



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:57 AM UTC

PDB ID : 5W97 / pdb_00005w97
Title : Crystal Structure of CO-bound Cytochrome c Oxidase determined by Serial Femtosecond X-Ray Crystallography at Room Temperature
Authors : Rousseau, D.L.; Yeh, S.-R.; Ishigami, I.; Zatsepin, N.A.; Grant, T.D.; Fromme, P.; Fromme, R.
Deposited on : 2017-06-22
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

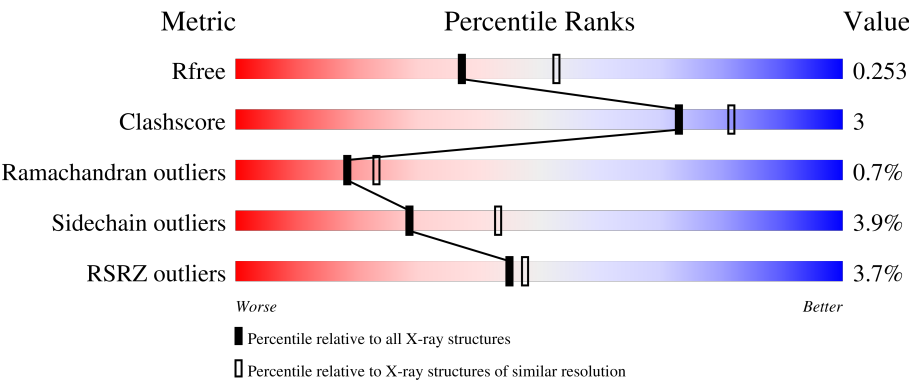
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



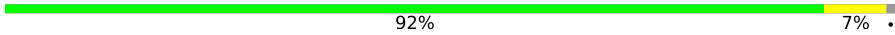
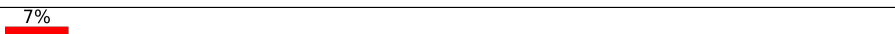
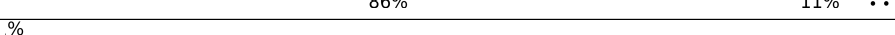
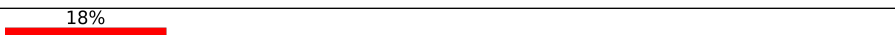
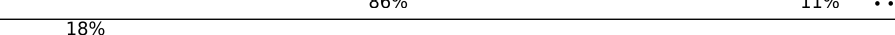
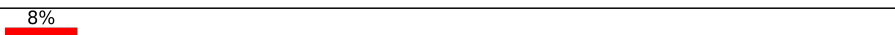
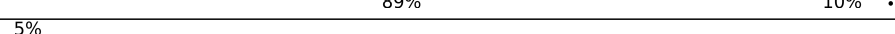
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	90%10%
1	a	514	% 87%12% .
2	B	227	% 83%16%
2	b	227	4% 87%12% .

Continued on next page...

Continued from previous page...

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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CMO	a	608	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32025 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 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	g	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

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

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

Continued on next page...

Continued from previous page...

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			

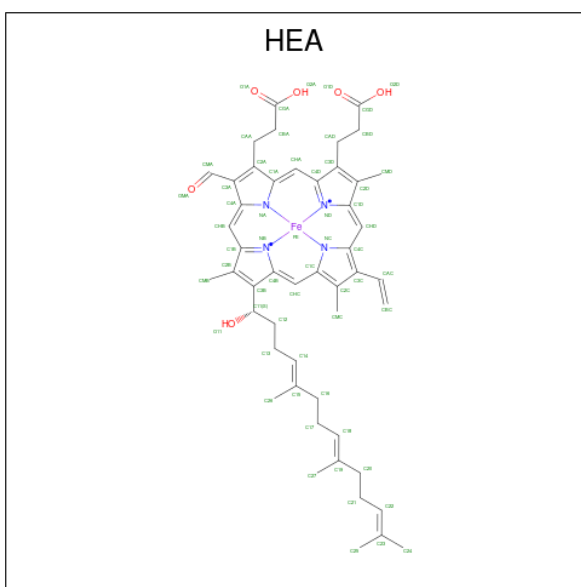
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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		

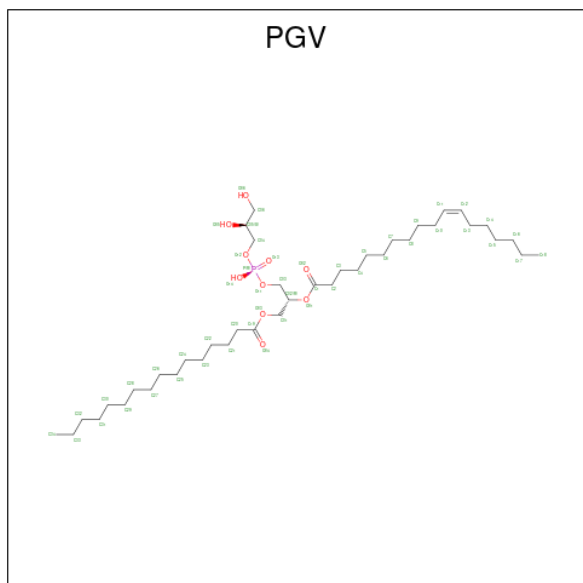
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

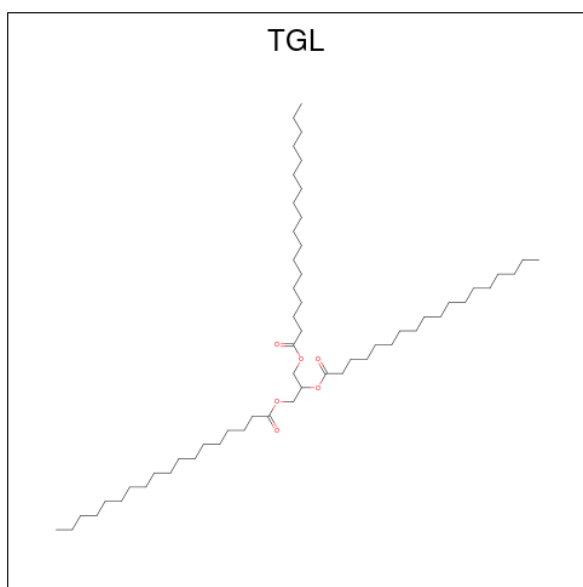
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	a	1	Total	Na	0	0
			1	1		

- 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).



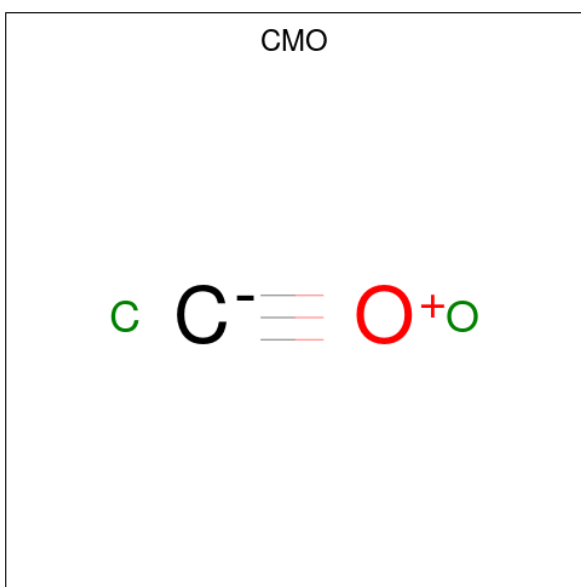
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	G	1	Total	C	O	P	0	0
			51	40	10	1		
18	a	1	Total	C	O	P	0	0
			51	40	10	1		
18	c	1	Total	C	O	P	0	0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



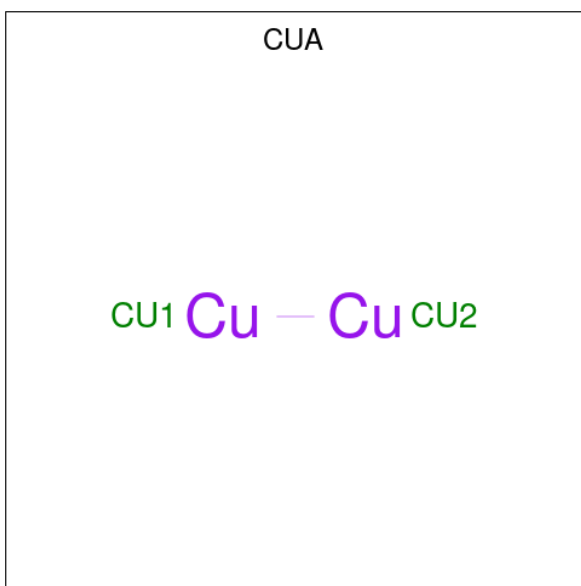
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	a	1	Total	C	O	0	0
			63	57	6		
19	i	1	Total	C	O	0	0
			63	57	6		
19	l	1	Total	C	O	0	0
			63	57	6		

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



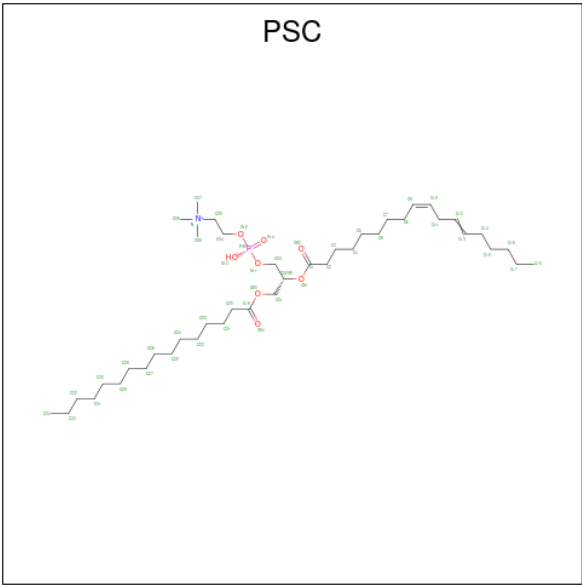
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			2	1	1		
20	a	1	Total	C	O	0	0
			2	1	1		

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



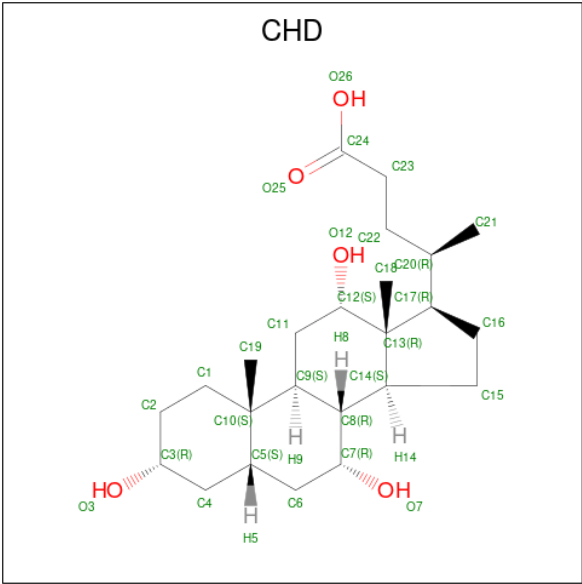
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	b	1	Total	Cu	0	0
			2	2		

- Molecule 22 is (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).



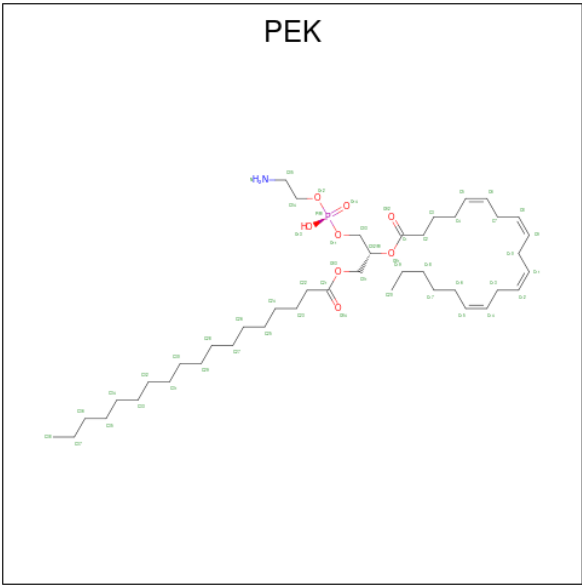
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
22	e	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



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

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



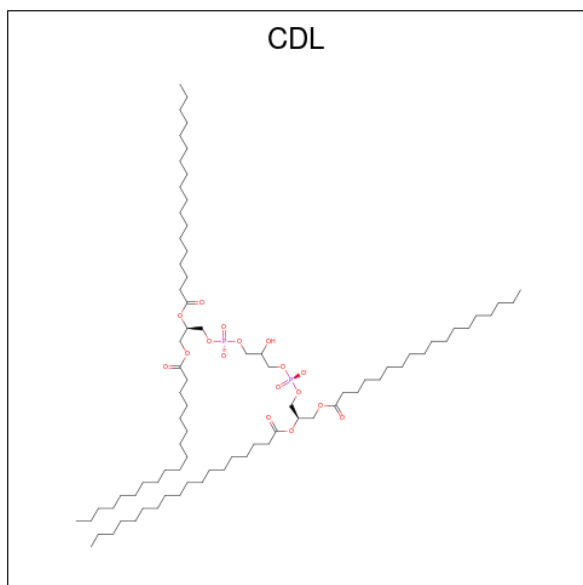
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

Continued on next page...

Continued from previous page...

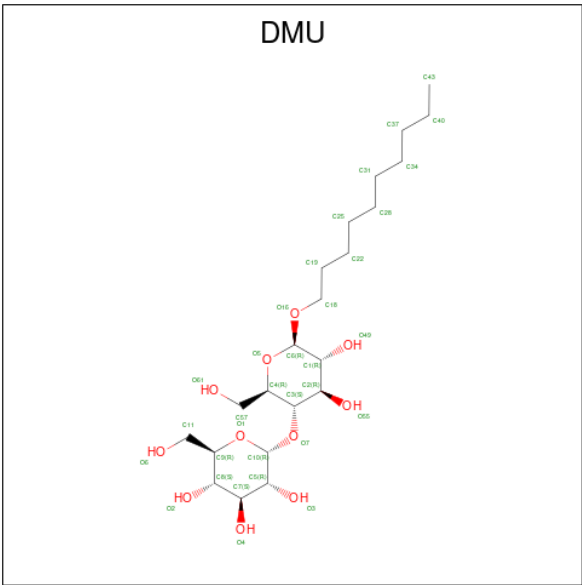
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	g	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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



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

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



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

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

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	197	Total	O	0	0
			197	197		
28	B	120	Total	O	0	0
			120	120		
28	C	81	Total	O	0	0
			81	81		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	D	85	Total 85	O 85	0	0
28	E	51	Total 51	O 51	0	0
28	F	66	Total 66	O 66	0	0
28	G	51	Total 51	O 51	0	0
28	H	33	Total 33	O 33	0	0
28	I	33	Total 33	O 33	0	0
28	J	26	Total 26	O 26	0	0
28	K	30	Total 30	O 30	0	0
28	L	35	Total 35	O 35	0	0
28	M	22	Total 22	O 22	0	0
28	a	140	Total 140	O 140	0	0
28	b	63	Total 63	O 63	0	0
28	c	59	Total 59	O 59	0	0
28	d	25	Total 25	O 25	0	0
28	e	36	Total 36	O 36	0	0
28	f	29	Total 29	O 29	0	0
28	g	29	Total 29	O 29	0	0
28	h	24	Total 24	O 24	0	0
28	i	14	Total 14	O 14	0	0
28	j	8	Total 8	O 8	0	0
28	k	8	Total 8	O 8	0	0

Continued on next page...

