



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2026 – 10:46 PM EDT

PDB ID : 5WAU / pdb_00005wau
Title : Crystal Structure of CO-bound Cytochrome c Oxidase determined by Synchrotron X-Ray Crystallography at 100 K
Authors : Fromme, R.; Ishigami, I.; Yeh, S.Y.; Zatsepin, N.; Grant, T.; Fromme, P.; Rousseau, D.
Deposited on : 2017-06-27
Resolution : 1.95 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

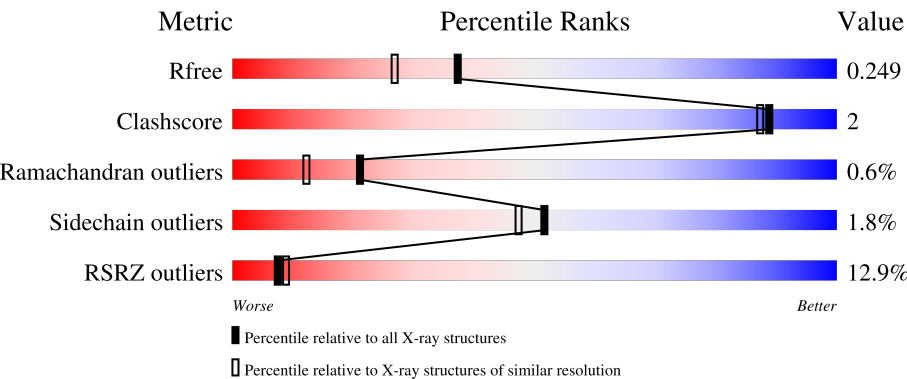
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	2% 94% 6%
1	a	514	7% 93% 7%
2	B	227	7% 92% 8%
2	b	227	13% 89% 10%

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Mol	Chain	Length	Quality of chain
3	C	261	
3	c	261	
4	D	147	
4	d	147	
5	E	109	
5	e	109	
6	F	98	
6	f	98	
7	G	85	
7	g	85	
8	H	85	
8	h	85	
9	I	73	
9	i	73	
10	J	59	
10	j	59	
11	K	56	
11	k	56	
12	L	47	
12	l	47	
13	M	46	
13	m	46	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32575 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	0	0
			4027	2691	623	678	35			
1	a	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	b	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	c	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	d	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	e	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	f	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	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	g	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	h	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	i	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	j	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	k	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

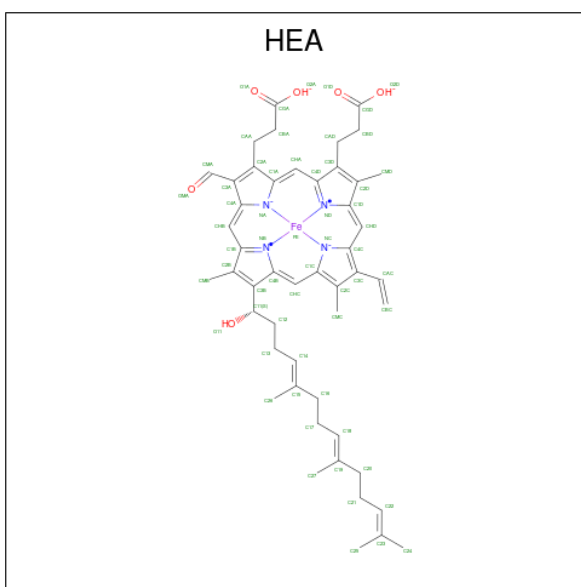
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	l	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	m	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 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	a	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	a	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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

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

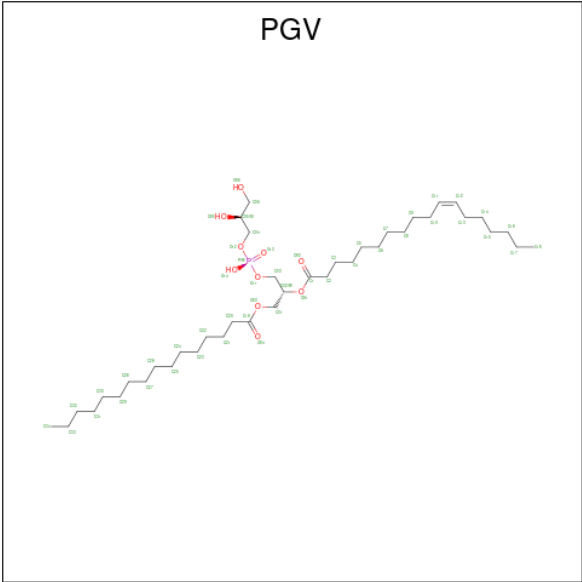
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

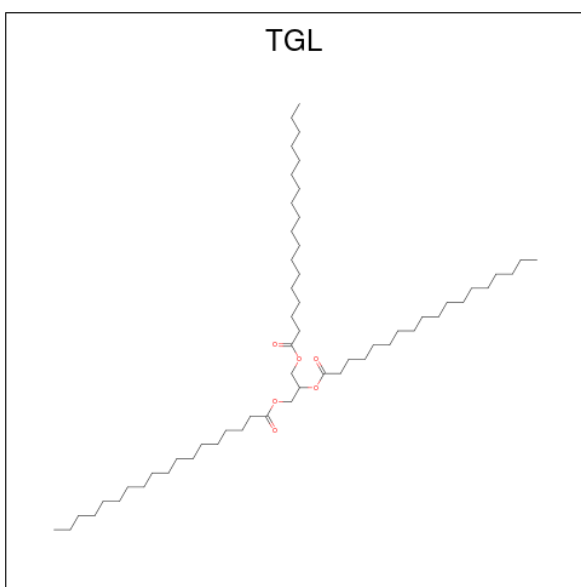
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	a	1	Total	Na	0	0
			1	1		

- Molecule 18 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



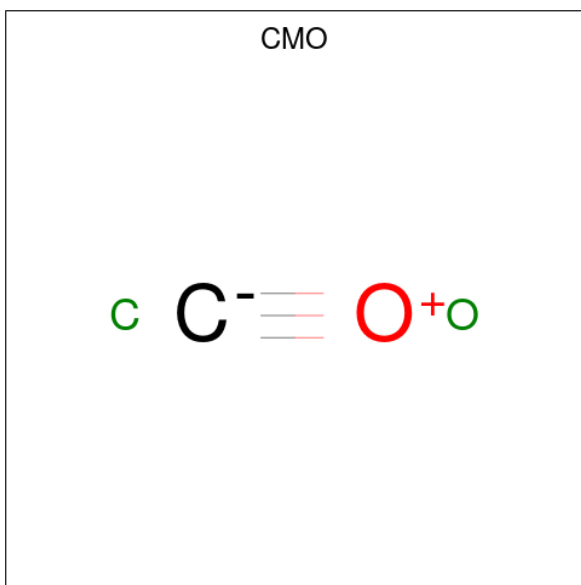
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	a	1	Total	C	O	P	0	0
			51	40	10	1		
18	a	1	Total	C	O	P	0	0
			51	40	10	1		
18	c	1	Total	C	O	P	0	0
			51	40	10	1		
18	c	1	Total	C	O	P	0	0
			51	40	10	1		

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



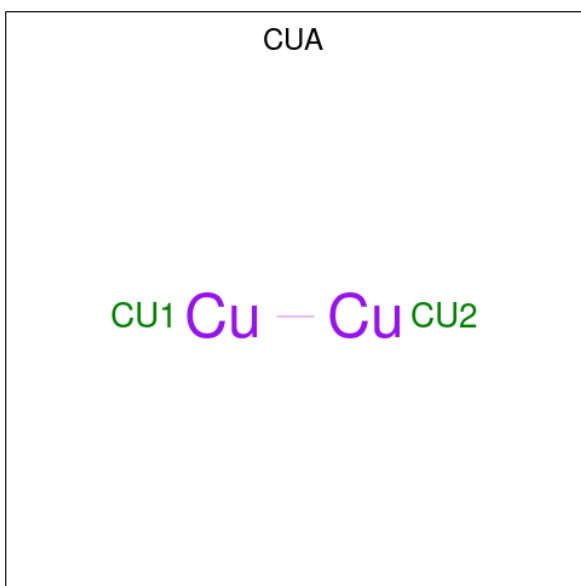
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	b	1	Total	C	O	0	0
			63	57	6		
19	d	1	Total	C	O	0	0
			63	57	6		
19	l	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



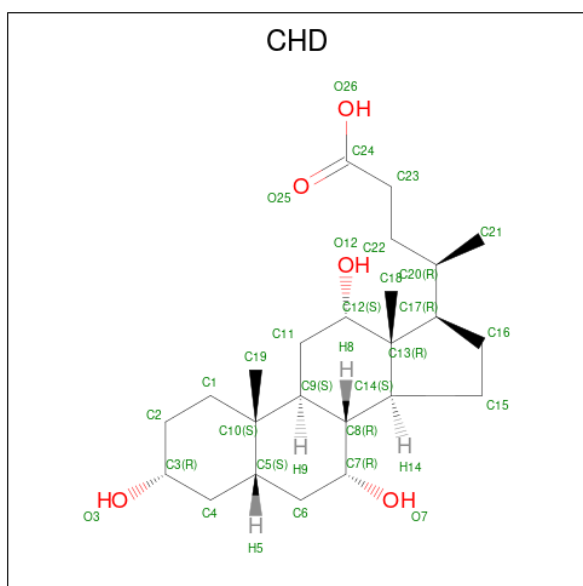
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			2	1	1		
20	a	1	Total	C	O	0	0
			2	1	1		

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



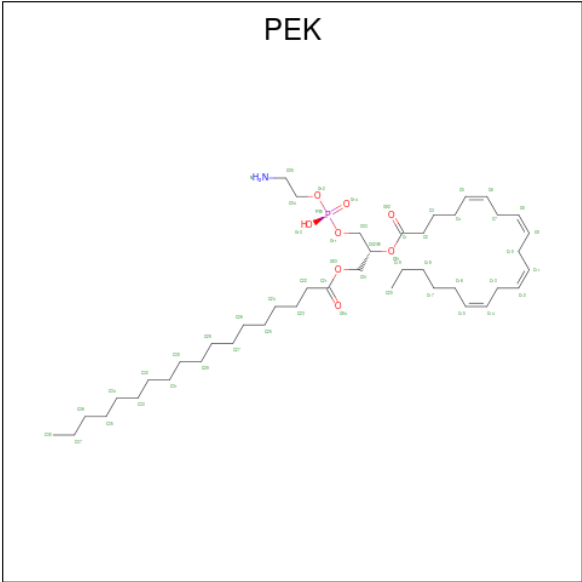
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	b	1	Total	Cu	0	0
			2	2		

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



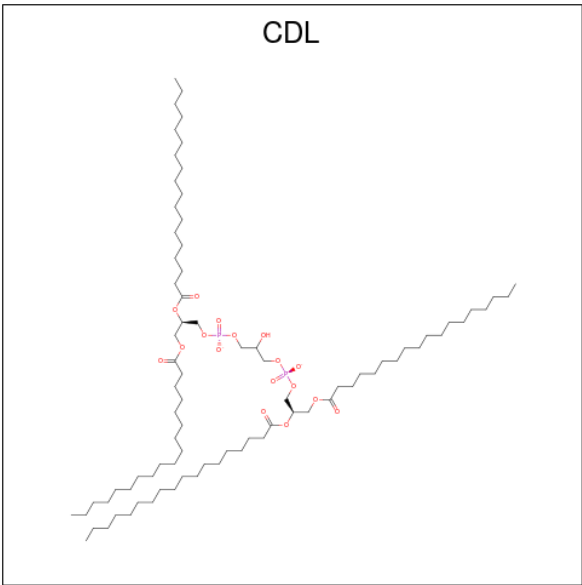
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	c	1	Total	C	O	0	0
			29	24	5		
22	c	1	Total	C	O	0	0
			29	24	5		
22	j	1	Total	C	O	0	0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

- Molecule 23 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



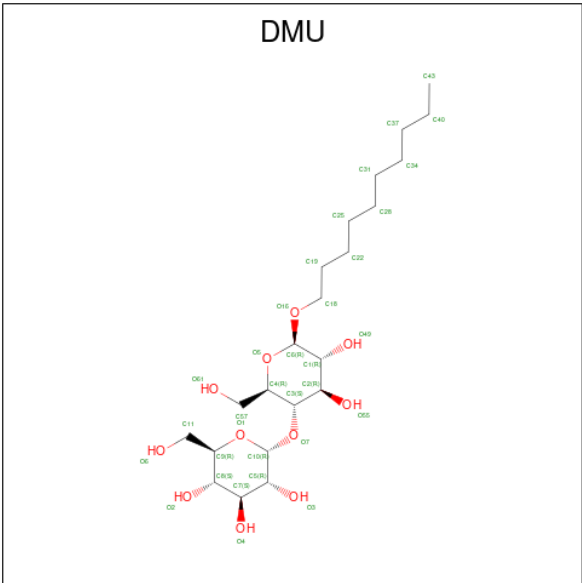
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



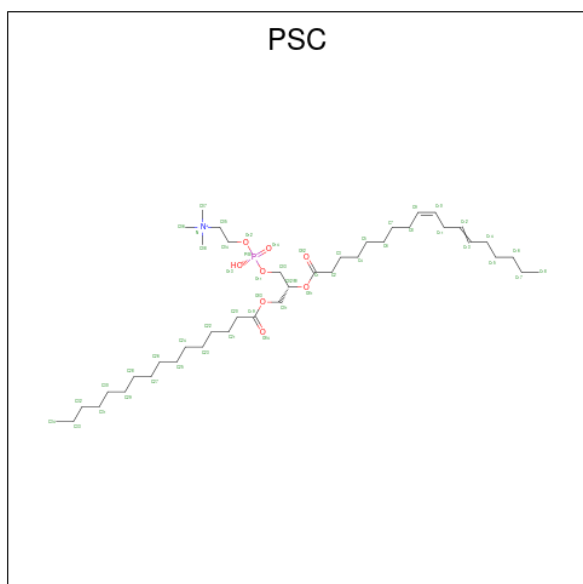
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	C	1	Total	C	O	P	0	0
			100	81	17	2		
24	G	1	Total	C	O	P	0	0
			100	81	17	2		
24	c	1	Total	C	O	P	0	0
			100	81	17	2		
24	g	1	Total	C	O	P	0	0
			100	81	17	2		

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



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



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

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

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	243	Total O 243 243	0	0
28	B	180	Total O 180 180	0	0
28	C	122	Total O 122 122	0	0
28	D	125	Total O 125 125	0	0
28	E	100	Total O 100 100	0	0
28	F	104	Total O 104 104	0	0
28	G	57	Total O 57 57	0	0
28	H	57	Total O 57 57	0	0
28	I	33	Total O 33 33	0	0
28	J	36	Total O 36 36	0	0
28	K	41	Total O 41 41	0	0
28	L	47	Total O 47 47	0	0
28	M	29	Total O 29 29	0	0
28	a	187	Total O 187 187	0	0
28	b	109	Total O 109 109	0	0
28	c	96	Total O 96 96	0	0
28	d	37	Total O 37 37	0	0
28	e	56	Total O 56 56	0	0
28	f	62	Total O 62 62	0	0
28	g	27	Total O 27 27	0	0
28	h	36	Total O 36 36	0	0
28	i	23	Total O 23 23	0	0

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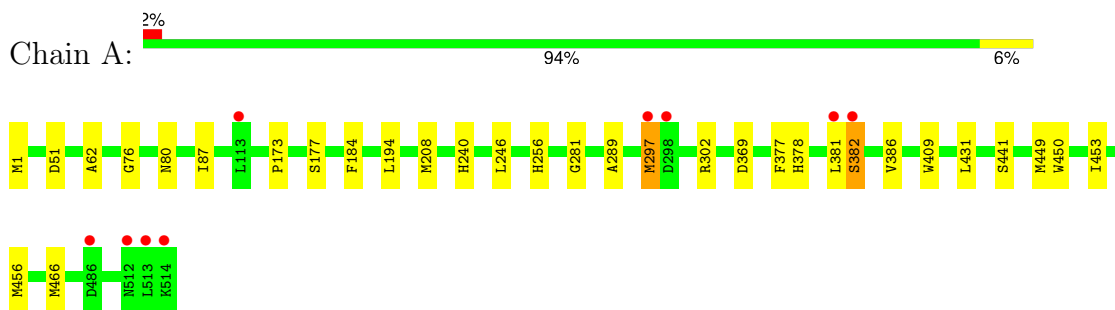
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	j	14	Total 14	O 14	0	0
28	k	7	Total 7	O 7	0	0
28	l	8	Total 8	O 8	0	0
28	m	5	Total 5	O 5	0	0

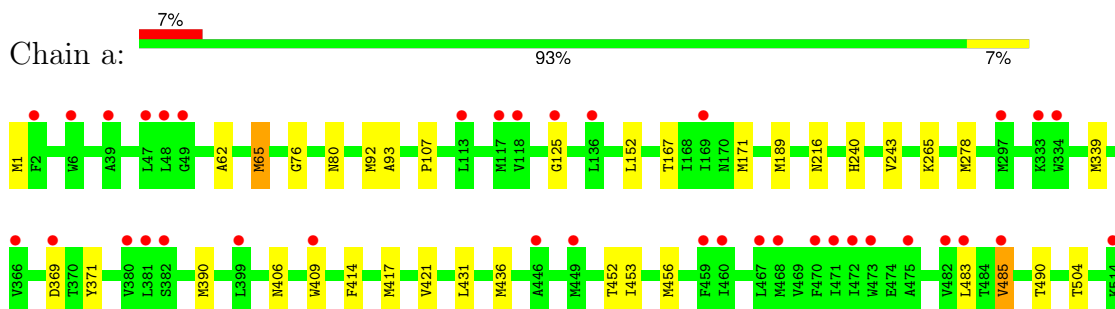
3 Residue-property plots [i](#)

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

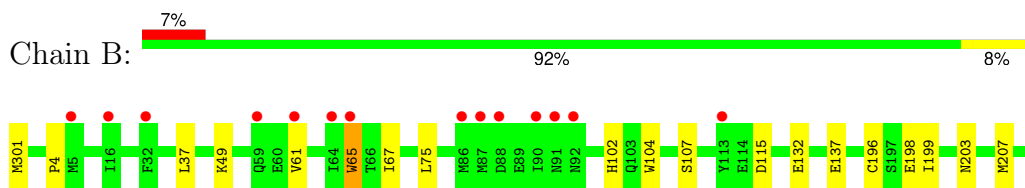
- Molecule 1: Cytochrome c oxidase subunit 1



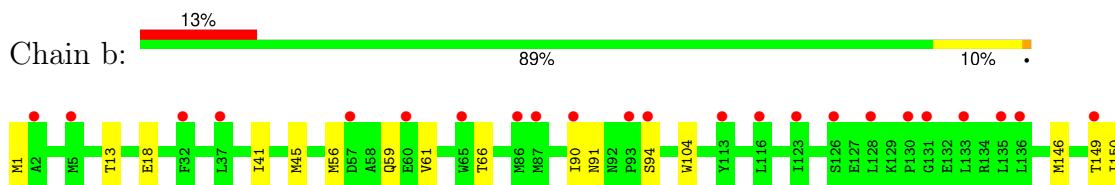
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2

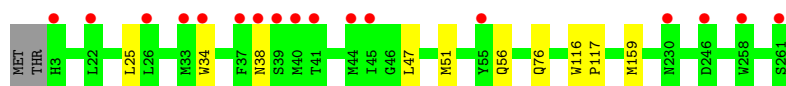




- Molecule 3: Cytochrome c oxidase subunit 3



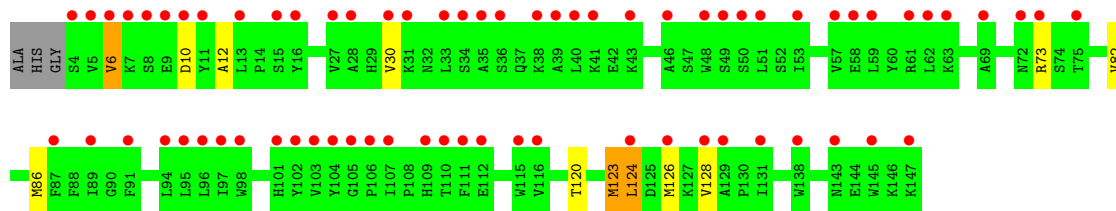
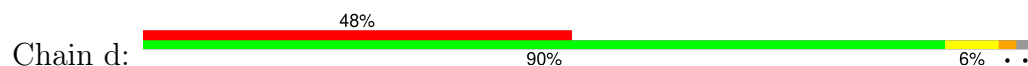
- Molecule 3: Cytochrome c oxidase subunit 3



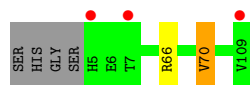
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



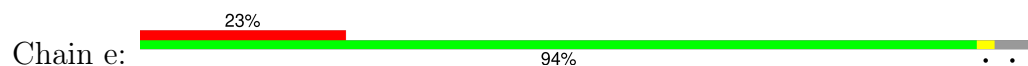
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

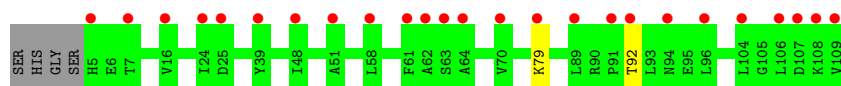


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



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

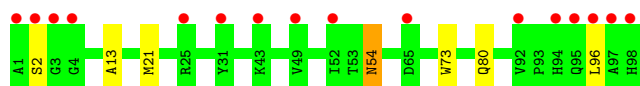




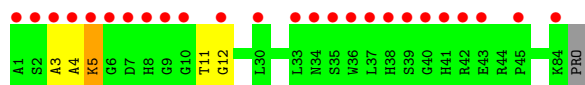
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



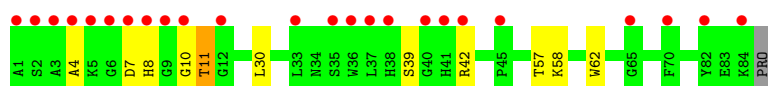
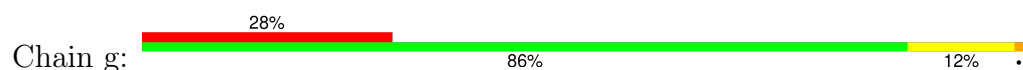
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



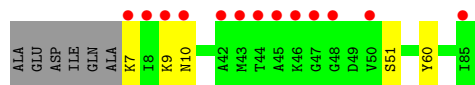
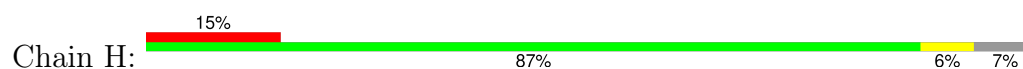
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



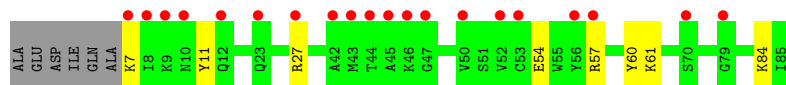
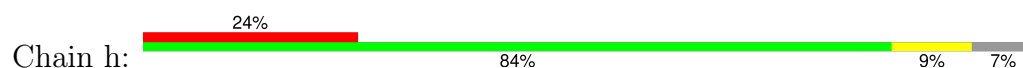
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



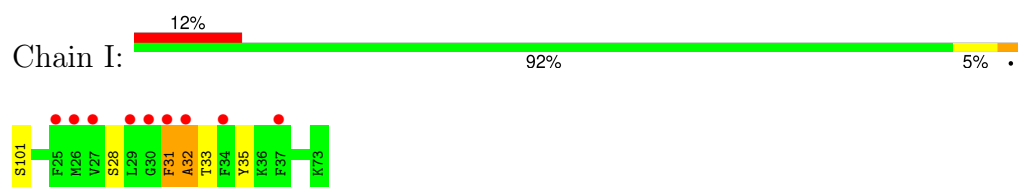
- Molecule 8: Cytochrome c oxidase subunit 6B1



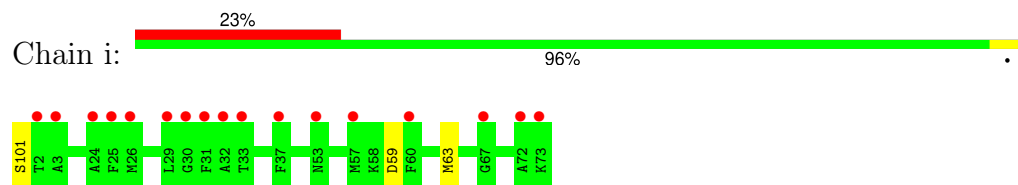
- Molecule 8: Cytochrome c oxidase subunit 6B1



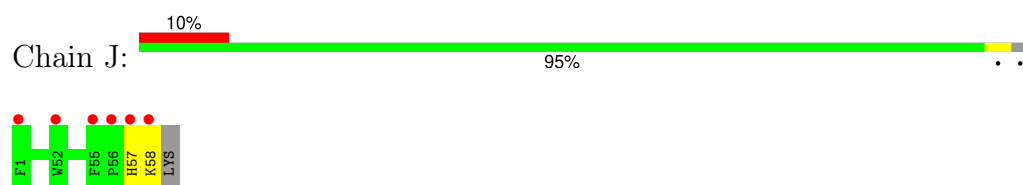
- Molecule 9: Cytochrome c oxidase subunit 6C



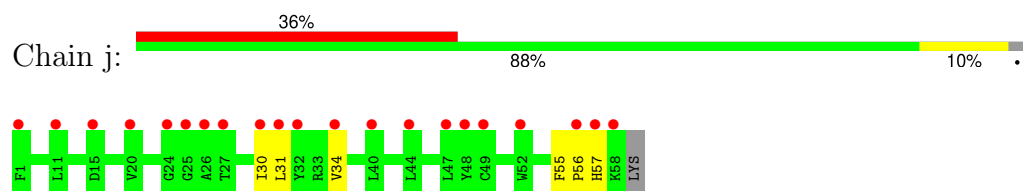
- Molecule 9: Cytochrome c oxidase subunit 6C



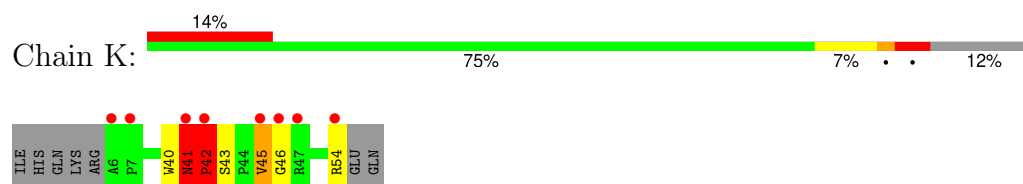
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



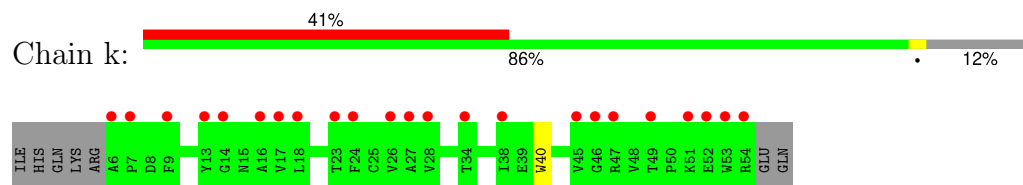
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



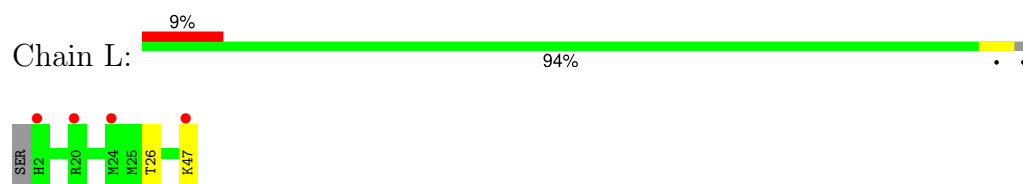
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



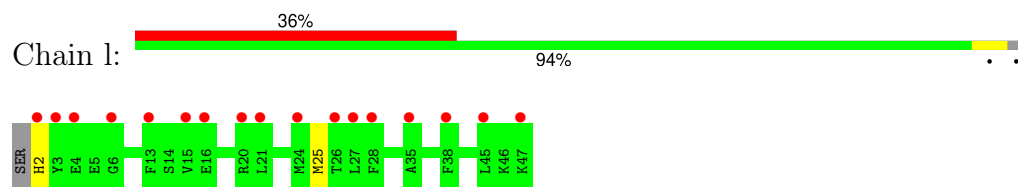
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



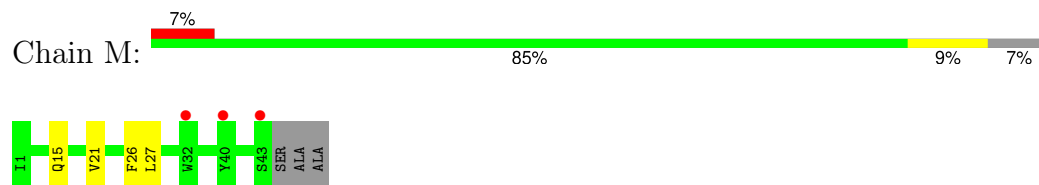
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



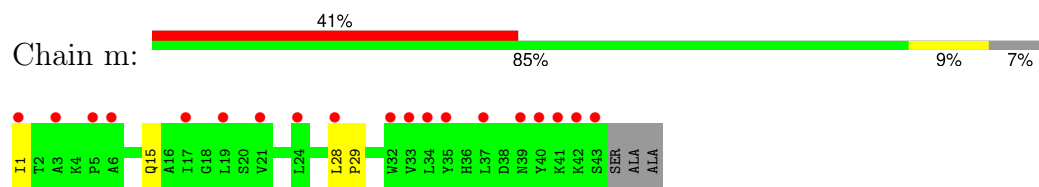
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	177.92Å 182.56Å 208.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 1.95 39.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.00-1.95) 94.3 (39.00-1.95)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.217 , 0.244 0.225 , 0.249	Depositor DCC
R_{free} test set	23097 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32575	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: FME, CU, PGV, MG, PSC, DMU, PEK, NA, TPO, CMO, CDL, ZN, TGL, HEA, CUA, CHD, SAC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.71	0/4156	0.95	2/5678 (0.0%)
1	a	0.67	0/4156	0.92	2/5678 (0.0%)
2	B	0.72	1/1860 (0.1%)	0.90	1/2534 (0.0%)
2	b	0.65	1/1860 (0.1%)	0.88	1/2534 (0.0%)
3	C	0.62	0/2197	0.90	0/3005
3	c	0.62	0/2197	0.83	0/3005
4	D	0.64	0/1229	0.83	0/1658
4	d	0.62	0/1229	0.93	1/1658 (0.1%)
5	E	0.66	0/871	0.89	0/1182
5	e	0.61	0/871	0.94	0/1182
6	F	0.72	0/765	0.84	1/1038 (0.1%)
6	f	0.65	0/765	0.83	0/1038
7	G	0.67	0/690	0.86	0/937
7	g	0.71	0/690	0.87	0/937
8	H	0.66	0/682	0.93	0/921
8	h	0.62	0/682	0.94	1/921 (0.1%)
9	I	0.60	0/605	0.85	1/802 (0.1%)
9	i	0.59	0/605	0.89	0/802
10	J	0.60	0/471	0.85	1/636 (0.2%)
10	j	0.67	0/471	0.88	0/636
11	K	0.72	0/398	1.34	4/546 (0.7%)
11	k	0.60	0/398	0.88	0/546
12	L	0.65	0/393	0.80	0/526
12	l	0.64	0/393	0.85	0/526
13	M	0.66	0/345	1.01	0/470
13	m	0.61	0/345	0.87	0/470
All	All	0.66	2/29324 (0.0%)	0.90	15/39866 (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
7	g	0	1
10	j	0	1
11	K	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	8.48	1.33	1.23
2	b	198	GLU	C-O	7.12	1.31	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	41	ASN	CA-C-N	-12.40	104.34	119.84
11	K	41	ASN	C-N-CA	-12.40	104.34	119.84
11	K	45	VAL	N-CA-C	6.49	117.17	110.36
1	A	240	HIS	N-CA-CB	6.43	118.00	110.42
9	I	31	PHE	N-CA-C	-5.86	102.38	110.35
1	a	240	HIS	N-CA-CB	5.63	117.06	110.42
11	K	41	ASN	CB-CA-C	5.59	121.19	110.17
4	d	123	MET	N-CA-C	-5.38	101.89	109.96
1	A	382	SER	N-CA-C	-5.36	105.13	110.97
8	h	54	GLU	N-CA-C	5.22	117.38	111.11
6	F	87	THR	N-CA-CB	5.22	117.68	110.17
2	b	59	GLN	N-CA-C	5.17	116.61	110.97
2	B	199	ILE	N-CA-CB	5.17	116.44	110.49
10	J	57	HIS	N-CA-C	5.15	117.50	109.52
1	a	125	GLY	N-CA-C	-5.06	106.35	112.48

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	41	ASN	Peptide
11	K	42	PRO	Peptide
11	K	46	GLY	Peptide
7	g	11	TPO	Peptide
10	j	55	PHE	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	4027	0	4001	28	0
1	a	4027	0	4001	29	0
2	B	1824	0	1833	13	0
2	b	1824	0	1833	9	0
3	C	2110	0	2027	4	0
3	c	2110	0	2027	6	0
4	D	1195	0	1183	2	0
4	d	1195	0	1183	9	0
5	E	852	0	845	1	0
5	e	852	0	845	0	0
6	F	748	0	728	2	0
6	f	748	0	728	3	0
7	G	675	0	644	1	0
7	g	675	0	643	7	0
8	H	662	0	623	0	0
8	h	662	0	623	1	0
9	I	601	0	613	4	0
9	i	601	0	613	3	0
10	J	460	0	459	0	0
10	j	460	0	459	2	0
11	K	384	0	366	11	0
11	k	384	0	366	2	0
12	L	380	0	380	1	0
12	l	380	0	380	1	0
13	M	335	0	352	8	0
13	m	335	0	352	3	0
14	A	120	0	108	2	0
14	a	120	0	108	1	0
15	A	1	0	0	0	0
15	a	1	0	0	0	0
16	A	1	0	0	0	0
16	a	1	0	0	0	0
17	A	1	0	0	0	0
17	a	1	0	0	0	0
18	A	102	0	152	0	0
18	C	102	0	152	0	0
18	a	102	0	152	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	c	102	0	152	0	0
19	A	126	0	220	0	0
19	D	63	0	110	0	0
19	b	63	0	110	0	0
19	d	63	0	110	0	0
19	l	63	0	110	1	0
20	A	2	0	0	0	0
20	a	2	0	0	1	0
21	B	2	0	0	0	0
21	b	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	0	0
22	G	29	0	39	0	0
22	J	29	0	39	0	0
22	c	58	0	78	0	0
22	j	29	0	39	0	0
23	C	106	0	154	0	0
23	G	53	0	77	1	0
23	c	159	0	231	0	0
24	C	100	0	156	0	0
24	G	100	0	156	0	0
24	c	100	0	156	0	0
24	g	100	0	156	0	0
25	C	33	0	42	0	0
25	M	33	0	42	0	0
25	c	33	0	42	3	0
25	m	33	0	42	0	0
26	E	52	0	80	0	0
26	b	52	0	80	0	0
27	F	1	0	0	0	0
27	f	1	0	0	0	0
28	A	243	0	0	1	0
28	B	180	0	0	0	0
28	C	122	0	0	0	0
28	D	125	0	0	0	0
28	E	100	0	0	0	0
28	F	104	0	0	0	0
28	G	57	0	0	0	0
28	H	57	0	0	0	0
28	I	33	0	0	1	0
28	J	36	0	0	0	0
28	K	41	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	L	47	0	0	0	0
28	M	29	0	0	0	0
28	a	187	0	0	1	0
28	b	109	0	0	1	0
28	c	96	0	0	1	0
28	d	37	0	0	0	0
28	e	56	0	0	0	0
28	f	62	0	0	0	0
28	g	27	0	0	0	0
28	h	36	0	0	1	0
28	i	23	0	0	0	0
28	j	14	0	0	0	0
28	k	7	0	0	0	0
28	l	8	0	0	0	0
28	m	5	0	0	0	0
All	All	32575	0	31317	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (117) 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)
2:B:4:PRO:HB3	11:K:42:PRO:CG	1.99	0.92
1:A:466:MET:CE	13:M:26:PHE:HB2	2.10	0.82
2:b:56:MET:SD	28:b:433:HOH:O	2.40	0.78
1:a:171:MET:SD	28:a:863:HOH:O	2.41	0.78
1:A:466:MET:HE3	13:M:26:PHE:CB	2.17	0.74
2:B:4:PRO:HB3	11:K:42:PRO:HG2	1.69	0.72
4:d:120:THR:O	4:d:123:MET:O	2.07	0.72
1:A:466:MET:HE3	13:M:26:PHE:HB2	1.72	0.72
11:K:54:ARG:C	28:K:102:HOH:O	2.34	0.71
25:c:309:DMU:H8	7:g:62:TRP:HA	1.72	0.70
25:c:309:DMU:H13	7:g:62:TRP:HB2	1.73	0.70
1:A:466:MET:HE1	13:M:27:LEU:HG	1.72	0.70
1:a:431:LEU:HB3	1:a:436:MET:HE2	1.75	0.69
6:F:75:HIS:H	6:F:80:GLN:HE22	1.40	0.68
2:B:4:PRO:HB3	11:K:42:PRO:HG3	1.80	0.63
1:A:51:ASP:OD2	1:A:441:SER:OG	2.17	0.62
4:d:82:VAL:HG12	4:d:86:MET:HE2	1.82	0.61
1:A:377:PHE:O	1:A:381:LEU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:456:MET:HE1	11:k:40:TRP:CH2	2.36	0.60
1:a:371:TYR:CD1	1:a:436:MET:HE3	2.37	0.59
2:b:186:SER:HB3	2:b:213:LEU:HD22	1.82	0.59
2:B:4:PRO:CB	11:K:42:PRO:HG2	2.32	0.59
3:C:91:VAL:O	3:C:95:THR:HG23	2.02	0.59
9:I:28:SER:O	9:I:31:PHE:O	2.21	0.59
1:a:167:THR:HA	1:a:171:MET:HE2	1.85	0.59
1:A:382:SER:O	1:A:386:VAL:HB	2.05	0.57
1:a:452:THR:HG22	1:a:456:MET:HE2	1.87	0.56
1:a:453:ILE:HA	1:a:456:MET:HE3	1.88	0.56
1:a:92:MET:C	1:a:171:MET:HE1	2.32	0.55
1:a:216:ASN:HD21	7:g:58:LYS:H	1.56	0.54
7:G:5:LYS:HB2	1:a:278:MET:HE2	1.90	0.54
1:a:167:THR:HG23	1:a:171:MET:CE	2.38	0.54
9:I:31:PHE:O	9:I:32:ALA:HB3	2.09	0.53
1:A:453:ILE:HA	1:A:456:MET:HE2	1.91	0.53
1:A:409:TRP:HE1	13:M:15:GLN:HE22	1.55	0.53
1:A:449:MET:HE3	1:A:450:TRP:CZ3	2.43	0.53
2:b:13:THR:HB	2:b:168:LEU:HD12	1.89	0.53
4:d:123:MET:O	4:d:124:LEU:HB2	2.07	0.53
2:b:149:THR:O	2:b:184:LEU:O	2.26	0.53
2:B:102:HIS:HE1	2:B:107:SER:OG	1.92	0.52
1:A:177:SER:HA	7:g:10:GLY:HA3	1.91	0.52
6:f:54:ASN:HD22	6:f:54:ASN:C	2.17	0.52
1:A:289:ALA:HB1	1:A:297:MET:HE1	1.91	0.51
1:a:406:ASN:HD21	18:a:606:PGV:H32	1.76	0.51
2:b:104:TRP:CG	2:b:203:ASN:HB2	2.46	0.51
1:A:184:PHE:H	1:A:256:HIS:HE1	1.58	0.51
1:A:246:LEU:HD13	1:A:381:LEU:HD21	1.92	0.51
2:B:4:PRO:CB	11:K:42:PRO:CG	2.81	0.51
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.51
3:C:161:GLN:HE21	23:G:101:PEK:H42	1.76	0.51
9:I:31:PHE:O	9:I:32:ALA:CB	2.60	0.50
1:A:87:ILE:O	1:A:173:PRO:HD3	2.13	0.49
2:B:49:LYS:O	4:D:20:ARG:NH2	2.40	0.49
2:b:146:MET:HE3	2:b:215:PRO:N	2.28	0.49
1:a:390:MET:HA	1:a:390:MET:HE3	1.95	0.48
4:d:123:MET:O	4:d:124:LEU:CB	2.60	0.48
6:F:85:CYS:SG	6:F:87:THR:HG23	2.54	0.48
1:A:297:MET:CG	1:A:302:ARG:HG3	2.43	0.48
1:a:485:VAL:HG23	13:m:1:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TRP:HD1	2:B:207:MET:CE	2.27	0.47
2:b:190:GLY:HA2	9:i:63:MET:HE1	1.95	0.47
1:A:194:LEU:CD2	7:g:4:ALA:HB1	2.45	0.47
1:a:456:MET:HE1	11:k:40:TRP:CZ3	2.49	0.47
1:A:184:PHE:H	1:A:256:HIS:CE1	2.33	0.47
4:d:6:VAL:HG13	4:d:10:ASP:CB	2.46	0.46
1:a:431:LEU:HD13	1:a:436:MET:HE1	1.98	0.46
2:b:41:ILE:O	2:b:45:MET:HG2	2.16	0.46
1:A:256:HIS:HD2	28:A:732:HOH:O	1.98	0.46
13:m:28:LEU:HB2	13:m:29:PRO:HD3	1.98	0.46
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.98	0.46
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.97	0.45
11:K:41:ASN:HB3	11:K:42:PRO:CD	2.47	0.45
11:K:41:ASN:HB3	11:K:42:PRO:HD3	1.98	0.45
1:a:93:ALA:N	1:a:171:MET:HE1	2.32	0.45
1:a:243:VAL:HG11	20:a:608:CMO:C	2.46	0.45
8:h:27:ARG:NH1	28:h:102:HOH:O	2.50	0.45
9:i:59:ASP:O	9:i:63:MET:HG3	2.16	0.45
1:a:76:GLY:O	1:a:80:ASN:HB2	2.17	0.45
3:C:76:GLN:O	3:C:80:ARG:HG3	2.16	0.45
3:c:116:TRP:HA	3:c:117:PRO:C	2.42	0.44
1:a:339:MET:HE2	1:a:414:PHE:CD2	2.51	0.44
11:K:40:TRP:O	11:K:42:PRO:HD3	2.17	0.44
4:d:6:VAL:HG13	4:d:10:ASP:HB2	1.99	0.44
1:A:409:TRP:HE1	13:M:15:GLN:NE2	2.16	0.44
1:a:107:PRO:HB3	3:c:25:LEU:HB2	2.00	0.44
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.53	0.44
3:c:56:GLN:NE2	10:j:31:LEU:HB3	2.33	0.43
3:c:47:LEU:O	3:c:51:MET:HG2	2.18	0.43
3:c:34:TRP:CH2	25:c:309:DMU:H25	2.54	0.43
1:A:466:MET:HE3	13:M:26:PHE:HB3	1.98	0.43
1:A:381:LEU:HG	14:A:602:HEA:HAC	2.01	0.42
1:a:65:MET:HA	1:a:65:MET:HE2	2.01	0.42
9:I:35:TYR:N	28:I:201:HOH:O	2.40	0.42
1:a:216:ASN:ND2	7:g:57:THR:H	2.18	0.42
5:E:66:ARG:O	5:E:70:VAL:HG13	2.19	0.41
1:A:76:GLY:O	1:A:80:ASN:HB2	2.19	0.41
1:a:417:MET:HE2	1:a:421:VAL:HG13	2.03	0.41
2:B:4:PRO:HB3	11:K:42:PRO:CB	2.50	0.41
4:D:145:TRP:CG	11:K:45:VAL:O	2.73	0.41
1:a:431:LEU:HD13	1:a:436:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.02	0.41
1:a:409:TRP:HE1	13:m:15:GLN:HE22	1.68	0.41
3:c:76:GLN:NE2	28:c:404:HOH:O	2.50	0.41
4:d:126:MET:HA	9:i:63:MET:HE3	2.03	0.41
2:B:61:VAL:CG1	2:B:65:TRP:CZ3	3.04	0.41
1:a:265:LYS:HB2	1:a:490:THR:HG21	2.01	0.41
1:a:483:LEU:HD22	4:d:6:VAL:HB	2.03	0.41
4:d:12:ALA:HA	6:f:73:TRP:CD1	2.56	0.41
12:l:25:MET:HG2	19:l:101:TGL:HA72	2.02	0.41
1:A:281:GLY:C	7:g:4:ALA:HB3	2.46	0.41
2:b:13:THR:HB	2:b:168:LEU:CD1	2.51	0.41
1:A:378:HIS:O	1:A:382:SER:HB3	2.21	0.40
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.03	0.40
10:j:30:ILE:O	10:j:34:VAL:HG23	2.21	0.40
1:a:62:ALA:HB2	14:a:601:HEA:HBD1	2.02	0.40
6:f:13:ALA:CB	6:f:21:MET:HE1	2.51	0.40
12:L:26:THR:HG21	13:M:21:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
1	a	512/514 (100%)	499 (98%)	13 (2%)	0	100	100
2	B	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
2	b	225/227 (99%)	215 (96%)	8 (4%)	2 (1%)	14	6
3	C	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	30	21
3	c	257/261 (98%)	250 (97%)	6 (2%)	1 (0%)	30	21
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	142/147 (97%)	135 (95%)	6 (4%)	1 (1%)	18	10
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	e	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	3	0
6	f	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	12	5
7	G	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	2	0
7	g	81/85 (95%)	72 (89%)	8 (10%)	1 (1%)	10	4
8	H	77/85 (91%)	69 (90%)	6 (8%)	2 (3%)	4	1
8	h	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	9	3
9	I	71/73 (97%)	69 (97%)	1 (1%)	1 (1%)	9	3
9	i	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	j	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	6	1
11	K	47/56 (84%)	43 (92%)	1 (2%)	3 (6%)	1	0
11	k	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	l	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	m	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3504/3614 (97%)	3371 (96%)	112 (3%)	21 (1%)	21	12

