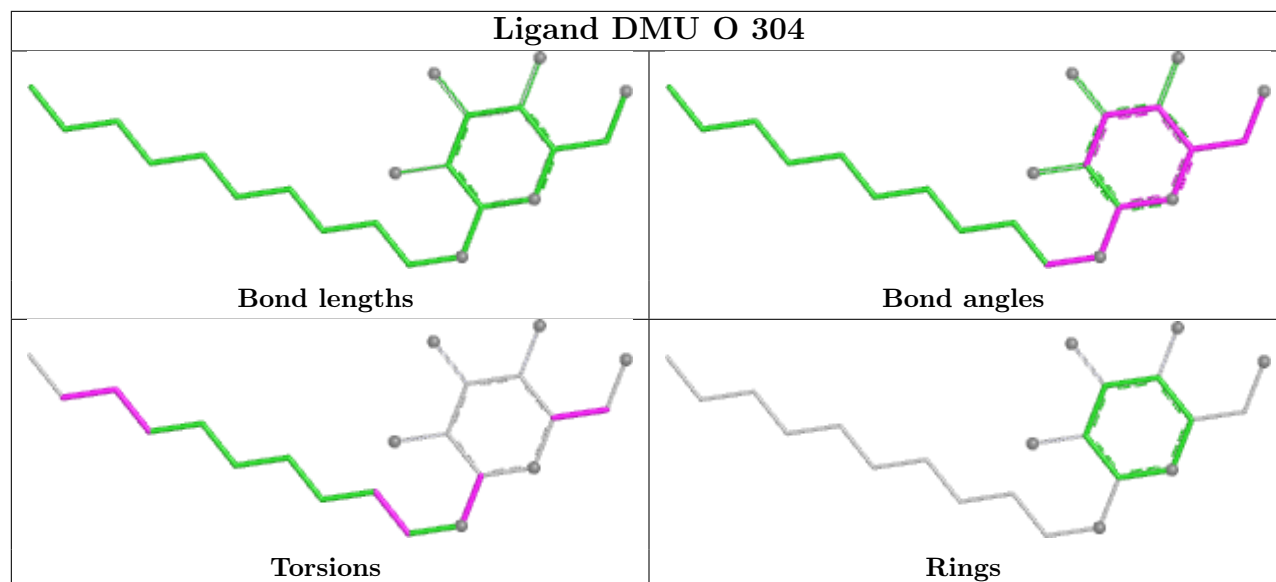


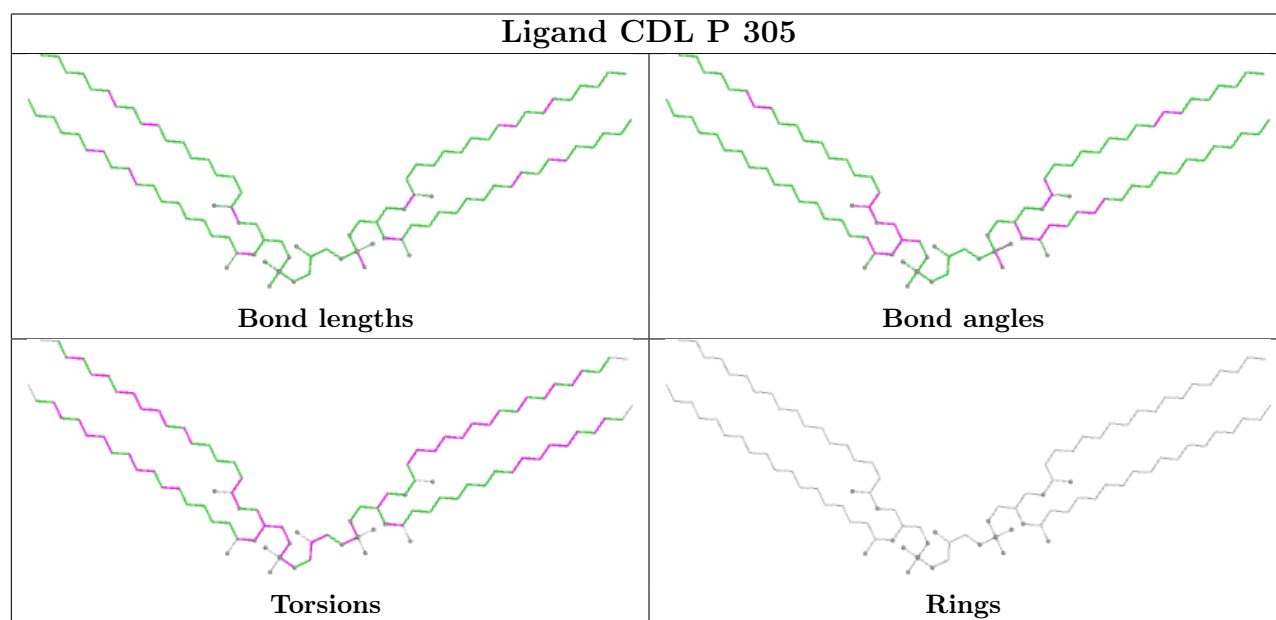
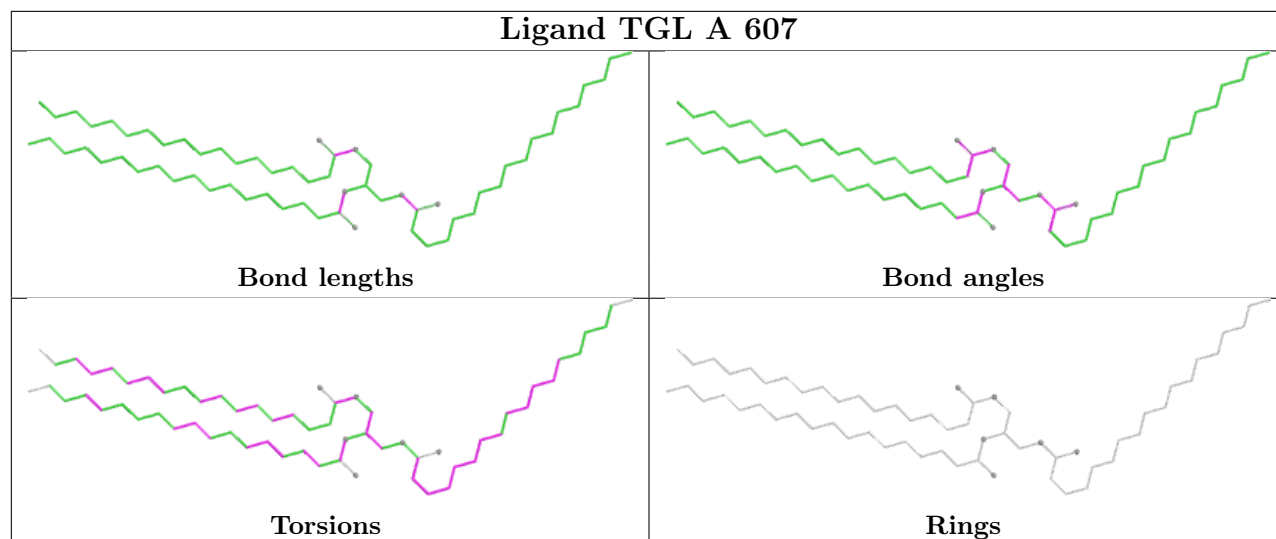


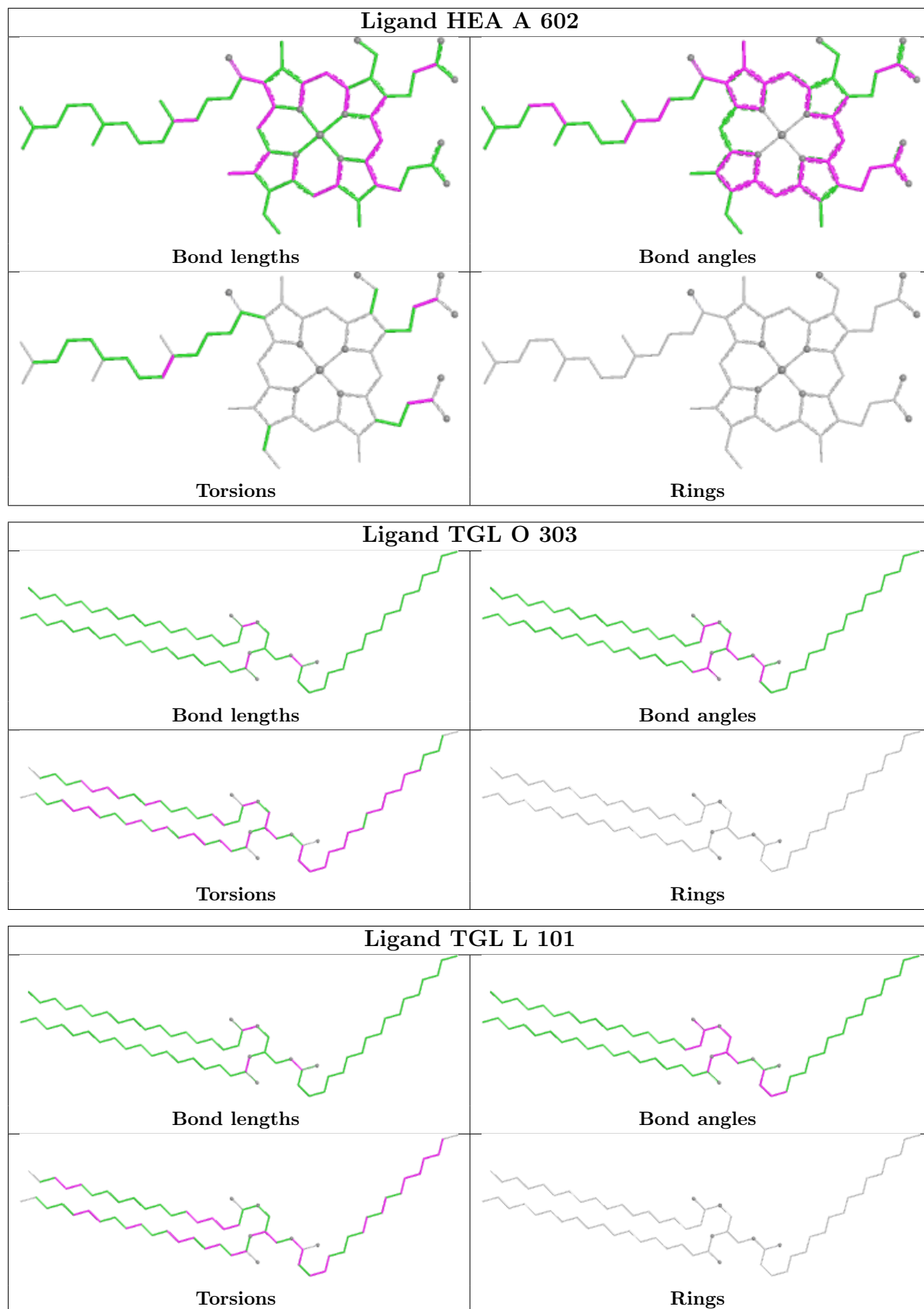


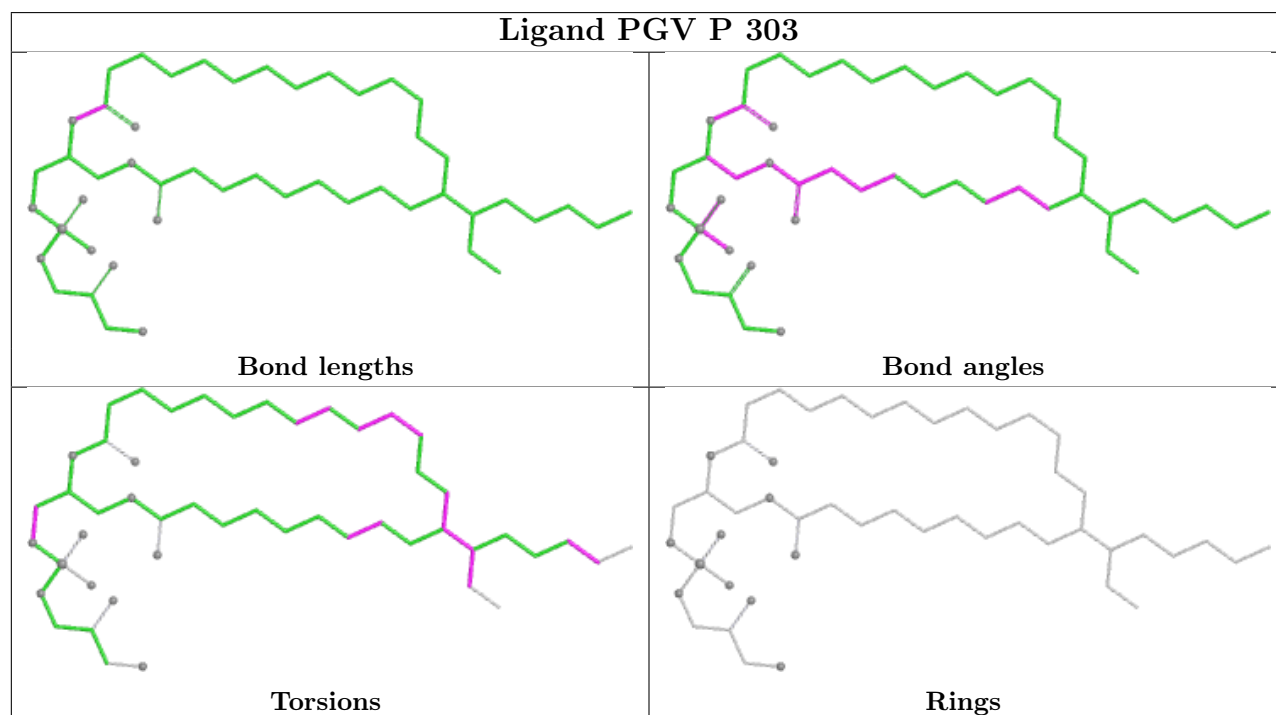
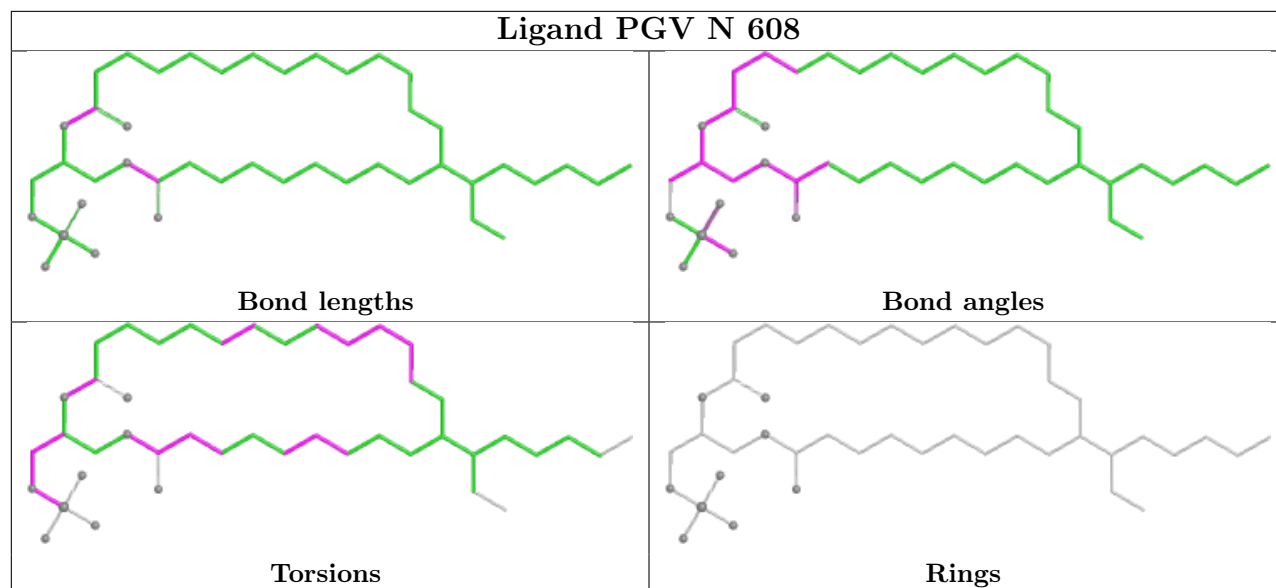