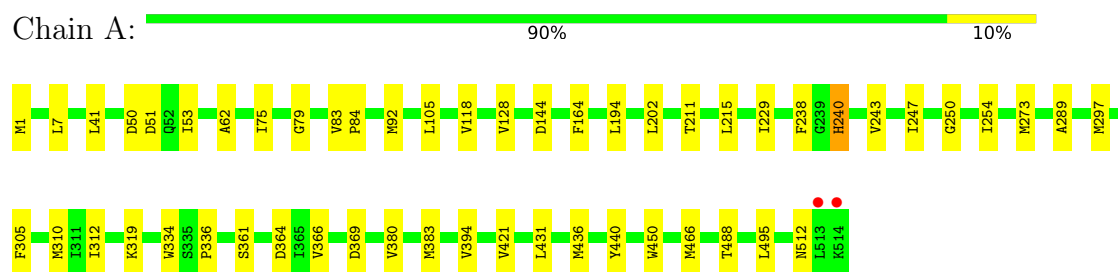
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	l	19	Total 19	O 19	0	0
28	m	7	Total 7	O 7	0	0

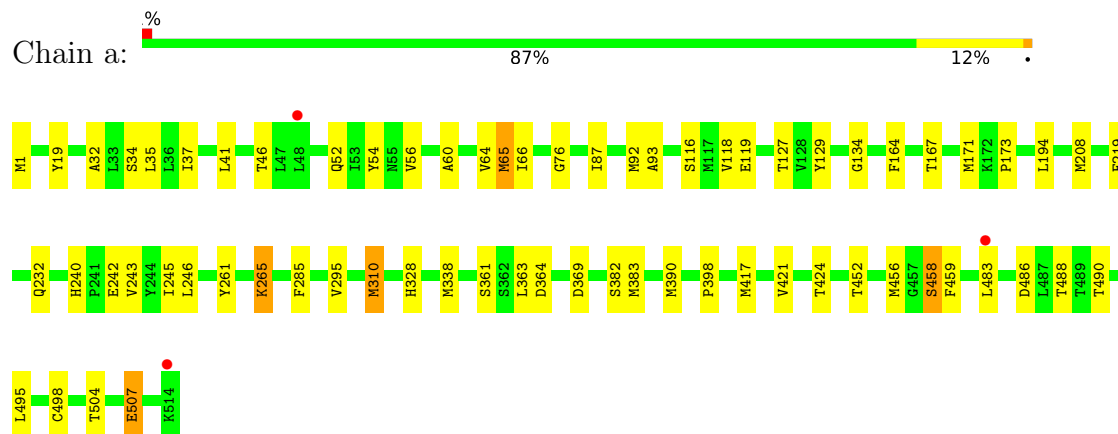
3 Residue-property plots

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

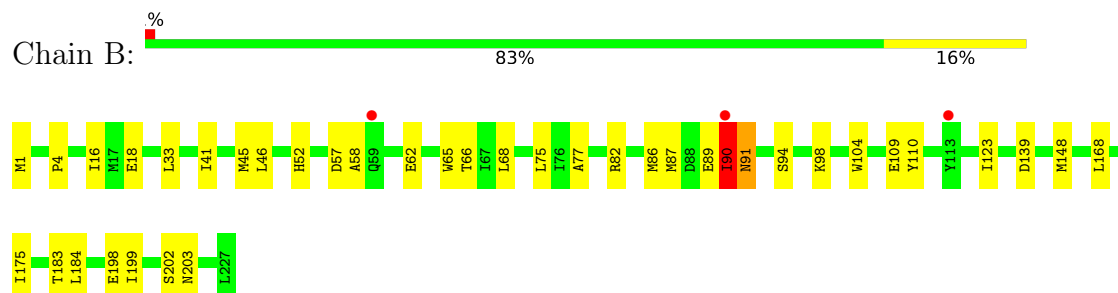
• Molecule 1: Cytochrome c oxidase subunit 1



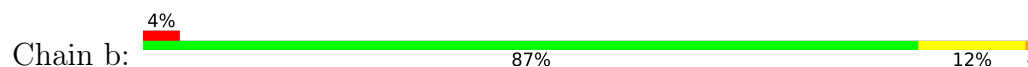
• Molecule 1: Cytochrome c oxidase subunit 1

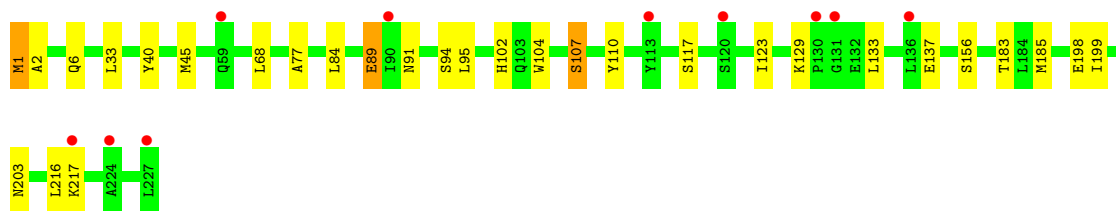


• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2





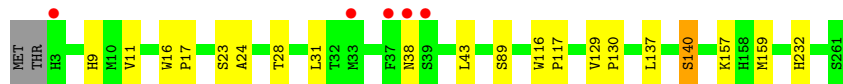
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 92% 7% .



- Molecule 3: Cytochrome c oxidase subunit 3

Chain c: 92% 7% .



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

Chain D: 88% 10% .



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

Chain d: 86% 11% ..



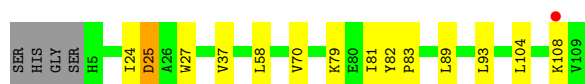
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E: 85% 10% ..

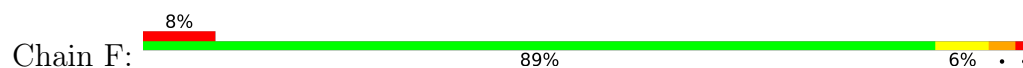


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

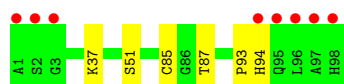
Chain e: 83% 12% ..



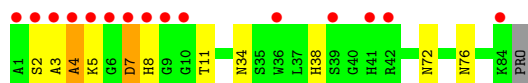
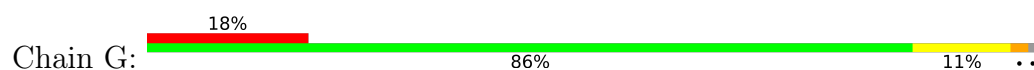
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



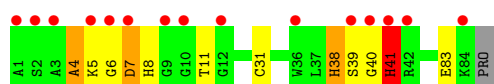
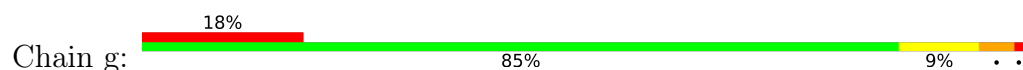
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



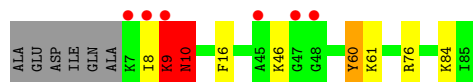
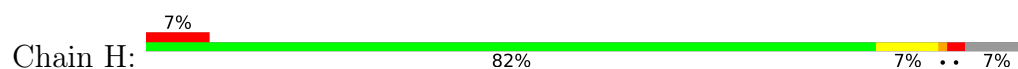
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



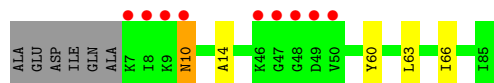
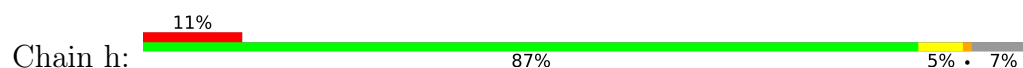
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



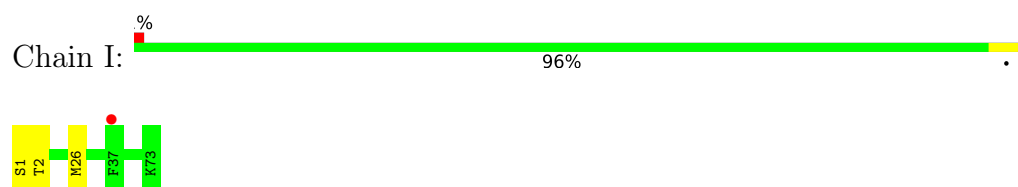
- Molecule 8: Cytochrome c oxidase subunit 6B1



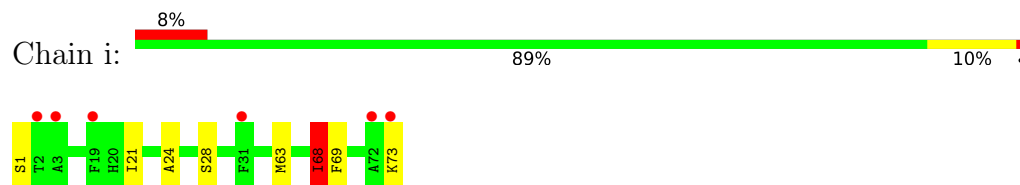
- Molecule 8: Cytochrome c oxidase subunit 6B1



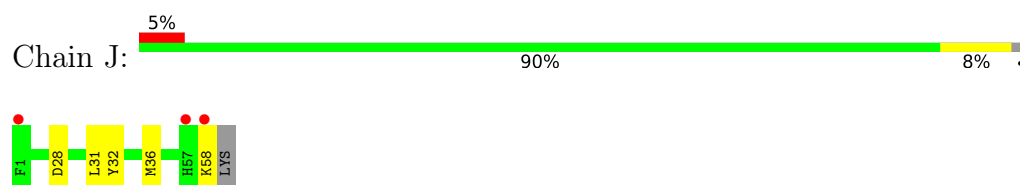
- Molecule 9: Cytochrome c oxidase subunit 6C



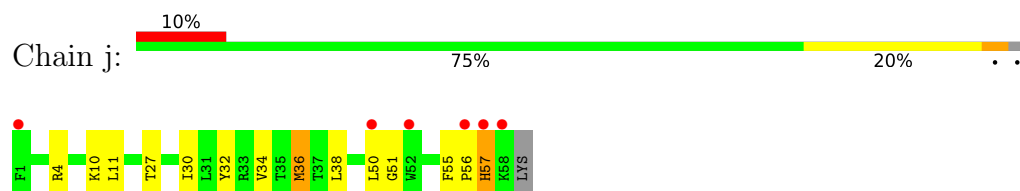
• Molecule 9: Cytochrome c oxidase subunit 6C



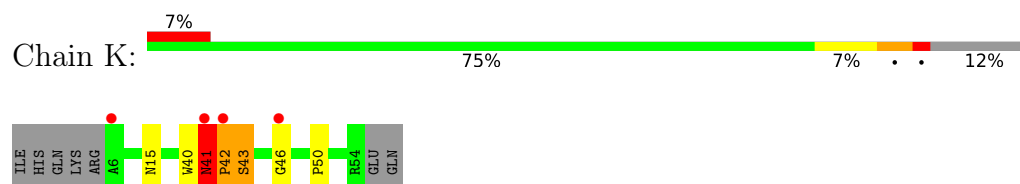
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



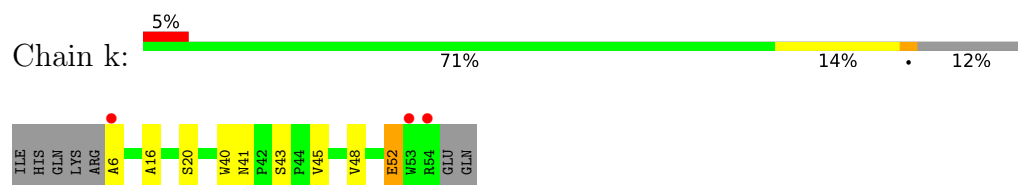
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



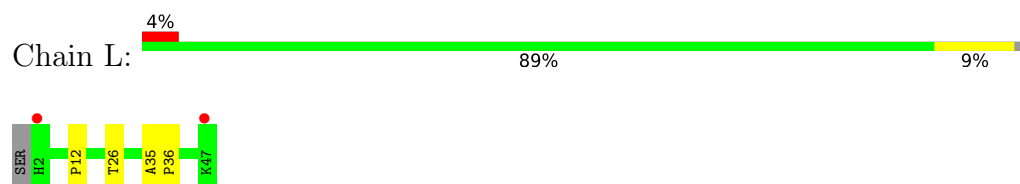
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



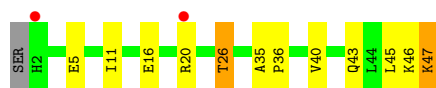
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



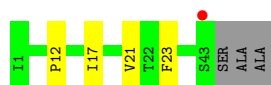
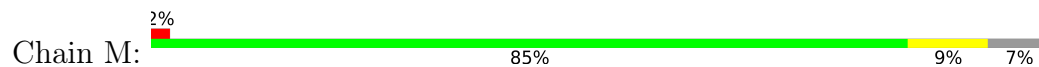
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



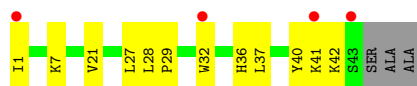
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	178.30Å 189.00Å 209.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.30 29.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.86-2.30) 99.9 (29.86-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.208 , 0.252 0.215 , 0.253	Depositor DCC
R_{free} test set	2994 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32025	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: PSC, PGV, MG, ZN, CU, CDL, FME, CUA, SAC, TGL, CHD, CMO, NA, TPO, HEA, PEK, DMU

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	0.95	1/4156 (0.0%)	1.03	6/5678 (0.1%)
1	a	0.87	1/4156 (0.0%)	1.01	2/5678 (0.0%)
2	B	0.97	1/1860 (0.1%)	1.05	2/2534 (0.1%)
2	b	0.88	1/1860 (0.1%)	1.00	1/2534 (0.0%)
3	C	0.91	1/2197 (0.0%)	0.96	1/3005 (0.0%)
3	c	0.83	0/2197	0.94	0/3005
4	D	0.86	0/1229	0.92	1/1658 (0.1%)
4	d	0.77	0/1229	0.97	2/1658 (0.1%)
5	E	0.82	0/871	0.96	0/1182
5	e	0.75	0/871	0.96	1/1182 (0.1%)
6	F	1.02	0/765	1.09	2/1038 (0.2%)
6	f	0.80	0/765	0.96	0/1038
7	G	0.94	1/690 (0.1%)	0.93	1/937 (0.1%)
7	g	0.89	0/690	0.92	0/937
8	H	0.90	0/682	1.10	1/921 (0.1%)
8	h	0.88	0/682	1.01	0/921
9	I	0.84	0/605	0.98	0/802
9	i	0.79	0/605	0.98	0/802
10	J	0.82	0/471	1.01	0/636
10	j	0.89	0/471	0.96	0/636
11	K	1.02	1/398 (0.3%)	1.70	4/546 (0.7%)
11	k	0.88	0/398	1.12	2/546 (0.4%)
12	L	0.95	1/393 (0.3%)	0.97	0/526
12	l	0.80	0/393	0.93	0/526
13	M	0.89	0/345	1.01	0/470
13	m	0.77	0/345	1.04	0/470
All	All	0.89	8/29324 (0.0%)	1.01	26/39866 (0.1%)

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
4	d	0	1
6	F	0	1
7	g	0	1
8	H	0	2
8	h	0	1
10	j	0	1
11	K	0	4
All	All	0	11

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	11.10	1.36	1.23
2	b	198	GLU	C-O	10.50	1.36	1.23
1	A	240	HIS	N-CA	-5.74	1.41	1.46
12	L	12	PRO	CA-C	5.52	1.57	1.52
1	a	240	HIS	C-O	-5.38	1.19	1.24
7	G	4	ALA	CA-C	5.30	1.59	1.52
11	K	41	ASN	C-O	5.04	1.29	1.24
3	C	10	MET	C-O	-5.03	1.17	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	41	ASN	CA-C-N	-20.18	93.00	120.25
11	K	41	ASN	C-N-CA	-20.18	93.00	120.25
3	C	152	MET	CG-SD-CE	7.73	117.90	100.90
1	A	105	LEU	CA-C-N	-6.83	113.34	120.38
1	A	105	LEU	C-N-CA	-6.83	113.34	120.38
1	A	436	MET	CA-C-N	-6.43	114.04	120.21
1	A	436	MET	C-N-CA	-6.43	114.04	120.21
7	G	7	ASP	N-CA-C	6.07	117.75	108.52
6	F	87	THR	N-CA-CB	5.96	118.76	110.17
1	A	240	HIS	N-CA-CB	5.91	117.39	110.42
2	B	202	SER	N-CA-C	5.90	118.47	111.33
6	F	92	VAL	CB-CA-C	5.83	116.62	111.08
11	k	6	ALA	CA-C-N	5.68	125.44	119.76
11	k	6	ALA	C-N-CA	5.68	125.44	119.76
2	b	89	GLU	N-CA-C	5.53	117.21	110.41
4	d	102	TYR	N-CA-C	5.50	119.69	112.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	43	SER	N-CA-CB	5.48	120.13	110.37
1	a	424	THR	CB-CA-C	-5.32	102.53	110.88
11	K	41	ASN	O-C-N	5.25	126.06	120.92
4	D	133	GLY	N-CA-C	5.22	118.81	112.49
2	B	199	ILE	N-CA-CB	5.17	116.43	110.49
1	a	507	GLU	N-CA-C	-5.17	101.19	109.04
4	d	133	GLY	N-CA-C	5.15	120.27	113.37
5	e	25	ASP	N-CA-CB	-5.11	102.30	110.63
1	A	380	VAL	N-CA-C	5.06	115.83	110.72
8	H	10	ASN	N-CA-C	5.04	121.54	110.80