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	38	ASN
6	F	95	GLN
6	F	96	LEU
11	K	41	ASN
11	K	42	PRO
11	K	43	SER
3	c	38	ASN
4	d	124	LEU
7	G	4	ALA
7	G	12	GLY
8	H	51	SER

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Mol	Chain	Res	Type
9	I	32	ALA
8	h	11	TYR
2	b	91	ASN
10	j	56	PRO
2	b	150	ILE
6	f	2	SER
7	g	8	HIS
6	F	97	ALA
7	G	3	ALA
8	H	10	ASN

5.3.2 Protein sidechains [i](#)

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	426/426 (100%)	424 (100%)	2 (0%)	81	82
1	a	426/426 (100%)	420 (99%)	6 (1%)	59	56
2	B	210/210 (100%)	205 (98%)	5 (2%)	43	36
2	b	210/210 (100%)	202 (96%)	8 (4%)	29	19
3	C	224/226 (99%)	223 (100%)	1 (0%)	84	85
3	c	224/226 (99%)	223 (100%)	1 (0%)	84	85
4	D	128/129 (99%)	127 (99%)	1 (1%)	73	74
4	d	128/129 (99%)	124 (97%)	4 (3%)	35	26
5	E	92/95 (97%)	91 (99%)	1 (1%)	65	64
5	e	92/95 (97%)	90 (98%)	2 (2%)	45	40
6	F	81/81 (100%)	79 (98%)	2 (2%)	42	34
6	f	81/81 (100%)	78 (96%)	3 (4%)	30	20
7	G	67/68 (98%)	66 (98%)	1 (2%)	57	54
7	g	67/68 (98%)	63 (94%)	4 (6%)	17	7
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	16
8	h	71/75 (95%)	66 (93%)	5 (7%)	14	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	47
9	i	57/57 (100%)	57 (100%)	0	100	100
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	43
10	j	49/50 (98%)	48 (98%)	1 (2%)	48	43
11	K	39/46 (85%)	39 (100%)	0	100	100
11	k	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	33
12	l	39/40 (98%)	38 (97%)	1 (3%)	40	33
13	M	37/38 (97%)	37 (100%)	0	100	100
13	m	37/38 (97%)	37 (100%)	0	100	100
All	All	3040/3082 (99%)	2986 (98%)	54 (2%)	51	47

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	MET
1	A	369	ASP
2	B	37	LEU
2	B	65	TRP
2	B	67	ILE
2	B	75	LEU
2	B	115	ASP
3	C	159	MET
4	D	4	SER
5	E	70	VAL
6	F	80	GLN
6	F	95	GLN
7	G	5	LYS
8	H	7	LYS
8	H	9	LYS
8	H	60	TYR
9	I	33	THR
10	J	58	LYS
12	L	47	LYS
1	a	65	MET
1	a	152	LEU
1	a	189	MET
1	a	369	ASP

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Mol	Chain	Res	Type
1	a	485	VAL
1	a	504	THR
2	b	18	GLU
2	b	61	VAL
2	b	66	THR
2	b	90	ILE
2	b	94	SER
2	b	168	LEU
2	b	213	LEU
2	b	217	LYS
3	c	159	MET
4	d	6	VAL
4	d	30	VAL
4	d	73	ARG
4	d	128	VAL
5	e	79	LYS
5	e	92	THR
6	f	54	ASN
6	f	80	GLN
6	f	96	LEU
7	g	7	ASP
7	g	30	LEU
7	g	39	SER
7	g	42	ARG
8	h	7	LYS
8	h	57	ARG
8	h	60	TYR
8	h	61	LYS
8	h	84	LYS
10	j	57	HIS
12	l	2	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	170	ASN
1	A	214	ASN
1	A	256	HIS
2	B	102	HIS
3	C	148	HIS
4	D	37	GLN

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Mol	Chain	Res	Type
4	D	101	HIS
6	F	80	GLN
8	H	31	GLN
10	J	9	GLN
13	M	15	GLN
1	a	216	ASN
2	b	59	GLN
2	b	91	ASN
3	c	3	HIS
3	c	56	GLN
4	d	32	ASN
6	f	54	ASN
8	h	23	GLN
8	h	25	GLN
8	h	28	ASN
8	h	32	ASN
10	j	21	HIS
10	j	29	ASN
13	m	15	GLN
13	m	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	TPO	G	11	7	8,10,11	1.39	1 (12%)	10,14,16	1.33	2 (20%)
2	FME	B	301	2	8,9,10	0.92	0	8,9,11	3.55	3 (37%)
1	FME	a	1	1	8,9,10	0.49	0	8,9,11	1.68	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SAC	I	101	9	7,8,9	1.58	1 (14%)	7,9,11	1.25	0
9	SAC	i	101	9	7,8,9	1.55	1 (14%)	7,9,11	1.03	0
1	FME	A	1	1	8,9,10	0.53	0	8,9,11	2.60	1 (12%)
7	TPO	g	11	7	8,10,11	1.16	1 (12%)	10,14,16	1.16	1 (10%)
2	FME	b	1	2	8,9,10	0.62	0	8,9,11	2.10	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
7	TPO	G	11	7	-	1/9/11/13	-
2	FME	B	301	2	-	1/7/9/11	-
1	FME	a	1	1	-	4/7/9/11	-
9	SAC	I	101	9	-	3/7/8/10	-
9	SAC	i	101	9	-	2/7/8/10	-
1	FME	A	1	1	-	4/7/9/11	-
7	TPO	g	11	7	-	4/9/11/13	-
2	FME	b	1	2	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	101	SAC	CA-N	3.99	1.52	1.46
9	i	101	SAC	CA-N	3.88	1.52	1.46
7	G	11	TPO	P-OG1	3.12	1.65	1.59
7	g	11	TPO	P-OG1	2.06	1.63	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FME	CA-N-CN	-8.81	109.27	122.82
1	A	1	FME	CA-N-CN	-6.68	112.55	122.82
2	b	1	FME	CA-N-CN	-4.54	115.84	122.82
1	a	1	FME	CA-N-CN	-3.81	116.96	122.82
2	B	301	FME	C-CA-N	3.24	115.75	109.50
2	B	301	FME	O1-CN-N	-2.75	118.22	125.32
7	g	11	TPO	P-OG1-CB	-2.60	116.26	123.33
2	b	1	FME	C-CA-N	2.56	114.45	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	11	TPO	P-OG1-CB	-2.37	116.89	123.33
7	G	11	TPO	CG2-CB-CA	-2.16	109.06	113.26

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	C-CA-CB-CG
2	B	301	FME	O1-CN-N-CA
9	I	101	SAC	CB-CA-N-C1A
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-OG1
9	i	101	SAC	O-C-CA-CB
9	I	101	SAC	C2A-C1A-N-CA
9	I	101	SAC	OAC-C1A-N-CA
9	i	101	SAC	N-CA-CB-OG
7	G	11	TPO	CB-OG1-P-O1P
1	A	1	FME	CA-CB-CG-SD
1	a	1	FME	C-CA-CB-CG
7	g	11	TPO	CB-OG1-P-O3P
1	A	1	FME	N-CA-CB-CG
1	a	1	FME	CB-CA-N-CN
7	g	11	TPO	O-C-CA-CB
7	g	11	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 8 are monoatomic - leaving 46 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	PGV	C	303	-	50,50,50	0.85	2 (4%)	53,56,56	0.81	1 (1%)
22	CHD	C	306	-	32,32,32	0.60	0	51,51,51	1.25	5 (9%)
25	DMU	c	309	-	34,34,34	0.96	2 (5%)	45,45,45	1.46	7 (15%)
18	PGV	c	302	-	50,50,50	1.06	2 (4%)	53,56,56	1.23	6 (11%)
24	CDL	C	305	-	99,99,99	1.00	4 (4%)	105,111,111	1.01	7 (6%)
22	CHD	c	308	-	32,32,32	0.52	0	51,51,51	1.07	3 (5%)
24	CDL	G	102	-	99,99,99	1.04	4 (4%)	105,111,111	0.96	6 (5%)
22	CHD	c	303	-	32,32,32	0.63	0	51,51,51	1.06	3 (5%)
19	TGL	A	608	-	62,62,62	1.10	3 (4%)	65,65,65	0.99	4 (6%)
22	CHD	J	101	-	32,32,32	0.68	0	51,51,51	2.10	16 (31%)
18	PGV	A	607	-	50,50,50	0.87	2 (4%)	53,56,56	0.87	3 (5%)
24	CDL	c	307	-	99,99,99	1.00	4 (4%)	105,111,111	1.04	6 (5%)
22	CHD	C	301	-	32,32,32	0.65	0	51,51,51	1.11	4 (7%)
18	PGV	c	306	-	50,50,50	0.90	2 (4%)	53,56,56	0.82	2 (3%)
25	DMU	m	101	-	34,34,34	0.49	0	45,45,45	0.97	4 (8%)
23	PEK	C	302	-	52,52,52	0.86	2 (3%)	55,57,57	0.97	4 (7%)
14	HEA	a	602	20,1	67,67,67	2.39	21 (31%)	81,103,103	2.35	28 (34%)
19	TGL	b	302	-	62,62,62	1.04	3 (4%)	65,65,65	0.96	4 (6%)
24	CDL	g	101	-	99,99,99	1.00	4 (4%)	105,111,111	1.04	7 (6%)
23	PEK	G	101	-	52,52,52	1.01	2 (3%)	55,57,57	1.15	4 (7%)
19	TGL	D	201	-	62,62,62	1.10	3 (4%)	65,65,65	0.96	5 (7%)
14	HEA	A	602	1	67,67,67	2.20	20 (29%)	81,103,103	2.55	34 (41%)
23	PEK	C	307	-	52,52,52	1.02	2 (3%)	55,57,57	0.86	3 (5%)
26	PSC	E	201	-	51,51,51	1.04	2 (3%)	57,59,59	1.84	10 (17%)
18	PGV	a	606	-	50,50,50	1.07	2 (4%)	53,56,56	1.18	5 (9%)
18	PGV	C	304	-	50,50,50	1.08	2 (4%)	53,56,56	1.01	4 (7%)
23	PEK	c	305	-	52,52,52	1.00	2 (3%)	55,57,57	0.93	3 (5%)
26	PSC	b	303	-	51,51,51	1.04	2 (3%)	57,59,59	1.79	11 (19%)
22	CHD	B	402	-	32,32,32	0.72	0	51,51,51	1.26	8 (15%)
20	CMO	A	610	15	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	601	1	67,67,67	2.17	25 (37%)	81,103,103	2.44	31 (38%)
18	PGV	A	606	-	50,50,50	1.04	2 (4%)	53,56,56	0.95	3 (5%)
18	PGV	a	607	-	50,50,50	0.85	2 (4%)	53,56,56	0.76	2 (3%)
19	TGL	A	609	-	62,62,62	1.04	3 (4%)	65,65,65	0.99	5 (7%)
19	TGL	d	201	-	62,62,62	1.10	3 (4%)	65,65,65	1.16	8 (12%)
20	CMO	a	608	14,15	0,1,1	-	-	-	-	-
14	HEA	a	601	1	67,67,67	2.36	23 (34%)	81,103,103	2.32	30 (37%)
21	CUA	B	401	2	0,1,1	-	-	-	-	-
23	PEK	c	304	-	52,52,52	0.89	2 (3%)	55,57,57	0.85	3 (5%)
22	CHD	j	101	-	32,32,32	0.58	0	51,51,51	1.40	10 (19%)
25	DMU	C	308	-	34,34,34	0.72	1 (2%)	45,45,45	1.25	6 (13%)
19	TGL	l	101	-	62,62,62	1.12	3 (4%)	65,65,65	1.11	5 (7%)
21	CUA	b	301	2	0,1,1	-	-	-	-	-
25	DMU	M	101	-	34,34,34	0.53	1 (2%)	45,45,45	0.75	0
23	PEK	c	301	-	52,52,52	0.99	2 (3%)	55,57,57	0.89	3 (5%)
22	CHD	G	103	-	32,32,32	0.67	0	51,51,51	1.11	4 (7%)

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
18	PGV	C	303	-	-	13/55/55/55	-
22	CHD	C	306	-	-	2/9/74/74	0/4/4/4
25	DMU	c	309	-	-	7/19/59/59	0/2/2/2
18	PGV	c	302	-	-	32/55/55/55	-
24	CDL	C	305	-	-	50/110/110/110	-
22	CHD	c	308	-	-	2/9/74/74	0/4/4/4
24	CDL	G	102	-	-	55/110/110/110	-
22	CHD	c	303	-	-	2/9/74/74	0/4/4/4
19	TGL	A	608	-	-	32/65/65/65	-
22	CHD	J	101	-	-	5/9/74/74	0/4/4/4
18	PGV	A	607	-	-	13/55/55/55	-
24	CDL	c	307	-	-	54/110/110/110	-
22	CHD	C	301	-	-	0/9/74/74	0/4/4/4
18	PGV	c	306	-	-	11/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DMU	m	101	-	-	4/19/59/59	0/2/2/2
23	PEK	C	302	-	-	21/56/56/56	-
14	HEA	a	602	20,1	-	5/36/76/76	-
19	TGL	b	302	-	-	33/65/65/65	-
24	CDL	g	101	-	-	54/110/110/110	-
23	PEK	G	101	-	-	24/56/56/56	-
19	TGL	D	201	-	-	29/65/65/65	-
14	HEA	A	602	1	-	5/36/76/76	-
23	PEK	C	307	-	-	17/56/56/56	-
26	PSC	E	201	-	-	21/55/55/55	-
18	PGV	a	606	-	-	27/55/55/55	-
18	PGV	C	304	-	-	25/55/55/55	-
23	PEK	c	305	-	-	24/56/56/56	-
26	PSC	b	303	-	-	24/55/55/55	-
22	CHD	B	402	-	-	2/9/74/74	0/4/4/4
14	HEA	A	601	1	-	4/36/76/76	-
18	PGV	A	606	-	-	22/55/55/55	-
18	PGV	a	607	-	-	12/55/55/55	-
19	TGL	A	609	-	-	39/65/65/65	-
19	TGL	d	201	-	-	38/65/65/65	-
14	HEA	a	601	1	-	3/36/76/76	-
23	PEK	c	304	-	-	16/56/56/56	-
22	CHD	j	101	-	-	8/9/74/74	0/4/4/4
25	DMU	C	308	-	-	3/19/59/59	0/2/2/2
19	TGL	l	101	-	-	33/65/65/65	-
25	DMU	M	101	-	-	5/19/59/59	0/2/2/2
23	PEK	c	301	-	-	22/56/56/56	-
22	CHD	G	103	-	-	2/9/74/74	0/4/4/4

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	602	HEA	FE-ND	6.09	2.13	1.94
14	a	601	HEA	C3B-C2B	5.51	1.47	1.34
14	a	601	HEA	FE-NB	5.33	2.11	1.94
14	a	602	HEA	C4A-NA	5.27	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	601	HEA	FE-ND	5.17	2.10	1.94
14	A	601	HEA	C3B-C2B	5.12	1.46	1.34
14	a	602	HEA	FE-NB	5.09	2.10	1.94
14	A	602	HEA	FE-ND	5.01	2.10	1.94
14	a	601	HEA	C1A-NA	4.94	1.48	1.39
26	b	303	PSC	O01-C1	4.91	1.48	1.34
18	a	606	PGV	O01-C1	4.91	1.48	1.34
18	C	304	PGV	O03-C19	4.88	1.47	1.33
19	A	608	TGL	OG1-CA1	4.87	1.47	1.33
19	l	101	TGL	OG3-CC1	4.84	1.47	1.33
19	l	101	TGL	OG2-CB1	4.80	1.47	1.34
26	E	201	PSC	O01-C1	4.80	1.47	1.34
14	A	601	HEA	C3D-C2D	4.79	1.47	1.36
18	A	606	PGV	O03-C19	4.79	1.47	1.33
18	a	606	PGV	O03-C19	4.78	1.47	1.33
24	G	102	CDL	OB8-CB7	4.76	1.47	1.33
18	c	302	PGV	O01-C1	4.74	1.47	1.34
14	A	601	HEA	FE-NC	4.74	2.10	1.95
23	C	307	PEK	O03-C21	4.67	1.47	1.33
19	d	201	TGL	OG2-CB1	4.67	1.47	1.34
24	c	307	CDL	OA6-CA5	4.66	1.47	1.34
23	c	301	PEK	O03-C21	4.64	1.46	1.33
24	G	102	CDL	OB6-CB5	4.63	1.47	1.34
14	a	602	HEA	C3B-C2B	4.62	1.45	1.34
23	G	101	PEK	O01-C1	4.61	1.47	1.34
19	D	201	TGL	OG2-CB1	4.59	1.47	1.34
23	C	307	PEK	O01-C1	4.59	1.47	1.34
19	D	201	TGL	OG1-CA1	4.58	1.46	1.33
24	G	102	CDL	OA8-CA7	4.58	1.46	1.33
18	C	304	PGV	O01-C1	4.56	1.47	1.34
23	c	305	PEK	O01-C1	4.56	1.47	1.34
19	A	608	TGL	OG3-CC1	4.55	1.46	1.33
14	a	602	HEA	C3A-C2A	4.54	1.47	1.37
19	l	101	TGL	OG1-CA1	4.54	1.46	1.33
23	c	305	PEK	O03-C21	4.53	1.46	1.33
18	c	302	PGV	O03-C19	4.53	1.46	1.33
24	c	307	CDL	OB6-CB5	4.52	1.47	1.34
14	A	602	HEA	C3B-C2B	4.51	1.45	1.34
24	g	101	CDL	OB6-CB5	4.50	1.47	1.34
19	d	201	TGL	OG1-CA1	4.50	1.46	1.33
24	C	305	CDL	OA6-CA5	4.49	1.47	1.34
24	c	307	CDL	OA8-CA7	4.49	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	101	PEK	O03-C21	4.48	1.46	1.33
24	g	101	CDL	OB8-CB7	4.47	1.46	1.33
19	D	201	TGL	OG3-CC1	4.47	1.46	1.33
14	A	602	HEA	FE-NC	4.47	2.09	1.95
19	b	302	TGL	OG2-CB1	4.46	1.46	1.34
24	g	101	CDL	OA8-CA7	4.45	1.46	1.33
19	A	609	TGL	OG1-CA1	4.44	1.46	1.33
24	C	305	CDL	OA8-CA7	4.44	1.46	1.33
19	b	302	TGL	OG1-CA1	4.43	1.46	1.33
14	a	602	HEA	CHD-C1D	4.40	1.47	1.38
26	b	303	PSC	O03-C19	4.40	1.46	1.33
14	A	602	HEA	C3D-C2D	4.38	1.46	1.36
19	d	201	TGL	OG3-CC1	4.37	1.46	1.33
24	c	307	CDL	OB8-CB7	4.37	1.46	1.33
26	E	201	PSC	O03-C19	4.36	1.46	1.33
14	A	602	HEA	CHD-C1D	4.36	1.47	1.38
14	a	601	HEA	C3D-C2D	4.35	1.46	1.36
24	C	305	CDL	OB8-CB7	4.34	1.46	1.33
24	g	101	CDL	OA6-CA5	4.34	1.46	1.34
23	c	304	PEK	O03-C21	4.33	1.46	1.33
19	A	609	TGL	OG2-CB1	4.32	1.46	1.34
14	a	602	HEA	CHB-C4A	4.32	1.46	1.38
23	c	301	PEK	O01-C1	4.27	1.46	1.34
19	b	302	TGL	OG3-CC1	4.26	1.45	1.33
14	a	602	HEA	C1A-NA	4.24	1.47	1.39
19	A	608	TGL	OG2-CB1	4.23	1.46	1.34
19	A	609	TGL	OG3-CC1	4.22	1.45	1.33
24	C	305	CDL	OB6-CB5	4.22	1.46	1.34
14	A	602	HEA	C4A-NA	4.21	1.47	1.39
24	G	102	CDL	OA6-CA5	4.21	1.46	1.34
14	a	602	HEA	CHC-C4B	4.16	1.46	1.38
14	A	602	HEA	C3A-C2A	4.15	1.46	1.37
14	a	602	HEA	CHA-C1A	4.11	1.46	1.38
18	c	306	PGV	O01-C1	4.10	1.45	1.34
18	A	606	PGV	O01-C1	4.08	1.45	1.34
14	a	601	HEA	CHD-C1D	4.06	1.46	1.38
14	a	601	HEA	CHA-C1A	4.04	1.46	1.38
14	a	601	HEA	C3A-C2A	4.01	1.46	1.37
14	A	602	HEA	CHB-C4A	4.01	1.46	1.38
14	A	602	HEA	C4D-ND	-3.97	1.31	1.38
14	A	601	HEA	FE-ND	3.96	2.07	1.94
14	a	602	HEA	CHC-C1C	3.92	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	601	HEA	CHC-C4B	3.91	1.46	1.38
14	a	601	HEA	CHD-C4C	3.91	1.48	1.39
14	a	602	HEA	C1B-NB	-3.84	1.31	1.38
18	c	306	PGV	O03-C19	3.82	1.44	1.33
14	A	602	HEA	C1B-NB	-3.82	1.31	1.38
14	A	601	HEA	C1A-NA	3.79	1.46	1.39
23	C	302	PEK	O03-C21	3.79	1.44	1.33
14	A	601	HEA	C4C-NC	-3.78	1.32	1.39
14	A	602	HEA	FE-NB	3.77	2.06	1.94
18	a	607	PGV	O03-C19	3.73	1.44	1.33
25	c	309	DMU	O5-C6	3.71	1.51	1.41
18	C	303	PGV	O01-C1	3.70	1.44	1.34
18	C	303	PGV	O03-C19	3.69	1.44	1.33
14	a	601	HEA	FE-NC	3.68	2.07	1.95
14	A	601	HEA	CHD-C1D	3.66	1.45	1.38
14	a	601	HEA	CHB-C4A	3.65	1.45	1.38
18	A	607	PGV	O03-C19	3.63	1.43	1.33
14	A	601	HEA	FE-NB	3.61	2.06	1.94
18	a	607	PGV	O01-C1	3.58	1.44	1.34
23	C	302	PEK	O01-C1	3.56	1.44	1.34
14	a	602	HEA	C3D-C2D	3.54	1.44	1.36
14	A	601	HEA	CHB-C4A	3.51	1.45	1.38
23	c	304	PEK	O01-C1	3.50	1.44	1.34
14	a	601	HEA	C1D-ND	-3.49	1.34	1.40
14	A	602	HEA	CHC-C4B	3.49	1.45	1.38
14	A	601	HEA	CHA-C1A	3.49	1.45	1.38
14	a	602	HEA	C4D-ND	-3.47	1.32	1.38
14	a	602	HEA	CHD-C4C	3.44	1.47	1.39
14	A	601	HEA	CHC-C4B	3.43	1.45	1.38
18	A	607	PGV	O01-C1	3.35	1.43	1.34
14	a	601	HEA	C4B-NB	-3.30	1.34	1.40
14	A	602	HEA	CHC-C1C	3.26	1.46	1.39
14	A	602	HEA	C4C-NC	-3.26	1.33	1.39
14	a	602	HEA	FE-NC	3.23	2.05	1.95
14	a	601	HEA	CHB-C1B	3.21	1.46	1.39
14	A	601	HEA	CHD-C4C	3.21	1.46	1.39
14	a	601	HEA	C11-C3B	-3.19	1.47	1.51
14	A	601	HEA	C3A-C2A	3.11	1.44	1.37
14	a	601	HEA	CHC-C1C	3.11	1.46	1.39
14	A	601	HEA	C4B-NB	-3.00	1.35	1.40
14	A	602	HEA	CHA-C1A	2.99	1.44	1.38
14	a	601	HEA	CHA-C4D	2.91	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	601	HEA	C4A-NA	2.90	1.45	1.39
25	c	309	DMU	O16-C6	2.84	1.44	1.40
14	A	601	HEA	C11-C3B	-2.78	1.48	1.51
14	A	601	HEA	C1C-C2C	2.76	1.49	1.43
14	a	601	HEA	C4D-ND	-2.76	1.33	1.38
14	A	601	HEA	CHB-C1B	2.69	1.45	1.39
14	a	601	HEA	C1C-C2C	2.66	1.49	1.43
25	C	308	DMU	O16-C6	2.60	1.44	1.40
14	a	602	HEA	C11-C3B	-2.52	1.48	1.51
14	A	602	HEA	CHA-C4D	2.52	1.44	1.39
14	a	602	HEA	C4C-NC	-2.50	1.34	1.39
14	A	601	HEA	CHC-C1C	2.50	1.45	1.39
14	A	602	HEA	CHB-C1B	2.48	1.44	1.39
14	a	602	HEA	CHB-C1B	2.46	1.44	1.39
14	a	601	HEA	C1B-NB	-2.46	1.34	1.38
14	A	602	HEA	C1C-C2C	2.45	1.48	1.43
14	A	601	HEA	O2D-CGD	-2.43	1.22	1.30
14	A	601	HEA	C1C-NC	-2.42	1.35	1.39
14	a	602	HEA	CHA-C4D	2.35	1.44	1.39
14	A	601	HEA	C1D-ND	-2.33	1.36	1.40
25	M	101	DMU	O16-C6	2.31	1.44	1.40
14	A	602	HEA	CHD-C4C	2.30	1.44	1.39
14	A	601	HEA	CHA-C4D	2.28	1.44	1.39
14	A	601	HEA	C4D-ND	-2.28	1.34	1.38
14	A	601	HEA	C4A-NA	2.25	1.43	1.39
14	A	601	HEA	C3C-C4C	2.23	1.49	1.42
14	a	602	HEA	C4B-C3B	2.21	1.48	1.44
14	A	602	HEA	C1A-NA	2.17	1.43	1.39
14	a	601	HEA	C1C-NC	-2.09	1.35	1.39

All (317) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C3D-C4D-ND	6.81	116.93	110.35
14	A	601	HEA	C3D-C4D-ND	6.53	116.66	110.35
26	E	201	PSC	C08-N-C06	-6.45	92.04	108.98
14	A	602	HEA	C2B-C1B-NB	6.35	117.24	109.90
26	b	303	PSC	C08-N-C06	-6.34	92.32	108.98
14	A	602	HEA	C2D-C1D-ND	6.33	117.12	109.84
26	E	201	PSC	C08-N-C07	-6.26	92.52	108.98
14	A	602	HEA	C1D-C2D-C3D	-6.26	100.40	106.98
14	A	601	HEA	C3C-C2C-C1C	-6.24	99.82	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	601	HEA	C3D-C4D-ND	6.15	116.30	110.35
26	b	303	PSC	C08-N-C07	-6.13	92.88	108.98
14	a	602	HEA	C3D-C4D-ND	5.89	116.04	110.35
14	a	601	HEA	C3C-C4C-NC	5.82	114.70	109.80
14	A	601	HEA	C2D-C1D-ND	5.77	116.47	109.84
18	a	606	PGV	O01-C1-C2	5.77	123.95	111.48
14	a	602	HEA	C2D-C1D-ND	5.71	116.41	109.84
14	a	601	HEA	C3C-C2C-C1C	-5.63	100.54	107.17
14	a	602	HEA	C1D-C2D-C3D	-5.59	101.10	106.98
24	c	307	CDL	OA6-CA5-C11	5.41	123.19	111.48
14	a	602	HEA	C2B-C1B-NB	5.39	116.13	109.90
14	A	602	HEA	C3C-C4C-NC	5.37	114.32	109.80
14	A	602	HEA	C3B-C4B-NB	5.37	116.02	109.84
22	J	101	CHD	C22-C20-C17	5.29	121.30	110.33
18	c	302	PGV	O01-C1-C2	5.28	122.90	111.48
14	A	602	HEA	C3C-C2C-C1C	-5.28	100.95	107.17
23	G	101	PEK	O01-C1-C2	5.26	122.87	111.48
19	l	101	TGL	OG2-CB1-CB2	5.18	122.69	111.48
14	a	601	HEA	C2B-C1B-NB	5.18	115.89	109.90
22	J	101	CHD	C6-C7-C8	5.14	117.11	111.50
14	a	602	HEA	C3C-C2C-C1C	-5.09	101.16	107.17
14	a	602	HEA	C3C-C4C-NC	5.09	114.08	109.80
24	g	101	CDL	OB6-CB5-C51	5.09	122.49	111.48
14	a	601	HEA	C3B-C4B-NB	5.02	115.61	109.84
14	a	602	HEA	C3B-C4B-NB	5.01	115.60	109.84
14	A	601	HEA	C2B-C1B-NB	4.99	115.67	109.90
22	J	101	CHD	C13-C17-C20	4.97	125.50	119.48
14	a	602	HEA	CAD-CBD-CGD	-4.95	100.53	113.67
14	A	601	HEA	C3C-C4C-NC	4.89	113.91	109.80
14	A	601	HEA	C1D-C2D-C3D	-4.85	101.87	106.98
14	a	601	HEA	C2D-C1D-ND	4.73	115.28	109.84
25	c	309	DMU	O16-C6-C1	4.73	115.45	108.27
26	E	201	PSC	O01-C1-C2	4.65	121.55	111.48
14	A	601	HEA	C3B-C4B-NB	4.65	115.19	109.84
24	C	305	CDL	OA6-CA5-C11	4.62	121.47	111.48
24	c	307	CDL	OB6-CB5-C51	4.35	120.89	111.48
19	d	201	TGL	OG2-CB1-CB2	4.33	120.85	111.48
14	a	601	HEA	C2C-C1C-NC	4.31	117.04	110.14
14	A	602	HEA	C2A-C1A-NA	4.30	114.47	110.32
26	E	201	PSC	C07-N-C06	4.27	120.20	108.98
19	b	302	TGL	OG2-CB1-CB2	4.18	120.53	111.48
26	E	201	PSC	C08-N-C05	-4.17	93.33	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	102	CDL	OB6-CB5-C51	4.13	120.41	111.48
23	C	302	PEK	O03-C21-C22	4.12	124.39	111.83
14	a	602	HEA	C2A-C1A-NA	4.10	114.28	110.32
22	J	101	CHD	C5-C6-C7	4.06	119.23	114.40
19	A	609	TGL	OG2-CB1-CB2	4.05	120.25	111.48
18	C	304	PGV	O03-C19-C20	4.05	124.17	111.83
14	A	601	HEA	C13-C12-C11	-4.01	107.98	114.39
19	D	201	TGL	OG2-CB1-CB2	4.01	120.16	111.48
14	A	601	HEA	C2C-C1C-NC	3.99	116.54	110.14
14	A	602	HEA	CMD-C2D-C1D	3.98	131.25	125.03
24	g	101	CDL	OA6-CA5-C11	3.97	120.07	111.48
26	b	303	PSC	C07-N-C06	3.87	119.15	108.98
23	c	305	PEK	O01-C1-C2	3.87	119.86	111.48
24	G	102	CDL	OA6-CA5-C11	3.87	119.85	111.48
26	b	303	PSC	C07-N-C05	3.80	125.03	109.91
18	c	302	PGV	O03-C19-C20	3.80	123.42	111.83
23	c	301	PEK	O01-C1-C2	3.79	119.69	111.48
14	a	601	HEA	C1D-C2D-C3D	-3.79	102.99	106.98
22	J	101	CHD	C6-C5-C4	-3.76	106.92	111.23
14	a	601	HEA	C1B-C2B-C3B	-3.76	102.44	106.80
22	C	306	CHD	C21-C20-C22	-3.75	104.53	110.34
14	A	601	HEA	C26-C15-C16	3.75	121.74	115.23
14	a	602	HEA	C4B-C3B-C2B	-3.74	101.15	107.44
14	A	601	HEA	O11-C11-C3B	-3.69	104.48	111.26
25	C	308	DMU	C6-O5-C4	3.67	120.88	113.72
23	C	307	PEK	O01-C1-C2	3.63	119.34	111.48
23	G	101	PEK	O03-C21-C22	3.63	122.90	111.83
14	A	602	HEA	CAD-CBD-CGD	-3.63	104.05	113.67
14	A	601	HEA	CMC-C2C-C3C	3.61	135.03	126.55
22	J	101	CHD	C6-C5-C10	3.59	116.48	112.66
25	c	309	DMU	C10-O1-C9	3.57	120.70	113.72
25	c	309	DMU	O5-C6-C1	3.57	117.70	110.37
14	A	602	HEA	C4B-C3B-C2B	-3.56	101.45	107.44
14	A	601	HEA	C1B-C2B-C3B	-3.56	102.67	106.80
14	a	601	HEA	C2A-C1A-NA	3.56	113.75	110.32
14	A	601	HEA	CMD-C2D-C1D	3.52	130.54	125.03
18	A	606	PGV	O03-C19-C20	3.50	122.51	111.83
18	C	304	PGV	O01-C1-C2	3.49	119.03	111.48
22	J	101	CHD	C21-C20-C17	-3.47	107.67	112.88
14	a	602	HEA	CMD-C2D-C1D	3.47	130.45	125.03
14	a	602	HEA	C2C-C1C-NC	3.46	115.69	110.14
24	C	305	CDL	OB6-CB5-C51	3.45	118.94	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C2A-C1A-NA	3.42	113.62	110.32
19	d	201	TGL	OG3-CC1-CC2	3.41	122.22	111.83
24	g	101	CDL	OA8-CA7-C31	3.39	122.17	111.83
14	a	601	HEA	C4D-C3D-C2D	-3.38	101.97	106.89
26	b	303	PSC	C08-N-C05	-3.33	96.66	109.91
14	a	601	HEA	C13-C12-C11	-3.33	109.07	114.39
14	A	602	HEA	CHD-C1D-C2D	-3.30	117.57	126.95
19	A	608	TGL	OG2-CB1-CB2	3.29	118.59	111.48
18	A	606	PGV	O01-C1-C2	3.26	118.53	111.48
14	A	602	HEA	C2C-C1C-NC	3.25	115.36	110.14
18	c	302	PGV	O03-C19-O04	-3.25	115.51	123.63
22	j	101	CHD	C21-C20-C17	3.24	117.75	112.88
14	a	601	HEA	C26-C15-C16	3.23	120.84	115.23
24	C	305	CDL	OA8-CA7-C31	3.23	121.67	111.83
24	G	102	CDL	OB8-CB7-C71	3.21	121.64	111.83
14	A	601	HEA	CHA-C4D-C3D	-3.19	120.12	124.77
22	B	402	CHD	C19-C10-C1	-3.19	103.24	108.31
14	a	602	HEA	CHD-C1D-C2D	-3.18	117.91	126.95
14	A	602	HEA	C4B-NB-C1B	-3.16	101.46	105.21
14	A	601	HEA	CHB-C1B-C2B	-3.16	120.04	125.03
24	C	305	CDL	OB8-CB7-C71	3.16	121.47	111.83
24	g	101	CDL	OB8-CB7-C71	3.15	121.45	111.83
14	a	601	HEA	CHB-C1B-C2B	-3.15	120.06	125.03
18	a	606	PGV	O03-C19-C20	3.14	121.41	111.83
22	B	402	CHD	C17-C13-C14	3.12	103.24	100.11
19	A	608	TGL	OG1-CA1-CA2	3.10	121.29	111.83
23	c	304	PEK	O03-C21-C22	3.09	121.25	111.83
14	A	602	HEA	C1B-C2B-C3B	-3.08	103.22	106.80
25	c	309	DMU	C18-O16-C6	-3.08	108.41	113.68
14	a	601	HEA	C3A-C2A-C1A	-3.08	104.13	107.05
25	m	101	DMU	O1-C9-C8	3.07	115.23	109.70
14	A	602	HEA	C1D-ND-C4D	-3.05	101.59	105.21
19	A	608	TGL	OG3-CC1-CC2	3.05	121.14	111.83
14	a	602	HEA	C4A-NA-C1A	-3.05	100.85	105.82
14	A	601	HEA	C3A-C2A-C1A	-3.04	104.17	107.05
14	a	601	HEA	CHA-C4D-C3D	-3.02	120.37	124.77
23	c	305	PEK	O03-C21-C22	3.01	121.01	111.83
26	b	303	PSC	O01-C1-C2	3.01	117.99	111.48
19	D	201	TGL	OG1-CA1-CA2	3.01	121.00	111.83
25	c	309	DMU	O1-C10-C5	3.00	116.54	110.37
24	C	305	CDL	OA6-CA5-OA7	-3.00	116.69	123.70
14	a	601	HEA	C4B-C3B-C2B	-2.99	102.41	107.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	302	TGL	OG1-CA1-CA2	2.98	120.93	111.83
14	A	601	HEA	C17-C18-C19	-2.98	120.80	127.62
24	c	307	CDL	OB8-CB7-C71	2.97	120.89	111.83
14	A	602	HEA	CAD-C3D-C4D	2.96	129.85	124.70
22	C	306	CHD	C19-C10-C1	-2.95	103.62	108.31
18	C	304	PGV	O03-C01-C02	2.95	116.89	108.40
14	a	602	HEA	CHC-C1C-C2C	-2.94	118.90	127.43
18	A	607	PGV	O03-C19-C20	2.93	120.75	111.83
19	l	101	TGL	OG1-CA1-CA2	2.93	120.75	111.83
14	A	602	HEA	C3A-C2A-C1A	-2.91	104.29	107.05
14	A	601	HEA	OMA-CMA-C3A	-2.88	119.12	125.62
18	c	306	PGV	O01-C1-C2	2.87	117.70	111.48
24	c	307	CDL	OA8-CA7-C31	2.86	120.55	111.83
26	b	303	PSC	O03-C19-C20	2.85	120.53	111.83
22	G	103	CHD	C22-C20-C17	2.85	116.23	110.33
19	b	302	TGL	OG3-CC1-CC2	2.83	120.47	111.83
23	c	304	PEK	O01-C1-C2	2.82	117.59	111.48
22	J	101	CHD	C17-C13-C14	-2.82	97.28	100.11
14	A	602	HEA	CHA-C4D-ND	-2.81	121.39	124.42
23	G	101	PEK	O03-C21-O04	-2.79	116.64	123.63
14	a	602	HEA	CMC-C2C-C3C	2.79	133.12	126.55
14	A	602	HEA	CMC-C2C-C3C	2.79	133.12	126.55
14	a	602	HEA	CHB-C1B-C2B	-2.78	120.63	125.03
14	A	602	HEA	CHB-C1B-C2B	-2.77	120.66	125.03
22	J	101	CHD	C5-C4-C3	2.76	116.87	112.71
19	d	201	TGL	OG1-CA1-CA2	2.76	120.24	111.83
14	A	601	HEA	C4D-C3D-C2D	-2.74	102.90	106.89
24	G	102	CDL	OA8-CA7-C31	2.73	120.15	111.83
25	C	308	DMU	C10-O1-C9	2.73	119.05	113.72
26	E	201	PSC	O03-C19-C20	2.72	120.14	111.83
24	C	305	CDL	OB8-CB7-OB9	-2.71	116.84	123.63
19	l	101	TGL	OG3-CC1-CC2	2.71	120.10	111.83
22	j	101	CHD	C6-C5-C4	-2.71	108.13	111.23
14	A	602	HEA	C4A-NA-C1A	-2.70	101.42	105.82
25	C	308	DMU	C6-C1-C2	2.68	115.65	110.01
22	c	303	CHD	C19-C10-C1	-2.67	104.06	108.31
23	C	302	PEK	O01-C1-C2	2.67	117.25	111.48
22	c	308	CHD	C6-C5-C4	-2.66	108.18	111.23
18	A	607	PGV	O03-C19-O04	-2.66	116.98	123.63
14	A	601	HEA	CAD-C3D-C4D	2.65	129.31	124.70
14	A	601	HEA	C1D-ND-C4D	-2.64	102.08	105.21
26	b	303	PSC	C02-O01-C1	2.64	124.12	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	602	HEA	OMA-CMA-C3A	-2.64	119.66	125.62
22	j	101	CHD	C9-C10-C5	2.64	112.17	108.51
19	d	201	TGL	CG2-OG2-CB1	2.63	124.09	117.80
14	A	602	HEA	C13-C12-C11	-2.62	110.20	114.39
19	d	201	TGL	OG2-CB1-OB1	-2.62	117.58	123.70
14	a	602	HEA	C1D-ND-C4D	-2.62	102.11	105.21
14	a	601	HEA	C4A-NA-C1A	-2.61	101.57	105.82
14	a	601	HEA	CHC-C1C-C2C	-2.59	119.90	127.43
19	d	201	TGL	OG2-CG2-CG1	2.58	117.59	108.34
22	G	103	CHD	C19-C10-C1	-2.58	104.21	108.31
26	E	201	PSC	C07-N-C05	2.56	120.10	109.91
14	a	602	HEA	CAD-C3D-C4D	2.56	129.16	124.70
14	a	601	HEA	CHB-C4A-NA	-2.54	121.69	124.45
22	J	101	CHD	C19-C10-C1	-2.54	104.27	108.31
14	A	601	HEA	C4B-C3B-C2B	-2.53	103.19	107.44
25	m	101	DMU	C7-C8-C9	2.53	114.82	110.23
24	G	102	CDL	OA6-CA5-OA7	-2.52	117.80	123.70
22	J	101	CHD	O7-C7-C6	-2.52	103.58	109.86
18	A	606	PGV	O03-C19-O04	-2.51	117.34	123.63
19	l	101	TGL	CG3-OG3-CC1	2.49	126.22	117.12
14	A	602	HEA	CHC-C4B-C3B	-2.49	119.52	125.80
14	a	601	HEA	OMA-CMA-C3A	-2.48	120.03	125.62
23	c	301	PEK	O03-C21-C22	2.47	119.37	111.83
22	C	301	CHD	C19-C10-C1	-2.47	104.38	108.31
14	A	601	HEA	O11-C11-C12	2.46	115.67	109.14
18	a	607	PGV	O01-C1-C2	2.46	116.81	111.48
22	B	402	CHD	C14-C13-C12	-2.46	105.17	107.42
14	A	602	HEA	CMB-C2B-C1B	2.45	128.87	125.03
22	J	101	CHD	C11-C12-C13	2.44	113.75	111.26
22	j	101	CHD	C10-C9-C8	2.44	114.55	111.84
19	D	201	TGL	OG2-CB1-OB1	-2.44	118.01	123.70
14	A	601	HEA	C4A-NA-C1A	-2.44	101.85	105.82
22	c	308	CHD	C19-C10-C1	-2.43	104.44	108.31
22	G	103	CHD	C11-C12-C13	2.43	113.74	111.26
14	A	601	HEA	CHD-C1D-C2D	-2.42	120.06	126.95
22	j	101	CHD	C19-C10-C5	-2.42	106.39	110.44
14	A	601	HEA	CHC-C1C-C2C	-2.41	120.42	127.43
22	C	306	CHD	C6-C5-C4	-2.41	108.48	111.23
23	C	307	PEK	O03-C21-C22	2.40	119.16	111.83
23	G	101	PEK	O01-C1-O02	-2.39	118.11	123.70
22	C	301	CHD	C6-C7-C8	2.39	114.11	111.50
18	c	302	PGV	C01-O03-C19	2.39	125.85	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	CHB-C4A-NA	-2.38	121.86	124.45
14	a	601	HEA	CMC-C2C-C3C	2.38	132.14	126.55
26	E	201	PSC	O01-C1-O02	-2.37	118.15	123.70
26	b	303	PSC	O01-C02-C01	2.37	116.86	108.34
22	c	303	CHD	C18-C13-C12	2.37	111.43	109.06
19	A	608	TGL	OG1-CA1-OA1	-2.37	117.70	123.63
22	B	402	CHD	O3-C3-C4	-2.37	105.13	109.84
24	g	101	CDL	OA8-CA7-OA9	-2.37	117.71	123.63
22	j	101	CHD	C5-C6-C7	-2.35	111.60	114.40
14	A	601	HEA	C25-C23-C24	2.35	119.99	114.59
24	G	102	CDL	OB6-CB5-OB7	-2.35	118.22	123.70
23	C	302	PEK	O01-C1-O02	-2.34	118.23	123.70
14	A	602	HEA	CHC-C1C-C2C	-2.34	120.63	127.43
22	C	301	CHD	C21-C20-C17	2.34	116.40	112.88
14	a	602	HEA	C1B-C2B-C3B	-2.34	104.09	106.80
24	c	307	CDL	OA6-CA5-OA7	-2.33	118.26	123.70
14	a	602	HEA	CHA-C4D-ND	-2.32	121.92	124.42
19	A	609	TGL	OG2-CB1-OB1	-2.32	118.29	123.70
14	a	602	HEA	CHC-C4B-C3B	-2.31	119.97	125.80
14	A	602	HEA	O2A-CGA-CBA	2.31	121.28	114.00
22	J	101	CHD	C13-C14-C8	2.30	117.64	114.72
26	E	201	PSC	C06-N-C05	2.30	119.06	109.91
24	g	101	CDL	OB6-CB5-OB7	-2.29	118.35	123.70
25	C	308	DMU	O7-C3-C2	2.29	113.04	107.23
24	C	305	CDL	OA8-CA7-OA9	-2.28	117.92	123.63
22	C	306	CHD	C21-C20-C17	2.28	116.31	112.88
22	B	402	CHD	C6-C7-C8	2.28	113.99	111.50
18	c	302	PGV	O01-C1-O02	-2.28	118.38	123.70
18	a	607	PGV	O03-C19-C20	2.28	118.78	111.83
22	j	101	CHD	O7-C7-C6	-2.27	104.21	109.86
22	j	101	CHD	O7-C7-C8	2.27	114.72	109.52
26	E	201	PSC	O03-C19-O04	-2.26	117.96	123.63
22	C	306	CHD	C18-C13-C12	2.26	111.32	109.06
23	c	304	PEK	O01-C1-O02	-2.26	118.43	123.70
19	d	201	TGL	OG3-CC1-OC1	-2.25	117.99	123.63
14	A	602	HEA	CBA-CAA-C2A	-2.25	106.31	112.53
25	C	308	DMU	O5-C6-C1	2.25	114.99	110.37
24	c	307	CDL	OB8-CB7-OB9	-2.24	118.01	123.63
14	a	601	HEA	O11-C11-C3B	-2.24	107.16	111.26
22	J	101	CHD	C19-C10-C5	-2.24	106.70	110.44
14	a	602	HEA	CBA-CAA-C2A	-2.23	106.36	112.53
23	C	307	PEK	C01-O03-C21	2.23	125.27	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	609	TGL	CG3-OG3-CC1	2.22	125.25	117.12
23	C	302	PEK	O03-C21-O04	-2.22	118.08	123.63
22	J	101	CHD	C9-C10-C5	2.22	111.59	108.51
18	a	606	PGV	O01-C1-O02	-2.21	118.53	123.70
22	B	402	CHD	C1-C10-C9	2.21	114.77	111.34
22	G	103	CHD	O26-C24-C23	2.21	120.97	114.00
14	A	602	HEA	CHB-C1B-NB	-2.20	122.05	124.42
23	c	305	PEK	O03-C21-O04	-2.20	118.13	123.63
14	a	601	HEA	CHD-C1D-C2D	-2.19	120.71	126.95
14	A	602	HEA	O1A-CGA-CBA	-2.19	116.14	123.09
25	C	308	DMU	C2-C3-C4	-2.19	106.07	110.93
14	a	601	HEA	CHA-C1A-C2A	-2.19	121.41	124.86
14	a	602	HEA	C27-C19-C20	2.18	119.00	115.23
19	A	609	TGL	OG3-CC1-CC2	2.17	118.44	111.83
14	a	601	HEA	CAA-CBA-CGA	-2.16	107.93	113.67
14	A	602	HEA	C4D-C3D-C2D	-2.16	103.74	106.89
19	D	201	TGL	OG3-CC1-CC2	2.16	118.41	111.83
25	c	309	DMU	C10-C5-C7	2.15	114.53	110.01
14	a	602	HEA	C3A-C2A-C1A	-2.15	105.01	107.05
14	a	602	HEA	C25-C23-C24	2.14	119.51	114.59
22	C	301	CHD	C18-C13-C12	2.13	111.19	109.06
14	A	602	HEA	CHA-C4D-C3D	-2.13	121.67	124.77
22	c	308	CHD	C11-C12-C13	2.13	113.43	111.26
14	A	601	HEA	CAA-CBA-CGA	-2.13	108.02	113.67
22	j	101	CHD	C13-C17-C20	2.13	122.06	119.48
22	J	101	CHD	C18-C13-C12	-2.12	106.93	109.06
19	A	609	TGL	OG1-CA1-CA2	2.12	118.29	111.83
22	B	402	CHD	C11-C12-C13	2.11	113.41	111.26
14	A	602	HEA	C4C-C3C-C2C	-2.11	104.68	107.30
25	m	101	DMU	O1-C10-C5	-2.11	106.04	110.37
18	A	607	PGV	O14-P-O13	2.11	122.24	112.44
18	C	304	PGV	O03-C19-O04	-2.10	118.37	123.63
14	a	602	HEA	CHA-C1A-C2A	-2.09	121.57	124.86
23	c	301	PEK	C01-O03-C21	2.08	124.73	117.12
22	j	101	CHD	C21-C20-C22	-2.08	107.12	110.34
14	a	601	HEA	CHC-C4B-C3B	-2.07	120.57	125.80
18	C	303	PGV	O01-C1-C2	2.07	115.96	111.48
18	c	306	PGV	O14-P-O13	2.07	122.07	112.44
19	l	101	TGL	OG1-CA1-OA1	-2.07	118.46	123.63
14	a	601	HEA	O2D-CGD-CBD	2.06	120.52	114.00
14	a	601	HEA	C25-C23-C24	2.05	119.32	114.59
26	b	303	PSC	C21-C20-C19	-2.05	106.18	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	606	PGV	O03-C01-C02	2.05	114.31	108.40
22	c	303	CHD	C6-C7-C8	2.05	113.74	111.50
19	b	302	TGL	OG2-CB1-OB1	-2.05	118.92	123.70
18	a	606	PGV	O03-C19-O04	-2.04	118.53	123.63
14	a	601	HEA	O2A-CGA-CBA	2.03	120.41	114.00
19	d	201	TGL	OG1-CA1-OA1	-2.03	118.56	123.63
19	D	201	TGL	CG3-OG3-CC1	2.02	124.50	117.12
14	A	602	HEA	OMA-CMA-C3A	-2.02	121.06	125.62
18	c	302	PGV	O03-C01-C02	2.01	114.19	108.40
25	c	309	DMU	O7-C10-O1	-2.01	105.41	110.69
24	g	101	CDL	OB8-CB7-OB9	-2.01	118.61	123.63
22	B	402	CHD	C6-C5-C4	-2.00	108.94	111.23
26	b	303	PSC	C01-O03-C19	2.00	124.44	117.12
25	m	101	DMU	O7-C10-C5	2.00	113.01	108.09