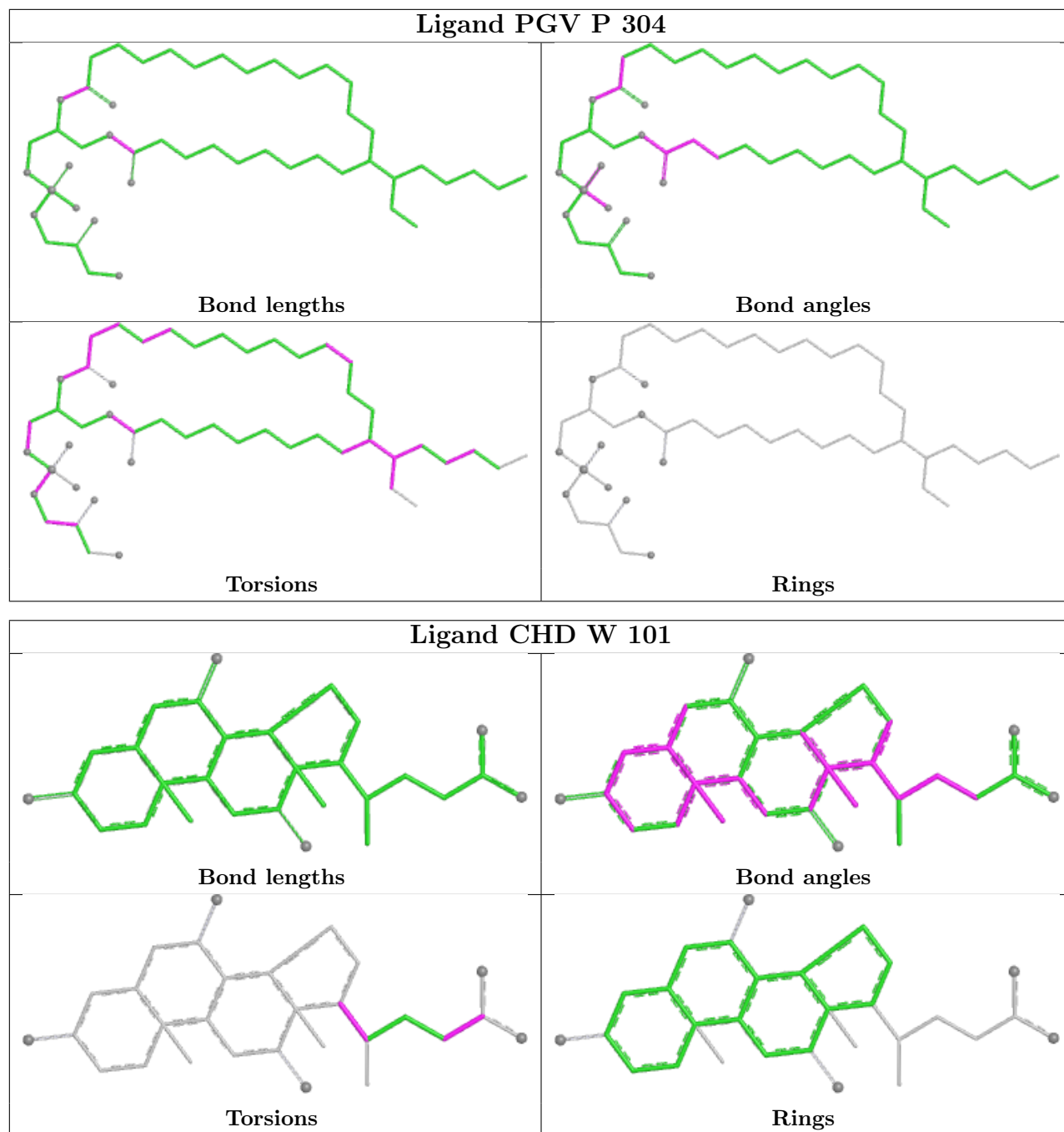




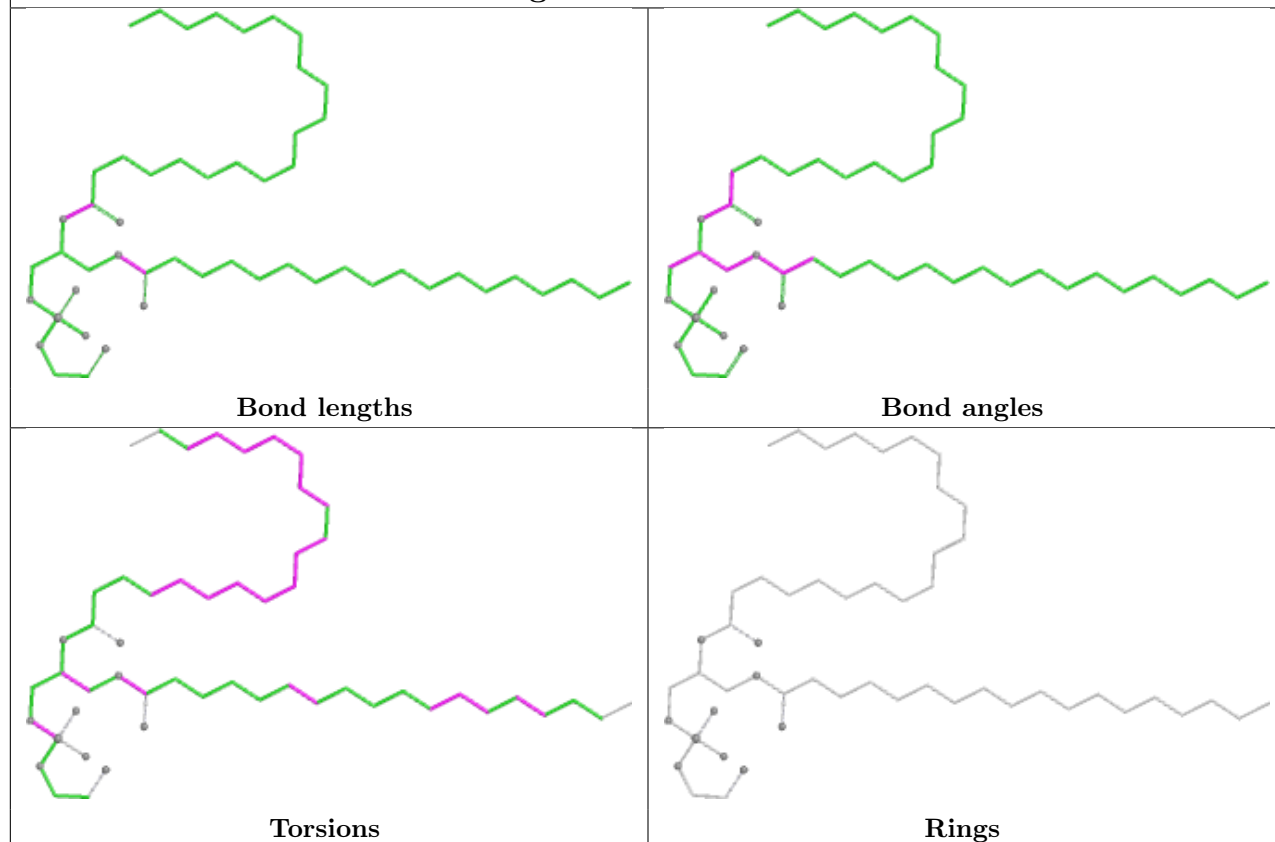




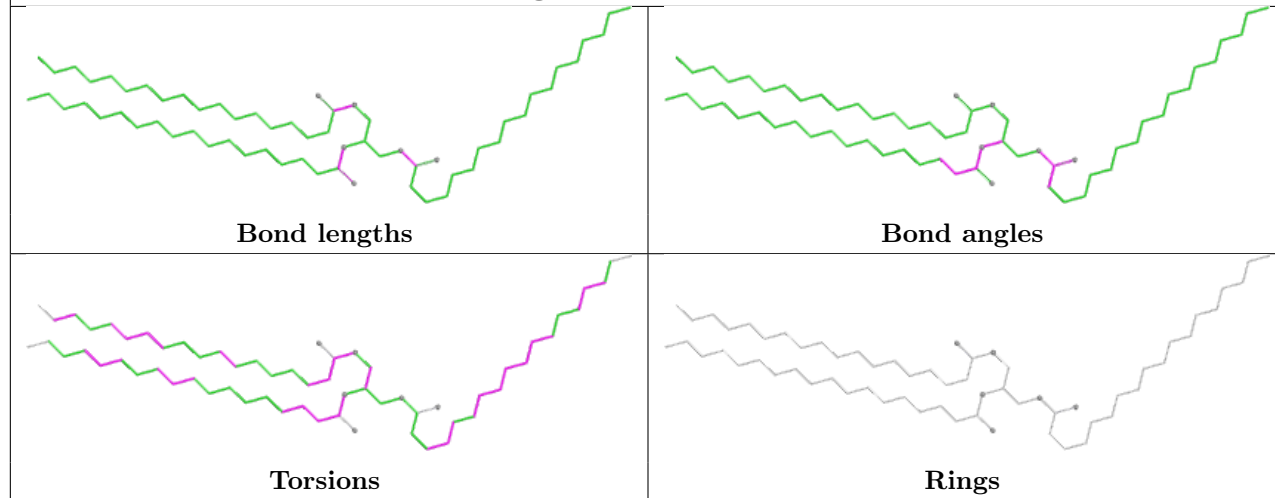


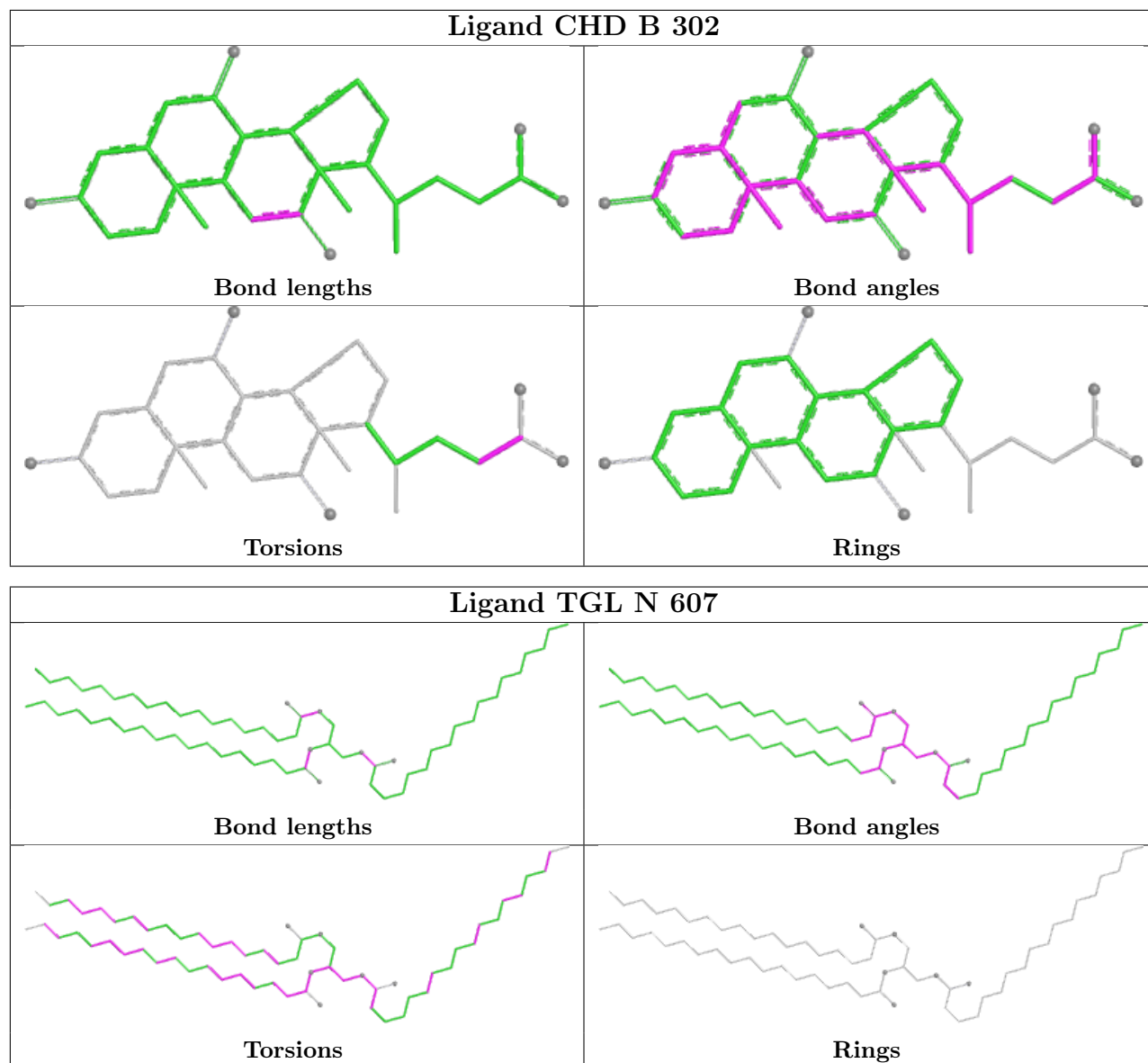


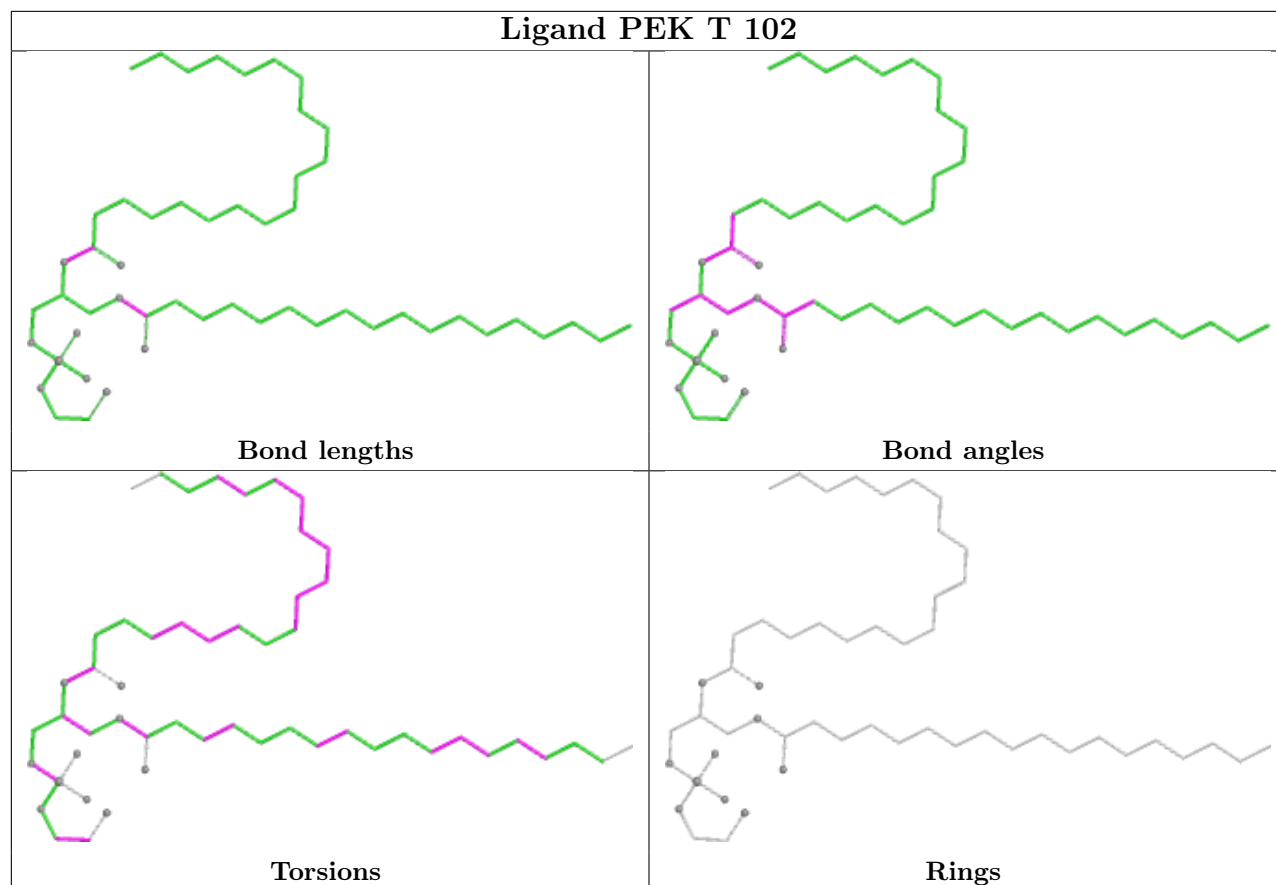
Ligand PEK G 103



Ligand TGL D 201







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%)	-0.59	4 (0%)	82 83	11, 25, 34, 79	10 (1%)
1	N	513/514 (99%)	-0.43	6 (1%)	76 77	14, 30, 40, 78	9 (1%)
2	B	226/227 (99%)	-0.03	12 (5%)	32 31	22, 32, 55, 85	2 (0%)
2	O	226/227 (99%)	0.29	14 (6%)	26 25	27, 38, 72, 110	0
3	C	259/261 (99%)	-0.31	4 (1%)	72 72	22, 29, 42, 77	3 (1%)
3	P	259/261 (99%)	-0.25	2 (0%)	82 83	25, 31, 47, 70	0
4	D	144/147 (97%)	0.32	6 (4%)	40 40	29, 39, 57, 86	0
4	Q	144/147 (97%)	0.88	17 (11%)	9 7	35, 48, 83, 162	0
5	E	105/109 (96%)	0.10	4 (3%)	44 44	32, 39, 69, 134	0
5	R	105/109 (96%)	0.30	4 (3%)	44 44	34, 46, 73, 145	0
6	F	98/98 (100%)	0.61	10 (10%)	12 10	26, 37, 120, 152	0
6	S	98/98 (100%)	0.79	9 (9%)	14 12	26, 39, 118, 159	0
7	G	83/85 (97%)	1.20	23 (27%)	1 1	26, 37, 109, 152	0
7	T	83/85 (97%)	1.21	20 (24%)	2 1	27, 41, 112, 149	0
8	H	79/85 (92%)	0.77	13 (16%)	4 3	28, 40, 91, 135	0
8	U	79/85 (92%)	1.05	15 (18%)	3 2	33, 44, 115, 144	0
9	I	72/73 (98%)	0.71	8 (11%)	10 8	32, 45, 68, 77	0
9	V	72/73 (98%)	1.06	11 (15%)	5 4	33, 51, 74, 128	0
10	J	58/59 (98%)	0.41	5 (8%)	16 14	29, 38, 68, 127	0
10	W	58/59 (98%)	0.57	5 (8%)	16 14	33, 44, 76, 146	0
11	K	49/56 (87%)	0.57	4 (8%)	17 15	32, 41, 62, 71	0
11	X	49/56 (87%)	0.90	7 (14%)	6 5	40, 51, 75, 93	0
12	L	46/47 (97%)	0.12	3 (6%)	25 23	26, 32, 54, 94	0
12	Y	46/47 (97%)	0.44	4 (8%)	16 14	33, 41, 68, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.51	6 (13%) 6 5	29, 34, 76, 123	0
13	Z	43/46 (93%)	0.81	7 (16%) 4 3	37, 45, 98, 153	0
All	All	3550/3614 (98%)	0.12	223 (6%) 26 24	11, 34, 70, 162	24 (0%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	22.1
6	S	97	ALA	11.4
4	Q	6	VAL	11.0
6	F	1	ALA	10.2
7	T	3	ALA	9.4
8	U	8	ILE	9.4
6	S	94	HIS	8.7
2	O	227	LEU	8.7
7	G	36	TRP	8.7
6	F	96	LEU	8.6
8	H	8	ILE	8.3
7	G	7	ASP	7.9
4	Q	4	SER	7.8
7	G	2	SER	7.5
7	T	36	TRP	7.5
8	H	47	GLY	7.5
7	G	9	GLY	6.9
6	F	97	ALA	6.9
6	S	98	HIS	6.8
7	T	2	SER	6.7
7	G	3	ALA	6.6
4	Q	5	VAL	6.5
2	B	59	GLN	6.3
5	R	109	VAL	6.0
7	T	84	LYS	6.0
9	V	2	THR	5.9
4	Q	8	SER	5.9
7	T	5	LYS	5.8
7	G	5	LYS	5.7
6	S	96	LEU	5.7
9	I	37	PHE	5.6
7	T	9	GLY	5.6
6	S	95	GLN	5.5
2	O	59	GLN	5.4

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Mol	Chain	Res	Type	RSRZ
7	G	10	GLY	5.4
7	G	8	HIS	5.3
2	B	113	TYR	5.3
2	O	113	TYR	5.2
6	F	94	HIS	5.2
7	T	8	HIS	5.2
7	T	4	ALA	5.2
6	S	3	GLY	5.1
8	U	47	GLY	5.1
8	U	45	ALA	5.1
7	G	4	ALA	4.9
4	Q	9	GLU	4.9
12	L	47	LYS	4.9
13	M	43	SER	4.8
2	O	65	TRP	4.8
2	O	226	MET	4.8
1	N	484	THR	4.8
8	U	48	GLY	4.8
8	H	7	LYS	4.7
9	V	36	LYS	4.6
7	G	1	ALA	4.6
7	T	1	ALA	4.6
7	T	7	ASP	4.6
7	G	37	LEU	4.5
8	U	44	THR	4.5
4	Q	7	LYS	4.4
6	F	2	SER	4.4
7	T	37	LEU	4.4
8	H	48	GLY	4.3
9	V	3	ALA	4.3
2	B	90	ILE	4.3
6	S	2	SER	4.3
9	V	37	PHE	4.2
11	X	6	ALA	4.2
12	L	2	HIS	4.2
1	N	113	LEU	4.2
7	T	10	GLY	4.2
11	K	6	ALA	4.2
10	W	52	TRP	4.1
10	W	58	LYS	4.1
5	R	5	HIS	4.1
8	H	9	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
11	X	7	PRO	4.0
4	D	4	SER	4.0
13	Z	43	SER	4.0
10	W	57	HIS	3.9
2	B	92	ASN	3.9
7	G	84	LYS	3.9
6	F	95	GLN	3.9
5	E	109	VAL	3.9
1	A	113	LEU	3.9
7	T	38	HIS	3.9
7	G	6	GLY	3.8
8	U	7	LYS	3.8
6	F	3	GLY	3.8
2	B	65	TRP	3.8
12	Y	47	LYS	3.8
13	Z	42	LYS	3.8
8	U	50	VAL	3.8
10	J	1	PHE	3.7
2	O	90	ILE	3.7
8	U	61	LYS	3.7
10	J	58	LYS	3.7
11	K	7	PRO	3.6
2	B	87	MET	3.6
8	U	9	LYS	3.6
4	Q	51	LEU	3.6
13	Z	41	LYS	3.6
13	M	40	TYR	3.5
11	X	47	ARG	3.5
10	J	56	PRO	3.5
7	T	40	GLY	3.5
6	S	93	PRO	3.5
7	G	41	HIS	3.5
7	G	39	SER	3.4
9	V	33	THR	3.4
1	A	514	LYS	3.4
13	M	42	LYS	3.4
3	C	3	HIS	3.4
6	F	98	HIS	3.4
12	Y	2	HIS	3.4