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	92	VAL	Peptide
8	H	10	ASN	Peptide
8	H	9	LYS	Peptide
11	K	40	TRP	Peptide
11	K	41	ASN	Peptide
11	K	42	PRO	Peptide
11	K	46	GLY	Peptide
4	d	7	LYS	Peptide
7	g	83	GLU	Peptide
8	h	10	ASN	Peptide
10	j	55	PHE	Peptide

5.2 Too-close contacts [i](#)

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	32	0
1	a	4027	0	4001	44	0
2	B	1824	0	1833	20	0
2	b	1824	0	1833	16	0
3	C	2110	0	2027	17	0
3	c	2110	0	2027	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1195	0	1183	8	0
4	d	1195	0	1183	6	0
5	E	852	0	845	5	0
5	e	852	0	845	4	0
6	F	748	0	728	6	0
6	f	748	0	728	2	0
7	G	675	0	643	5	0
7	g	675	0	643	5	0
8	H	662	0	623	3	0
8	h	662	0	623	1	0
9	I	601	0	613	0	0
9	i	601	0	613	4	0
10	J	460	0	459	2	0
10	j	460	0	459	3	0
11	K	384	0	366	5	0
11	k	384	0	366	5	0
12	L	380	0	380	1	0
12	l	380	0	380	7	0
13	M	335	0	352	4	0
13	m	335	0	352	6	0
14	A	120	0	108	5	0
14	a	120	0	108	5	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	2	0
18	C	102	0	152	1	0
18	G	51	0	76	0	0
18	a	51	0	76	0	0
18	c	102	0	152	0	0
19	A	63	0	110	0	0
19	D	63	0	110	0	0
19	L	63	0	110	0	0
19	a	63	0	110	0	0
19	i	63	0	110	0	0
19	l	63	0	110	0	0
20	A	2	0	0	0	0
20	a	2	0	0	2	0
21	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	b	2	0	0	0	0
22	B	52	0	80	0	0
22	e	52	0	80	0	0
23	B	29	0	39	1	0
23	C	58	0	78	1	0
23	J	29	0	39	0	0
23	b	29	0	39	1	0
23	c	58	0	78	2	0
23	j	29	0	39	0	0
24	C	159	0	231	3	0
24	G	53	0	77	0	0
24	c	53	0	77	0	0
24	g	53	0	77	0	0
25	C	100	0	156	0	0
25	G	100	0	156	0	0
25	c	100	0	156	0	0
25	g	100	0	156	1	0
26	C	33	0	42	1	0
26	M	33	0	42	0	0
26	c	33	0	42	0	0
26	m	33	0	42	1	0
27	F	1	0	0	0	0
27	f	1	0	0	0	0
28	A	197	0	0	1	0
28	B	120	0	0	1	0
28	C	81	0	0	1	0
28	D	85	0	0	2	0
28	E	51	0	0	0	0
28	F	66	0	0	1	0
28	G	51	0	0	0	0
28	H	33	0	0	0	0
28	I	33	0	0	0	0
28	J	26	0	0	0	0
28	K	30	0	0	1	0
28	L	35	0	0	0	0
28	M	22	0	0	0	0
28	a	140	0	0	1	0
28	b	63	0	0	0	0
28	c	59	0	0	1	0
28	d	25	0	0	0	0
28	e	36	0	0	0	0
28	f	29	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	g	29	0	0	0	0
28	h	24	0	0	0	0
28	i	14	0	0	0	0
28	j	8	0	0	0	0
28	k	8	0	0	0	0
28	l	19	0	0	0	0
28	m	7	0	0	0	0
All	All	32025	0	31316	199	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 3.

All (199) 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)
3:C:152:MET:HE2	3:C:232:HIS:NE2	1.63	1.12
1:A:273:MET:HE1	1:A:319:LYS:HA	1.51	0.93
3:C:152:MET:CE	3:C:232:HIS:NE2	2.35	0.90
2:B:89:GLU:O	2:B:91:ASN:ND2	2.09	0.85
1:A:273:MET:HE2	1:A:273:MET:HA	1.58	0.84
5:E:56:ARG:HH21	5:E:59:ASN:HD22	1.26	0.82
7:G:72:ASN:H	7:G:76:ASN:HD22	1.27	0.82
1:a:167:THR:HG23	1:a:171:MET:HE3	1.59	0.82
3:C:148:HIS:NE2	3:C:152:MET:CE	2.45	0.79
1:a:167:THR:HG23	1:a:171:MET:CE	2.13	0.78
3:C:148:HIS:NE2	3:C:152:MET:HE3	2.00	0.77
24:C:302:PEK:HN2	7:G:76:ASN:HD21	1.33	0.76
1:a:328:HIS:HA	2:b:45:MET:CE	2.19	0.73
1:A:289:ALA:HB1	1:A:297:MET:HE1	1.72	0.71
1:a:328:HIS:ND1	2:b:45:MET:HE1	2.07	0.70
11:K:15:ASN:OD1	28:K:101:HOH:O	2.11	0.68
1:a:167:THR:HA	1:a:171:MET:HE2	1.76	0.67
6:F:85:CYS:SG	6:F:87:THR:HG23	2.34	0.66
1:a:232:GLN:HE22	1:a:295:VAL:HG11	1.59	0.66
1:a:452:THR:HG22	1:a:456:MET:HE3	1.77	0.66
4:D:34:SER:H	4:D:37:GLN:HE21	1.43	0.66
1:a:65:MET:HA	1:a:65:MET:HE2	1.77	0.66
2:b:2:ALA:HA	2:b:6:GLN:HE22	1.61	0.65
7:G:34:ASN:HD21	7:G:38:HIS:CE1	2.15	0.65
1:A:310:MET:HE1	2:B:77:ALA:HB2	1.80	0.64
14:A:601:HEA:HMC3	14:A:601:HEA:HBC1	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:85:CYS:SG	6:f:87:THR:HG22	2.38	0.63
3:C:148:HIS:NE2	3:C:152:MET:HE2	2.14	0.61
12:l:26:THR:HG21	13:m:21:VAL:HG12	1.83	0.61
1:a:390:MET:HA	1:a:390:MET:HE3	1.82	0.61
10:j:30:ILE:O	10:j:34:VAL:HG23	2.01	0.60
1:A:466:MET:HE3	13:M:23:PHE:CG	2.36	0.60
7:G:72:ASN:H	7:G:76:ASN:ND2	1.97	0.60
11:K:41:ASN:N	11:K:42:PRO:HD3	2.17	0.59
1:a:127:THR:HB	1:a:129:TYR:CE1	2.38	0.59
2:B:41:ILE:O	2:B:45:MET:HG2	2.04	0.58
14:a:601:HEA:HMC1	14:a:601:HEA:HBC1	1.86	0.57
1:a:328:HIS:CA	2:b:45:MET:CE	2.82	0.57
8:h:14:ALA:HB3	8:h:63:LEU:HD21	1.86	0.57
6:F:25:ARG:NH1	28:F:201:HOH:O	2.21	0.56
1:a:261:TYR:HB2	1:a:338:MET:HE2	1.87	0.56
6:F:95:GLN:HE21	6:F:96:LEU:N	2.04	0.56
2:b:33:LEU:HD12	9:i:28:SER:HB3	1.87	0.56
23:c:302:CHD:H212	23:c:302:CHD:H12	1.88	0.56
1:A:336:PRO:HB2	1:A:394:VAL:HG11	1.87	0.56
3:C:148:HIS:CE1	3:C:152:MET:HE3	2.39	0.56
1:a:265:LYS:HB2	1:a:490:THR:HG21	1.89	0.55
4:D:34:SER:H	4:D:37:GLN:NE2	2.04	0.55
2:b:89:GLU:O	2:b:91:ASN:OD1	2.25	0.54
2:B:18:GLU:OE2	28:B:401:HOH:O	2.18	0.54
1:a:52:GLN:O	1:a:56:VAL:HG23	2.08	0.54
1:a:243:VAL:HG21	20:a:608:CMO:O	2.07	0.54
10:J:32:TYR:CE1	10:J:36:MET:HE3	2.43	0.54
1:a:310:MET:HE3	2:b:77:ALA:HB2	1.90	0.53
11:k:16:ALA:O	11:k:20:SER:OG	2.24	0.53
1:a:261:TYR:CB	1:a:338:MET:HE2	2.39	0.53
2:B:90:ILE:HD13	8:H:16:PHE:CG	2.43	0.53
6:F:93:PRO:C	6:F:95:GLN:N	2.66	0.52
1:A:211:THR:HG22	1:A:215:LEU:HD12	1.90	0.52
1:A:273:MET:HE2	1:A:273:MET:CA	2.35	0.52
2:b:102:HIS:NE2	2:b:107:SER:OG	2.40	0.52
5:e:37:VAL:HG11	5:e:70:VAL:HG21	1.92	0.52
4:d:33:LEU:HD22	4:d:62:LEU:HD13	1.92	0.51
1:a:92:MET:C	1:a:171:MET:HE1	2.35	0.51
3:c:9:HIS:CE1	3:c:11:VAL:HG22	2.46	0.51
3:C:76:GLN:OE1	28:C:401:HOH:O	2.18	0.51
13:M:17:ILE:O	13:M:21:VAL:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:34:SER:HA	1:a:37:ILE:HD12	1.92	0.50
23:b:301:CHD:H212	23:b:301:CHD:H12	1.93	0.50
1:A:240:HIS:O	1:A:243:VAL:HG22	2.11	0.50
1:a:364:ASP:OD1	14:a:602:HEA:O1A	2.29	0.49
2:b:123:ILE:HD12	2:b:137:GLU:HB3	1.92	0.49
3:c:232:HIS:NE2	28:c:401:HOH:O	2.12	0.49
4:d:137:LYS:HD3	11:k:45:VAL:HG21	1.94	0.49
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.48	0.49
8:H:9:LYS:HE3	8:H:10:ASN:N	2.28	0.49
7:g:6:GLY:O	7:g:7:ASP:HB2	2.12	0.49
2:B:94:SER:HB2	2:B:148:MET:HE3	1.94	0.49
1:a:328:HIS:CA	2:b:45:MET:HE2	2.42	0.49
2:b:199:ILE:HG23	2:b:199:ILE:O	2.12	0.49
9:i:63:MET:HB3	9:i:68:ILE:HD11	1.93	0.48
11:k:43:SER:OG	11:k:45:VAL:HG12	2.12	0.48
1:a:127:THR:HB	1:a:129:TYR:CD1	2.48	0.48
1:a:93:ALA:N	1:a:171:MET:HE1	2.29	0.48
13:m:28:LEU:HB2	13:m:29:PRO:HD3	1.96	0.48
1:A:202:LEU:HD22	1:A:238:PHE:CE2	2.49	0.48
3:C:47:LEU:O	3:C:51:MET:HG2	2.14	0.48
1:a:66:ILE:HG23	1:a:246:LEU:HD11	1.95	0.48
5:E:49:ASP:OD2	5:E:92:THR:OG1	2.25	0.47
1:A:144:ASP:OD2	3:C:36:HIS:HE1	1.98	0.47
13:m:1:ILE:HG23	13:m:1:ILE:O	2.13	0.47
1:A:75:ILE:O	1:A:79:GLY:HA3	2.15	0.47
2:b:1:FME:HE1	2:b:133:LEU:HD22	1.96	0.47
1:A:310:MET:CE	2:B:77:ALA:HB2	2.46	0.46
4:d:121:LYS:HD2	11:k:52:GLU:HA	1.97	0.46
23:B:303:CHD:H212	23:B:303:CHD:H12	1.98	0.46
4:D:131:ILE:N	4:D:131:ILE:HD12	2.31	0.46
11:k:40:TRP:O	11:k:41:ASN:C	2.58	0.46
1:a:35:LEU:HD23	1:a:458:SER:HB3	1.98	0.46
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.97	0.45
7:g:31:CYS:SG	25:g:103:CDL:H532	2.56	0.45
1:a:60:ALA:O	1:a:64:VAL:HG23	2.16	0.45
1:a:242:GLU:HA	1:a:245:ILE:HD12	1.97	0.45
5:E:81:ILE:O	5:E:85:VAL:HG23	2.17	0.45
1:a:87:ILE:O	1:a:173:PRO:HD3	2.17	0.45
7:g:40:GLY:O	7:g:41:HIS:C	2.59	0.45
2:B:90:ILE:HD12	2:B:91:ASN:N	2.32	0.45
12:l:36:PRO:O	12:l:40:VAL:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:MET:HE2	26:C:307:DMU:H29	1.98	0.45
1:a:488:THR:HB	1:a:495:LEU:HD13	1.98	0.45
10:j:32:TYR:CE1	10:j:36:MET:HG3	2.51	0.45
4:D:131:ILE:HG22	4:D:132:GLN:HG3	1.99	0.45
4:D:100:LYS:NZ	28:D:304:HOH:O	2.49	0.45
1:a:92:MET:HE1	1:a:164:PHE:CD1	2.52	0.45
1:a:383:MET:HG2	1:a:421:VAL:HG21	1.98	0.45
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.82	0.44
3:C:116:TRP:HA	3:C:117:PRO:C	2.41	0.44
1:a:41:LEU:HD11	1:a:54:TYR:OH	2.17	0.44
5:E:20:ASN:O	5:E:21:LYS:C	2.60	0.44
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.99	0.44
1:a:32:ALA:HB3	12:l:36:PRO:HG2	2.00	0.44
3:c:116:TRP:HA	3:c:117:PRO:C	2.41	0.44
14:A:602:HEA:HMC1	14:A:602:HEA:HBC1	1.99	0.44
2:B:58:ALA:O	2:B:62:GLU:HG3	2.18	0.44
1:a:19:TYR:CD1	1:a:76:GLY:HA3	2.53	0.44
3:c:16:TRP:N	3:c:17:PRO:CD	2.80	0.44
13:m:32:TRP:HD1	13:m:36:HIS:CE1	2.36	0.44
3:c:31:LEU:HD12	3:c:43:LEU:HD13	1.99	0.44
10:j:11:LEU:C	10:j:11:LEU:HD13	2.43	0.44
1:A:194:LEU:HD23	7:g:4:ALA:HB1	2.00	0.44
3:C:160:LEU:HD13	23:C:306:CHD:H181	2.00	0.44
4:d:82:VAL:HG12	4:d:86:MET:HE2	2.00	0.44
4:D:23:PRO:HG3	5:E:70:VAL:HG21	1.99	0.44
2:B:4:PRO:HB2	11:K:43:SER:HA	1.99	0.43
1:A:50:ASP:HB3	1:A:53:ILE:HD12	2.00	0.43
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.53	0.43
5:e:24:ILE:O	5:e:58:LEU:HD21	2.19	0.43
1:A:144:ASP:OD2	3:C:36:HIS:CE1	2.71	0.43
1:A:383:MET:HE2	1:A:421:VAL:HB	2.00	0.43
1:A:488:THR:HB	1:A:495:LEU:HD13	2.00	0.43
1:a:65:MET:HA	1:a:65:MET:CE	2.47	0.43
12:l:45:LEU:O	12:l:47:LYS:N	2.52	0.43
4:D:125:ASP:O	28:D:301:HOH:O	2.21	0.43
14:a:602:HEA:HBC1	14:a:602:HEA:HMC3	2.01	0.43
1:A:289:ALA:HB3	1:A:305:PHE:CD2	2.53	0.43
2:B:168:LEU:HD23	2:B:184:LEU:HG	2.00	0.43
11:K:41:ASN:O	11:K:42:PRO:C	2.59	0.43
12:l:45:LEU:HD21	13:m:40:TYR:CD1	2.53	0.43
1:A:41:LEU:HD21	1:A:440:TYR:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:24:ALA:O	3:c:28:THR:OG1	2.33	0.43
23:c:306:CHD:H212	23:c:306:CHD:H12	2.00	0.43
7:g:38:HIS:O	7:g:40:GLY:N	2.52	0.43
1:a:134:GLY:C	28:a:720:HOH:O	2.60	0.43
1:a:398:PRO:O	1:a:498:CYS:HB3	2.19	0.43
14:a:602:HEA:C1A	20:a:608:CMO:C	2.94	0.43
9:i:68:ILE:HD12	9:i:69:PHE:CD1	2.54	0.43
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	2.01	0.42
1:A:83:VAL:HB	1:A:84:PRO:HD3	2.01	0.42
1:a:194:LEU:HD22	1:a:285:PHE:CE2	2.54	0.42
2:b:104:TRP:CG	2:b:203:ASN:HB2	2.55	0.42
7:G:34:ASN:ND2	7:G:38:HIS:CE1	2.86	0.42
2:B:123:ILE:HD11	2:B:139:ASP:HA	2.00	0.42
3:c:129:VAL:N	3:c:130:PRO:CD	2.82	0.42
3:c:137:LEU:O	3:c:140:SER:HB3	2.18	0.42
12:l:35:ALA:HB3	12:l:36:PRO:HD3	2.01	0.42
1:A:247:ILE:HB	14:A:602:HEA:HBC1	2.01	0.42
2:b:104:TRP:CD2	2:b:203:ASN:HB2	2.55	0.42
1:a:507:GLU:OE1	6:f:51:SER:HA	2.19	0.42
3:C:91:VAL:HG13	24:C:309:PEK:H162	2.02	0.42
1:a:129:TYR:CZ	1:a:232:GLN:HG2	2.55	0.42
18:A:606:PGV:H202	13:M:12:PRO:HG3	2.02	0.41
6:F:91:LEU:HD23	6:F:93:PRO:HD3	2.03	0.41
1:A:92:MET:HE1	1:A:164:PHE:CD1	2.55	0.41
1:A:364:ASP:OD1	14:A:602:HEA:O1A	2.37	0.41
6:F:39:THR:H	6:F:47:ASN:ND2	2.18	0.41
1:a:208:MET:HE3	1:a:219:PHE:CD1	2.55	0.41
5:e:25:ASP:OD1	5:e:27:TRP:N	2.49	0.41
1:a:459:PHE:HB3	4:d:92:THR:HG23	2.02	0.41
1:A:250:GLY:O	1:A:254:ILE:HG12	2.21	0.41
2:B:16:ILE:HD11	2:B:87:MET:HG3	2.03	0.41
14:a:602:HEA:HBC1	14:a:602:HEA:CMC	2.51	0.41
2:B:82:ARG:CZ	2:B:86:MET:HE1	2.51	0.41
2:B:94:SER:CB	2:B:148:MET:HE3	2.51	0.41
2:B:98:LYS:HB2	2:B:109:GLU:HB2	2.03	0.41
8:H:60:TYR:CD1	8:H:60:TYR:C	2.99	0.41
13:m:27:LEU:HD22	26:m:401:DMU:H14	2.03	0.41
1:A:512:ASN:ND2	28:A:703:HOH:O	2.40	0.41
18:A:607:PGV:H331	24:C:302:PEK:H382	2.03	0.41
3:C:173:PHE:CD1	3:C:173:PHE:C	2.99	0.41
1:a:361:SER:OG	2:b:84:LEU:HD13	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:40:TYR:CD1	9:i:24:ALA:HB2	2.56	0.40
5:e:82:TYR:HB3	5:e:83:PRO:HD3	2.03	0.40
1:A:466:MET:CE	13:M:23:PHE:CG	3.03	0.40
3:C:63:ARG:HH22	10:J:28:ASP:CG	2.30	0.40
3:C:210:ILE:HD13	18:C:303:PGV:H302	2.02	0.40
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.57	0.40
4:d:6:VAL:HG22	4:d:11:TYR:HA	2.04	0.40
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.04	0.40
1:a:116:SER:O	12:l:43:GLN:NE2	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
1	a	512/514 (100%)	495 (97%)	16 (3%)	1 (0%)	43	55
2	B	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	30	38
2	b	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	30	38
3	c	257/261 (98%)	248 (96%)	8 (3%)	1 (0%)	30	38
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	d	142/147 (97%)	133 (94%)	8 (6%)	1 (1%)	18	23
5	E	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
5	e	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	5	4
6	f	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	5	4
7	G	81/85 (95%)	71 (88%)	7 (9%)	3 (4%)	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	81/85 (95%)	66 (82%)	9 (11%)	6 (7%)	1	0
8	H	77/85 (91%)	72 (94%)	3 (4%)	2 (3%)	4	3
8	h	77/85 (91%)	73 (95%)	4 (5%)	0	100	100
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	i	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	9	9
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	j	56/59 (95%)	53 (95%)	0	3 (5%)	1	1
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	k	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	l	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	5	4
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	m	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	4	4
All	All	3504/3614 (97%)	3355 (96%)	123 (4%)	26 (1%)	18	23