There are no chirality outliers.

All (800) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C03-O11-P-O12
18	C	304	PGV	C03-O11-P-O12
18	C	304	PGV	C02-C03-O11-P
18	C	304	PGV	O12-C04-C05-C06
18	C	304	PGV	C04-C05-C06-O06
18	a	606	PGV	O02-C1-O01-C02
18	a	606	PGV	C2-C1-O01-C02
18	c	302	PGV	C03-O11-P-O12
18	c	302	PGV	C03-O11-P-O14
18	c	302	PGV	C04-O12-P-O14
18	c	302	PGV	O12-C04-C05-C06
18	c	302	PGV	O04-C19-O03-C01
18	c	302	PGV	C20-C19-O03-C01
19	D	201	TGL	CB2-CB1-OG2-CG2
19	d	201	TGL	CB2-CB1-OG2-CG2
23	C	307	PEK	O12-C04-C05-N
23	G	101	PEK	C03-O11-P-O13
23	G	101	PEK	C2-C1-O01-C02
23	G	101	PEK	C6-C7-C8-C9
23	c	305	PEK	C03-O11-P-O12
23	c	305	PEK	C03-O11-P-O14
23	c	305	PEK	C04-O12-P-O11
23	c	305	PEK	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
24	C	305	CDL	C1-CA2-OA2-PA1
24	C	305	CDL	CA2-OA2-PA1-OA3
24	C	305	CDL	C11-CA5-OA6-CA4
24	G	102	CDL	CB2-C1-CA2-OA2
24	G	102	CDL	CA3-OA5-PA1-OA2
24	G	102	CDL	CA3-OA5-PA1-OA4
24	G	102	CDL	OA7-CA5-OA6-CA4
24	G	102	CDL	C11-CA5-OA6-CA4
24	G	102	CDL	CB3-OB5-PB2-OB2
24	G	102	CDL	CB3-OB5-PB2-OB4
24	G	102	CDL	C51-CB5-OB6-CB4
24	c	307	CDL	C1-CA2-OA2-PA1
24	c	307	CDL	CA2-OA2-PA1-OA3
24	c	307	CDL	CA2-OA2-PA1-OA4
24	c	307	CDL	CA2-OA2-PA1-OA5
24	c	307	CDL	CA3-OA5-PA1-OA2
24	c	307	CDL	CA3-OA5-PA1-OA3
24	c	307	CDL	CA3-OA5-PA1-OA4
24	c	307	CDL	OA7-CA5-OA6-CA4
24	c	307	CDL	C11-CA5-OA6-CA4
24	c	307	CDL	CB3-OB5-PB2-OB3
24	g	101	CDL	OA7-CA5-OA6-CA4
24	g	101	CDL	C11-CA5-OA6-CA4
24	g	101	CDL	CB2-OB2-PB2-OB3
26	E	201	PSC	C04-O12-P-O14
26	E	201	PSC	C2-C1-O01-C02
26	b	303	PSC	C03-O11-P-O12
26	b	303	PSC	C03-O11-P-O13
26	b	303	PSC	C01-C02-O01-C1
26	b	303	PSC	O12-C04-C05-N
26	b	303	PSC	O04-C19-O03-C01
26	b	303	PSC	C20-C19-O03-C01
19	b	302	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	CA2-CA1-OG1-CG1
19	A	608	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	OA1-CA1-OG1-CG1
19	d	201	TGL	OA1-CA1-OG1-CG1
24	g	101	CDL	OA9-CA7-OA8-CA6
18	c	302	PGV	O02-C1-O01-C02
19	A	608	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	OB1-CB1-OG2-CG2
19	d	201	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
23	c	305	PEK	O02-C1-O01-C02
24	C	305	CDL	OA7-CA5-OA6-CA4
24	G	102	CDL	OB7-CB5-OB6-CB4
26	E	201	PSC	O02-C1-O01-C02
19	A	608	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	CC2-CC1-OG3-CG3
19	b	302	TGL	CC2-CC1-OG3-CG3
19	d	201	TGL	CA2-CA1-OG1-CG1
24	G	102	CDL	C71-CB7-OB8-CB6
24	g	101	CDL	C31-CA7-OA8-CA6
19	A	608	TGL	CB2-CB1-OG2-CG2
23	c	305	PEK	C2-C1-O01-C02
19	D	201	TGL	OC1-CC1-OG3-CG3
24	C	305	CDL	C31-CA7-OA8-CA6
24	g	101	CDL	C71-CB7-OB8-CB6
18	a	606	PGV	O04-C19-O03-C01
24	C	305	CDL	OA9-CA7-OA8-CA6
24	G	102	CDL	OB9-CB7-OB8-CB6
24	g	101	CDL	OB9-CB7-OB8-CB6
23	G	101	PEK	O02-C1-O01-C02
18	C	304	PGV	O12-C04-C05-O05
18	a	606	PGV	O12-C04-C05-O05
18	c	302	PGV	O12-C04-C05-O05
24	G	102	CDL	O1-C1-CA2-OA2
24	C	305	CDL	C71-CB7-OB8-CB6
26	E	201	PSC	C20-C19-O03-C01
18	c	302	PGV	C2-C1-O01-C02
19	d	201	TGL	CA1-CA2-CA3-CA4
25	C	308	DMU	O6-C11-C9-O1
18	a	606	PGV	C20-C19-O03-C01
24	C	305	CDL	OB9-CB7-OB8-CB6
26	E	201	PSC	O04-C19-O03-C01
25	c	309	DMU	O5-C6-O16-C18
25	M	101	DMU	O6-C11-C9-O1
19	l	101	TGL	CA3-CA4-CA5-CA6
19	d	201	TGL	CC1-CC2-CC3-CC4
22	C	306	CHD	C17-C20-C22-C23
22	j	101	CHD	C17-C20-C22-C23
25	c	309	DMU	O5-C4-C57-O61
18	c	306	PGV	C27-C28-C29-C30
22	C	306	CHD	C21-C20-C22-C23
18	a	606	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
25	M	101	DMU	O6-C11-C9-C8
19	d	201	TGL	C13-C14-C29-C30
18	A	607	PGV	C29-C30-C31-C32
25	c	309	DMU	C3-C4-C57-O61
25	c	309	DMU	C1-C6-O16-C18
24	G	102	CDL	CB5-C51-C52-C53
24	g	101	CDL	OA6-CA4-CA6-OA8
24	G	102	CDL	C31-CA7-OA8-CA6
24	g	101	CDL	CA7-C31-C32-C33
24	g	101	CDL	CB7-C71-C72-C73
23	G	101	PEK	C21-C22-C23-C24
24	C	305	CDL	CB7-C71-C72-C73
24	c	307	CDL	CB7-C71-C72-C73
18	A	606	PGV	C2-C1-O01-C02
22	j	101	CHD	C21-C20-C22-C23
18	C	304	PGV	C1-C2-C3-C4
23	c	305	PEK	C1-C2-C3-C4
24	G	102	CDL	CB7-C71-C72-C73
26	b	303	PSC	C19-C20-C21-C22
24	G	102	CDL	OA9-CA7-OA8-CA6
19	b	302	TGL	CA1-CA2-CA3-CA4
23	C	302	PEK	C1-C2-C3-C4
24	G	102	CDL	C73-C74-C75-C76
24	C	305	CDL	C51-CB5-OB6-CB4
18	A	606	PGV	O02-C1-O01-C02
24	C	305	CDL	OB7-CB5-OB6-CB4
24	c	307	CDL	C31-CA7-OA8-CA6
19	b	302	TGL	CC1-CC2-CC3-CC4
19	A	609	TGL	CB2-CB1-OG2-CG2
23	c	301	PEK	C2-C1-O01-C02
19	A	609	TGL	OB1-CB1-OG2-CG2
23	c	301	PEK	O02-C1-O01-C02
25	C	308	DMU	O6-C11-C9-C8
24	g	101	CDL	CB5-C51-C52-C53
24	c	307	CDL	OA9-CA7-OA8-CA6
19	d	201	TGL	CG1-CG2-OG2-CB1
18	c	302	PGV	C6-C7-C8-C9
19	l	101	TGL	CA2-CA1-OG1-CG1
26	E	201	PSC	C04-C05-N-C06
19	A	609	TGL	C11-C12-C13-C14
18	a	606	PGV	C26-C27-C28-C29
19	A	609	TGL	C12-C13-C14-C29

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Mol	Chain	Res	Type	Atoms
23	c	305	PEK	C28-C29-C30-C31
24	c	307	CDL	C63-C64-C65-C66
24	g	101	CDL	C82-C83-C84-C85
19	l	101	TGL	CC4-CC5-CC6-CC7
23	c	301	PEK	C29-C30-C31-C32
25	m	101	DMU	C19-C22-C25-C28
19	b	302	TGL	CA2-CA1-OG1-CG1
18	A	607	PGV	C6-C7-C8-C9
19	A	609	TGL	CC9-C15-C16-C17
19	A	609	TGL	C16-C17-C18-C19
23	C	302	PEK	C30-C31-C32-C33
24	G	102	CDL	C14-C15-C16-C17
18	C	304	PGV	O05-C05-C06-O06
18	c	302	PGV	C23-C24-C25-C26
19	A	609	TGL	C10-C11-C12-C13
24	C	305	CDL	C53-C54-C55-C56
24	G	102	CDL	C79-C80-C81-C82
24	c	307	CDL	C39-C40-C41-C42
18	a	606	PGV	C7-C8-C9-C10
19	d	201	TGL	CA4-CA5-CA6-CA7
24	G	102	CDL	C83-C84-C85-C86
22	J	101	CHD	C13-C17-C20-C22
19	A	609	TGL	C16-C15-CC9-CC8
24	C	305	CDL	C41-C42-C43-C44
19	l	101	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	CA9-C20-C21-C22
19	d	201	TGL	C23-C24-C25-C26
19	A	609	TGL	CC1-CC2-CC3-CC4
19	D	201	TGL	CA1-CA2-CA3-CA4
18	A	607	PGV	C4-C5-C6-C7
19	b	302	TGL	CA3-CA4-CA5-CA6
19	b	302	TGL	C16-C17-C18-C19
19	l	101	TGL	CC5-CC6-CC7-CC8
24	C	305	CDL	C57-C58-C59-C60
24	c	307	CDL	C78-C79-C80-C81
24	G	102	CDL	C19-C20-C21-C22
18	c	306	PGV	C19-C20-C21-C22
18	A	606	PGV	C7-C8-C9-C10
18	c	302	PGV	C24-C25-C26-C27
19	D	201	TGL	CA4-CA5-CA6-CA7
24	G	102	CDL	C22-C23-C24-C25
24	G	102	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
23	G	101	PEK	C28-C29-C30-C31
19	A	608	TGL	C24-C25-C26-C27
23	c	305	PEK	C29-C30-C31-C32
24	G	102	CDL	C37-C38-C39-C40
18	A	606	PGV	C5-C6-C7-C8
18	c	302	PGV	C20-C21-C22-C23
19	b	302	TGL	CB2-CB3-CB4-CB5
24	C	305	CDL	C40-C41-C42-C43
24	C	305	CDL	C61-C62-C63-C64
24	G	102	CDL	C11-C12-C13-C14
18	C	304	PGV	C13-C14-C15-C16
18	c	302	PGV	C5-C6-C7-C8
19	b	302	TGL	CB3-CB4-CB5-CB6
23	C	302	PEK	C22-C23-C24-C25
18	C	304	PGV	C26-C27-C28-C29
19	A	609	TGL	CB2-CB3-CB4-CB5
19	D	201	TGL	C11-C12-C13-C14
23	c	301	PEK	C24-C25-C26-C27
18	a	607	PGV	C19-C20-C21-C22
18	c	302	PGV	C7-C8-C9-C10
24	c	307	CDL	C40-C41-C42-C43
19	A	608	TGL	C19-C33-C34-C35
19	l	101	TGL	C17-C18-C19-C33
23	G	101	PEK	C16-C17-C18-C19
19	d	201	TGL	CA6-CA7-CA8-CA9
23	c	305	PEK	C25-C26-C27-C28
19	A	608	TGL	CB7-CB8-CB9-C10
19	d	201	TGL	C16-C17-C18-C19
19	l	101	TGL	C10-C11-C12-C13
19	b	302	TGL	OA1-CA1-OG1-CG1
19	l	101	TGL	OA1-CA1-OG1-CG1
18	C	304	PGV	C30-C31-C32-C33
19	D	201	TGL	C24-C25-C26-C27
19	l	101	TGL	OB1-CB1-OG2-CG2
23	c	304	PEK	C24-C25-C26-C27
24	c	307	CDL	C11-C12-C13-C14
18	C	304	PGV	C7-C8-C9-C10
25	c	309	DMU	C22-C25-C28-C31
26	E	201	PSC	C23-C24-C25-C26
18	A	607	PGV	C19-C20-C21-C22
19	l	101	TGL	C15-C16-C17-C18
23	c	305	PEK	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	c	307	CDL	C43-C44-C45-C46
24	g	101	CDL	C22-C23-C24-C25
23	C	307	PEK	C27-C28-C29-C30
23	C	307	PEK	C29-C30-C31-C32
24	c	307	CDL	C56-C57-C58-C59
24	c	307	CDL	C74-C75-C76-C77
25	M	101	DMU	C28-C31-C34-C37
22	J	101	CHD	C13-C17-C20-C21
24	g	101	CDL	C51-CB5-OB6-CB4
23	c	304	PEK	C1-C2-C3-C4
23	C	302	PEK	C26-C27-C28-C29
19	b	302	TGL	C20-C21-C22-C23
19	d	201	TGL	CA9-C20-C21-C22
18	A	606	PGV	C12-C13-C14-C15
19	b	302	TGL	C16-C15-CC9-CC8
18	C	304	PGV	C20-C21-C22-C23
23	c	301	PEK	C34-C35-C36-C37
24	c	307	CDL	C35-C36-C37-C38
19	D	201	TGL	C18-C19-C33-C34
19	d	201	TGL	C21-C20-CA9-CA8
23	C	307	PEK	C31-C32-C33-C34
24	C	305	CDL	C36-C37-C38-C39
19	A	609	TGL	C23-C24-C25-C26
19	D	201	TGL	C21-C22-C23-C24
23	c	304	PEK	C34-C35-C36-C37
24	G	102	CDL	C40-C41-C42-C43
23	c	304	PEK	C2-C1-O01-C02
24	c	307	CDL	C51-CB5-OB6-CB4
22	J	101	CHD	C16-C17-C20-C21
19	A	609	TGL	CA9-C20-C21-C22
24	G	102	CDL	C54-C55-C56-C57
24	g	101	CDL	C31-C32-C33-C34
26	E	201	PSC	C21-C22-C23-C24
18	C	303	PGV	C19-C20-C21-C22
18	C	304	PGV	C27-C28-C29-C30
19	A	608	TGL	C16-C17-C18-C19
19	A	608	TGL	CA9-C20-C21-C22
19	l	101	TGL	CA2-CA3-CA4-CA5
18	A	606	PGV	C11-C10-C9-C8
18	A	607	PGV	C12-C13-C14-C15
18	C	304	PGV	C11-C10-C9-C8
19	b	302	TGL	OG1-CG1-CG2-OG2

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Mol	Chain	Res	Type	Atoms
19	l	101	TGL	OG1-CG1-CG2-OG2
23	c	305	PEK	O03-C01-C02-O01
18	c	306	PGV	C7-C8-C9-C10
19	d	201	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	CA2-CA3-CA4-CA5
24	g	101	CDL	C80-C81-C82-C83
18	c	302	PGV	C14-C15-C16-C17
19	l	101	TGL	CC3-CC4-CC5-CC6
24	g	101	CDL	C16-C17-C18-C19
18	a	606	PGV	C3-C4-C5-C6
23	C	302	PEK	C31-C32-C33-C34
24	c	307	CDL	C54-C55-C56-C57
26	E	201	PSC	C2-C3-C4-C5
19	A	608	TGL	C13-C14-C29-C30
19	A	608	TGL	CC4-CC5-CC6-CC7
19	b	302	TGL	CA9-C20-C21-C22
19	l	101	TGL	CA4-CA5-CA6-CA7
24	G	102	CDL	C32-C33-C34-C35
18	C	303	PGV	C7-C8-C9-C10
19	d	201	TGL	CB7-CB8-CB9-C10
22	j	101	CHD	C13-C17-C20-C21
19	A	608	TGL	CB6-CB7-CB8-CB9
18	C	304	PGV	C29-C30-C31-C32
18	c	302	PGV	C4-C5-C6-C7
19	d	201	TGL	C18-C19-C33-C34
24	c	307	CDL	OA5-CA3-CA4-CA6
24	c	307	CDL	OB7-CB5-OB6-CB4
24	G	102	CDL	C34-C35-C36-C37
18	a	607	PGV	C7-C8-C9-C10
19	A	609	TGL	C17-C18-C19-C33
19	d	201	TGL	C11-C12-C13-C14
24	C	305	CDL	C79-C80-C81-C82
24	G	102	CDL	C56-C57-C58-C59
24	C	305	CDL	CA5-C11-C12-C13
19	l	101	TGL	C11-C12-C13-C14
18	C	304	PGV	O03-C01-C02-C03
19	D	201	TGL	OG1-CG1-CG2-CG3
19	b	302	TGL	OG1-CG1-CG2-CG3
19	d	201	TGL	OG1-CG1-CG2-CG3
19	d	201	TGL	CG1-CG2-CG3-OG3
24	C	305	CDL	CB3-CB4-CB6-OB8
24	g	101	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
19	A	609	TGL	CB4-CB5-CB6-CB7
19	l	101	TGL	CB6-CB7-CB8-CB9
23	c	301	PEK	C23-C24-C25-C26
24	G	102	CDL	C20-C21-C22-C23
18	A	607	PGV	C11-C10-C9-C8
18	C	303	PGV	C11-C10-C9-C8
23	c	305	PEK	C15-C16-C17-C18
24	c	307	CDL	C81-C82-C83-C84
24	g	101	CDL	C35-C36-C37-C38
19	l	101	TGL	CC1-CC2-CC3-CC4
19	l	101	TGL	CB3-CB4-CB5-CB6
19	d	201	TGL	OC1-CC1-OG3-CG3
18	C	304	PGV	C4-C5-C6-C7
19	D	201	TGL	CC6-CC7-CC8-CC9
18	c	306	PGV	C1-C2-C3-C4
18	A	606	PGV	C29-C30-C31-C32
23	C	307	PEK	C28-C29-C30-C31
24	G	102	CDL	C33-C34-C35-C36
24	G	102	CDL	C58-C59-C60-C61
19	D	201	TGL	C16-C17-C18-C19
19	l	101	TGL	C14-C29-C30-C31
24	g	101	CDL	C36-C37-C38-C39
23	G	101	PEK	C34-C35-C36-C37
26	b	303	PSC	C22-C23-C24-C25
23	C	302	PEK	C2-C3-C4-C5
23	G	101	PEK	C2-C3-C4-C5
23	c	301	PEK	C15-C16-C17-C18
23	c	304	PEK	C2-C3-C4-C5
18	a	607	PGV	C5-C6-C7-C8
19	A	609	TGL	CA6-CA7-CA8-CA9
19	b	302	TGL	CC2-CC3-CC4-CC5
26	b	303	PSC	C23-C24-C25-C26
18	C	304	PGV	C3-C4-C5-C6
18	c	302	PGV	C29-C30-C31-C32
24	C	305	CDL	C56-C57-C58-C59
24	G	102	CDL	C81-C82-C83-C84
18	a	606	PGV	C4-C5-C6-C7
19	d	201	TGL	CB6-CB7-CB8-CB9
18	C	303	PGV	C24-C25-C26-C27
18	a	607	PGV	C29-C30-C31-C32
24	C	305	CDL	C34-C35-C36-C37
18	a	606	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
18	a	607	PGV	C23-C24-C25-C26
23	C	307	PEK	C22-C23-C24-C25
24	g	101	CDL	C72-C73-C74-C75
24	g	101	CDL	C73-C74-C75-C76
18	C	304	PGV	O03-C01-C02-O01
18	A	606	PGV	C2-C3-C4-C5
19	l	101	TGL	C21-C22-C23-C24
24	c	307	CDL	C64-C65-C66-C67
24	g	101	CDL	C42-C43-C44-C45
26	b	303	PSC	C04-C05-N-C07
19	D	201	TGL	CC5-CC6-CC7-CC8
23	c	305	PEK	C23-C24-C25-C26
23	C	302	PEK	C17-C18-C19-C20
18	c	302	PGV	C12-C13-C14-C15
18	c	302	PGV	C30-C31-C32-C33
18	A	606	PGV	C14-C15-C16-C17
19	A	608	TGL	CA7-CA8-CA9-C20
18	C	304	PGV	C22-C23-C24-C25
19	d	201	TGL	CB5-CB6-CB7-CB8
19	D	201	TGL	CB7-CB8-CB9-C10
23	C	302	PEK	C34-C35-C36-C37
23	G	101	PEK	C25-C26-C27-C28
24	C	305	CDL	C83-C84-C85-C86
24	g	101	CDL	C53-C54-C55-C56
24	g	101	CDL	OB7-CB5-OB6-CB4
25	c	309	DMU	C19-C18-O16-C6
18	c	302	PGV	C9-C10-C11-C12
24	c	307	CDL	C55-C56-C57-C58
26	b	303	PSC	C28-C29-C30-C31
23	c	305	PEK	C02-C03-O11-P
19	A	609	TGL	CC3-CC4-CC5-CC6
19	D	201	TGL	C12-C13-C14-C29
19	A	609	TGL	CC2-CC1-OG3-CG3
18	C	303	PGV	C22-C23-C24-C25
19	A	608	TGL	C15-C16-C17-C18
19	b	302	TGL	C11-C12-C13-C14
18	A	606	PGV	C4-C5-C6-C7
19	d	201	TGL	CC4-CC5-CC6-CC7
24	g	101	CDL	C76-C77-C78-C79
18	A	606	PGV	C01-C02-C03-O11
23	G	101	PEK	C01-C02-C03-O11
23	c	301	PEK	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
24	C	305	CDL	OB5-CB3-CB4-CB6
24	g	101	CDL	OA5-CA3-CA4-CA6
24	g	101	CDL	OB5-CB3-CB4-CB6
19	b	302	TGL	C13-C14-C29-C30
19	d	201	TGL	CA3-CA4-CA5-CA6
19	A	608	TGL	C29-C30-C31-C32
23	G	101	PEK	C17-C18-C19-C20
26	b	303	PSC	C15-C16-C17-C18
26	b	303	PSC	C31-C32-C33-C34
19	d	201	TGL	C21-C22-C23-C24
19	d	201	TGL	C33-C34-C35-C36
24	G	102	CDL	C24-C25-C26-C27
25	m	101	DMU	C34-C37-C40-C43
24	g	101	CDL	C43-C44-C45-C46
24	C	305	CDL	C24-C25-C26-C27
24	c	307	CDL	C20-C21-C22-C23
19	D	201	TGL	C13-C14-C29-C30
19	d	201	TGL	CB3-CB4-CB5-CB6
19	l	101	TGL	OG1-CG1-CG2-CG3
23	c	305	PEK	O03-C01-C02-C03
24	G	102	CDL	CB3-CB4-CB6-OB8
18	c	302	PGV	C22-C23-C24-C25
19	A	609	TGL	C20-C21-C22-C23
19	b	302	TGL	C25-C26-C27-C28
18	a	606	PGV	C13-C14-C15-C16
24	c	307	CDL	C18-C19-C20-C21
24	g	101	CDL	C32-C33-C34-C35
19	A	608	TGL	CB9-C10-C11-C12
18	A	606	PGV	O01-C02-C03-O11
24	c	307	CDL	OA5-CA3-CA4-OA6
24	g	101	CDL	OA5-CA3-CA4-OA6
19	A	608	TGL	CA4-CA5-CA6-CA7
19	D	201	TGL	CA7-CA8-CA9-C20
24	g	101	CDL	C1-CA2-OA2-PA1
23	G	101	PEK	C26-C27-C28-C29
18	c	306	PGV	C31-C32-C33-C34
19	l	101	TGL	CB9-C10-C11-C12
24	C	305	CDL	C13-C14-C15-C16
24	c	307	CDL	C23-C24-C25-C26
18	c	302	PGV	O03-C01-C02-O01
19	A	608	TGL	OG2-CG2-CG3-OG3
19	d	201	TGL	OG2-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
26	b	303	PSC	O03-C01-C02-O01
23	C	302	PEK	C11-C10-C9-C8
23	C	302	PEK	C9-C10-C11-C12
23	C	307	PEK	C5-C6-C7-C8
23	C	307	PEK	C12-C13-C14-C15
23	G	101	PEK	C5-C6-C7-C8
23	G	101	PEK	C9-C10-C11-C12
23	c	301	PEK	C11-C10-C9-C8
23	c	301	PEK	C11-C12-C13-C14
23	c	301	PEK	C12-C13-C14-C15
23	c	304	PEK	C12-C13-C14-C15
23	c	305	PEK	C5-C6-C7-C8
18	A	607	PGV	C5-C6-C7-C8
23	c	304	PEK	O02-C1-O01-C02
18	a	606	PGV	C24-C25-C26-C27
23	c	304	PEK	C23-C24-C25-C26
24	C	305	CDL	C37-C38-C39-C40
18	C	303	PGV	C13-C14-C15-C16
19	D	201	TGL	CA5-CA6-CA7-CA8
19	l	101	TGL	CB1-CB2-CB3-CB4
23	C	302	PEK	C2-C1-O01-C02
24	g	101	CDL	C63-C64-C65-C66
18	a	606	PGV	C11-C10-C9-C8
19	A	609	TGL	CA5-CA6-CA7-CA8
23	G	101	PEK	C35-C36-C37-C38
18	c	306	PGV	C29-C30-C31-C32
19	d	201	TGL	CC5-CC6-CC7-CC8
24	C	305	CDL	C81-C82-C83-C84
26	b	303	PSC	C2-C1-O01-C02
24	C	305	CDL	C33-C34-C35-C36
18	C	303	PGV	C1-C2-C3-C4
19	l	101	TGL	C25-C26-C27-C28
18	c	302	PGV	C27-C28-C29-C30
19	D	201	TGL	C22-C23-C24-C25
19	b	302	TGL	C12-C13-C14-C29
19	b	302	TGL	CC7-CC8-CC9-C15
24	G	102	CDL	C61-C62-C63-C64
24	g	101	CDL	C78-C79-C80-C81
23	c	301	PEK	C1-C2-C3-C4
19	l	101	TGL	CC6-CC7-CC8-CC9
23	C	307	PEK	C30-C31-C32-C33
19	A	609	TGL	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
23	G	101	PEK	C31-C32-C33-C34
26	b	303	PSC	O02-C1-O01-C02
23	C	302	PEK	C28-C29-C30-C31
19	A	609	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	CC3-CC4-CC5-CC6
19	b	302	TGL	C21-C20-CA9-CA8
18	c	302	PGV	C11-C10-C9-C8
19	A	609	TGL	C14-C29-C30-C31
23	G	101	PEK	O01-C02-C03-O11
23	c	301	PEK	O01-C02-C03-O11
24	C	305	CDL	OB5-CB3-CB4-OB6
26	E	201	PSC	O01-C02-C03-O11
19	A	608	TGL	CG1-CG2-CG3-OG3
24	c	307	CDL	CB3-CB4-CB6-OB8
24	G	102	CDL	C84-C85-C86-C87
24	c	307	CDL	C42-C43-C44-C45
23	C	307	PEK	C05-C04-O12-P
23	c	304	PEK	C25-C26-C27-C28
24	c	307	CDL	C51-C52-C53-C54
19	d	201	TGL	OG1-CG1-CG2-OG2
19	l	101	TGL	OG2-CG2-CG3-OG3
23	C	307	PEK	O03-C01-C02-O01
24	G	102	CDL	OB6-CB4-CB6-OB8
24	g	101	CDL	OB6-CB4-CB6-OB8
18	C	304	PGV	C24-C25-C26-C27
18	A	607	PGV	C7-C8-C9-C10
18	a	606	PGV	C28-C29-C30-C31
19	d	201	TGL	C11-C10-CB9-CB8
23	c	305	PEK	C24-C25-C26-C27
23	C	302	PEK	C24-C25-C26-C27
24	c	307	CDL	C17-C18-C19-C20
18	C	304	PGV	C31-C32-C33-C34
26	E	201	PSC	O12-C04-C05-N
19	b	302	TGL	C19-C33-C34-C35
24	C	305	CDL	C77-C78-C79-C80
24	c	307	CDL	C37-C38-C39-C40
22	j	101	CHD	C16-C17-C20-C22
25	c	309	DMU	O6-C11-C9-O1
19	A	609	TGL	C24-C25-C26-C27
19	D	201	TGL	C10-C11-C12-C13
26	E	201	PSC	C01-C02-C03-O11
24	G	102	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
19	l	101	TGL	CC7-CC8-CC9-C15
23	c	304	PEK	C16-C17-C18-C19
25	m	101	DMU	O16-C18-C19-C22
19	l	101	TGL	CB4-CB5-CB6-CB7
18	c	306	PGV	C02-C03-O11-P
19	b	302	TGL	OB1-CB1-OG2-CG2
23	C	302	PEK	O02-C1-O01-C02
24	g	101	CDL	OB5-CB3-CB4-OB6
19	b	302	TGL	CB2-CB1-OG2-CG2
18	c	302	PGV	C3-C4-C5-C6
19	b	302	TGL	CA6-CA7-CA8-CA9
19	A	608	TGL	C21-C20-CA9-CA8
19	D	201	TGL	OG1-CG1-CG2-OG2
24	c	307	CDL	OB6-CB4-CB6-OB8
18	a	606	PGV	C20-C21-C22-C23
18	c	302	PGV	O03-C01-C02-C03
24	c	307	CDL	CA3-CA4-CA6-OA8
19	D	201	TGL	CC7-CC8-CC9-C15
24	g	101	CDL	C17-C18-C19-C20
23	c	301	PEK	C30-C31-C32-C33
18	a	607	PGV	C4-C5-C6-C7
24	g	101	CDL	C12-C13-C14-C15
23	c	304	PEK	C31-C32-C33-C34
18	A	606	PGV	C03-O11-P-O13
18	C	304	PGV	C03-O11-P-O13
18	a	606	PGV	C04-O12-P-O13
23	G	101	PEK	C03-O11-P-O12
23	G	101	PEK	C03-O11-P-O14
23	c	301	PEK	C03-O11-P-O14
23	c	301	PEK	C04-O12-P-O14
23	c	304	PEK	O12-C04-C05-N
24	C	305	CDL	CA3-OA5-PA1-OA2
24	C	305	CDL	CA3-OA5-PA1-OA3
24	C	305	CDL	CA3-OA5-PA1-OA4
24	C	305	CDL	CB2-OB2-PB2-OB3
24	C	305	CDL	CB2-OB2-PB2-OB4
24	C	305	CDL	CB2-OB2-PB2-OB5
24	G	102	CDL	CB2-OB2-PB2-OB3
24	g	101	CDL	CB3-OB5-PB2-OB3
26	E	201	PSC	C03-O11-P-O14
26	b	303	PSC	C04-O12-P-O14
18	C	303	PGV	C02-C03-O11-P

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Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C1-C2-C3-C4
19	d	201	TGL	CB2-CB3-CB4-CB5
24	g	101	CDL	C61-C62-C63-C64
24	C	305	CDL	C42-C43-C44-C45
18	C	303	PGV	C28-C29-C30-C31
19	A	609	TGL	CG1-CG2-OG2-CB1
19	d	201	TGL	CC2-CC3-CC4-CC5
19	l	101	TGL	OG2-CB1-CB2-CB3
23	c	301	PEK	C21-C22-C23-C24
18	c	306	PGV	C20-C21-C22-C23
24	G	102	CDL	C74-C75-C76-C77
19	A	608	TGL	CC6-CC7-CC8-CC9
26	E	201	PSC	C7-C8-C9-C10
18	a	607	PGV	C30-C31-C32-C33
24	g	101	CDL	C33-C34-C35-C36
23	C	302	PEK	C33-C34-C35-C36
19	l	101	TGL	CA6-CA7-CA8-CA9
24	C	305	CDL	OB6-CB4-CB6-OB8
19	A	608	TGL	C22-C23-C24-C25
23	C	302	PEK	O03-C21-C22-C23
18	A	606	PGV	C21-C22-C23-C24
18	a	607	PGV	C12-C13-C14-C15
19	l	101	TGL	CG1-CG2-CG3-OG3
26	b	303	PSC	O03-C01-C02-C03
18	a	606	PGV	C5-C6-C7-C8
19	A	609	TGL	CA3-CA4-CA5-CA6
19	b	302	TGL	C29-C30-C31-C32
24	C	305	CDL	C12-C13-C14-C15
19	d	201	TGL	C20-C21-C22-C23
24	g	101	CDL	C59-C60-C61-C62
19	A	609	TGL	C33-C34-C35-C36
19	A	608	TGL	CC7-CC8-CC9-C15
25	m	101	DMU	C28-C31-C34-C37
18	C	303	PGV	C31-C32-C33-C34
19	D	201	TGL	C29-C30-C31-C32
26	E	201	PSC	C12-C13-C14-C15
23	c	305	PEK	C17-C18-C19-C20
24	c	307	CDL	C14-C15-C16-C17
18	a	607	PGV	C27-C28-C29-C30
19	A	609	TGL	C25-C26-C27-C28
24	c	307	CDL	C60-C61-C62-C63
19	A	608	TGL	C12-C13-C14-C29