12	Y	20	ARG	3.4
8	U	43	MET	3.4
7	T	39	SER	3.3

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Mol	Chain	Res	Type	RSRZ
5	E	5	HIS	3.3
13	Z	38	ASP	3.3
8	H	10	ASN	3.3
4	D	11	TYR	3.3
1	A	297	MET	3.2
8	U	46	LYS	3.2
9	V	29	LEU	3.2
2	O	129	LYS	3.2
9	V	30	GLY	3.2
2	B	91	ASN	3.2
13	Z	39	ASN	3.2
8	H	46	LYS	3.2
2	O	32	PHE	3.2
4	Q	33	LEU	3.1
7	G	38	HIS	3.1
7	G	12	GLY	3.1
7	G	33	LEU	3.1
4	Q	11	TYR	3.0
4	Q	46	ALA	3.0
2	B	16	ILE	3.0
4	Q	17	VAL	2.9
4	Q	10	ASP	2.9
9	V	73	LYS	2.9
7	T	42	ARG	2.9
13	Z	40	TYR	2.9
4	Q	143	ASN	2.9
7	T	35	SER	2.9
1	N	513	LEU	2.9
3	C	37	PHE	2.8
3	P	37	PHE	2.8
9	I	36	LYS	2.8
9	V	26	MET	2.8
7	T	12	GLY	2.8
11	K	47	ARG	2.7
11	K	54	ARG	2.7
9	I	33	THR	2.7
8	H	50	VAL	2.7
1	N	512	ASN	2.7
8	U	42	ALA	2.7
7	G	40	GLY	2.7
4	Q	72	ASN	2.7
2	B	60	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	8	SER	2.7
4	Q	35	ALA	2.6
9	I	73	LYS	2.6
13	M	41	LYS	2.6
9	I	29	LEU	2.6
2	O	221	LYS	2.6
5	E	7	THR	2.6
8	U	10	ASN	2.6
10	W	1	PHE	2.6
8	H	45	ALA	2.6
13	M	39	ASN	2.6
2	O	91	ASN	2.5
2	O	217	LYS	2.5
9	I	30	GLY	2.5
2	O	57	ASP	2.5
4	Q	147	LYS	2.5
13	Z	19	LEU	2.4
1	N	514	LYS	2.4
8	H	44	THR	2.4
7	T	6	GLY	2.4
9	I	26	MET	2.4
10	J	55	PHE	2.4
7	G	35	SER	2.4
10	W	55	PHE	2.4
8	H	42	ALA	2.4
11	X	19	ALA	2.4
2	O	92	ASN	2.4
4	D	5	VAL	2.4
1	N	297[A]	MET	2.4
9	V	10	ARG	2.3
3	C	44	MET	2.3
6	F	92	VAL	2.3
8	U	52	VAL	2.3
3	C	38	ASN	2.3
2	O	87	MET	2.3
4	Q	87	PHE	2.2
6	F	93	PRO	2.2
7	G	45	PRO	2.2
5	E	108	LYS	2.2
7	G	42	ARG	2.2
9	I	2	THR	2.2
7	T	33	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	57	ASP	2.2
11	X	52	GLU	2.2
11	X	20	SER	2.2
7	G	70	PHE	2.2
5	R	9	GLU	2.2
12	L	24	MET	2.1
4	D	9	GLU	2.1
4	D	17	VAL	2.1
8	H	43	MET	2.1
3	P	107	ALA	2.1
10	J	52	TRP	2.1
1	A	513	LEU	2.1
11	X	54	ARG	2.1
2	B	55	THR	2.1
9	V	32	ALA	2.1
5	R	108	LYS	2.0
2	B	37	LEU	2.0
13	M	38	ASP	2.0
8	H	84	LYS	2.0
12	Y	26	THR	2.0
8	U	11	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.31	0.23	147,152,161,162	0
7	TPO	G	11	11/12	0.57	0.38	90,120,150,166	0
7	TPO	T	11	11/12	0.65	0.30	103,113,156,158	0
9	SAC	I	1	9/10	0.68	0.23	65,84,106,118	0
1	FME	N	1	10/11	0.91	0.14	40,54,91,104	0
1	FME	A	1	10/11	0.94	0.12	36,39,76,103	0
2	FME	B	1	10/11	0.97	0.10	17,34,75,76	0
2	FME	O	1	10/11	0.97	0.09	30,39,45,76	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($\text{\AA}^2$)	Q<0.9
24	PEK	G	103	53/53	0.71	0.26	46,95,133,145	0
26	DMU	P	307	33/33	0.71	0.21	60,110,126,129	0
20	PGV	P	304	51/51	0.72	0.24	43,78,120,149	0
23	CHD	J	101	29/29	0.72	0.23	73,104,110,113	0
24	PEK	T	102	53/53	0.73	0.25	47,94,128,138	0
23	CHD	W	101	29/29	0.73	0.22	81,107,119,120	0
26	DMU	C	307	33/33	0.74	0.21	58,102,122,124	0
25	CDL	T	103	100/100	0.74	0.23	52,88,125,150	0
20	PGV	N	608	46/51	0.75	0.25	40,83,127,143	0
24	PEK	T	101	53/53	0.75	0.24	40,80,124,154	0
24	PEK	G	101	50/53	0.75	0.24	46,82,118,145	0
26	DMU	W	102	32/33	0.75	0.21	50,80,104,115	0
19	TGL	D	201	63/63	0.76	0.24	41,71,103,117	0
19	TGL	Q	201	63/63	0.76	0.25	49,77,107,112	0
25	CDL	G	102	100/100	0.77	0.23	46,88,122,152	0
20	PGV	C	304	51/51	0.78	0.25	44,88,114,150	0
20	PGV	A	609	51/51	0.78	0.25	43,77,132,157	0
27	PSC	R	201	52/52	0.78	0.27	44,94,141,175	0
25	CDL	P	305	100/100	0.79	0.24	41,90,124,138	0
19	TGL	A	607	63/63	0.79	0.23	47,73,96,105	0
25	CDL	C	305	100/100	0.80	0.23	41,86,116,128	0
19	TGL	O	303	63/63	0.80	0.21	52,76,99,106	0
19	TGL	L	101	63/63	0.80	0.23	33,63,97,113	0
19	TGL	N	607	63/63	0.80	0.25	45,69,101,121	0
21	EDO	N	615	4/4	0.81	0.24	46,68,84,87	0
27	PSC	E	201	52/52	0.81	0.27	42,95,144,175	0
21	EDO	S	103	4/4	0.81	0.26	40,50,56,68	0
21	EDO	Q	203	4/4	0.82	0.22	41,46,57,69	0
21	EDO	P	308	4/4	0.84	0.18	53,62,69,87	0
26	DMU	O	304	22/33	0.86	0.15	43,69,95,113	0
21	EDO	N	610	4/4	0.87	0.20	39,45,49,55	0
23	CHD	C	306	29/29	0.87	0.13	42,54,66,104	0