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	96	LEU
8	H	10	ASN
7	g	4	ALA
12	l	46	LYS
2	B	90	ILE
3	C	38	ASN
7	G	4	ALA
1	a	119	GLU
4	d	8	SER
7	g	7	ASP
7	g	8	HIS
9	i	68	ILE
7	G	8	HIS
3	c	38	ASN
6	f	94	HIS
7	g	39	SER
10	j	57	HIS
7	G	3	ALA
7	g	41	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	g	5	LYS
13	m	42	LYS
6	F	93	PRO
10	j	51	GLY
10	j	56	PRO
8	H	8	ILE
6	f	93	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	418 (98%)	8 (2%)	50	69
1	a	426/426 (100%)	413 (97%)	13 (3%)	35	52
2	B	210/210 (100%)	199 (95%)	11 (5%)	21	31
2	b	210/210 (100%)	198 (94%)	12 (6%)	18	27
3	C	224/226 (99%)	222 (99%)	2 (1%)	70	84
3	c	224/226 (99%)	219 (98%)	5 (2%)	45	65
4	D	128/129 (99%)	123 (96%)	5 (4%)	28	43
4	d	128/129 (99%)	121 (94%)	7 (6%)	19	28
5	E	92/95 (97%)	88 (96%)	4 (4%)	26	39
5	e	92/95 (97%)	86 (94%)	6 (6%)	15	22
6	F	81/81 (100%)	77 (95%)	4 (5%)	22	34
6	f	81/81 (100%)	80 (99%)	1 (1%)	63	79
7	G	67/68 (98%)	64 (96%)	3 (4%)	24	37
7	g	67/68 (98%)	65 (97%)	2 (3%)	36	53
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	13
8	h	71/75 (95%)	68 (96%)	3 (4%)	26	40
9	I	57/57 (100%)	55 (96%)	2 (4%)	32	48
9	i	57/57 (100%)	54 (95%)	3 (5%)	20	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	41
10	j	49/50 (98%)	42 (86%)	7 (14%)	3	3
11	K	39/46 (85%)	39 (100%)	0	100	100
11	k	39/46 (85%)	37 (95%)	2 (5%)	21	32
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	59
12	l	39/40 (98%)	33 (85%)	6 (15%)	2	3
13	M	37/38 (97%)	37 (100%)	0	100	100
13	m	37/38 (97%)	34 (92%)	3 (8%)	11	14
All	All	3040/3082 (99%)	2922 (96%)	118 (4%)	28	43

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	51	ASP
1	A	118	VAL
1	A	128	VAL
1	A	312	ILE
1	A	361	SER
1	A	366	VAL
1	A	369	ASP
2	B	33	LEU
2	B	52	HIS
2	B	57	ASP
2	B	65	TRP
2	B	66	THR
2	B	68	LEU
2	B	75	LEU
2	B	90	ILE
2	B	91	ASN
2	B	110	TYR
2	B	183	THR
3	C	33	MET
3	C	179	SER
4	D	36	SER
4	D	47	SER
4	D	49	SER
4	D	50	SER
4	D	63	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	9	GLU
5	E	46	LYS
5	E	70	VAL
5	E	79	LYS
6	F	37	LYS
6	F	87	THR
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	5	LYS
7	G	7	ASP
8	H	9	LYS
8	H	46	LYS
8	H	60	TYR
8	H	61	LYS
8	H	76	ARG
8	H	84	LYS
9	I	2	THR
9	I	26	MET
10	J	31	LEU
10	J	58	LYS
12	L	26	THR
1	a	46	THR
1	a	65	MET
1	a	118	VAL
1	a	265	LYS
1	a	310	MET
1	a	363	LEU
1	a	369	ASP
1	a	382	SER
1	a	417	MET
1	a	458	SER
1	a	483	LEU
1	a	486	ASP
1	a	504	THR
2	b	68	LEU
2	b	94	SER
2	b	95	LEU
2	b	107	SER
2	b	110	TYR
2	b	117	SER
2	b	129	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	156	SER
2	b	183	THR
2	b	185	MET
2	b	216	LEU
2	b	217	LYS
3	c	23	SER
3	c	89	SER
3	c	140	SER
3	c	157	LYS
3	c	159	MET
4	d	5	VAL
4	d	33	LEU
4	d	47	SER
4	d	94	LEU
4	d	110	THR
4	d	121	LYS
4	d	131	ILE
5	e	79	LYS
5	e	81	ILE
5	e	89	LEU
5	e	93	LEU
5	e	104	LEU
5	e	108	LYS
6	f	37	LYS
7	g	38	HIS
7	g	41	HIS
8	h	10	ASN
8	h	60	TYR
8	h	66	ILE
9	i	21	ILE
9	i	68	ILE
9	i	73	LYS
10	j	4	ARG
10	j	10	LYS
10	j	27	THR
10	j	36	MET
10	j	38	LEU
10	j	50	LEU
10	j	57	HIS
11	k	48	VAL
11	k	52	GLU
12	l	5	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	l	11	ILE
12	l	16	GLU
12	l	20	ARG
12	l	26	THR
12	l	47	LYS
13	m	7	LYS
13	m	37	LEU
13	m	41	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	138	HIS
1	A	232	GLN
1	A	428	GLN
2	B	91	ASN
2	B	140	ASN
3	C	36	HIS
3	C	38	ASN
4	D	29	HIS
4	D	37	GLN
4	D	72	ASN
4	D	76	ASN
4	D	119	GLN
5	E	59	ASN
6	F	32	ASN
6	F	47	ASN
6	F	54	ASN
6	F	66	ASN
6	F	95	GLN
7	G	38	HIS
7	G	51	HIS
7	G	76	ASN
8	H	25	GLN
8	H	28	ASN
8	H	31	GLN
8	H	32	ASN
8	H	37	HIS
9	I	8	GLN
10	J	9	GLN
11	K	41	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	99	ASN
1	a	170	ASN
1	a	232	GLN
1	a	331	ASN
1	a	422	ASN
1	a	512	ASN
2	b	6	GLN
3	c	76	GLN
3	c	161	GLN
4	d	32	ASN
4	d	72	ASN
4	d	132	GLN
4	d	143	ASN
5	e	78	HIS
6	f	32	ASN
6	f	88	HIS
8	h	32	ASN
8	h	37	HIS
9	i	8	GLN
12	l	2	HIS
12	l	17	ASN
13	m	15	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	a	1	1	8,9,10	0.54	0	8,9,11	1.81	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	b	1	2	8,9,10	0.62	0	8,9,11	2.33	2 (25%)
7	TPO	g	11	7	8,10,11	1.39	1 (12%)	10,14,16	0.78	0
7	TPO	G	11	7	8,10,11	1.58	2 (25%)	10,14,16	0.95	0
1	FME	A	1	1	8,9,10	0.55	0	8,9,11	2.59	3 (37%)
9	SAC	I	1	9	7,8,9	1.49	1 (14%)	7,9,11	1.01	0
9	SAC	i	1	9	7,8,9	1.79	1 (14%)	7,9,11	1.97	2 (28%)
2	FME	B	1	2	8,9,10	1.00	0	8,9,11	3.70	4 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	a	1	1	-	5/7/9/11	-
2	FME	b	1	2	-	1/7/9/11	-
7	TPO	g	11	7	-	5/9/11/13	-
7	TPO	G	11	7	-	5/9/11/13	-
1	FME	A	1	1	-	5/7/9/11	-
9	SAC	I	1	9	-	1/7/8/10	-
9	SAC	i	1	9	-	2/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	1	SAC	CA-N	4.22	1.52	1.46
9	I	1	SAC	CA-N	3.41	1.51	1.46
7	G	11	TPO	P-OG1	2.91	1.64	1.59
7	G	11	TPO	CB-CA	2.67	1.59	1.53
7	g	11	TPO	P-OG1	2.52	1.63	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-8.96	109.04	122.82
1	A	1	FME	CA-N-CN	-6.41	112.97	122.82
2	b	1	FME	CA-N-CN	-5.22	114.80	122.82
1	a	1	FME	CA-N-CN	-4.24	116.30	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	1	SAC	C-CA-N	3.30	115.86	109.50
2	B	1	FME	CB-CA-N	3.14	116.24	110.52
2	B	1	FME	C-CA-N	3.02	115.32	109.50
2	b	1	FME	C-CA-N	2.82	114.94	109.50
2	B	1	FME	O1-CN-N	-2.82	118.04	125.32
9	i	1	SAC	OAC-C1A-C2A	-2.73	117.19	122.05
1	A	1	FME	C-CA-N	-2.27	105.13	109.50
1	A	1	FME	O-C-CA	-2.26	118.96	124.77
1	a	1	FME	O-C-CA	-2.19	119.14	124.77

There are no chirality outliers.

All (25) 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	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	O-C-CA-CB
1	a	1	FME	O1-CN-N-CA
1	a	1	FME	C-CA-CB-CG
2	b	1	FME	O1-CN-N-CA
7	g	11	TPO	N-CA-CB-OG1
1	a	1	FME	CA-CB-CG-SD
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	CA-CB-CG-SD
7	G	11	TPO	CG2-CB-OG1-P
1	A	1	FME	CB-CG-SD-CE
1	a	1	FME	CB-CG-SD-CE
7	g	11	TPO	CG2-CB-OG1-P
9	i	1	SAC	N-CA-CB-OG
7	G	11	TPO	CB-OG1-P-O3P
9	i	1	SAC	C-CA-CB-OG
7	g	11	TPO	CB-OG1-P-O1P
1	a	1	FME	N-CA-CB-CG
7	g	11	TPO	CB-OG1-P-O2P
7	g	11	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	b	1	FME	1	0