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Mol	Chain	Res	Type	Atoms
25	M	101	DMU	C19-C22-C25-C28
24	c	307	CDL	C38-C39-C40-C41
18	a	606	PGV	C15-C16-C17-C18
23	G	101	PEK	C3-C4-C5-C6
22	j	101	CHD	C22-C23-C24-O25
24	C	305	CDL	CA3-CA4-OA6-CA5
24	C	305	CDL	CA6-CA4-OA6-CA5
26	b	303	PSC	C30-C31-C32-C33
19	A	608	TGL	CA2-CA3-CA4-CA5
19	l	101	TGL	CA1-CA2-CA3-CA4
22	B	402	CHD	C22-C23-C24-O25
24	g	101	CDL	C74-C75-C76-C77
14	A	601	HEA	CAD-CBD-CGD-O1D
22	c	308	CHD	C22-C23-C24-O25
23	C	307	PEK	C17-C18-C19-C20
26	b	303	PSC	C02-C03-O11-P
25	M	101	DMU	C22-C25-C28-C31
24	G	102	CDL	C39-C40-C41-C42
22	J	101	CHD	C22-C23-C24-O25
19	A	609	TGL	CC7-CC8-CC9-C15
19	A	609	TGL	C18-C19-C33-C34
14	A	602	HEA	CAA-CBA-CGA-O1A
22	G	103	CHD	C22-C23-C24-O26
14	a	601	HEA	CAD-CBD-CGD-O1D
23	C	302	PEK	C5-C6-C7-C8
23	C	307	PEK	C11-C10-C9-C8
23	c	301	PEK	C6-C7-C8-C9
23	c	304	PEK	C5-C6-C7-C8
23	c	304	PEK	C9-C10-C11-C12
23	c	305	PEK	C11-C10-C9-C8
23	C	307	PEK	C34-C35-C36-C37
26	b	303	PSC	C26-C27-C28-C29
24	C	305	CDL	C22-C23-C24-C25
22	B	402	CHD	C22-C23-C24-O26
22	G	103	CHD	C22-C23-C24-O25
24	G	102	CDL	C16-C17-C18-C19
24	g	101	CDL	C60-C61-C62-C63
24	G	102	CDL	C12-C13-C14-C15
23	c	301	PEK	C27-C28-C29-C30
18	A	607	PGV	C25-C26-C27-C28
26	E	201	PSC	C30-C31-C32-C33
14	a	601	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	606	PGV	O04-C19-O03-C01
19	b	302	TGL	CC6-CC7-CC8-CC9
24	C	305	CDL	C39-C40-C41-C42
24	g	101	CDL	C11-C12-C13-C14
23	C	307	PEK	O03-C01-C02-C03
24	g	101	CDL	CB3-CB4-CB6-OB8
14	A	602	HEA	CAD-CBD-CGD-O1D
18	c	302	PGV	C13-C14-C15-C16
22	j	101	CHD	C22-C23-C24-O26
24	G	102	CDL	C64-C65-C66-C67
24	G	102	CDL	OB5-CB3-CB4-OB6
14	A	601	HEA	C26-C15-C16-C17
19	b	302	TGL	CB4-CB5-CB6-CB7
14	a	602	HEA	CAD-CBD-CGD-O2D
24	G	102	CDL	C36-C37-C38-C39
18	A	607	PGV	C9-C10-C11-C12
18	C	303	PGV	C11-C12-C13-C14
18	c	302	PGV	C11-C12-C13-C14
24	C	305	CDL	C32-C31-CA7-OA8
18	a	607	PGV	C26-C27-C28-C29
14	A	601	HEA	CAD-CBD-CGD-O2D
23	c	304	PEK	O03-C21-C22-C23
23	c	301	PEK	C32-C33-C34-C35
18	C	304	PGV	C01-C02-C03-O11
24	g	101	CDL	C52-C51-CB5-OB6
18	C	303	PGV	C05-C04-O12-P
22	c	308	CHD	C22-C23-C24-O26
24	C	305	CDL	C20-C21-C22-C23
14	A	602	HEA	CAA-CBA-CGA-O2A
14	A	602	HEA	CAD-CBD-CGD-O2D
26	E	201	PSC	C26-C27-C28-C29
18	a	607	PGV	C11-C12-C13-C14
24	G	102	CDL	C44-C45-C46-C47
24	G	102	CDL	C38-C39-C40-C41
22	J	101	CHD	C22-C23-C24-O26
18	A	607	PGV	C13-C14-C15-C16
19	A	608	TGL	CB4-CB5-CB6-CB7
18	A	606	PGV	C20-C19-O03-C01
19	l	101	TGL	C24-C25-C26-C27
18	c	306	PGV	C9-C10-C11-C12
23	c	301	PEK	C14-C15-C16-C17
23	c	305	PEK	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	609	TGL	CB9-C10-C11-C12
24	c	307	CDL	C76-C77-C78-C79
24	C	305	CDL	C18-C19-C20-C21
26	b	303	PSC	C12-C13-C14-C15
23	G	101	PEK	C1-C2-C3-C4
24	g	101	CDL	C40-C41-C42-C43
18	c	306	PGV	C11-C12-C13-C14
14	a	602	HEA	CAA-CBA-CGA-O1A
24	G	102	CDL	C17-C18-C19-C20
18	A	606	PGV	C6-C7-C8-C9
23	C	302	PEK	C25-C26-C27-C28
18	a	606	PGV	C6-C7-C8-C9
26	E	201	PSC	C3-C4-C5-C6
19	A	609	TGL	OG2-CB1-CB2-CB3
24	g	101	CDL	C81-C82-C83-C84
23	G	101	PEK	O03-C01-C02-O01
19	A	608	TGL	C10-C11-C12-C13
19	A	608	TGL	C20-C21-C22-C23
18	A	606	PGV	C9-C10-C11-C12
18	a	607	PGV	C9-C10-C11-C12
26	b	303	PSC	C7-C8-C9-C10
24	C	305	CDL	C73-C74-C75-C76
24	g	101	CDL	C79-C80-C81-C82
24	C	305	CDL	C52-C51-CB5-OB6
24	g	101	CDL	C72-C71-CB7-OB8
18	c	306	PGV	C30-C31-C32-C33
18	A	606	PGV	C11-C12-C13-C14
18	a	606	PGV	C9-C10-C11-C12
23	C	307	PEK	C14-C15-C16-C17
23	c	301	PEK	C3-C4-C5-C6
14	a	602	HEA	CAD-CBD-CGD-O1D
14	A	602	HEA	C3B-C11-C12-C13
24	g	101	CDL	C84-C85-C86-C87
23	c	305	PEK	C14-C15-C16-C17
24	c	307	CDL	C12-C11-CA5-OA6
19	A	608	TGL	CB3-CB4-CB5-CB6
19	A	609	TGL	CB7-CB8-CB9-C10
18	c	302	PGV	O01-C1-C2-C3
19	b	302	TGL	OG1-CA1-CA2-CA3
19	d	201	TGL	OG2-CB1-CB2-CB3
19	b	302	TGL	C24-C25-C26-C27
24	g	101	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
18	a	606	PGV	C29-C30-C31-C32
18	C	303	PGV	C26-C27-C28-C29
24	G	102	CDL	C72-C71-CB7-OB8
19	A	608	TGL	C14-C29-C30-C31
19	A	609	TGL	CG1-CG2-CG3-OG3
24	G	102	CDL	C63-C64-C65-C66
24	c	307	CDL	C13-C14-C15-C16
18	C	304	PGV	C5-C6-C7-C8
14	a	602	HEA	C26-C15-C16-C17
23	c	305	PEK	O01-C1-C2-C3
26	E	201	PSC	O03-C19-C20-C21
22	c	303	CHD	C22-C23-C24-O26
26	E	201	PSC	C02-C01-O03-C19
19	A	609	TGL	OG3-CC1-CC2-CC3
14	a	602	HEA	CAA-CBA-CGA-O2A
19	d	201	TGL	C19-C33-C34-C35
24	G	102	CDL	C82-C83-C84-C85
24	c	307	CDL	C82-C83-C84-C85
19	A	609	TGL	CC6-CC7-CC8-CC9
24	G	102	CDL	C51-C52-C53-C54
19	A	609	TGL	CG3-CG2-OG2-CB1
19	A	609	TGL	OB1-CB1-CB2-CB3
19	A	608	TGL	CC3-CC4-CC5-CC6
24	g	101	CDL	C72-C71-CB7-OB9
26	b	303	PSC	C29-C30-C31-C32
26	E	201	PSC	O04-C19-C20-C21
18	a	606	PGV	C23-C24-C25-C26
24	c	307	CDL	C52-C51-CB5-OB6
19	A	609	TGL	CA4-CA5-CA6-CA7
22	j	101	CHD	C13-C17-C20-C22
24	C	305	CDL	C52-C51-CB5-OB7
24	c	307	CDL	C12-C11-CA5-OA7
19	A	608	TGL	C33-C34-C35-C36
22	c	303	CHD	C22-C23-C24-O25
18	a	606	PGV	O03-C19-C20-C21
22	j	101	CHD	C16-C17-C20-C21
24	c	307	CDL	O1-C1-CA2-OA2
18	a	606	PGV	C21-C22-C23-C24
14	a	601	HEA	C26-C15-C16-C17
23	C	302	PEK	O01-C1-C2-C3
23	C	307	PEK	O01-C1-C2-C3
14	A	601	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	c	307	CDL	CB2-C1-CA2-OA2
18	c	302	PGV	O02-C1-C2-C3
19	d	201	TGL	OB1-CB1-CB2-CB3
23	c	304	PEK	O01-C1-C2-C3
23	C	302	PEK	C3-C4-C5-C6
18	c	302	PGV	C25-C26-C27-C28
19	b	302	TGL	OA1-CA1-CA2-CA3
18	A	606	PGV	O01-C1-C2-C3
18	A	607	PGV	O03-C19-C20-C21
23	c	305	PEK	O02-C1-C2-C3
18	a	606	PGV	C1-C2-C3-C4
19	b	302	TGL	CC4-CC5-CC6-CC7
25	C	308	DMU	C4-C3-O7-C10
19	A	609	TGL	OC1-CC1-CC2-CC3
24	c	307	CDL	C52-C51-CB5-OB7
23	G	101	PEK	O01-C1-C2-C3
24	c	307	CDL	C21-C22-C23-C24
24	c	307	CDL	CB5-C51-C52-C53
18	A	607	PGV	O04-C19-C20-C21
18	a	606	PGV	O04-C19-C20-C21
23	C	302	PEK	O02-C1-C2-C3

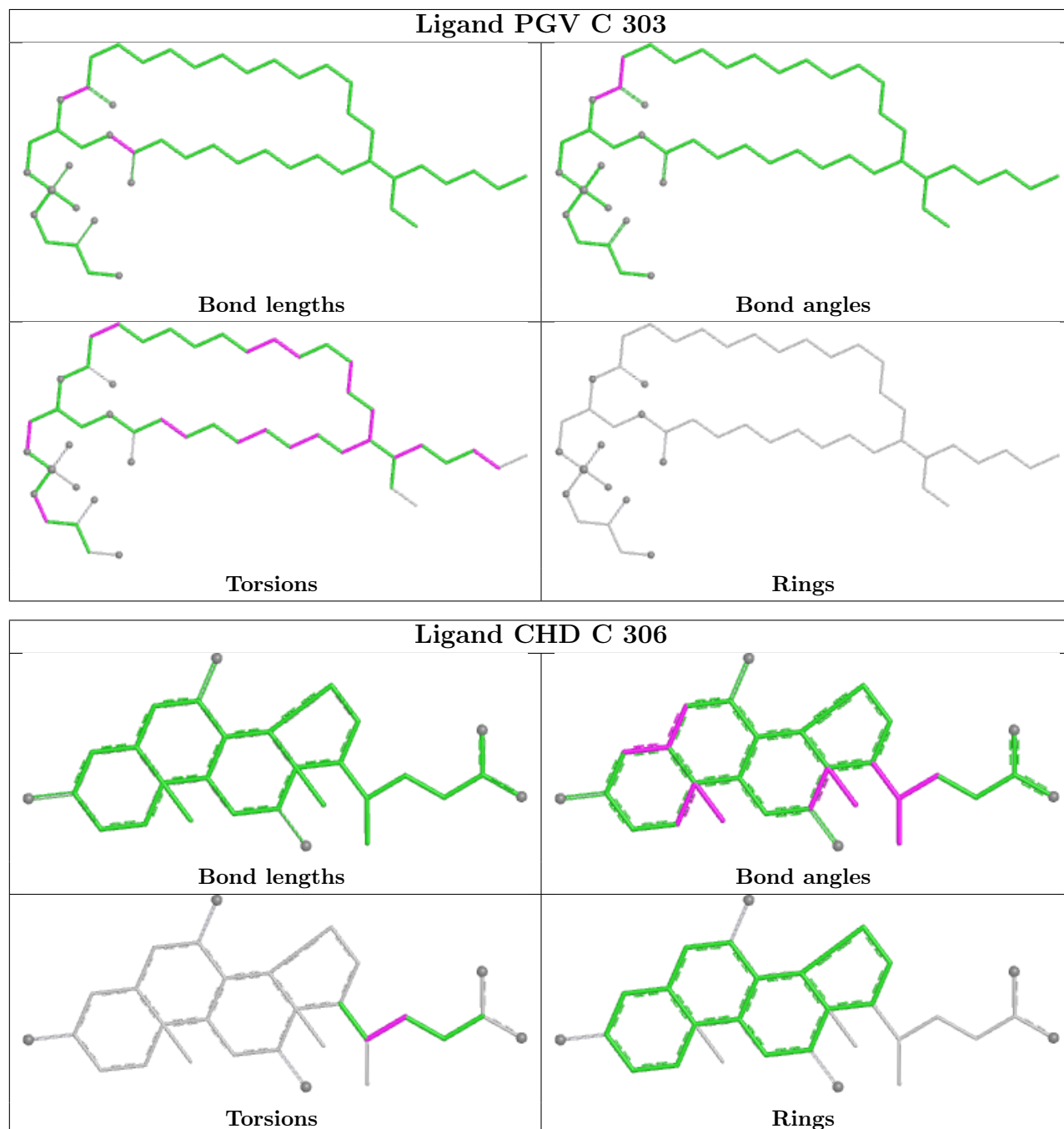
There are no ring outliers.

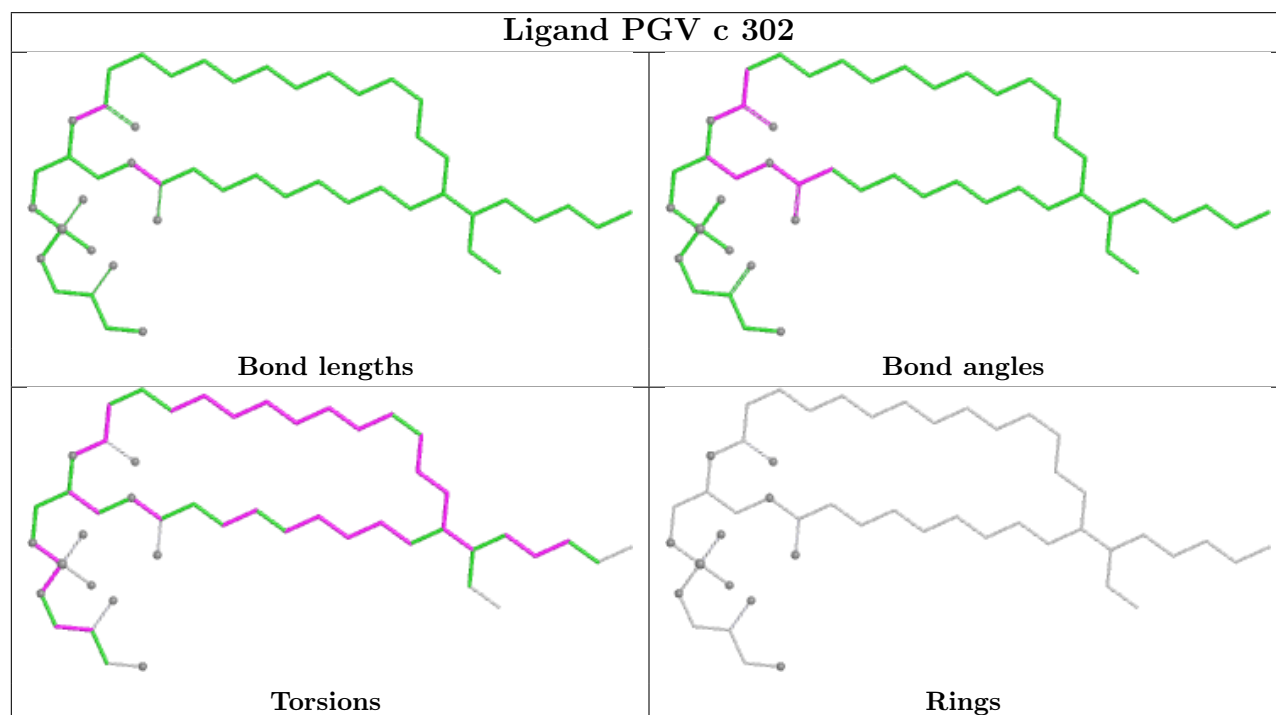
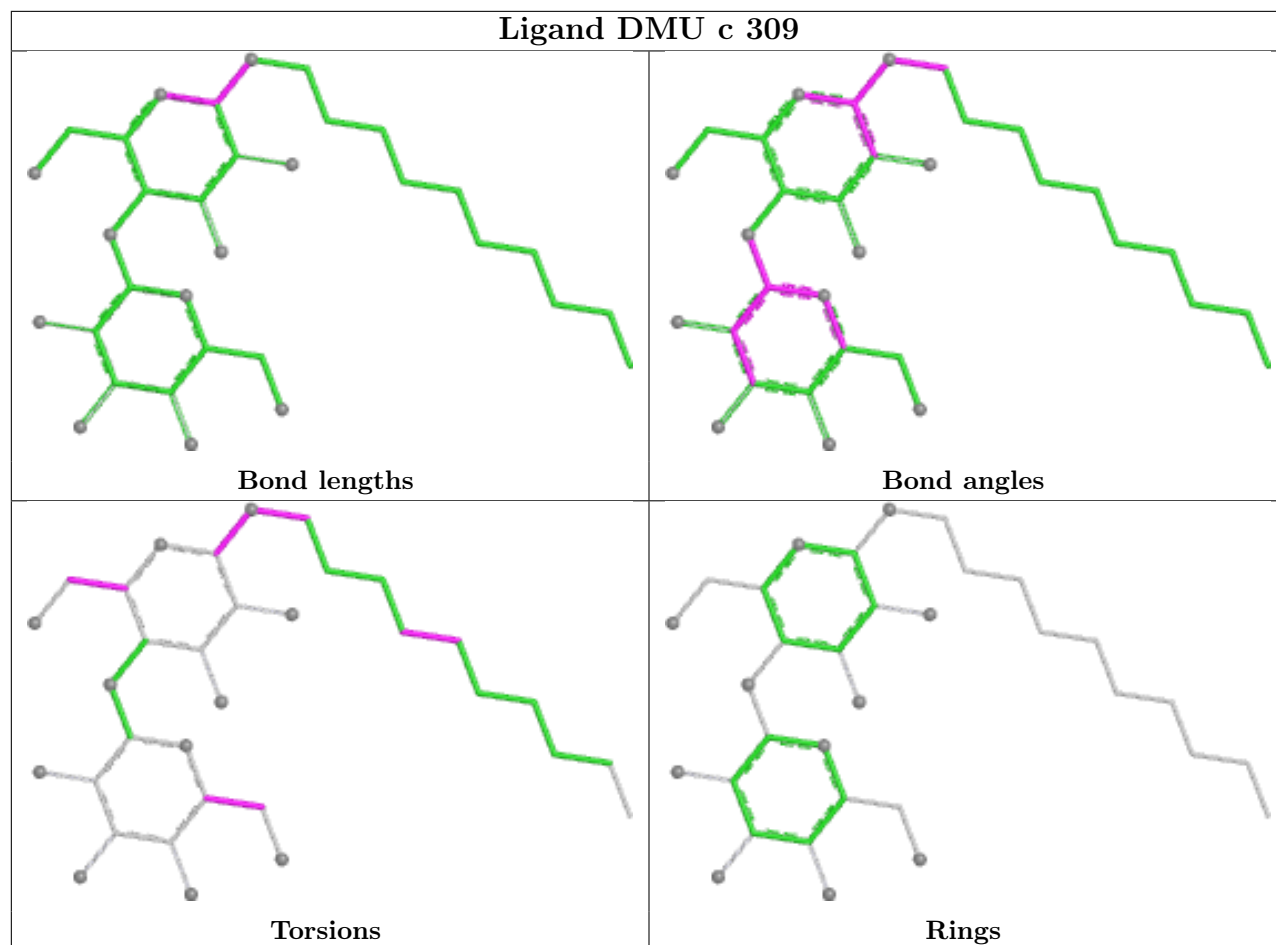
8 monomers are involved in 10 short contacts:

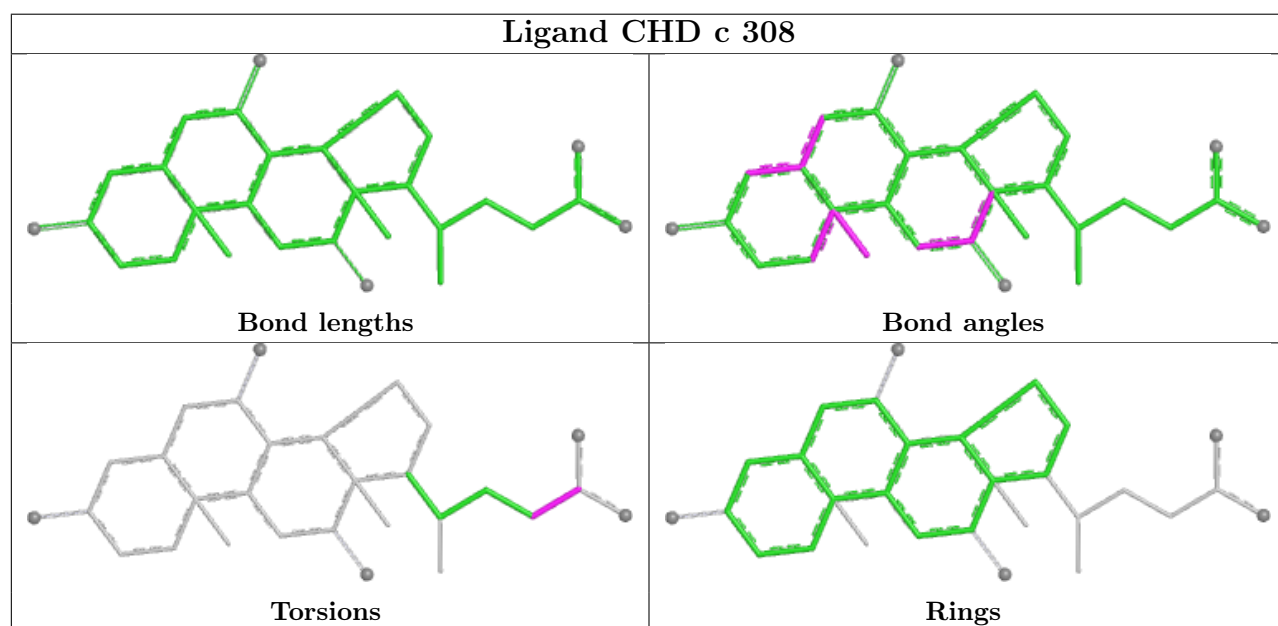
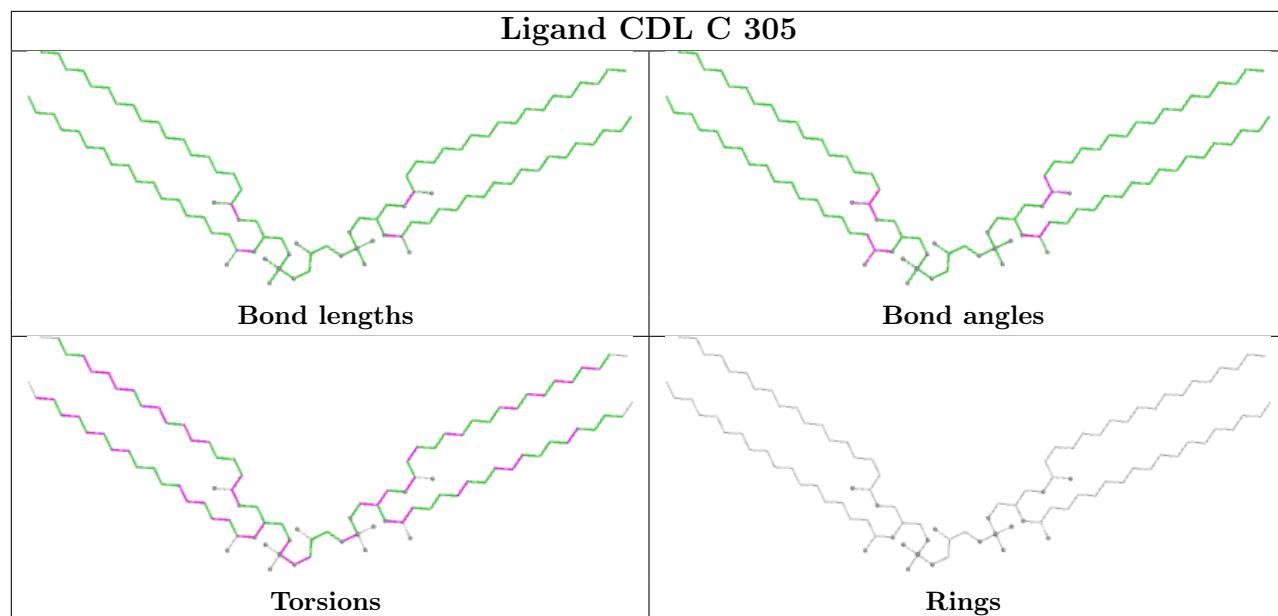
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	309	DMU	3	0
23	G	101	PEK	1	0
14	A	602	HEA	1	0
18	a	606	PGV	1	0
14	A	601	HEA	1	0
20	a	608	CMO	1	0
14	a	601	HEA	1	0
19	l	101	TGL	1	0

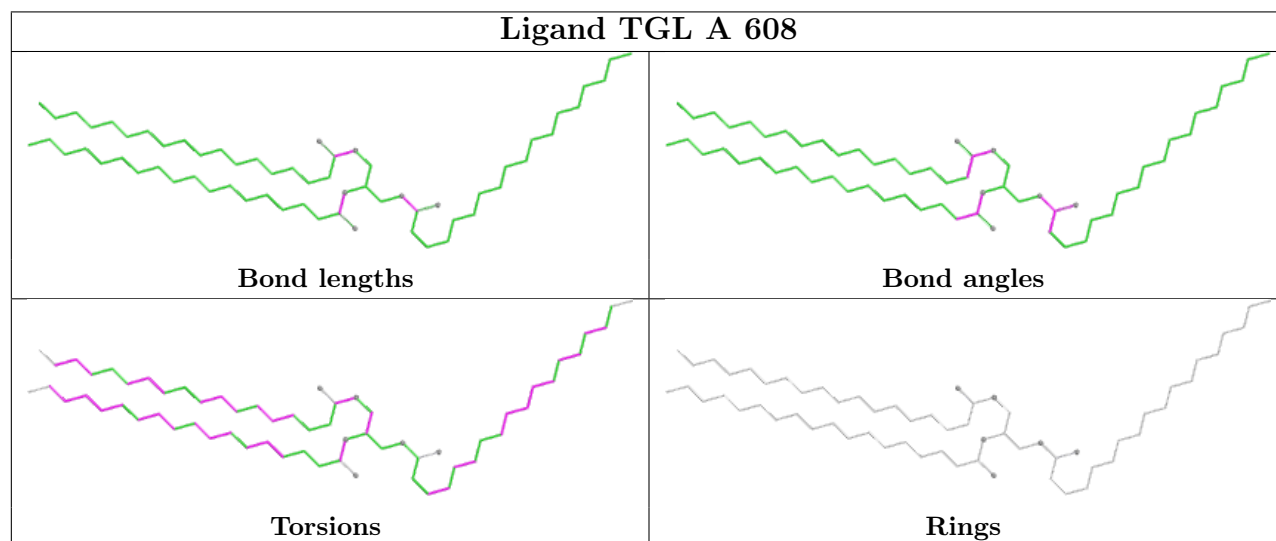
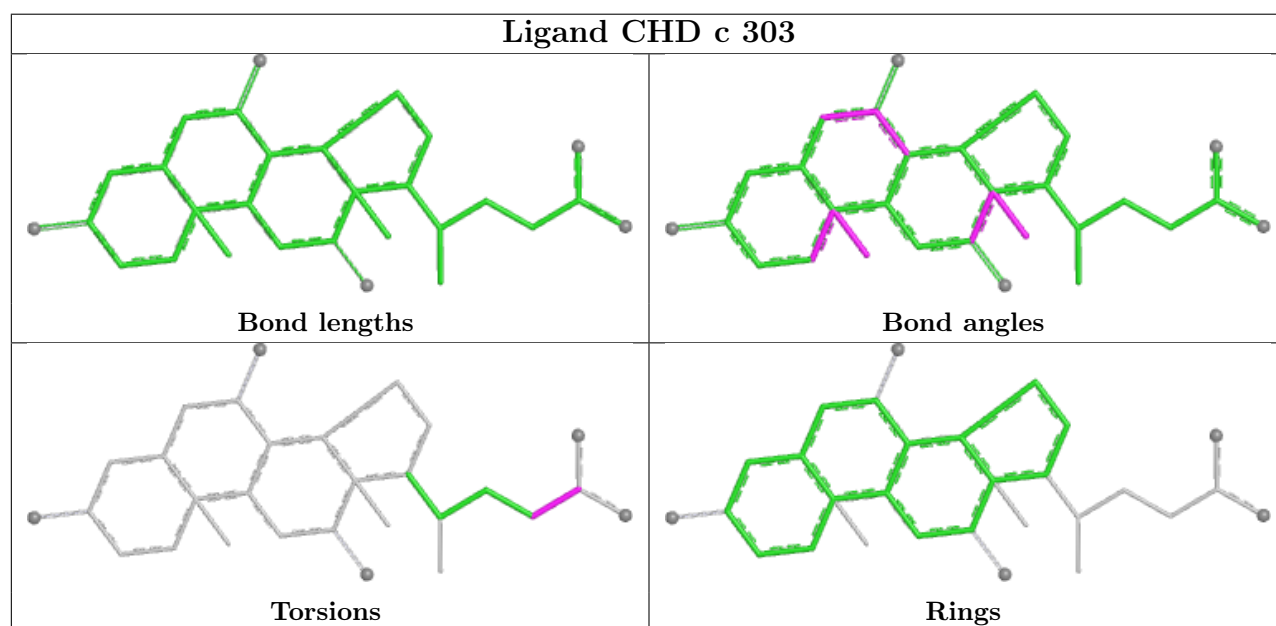
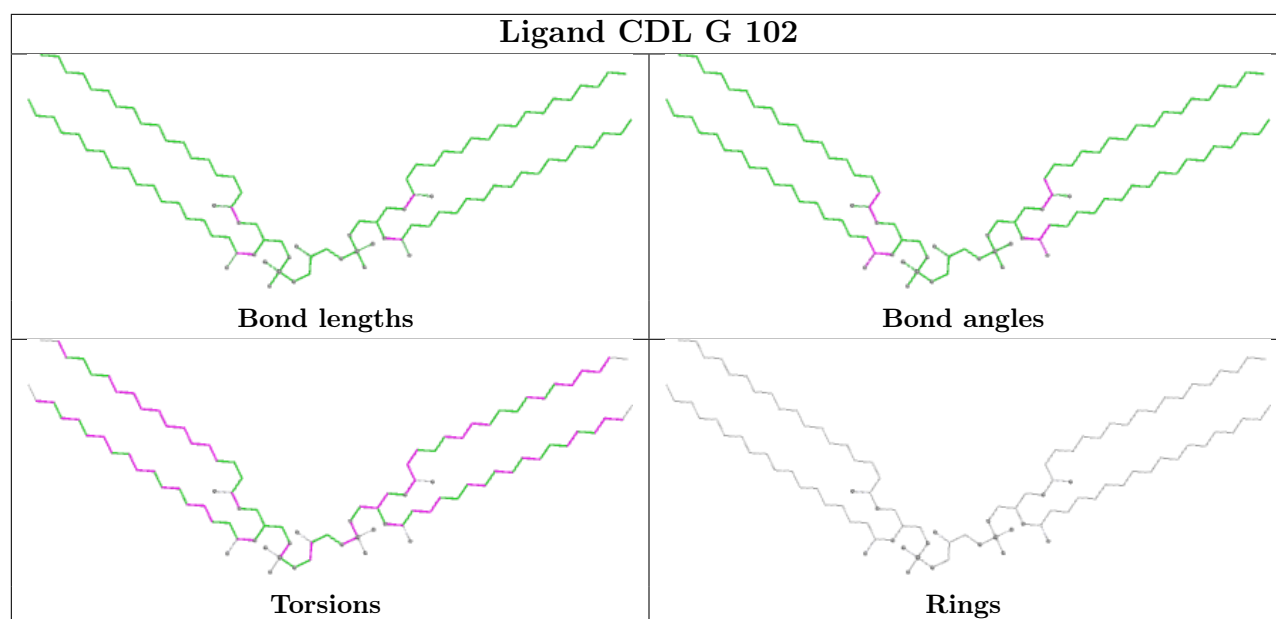
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

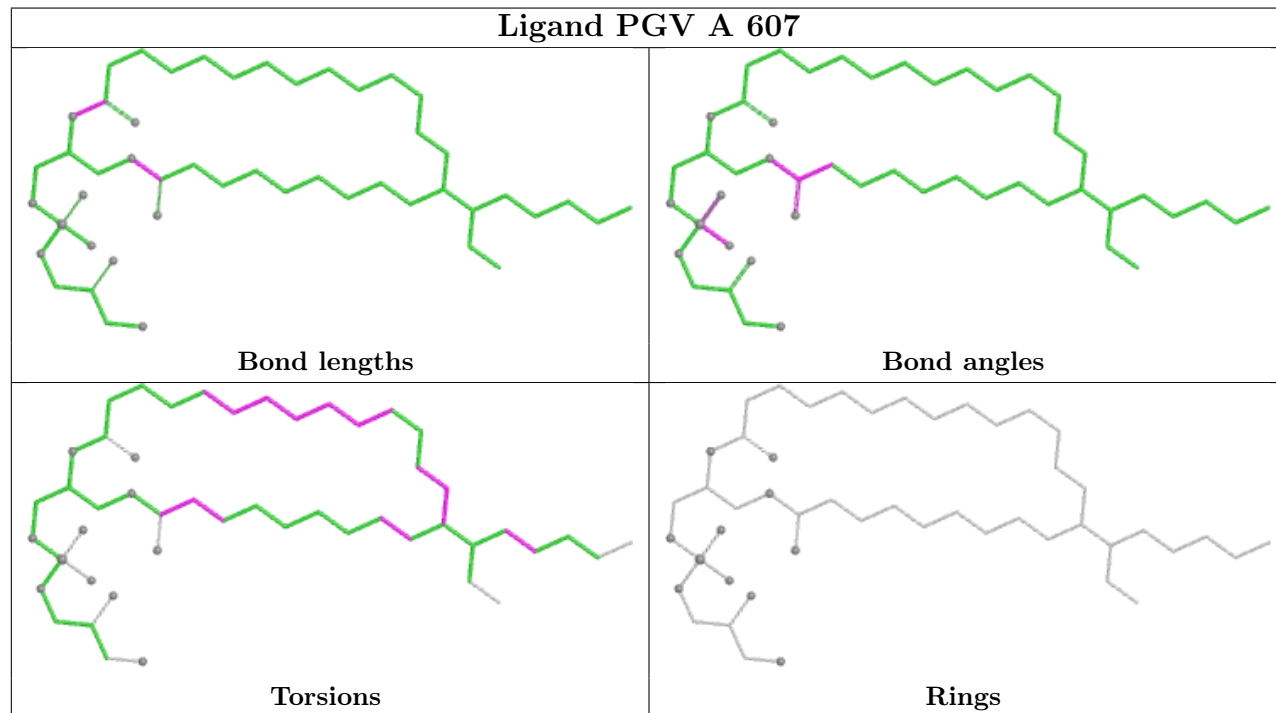
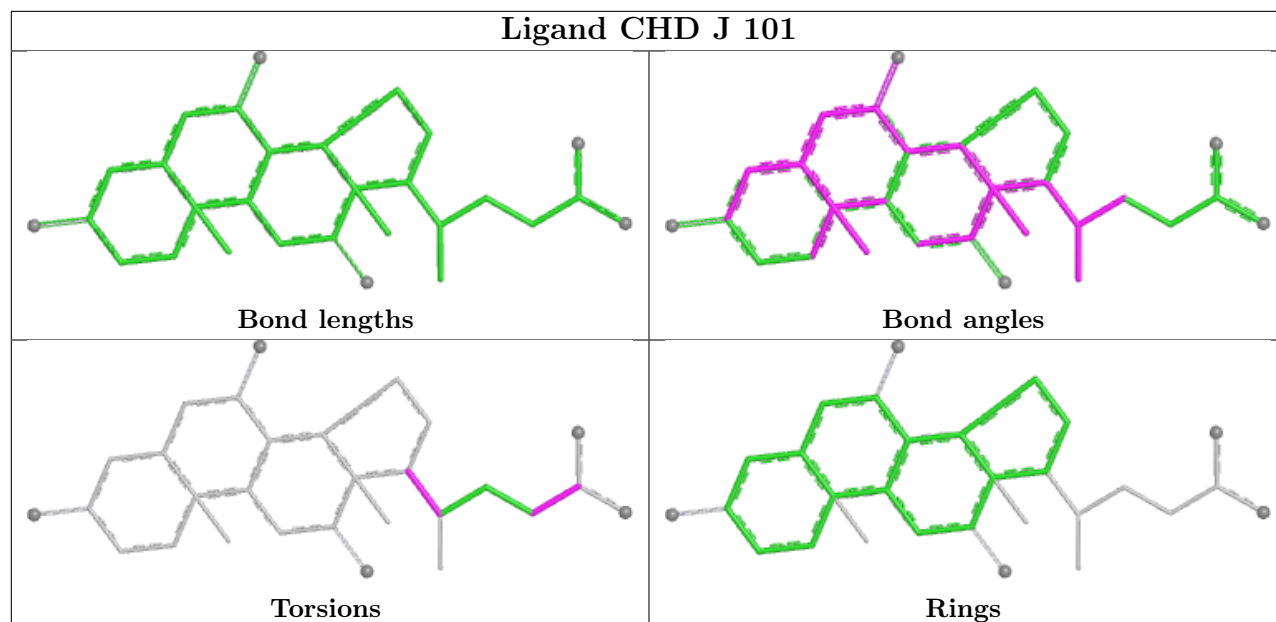
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

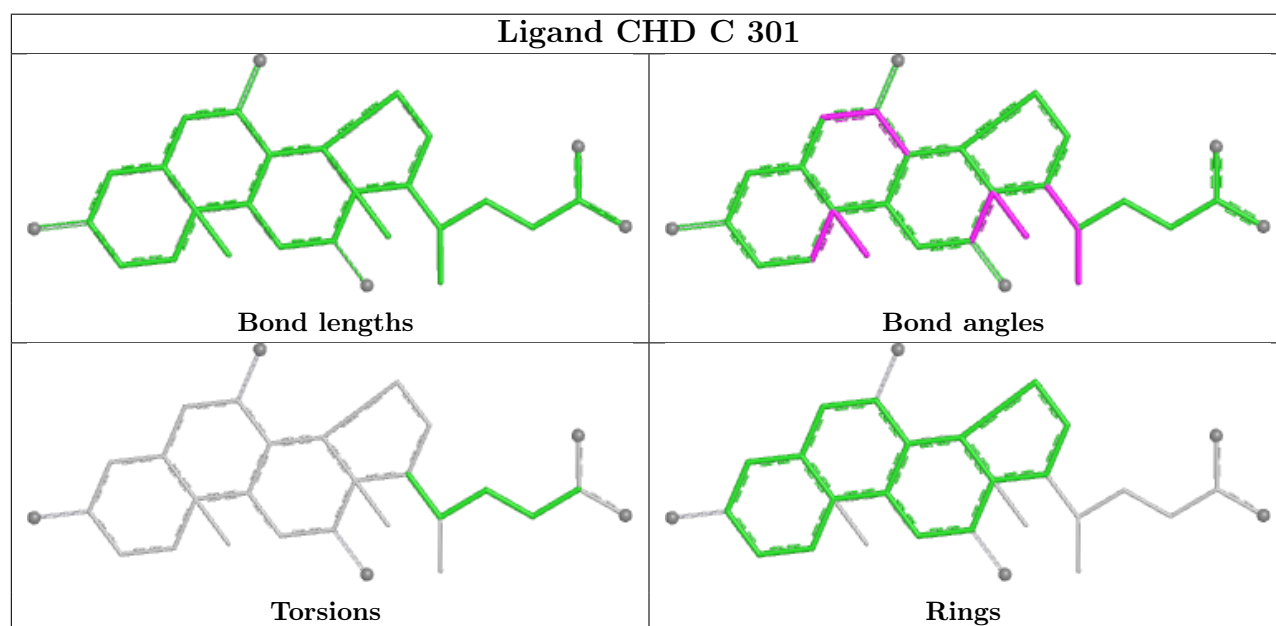
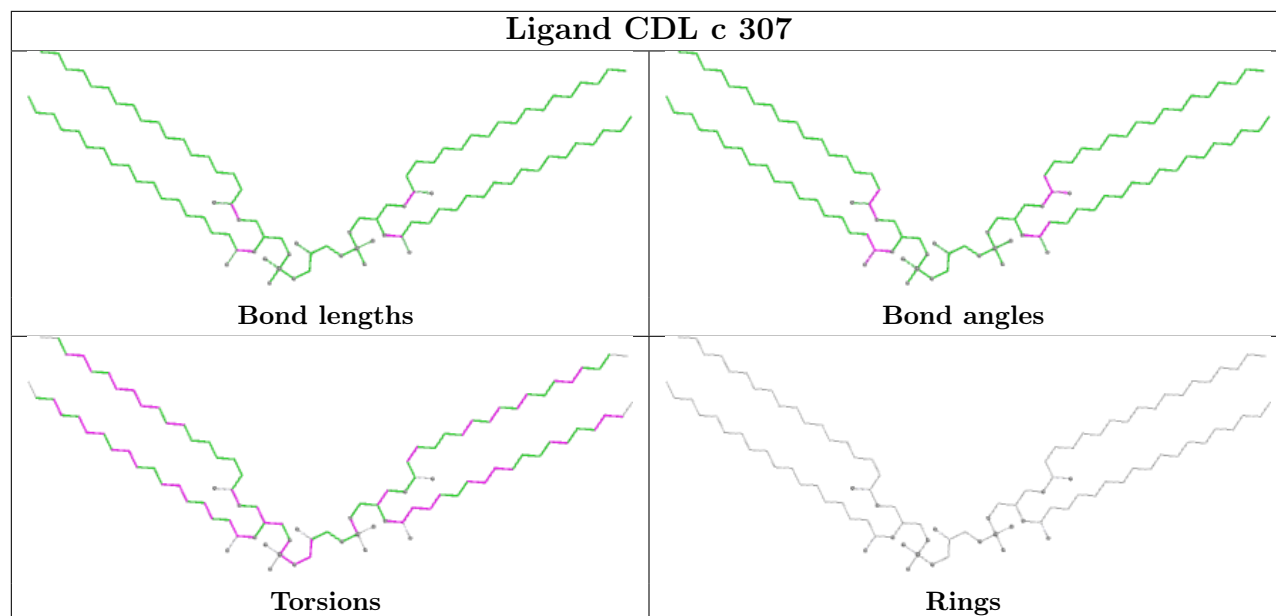