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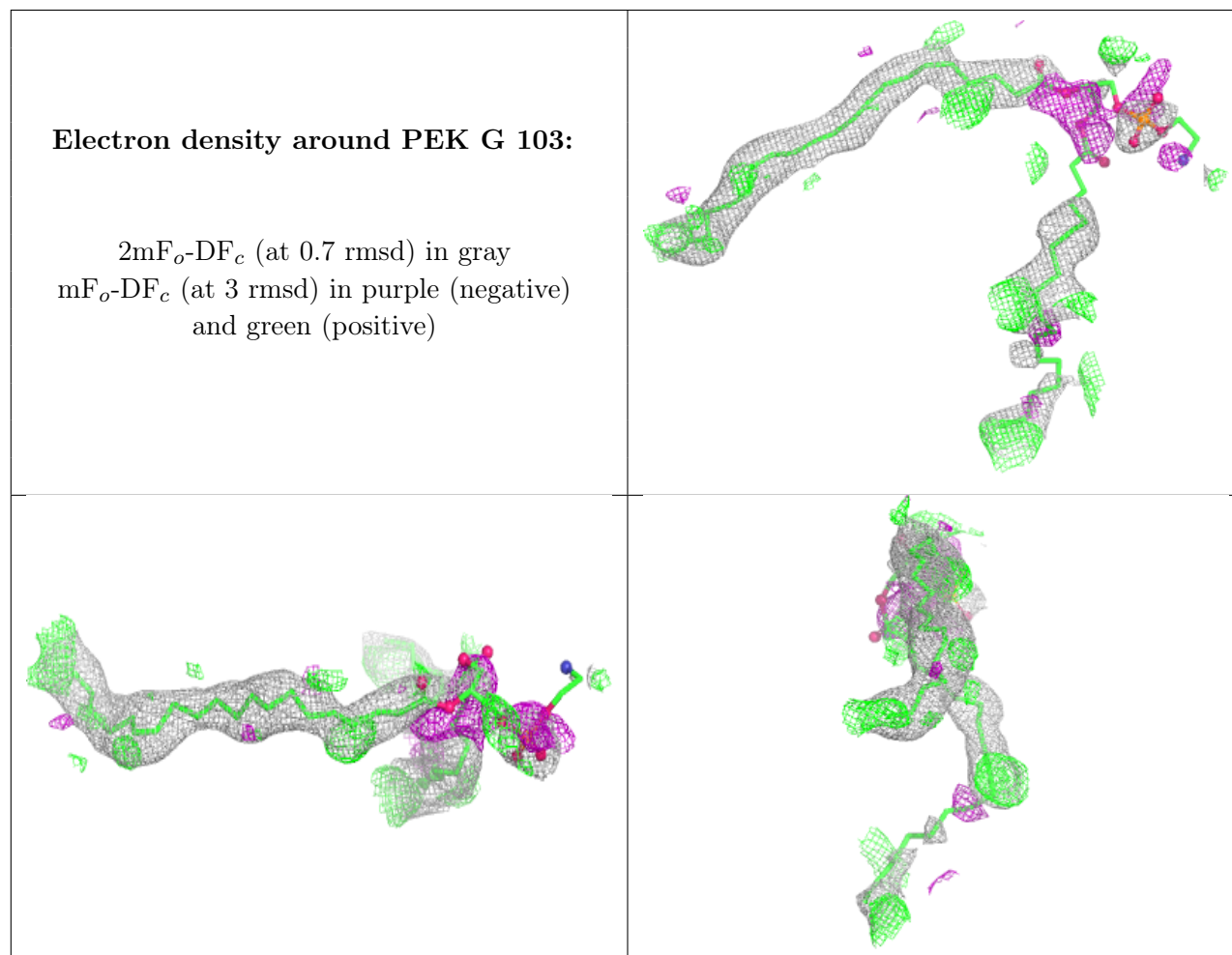
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	DMU	Z	101	33/33	0.89	0.14	46,58,88,96	0
21	EDO	Q	202	4/4	0.90	0.14	35,43,43,59	0
23	CHD	P	306	29/29	0.90	0.12	46,57,72,86	0
21	EDO	A	613	4/4	0.90	0.15	34,42,61,62	0
21	EDO	O	306	4/4	0.91	0.16	43,43,53,53	0
26	DMU	M	101	33/33	0.92	0.11	36,48,66,80	0
21	EDO	A	611	4/4	0.93	0.13	29,30,33,47	0
21	EDO	N	613	4/4	0.93	0.12	40,47,52,58	0
21	EDO	N	612	4/4	0.94	0.14	33,47,64,72	0
24	PEK	P	302	53/53	0.94	0.15	31,53,96,104	0
24	PEK	C	302	53/53	0.94	0.13	26,46,92,97	0
21	EDO	P	309	4/4	0.94	0.12	37,41,42,53	0
20	PGV	P	303	51/51	0.95	0.12	24,36,88,99	0
20	PGV	N	609	51/51	0.96	0.11	23,35,75,81	0
21	EDO	A	612	4/4	0.96	0.14	31,38,51,57	0
21	EDO	N	611	4/4	0.96	0.08	31,32,32,40	0
21	EDO	O	305	4/4	0.96	0.08	32,33,36,36	0
21	EDO	N	614	4/4	0.97	0.07	26,33,35,37	0
21	EDO	S	104	4/4	0.97	0.08	40,40,47,58	0
23	CHD	C	301	29/29	0.97	0.06	24,29,35,38	0
20	PGV	C	303	51/51	0.97	0.10	20,33,83,93	0
21	EDO	C	308	4/4	0.97	0.09	34,40,48,56	0
23	CHD	O	302	29/29	0.97	0.06	24,28,36,41	0
23	CHD	P	301	29/29	0.97	0.06	24,31,35,37	0
20	PGV	A	608	51/51	0.97	0.10	20,31,73,85	0
21	EDO	S	102	4/4	0.97	0.07	26,27,29,30	0
18	NA	N	606	1/1	0.98	0.09	34,34,34,34	0
14	HEA	N	601	60/60	0.98	0.06	21,27,44,47	0
21	EDO	B	303	4/4	0.98	0.05	27,27,29,31	0
15	NO	A	603	2/2	0.98	0.06	20,20,20,25	0
21	EDO	F	102	4/4	0.98	0.05	25,25,26,27	0
21	EDO	A	610	4/4	0.98	0.07	24,24,26,29	0
23	CHD	B	302	29/29	0.98	0.05	24,28,35,40	0
18	NA	A	606	1/1	0.98	0.10	29,29,29,29	0
14	HEA	A	601	60/60	0.99	0.05	16,22,37,41	0
14	HEA	N	602	60/60	0.99	0.05	21,25,31,37	0
14	HEA	A	602	60/60	0.99	0.05	17,21,28,34	0
15	NO	N	603	2/2	0.99	0.04	26,26,26,27	0
16	CU	A	604	1/1	1.00	0.01	22,22,22,22	0
16	CU	N	604	1/1	1.00	0.01	24,24,24,24	0
22	CUA	B	301	2/2	1.00	0.01	23,23,23,23	0
22	CUA	O	301	2/2	1.00	0.02	28,28,28,28	0

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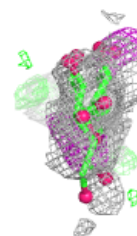
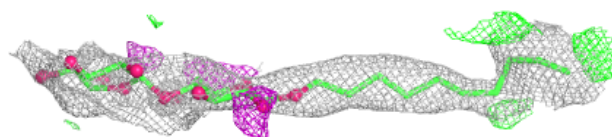
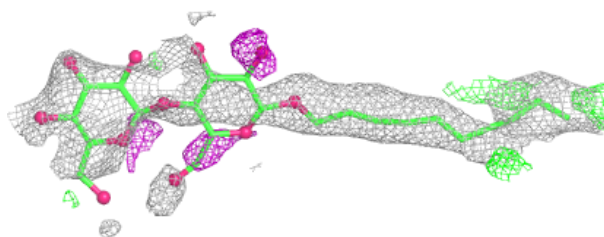
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	MG	A	605	1/1	1.00	0.05	19,19,19,19	0
17	MG	N	605	1/1	1.00	0.07	24,24,24,24	0
28	ZN	F	101	1/1	1.00	0.04	29,29,29,29	0
28	ZN	S	101	1/1	1.00	0.03	31,31,31,31	0

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.

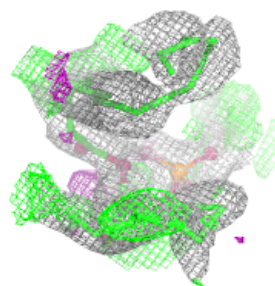
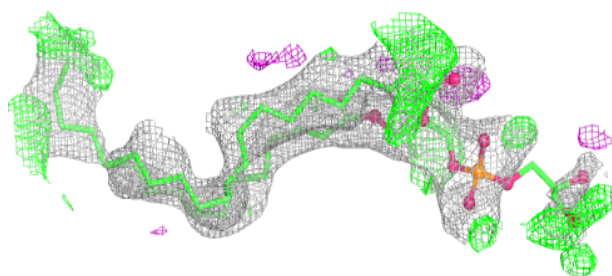
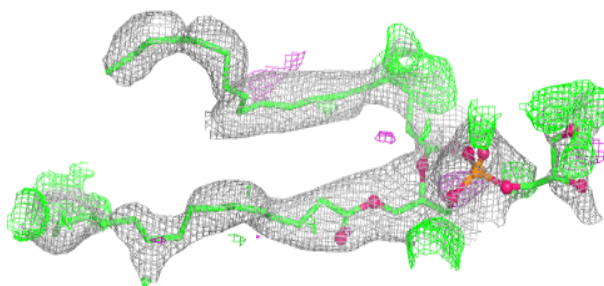


Electron density around DMU P 307:

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

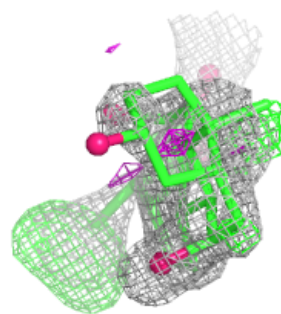
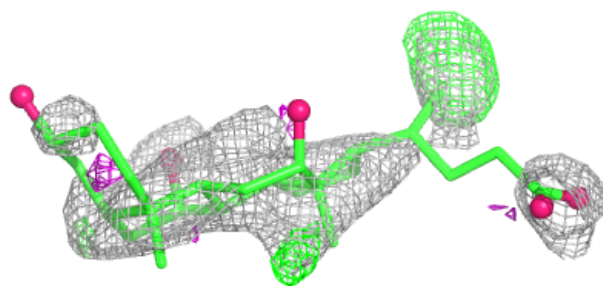
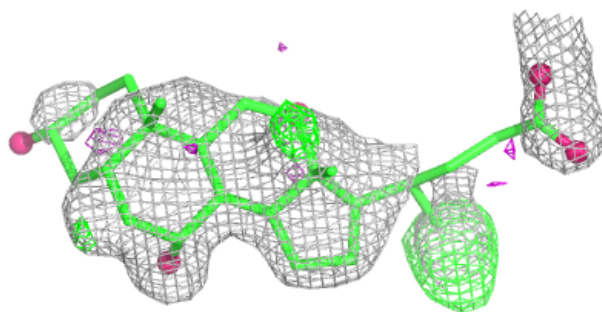
**Electron density around PGV P 304:**

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



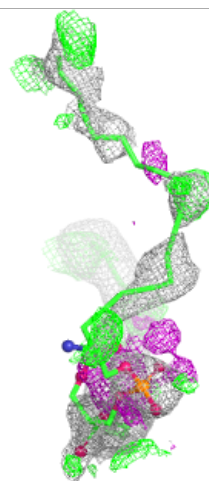
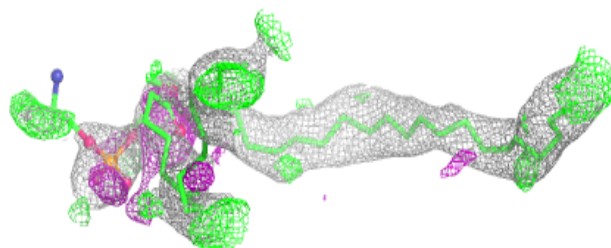
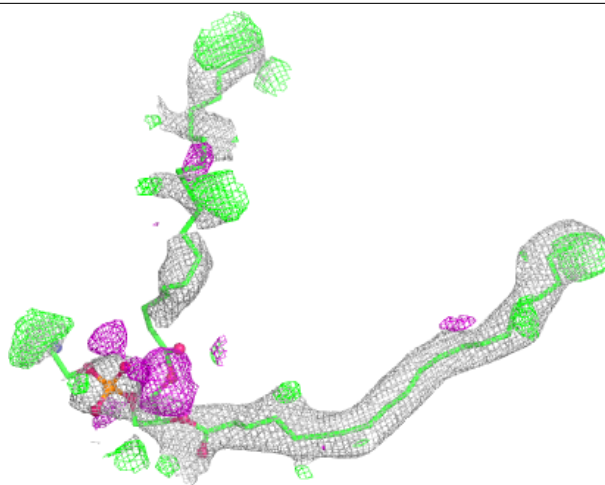
Electron density around CHD J 101:

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



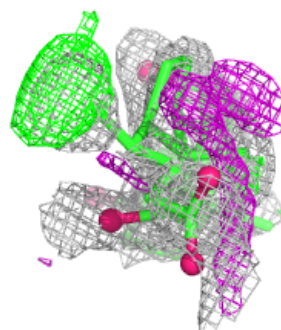
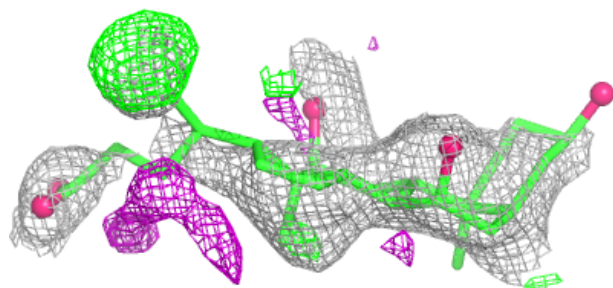
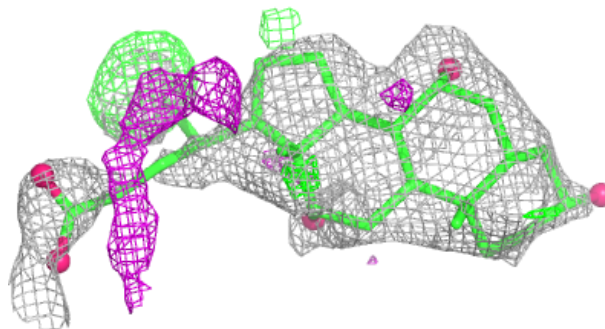
Electron density around PEK T 102:

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

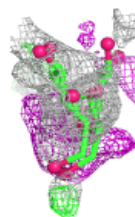
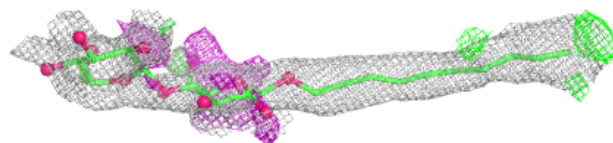
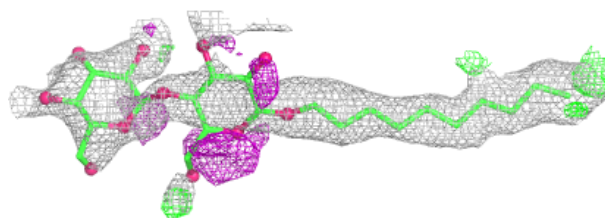


Electron density around CHD W 101:

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

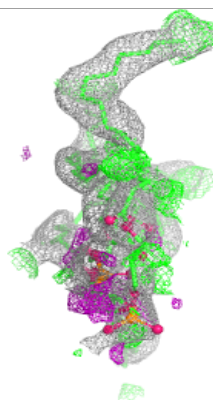
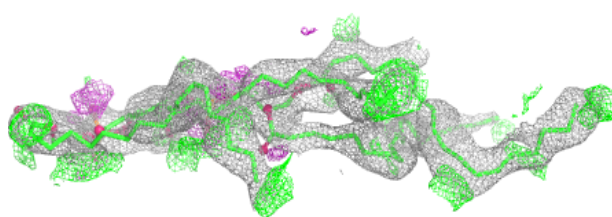
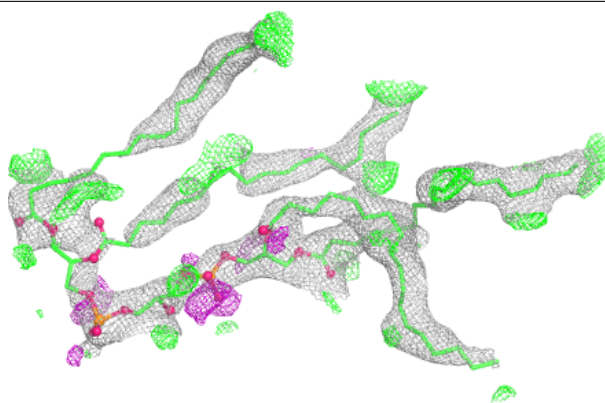
**Electron density around DMU C 307:**

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

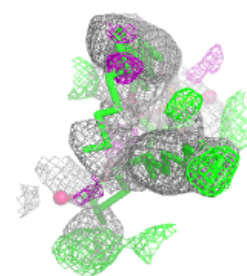
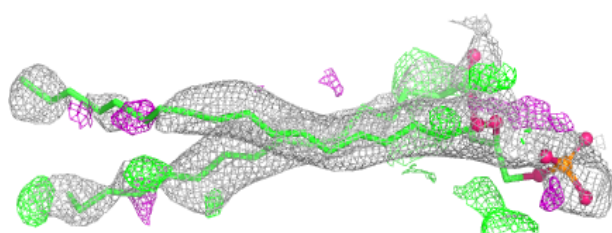
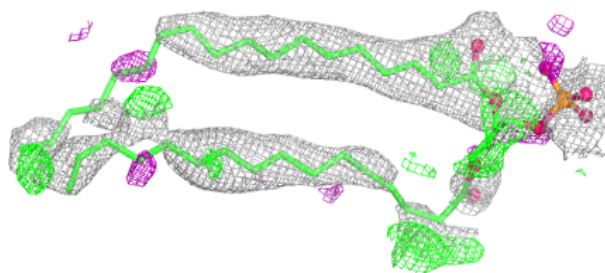


Electron density around CDL T 103:

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

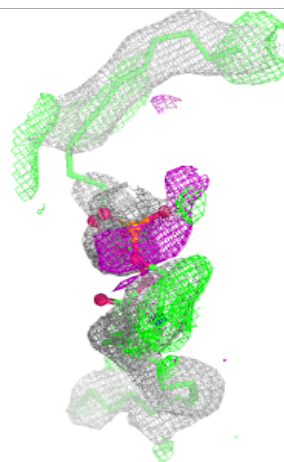
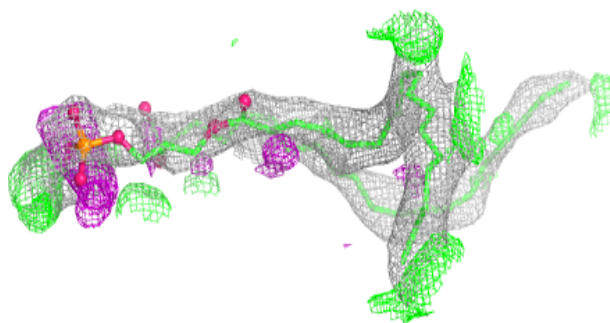
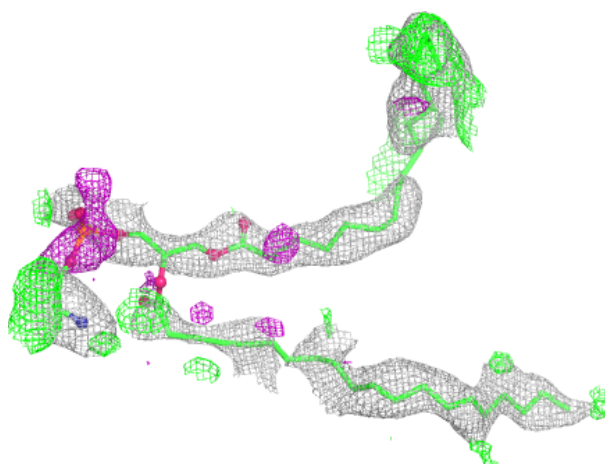
**Electron density around PGV N 608:**

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



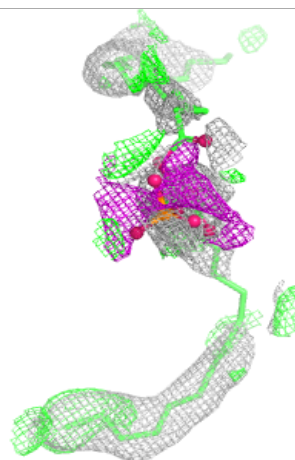
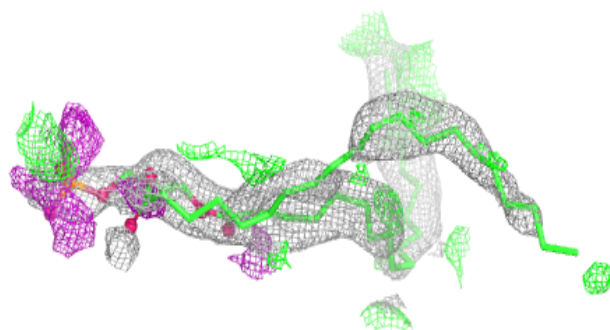
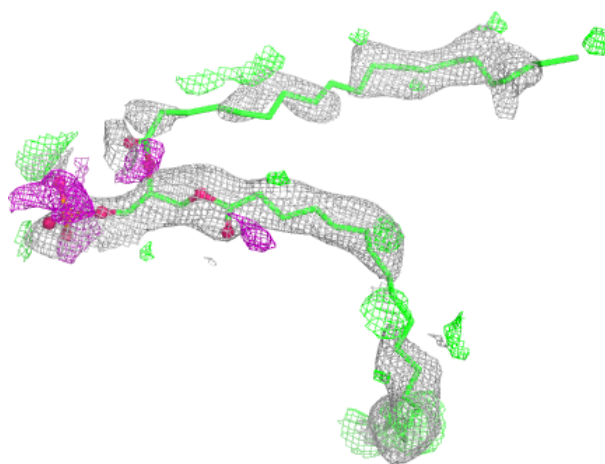
Electron density around PEK T 101:

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



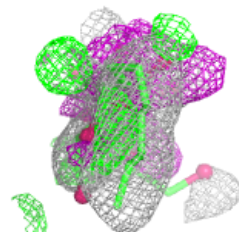
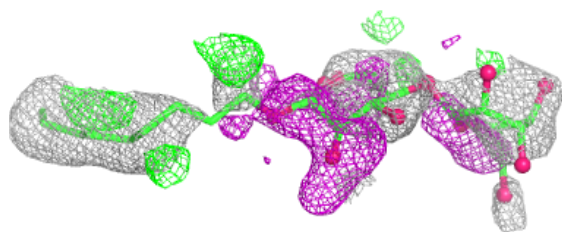
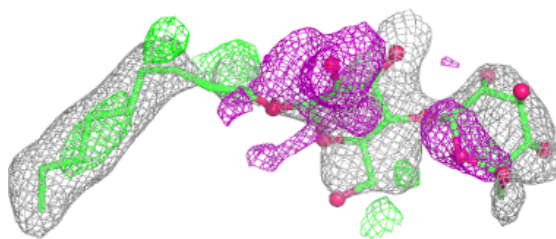
Electron density around PEK G 101:

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



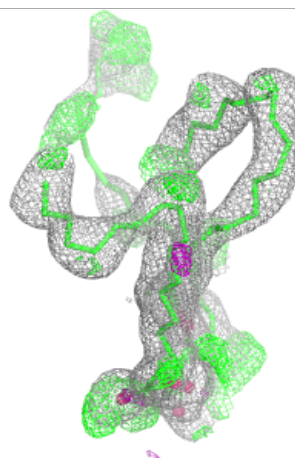
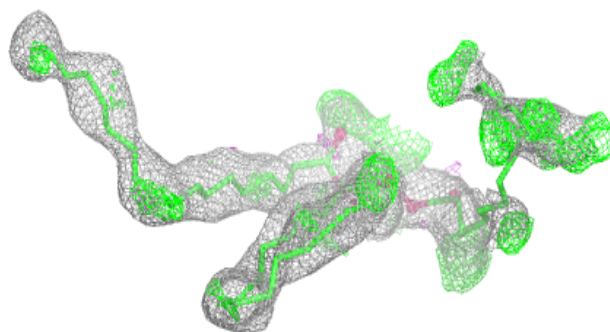
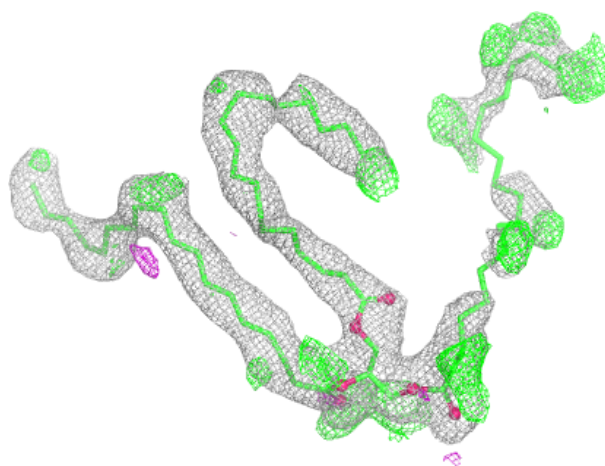
Electron density around DMU W 102:

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



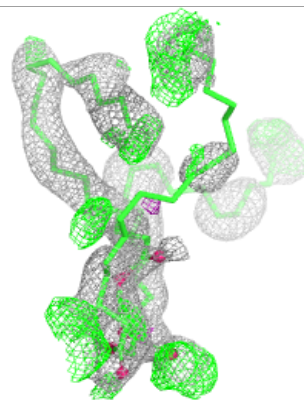
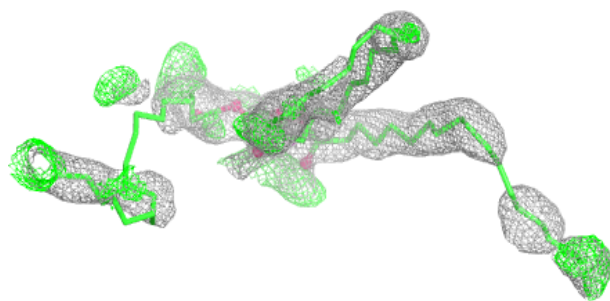
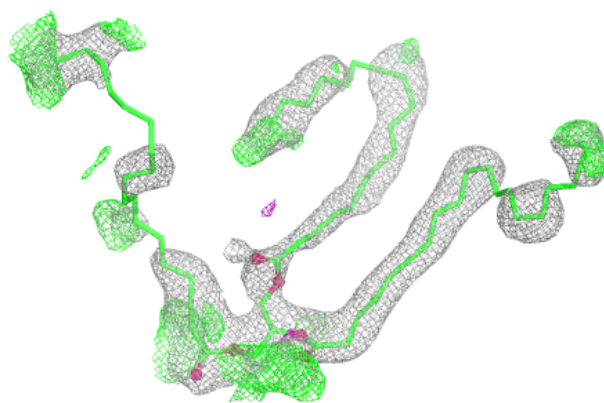
Electron density around TGL D 201:

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

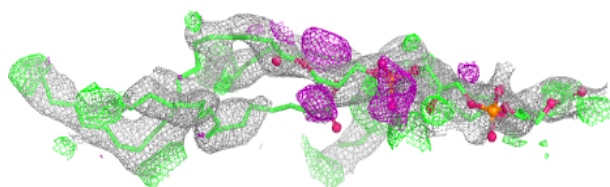
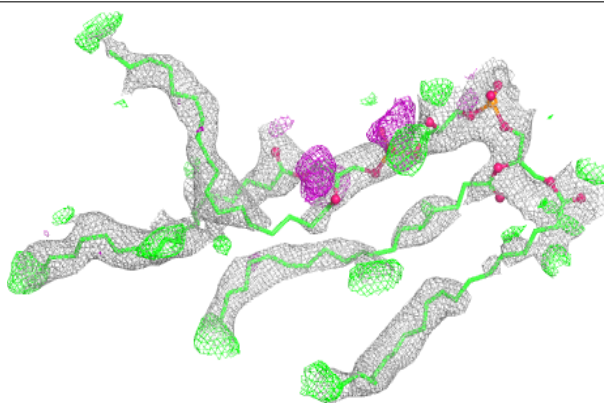


Electron density around TGL Q 201:

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

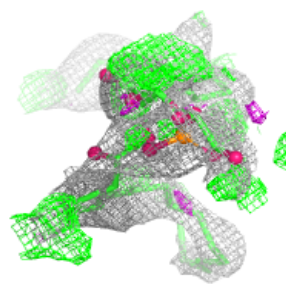
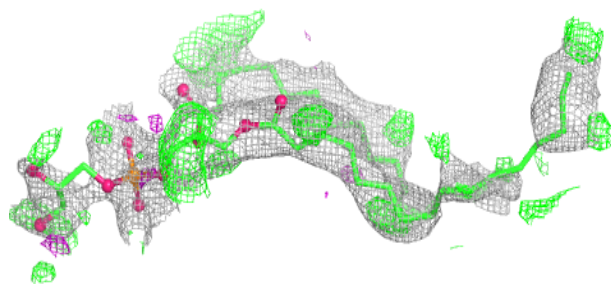
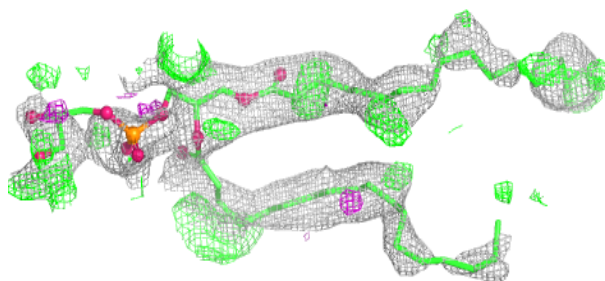
**Electron density around CDL G 102:**

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

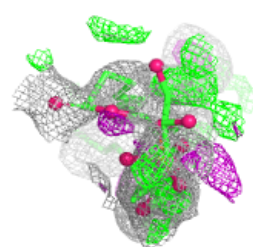
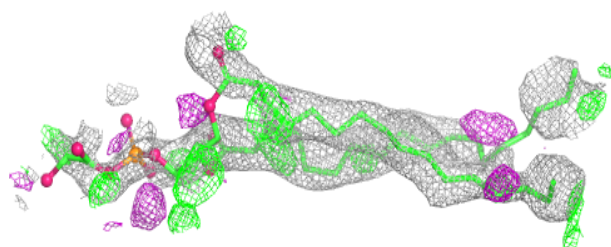
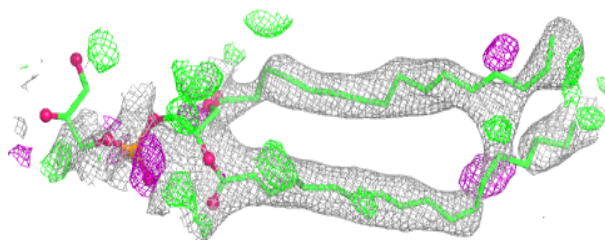


Electron density around PGV C 304:

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

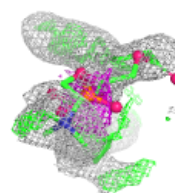
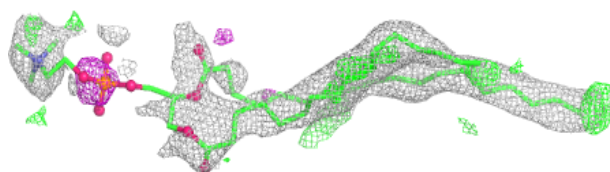
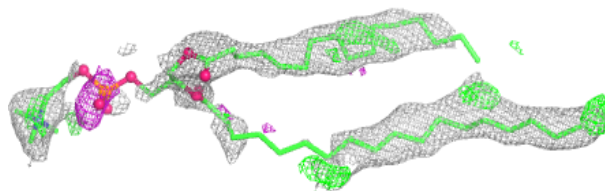
**Electron density around PGV A 609:**

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



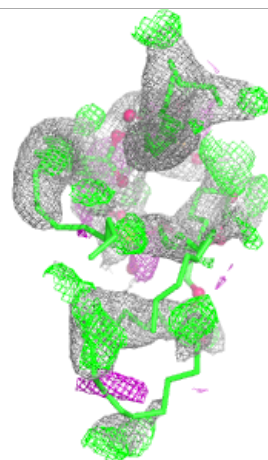
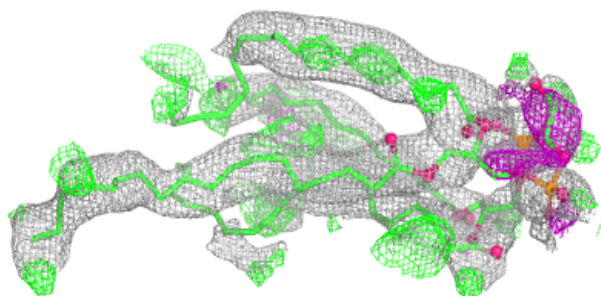
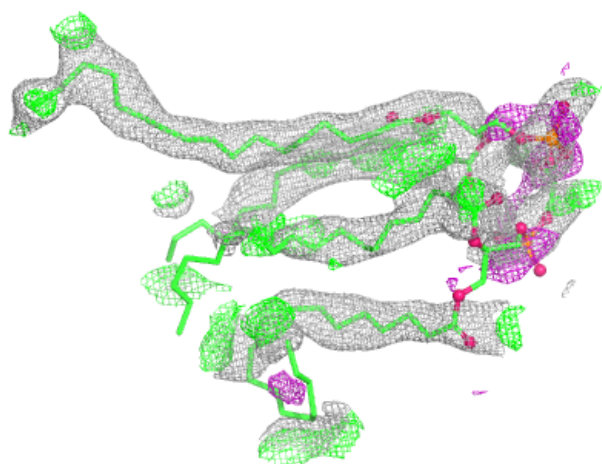
Electron density around PSC R 201:

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



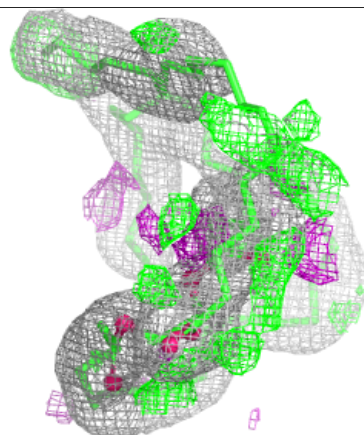
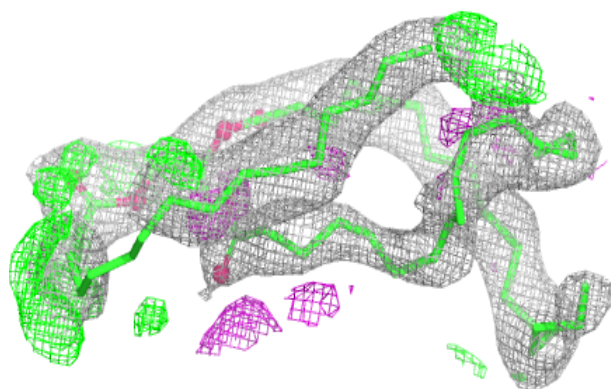
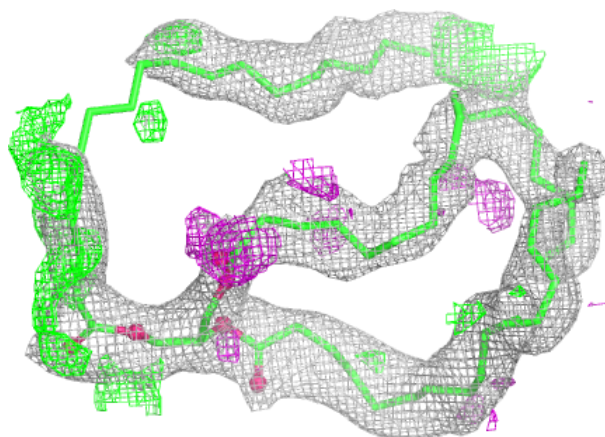
Electron density around CDL P 305:

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



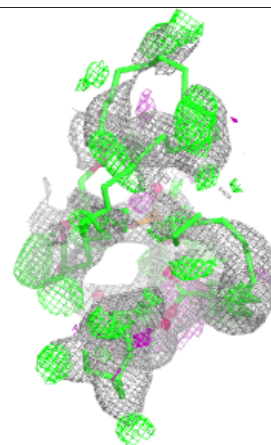
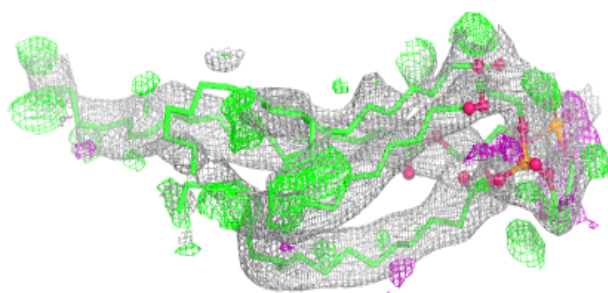
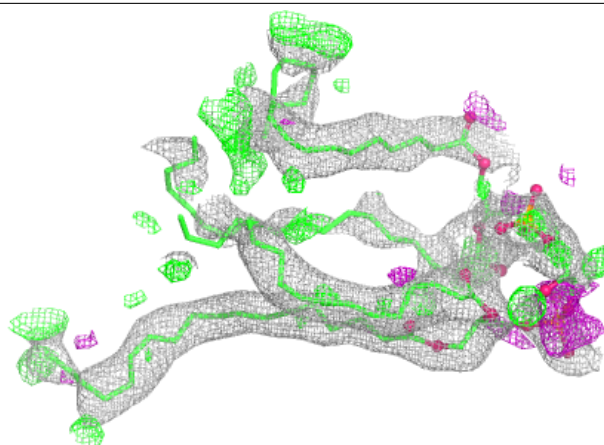
Electron density around TGL A 607:

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

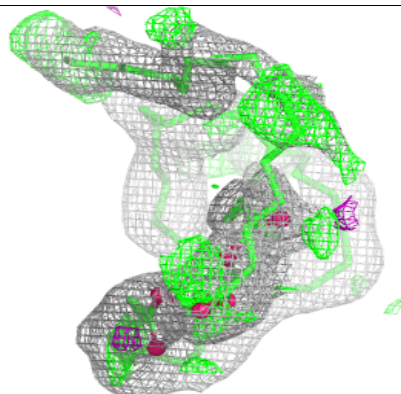
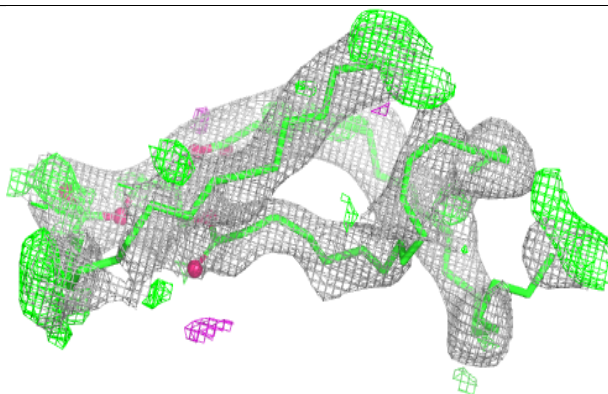
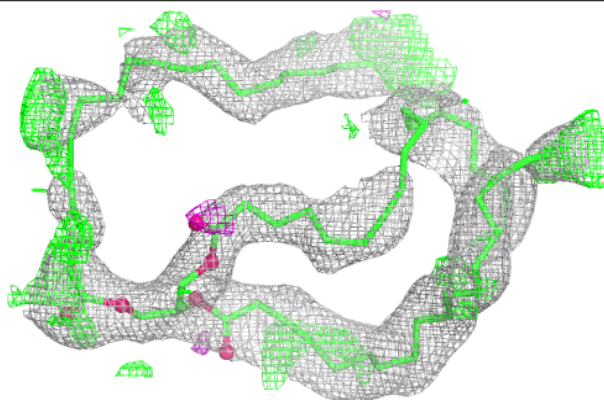


Electron density around CDL C 305:

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

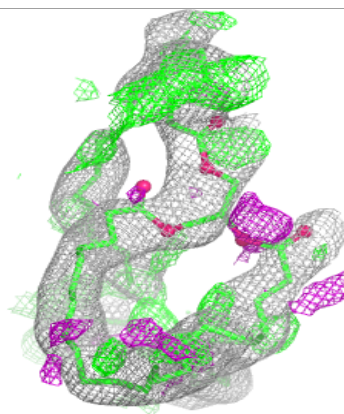
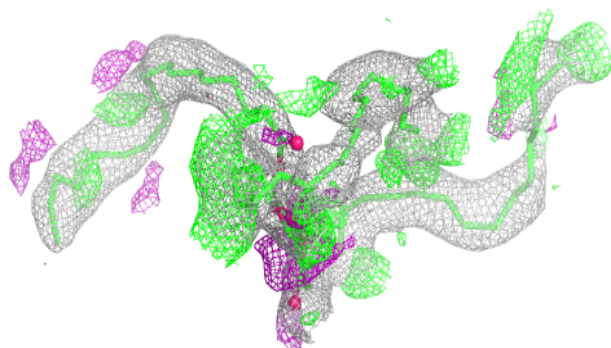
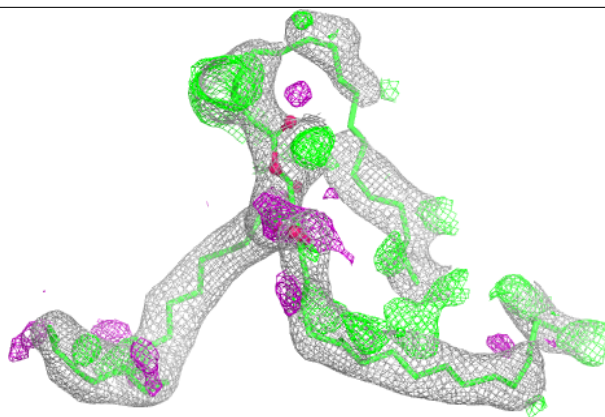
**Electron density around TGL O 303:**