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	$\# Z > 2$
26	DMU	C	307	-	34,34,34	0.99	1 (2%)	45,45,45	1.47	8 (17%)
19	TGL	i	101	-	62,62,62	1.05	3 (4%)	65,65,65	1.24	5 (7%)
20	CMO	A	609	14	0,1,1	-	-	-	-	-
23	CHD	c	306	-	32,32,32	0.60	0	51,51,51	1.49	13 (25%)
23	CHD	C	306	-	32,32,32	0.56	0	51,51,51	1.24	5 (9%)
24	PEK	C	308	-	52,52,52	1.01	2 (3%)	55,57,57	1.20	4 (7%)
18	PGV	A	606	-	50,50,50	1.27	2 (4%)	53,56,56	1.31	8 (15%)
25	CDL	G	101	-	99,99,99	1.09	4 (4%)	105,111,111	0.96	6 (5%)
19	TGL	A	608	-	62,62,62	1.29	3 (4%)	65,65,65	1.32	6 (9%)
25	CDL	C	305	-	99,99,99	1.03	4 (4%)	105,111,111	1.13	10 (9%)
18	PGV	C	303	-	50,50,50	0.87	2 (4%)	53,56,56	0.92	3 (5%)
21	CUA	B	301	2	0,1,1	-	-	-	-	-
14	HEA	a	601	1	67,67,67	2.33	24 (35%)	81,103,103	2.47	29 (35%)
19	TGL	a	606	-	62,62,62	1.17	3 (4%)	65,65,65	0.96	4 (6%)
25	CDL	g	103	-	99,99,99	1.08	4 (4%)	105,111,111	0.96	7 (6%)
19	TGL	L	101	-	62,62,62	1.11	3 (4%)	65,65,65	1.05	4 (6%)
26	DMU	M	101	-	34,34,34	0.47	0	45,45,45	1.05	4 (8%)
23	CHD	C	301	-	32,32,32	0.86	0	51,51,51	1.22	3 (5%)
18	PGV	a	607	-	50,50,50	1.09	2 (4%)	53,56,56	0.98	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	TGL	l	101	-	62,62,62	1.17	3 (4%)	65,65,65	1.18	5 (7%)
24	PEK	g	102	-	52,52,52	0.90	3 (5%)	55,57,57	0.86	2 (3%)
23	CHD	c	302	-	32,32,32	0.80	0	51,51,51	1.60	12 (23%)
18	PGV	c	304	-	50,50,50	0.90	2 (4%)	53,56,56	1.06	3 (5%)
21	CUA	b	302	2	0,1,1	-	-	-	-	-
23	CHD	J	101	-	32,32,32	0.84	0	51,51,51	2.02	12 (23%)
24	PEK	C	302	-	52,52,52	0.97	4 (7%)	55,57,57	0.98	2 (3%)
23	CHD	b	301	-	32,32,32	0.81	0	51,51,51	1.55	12 (23%)
14	HEA	A	602	1,20	67,67,67	2.08	24 (35%)	81,103,103	2.50	30 (37%)
24	PEK	G	102	-	52,52,52	1.11	2 (3%)	55,57,57	0.92	4 (7%)
18	PGV	A	607	-	50,50,50	0.74	2 (4%)	53,56,56	0.96	3 (5%)
14	HEA	a	602	1,20	67,67,67	2.14	20 (29%)	81,103,103	2.59	31 (38%)
18	PGV	c	301	-	50,50,50	0.79	2 (4%)	53,56,56	0.86	2 (3%)
23	CHD	j	101	-	32,32,32	0.82	0	51,51,51	2.03	12 (23%)
26	DMU	m	401	-	34,34,34	0.52	0	45,45,45	1.14	3 (6%)
14	HEA	A	601	1	67,67,67	2.30	27 (40%)	81,103,103	2.34	29 (35%)
18	PGV	G	103	-	50,50,50	1.08	2 (4%)	53,56,56	1.00	4 (7%)
20	CMO	a	608	14	0,1,1	-	-	-	-	-
18	PGV	C	304	-	50,50,50	1.15	2 (4%)	53,56,56	1.16	3 (5%)
23	CHD	B	303	-	32,32,32	1.02	1 (3%)	51,51,51	1.22	8 (15%)
22	PSC	e	201	-	51,51,51	1.07	2 (3%)	57,59,59	1.83	10 (17%)
24	PEK	c	303	-	52,52,52	1.10	2 (3%)	55,57,57	1.05	3 (5%)
25	CDL	c	305	-	99,99,99	1.09	4 (4%)	105,111,111	1.10	8 (7%)
19	TGL	D	201	-	62,62,62	1.29	3 (4%)	65,65,65	1.26	6 (9%)
22	PSC	B	302	-	51,51,51	1.08	2 (3%)	57,59,59	1.90	9 (15%)
24	PEK	C	309	-	52,52,52	1.15	2 (3%)	55,57,57	0.97	4 (7%)
26	DMU	c	307	-	34,34,34	0.82	1 (2%)	45,45,45	1.13	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DMU	C	307	-	-	7/19/59/59	0/2/2/2
19	TGL	i	101	-	-	23/65/65/65	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	c	306	-	-	1/9/74/74	0/4/4/4
23	CHD	C	306	-	-	2/9/74/74	0/4/4/4
24	PEK	C	308	-	-	20/56/56/56	-
18	PGV	A	606	-	-	31/55/55/55	-
25	CDL	G	101	-	-	57/110/110/110	-
19	TGL	A	608	-	-	33/65/65/65	-
25	CDL	C	305	-	-	44/110/110/110	-
18	PGV	C	303	-	-	12/55/55/55	-
14	HEA	a	601	1	-	3/36/76/76	-
19	TGL	a	606	-	-	29/65/65/65	-
25	CDL	g	103	-	-	54/110/110/110	-
19	TGL	L	101	-	-	38/65/65/65	-
26	DMU	M	101	-	-	3/19/59/59	0/2/2/2
23	CHD	C	301	-	-	3/9/74/74	0/4/4/4
18	PGV	a	607	-	-	21/55/55/55	-
19	TGL	l	101	-	-	33/65/65/65	-
24	PEK	g	102	-	-	17/56/56/56	-
23	CHD	c	302	-	-	2/9/74/74	0/4/4/4
18	PGV	c	304	-	-	14/55/55/55	-
23	CHD	J	101	-	-	6/9/74/74	0/4/4/4
24	PEK	C	302	-	-	13/56/56/56	-
23	CHD	b	301	-	-	3/9/74/74	0/4/4/4
14	HEA	A	602	1,20	-	4/36/76/76	-
24	PEK	G	102	-	-	22/56/56/56	-
18	PGV	A	607	-	-	16/55/55/55	-
14	HEA	a	602	1,20	-	5/36/76/76	-
18	PGV	c	301	-	-	18/55/55/55	-
23	CHD	j	101	-	-	7/9/74/74	0/4/4/4
26	DMU	m	401	-	-	6/19/59/59	0/2/2/2
14	HEA	A	601	1	-	3/36/76/76	-
18	PGV	G	103	-	-	27/55/55/55	-
18	PGV	C	304	-	-	24/55/55/55	-
23	CHD	B	303	-	-	2/9/74/74	0/4/4/4
22	PSC	e	201	-	-	23/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEK	c	303	-	-	25/56/56/56	-
25	CDL	c	305	-	-	54/110/110/110	-
19	TGL	D	201	-	-	31/65/65/65	-
22	PSC	B	302	-	-	29/55/55/55	-
24	PEK	C	309	-	-	25/56/56/56	-
26	DMU	c	307	-	-	11/19/59/59	0/2/2/2

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	608	TGL	OG1-CA1	6.09	1.51	1.33
14	a	601	HEA	C3B-C2B	5.74	1.47	1.34
14	A	601	HEA	C3D-C2D	5.57	1.48	1.36
19	D	201	TGL	OG2-CB1	5.55	1.50	1.34
14	a	601	HEA	FE-NB	5.48	2.11	1.94
18	A	606	PGV	O03-C19	5.35	1.48	1.33
19	A	608	TGL	OG2-CB1	5.26	1.49	1.34
19	D	201	TGL	OG3-CC1	5.24	1.48	1.33
14	A	601	HEA	C3B-C2B	5.14	1.46	1.34
24	C	309	PEK	O01-C1	5.12	1.48	1.34
24	G	102	PEK	O03-C21	5.09	1.48	1.33
14	a	602	HEA	C11-C3B	-5.09	1.45	1.51
19	l	101	TGL	OG3-CC1	5.05	1.48	1.33
24	C	309	PEK	O03-C21	5.05	1.48	1.33
19	L	101	TGL	OG2-CB1	5.01	1.48	1.34
19	a	606	TGL	OG2-CB1	4.98	1.48	1.34
24	c	303	PEK	O01-C1	4.95	1.48	1.34
14	a	601	HEA	FE-ND	4.94	2.10	1.94
18	C	304	PGV	O03-C19	4.91	1.47	1.33
25	g	103	CDL	OB6-CB5	4.91	1.48	1.34
18	a	607	PGV	O03-C19	4.83	1.47	1.33
25	c	305	CDL	OB8-CB7	4.81	1.47	1.33
24	c	303	PEK	O03-C21	4.81	1.47	1.33
25	G	101	CDL	OB8-CB7	4.79	1.47	1.33
18	A	606	PGV	O01-C1	4.78	1.47	1.34
24	G	102	PEK	O01-C1	4.75	1.47	1.34
18	C	304	PGV	O01-C1	4.75	1.47	1.34
22	e	201	PSC	O03-C19	4.75	1.47	1.33
19	i	101	TGL	OG2-CB1	4.74	1.47	1.34
25	c	305	CDL	OB6-CB5	4.73	1.47	1.34
25	C	305	CDL	OA6-CA5	4.73	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	FE-NB	4.72	2.09	1.94
19	l	101	TGL	OG2-CB1	4.72	1.47	1.34
25	c	305	CDL	OA8-CA7	4.70	1.47	1.33
22	e	201	PSC	O01-C1	4.70	1.47	1.34
19	a	606	TGL	OG3-CC1	4.69	1.47	1.33
18	G	103	PGV	O01-C1	4.69	1.47	1.34
22	B	302	PSC	O01-C1	4.69	1.47	1.34
19	L	101	TGL	OG3-CC1	4.67	1.47	1.33
19	i	101	TGL	OG1-CA1	4.67	1.46	1.33
24	C	308	PEK	O01-C1	4.64	1.47	1.34
14	A	601	HEA	FE-NC	4.63	2.10	1.95
25	G	101	CDL	OB6-CB5	4.63	1.47	1.34
25	g	103	CDL	OA6-CA5	4.61	1.47	1.34
19	D	201	TGL	OG1-CA1	4.59	1.46	1.33
25	c	305	CDL	OA6-CA5	4.58	1.47	1.34
22	B	302	PSC	O03-C19	4.58	1.46	1.33
19	a	606	TGL	OG1-CA1	4.57	1.46	1.33
14	a	601	HEA	C11-C3B	-4.56	1.45	1.51
18	G	103	PGV	O03-C19	4.55	1.46	1.33
25	C	305	CDL	OB8-CB7	4.54	1.46	1.33
25	g	103	CDL	OB8-CB7	4.50	1.46	1.33
14	A	602	HEA	C3B-C2B	4.50	1.45	1.34
14	a	602	HEA	FE-NB	4.49	2.08	1.94
25	g	103	CDL	OA8-CA7	4.48	1.46	1.33
14	a	602	HEA	C4B-NB	-4.48	1.32	1.40
25	G	101	CDL	OA6-CA5	4.47	1.46	1.34
14	A	601	HEA	C11-C3B	-4.46	1.45	1.51
24	C	308	PEK	O03-C21	4.45	1.46	1.33
14	A	602	HEA	C3D-C2D	4.43	1.46	1.36
19	l	101	TGL	OG1-CA1	4.43	1.46	1.33
25	G	101	CDL	OA8-CA7	4.39	1.46	1.33
14	A	602	HEA	FE-NC	4.39	2.09	1.95
14	a	602	HEA	FE-ND	4.34	2.08	1.94
25	C	305	CDL	OA8-CA7	4.30	1.45	1.33
14	a	602	HEA	C1D-ND	-4.26	1.32	1.40
14	A	601	HEA	C4B-NB	-4.26	1.32	1.40
14	a	601	HEA	C3D-C2D	4.25	1.45	1.36
14	A	601	HEA	FE-ND	4.20	2.07	1.94
18	C	303	PGV	O01-C1	4.16	1.46	1.34
14	a	602	HEA	C3D-C2D	4.13	1.45	1.36
19	A	608	TGL	OG3-CC1	4.12	1.45	1.33
14	a	602	HEA	C1C-NC	-4.09	1.31	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	607	PGV	O01-C1	4.09	1.45	1.34
24	C	302	PEK	O03-C21	4.07	1.45	1.33
14	a	601	HEA	C3A-C2A	4.06	1.46	1.37
14	a	602	HEA	C3B-C2B	4.02	1.43	1.34
14	A	602	HEA	FE-NB	4.00	2.07	1.94
14	a	601	HEA	C4B-NB	-3.98	1.33	1.40
14	a	601	HEA	CHA-C1A	3.94	1.46	1.38
14	a	602	HEA	CHB-C4A	3.91	1.46	1.38
14	a	602	HEA	C4C-NC	-3.90	1.32	1.39
25	C	305	CDL	OB6-CB5	3.88	1.45	1.34
18	c	304	PGV	O01-C1	3.83	1.45	1.34
14	A	601	HEA	C1D-ND	-3.83	1.33	1.40
19	L	101	TGL	OG1-CA1	3.81	1.44	1.33
14	a	601	HEA	C1D-ND	-3.80	1.33	1.40
14	a	602	HEA	C4D-ND	-3.77	1.31	1.38
14	a	601	HEA	CHD-C1D	3.77	1.46	1.38
14	a	601	HEA	C1A-NA	3.76	1.46	1.39
14	A	601	HEA	CHD-C1D	3.73	1.46	1.38
18	c	304	PGV	O03-C19	3.73	1.44	1.33
14	A	601	HEA	C3A-C2A	3.69	1.45	1.37
14	a	601	HEA	CHB-C4A	3.66	1.45	1.38
14	A	601	HEA	C4C-NC	-3.65	1.32	1.39
14	a	602	HEA	C3A-C2A	3.65	1.45	1.37
14	A	601	HEA	CHA-C1A	3.61	1.45	1.38
24	g	102	PEK	O03-C21	3.60	1.43	1.33
14	a	601	HEA	CHC-C1C	3.59	1.47	1.39
24	g	102	PEK	O01-C1	3.59	1.44	1.34
14	A	602	HEA	C1D-ND	-3.58	1.34	1.40
26	C	307	DMU	O16-C6	3.52	1.46	1.40
24	C	302	PEK	O01-C1	3.49	1.44	1.34
14	a	601	HEA	C4A-NA	3.45	1.46	1.39
14	A	602	HEA	C1B-NB	-3.43	1.32	1.38
14	A	601	HEA	CHB-C4A	3.42	1.45	1.38
18	c	301	PGV	O01-C1	3.41	1.43	1.34
14	A	602	HEA	CHC-C4B	3.35	1.45	1.38
14	A	602	HEA	CHC-C1C	3.33	1.46	1.39
18	C	303	PGV	O03-C19	3.32	1.43	1.33
14	a	601	HEA	FE-NC	3.30	2.06	1.95
19	i	101	TGL	OG3-CC1	3.30	1.43	1.33
18	c	301	PGV	O03-C19	3.28	1.42	1.33
14	A	602	HEA	C4C-NC	-3.25	1.33	1.39
14	A	602	HEA	CHD-C1D	3.25	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C4B-NB	-3.17	1.34	1.40
18	A	607	PGV	O03-C19	3.14	1.42	1.33
14	A	602	HEA	FE-ND	3.11	2.04	1.94
24	C	302	PEK	O01-C02	-3.07	1.39	1.46
14	A	602	HEA	C3A-C2A	3.06	1.44	1.37
14	A	601	HEA	CHC-C1C	3.06	1.46	1.39
14	a	602	HEA	C4A-NA	3.03	1.45	1.39
14	A	602	HEA	C4D-ND	-3.00	1.33	1.38
14	A	602	HEA	C11-C3B	-2.97	1.47	1.51
26	c	307	DMU	O16-C6	2.96	1.45	1.40
14	A	601	HEA	CHB-C1B	2.96	1.45	1.39
14	A	602	HEA	CHA-C1A	2.92	1.44	1.38
14	a	601	HEA	C4C-NC	-2.88	1.34	1.39
18	A	607	PGV	O01-C1	2.87	1.42	1.34
14	a	601	HEA	CHC-C4B	2.85	1.44	1.38
14	A	601	HEA	CHC-C4B	2.84	1.44	1.38
14	A	602	HEA	CHB-C4A	2.84	1.43	1.38
14	a	602	HEA	CHC-C1C	2.80	1.45	1.39
14	A	602	HEA	C1C-NC	-2.75	1.34	1.39
14	A	602	HEA	CHA-C4D	2.73	1.45	1.39
14	A	602	HEA	CHB-C1B	2.72	1.45	1.39
14	a	601	HEA	C4D-ND	-2.69	1.33	1.38
14	a	602	HEA	CHD-C4C	2.64	1.45	1.39
14	A	602	HEA	CHD-C4C	2.61	1.45	1.39
14	A	601	HEA	C1B-C2B	2.61	1.49	1.44
14	A	601	HEA	C4D-ND	-2.60	1.33	1.38
14	a	602	HEA	CHD-C1D	2.59	1.43	1.38
14	a	601	HEA	CHD-C4C	2.58	1.45	1.39
14	a	602	HEA	FE-NC	2.55	2.03	1.95
14	a	601	HEA	CHA-C4D	2.51	1.44	1.39
23	B	303	CHD	C13-C14	-2.50	1.51	1.55
14	a	602	HEA	CHC-C4B	2.50	1.43	1.38
14	A	601	HEA	C1C-C2C	2.48	1.48	1.43
14	a	601	HEA	C1C-C2C	2.46	1.48	1.43
14	A	602	HEA	C1C-C2C	2.45	1.48	1.43
14	a	601	HEA	C1C-NC	-2.44	1.35	1.39
24	g	102	PEK	O03-C01	-2.44	1.39	1.45
14	a	602	HEA	C1B-NB	-2.42	1.34	1.38
14	A	602	HEA	C1D-C2D	2.41	1.49	1.44
14	A	601	HEA	O1A-CGA	2.32	1.29	1.22
14	A	601	HEA	C1A-NA	2.31	1.44	1.39
14	A	601	HEA	C1C-NC	-2.30	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C1B-NB	-2.25	1.34	1.38
14	a	601	HEA	C4B-C3B	2.24	1.48	1.44
14	a	601	HEA	CHB-C1B	2.19	1.44	1.39
14	A	602	HEA	C4D-C3D	2.18	1.48	1.45
14	a	602	HEA	CHA-C1A	2.18	1.42	1.38
14	A	601	HEA	FE-NA	2.15	2.02	1.95
14	A	601	HEA	C4B-C3B	2.13	1.48	1.44
14	A	601	HEA	C4A-NA	2.09	1.43	1.39
14	A	601	HEA	CHA-C4D	2.05	1.43	1.39
24	C	302	PEK	O03-C01	-2.05	1.40	1.45