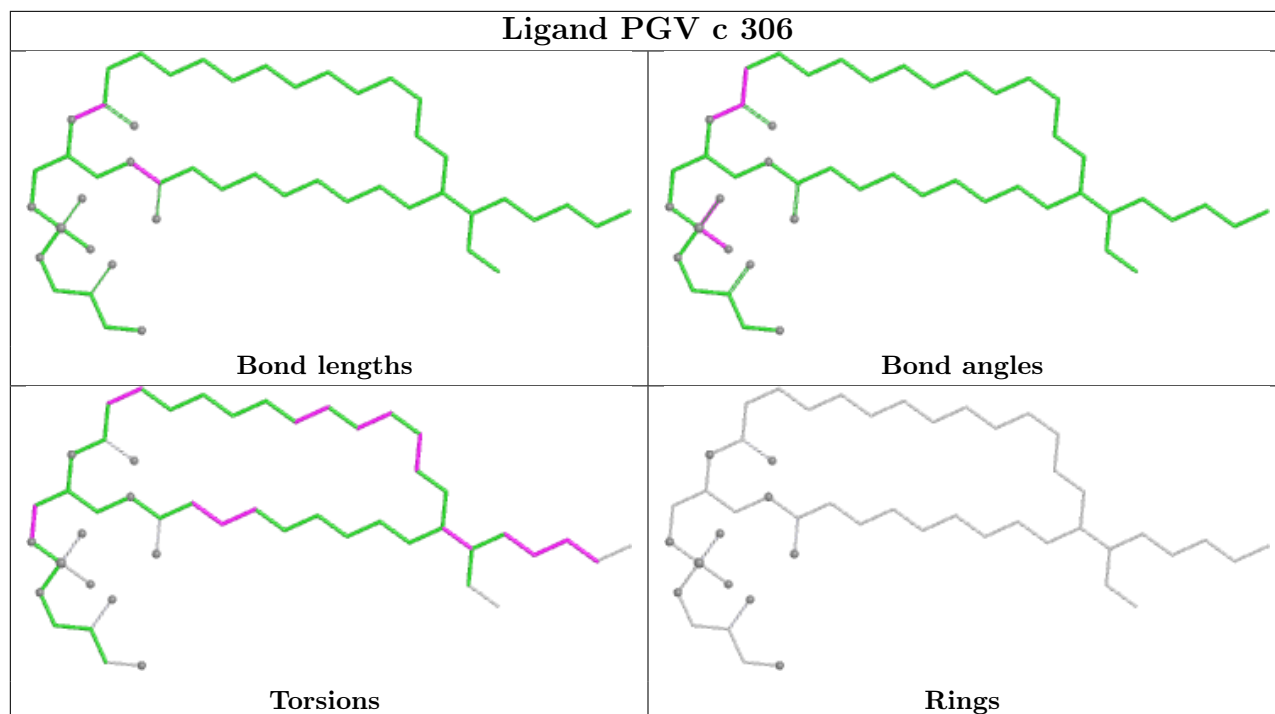




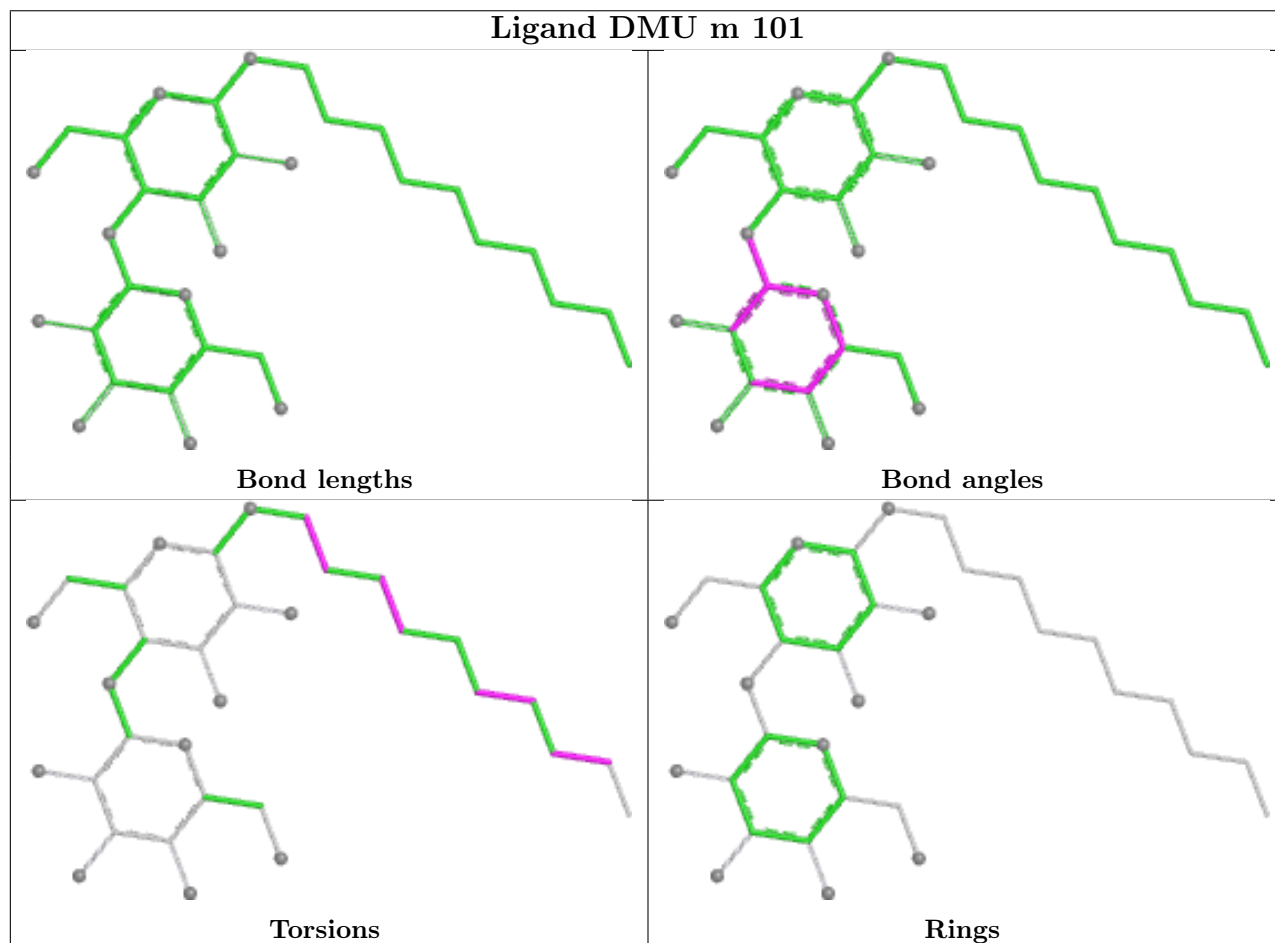


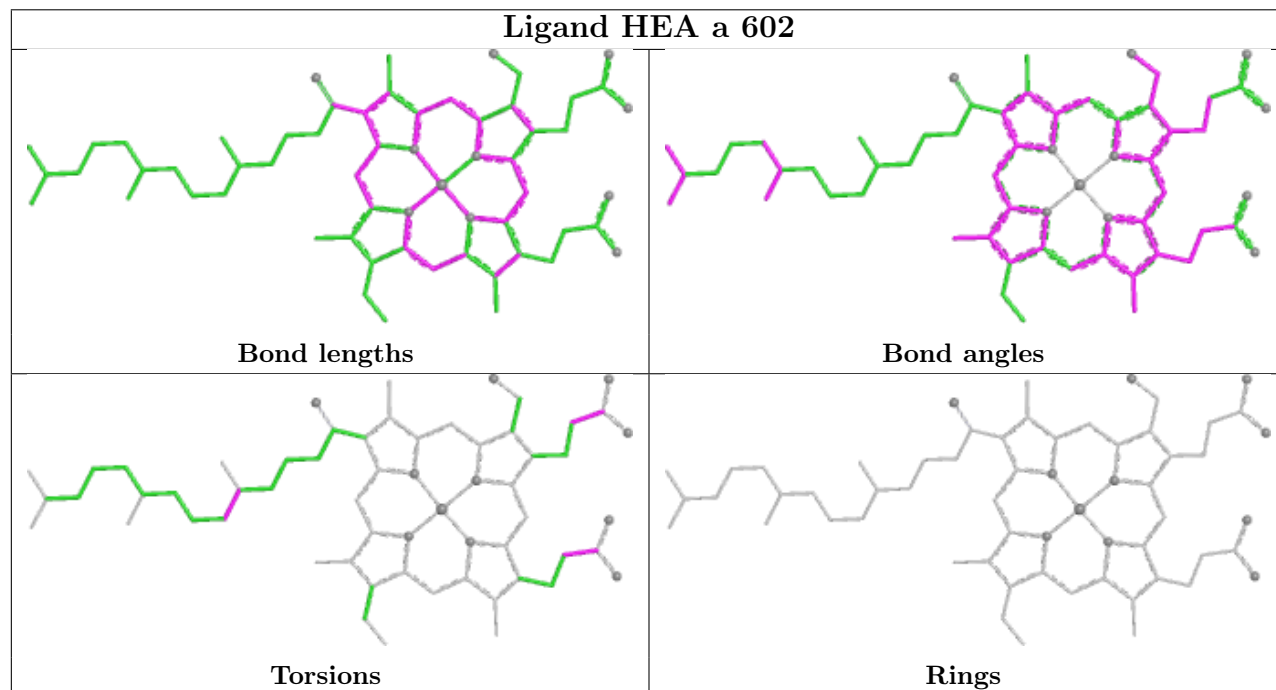
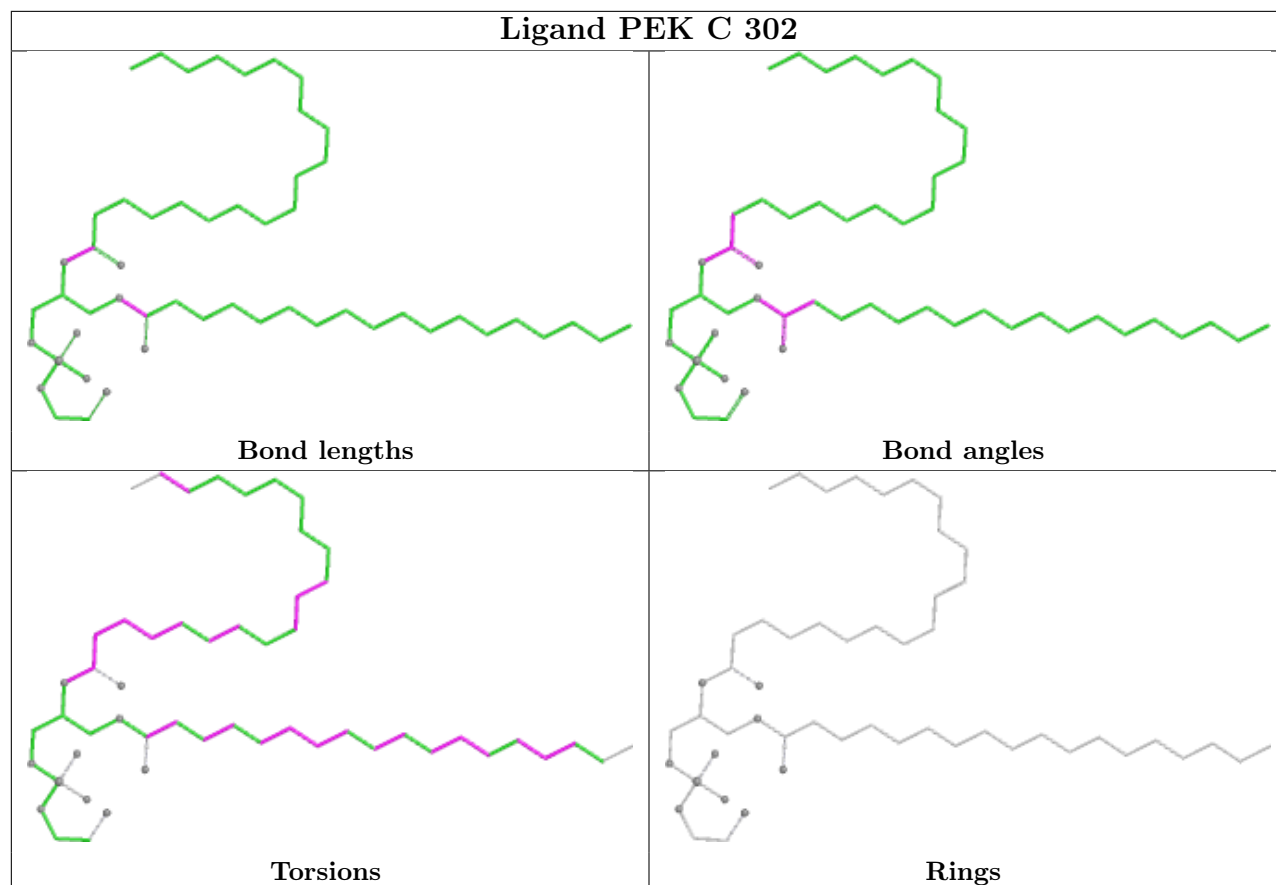


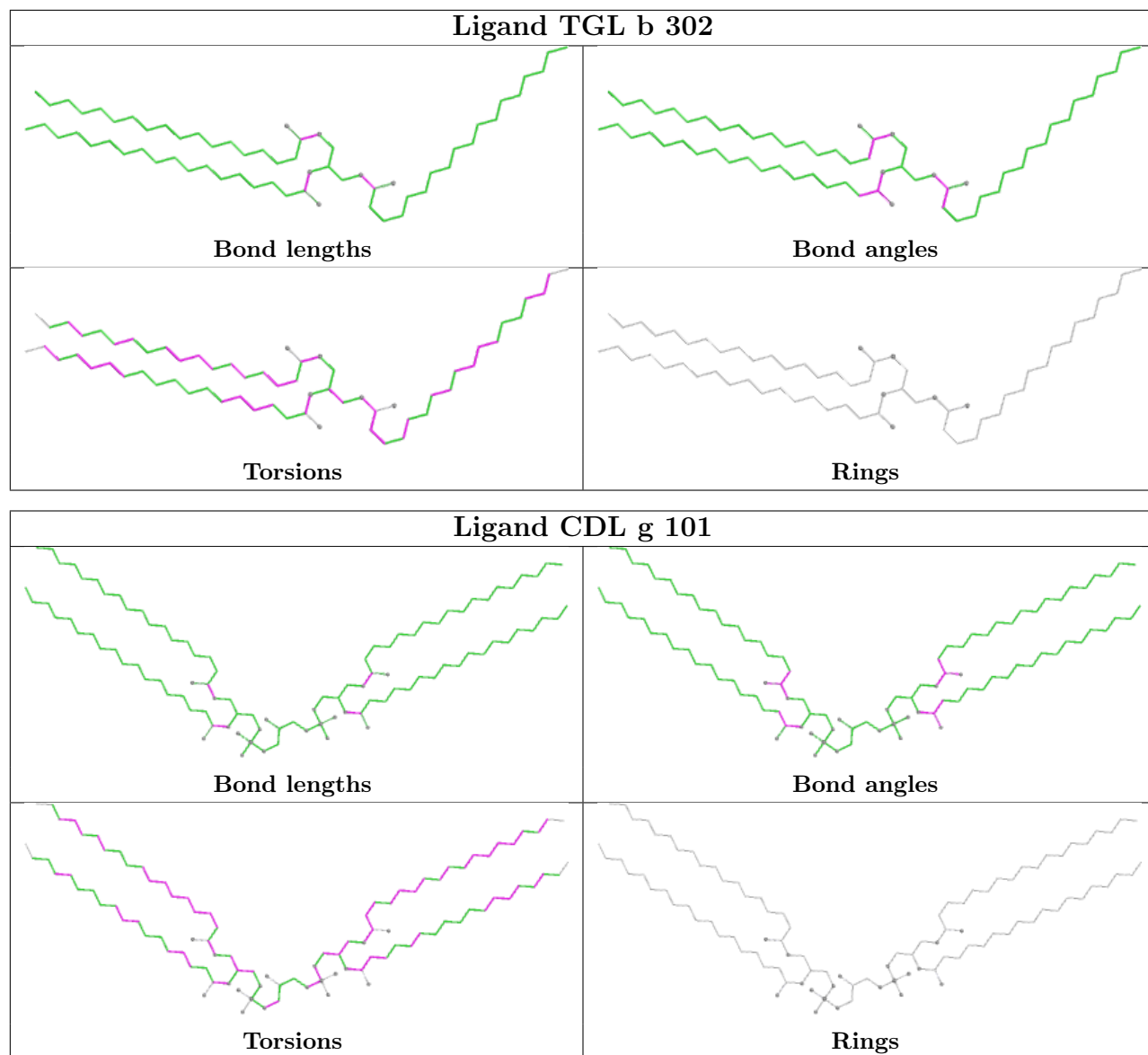
Ligand PGV c 306

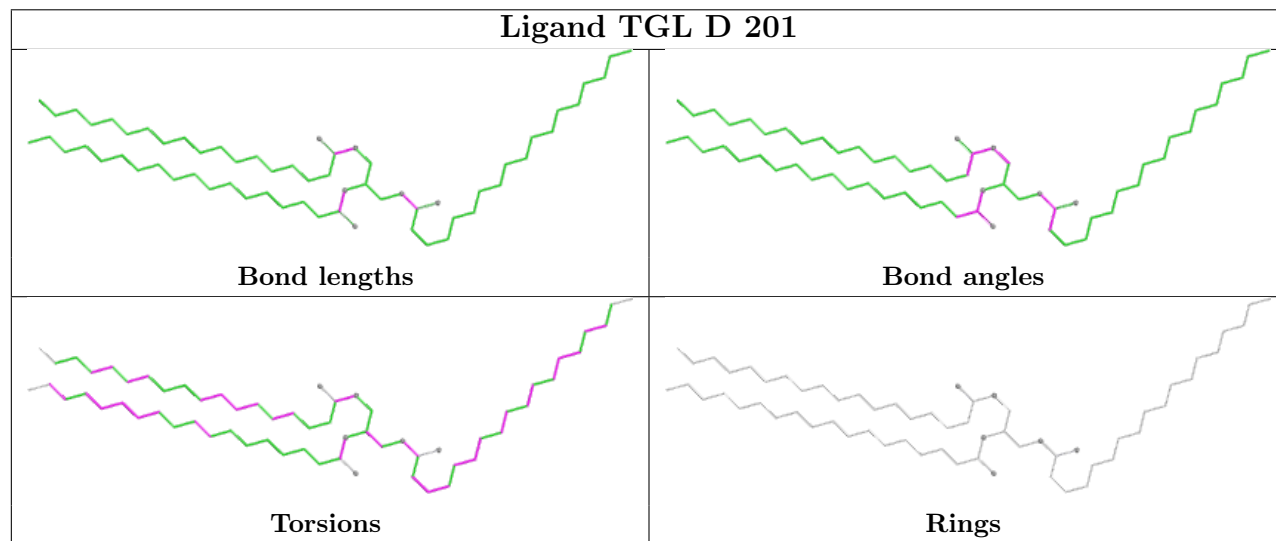
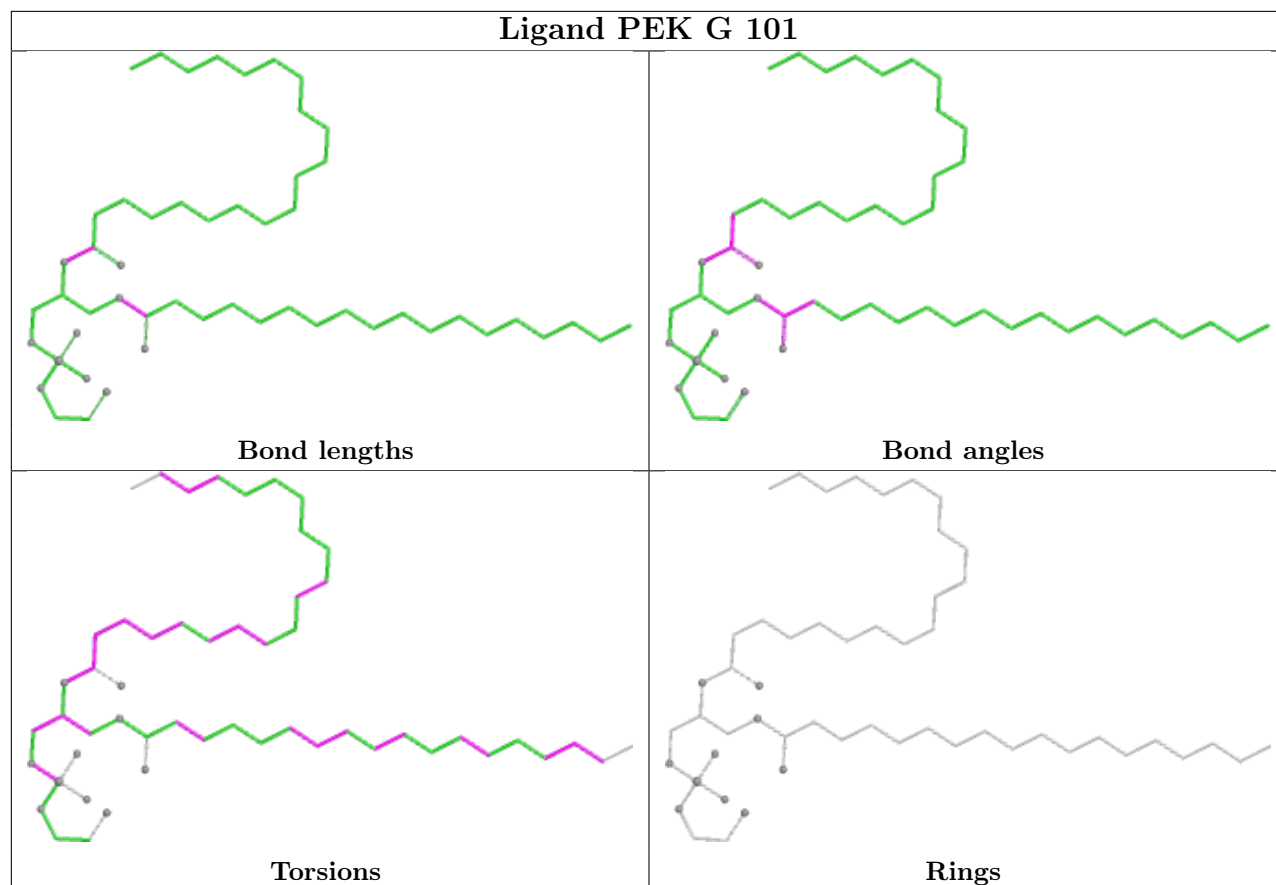


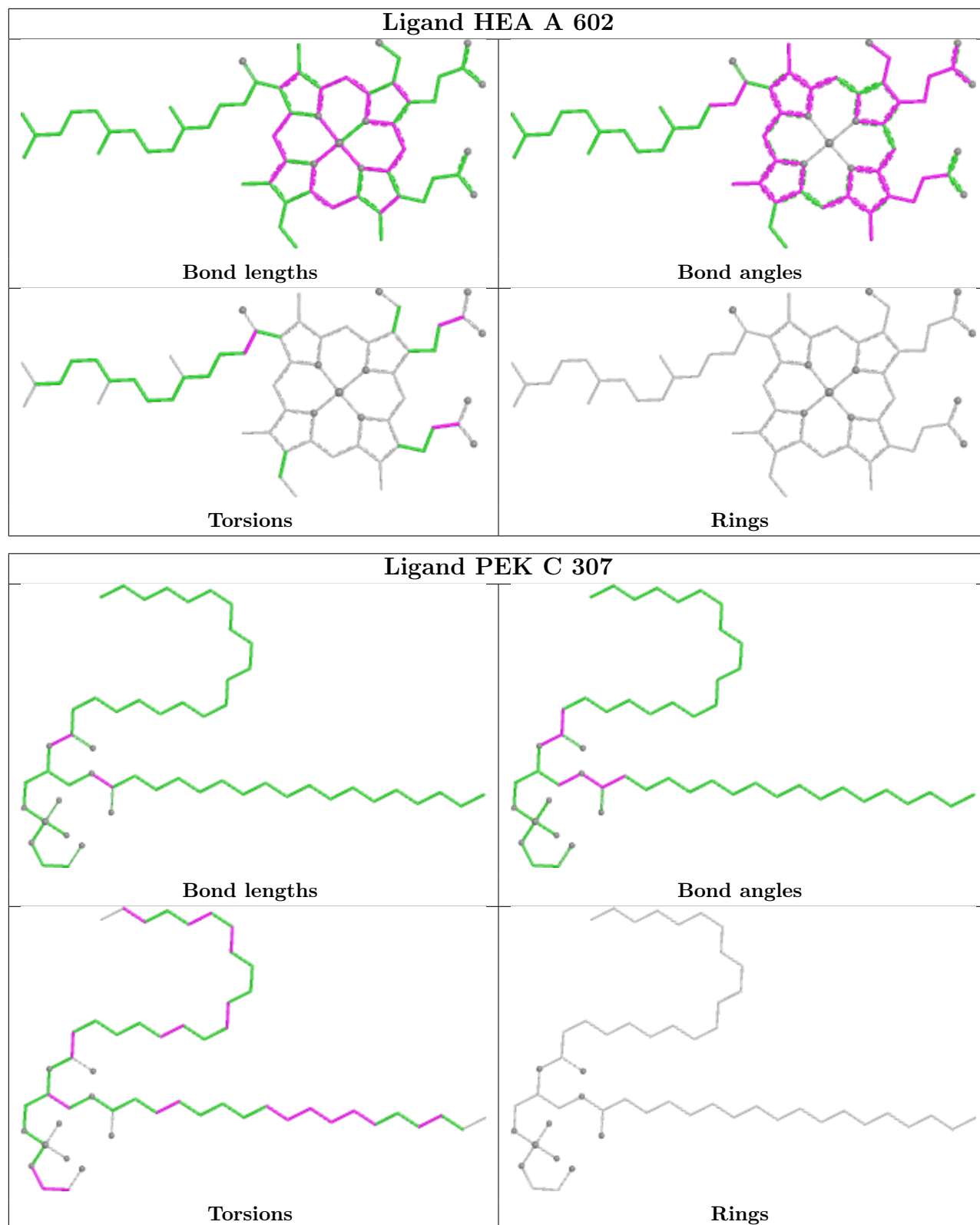
Ligand DMU m 101



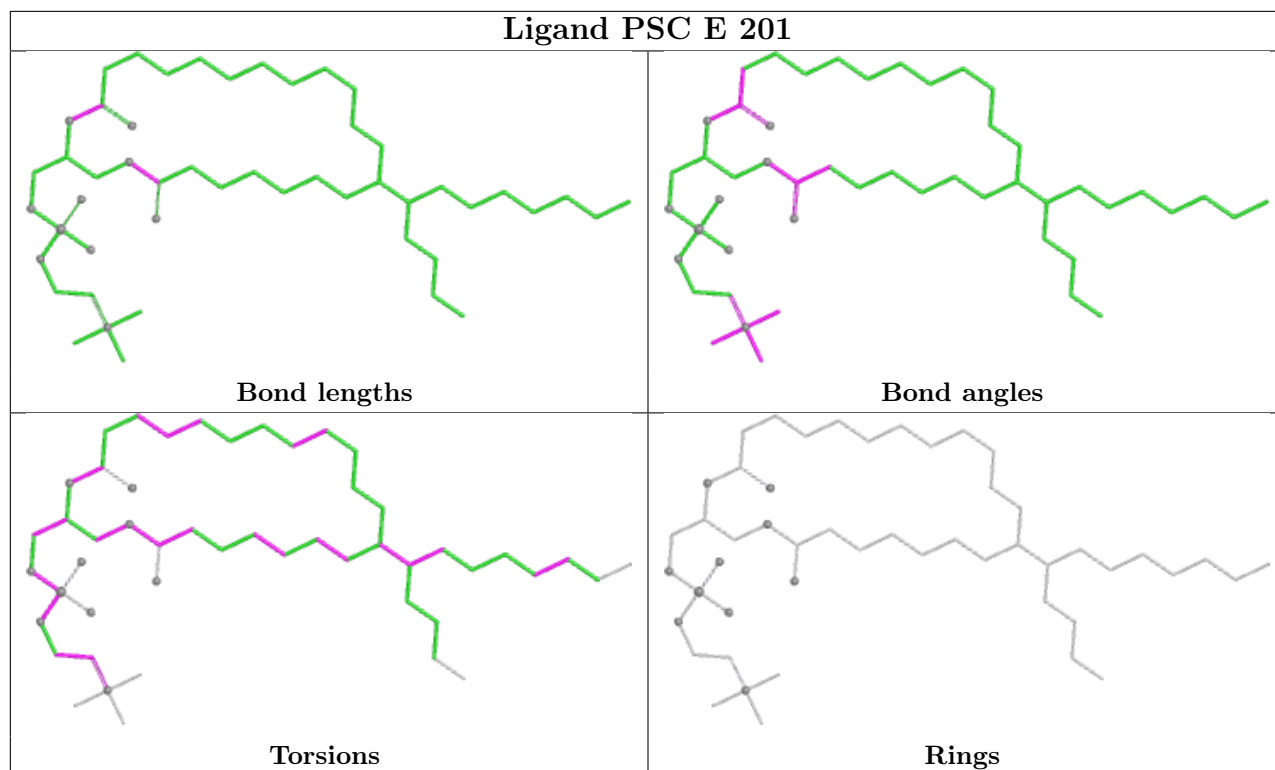




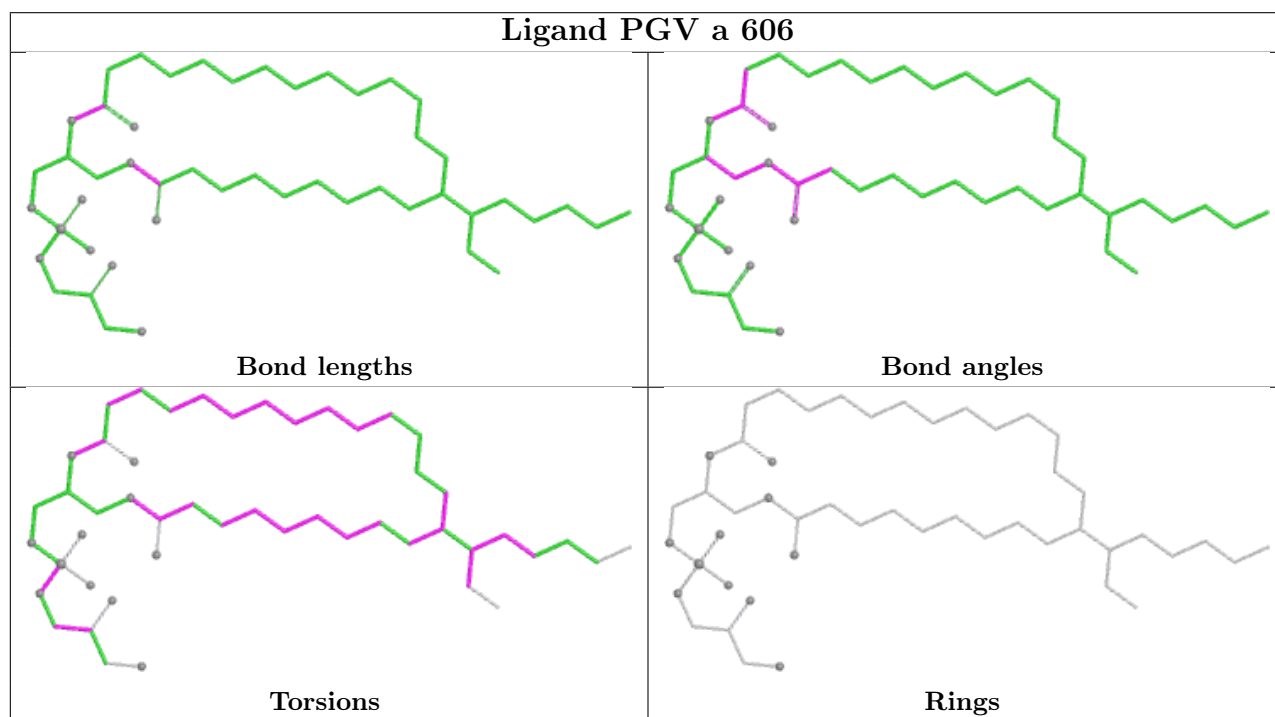


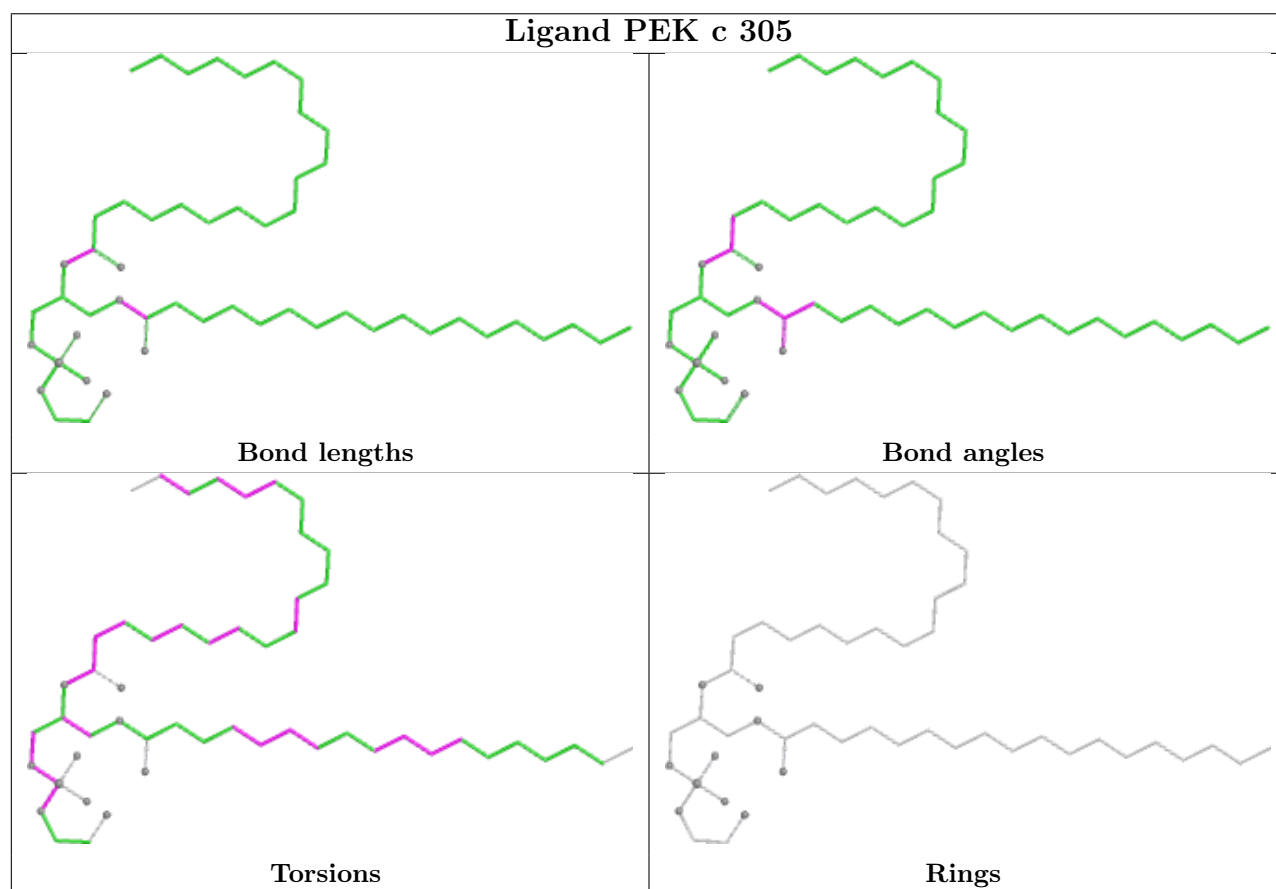
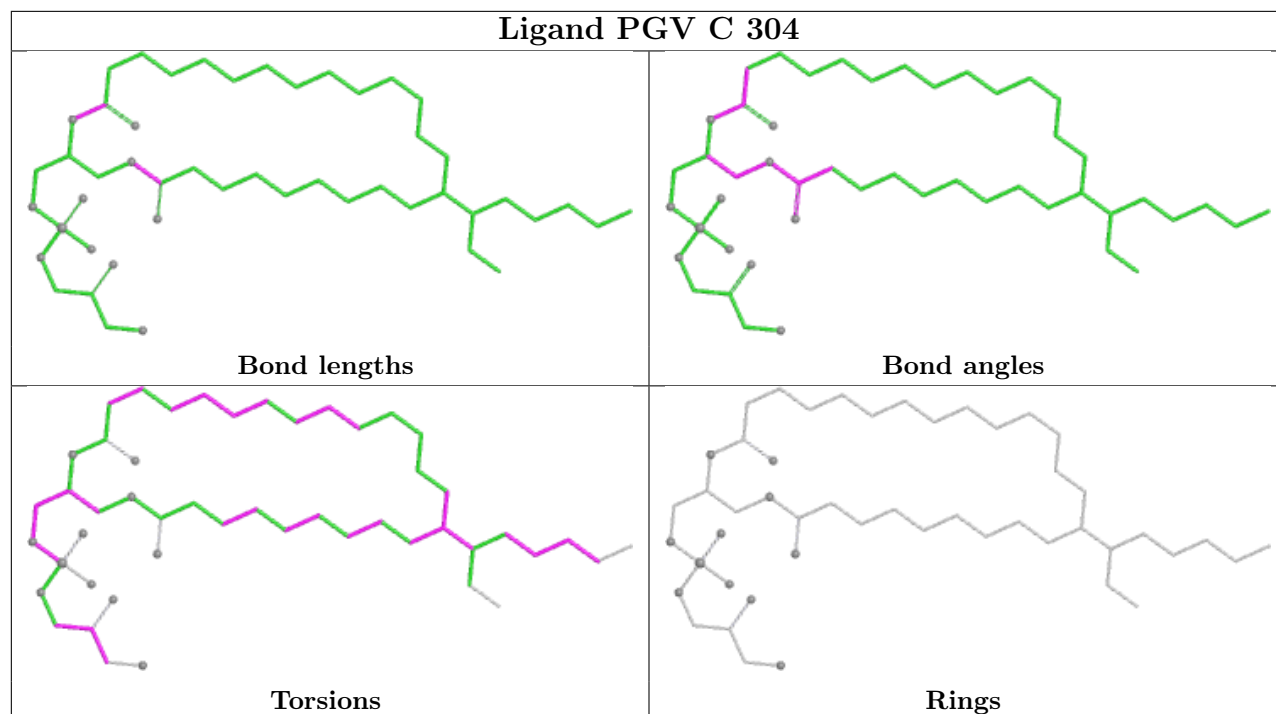