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

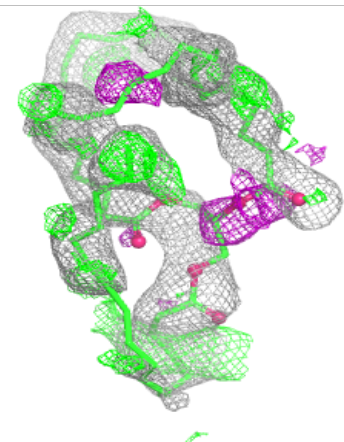
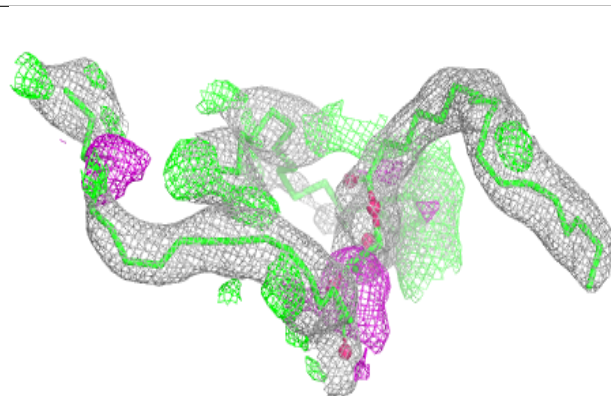
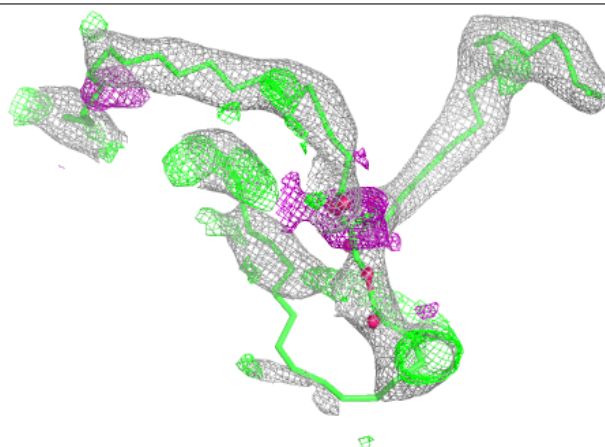


Electron density around TGL L 101:

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

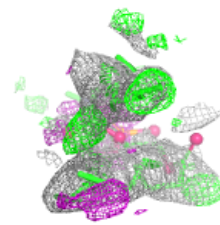
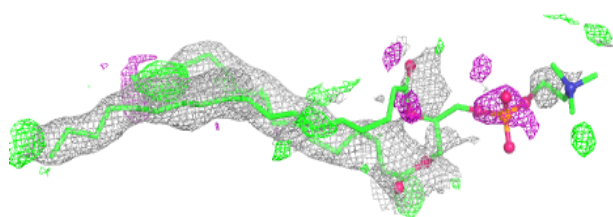
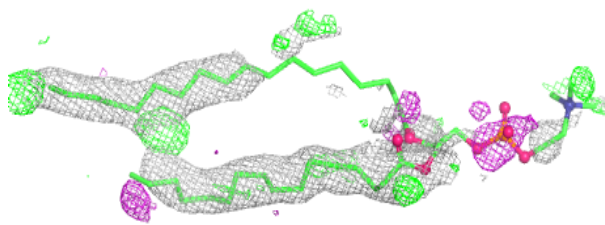
**Electron density around TGL N 607:**

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

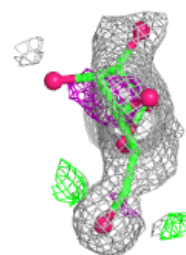
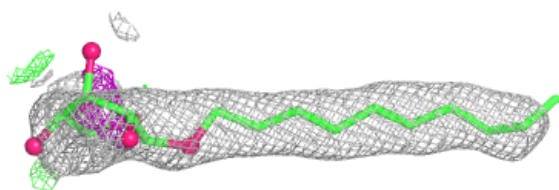
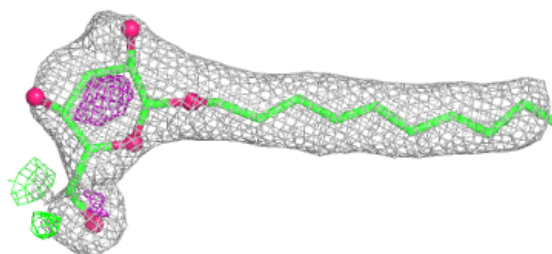


Electron density around PSC E 201:

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

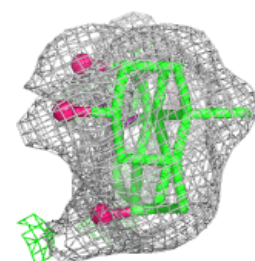
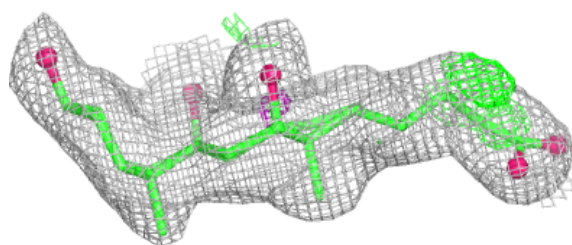
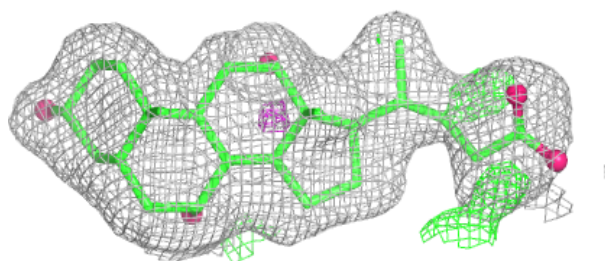
**Electron density around DMU O 304:**

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

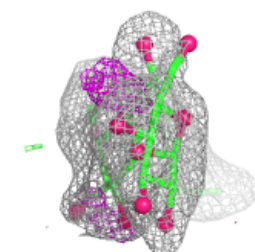
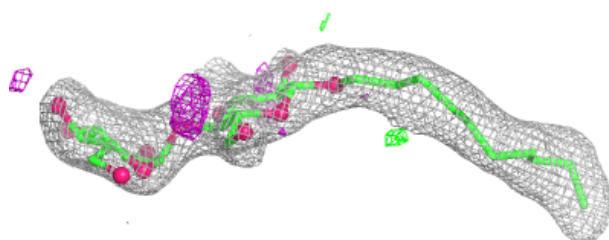
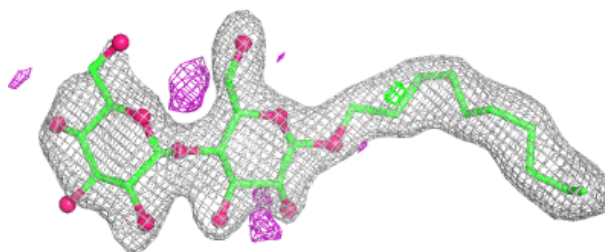


Electron density around CHD C 306:

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

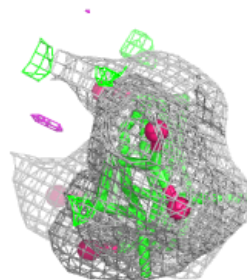
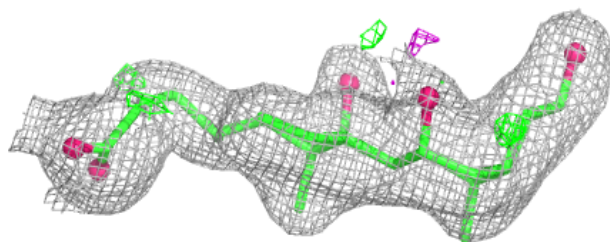
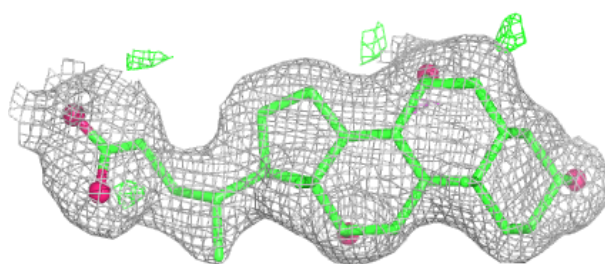
**Electron density around DMU Z 101:**

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

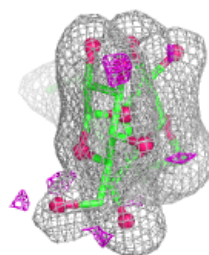
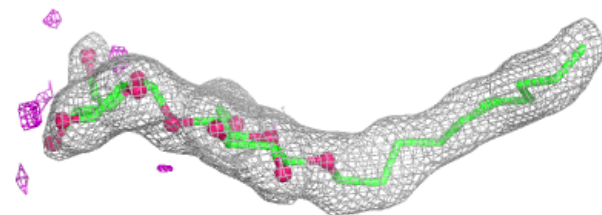
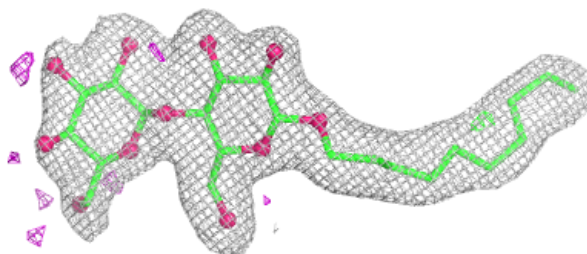


Electron density around CHD P 306:

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

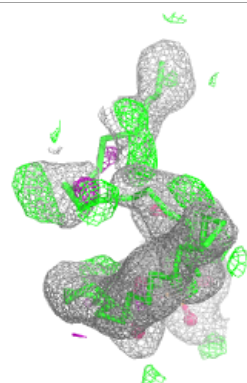
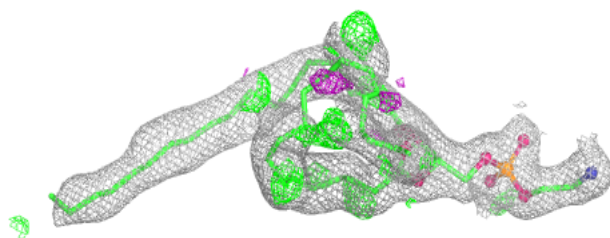
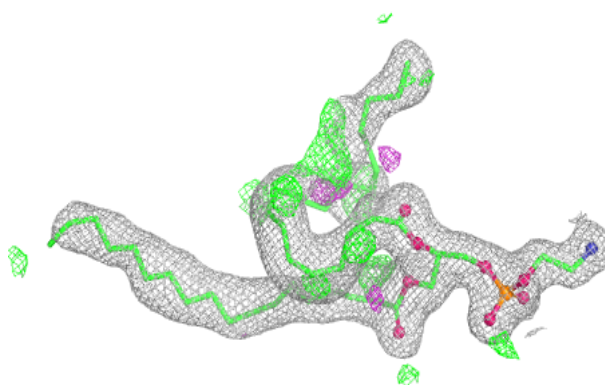
**Electron density around DMU M 101:**

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

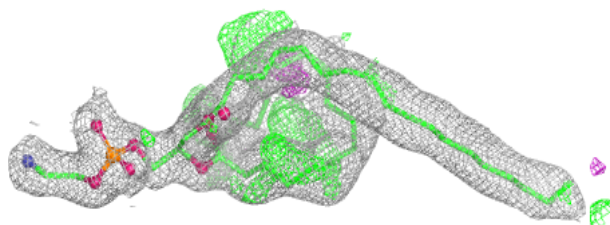
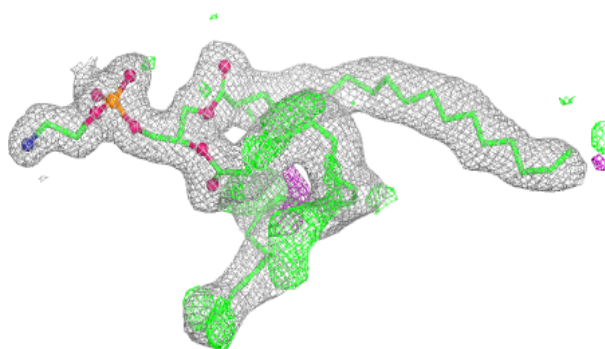


Electron density around PEK P 302:

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

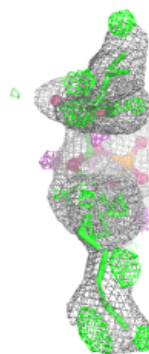
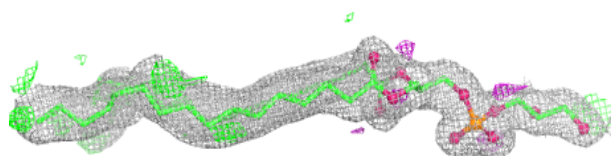
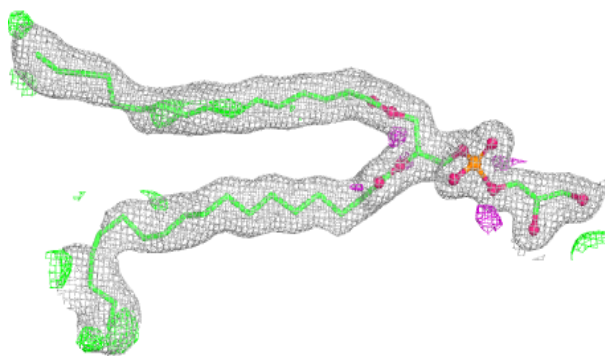
**Electron density around PEK C 302:**

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

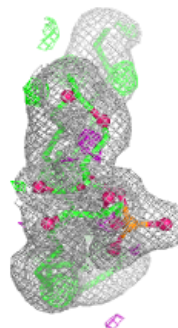
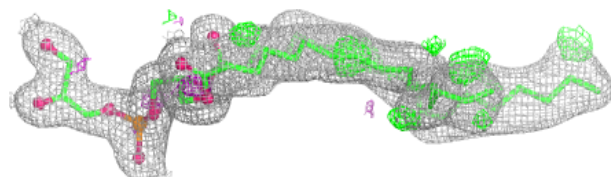
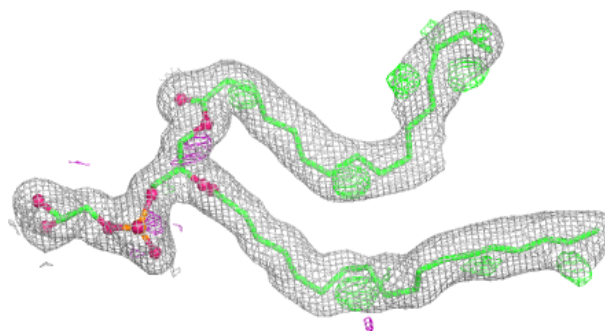


Electron density around PGV P 303:

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

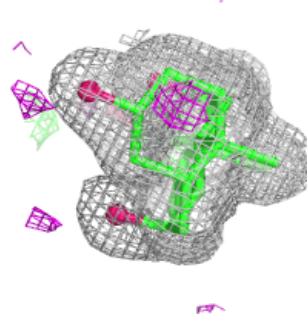
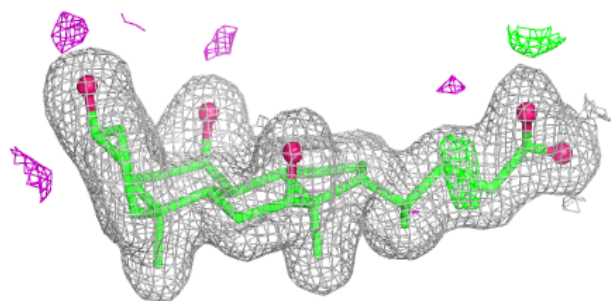
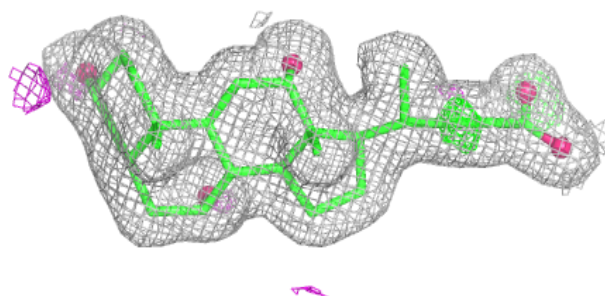
**Electron density around PGV N 609:**

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

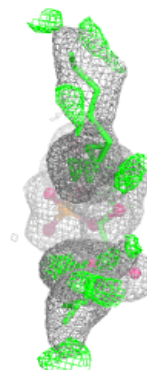
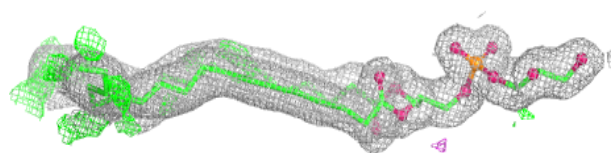
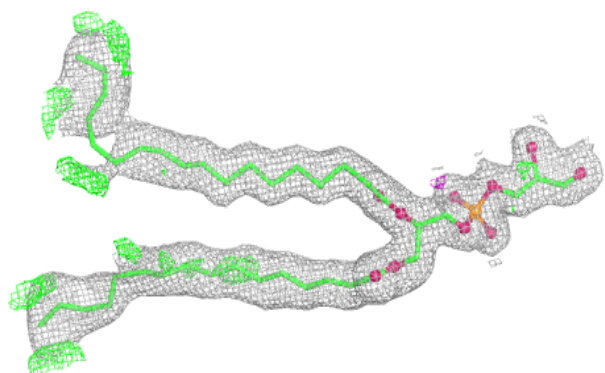


Electron density around CHD C 301:

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

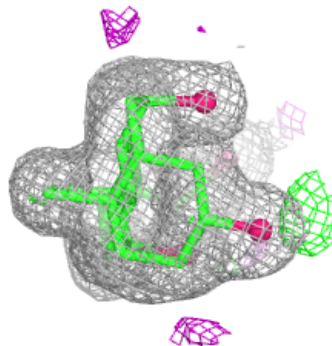
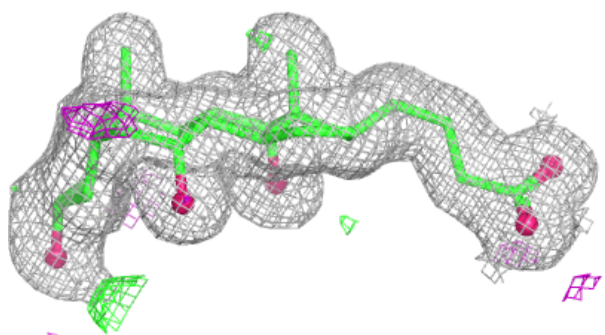
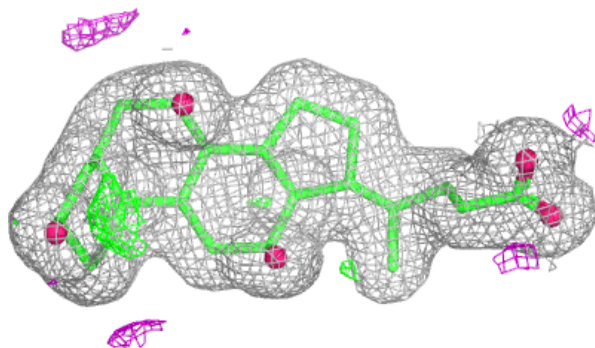
**Electron density around PGV C 303:**

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

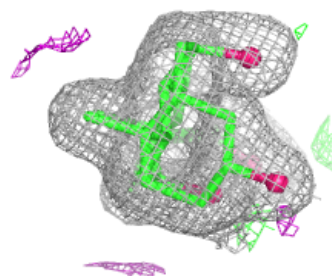
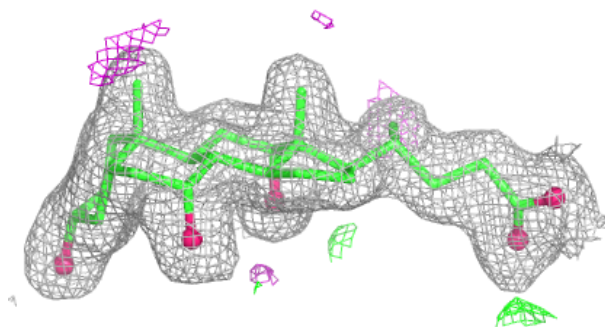
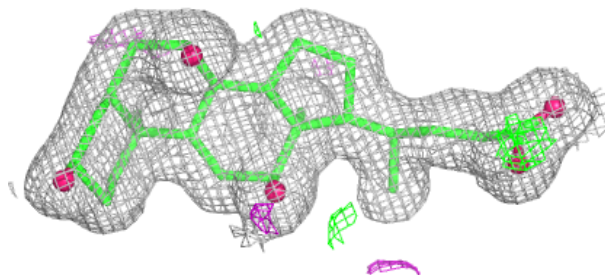


Electron density around CHD O 302:

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

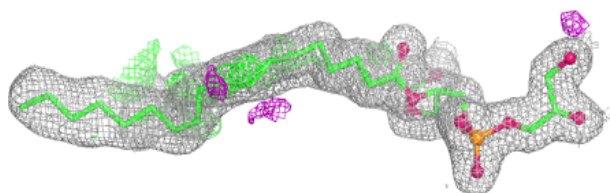
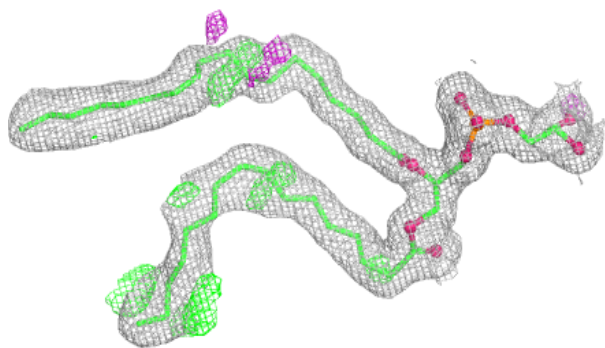
**Electron density around CHD P 301:**

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

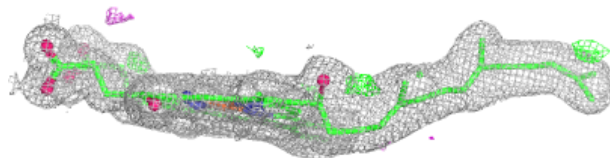
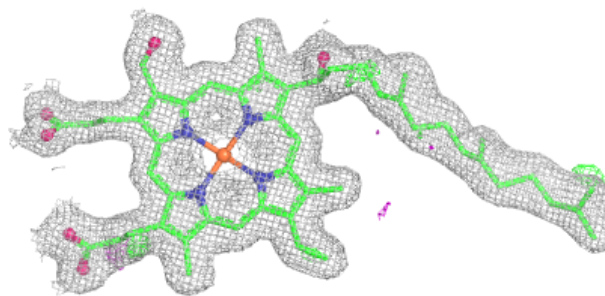


Electron density around PGV A 608:

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

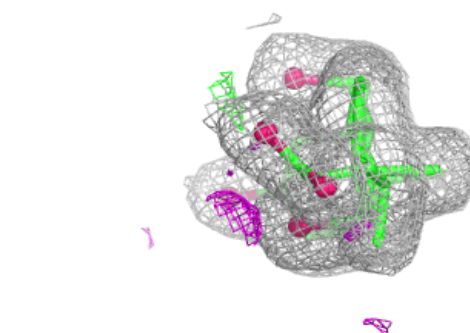
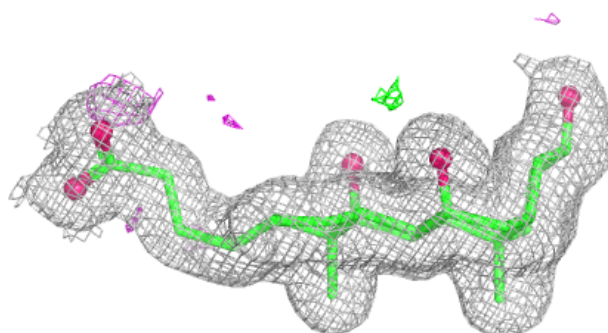
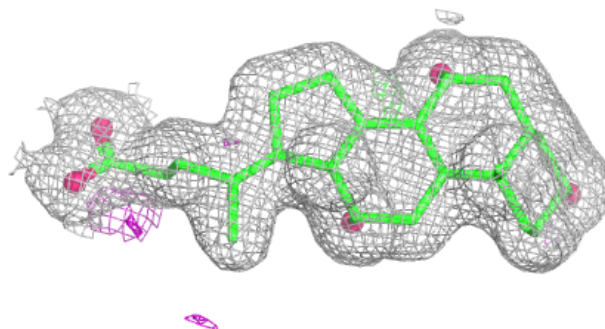
**Electron density around HEA N 601:**

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

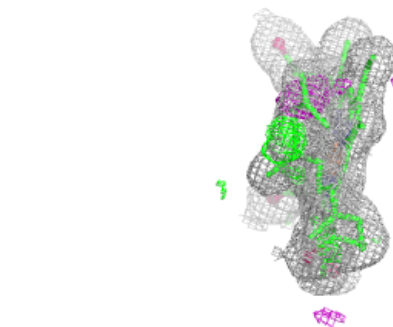
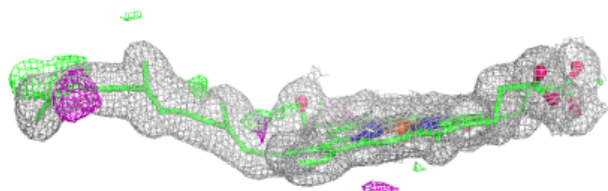
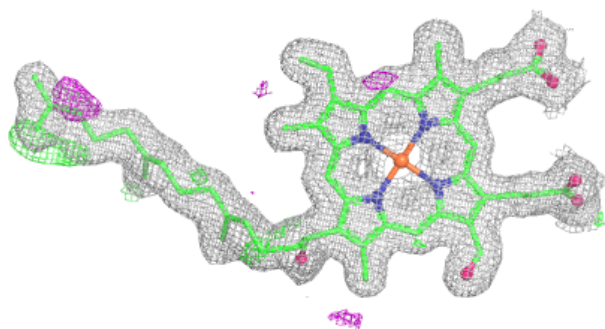


Electron density around CHD B 302:

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

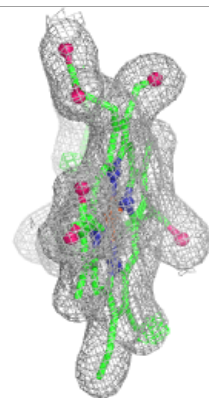
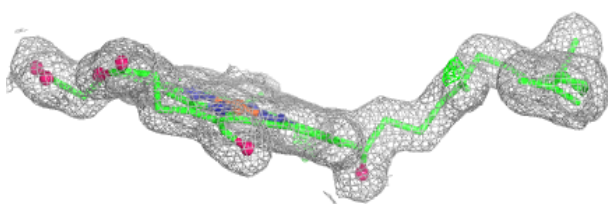
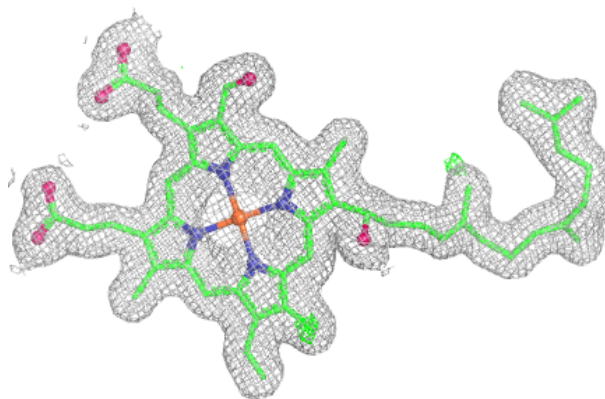
**Electron density around HEA A 601:**

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

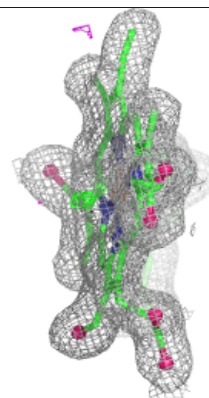
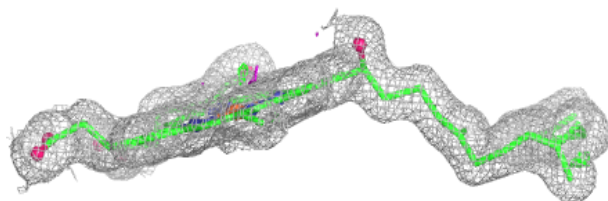
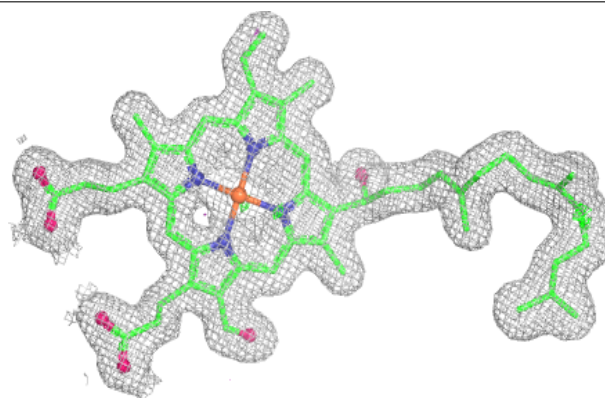


Electron density around HEA N 602:

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

**Electron density around HEA A 602:**

$2mF_o-DF_c$ (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.