All (343) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	302	PSC	C08-N-C07	-7.27	89.88	108.98
14	a	602	HEA	C3D-C4D-ND	7.23	117.33	110.35
14	a	601	HEA	C3D-C4D-ND	6.93	117.05	110.35
14	a	602	HEA	C2D-C1D-ND	6.66	117.50	109.84
22	B	302	PSC	C08-N-C06	-6.51	91.89	108.98
19	i	101	TGL	OG2-CB1-CB2	6.28	125.07	111.48
14	a	601	HEA	C2B-C1B-NB	6.16	117.02	109.90
22	e	201	PSC	C08-N-C07	-6.10	92.96	108.98
14	a	602	HEA	C2B-C1B-NB	6.09	116.94	109.90
14	A	601	HEA	C2B-C1B-NB	6.06	116.91	109.90
14	A	601	HEA	C3C-C2C-C1C	-6.04	100.05	107.17
14	a	602	HEA	C1D-C2D-C3D	-6.01	100.66	106.98
14	A	602	HEA	C2B-C1B-NB	6.01	116.85	109.90
22	e	201	PSC	C08-N-C06	-5.99	93.25	108.98
14	A	602	HEA	C3D-C4D-ND	5.97	116.13	110.35
14	a	601	HEA	C13-C12-C11	-5.92	104.94	114.39
19	D	201	TGL	OG2-CB1-CB2	5.91	124.28	111.48
23	J	101	CHD	C6-C5-C10	5.81	118.84	112.66
14	A	602	HEA	C3B-C4B-NB	5.70	116.39	109.84
19	A	608	TGL	OG2-CB1-CB2	5.66	123.73	111.48
22	B	302	PSC	C07-N-C06	5.64	123.79	108.98
19	l	101	TGL	OG2-CB1-CB2	5.63	123.66	111.48
14	A	601	HEA	C3D-C4D-ND	5.61	115.77	110.35
23	j	101	CHD	C6-C5-C10	5.59	118.61	112.66
14	A	602	HEA	C3C-C4C-NC	5.59	114.50	109.80
24	C	308	PEK	O01-C1-C2	5.55	123.48	111.48
14	a	602	HEA	C3C-C4C-NC	5.54	114.47	109.80
14	A	601	HEA	C3B-C4B-NB	5.51	116.17	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	101	CHD	C9-C10-C5	5.38	115.98	108.51
25	C	305	CDL	OA6-CA5-C11	5.37	123.09	111.48
14	a	601	HEA	C3B-C4B-NB	5.34	115.98	109.84
14	A	601	HEA	C1B-C2B-C3B	-5.30	100.66	106.80
14	A	601	HEA	C1D-C2D-C3D	-5.25	101.45	106.98
14	a	601	HEA	C2D-C1D-ND	5.20	115.82	109.84
14	a	602	HEA	C2A-C1A-NA	5.15	115.29	110.32
14	a	601	HEA	C3C-C2C-C1C	-5.12	101.13	107.17
14	A	602	HEA	C2D-C1D-ND	5.05	115.65	109.84
14	A	601	HEA	C13-C12-C11	-5.04	106.35	114.39
23	J	101	CHD	C6-C7-C8	5.03	116.99	111.50
22	e	201	PSC	O01-C1-C2	5.02	122.35	111.48
14	A	602	HEA	C3C-C2C-C1C	-5.01	101.26	107.17
23	J	101	CHD	C22-C20-C17	5.00	120.70	110.33
14	a	601	HEA	C1B-C2B-C3B	-4.99	101.02	106.80
14	a	601	HEA	O11-C11-C3B	-4.97	102.14	111.26
14	A	602	HEA	C2A-C1A-NA	4.97	115.12	110.32
25	c	305	CDL	OB6-CB5-C51	4.93	122.15	111.48
25	g	103	CDL	OB6-CB5-C51	4.84	121.95	111.48
14	a	601	HEA	C3C-C4C-NC	4.81	113.85	109.80
14	a	602	HEA	C3C-C2C-C1C	-4.78	101.54	107.17
14	a	602	HEA	C3B-C4B-NB	4.77	115.32	109.84
23	j	101	CHD	C13-C17-C20	4.67	125.14	119.48
14	A	601	HEA	C2D-C1D-ND	4.67	115.21	109.84
25	c	305	CDL	OA6-CA5-C11	4.64	121.52	111.48
14	A	602	HEA	C1D-C2D-C3D	-4.63	102.11	106.98
18	C	304	PGV	O03-C19-C20	4.57	125.78	111.83
14	A	601	HEA	C3C-C4C-NC	4.52	113.61	109.80
25	G	101	CDL	OA6-CA5-C11	4.47	121.16	111.48
18	C	304	PGV	O01-C1-C2	4.47	121.14	111.48
14	a	602	HEA	C3A-C2A-C1A	-4.45	102.84	107.05
14	A	602	HEA	CAD-CBD-CGD	-4.44	101.89	113.67
24	c	303	PEK	O03-C21-C22	4.37	125.17	111.83
23	j	101	CHD	C22-C20-C17	4.37	119.39	110.33
18	a	607	PGV	O01-C1-C2	4.36	120.90	111.48
25	C	305	CDL	OB6-CB5-C51	4.32	120.83	111.48
14	A	602	HEA	C3A-C2A-C1A	-4.32	102.96	107.05
25	g	103	CDL	OA6-CA5-C11	4.24	120.66	111.48
18	A	606	PGV	O03-C19-C20	4.20	124.64	111.83
14	a	602	HEA	CAD-CBD-CGD	-4.20	102.53	113.67
14	A	602	HEA	CMD-C2D-C1D	4.15	131.53	125.03
23	j	101	CHD	C5-C6-C7	4.15	119.34	114.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	302	PSC	O01-C1-C2	4.14	120.43	111.48
23	J	101	CHD	C5-C6-C7	4.11	119.29	114.40
26	m	401	DMU	C7-C8-C9	4.09	117.65	110.23
18	A	606	PGV	C02-O01-C1	4.07	127.54	117.80
18	G	103	PGV	O03-C19-C20	4.02	124.10	111.83
14	a	602	HEA	C1B-C2B-C3B	-3.94	102.23	106.80
25	c	305	CDL	OB8-CB7-C71	3.94	123.83	111.83
25	G	101	CDL	OB6-CB5-C51	3.93	119.98	111.48
23	c	302	CHD	C22-C20-C17	3.89	118.40	110.33
14	A	602	HEA	C1B-C2B-C3B	-3.89	102.30	106.80
23	C	306	CHD	C6-C5-C4	-3.88	106.79	111.23
14	A	602	HEA	CHA-C4D-C3D	-3.86	119.14	124.77
19	L	101	TGL	OG2-CB1-CB2	3.84	119.78	111.48
14	a	601	HEA	C1D-C2D-C3D	-3.83	102.95	106.98
19	a	606	TGL	OG2-CB1-CB2	3.80	119.70	111.48
14	A	602	HEA	C13-C12-C11	-3.80	108.32	114.39
18	C	303	PGV	O03-C19-O04	-3.79	114.14	123.63
24	C	309	PEK	O01-C1-C2	3.77	119.63	111.48
22	e	201	PSC	C07-N-C06	3.77	118.87	108.98
23	b	301	CHD	C13-C17-C20	-3.76	114.92	119.48
19	a	606	TGL	OG3-CC1-CC2	3.76	123.31	111.83
14	a	601	HEA	C2A-C1A-NA	3.75	113.95	110.32
19	D	201	TGL	OG1-CA1-CA2	3.73	123.20	111.83
22	e	201	PSC	O03-C19-C20	3.73	123.19	111.83
19	A	608	TGL	OG3-CC1-CC2	3.72	123.19	111.83
26	C	307	DMU	C10-C5-C7	3.69	117.76	110.01
14	a	601	HEA	C4D-C3D-C2D	-3.67	101.55	106.89
22	e	201	PSC	C08-N-C05	-3.67	95.34	109.91
23	J	101	CHD	C13-C17-C20	3.66	123.92	119.48
14	a	602	HEA	CHB-C1B-C2B	-3.65	119.27	125.03
24	C	302	PEK	O01-C1-C2	3.64	119.36	111.48
18	c	304	PGV	O01-C1-C2	3.63	119.33	111.48
24	c	303	PEK	O01-C1-C2	3.62	119.31	111.48
19	A	608	TGL	OG1-CA1-CA2	3.60	122.80	111.83
14	A	602	HEA	C2C-C1C-NC	3.58	115.88	110.14
19	D	201	TGL	OG3-CC1-CC2	3.55	122.67	111.83
23	C	306	CHD	C4-C5-C10	3.52	116.41	112.66
24	c	303	PEK	O03-C21-O04	-3.44	115.02	123.63
14	A	602	HEA	CAD-C3D-C4D	3.43	130.67	124.70
23	J	101	CHD	C6-C5-C4	-3.42	107.32	111.23
25	C	305	CDL	OB8-CB7-C71	3.41	122.23	111.83
14	a	601	HEA	CHA-C4D-C3D	-3.39	119.83	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	606	PGV	O01-C1-C2	3.37	118.77	111.48
22	e	201	PSC	C07-N-C05	3.32	123.09	109.91
14	a	601	HEA	C12-C11-C3B	3.30	117.29	112.12
25	c	305	CDL	OA8-CA7-C31	3.30	121.89	111.83
24	C	308	PEK	O03-C21-C22	3.30	121.89	111.83
24	G	102	PEK	O01-C1-C2	3.29	118.60	111.48
26	c	307	DMU	C6-C1-C2	3.29	116.92	110.01
14	a	602	HEA	O11-C11-C3B	-3.28	105.24	111.26
23	c	302	CHD	O26-C24-C23	3.25	124.27	114.00
26	C	307	DMU	C8-C7-C5	3.25	116.53	110.83
14	A	601	HEA	C2C-C1C-NC	3.24	115.34	110.14
14	a	602	HEA	CHA-C4D-C3D	-3.23	120.06	124.77
14	a	601	HEA	CHB-C1B-C2B	-3.23	119.93	125.03
23	b	301	CHD	C6-C5-C4	-3.22	107.55	111.23
14	A	601	HEA	CHA-C4D-C3D	-3.20	120.11	124.77
14	a	602	HEA	CMD-C2D-C1D	3.19	130.02	125.03
24	C	308	PEK	O03-C21-O04	-3.14	115.77	123.63
14	A	602	HEA	C4B-C3B-C2B	-3.09	102.24	107.44
23	c	302	CHD	C13-C17-C20	-3.08	115.76	119.48
19	A	608	TGL	OG3-CG3-CG2	3.07	117.24	108.40
14	A	602	HEA	CHB-C1B-C2B	-3.06	120.19	125.03
18	G	103	PGV	O01-C1-C2	3.06	118.11	111.48
14	a	601	HEA	C3A-C2A-C1A	-3.04	104.17	107.05
24	G	102	PEK	O03-C21-C22	3.04	121.11	111.83
14	A	602	HEA	C4D-C3D-C2D	-3.04	102.47	106.89
19	D	201	TGL	OG2-CB1-OB1	-3.04	116.60	123.70
19	l	101	TGL	OG3-CC1-CC2	3.04	121.09	111.83
14	A	602	HEA	C4A-NA-C1A	-3.02	100.89	105.82
26	M	101	DMU	O49-C1-C6	-3.02	102.88	110.08
19	i	101	TGL	OG2-CB1-OB1	-3.01	116.67	123.70
23	c	302	CHD	O25-C24-C23	-2.98	113.64	123.09
26	C	307	DMU	C2-C3-C4	-2.98	104.32	110.93
25	C	305	CDL	OA6-CA5-OA7	-2.98	116.74	123.70
14	A	601	HEA	CMB-C2B-C1B	2.98	129.69	125.03
19	i	101	TGL	OG3-CC1-CC2	2.97	120.88	111.83
26	C	307	DMU	O7-C3-C2	2.96	114.76	107.23
25	C	305	CDL	OA8-CA7-C31	2.96	120.85	111.83
26	C	307	DMU	C18-O16-C6	2.95	118.72	113.68
22	B	302	PSC	C08-N-C05	-2.95	98.19	109.91
14	a	602	HEA	C2C-C1C-NC	2.95	114.87	110.14
25	c	305	CDL	OB6-CB5-OB7	-2.94	116.82	123.70
14	a	601	HEA	C2C-C1C-NC	2.94	114.86	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	607	PGV	O01-C1-C2	2.94	117.85	111.48
14	a	602	HEA	C4D-C3D-C2D	-2.93	102.62	106.89
18	A	606	PGV	O03-C01-C02	2.93	116.84	108.40
23	c	306	CHD	C4-C3-C2	-2.92	107.05	110.62
18	C	304	PGV	O03-C19-O04	-2.92	116.32	123.63
23	j	101	CHD	C6-C5-C4	-2.91	107.90	111.23
14	A	601	HEA	CHB-C1B-C2B	-2.90	120.44	125.03
23	C	306	CHD	C4-C3-C2	-2.90	107.08	110.62
22	B	302	PSC	C06-N-C05	2.90	121.45	109.91
19	L	101	TGL	OG3-CC1-CC2	2.89	120.65	111.83
14	A	602	HEA	O11-C11-C3B	-2.86	106.02	111.26
19	i	101	TGL	OG1-CA1-CA2	2.84	120.50	111.83
23	j	101	CHD	C1-C2-C3	2.84	114.24	110.48
19	l	101	TGL	OG1-CA1-CA2	2.83	120.47	111.83
14	a	602	HEA	CAA-C2A-C1A	2.83	130.60	124.85
23	J	101	CHD	C16-C17-C20	2.82	116.45	112.18
22	e	201	PSC	C01-O03-C19	2.82	127.42	117.12