Ligand PSC E 201

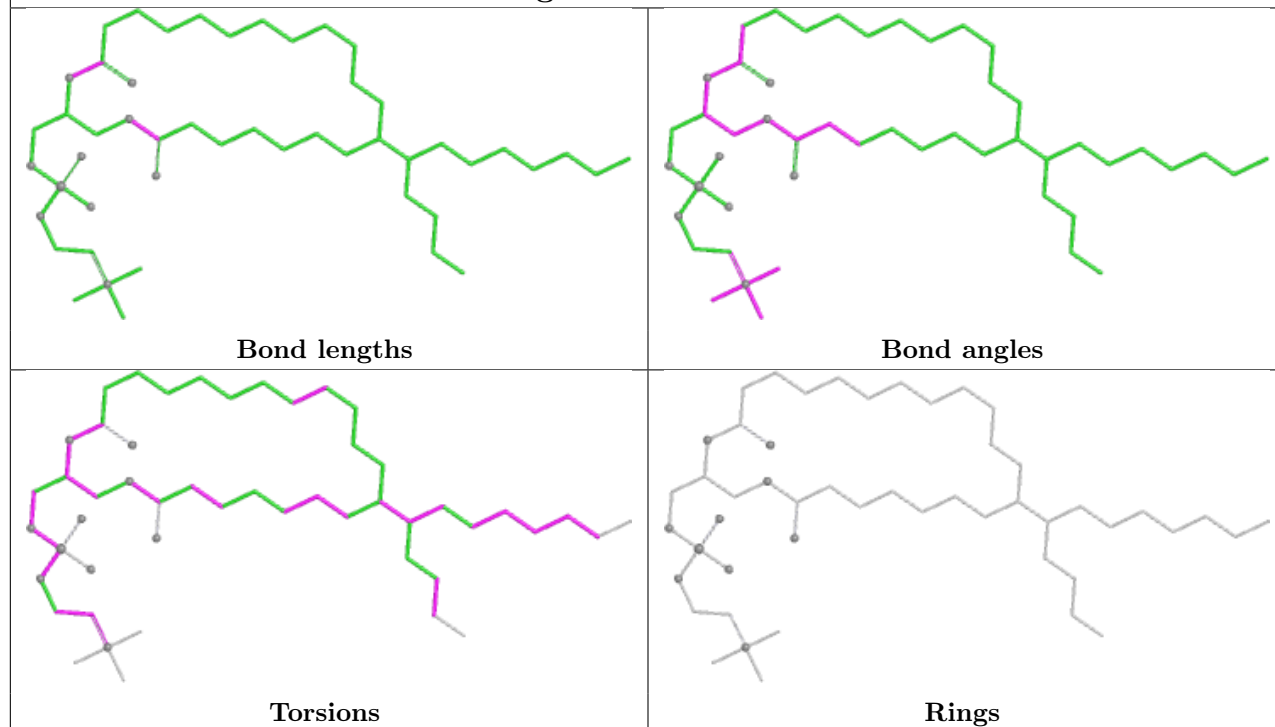


Ligand PGV a 606

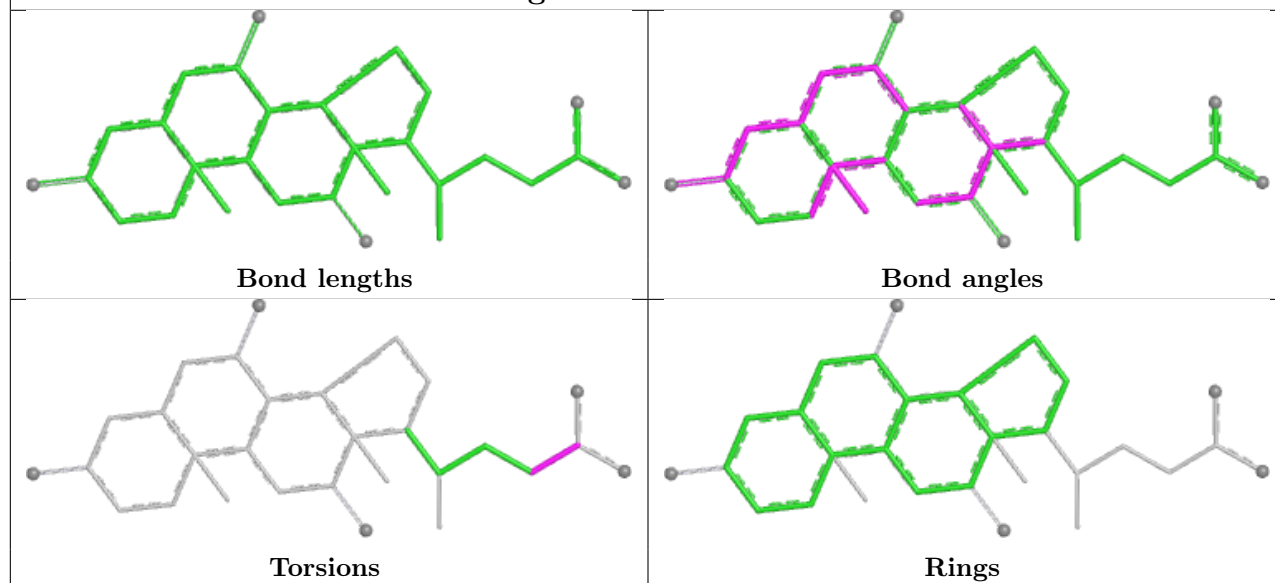


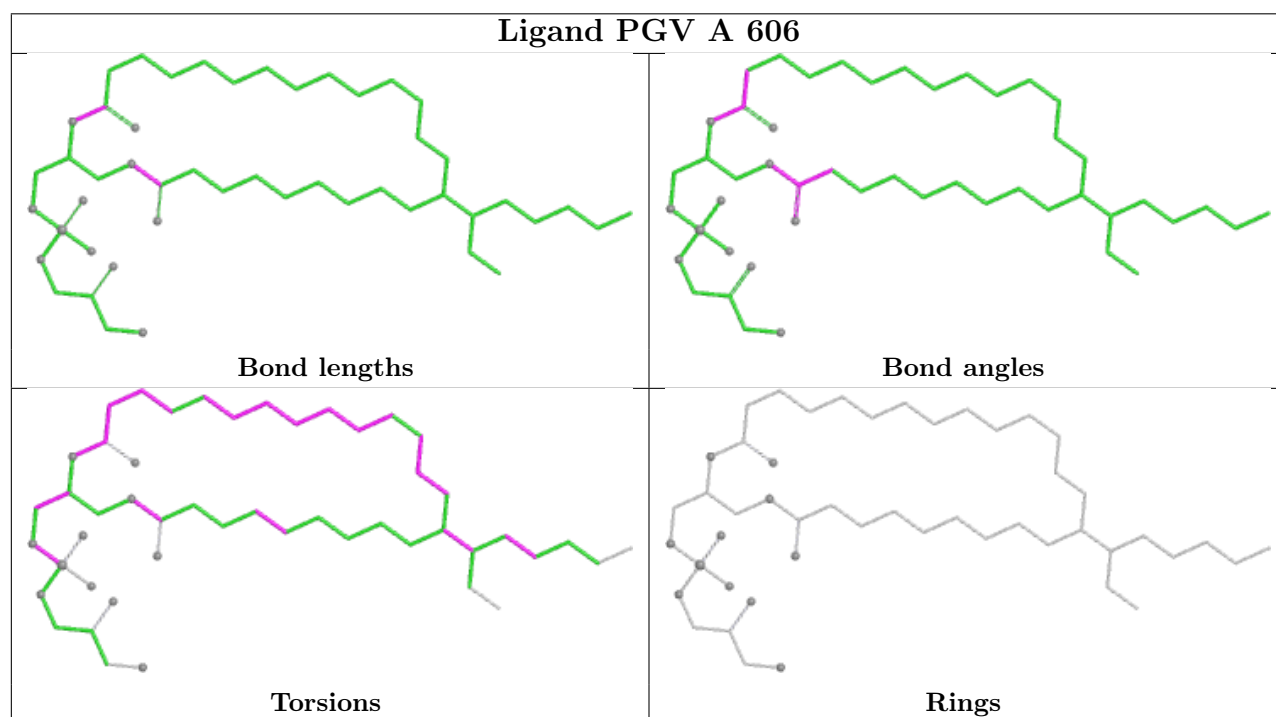
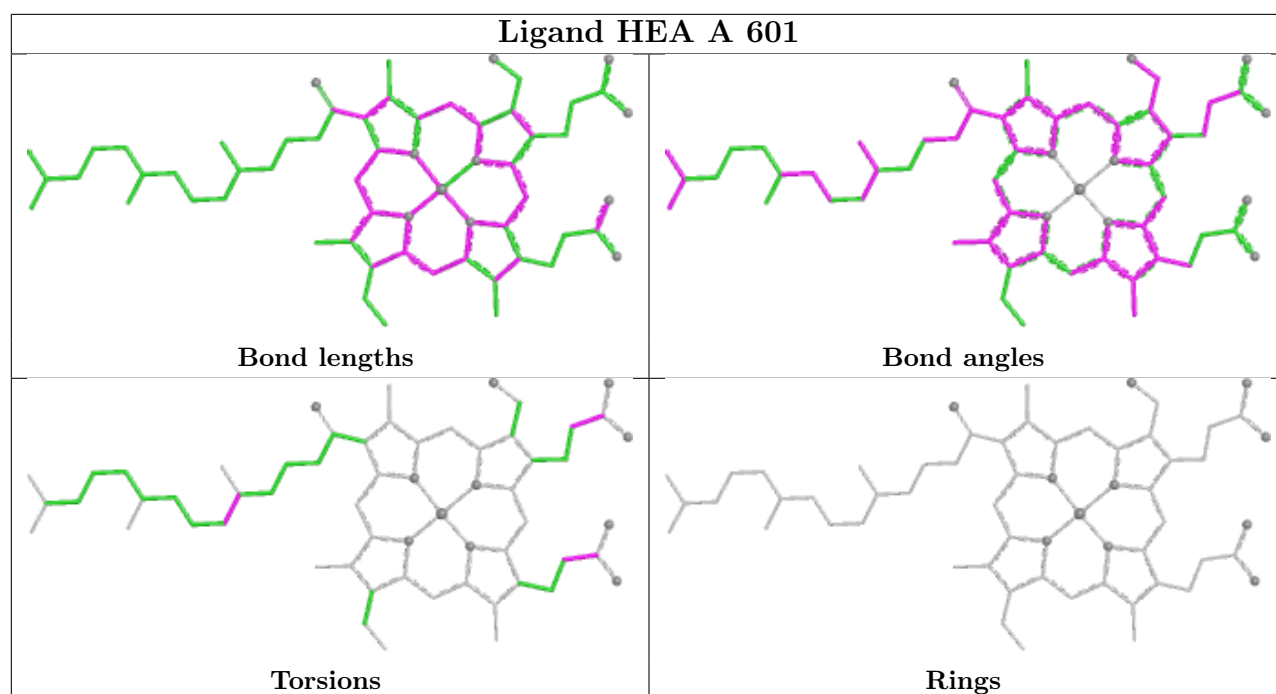


Ligand PSC b 303

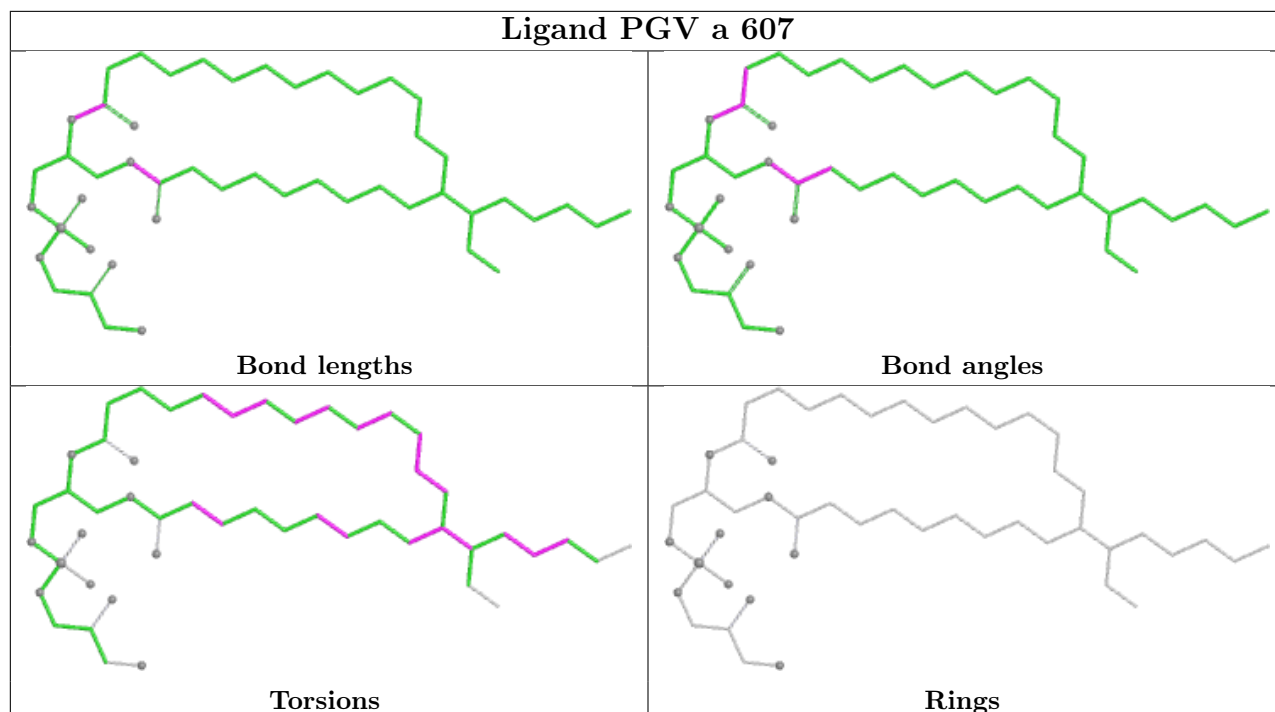


Ligand CHD B 402

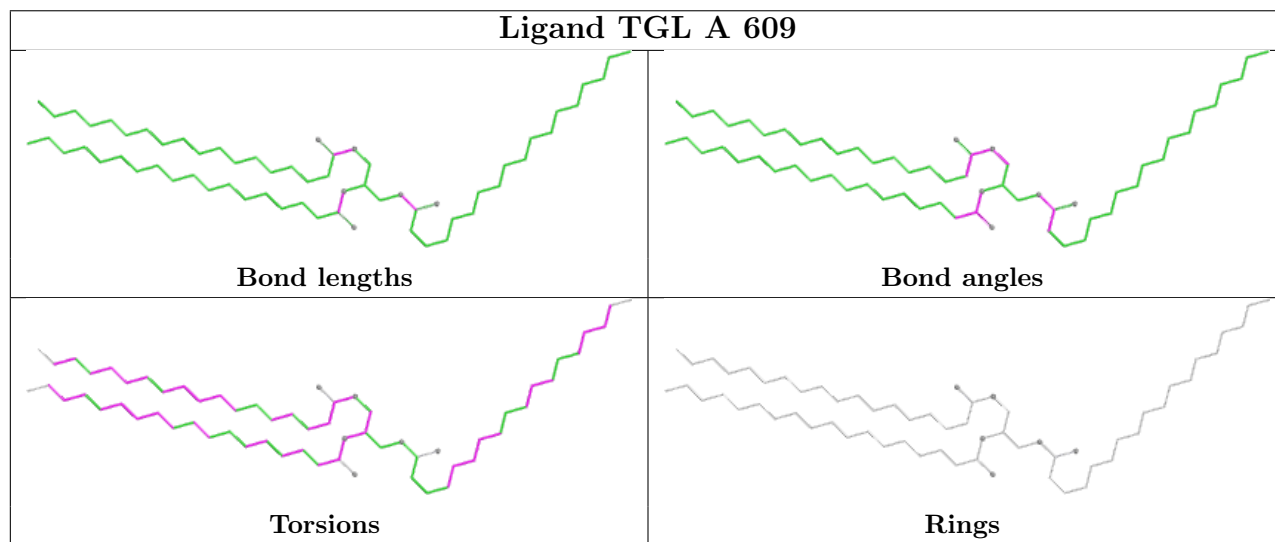


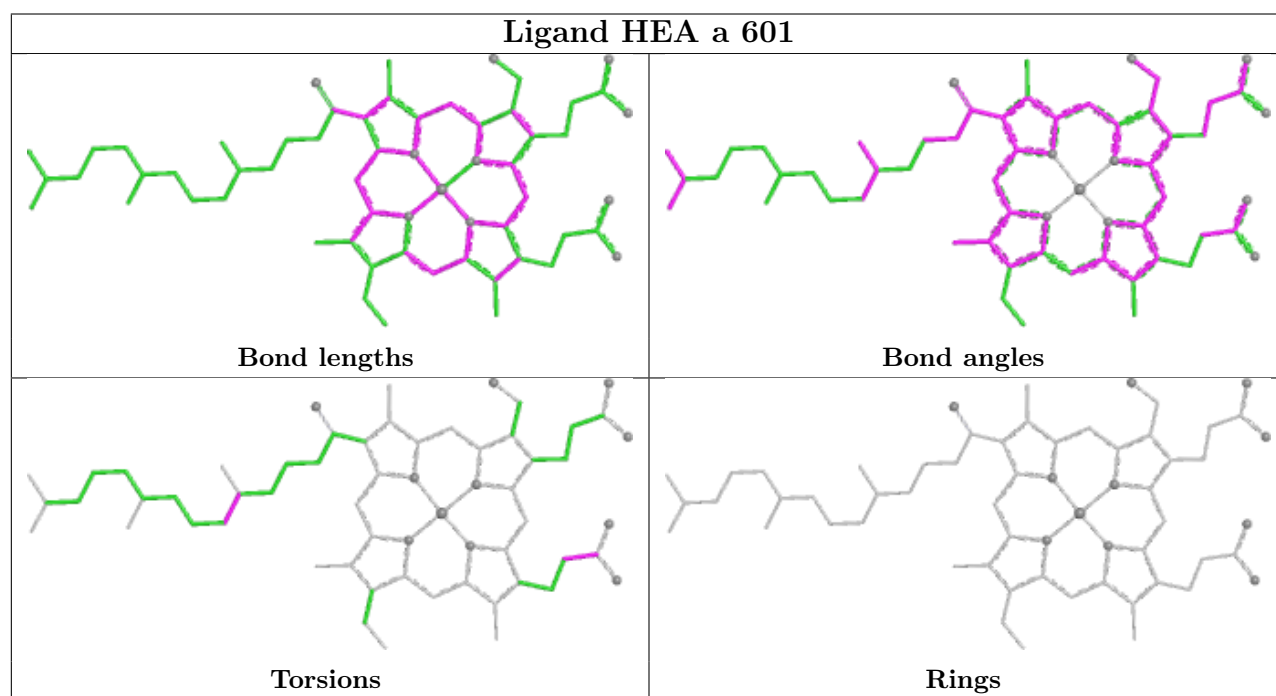
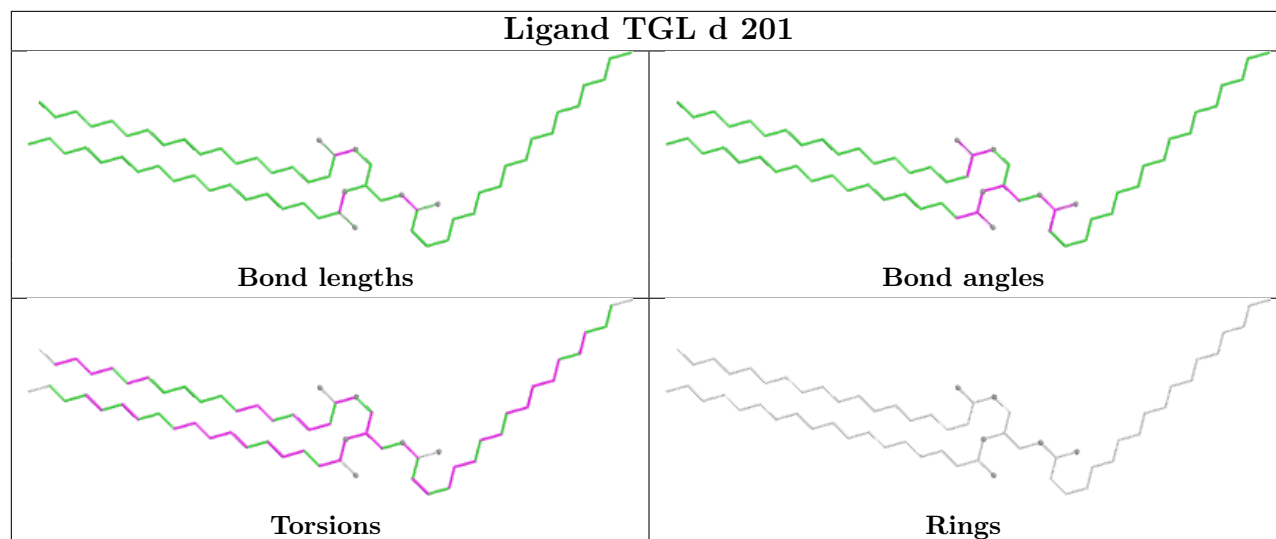


Ligand PGV a 607

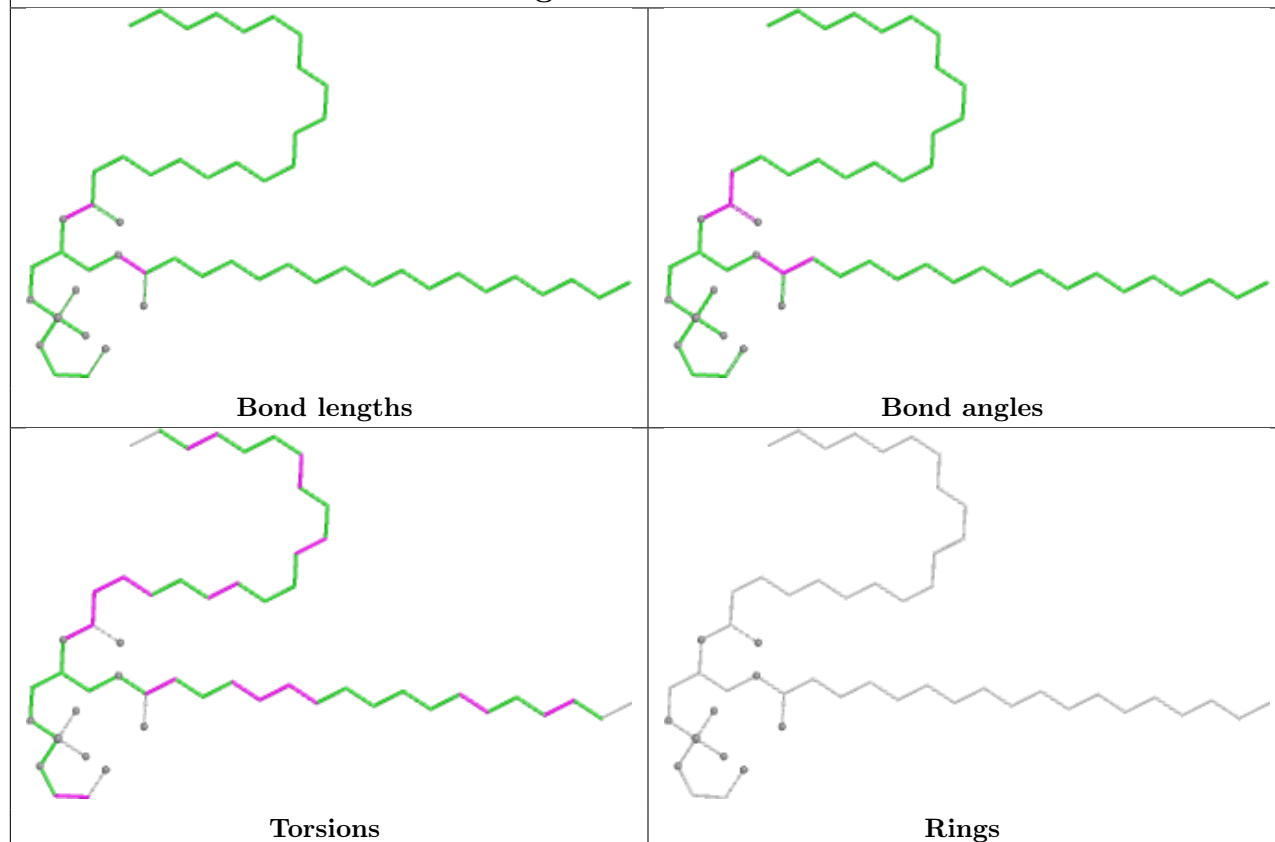


Ligand TGL A 609

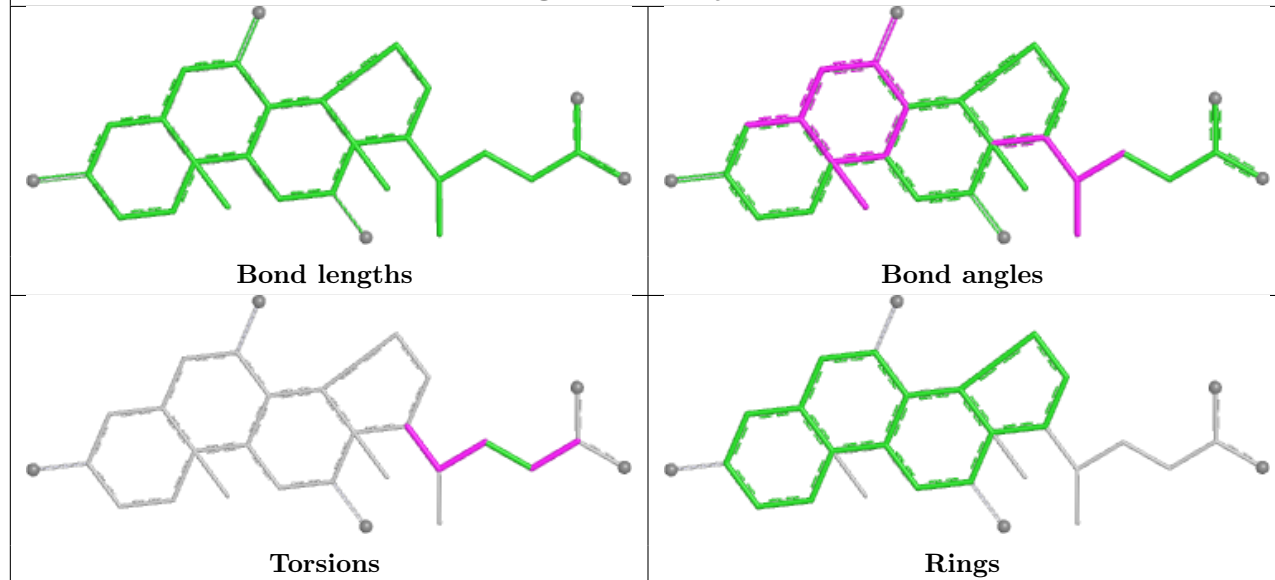


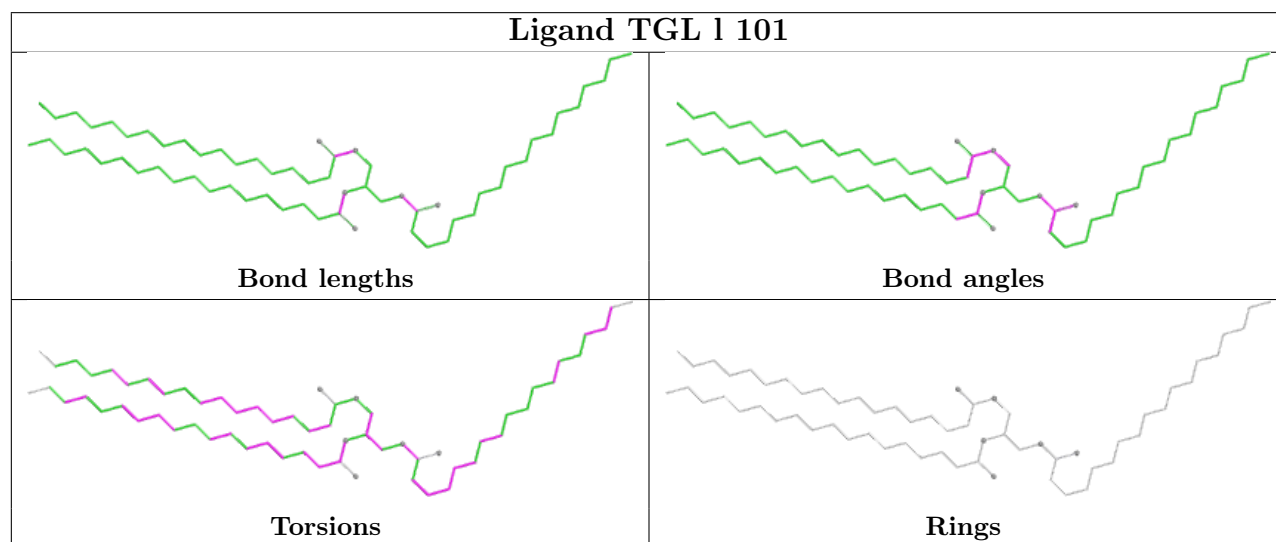
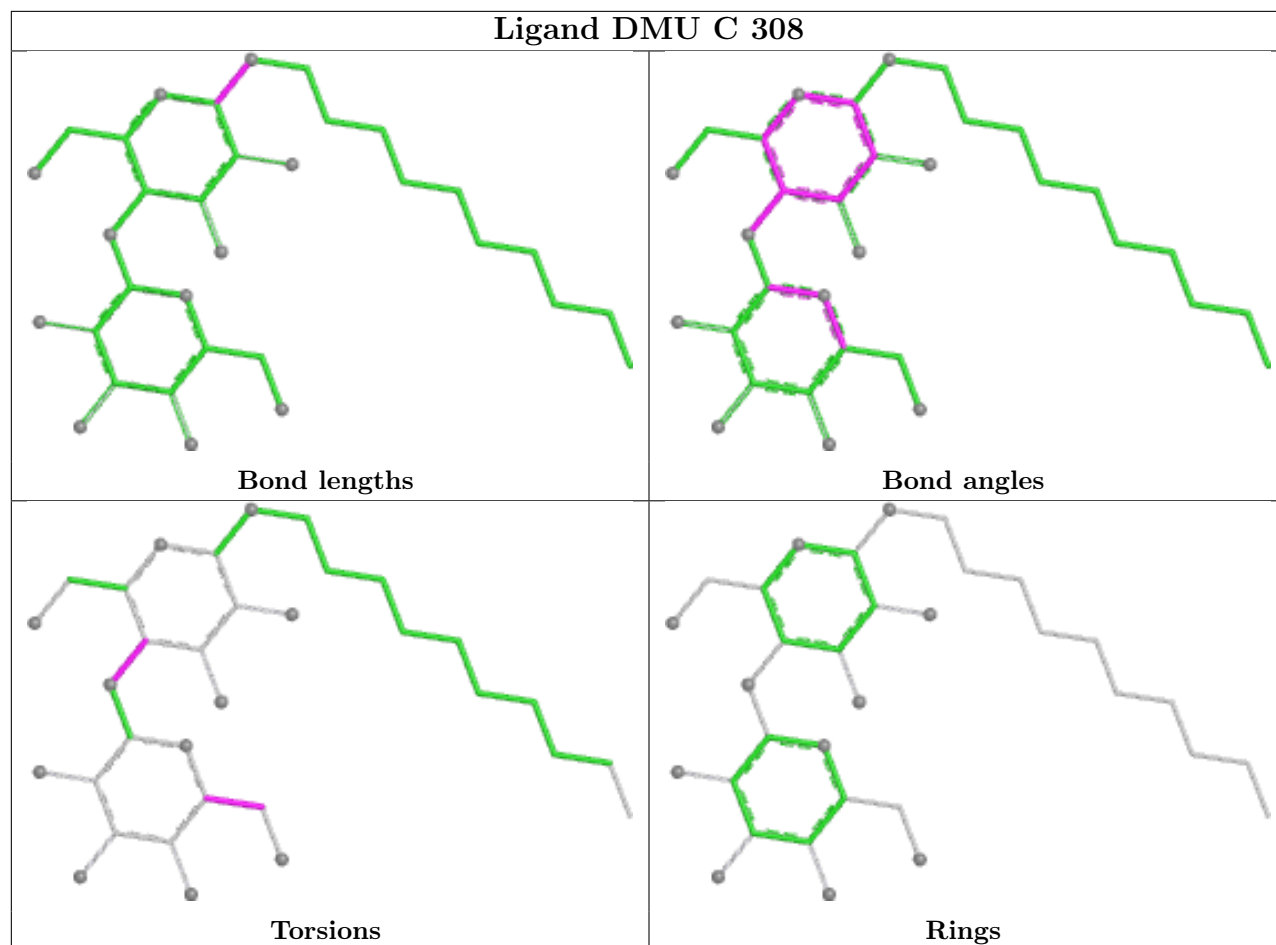


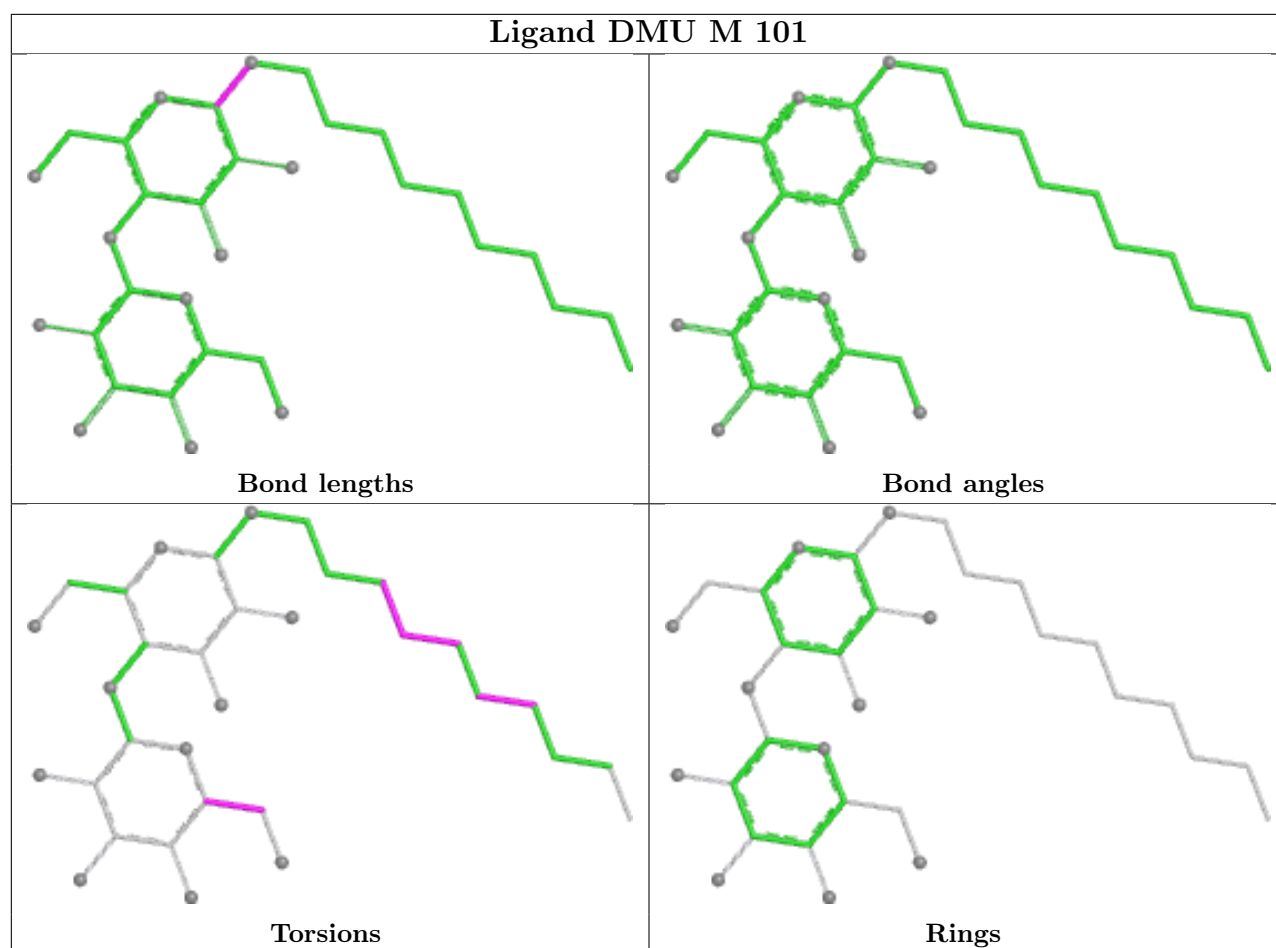
Ligand PEK c 304

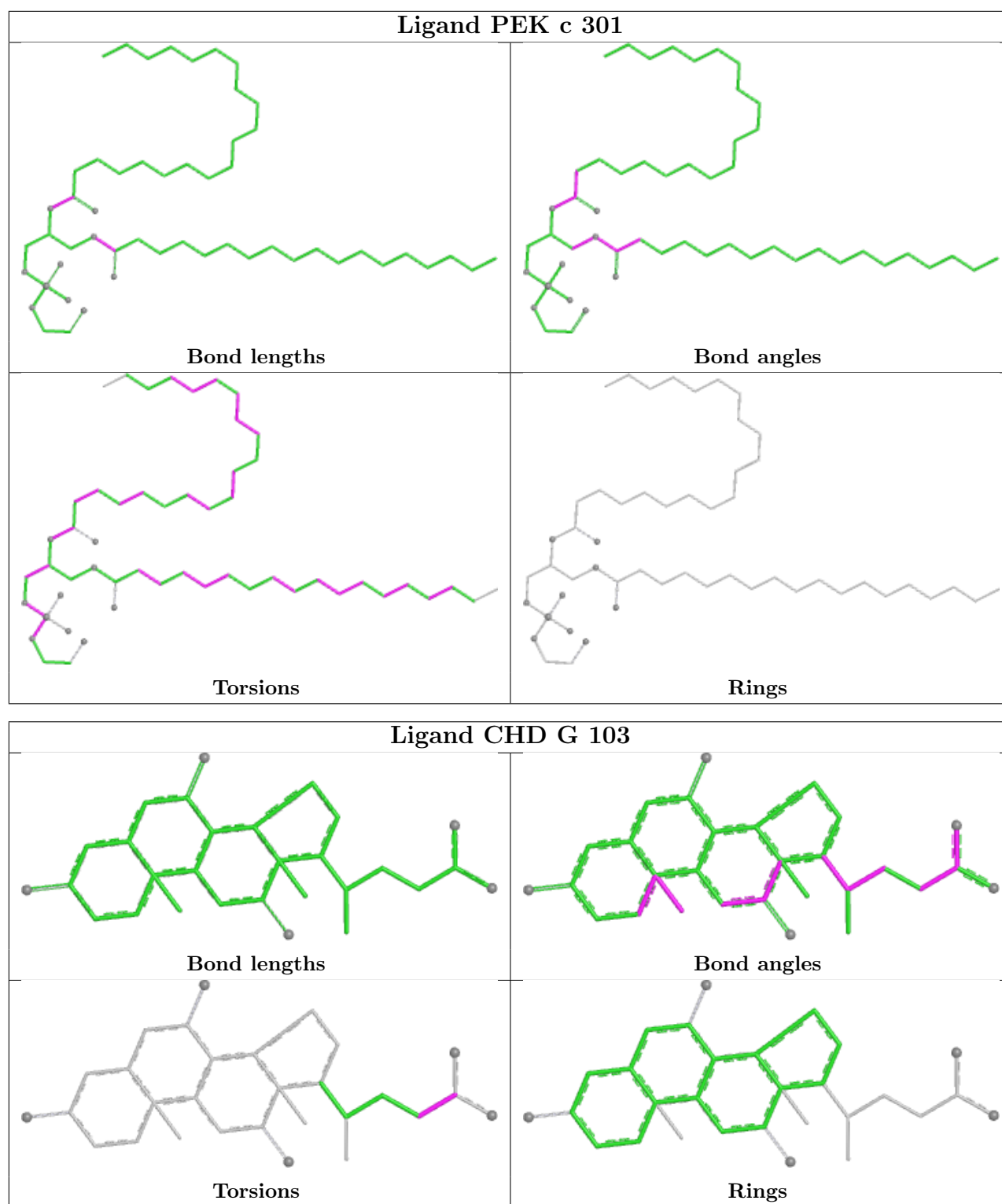


Ligand CHD j 101









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.06	9 (1%) 67 75	21, 27, 36, 72	0
1	a	513/514 (99%)	0.83	37 (7%) 21 25	27, 39, 52, 76	0
2	B	226/227 (99%)	0.50	15 (6%) 24 28	23, 34, 55, 89	0
2	b	226/227 (99%)	1.24	30 (13%) 7 8	35, 45, 70, 104	0
3	C	259/261 (99%)	0.24	9 (3%) 47 53	26, 32, 44, 79	0
3	c	259/261 (99%)	0.76	17 (6%) 24 28	30, 39, 55, 79	0
4	D	144/147 (97%)	0.63	6 (4%) 40 47	29, 37, 53, 77	0
4	d	144/147 (97%)	2.19	70 (48%) 0 0	46, 58, 90, 147	0
5	E	105/109 (96%)	0.51	3 (2%) 53 60	32, 40, 60, 107	0
5	e	105/109 (96%)	1.43	25 (23%) 2 2	39, 51, 70, 105	0
6	F	98/98 (100%)	1.18	13 (13%) 7 8	27, 38, 87, 129	0
6	f	98/98 (100%)	1.66	16 (16%) 4 5	34, 48, 103, 143	0
7	G	83/85 (97%)	1.63	25 (30%) 1 1	30, 40, 106, 141	0
7	g	83/85 (97%)	1.96	24 (28%) 1 1	32, 49, 103, 118	0
8	H	79/85 (92%)	1.25	13 (16%) 4 4	29, 42, 89, 120	0
8	h	79/85 (92%)	1.61	20 (25%) 1 1	40, 52, 97, 116	0
9	I	72/73 (98%)	0.99	9 (12%) 8 9	32, 45, 63, 75	0
9	i	72/73 (98%)	1.48	17 (23%) 2 2	37, 54, 73, 90	0
10	J	58/59 (98%)	0.93	6 (10%) 12 13	30, 42, 64, 110	0
10	j	58/59 (98%)	2.01	21 (36%) 1 0	42, 53, 77, 130	0
11	K	49/56 (87%)	1.30	8 (16%) 4 5	31, 41, 58, 73	0
11	k	49/56 (87%)	1.98	23 (46%) 0 0	53, 60, 79, 91	0
12	L	46/47 (97%)	0.64	4 (8%) 16 18	28, 34, 54, 88	0
12	l	46/47 (97%)	1.90	17 (36%) 1 0	44, 52, 72, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.72	3 (6%) 22 26	31, 35, 62, 88	0
13	m	43/46 (93%)	2.10	19 (44%) 0 0	47, 57, 87, 117	0
All	All	3550/3614 (98%)	0.90	459 (12%) 7 9	21, 40, 73, 147	0

All (459) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	f	1	ALA	12.9
6	F	1	ALA	12.3
6	F	96	LEU	11.9
6	f	96	LEU	11.9
6	f	97	ALA	11.7
4	d	6	VAL	10.6
2	b	90	ILE	10.1
7	G	9	GLY	9.8
7	g	1	ALA	8.8
7	G	3	ALA	8.6
7	g	3	ALA	8.5
8	h	8	ILE	8.3
8	H	8	ILE	8.0
11	K	42	PRO	7.7
4	d	5	VAL	7.6
6	F	97	ALA	7.6
7	G	5	LYS	7.5
7	g	10	GLY	7.4
5	e	109	VAL	7.3
7	G	1	ALA	7.2
7	g	36	TRP	7.1
2	B	90	ILE	6.9
7	g	5	LYS	6.8
10	j	58	LYS	6.8
7	G	4	ALA	6.7
7	g	9	GLY	6.7
7	g	4	ALA	6.6
6	f	98	HIS	6.5
6	f	95	GLN	6.5
4	d	33	LEU	6.2
6	F	2	SER	6.2
7	g	37	LEU	6.1
7	G	2	SER	6.0
3	C	3	HIS	5.9