14	a	602	HEA	C1D-ND-C4D	-2.82	101.87	105.21
23	c	302	CHD	C1-C2-C3	-2.81	106.76	110.48
18	G	103	PGV	O03-C19-O04	-2.81	116.60	123.63
14	A	601	HEA	C2A-C1A-NA	2.80	113.03	110.32
23	j	101	CHD	C10-C9-C8	2.80	114.96	111.84
19	D	201	TGL	OG1-CA1-OA1	-2.79	116.64	123.63
23	j	101	CHD	C19-C10-C1	-2.79	103.88	108.31
23	J	101	CHD	C11-C9-C8	2.78	115.01	110.89
19	l	101	TGL	OG2-CB1-OB1	-2.78	117.20	123.70
25	C	305	CDL	CB4-OB6-CB5	-2.78	111.15	117.80
25	G	101	CDL	OA6-CA5-OA7	-2.77	117.23	123.70
23	c	306	CHD	C11-C9-C8	-2.76	106.81	110.89
14	A	601	HEA	C13-C14-C15	-2.76	121.31	127.62
23	j	101	CHD	C13-C14-C8	2.75	118.20	114.72
25	g	103	CDL	OA8-CA7-C31	2.74	120.20	111.83
24	C	309	PEK	C01-O03-C21	2.73	127.11	117.12
24	C	302	PEK	O01-C1-O02	-2.73	117.31	123.70
23	b	301	CHD	C22-C20-C17	2.73	115.99	110.33
14	a	602	HEA	C4C-C3C-C2C	-2.73	103.91	107.30
14	A	601	HEA	O2D-CGD-CBD	2.72	122.61	114.00
26	C	307	DMU	C6-C1-C2	2.72	115.73	110.01
25	G	101	CDL	OA8-CA7-C31	2.72	120.12	111.83
23	J	101	CHD	O26-C24-C23	2.72	122.58	114.00
14	a	602	HEA	C4B-C3B-C2B	-2.70	102.90	107.44
23	B	303	CHD	C19-C10-C1	-2.70	104.02	108.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	m	401	DMU	O1-C9-C8	2.67	114.51	109.70
26	M	101	DMU	C18-O16-C6	-2.66	109.13	113.68
22	B	302	PSC	O03-C19-C20	2.66	119.93	111.83
18	A	606	PGV	O03-C19-O04	-2.64	117.03	123.63
25	G	101	CDL	OB8-CB7-C71	2.64	119.87	111.83
18	a	607	PGV	O03-C19-C20	2.62	119.83	111.83
23	J	101	CHD	C19-C10-C1	-2.62	104.14	108.31
18	c	304	PGV	O01-C1-O02	-2.61	117.59	123.70
14	a	602	HEA	O1D-CGD-CBD	-2.60	114.84	123.09
18	C	303	PGV	O01-C1-C2	2.60	117.11	111.48
23	b	301	CHD	C1-C10-C9	2.60	115.38	111.34
19	L	101	TGL	OG3-CC1-OC1	-2.60	117.12	123.63
23	c	306	CHD	C1-C10-C9	2.60	115.37	111.34
26	M	101	DMU	O1-C10-C5	-2.58	105.07	110.37
22	B	302	PSC	C04-C05-N	2.58	124.10	115.82
14	A	601	HEA	C4D-C3D-C2D	-2.58	103.14	106.89
25	C	305	CDL	OB6-CB5-OB7	-2.58	117.68	123.70
14	A	602	HEA	C4B-NB-C1B	-2.57	102.16	105.21
14	a	601	HEA	CAD-C3D-C4D	2.56	129.16	124.70
23	c	306	CHD	C23-C22-C20	-2.55	109.69	114.46
14	A	601	HEA	O1D-CGD-CBD	-2.55	115.00	123.09
23	B	303	CHD	C5-C6-C7	2.55	117.43	114.40
19	A	608	TGL	CG1-OG1-CA1	2.54	126.42	117.12
23	b	301	CHD	C4-C5-C10	2.54	115.36	112.66
24	C	308	PEK	O01-C1-O02	-2.54	117.78	123.70
23	c	306	CHD	C10-C9-C8	2.53	114.66	111.84
14	A	602	HEA	CHD-C1D-C2D	-2.52	119.78	126.95
19	i	101	TGL	OG3-CG3-CG2	2.52	115.66	108.40
22	e	201	PSC	O01-C1-O02	-2.52	117.82	123.70
14	a	602	HEA	C4A-NA-C1A	-2.51	101.72	105.82
14	a	602	HEA	CHD-C1D-C2D	-2.51	119.82	126.95
25	G	101	CDL	OB6-CB5-OB7	-2.50	117.85	123.70
18	a	607	PGV	O01-C1-O02	-2.50	117.87	123.70
14	a	602	HEA	CHC-C1C-C2C	-2.50	120.18	127.43
14	A	601	HEA	CHD-C1D-C2D	-2.49	119.86	126.95
14	a	601	HEA	C4B-C3B-C2B	-2.49	103.25	107.44
25	C	305	CDL	O1-C1-CB2	2.49	118.30	109.70
23	c	306	CHD	C6-C5-C4	-2.49	108.38	111.23
26	c	307	DMU	C1-C2-C3	2.48	115.31	109.68
23	c	302	CHD	C6-C7-C8	2.46	114.19	111.50
22	e	201	PSC	O03-C19-O04	-2.46	117.47	123.63
23	c	306	CHD	C9-C10-C5	2.46	111.93	108.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	301	CHD	C5-C4-C3	2.46	116.42	112.71
19	a	606	TGL	OG3-CC1-OC1	-2.46	117.48	123.63
18	c	304	PGV	O03-C19-O04	-2.46	117.48	123.63
14	a	602	HEA	C26-C15-C16	2.45	119.48	115.23
14	A	602	HEA	O1A-CGA-CBA	-2.43	115.38	123.09
24	C	309	PEK	O03-C01-C02	2.43	115.40	108.40
23	B	303	CHD	O26-C24-C23	2.43	121.67	114.00
19	A	608	TGL	CC3-CC2-CC1	-2.42	104.81	113.69
14	a	602	HEA	CHA-C1A-C2A	-2.42	121.04	124.86
25	g	103	CDL	OB8-CB7-OB9	-2.42	117.57	123.63
14	A	601	HEA	C3A-C2A-C1A	-2.41	104.76	107.05
14	a	602	HEA	OMA-CMA-C3A	-2.41	120.18	125.62
14	a	601	HEA	CHD-C1D-C2D	-2.40	120.12	126.95
25	C	305	CDL	OB8-CB7-OB9	-2.40	117.62	123.63
25	c	305	CDL	OA8-CA7-OA9	-2.39	117.64	123.63
23	b	301	CHD	C18-C13-C12	-2.39	106.67	109.06
14	A	601	HEA	CMC-C2C-C1C	2.38	129.04	125.42
24	G	102	PEK	C01-O03-C21	2.37	125.80	117.12
23	j	101	CHD	C14-C13-C12	-2.37	105.25	107.42
18	c	301	PGV	O01-C1-C2	2.37	116.60	111.48
24	C	309	PEK	O03-C21-C22	2.37	119.05	111.83
14	A	601	HEA	C4B-C3B-C2B	-2.36	103.47	107.44
19	l	101	TGL	CG3-OG3-CC1	2.36	125.75	117.12
23	c	306	CHD	C2-C1-C10	2.36	116.72	112.74
19	L	101	TGL	OG3-CG3-CG2	2.36	115.19	108.40
23	c	302	CHD	C19-C10-C1	-2.35	104.56	108.31
18	A	607	PGV	O03-C19-C20	2.35	119.00	111.83
23	C	301	CHD	C19-C10-C1	-2.34	104.59	108.31
26	C	307	DMU	O5-C4-C57	2.34	112.23	106.44
14	a	602	HEA	C4B-NB-C1B	-2.33	102.44	105.21
23	j	101	CHD	C6-C7-C8	2.33	114.05	111.50
14	a	601	HEA	CHC-C1C-C2C	-2.33	120.66	127.43
23	C	306	CHD	C9-C10-C5	2.32	111.73	108.51
18	A	607	PGV	O01-C1-O02	-2.31	118.30	123.70
14	A	602	HEA	O2A-CGA-CBA	2.31	121.30	114.00
18	C	303	PGV	O03-C19-C20	2.31	118.86	111.83
14	a	601	HEA	O2D-CGD-CBD	2.30	121.27	114.00
14	A	601	HEA	CHC-C1C-C2C	-2.30	120.75	127.43
23	b	301	CHD	C11-C12-C13	2.30	113.60	111.26
23	J	101	CHD	C21-C20-C17	-2.30	109.43	112.88
23	c	306	CHD	O25-C24-C23	-2.30	115.80	123.09
24	g	102	PEK	O03-C21-O04	-2.29	117.89	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	102	PEK	O01-C1-C2	2.28	116.40	111.48
23	c	302	CHD	C18-C13-C12	2.28	111.33	109.06
25	c	305	CDL	OB8-CB7-OB9	-2.27	117.94	123.63
18	A	606	PGV	O01-C02-C03	2.27	116.47	108.34
23	B	303	CHD	C22-C20-C17	2.26	115.02	110.33
23	c	306	CHD	C1-C2-C3	2.26	113.47	110.48
23	b	301	CHD	C19-C10-C1	-2.26	104.72	108.31
24	G	102	PEK	O03-C01-C02	2.25	114.89	108.40
14	A	602	HEA	CHC-C1C-C2C	-2.24	120.92	127.43
23	B	303	CHD	C6-C5-C4	-2.24	108.67	111.23
19	D	201	TGL	CG3-OG3-CC1	2.23	125.29	117.12
14	A	601	HEA	O1A-CGA-CBA	-2.23	116.01	123.09
18	G	103	PGV	O03-C01-C02	2.21	114.76	108.40
14	a	601	HEA	C1D-ND-C4D	-2.21	102.59	105.21
14	A	602	HEA	C4C-C3C-C2C	-2.20	104.57	107.30
23	c	302	CHD	C14-C13-C12	-2.19	105.41	107.42
26	M	101	DMU	O1-C9-C11	2.19	111.87	106.44
26	C	307	DMU	C10-O1-C9	2.18	117.98	113.72
23	c	302	CHD	C11-C9-C8	2.18	114.12	110.89
25	g	103	CDL	OA8-CA7-OA9	-2.17	118.20	123.63
25	g	103	CDL	OA6-CA5-OA7	-2.16	118.66	123.70
14	a	601	HEA	C4A-NA-C1A	-2.16	102.30	105.82
23	B	303	CHD	C11-C12-C13	2.16	113.46	111.26
22	B	302	PSC	O03-C01-C02	2.15	114.61	108.40
14	A	602	HEA	C26-C15-C16	2.15	118.97	115.23
25	C	305	CDL	OA8-CA7-OA9	-2.14	118.26	123.63
14	a	601	HEA	OMA-CMA-C3A	-2.14	120.80	125.62
25	c	305	CDL	OA6-CA5-OA7	-2.14	118.71	123.70
23	b	301	CHD	C1-C10-C5	-2.13	104.68	107.75
14	a	601	HEA	C4B-NB-C1B	-2.13	102.68	105.21
23	b	301	CHD	O26-C24-C23	2.13	120.72	114.00
23	B	303	CHD	C1-C10-C9	2.13	114.64	111.34
23	c	302	CHD	C5-C4-C3	-2.12	109.50	112.71
14	A	601	HEA	CAD-C3D-C4D	2.12	128.40	124.70
23	J	101	CHD	C18-C13-C17	2.12	114.53	111.20
14	a	601	HEA	CHC-C4B-NB	-2.12	121.75	124.37
23	C	306	CHD	C19-C10-C1	-2.12	104.94	108.31
14	A	601	HEA	O11-C11-C3B	-2.12	107.38	111.26
23	b	301	CHD	C18-C13-C14	2.11	114.51	111.20
14	A	602	HEA	CHB-C4A-NA	-2.10	122.16	124.45
26	m	401	DMU	O1-C10-C5	-2.10	106.06	110.37
18	c	301	PGV	C02-O01-C1	-2.09	112.80	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	CMD-C2D-C1D	2.08	128.28	125.03
23	c	306	CHD	C19-C10-C9	-2.08	108.38	111.18
14	A	601	HEA	C4B-NB-C1B	-2.07	102.75	105.21
14	A	601	HEA	CHC-C4B-C3B	-2.07	120.59	125.80
14	a	601	HEA	C4C-C3C-C2C	-2.06	104.74	107.30
25	g	103	CDL	OB8-CB7-C71	2.06	118.12	111.83
14	a	602	HEA	C27-C19-C20	2.06	118.80	115.23
14	a	601	HEA	CBA-CAA-C2A	-2.06	106.84	112.53
18	A	606	PGV	C21-C20-C19	2.05	121.22	113.69
18	A	606	PGV	C01-O03-C19	2.05	124.62	117.12
19	a	606	TGL	OG1-CA1-CA2	2.05	118.07	111.83
14	a	602	HEA	O11-C11-C12	2.04	114.54	109.14
23	c	306	CHD	C11-C9-C10	2.03	115.77	113.70
26	c	307	DMU	C18-O16-C6	2.03	117.15	113.68
23	B	303	CHD	O25-C24-C23	-2.02	116.70	123.09
14	A	602	HEA	CHC-C4B-C3B	-2.02	120.72	125.80
23	C	301	CHD	C21-C20-C22	-2.01	107.22	110.34
18	a	607	PGV	O03-C01-C02	2.01	114.20	108.40
23	c	302	CHD	C11-C12-C13	2.01	113.31	111.26
23	C	301	CHD	O7-C7-C8	2.01	114.12	109.52
23	c	306	CHD	C4-C5-C10	2.01	114.79	112.66