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Mol	Chain	Res	Type	RSRZ
4	d	128	VAL	5.9
6	f	2	SER	5.9
7	G	6	GLY	5.8
6	F	98	HIS	5.8
10	j	57	HIS	5.8
7	g	2	SER	5.8
7	g	6	GLY	5.6
6	f	94	HIS	5.6
4	d	4	SER	5.5
7	G	8	HIS	5.5
7	G	7	ASP	5.5
8	H	45	ALA	5.5
7	G	10	GLY	5.5
7	G	36	TRP	5.3
6	F	94	HIS	5.3
9	I	37	PHE	5.3
8	H	47	GLY	5.2
4	d	48	TRP	5.2
4	d	7	LYS	5.2
3	c	37	PHE	5.1
1	a	113	LEU	5.1
2	b	113	TYR	5.0
6	F	3	GLY	4.9
10	j	52	TRP	4.8
2	B	91	ASN	4.7
4	d	35	ALA	4.6
13	m	43	SER	4.6
3	c	3	HIS	4.6
2	b	65	TRP	4.5
9	i	37	PHE	4.5
8	h	45	ALA	4.5
6	f	3	GLY	4.5
1	A	513	LEU	4.4
12	L	2	HIS	4.4
11	k	6	ALA	4.4
8	H	9	LYS	4.3
12	l	45	LEU	4.3
7	g	84	LYS	4.3
8	h	7	LYS	4.3
4	d	124	LEU	4.2
7	G	37	LEU	4.2
8	H	50	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
4	d	46	ALA	4.2
9	i	3	ALA	4.2
13	M	43	SER	4.2
9	i	26	MET	4.2
4	d	40	LEU	4.2
7	g	8	HIS	4.1
7	G	45	PRO	4.1
2	B	87	MET	4.1
12	l	47	LYS	4.1
10	J	52	TRP	4.1
7	g	38	HIS	4.1
4	d	59	LEU	4.0
13	m	1	ILE	4.0
4	d	8	SER	4.0
6	F	95	GLN	4.0
8	h	44	THR	3.9
6	f	43	LYS	3.9
1	a	297	MET	3.9
2	b	227	LEU	3.9
5	e	92	THR	3.9
8	h	9	LYS	3.9
9	i	2	THR	3.9
8	H	7	LYS	3.8
10	j	24	GLY	3.8
4	d	10	ASP	3.8
3	c	44	MET	3.8
1	A	514	LYS	3.8
10	J	57	HIS	3.8
13	m	32	TRP	3.8
11	k	7	PRO	3.8
2	B	113	TYR	3.7
8	h	10	ASN	3.7
3	c	33	MET	3.7
4	d	102	TYR	3.7
10	j	48	TYR	3.7
9	I	32	ALA	3.7
13	m	40	TYR	3.7
9	i	73	LYS	3.7
2	b	93	PRO	3.7
10	j	44	LEU	3.6
11	K	6	ALA	3.6
4	d	9	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
7	G	38	HIS	3.6
11	K	7	PRO	3.6
4	d	87	PHE	3.6
7	G	84	LYS	3.6
8	H	44	THR	3.5
5	E	109	VAL	3.5
8	h	50	VAL	3.5
7	g	42	ARG	3.5
2	b	130	PRO	3.5
10	j	56	PRO	3.5
2	B	65	TRP	3.5
3	c	38	ASN	3.5
3	c	230	ASN	3.5
7	G	41	HIS	3.4
7	g	7	ASP	3.4
10	j	27	THR	3.4
11	K	46	GLY	3.4
7	g	41	HIS	3.4
10	j	30	ILE	3.4
4	D	4	SER	3.4
11	k	23	THR	3.4
12	L	24	MET	3.4
4	d	58	GLU	3.3
7	g	12	GLY	3.3
5	e	96	LEU	3.3
3	c	34	TRP	3.3
12	l	24	MET	3.3
10	J	58	LYS	3.3
12	l	2	HIS	3.3
5	e	25	ASP	3.3
8	h	46	LYS	3.3
4	D	147	LYS	3.3
4	d	57	VAL	3.3
5	E	5	HIS	3.3
8	H	42	ALA	3.3
7	g	70	PHE	3.3
1	a	473	TRP	3.3
4	d	53	ILE	3.2
10	j	32	TYR	3.2
8	h	27	ARG	3.2
10	J	1	PHE	3.2
12	l	38	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	382	SER	3.2
2	b	131	GLY	3.2
4	d	129	ALA	3.2
3	C	38	ASN	3.2
3	c	40	MET	3.2
11	K	41	ASN	3.2
10	J	55	PHE	3.1
13	m	41	LYS	3.1
11	k	54	ARG	3.1
1	a	381	LEU	3.1
2	b	128	LEU	3.1
12	l	15	VAL	3.1
12	l	20	ARG	3.1
10	J	56	PRO	3.1
2	b	201	GLY	3.1
4	d	97	ILE	3.1
7	G	40	GLY	3.1
4	d	13	LEU	3.1
4	d	39	ALA	3.1
2	b	126	SER	3.0
5	E	7	THR	3.0
8	h	42	ALA	3.0
10	j	26	ALA	3.0
13	m	6	ALA	3.0
9	I	26	MET	3.0
1	a	382	SER	3.0
13	m	17	ILE	3.0
4	d	95	LEU	3.0
4	d	110	THR	3.0
7	g	45	PRO	3.0
1	A	113	LEU	2.9
3	c	26	LEU	2.9
4	d	62	LEU	2.9
2	b	202	SER	2.9
1	A	486	ASP	2.9
7	g	40	GLY	2.9
11	k	52	GLU	2.9
4	d	115	TRP	2.9
11	k	13	TYR	2.9
1	a	334	TRP	2.9
10	j	15	ASP	2.9
5	e	7	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	a	2	PHE	2.8
1	a	136	LEU	2.8
7	G	34	ASN	2.8
8	H	10	ASN	2.8
11	k	51	LYS	2.8
2	b	87	MET	2.8
8	H	43	MET	2.8
9	I	25	PHE	2.8
6	F	22	LEU	2.8
10	j	40	LEU	2.8
3	c	258	TRP	2.8
1	A	298	ASP	2.8
2	B	88	ASP	2.8
4	d	28	ALA	2.8
4	d	111	PHE	2.8
8	H	48	GLY	2.8
7	g	33	LEU	2.8
4	d	145	TRP	2.8
1	a	485	VAL	2.8
4	d	103	VAL	2.8
2	b	224	ALA	2.7
9	i	72	ALA	2.7
4	d	147	LYS	2.7
12	L	47	LYS	2.7
5	e	106	LEU	2.7
9	I	29	LEU	2.7
2	b	57	ASP	2.7
4	d	30	VAL	2.7
13	m	42	LYS	2.7
1	A	297	MET	2.7
2	b	37	LEU	2.7
6	F	52	ILE	2.7
7	G	42	ARG	2.7
7	g	35	SER	2.7
3	C	230	ASN	2.7
11	k	45	VAL	2.7
12	l	35	ALA	2.7
8	h	47	GLY	2.7
4	d	61	ARG	2.7
7	G	30	LEU	2.7
4	d	27	VAL	2.7
11	k	26	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
9	i	30	GLY	2.6
1	a	369	ASP	2.6
4	d	98	TRP	2.6
13	m	35	TYR	2.6
2	b	183	THR	2.6
4	d	91	PHE	2.6
2	B	16	ILE	2.6
4	d	89	ILE	2.6
1	a	118	VAL	2.6
9	I	27	VAL	2.6
2	B	92	ASN	2.6
2	b	32	PHE	2.6
9	I	34	PHE	2.6
10	j	1	PHE	2.6
11	k	9	PHE	2.6
11	k	24	PHE	2.6
2	b	133	LEU	2.6
1	a	125	GLY	2.6
7	G	39	SER	2.6
1	a	459	PHE	2.6
4	d	31	LYS	2.6
1	a	39	ALA	2.6
4	d	116	VAL	2.6
8	h	52	VAL	2.6
4	d	36	SER	2.6
2	b	149	THR	2.6
1	a	470	PHE	2.5
5	e	61	PHE	2.5
2	b	135	LEU	2.5
4	d	51	LEU	2.5
13	m	19	LEU	2.5
11	k	53	TRP	2.5
5	e	48	ILE	2.5
10	j	25	GLY	2.5
10	j	20	VAL	2.5
11	k	34	THR	2.5
2	b	5	MET	2.5
3	C	44	MET	2.5
4	D	9	GLU	2.5
10	j	47	LEU	2.5
1	a	169	ILE	2.5
11	K	47	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
12	l	26	THR	2.5
1	a	333	LYS	2.5
10	j	49	CYS	2.5
2	b	116	LEU	2.5
12	l	13	PHE	2.5
13	m	24	LEU	2.5
4	d	72	ASN	2.5
4	D	19	ARG	2.5
11	k	28	VAL	2.5
9	i	67	GLY	2.4
13	M	40	TYR	2.4
1	a	48	LEU	2.4
13	m	37	LEU	2.4
3	c	39	SER	2.4
2	B	86	MET	2.4
2	b	86	MET	2.4
3	c	45	ILE	2.4
1	a	380	VAL	2.4
2	B	61	VAL	2.4
11	K	45	VAL	2.4
1	A	512	ASN	2.4
4	d	101	HIS	2.4
5	e	5	HIS	2.4
8	h	53	CYS	2.4
4	d	34	SER	2.4
4	d	96	LEU	2.4
4	d	104	TYR	2.4
9	i	29	LEU	2.4
3	C	37	PHE	2.4
1	a	514	LYS	2.4
5	e	108	LYS	2.4
5	e	51	ALA	2.4
4	d	73	ARG	2.4
6	F	93	PRO	2.4
3	C	258	TRP	2.4
6	f	92	VAL	2.4
12	l	16	GLU	2.4
11	k	46	GLY	2.4
7	G	35	SER	2.4
1	a	47	LEU	2.4
11	k	18	LEU	2.4
12	l	28	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	a	471	ILE	2.4
2	b	123	ILE	2.4
13	m	39	ASN	2.4
9	I	30	GLY	2.4
13	m	21	VAL	2.4
1	a	409	TRP	2.4
8	h	70	SER	2.4
4	d	94	LEU	2.3
12	l	21	LEU	2.3
4	d	11	TYR	2.3
12	l	3	TYR	2.3
5	e	64	ALA	2.3
13	m	3	ALA	2.3
5	e	91	PRO	2.3
1	a	6	TRP	2.3
6	F	64	GLU	2.3
7	G	43	GLU	2.3
5	e	94	ASN	2.3
9	i	53	ASN	2.3
9	i	32	ALA	2.3
2	b	94	SER	2.3
11	k	47	ARG	2.3
6	f	49	VAL	2.3
2	B	59	GLN	2.3
5	e	104	LEU	2.3
2	b	152	MET	2.3
9	i	57	MET	2.3
2	B	32	PHE	2.3
2	b	218	TYR	2.3
5	e	79	LYS	2.3
2	b	2	ALA	2.3
1	a	460	ILE	2.3
4	d	107	ILE	2.3
8	H	85	ILE	2.3
8	h	57	ARG	2.3
4	d	50	SER	2.3
1	a	482	VAL	2.3
5	e	16	VAL	2.3
1	a	467	LEU	2.3
2	B	5	MET	2.3
4	d	38	LYS	2.3
7	G	33	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	a	49	GLY	2.2
7	g	82	TYR	2.2
12	l	6	GLY	2.2
5	e	63	SER	2.2
6	f	65	ASP	2.2
10	j	34	VAL	2.2
1	a	117	MET	2.2
4	d	41	LYS	2.2
1	A	381	LEU	2.2
1	a	483	LEU	2.2
12	l	4	GLU	2.2
3	C	246	ASP	2.2
3	C	261	SER	2.2
4	d	106	PRO	2.2
11	k	16	ALA	2.2
1	a	366	VAL	2.2
11	k	17	VAL	2.2
2	b	136	LEU	2.2
3	c	22	LEU	2.2
10	j	31	LEU	2.2
13	m	28	LEU	2.2
9	i	31	PHE	2.2
5	e	24	ILE	2.2
11	k	38	ILE	2.2
4	d	63	LYS	2.2
4	d	138	TRP	2.2
3	c	246	ASP	2.2
11	k	14	GLY	2.2
13	m	5	PRO	2.2
6	F	54	ASN	2.1
9	i	25	PHE	2.1
3	c	55	TYR	2.1
4	d	16	TYR	2.1
1	a	472	ILE	2.1
4	d	131	ILE	2.1
6	f	52	ILE	2.1
13	M	32	TRP	2.1
9	i	33	THR	2.1
3	c	261	SER	2.1
4	d	49	SER	2.1
1	a	399	LEU	2.1
11	K	54	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	126	MET	2.1
1	a	446	ALA	2.1
4	d	75	THR	2.1
4	d	105	GLY	2.1
12	L	20	ARG	2.1
1	a	468	MET	2.1
8	h	43	MET	2.1
2	B	227	LEU	2.1
13	m	34	LEU	2.1
9	I	31	PHE	2.1
4	d	15	SER	2.1
3	C	236	GLU	2.1
8	H	46	LYS	2.1
6	f	4	GLY	2.1
7	G	12	GLY	2.1
4	d	109	HIS	2.1
4	d	143	ASN	2.1
5	e	70	VAL	2.1
8	h	12	GLN	2.1
8	h	23	GLN	2.1
5	e	58	LEU	2.1
5	e	89	LEU	2.1
10	j	11	LEU	2.1
9	i	24	ALA	2.1
5	e	107	ASP	2.1
6	f	25	ARG	2.1
4	d	43	LYS	2.0
4	d	112	GLU	2.0
5	e	39	TYR	2.0
4	D	143	ASN	2.0
4	D	5	VAL	2.0
13	m	33	VAL	2.0
12	l	27	LEU	2.0
1	a	475	ALA	2.0
4	d	69	ALA	2.0
5	e	62	ALA	2.0
11	k	27	ALA	2.0
2	b	60	GLU	2.0
1	a	449	MET	2.0
2	B	64	ILE	2.0
9	i	60	PHE	2.0
3	c	41	THR	2.0

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Mol	Chain	Res	Type	RSRZ
7	g	65	GLY	2.0
8	h	79	GLY	2.0
11	k	49	THR	2.0
6	f	31	TYR	2.0
8	h	56	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	g	11	11/12	0.39	0.31	88,116,130,131	0
9	SAC	i	101	9/10	0.46	0.18	100,104,108,108	0
7	TPO	G	11	11/12	0.66	0.25	64,95,111,114	0
9	SAC	I	101	9/10	0.74	0.17	64,68,76,79	0
1	FME	a	1	10/11	0.82	0.21	55,69,82,85	0
1	FME	A	1	10/11	0.83	0.19	39,49,82,85	0
2	FME	B	301	10/11	0.94	0.09	30,33,43,46	0
2	FME	b	1	10/11	0.94	0.12	45,47,58,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	DMU	c	309	33/33	0.50	0.31	100,119,130,133	0
18	PGV	c	302	51/51	0.66	0.31	63,84,114,117	0
19	TGL	D	201	63/63	0.67	0.32	61,78,87,94	0
23	PEK	C	307	53/53	0.68	0.28	59,86,146,157	0
18	PGV	a	606	51/51	0.69	0.31	62,89,129,134	0

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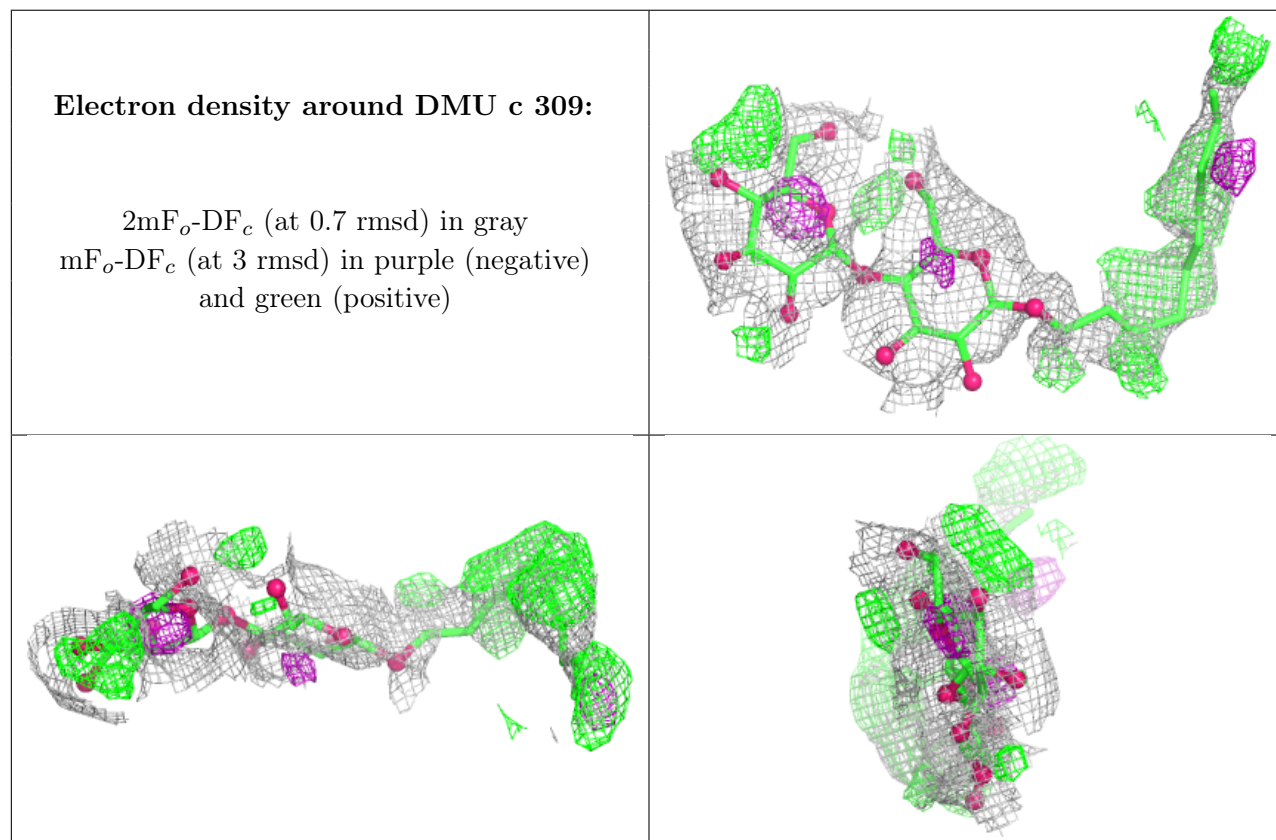
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	DMU	C	308	33/33	0.70	0.23	70,94,111,112	0
23	PEK	c	301	53/53	0.72	0.26	58,93,150,158	0
24	CDL	G	102	100/100	0.72	0.31	62,96,130,139	0
18	PGV	A	606	51/51	0.72	0.29	48,77,123,129	0
23	PEK	G	101	53/53	0.72	0.28	61,84,119,130	0
23	PEK	c	305	53/53	0.73	0.30	63,90,111,120	0
18	PGV	C	304	51/51	0.73	0.30	64,90,105,109	0
16	MG	a	604	1/1	0.73	0.13	47,47,47,47	0
22	CHD	J	101	29/29	0.73	0.21	64,70,84,86	0
19	TGL	A	608	63/63	0.74	0.29	55,79,96,100	0
19	TGL	d	201	63/63	0.74	0.31	67,81,103,111	0
26	PSC	b	303	52/52	0.74	0.33	53,96,136,144	0
24	CDL	g	101	100/100	0.75	0.30	66,102,140,149	0
19	TGL	b	302	63/63	0.75	0.27	68,86,96,97	0
19	TGL	l	101	63/63	0.75	0.32	63,80,110,114	0
24	CDL	c	307	100/100	0.75	0.27	62,96,126,135	0
19	TGL	A	609	63/63	0.76	0.28	50,68,89,94	0
26	PSC	E	201	52/52	0.77	0.27	53,101,160,171	0
24	CDL	C	305	100/100	0.78	0.23	53,87,111,114	0
22	CHD	j	101	29/29	0.82	0.17	86,90,99,103	0
25	DMU	m	101	33/33	0.82	0.19	70,81,91,94	0
22	CHD	c	308	29/29	0.87	0.13	59,62,68,69	0
22	CHD	C	306	29/29	0.90	0.12	50,54,62,64	0
25	DMU	M	101	33/33	0.91	0.12	39,48,58,63	0
23	PEK	c	304	53/53	0.92	0.18	41,63,99,101	0
23	PEK	C	302	53/53	0.93	0.16	31,53,83,89	0
18	PGV	c	306	51/51	0.93	0.14	32,46,82,85	0
22	CHD	B	402	29/29	0.94	0.08	31,32,36,41	0
22	CHD	C	301	29/29	0.94	0.08	31,34,36,38	0
18	PGV	a	607	51/51	0.94	0.14	32,48,74,83	0
22	CHD	G	103	29/29	0.94	0.08	32,35,38,41	0
17	NA	a	605	1/1	0.94	0.07	48,48,48,48	0
22	CHD	c	303	29/29	0.94	0.09	34,36,40,41	0
17	NA	A	605	1/1	0.94	0.14	28,28,28,28	0
20	CMO	a	608	2/2	0.94	0.21	65,65,65,69	0
16	MG	A	604	1/1	0.95	0.06	27,27,27,27	0
18	PGV	A	607	51/51	0.95	0.13	25,42,65,69	0
18	PGV	C	303	51/51	0.95	0.12	27,39,70,76	0
14	HEA	a	602	60/60	0.96	0.10	29,32,40,43	0
20	CMO	A	610	2/2	0.96	0.18	46,46,46,46	0
14	HEA	a	601	60/60	0.96	0.12	32,37,55,62	0
21	CUA	b	301	2/2	0.96	0.05	36,36,36,38	0

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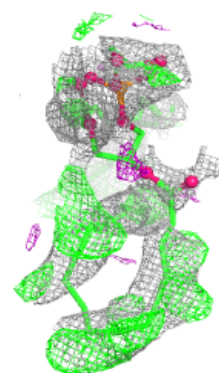
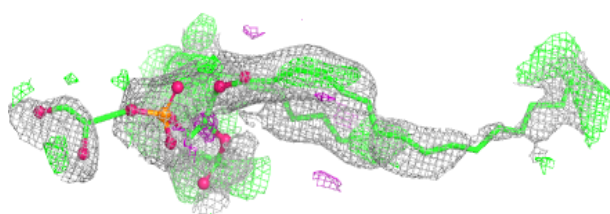
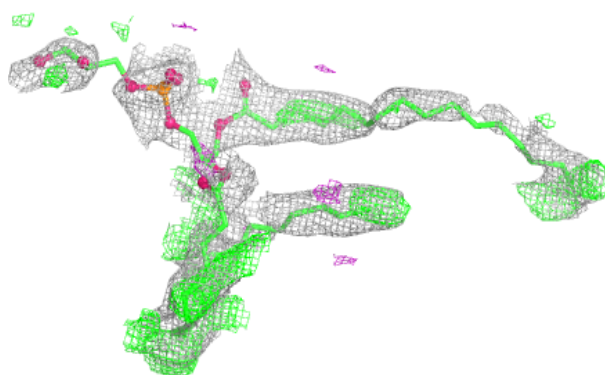
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	HEA	A	602	60/60	0.98	0.07	22,24,33,35	0
21	CUA	B	401	2/2	0.98	0.03	24,24,24,24	0
14	HEA	A	601	60/60	0.98	0.07	21,23,45,50	0
27	ZN	F	101	1/1	0.98	0.03	33,33,33,33	0
15	CU	a	603	1/1	0.99	0.02	34,34,34,34	0
27	ZN	f	101	1/1	0.99	0.03	41,41,41,41	0
15	CU	A	603	1/1	1.00	0.01	25,25,25,25	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.

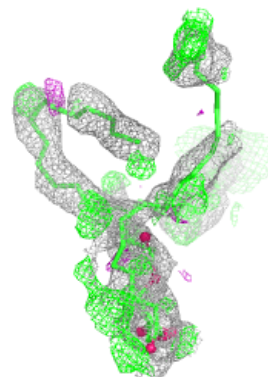
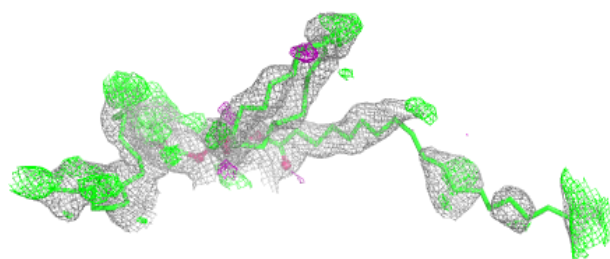
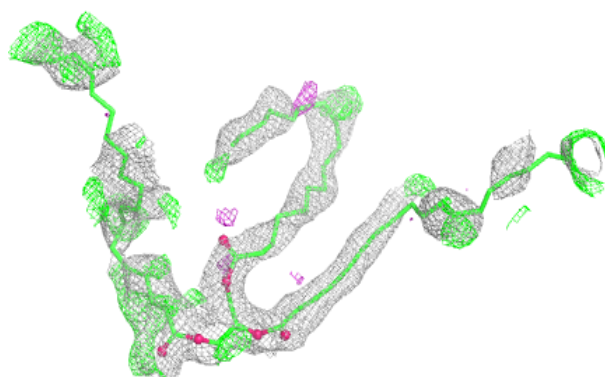


Electron density around PGV c 302:

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

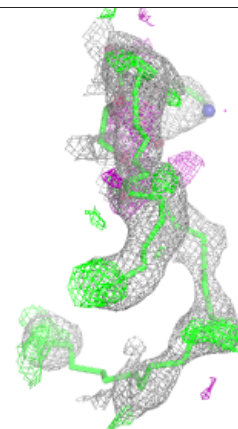
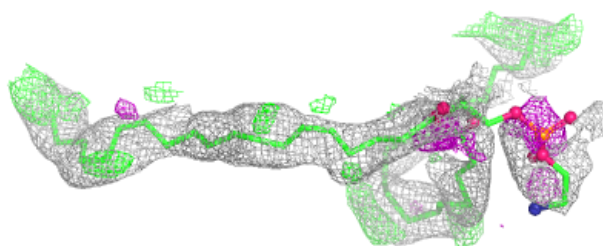
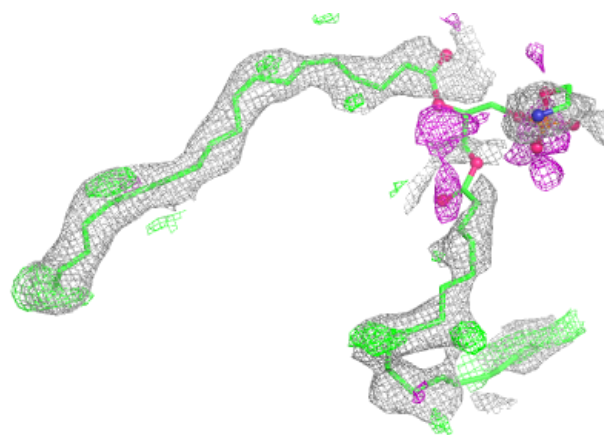
**Electron density around TGL D 201:**

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

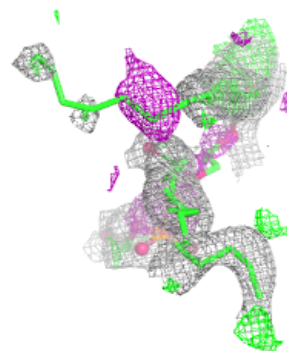
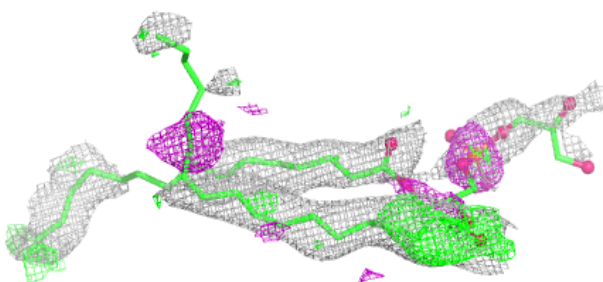
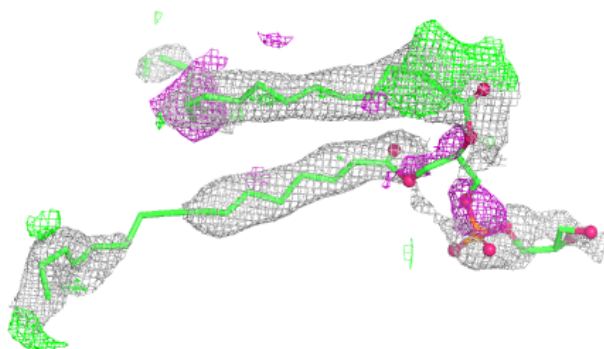


Electron density around PEK C 307:

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

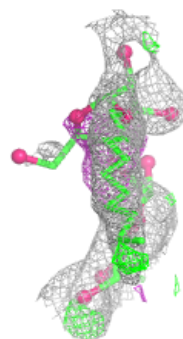
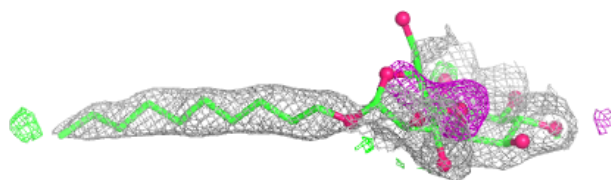
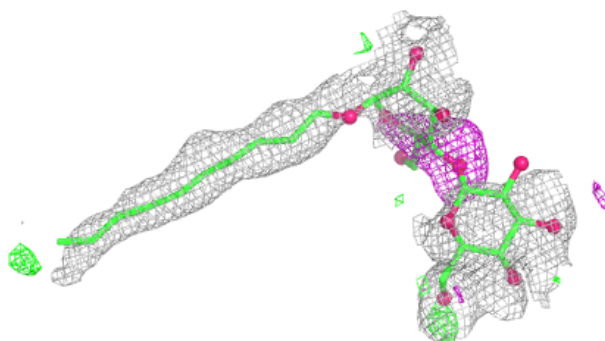
**Electron density around PGV a 606:**

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



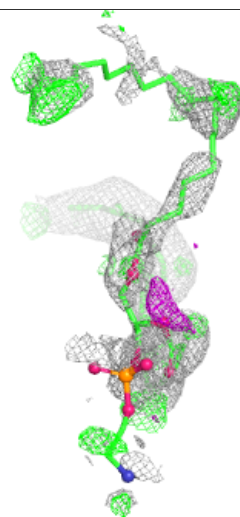
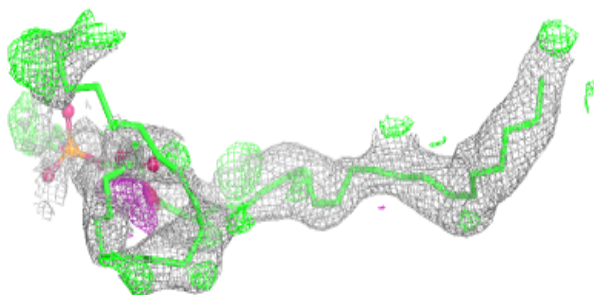
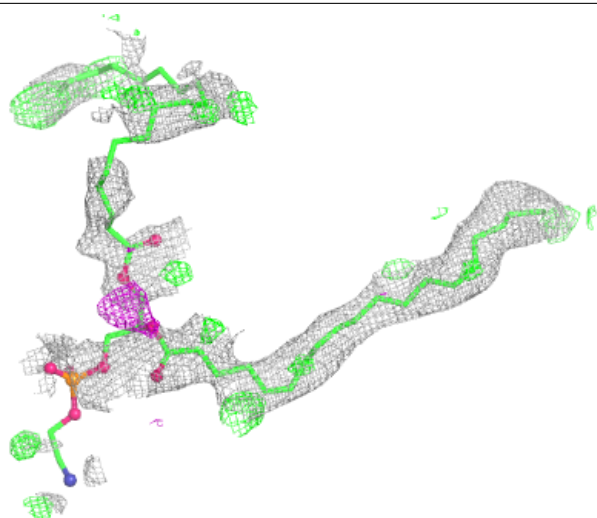
Electron density around DMU C 308:

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



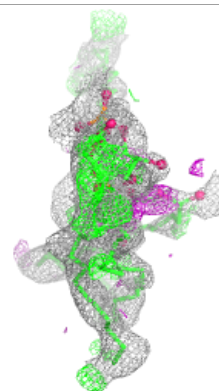
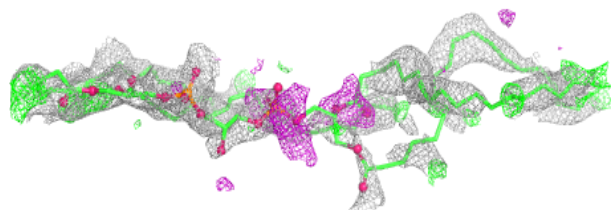
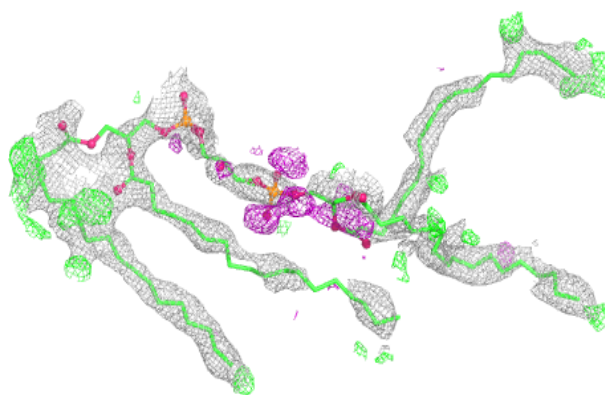
Electron density around PEK c 301:

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

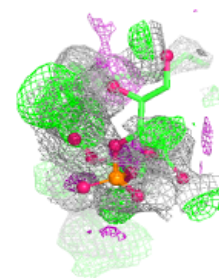
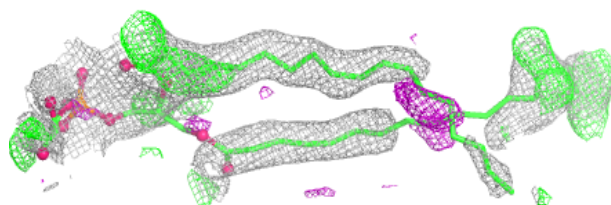
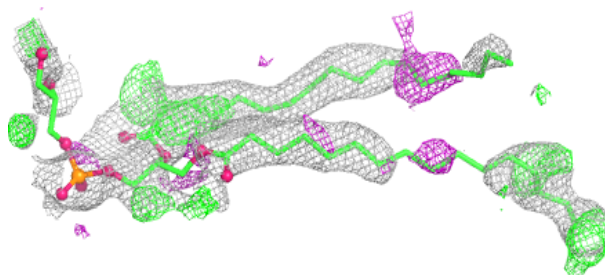


Electron density around CDL G 102:

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

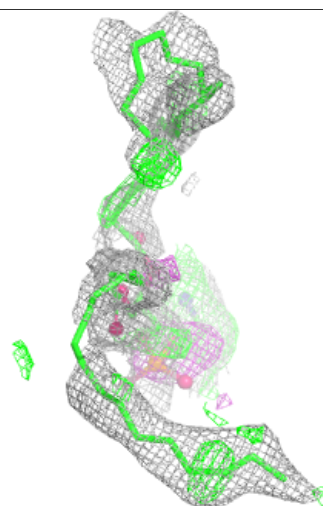
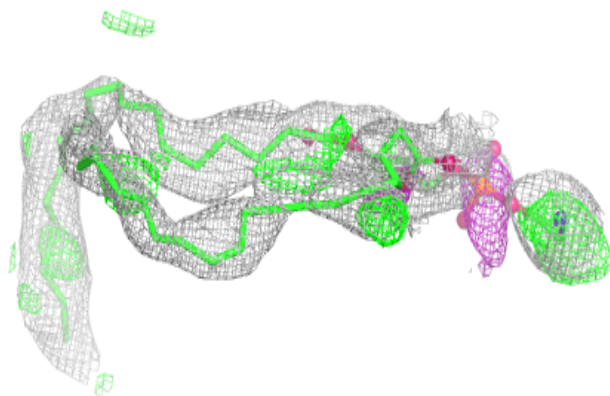
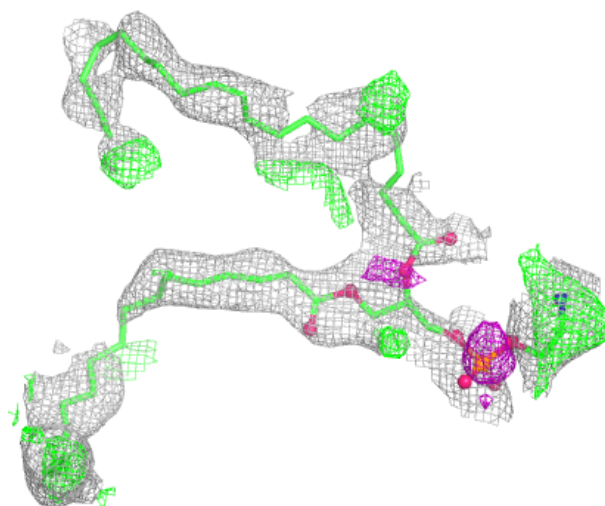
**Electron density around PGV A 606:**

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



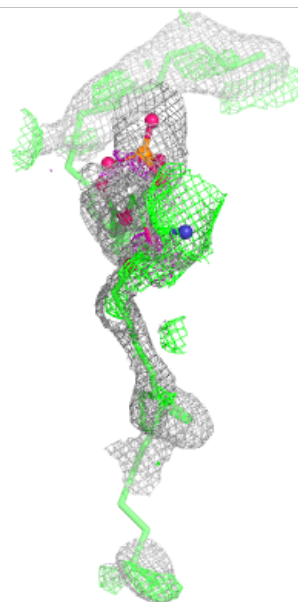
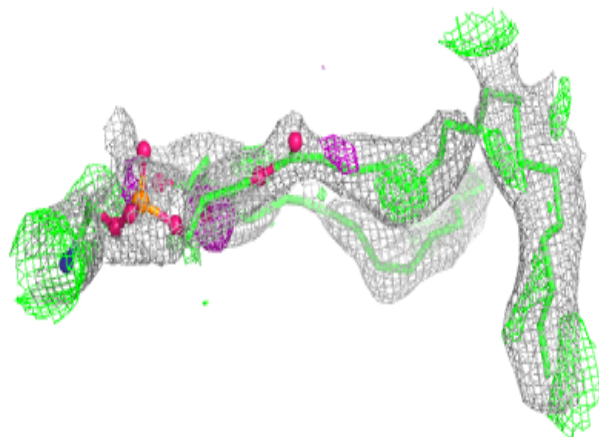
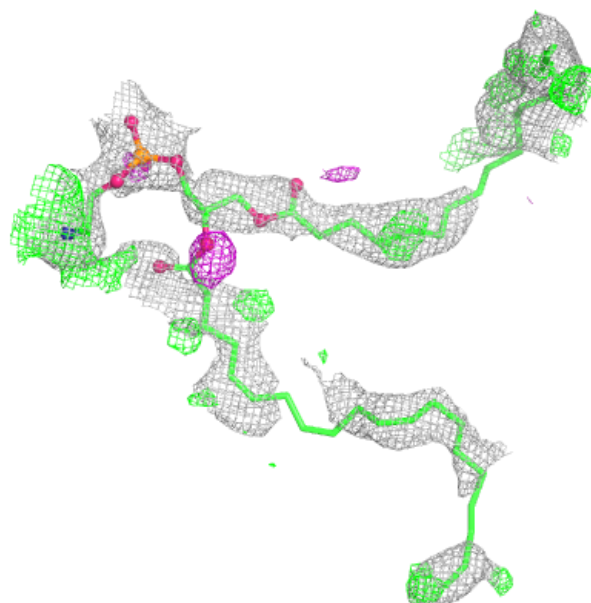
Electron density around PEK G 101:

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



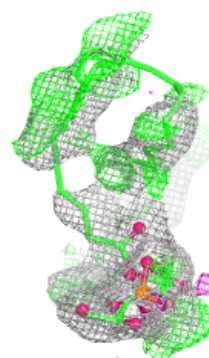
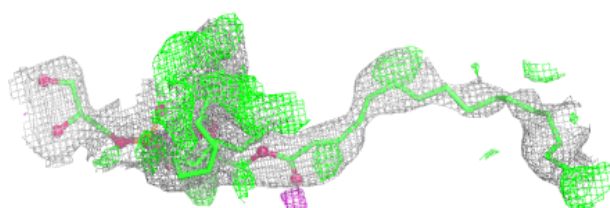
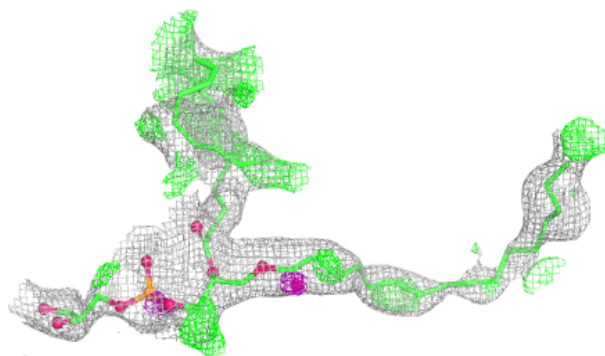
Electron density around PEK c 305:

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

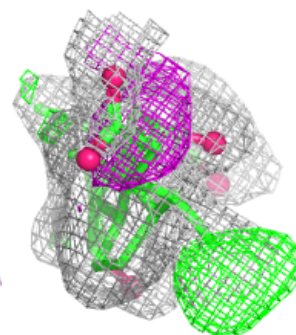
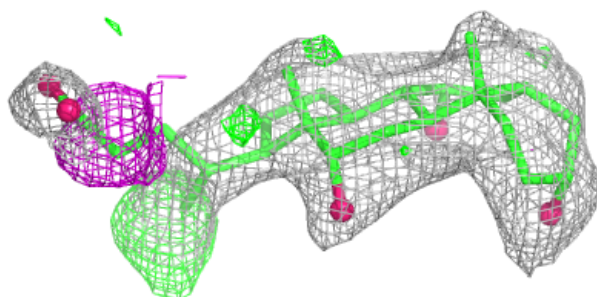
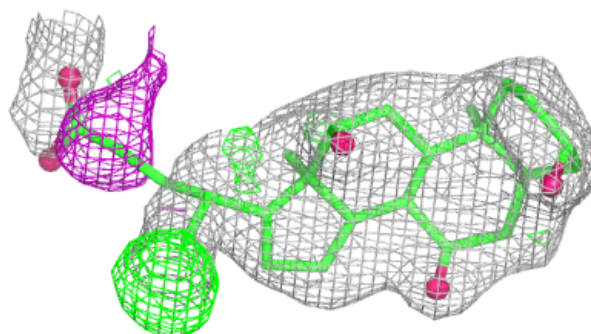


Electron density around PGV C 304:

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

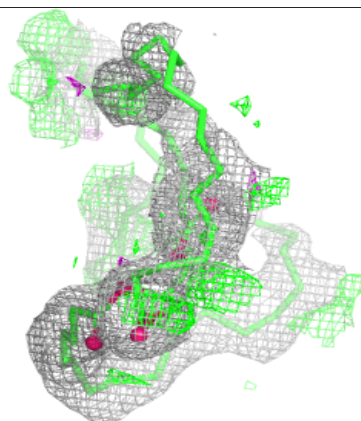
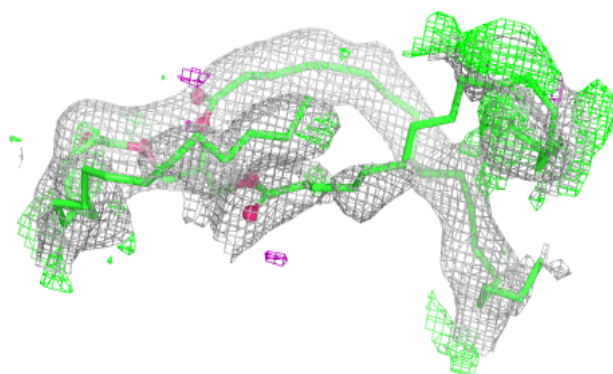
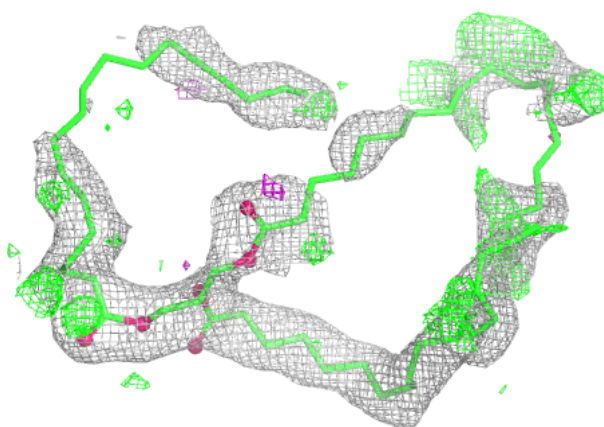
**Electron density around CHD J 101:**

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

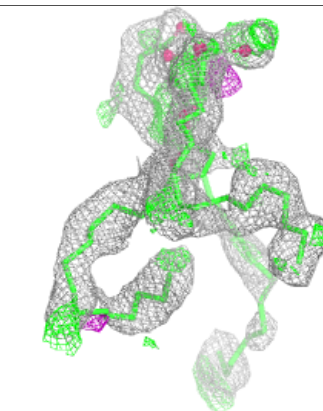
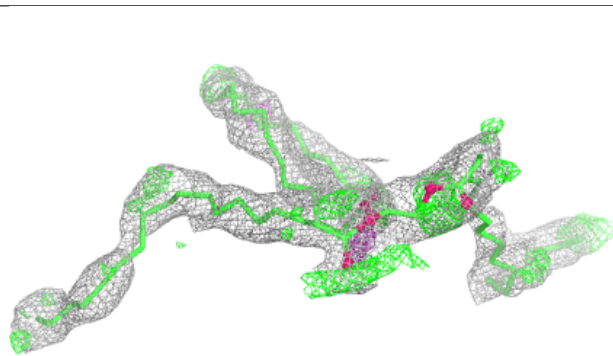
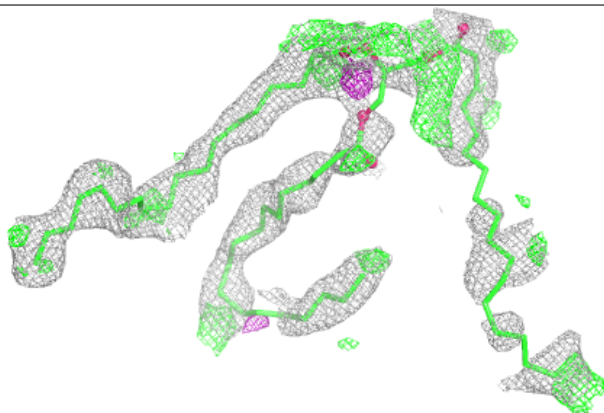


Electron density around TGL A 608:

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

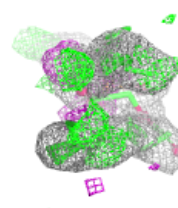
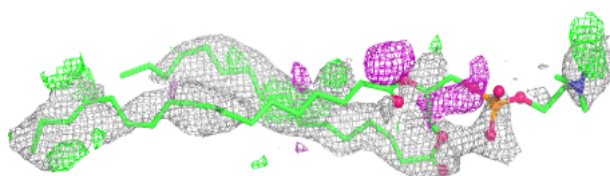
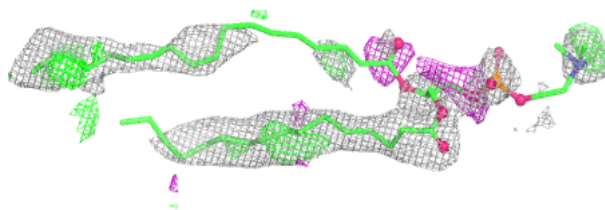
**Electron density around TGL d 201:**

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

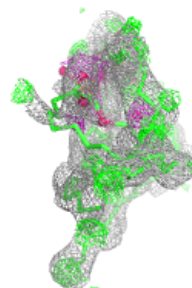
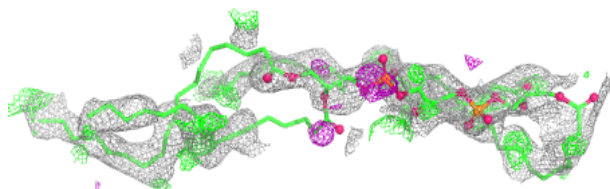
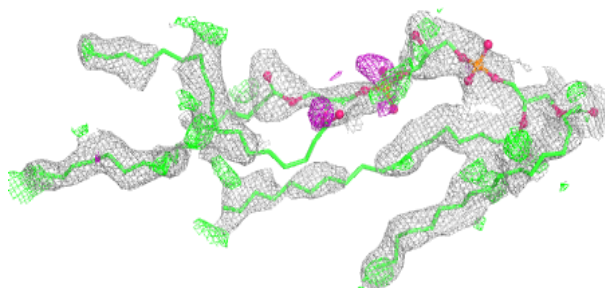


Electron density around PSC b 303:

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

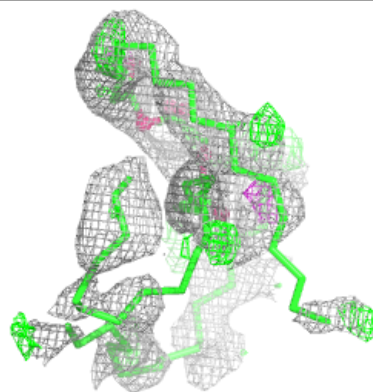
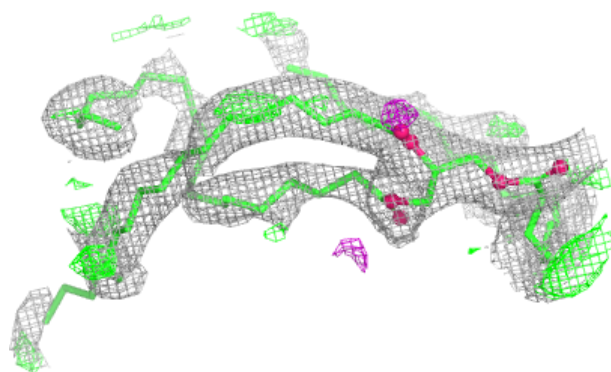
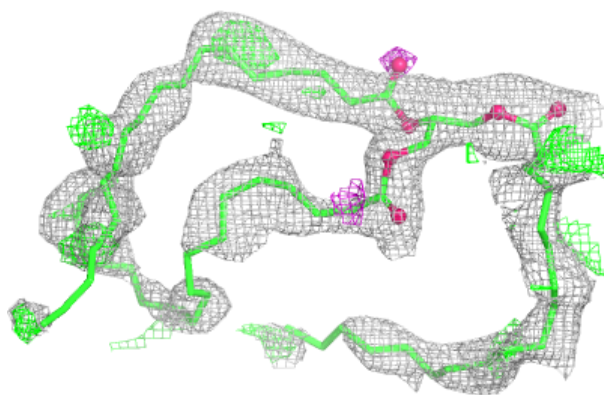
**Electron density around CDL g 101:**

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



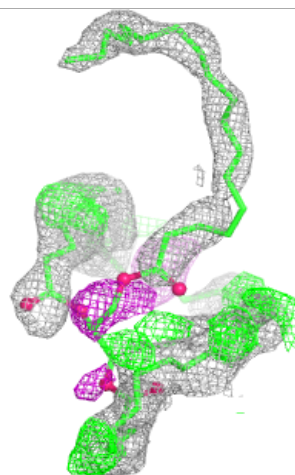
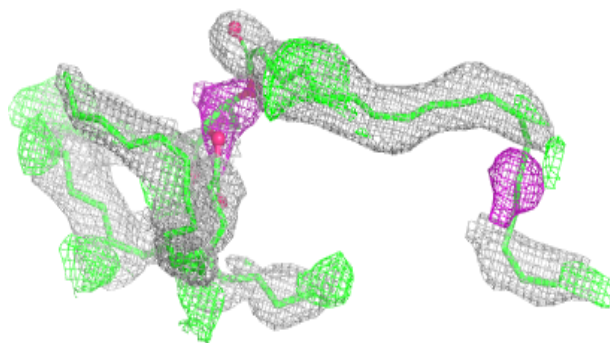
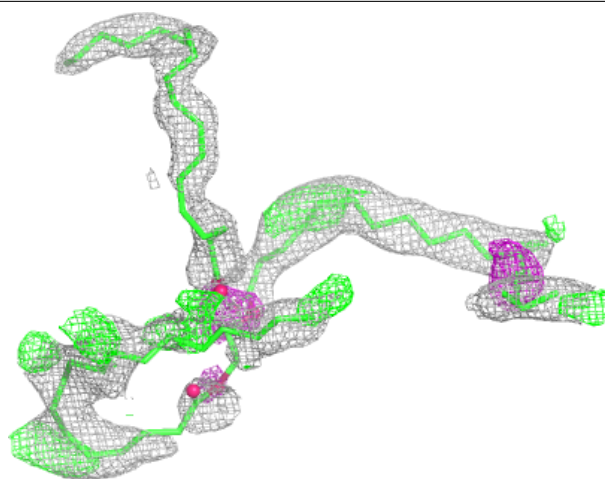
Electron density around TGL b 302:

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



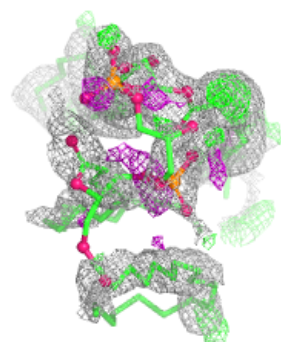
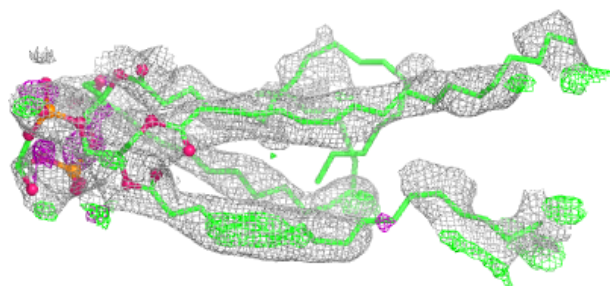
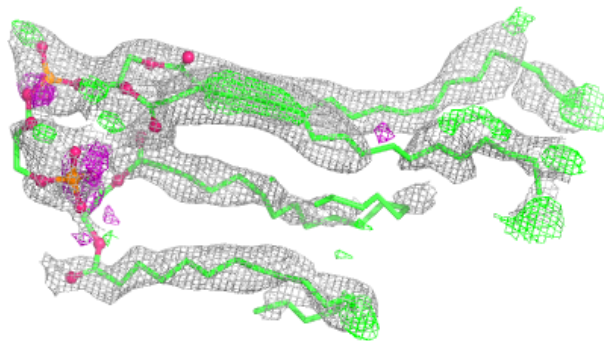
Electron density around TGL 1 101:

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



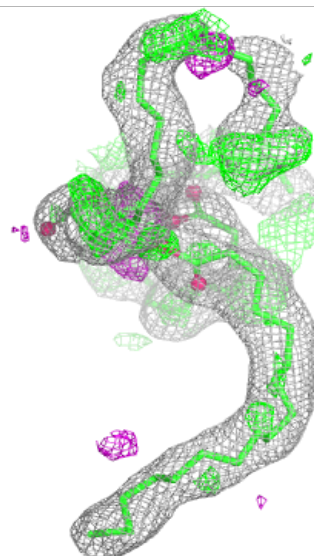
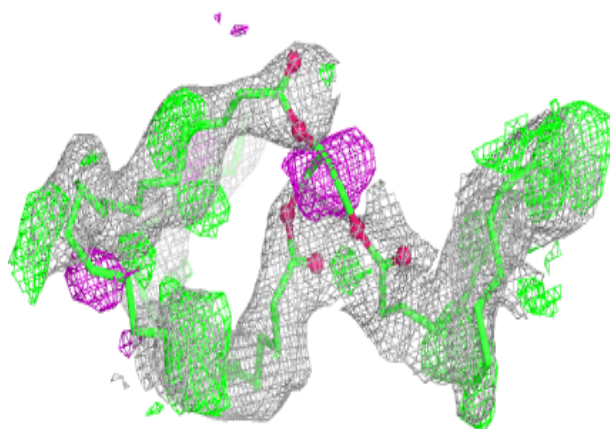
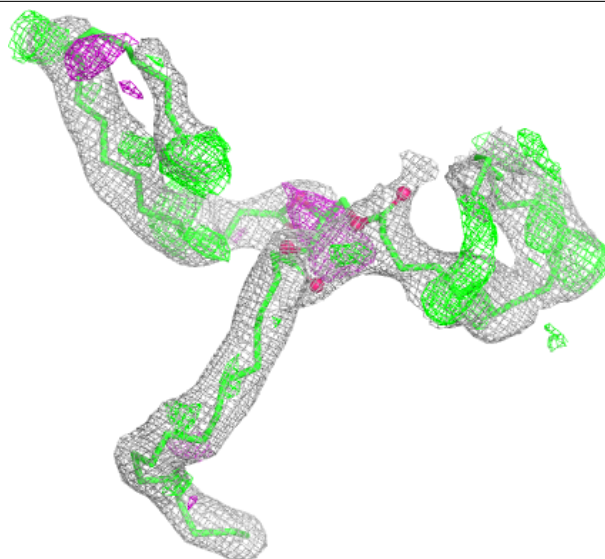
Electron density around CDL c 307:

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



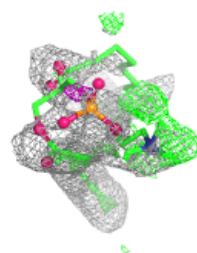
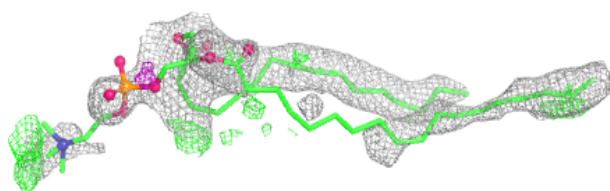
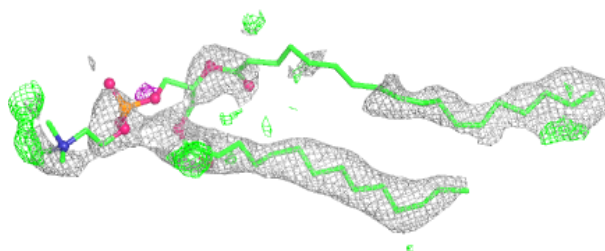
Electron density around TGL A 609:

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

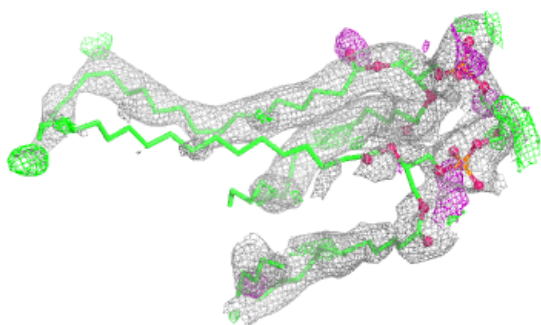
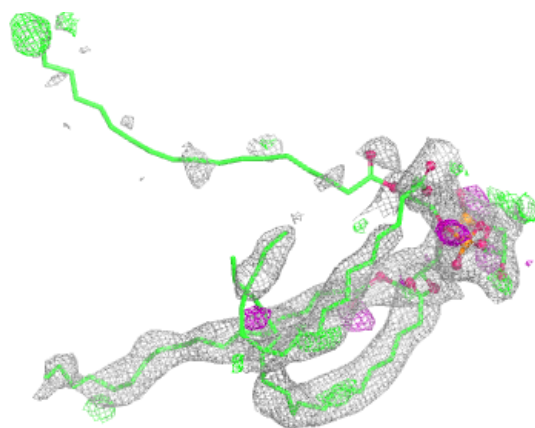


Electron density around PSC E 201:

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

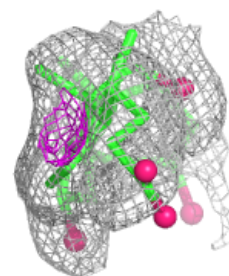
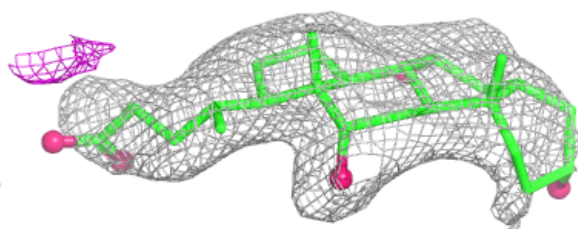
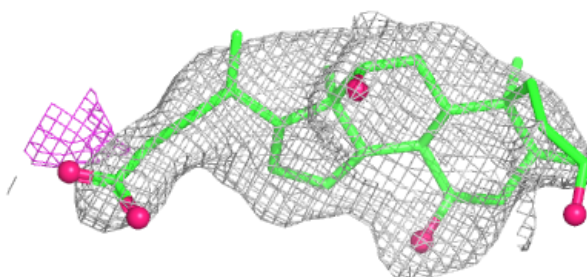
**Electron density around CDL C 305:**

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

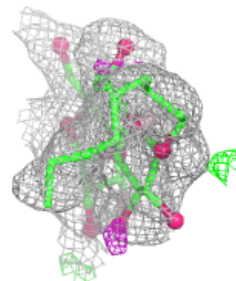
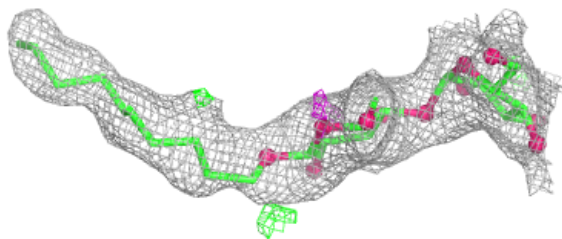
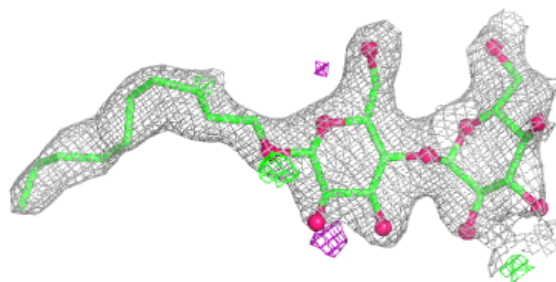


Electron density around CHD j 101:

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

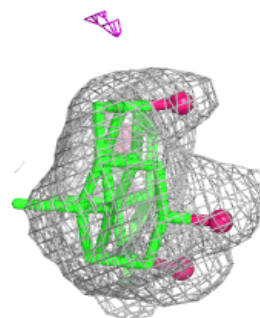
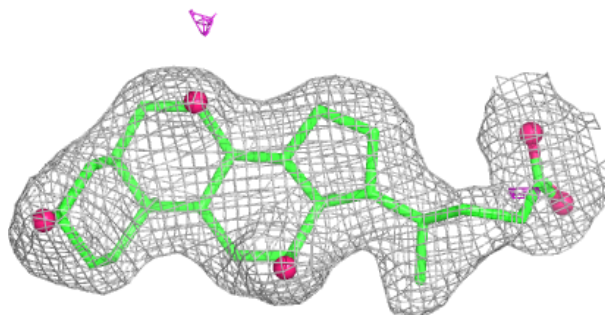
**Electron density around DMU m 101:**

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

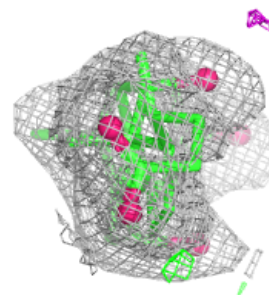
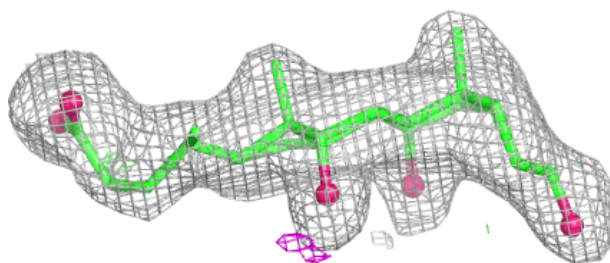
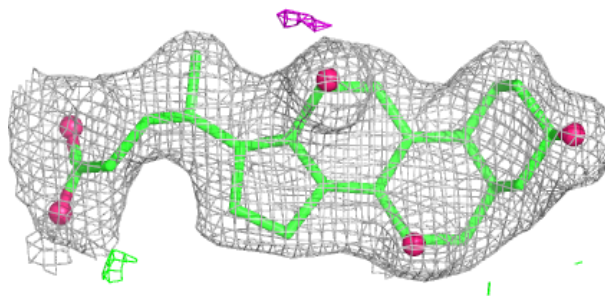


Electron density around CHD c 308:

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

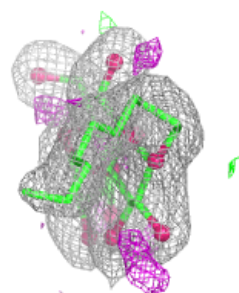
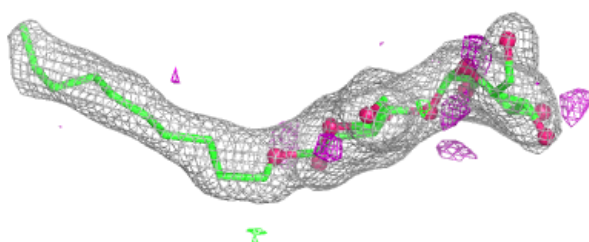
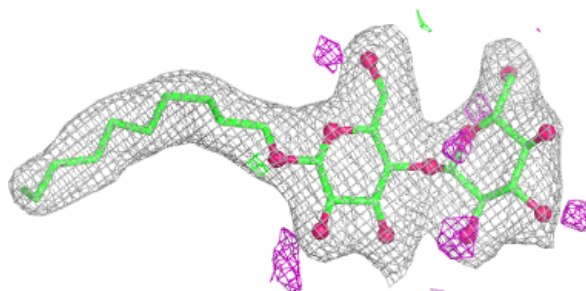
**Electron density around CHD C 306:**

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

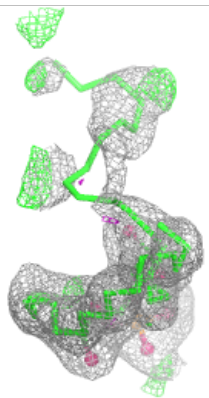
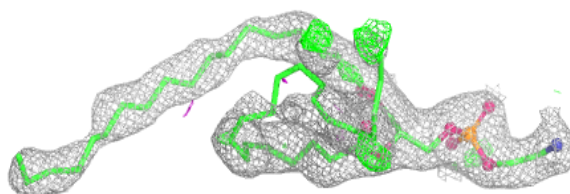
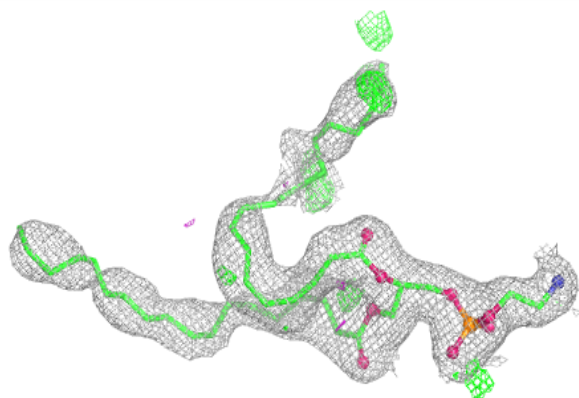


Electron density around DMU M 101:

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

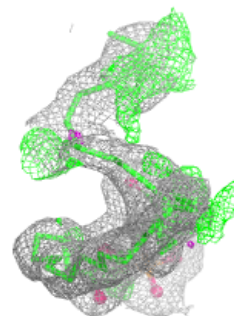
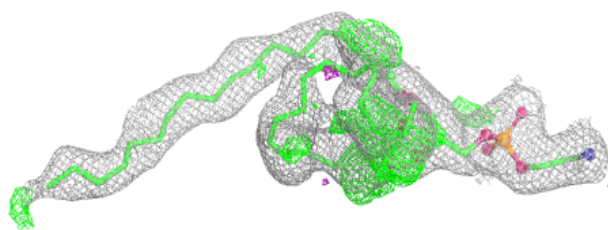
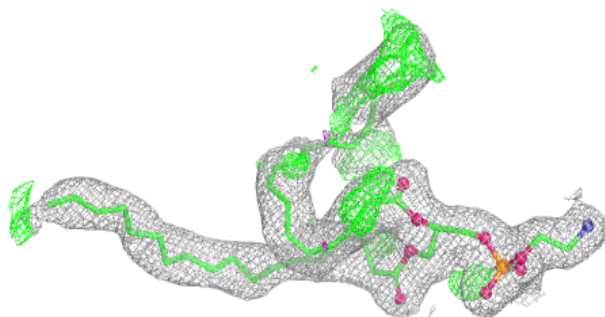
**Electron density around PEK c 304:**

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

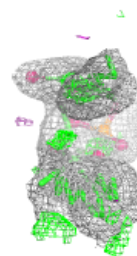
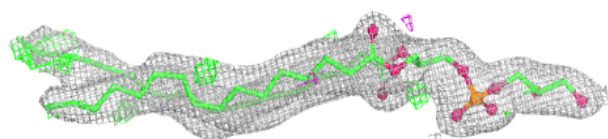
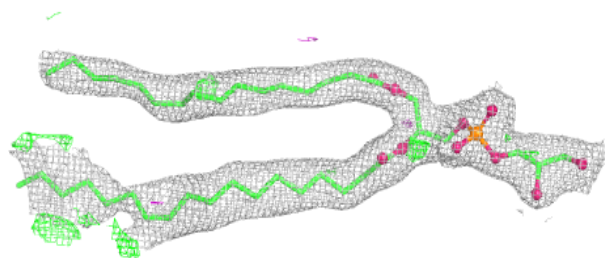


Electron density around PEK C 302:

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

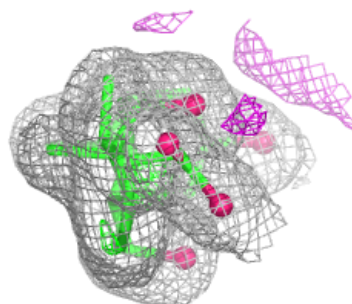
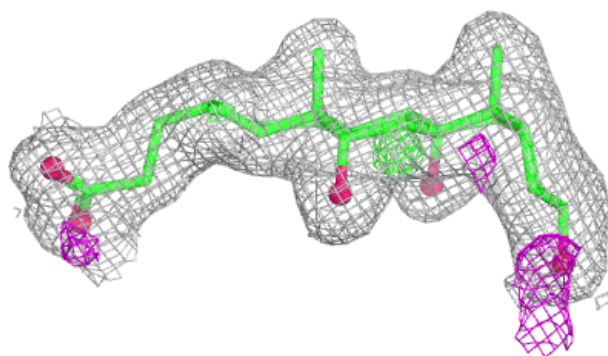
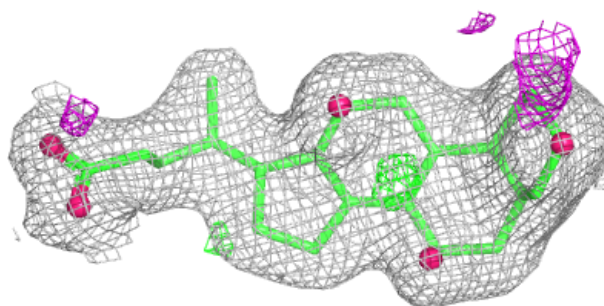
**Electron density around PGV c 306:**

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

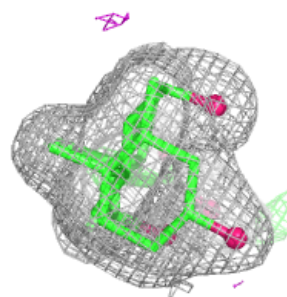
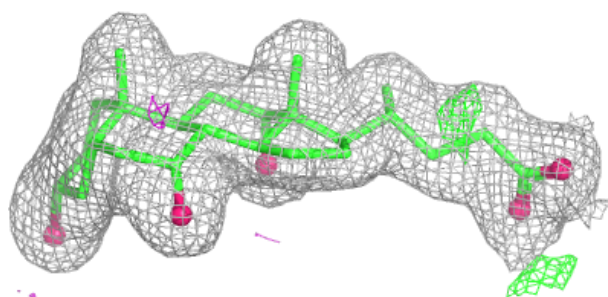
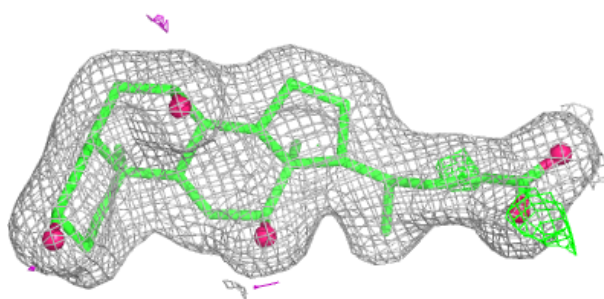


Electron density around CHD B 402:

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

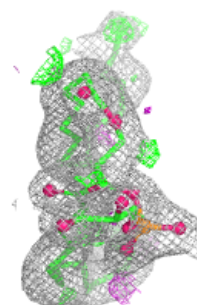
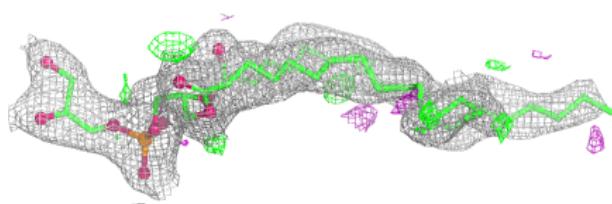
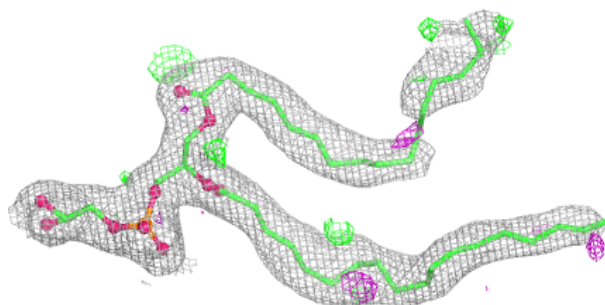
**Electron density around CHD C 301:**

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

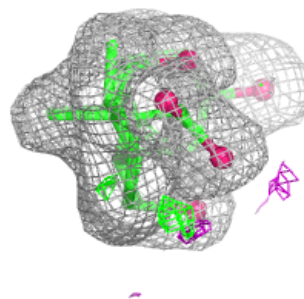
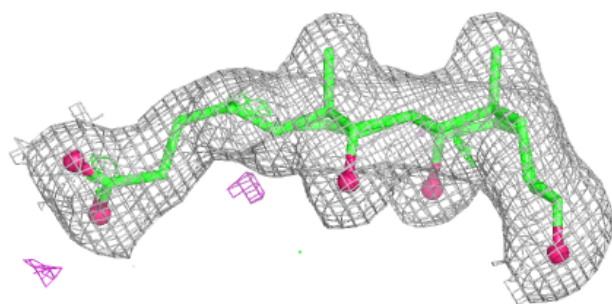
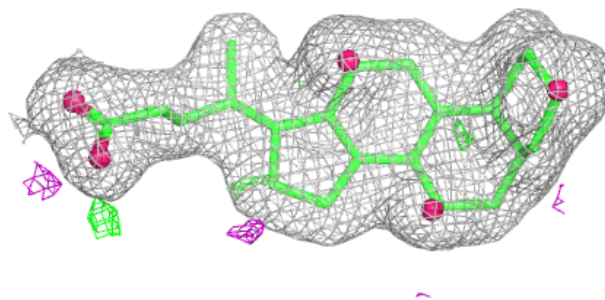


Electron density around PGV a 607:

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

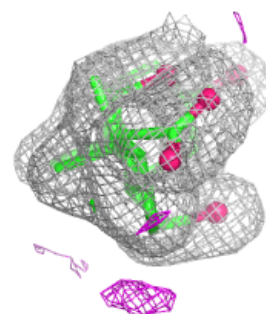
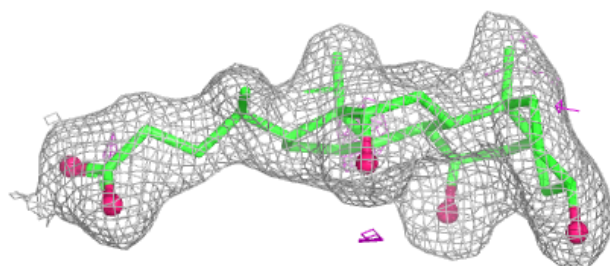
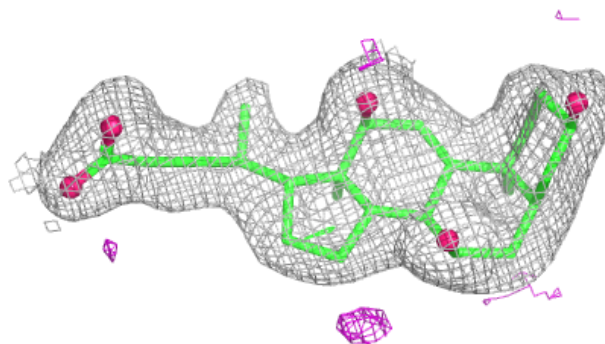
**Electron density around CHD G 103:**

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

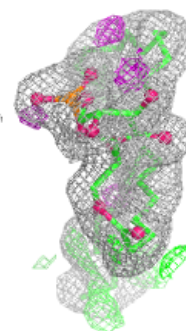
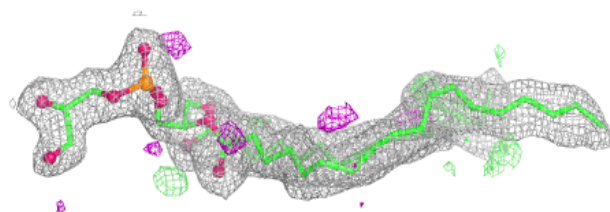
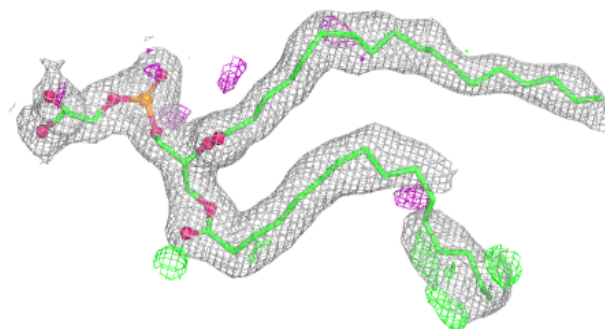


Electron density around CHD c 303:

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

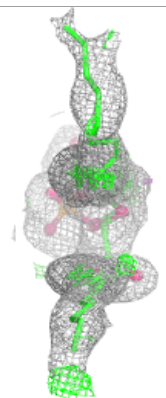
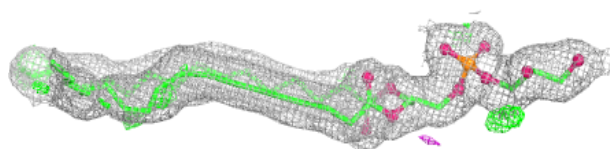
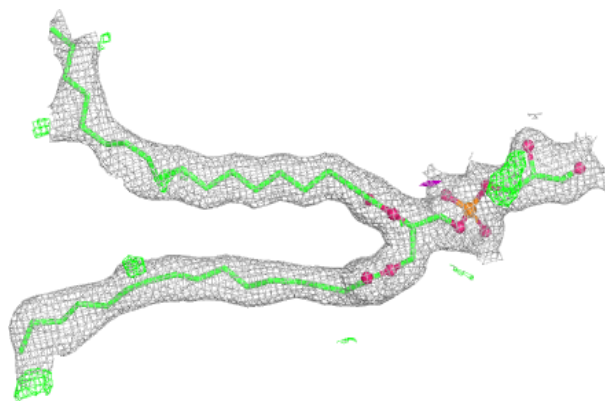
**Electron density around PGV A 607:**

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

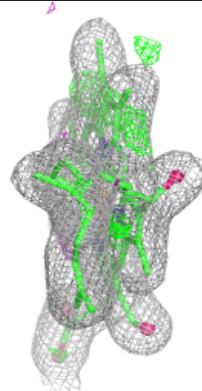
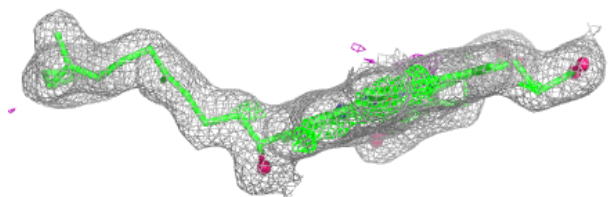
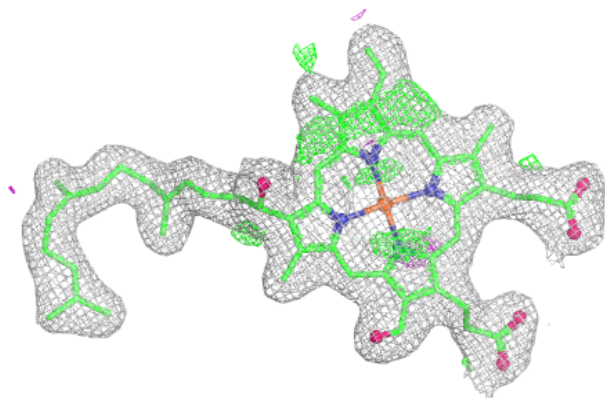


Electron density around PGV C 303:

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

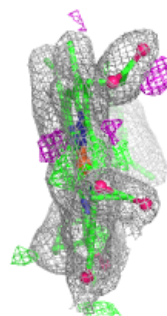
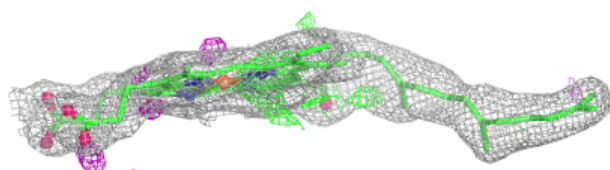
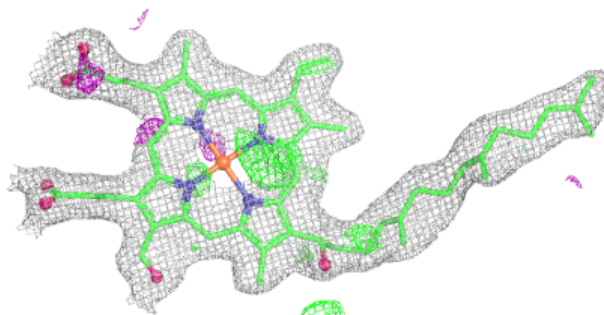
**Electron density around HEA a 602:**

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

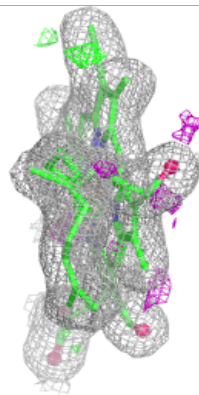
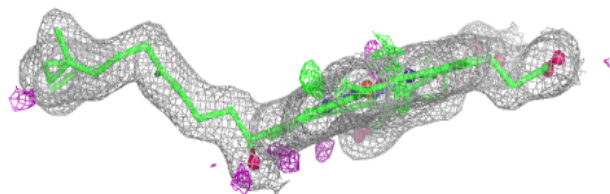
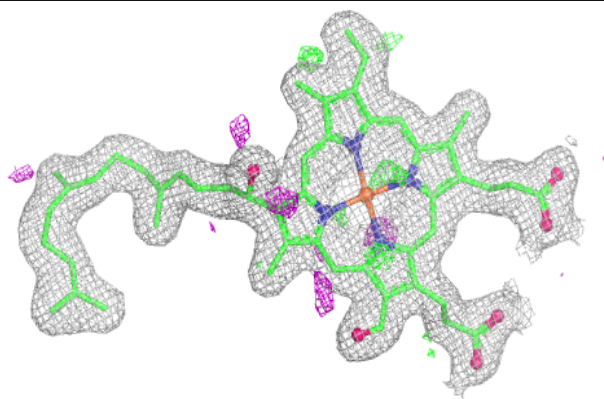


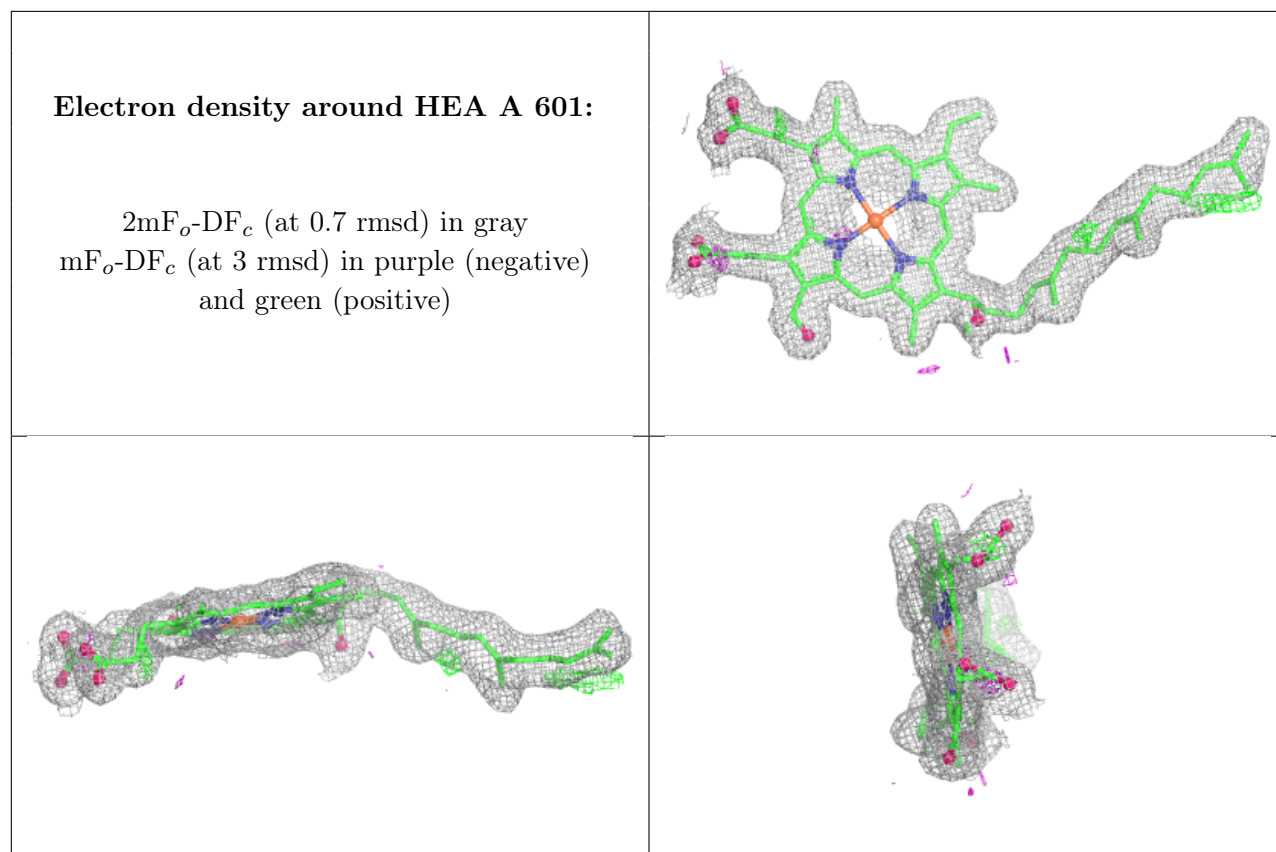
Electron density around HEA a 601:

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

**Electron density around HEA A 602:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.