There are no chirality outliers.

All (801) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C03-O11-P-O12
18	A	606	PGV	C03-O11-P-O13
18	A	606	PGV	C03-O11-P-O14
18	A	606	PGV	O12-C04-C05-O05
18	C	304	PGV	C03-O11-P-O12
18	C	304	PGV	C03-O11-P-O13
18	C	304	PGV	C03-O11-P-O14
18	C	304	PGV	C04-O12-P-O11
18	C	304	PGV	C04-O12-P-O13
18	C	304	PGV	C04-O12-P-O14
18	G	103	PGV	C03-O11-P-O12
18	G	103	PGV	C03-O11-P-O13
18	G	103	PGV	C04-C05-C06-O06
18	a	607	PGV	C03-O11-P-O12
18	a	607	PGV	C03-O11-P-O14
18	a	607	PGV	C04-O12-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	607	PGV	C04-O12-P-O14
18	a	607	PGV	C2-C1-O01-C02
19	A	608	TGL	CB2-CB1-OG2-CG2
19	A	608	TGL	OB1-CB1-OG2-CG2
19	L	101	TGL	CB2-CB1-OG2-CG2
19	a	606	TGL	CB2-CB1-OG2-CG2
22	B	302	PSC	C04-O12-P-O11
22	B	302	PSC	C04-O12-P-O13
22	B	302	PSC	O12-C04-C05-N
22	B	302	PSC	C05-C04-O12-P
22	e	201	PSC	C03-O11-P-O13
22	e	201	PSC	C04-O12-P-O11
22	e	201	PSC	C04-O12-P-O14
22	e	201	PSC	O02-C1-O01-C02
22	e	201	PSC	O04-C19-O03-C01
22	e	201	PSC	C20-C19-O03-C01
24	C	308	PEK	C04-O12-P-O11
24	C	308	PEK	C04-O12-P-O14
24	C	308	PEK	O02-C1-O01-C02
24	C	308	PEK	C2-C1-O01-C02
24	C	309	PEK	C04-O12-P-O11
24	C	309	PEK	C04-O12-P-O13
24	C	309	PEK	O12-C04-C05-N
24	G	102	PEK	C03-O11-P-O12
24	G	102	PEK	C03-O11-P-O14
24	c	303	PEK	C04-O12-P-O14
24	c	303	PEK	C2-C1-O01-C02
24	g	102	PEK	C9-C10-C11-C12
25	C	305	CDL	C1-CA2-OA2-PA1
25	C	305	CDL	OA7-CA5-OA6-CA4
25	C	305	CDL	C11-CA5-OA6-CA4
25	C	305	CDL	CB3-OB5-PB2-OB3
25	G	101	CDL	CA2-C1-CB2-OB2
25	G	101	CDL	CA2-OA2-PA1-OA4
25	G	101	CDL	CA2-OA2-PA1-OA5
25	G	101	CDL	CA3-OA5-PA1-OA2
25	G	101	CDL	CA3-OA5-PA1-OA3
25	G	101	CDL	OA7-CA5-OA6-CA4
25	G	101	CDL	CB3-OB5-PB2-OB2
25	G	101	CDL	CB3-OB5-PB2-OB3
25	G	101	CDL	CB3-OB5-PB2-OB4
25	c	305	CDL	C1-CA2-OA2-PA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	305	CDL	CA2-OA2-PA1-OA3
25	c	305	CDL	CA2-OA2-PA1-OA4
25	c	305	CDL	CA2-OA2-PA1-OA5
25	c	305	CDL	CA3-OA5-PA1-OA2
25	c	305	CDL	CA3-OA5-PA1-OA4
25	c	305	CDL	C11-CA5-OA6-CA4
25	c	305	CDL	CB3-OB5-PB2-OB2
25	c	305	CDL	CB3-OB5-PB2-OB3
25	c	305	CDL	CB3-OB5-PB2-OB4
25	g	103	CDL	CA2-OA2-PA1-OA3
25	g	103	CDL	CA3-OA5-PA1-OA3
25	g	103	CDL	OA7-CA5-OA6-CA4
25	g	103	CDL	CB2-OB2-PB2-OB5
25	g	103	CDL	OB6-CB4-CB6-OB8
26	c	307	DMU	O5-C6-O16-C18
19	a	606	TGL	CC2-CC1-OG3-CG3
18	G	103	PGV	O04-C19-O03-C01
19	a	606	TGL	OC1-CC1-OG3-CG3
25	G	101	CDL	OB9-CB7-OB8-CB6
24	C	308	PEK	O04-C21-O03-C01
18	a	607	PGV	O02-C1-O01-C02
19	L	101	TGL	OB1-CB1-OG2-CG2
19	a	606	TGL	OB1-CB1-OG2-CG2
24	c	303	PEK	O02-C1-O01-C02
25	c	305	CDL	OA7-CA5-OA6-CA4
18	G	103	PGV	C20-C19-O03-C01
25	G	101	CDL	C31-CA7-OA8-CA6
22	e	201	PSC	C2-C1-O01-C02
25	G	101	CDL	C11-CA5-OA6-CA4
25	g	103	CDL	C11-CA5-OA6-CA4
19	D	201	TGL	OC1-CC1-OG3-CG3
19	L	101	TGL	CA2-CA1-OG1-CG1
24	C	308	PEK	C22-C21-O03-C01
24	g	102	PEK	C22-C21-O03-C01
25	G	101	CDL	C71-CB7-OB8-CB6
19	l	101	TGL	OA1-CA1-OG1-CG1
25	G	101	CDL	OA9-CA7-OA8-CA6
18	C	304	PGV	O02-C1-O01-C02
25	C	305	CDL	O1-C1-CB2-OB2
25	G	101	CDL	O1-C1-CB2-OB2
19	A	608	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	CC2-CC1-OG3-CG3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	g	103	CDL	C31-CA7-OA8-CA6
18	C	304	PGV	C2-C1-O01-C02
19	i	101	TGL	CB2-CB1-OG2-CG2
24	g	102	PEK	O04-C21-O03-C01
19	l	101	TGL	CA2-CA1-OG1-CG1
25	C	305	CDL	C31-CA7-OA8-CA6
19	L	101	TGL	OA1-CA1-OG1-CG1
25	g	103	CDL	OA9-CA7-OA8-CA6
23	J	101	CHD	C13-C17-C20-C22
23	j	101	CHD	C13-C17-C20-C22
25	C	305	CDL	OA9-CA7-OA8-CA6
26	c	307	DMU	O5-C4-C57-O61
25	G	101	CDL	C51-CB5-OB6-CB4
19	A	608	TGL	OC1-CC1-OG3-CG3
19	i	101	TGL	OB1-CB1-OG2-CG2
18	A	606	PGV	O12-C04-C05-C06
25	C	305	CDL	CA2-C1-CB2-OB2
19	D	201	TGL	CA2-CA1-OG1-CG1
25	c	305	CDL	C31-CA7-OA8-CA6
26	c	307	DMU	C3-C4-C57-O61
26	m	401	DMU	C3-C4-C57-O61
26	c	307	DMU	C1-C6-O16-C18
18	C	304	PGV	O12-C04-C05-O05
25	g	103	CDL	O1-C1-CA2-OA2
25	c	305	CDL	OA9-CA7-OA8-CA6
23	C	306	CHD	C17-C20-C22-C23
23	j	101	CHD	C17-C20-C22-C23
23	J	101	CHD	C17-C20-C22-C23
18	a	607	PGV	C20-C19-O03-C01
25	C	305	CDL	C71-CB7-OB8-CB6
24	C	308	PEK	C21-C22-C23-C24
25	G	101	CDL	OB7-CB5-OB6-CB4
26	m	401	DMU	O6-C11-C9-C8
24	C	302	PEK	C1-C2-C3-C4
19	D	201	TGL	OA1-CA1-OG1-CG1
23	b	301	CHD	C17-C20-C22-C23
26	C	307	DMU	O1-C10-O7-C3
23	J	101	CHD	C21-C20-C22-C23
18	a	607	PGV	C1-C2-C3-C4
19	L	101	TGL	CA1-CA2-CA3-CA4
19	i	101	TGL	CC1-CC2-CC3-CC4
25	C	305	CDL	CB7-C71-C72-C73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	305	CDL	CB7-C71-C72-C73
18	G	103	PGV	C1-C2-C3-C4
18	c	301	PGV	C19-C20-C21-C22
19	D	201	TGL	CA1-CA2-CA3-CA4
23	C	306	CHD	C21-C20-C22-C23
23	j	101	CHD	C21-C20-C22-C23
26	m	401	DMU	O5-C4-C57-O61
19	L	101	TGL	CC2-CC1-OG3-CG3
25	g	103	CDL	C71-CB7-OB8-CB6
18	G	103	PGV	C2-C1-O01-C02
25	C	305	CDL	C51-CB5-OB6-CB4
18	G	103	PGV	O02-C1-O01-C02
19	D	201	TGL	OB1-CB1-OG2-CG2
25	C	305	CDL	OB7-CB5-OB6-CB4
25	g	103	CDL	CB2-C1-CA2-OA2
22	B	302	PSC	C20-C19-O03-C01
19	D	201	TGL	CB2-CB1-OG2-CG2
18	c	301	PGV	C1-C2-C3-C4
18	a	607	PGV	O04-C19-O03-C01
19	L	101	TGL	OC1-CC1-OG3-CG3
18	A	606	PGV	C04-C05-C06-O06
18	A	606	PGV	C03-C02-O01-C1
25	C	305	CDL	OB9-CB7-OB8-CB6
25	c	305	CDL	OB7-CB5-OB6-CB4
25	c	305	CDL	C51-CB5-OB6-CB4
25	G	101	CDL	CB5-C51-C52-C53
25	c	305	CDL	C16-C17-C18-C19
18	c	301	PGV	C7-C8-C9-C10
19	A	608	TGL	C18-C19-C33-C34
19	L	101	TGL	CB3-CB4-CB5-CB6
19	L	101	TGL	C11-C10-CB9-CB8
19	i	101	TGL	C11-C12-C13-C14
19	l	101	TGL	CC9-C15-C16-C17
24	c	303	PEK	C16-C17-C18-C19
19	D	201	TGL	C18-C19-C33-C34
19	a	606	TGL	C21-C20-CA9-CA8
24	C	309	PEK	C27-C28-C29-C30
25	c	305	CDL	C59-C60-C61-C62
25	g	103	CDL	OB9-CB7-OB8-CB6
18	A	607	PGV	C22-C23-C24-C25
24	G	102	PEK	C29-C30-C31-C32
25	G	101	CDL	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	G	101	CDL	C80-C81-C82-C83
25	c	305	CDL	C43-C44-C45-C46
25	g	103	CDL	C52-C53-C54-C55
26	c	307	DMU	C25-C28-C31-C34
18	G	103	PGV	O05-C05-C06-O06
18	A	606	PGV	C5-C6-C7-C8
19	A	608	TGL	C15-C16-C17-C18
19	l	101	TGL	C20-C21-C22-C23
25	G	101	CDL	C32-C33-C34-C35
25	C	305	CDL	C16-C17-C18-C19
19	l	101	TGL	CC3-CC4-CC5-CC6
19	l	101	TGL	CB2-CB1-OG2-CG2
25	C	305	CDL	C32-C33-C34-C35
18	a	607	PGV	O12-C04-C05-O05
18	C	303	PGV	C19-C20-C21-C22
19	L	101	TGL	CC1-CC2-CC3-CC4
19	l	101	TGL	CA5-CA6-CA7-CA8
19	l	101	TGL	CA3-CA4-CA5-CA6
22	e	201	PSC	C29-C30-C31-C32
26	c	307	DMU	C28-C31-C34-C37
19	L	101	TGL	C22-C23-C24-C25
26	C	307	DMU	C3-C4-C57-O61
23	J	101	CHD	C13-C17-C20-C21
24	C	302	PEK	C16-C17-C18-C19
22	B	302	PSC	O04-C19-O03-C01
18	G	103	PGV	C5-C6-C7-C8
19	D	201	TGL	CA9-C20-C21-C22
25	c	305	CDL	C52-C53-C54-C55
18	G	103	PGV	C7-C8-C9-C10
25	g	103	CDL	C56-C57-C58-C59
19	i	101	TGL	CC2-CC1-OG3-CG3
19	i	101	TGL	CC3-CC4-CC5-CC6
25	C	305	CDL	C12-C13-C14-C15
25	C	305	CDL	C33-C34-C35-C36
25	G	101	CDL	C34-C35-C36-C37
25	g	103	CDL	C19-C20-C21-C22
19	D	201	TGL	CC6-CC7-CC8-CC9
25	C	305	CDL	C22-C23-C24-C25
25	c	305	CDL	C41-C42-C43-C44
25	g	103	CDL	C13-C14-C15-C16
25	g	103	CDL	C31-C32-C33-C34
25	g	103	CDL	C59-C60-C61-C62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	g	103	CDL	C80-C81-C82-C83
19	a	606	TGL	C10-C11-C12-C13
25	G	101	CDL	C56-C57-C58-C59
25	c	305	CDL	C56-C57-C58-C59
25	g	103	CDL	C53-C54-C55-C56
18	C	304	PGV	C5-C6-C7-C8
19	l	101	TGL	CC7-CC8-CC9-C15
24	c	303	PEK	C25-C26-C27-C28
26	m	401	DMU	C25-C28-C31-C34
23	j	101	CHD	C16-C17-C20-C21
25	C	305	CDL	C51-C52-C53-C54
26	c	307	DMU	C22-C25-C28-C31
25	c	305	CDL	CA5-C11-C12-C13
25	g	103	CDL	CA5-C11-C12-C13
18	C	304	PGV	C22-C23-C24-C25
25	g	103	CDL	C51-CB5-OB6-CB4
19	a	606	TGL	C15-C16-C17-C18
25	c	305	CDL	C63-C64-C65-C66
19	D	201	TGL	CA7-CA8-CA9-C20
25	G	101	CDL	C14-C15-C16-C17
24	c	303	PEK	C28-C29-C30-C31
18	c	301	PGV	C26-C27-C28-C29
19	A	608	TGL	CA4-CA5-CA6-CA7
25	G	101	CDL	C37-C38-C39-C40
25	G	101	CDL	C79-C80-C81-C82
23	j	101	CHD	C13-C17-C20-C21
19	L	101	TGL	CC9-C15-C16-C17
19	L	101	TGL	C15-C16-C17-C18
24	C	308	PEK	C24-C25-C26-C27
25	C	305	CDL	CA7-C31-C32-C33
25	g	103	CDL	C14-C15-C16-C17
23	J	101	CHD	C16-C17-C20-C22
19	A	608	TGL	CC9-C15-C16-C17
19	D	201	TGL	C17-C18-C19-C33
24	C	308	PEK	C33-C34-C35-C36
24	C	309	PEK	C28-C29-C30-C31
25	c	305	CDL	C77-C78-C79-C80
19	a	606	TGL	CC7-CC8-CC9-C15
25	c	305	CDL	C75-C76-C77-C78
18	c	304	PGV	C23-C24-C25-C26
19	l	101	TGL	CB4-CB5-CB6-CB7
25	C	305	CDL	C81-C82-C83-C84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	G	103	PGV	C21-C22-C23-C24
19	i	101	TGL	CB5-CB6-CB7-CB8
19	l	101	TGL	C19-C33-C34-C35
24	g	102	PEK	C30-C31-C32-C33
25	G	101	CDL	C23-C24-C25-C26
25	c	305	CDL	C36-C37-C38-C39
18	A	606	PGV	C2-C1-O01-C02
22	B	302	PSC	C2-C1-O01-C02
24	G	102	PEK	C2-C1-O01-C02
25	g	103	CDL	CA7-C31-C32-C33
19	l	101	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	CA2-CA3-CA4-CA5
19	i	101	TGL	C20-C21-C22-C23
25	g	103	CDL	C54-C55-C56-C57
19	L	101	TGL	C23-C24-C25-C26
18	G	103	PGV	C27-C28-C29-C30
19	D	201	TGL	CB7-CB8-CB9-C10
25	C	305	CDL	C58-C59-C60-C61
19	D	201	TGL	CB6-CB7-CB8-CB9
23	c	306	CHD	C20-C22-C23-C24
22	B	302	PSC	C24-C25-C26-C27
22	e	201	PSC	C04-C05-N-C07
19	L	101	TGL	C14-C29-C30-C31
19	a	606	TGL	CB5-CB6-CB7-CB8
25	c	305	CDL	C39-C40-C41-C42
19	l	101	TGL	CC6-CC7-CC8-CC9
23	j	101	CHD	C16-C17-C20-C22
18	G	103	PGV	C4-C5-C6-C7
19	i	101	TGL	C13-C14-C29-C30
19	A	608	TGL	C11-C10-CB9-CB8
19	L	101	TGL	CB6-CB7-CB8-CB9
24	C	309	PEK	C26-C27-C28-C29
25	g	103	CDL	CB7-C71-C72-C73
22	B	302	PSC	C2-C3-C4-C5
18	C	304	PGV	O01-C02-C03-O11
19	i	101	TGL	C15-C16-C17-C18
19	L	101	TGL	CC3-CC4-CC5-CC6
22	e	201	PSC	C27-C28-C29-C30
24	C	308	PEK	C22-C23-C24-C25
22	B	302	PSC	C1-C2-C3-C4
18	C	303	PGV	C21-C22-C23-C24
19	L	101	TGL	CB2-CB3-CB4-CB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	O03-C01-C02-O01
18	G	103	PGV	C12-C13-C14-C15
24	c	303	PEK	C2-C3-C4-C5
18	a	607	PGV	C6-C7-C8-C9
18	c	301	PGV	C2-C3-C4-C5
19	A	608	TGL	CC4-CC5-CC6-CC7
19	A	608	TGL	C20-C21-C22-C23
18	A	607	PGV	C27-C28-C29-C30
19	L	101	TGL	C17-C18-C19-C33
19	i	101	TGL	CC7-CC8-CC9-C15
19	i	101	TGL	C16-C17-C18-C19
18	A	606	PGV	C20-C21-C22-C23
18	G	103	PGV	C24-C25-C26-C27
19	i	101	TGL	CA4-CA5-CA6-CA7
19	L	101	TGL	C21-C22-C23-C24
18	A	606	PGV	O02-C1-O01-C02
22	B	302	PSC	O02-C1-O01-C02
18	C	304	PGV	O12-C04-C05-C06
22	e	201	PSC	C28-C29-C30-C31
25	C	305	CDL	C36-C37-C38-C39
25	G	101	CDL	C19-C20-C21-C22
25	g	103	CDL	C62-C63-C64-C65
19	L	101	TGL	C16-C15-CC9-CC8
25	g	103	CDL	C34-C35-C36-C37
25	G	101	CDL	C11-C12-C13-C14
25	C	305	CDL	C41-C42-C43-C44
18	c	304	PGV	C7-C8-C9-C10
25	C	305	CDL	C43-C44-C45-C46
19	i	101	TGL	OC1-CC1-OG3-CG3
23	J	101	CHD	C16-C17-C20-C21
18	A	607	PGV	C5-C6-C7-C8
19	D	201	TGL	C10-C11-C12-C13
19	a	606	TGL	C19-C33-C34-C35
25	G	101	CDL	C72-C73-C74-C75
18	a	607	PGV	C3-C4-C5-C6
18	A	606	PGV	C11-C10-C9-C8
18	C	303	PGV	C11-C10-C9-C8
18	c	304	PGV	C12-C13-C14-C15
22	e	201	PSC	C6-C7-C8-C9
24	C	309	PEK	C01-C02-C03-O11
25	g	103	CDL	OB5-CB3-CB4-CB6
24	G	102	PEK	O02-C1-O01-C02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	g	103	CDL	OB7-CB5-OB6-CB4
24	c	303	PEK	C34-C35-C36-C37
18	A	607	PGV	C19-C20-C21-C22
25	c	305	CDL	C62-C63-C64-C65
18	C	304	PGV	C20-C21-C22-C23
19	L	101	TGL	C12-C13-C14-C29
18	A	606	PGV	O03-C01-C02-C03
19	D	201	TGL	OG1-CG1-CG2-CG3
25	C	305	CDL	CB3-CB4-CB6-OB8
25	G	101	CDL	CB3-CB4-CB6-OB8
25	g	103	CDL	C37-C38-C39-C40
26	C	307	DMU	O6-C11-C9-O1
18	c	301	PGV	C12-C13-C14-C15
19	A	608	TGL	CB6-CB7-CB8-CB9
19	A	608	TGL	C22-C23-C24-C25
22	B	302	PSC	C23-C24-C25-C26
24	C	302	PEK	C25-C26-C27-C28
18	C	303	PGV	C24-C25-C26-C27
19	L	101	TGL	CB5-CB6-CB7-CB8
19	L	101	TGL	C11-C12-C13-C14
19	i	101	TGL	CA6-CA7-CA8-CA9
19	i	101	TGL	CB2-CB3-CB4-CB5
19	A	608	TGL	CC3-CC4-CC5-CC6
19	l	101	TGL	CB9-C10-C11-C12
24	C	309	PEK	C31-C32-C33-C34
19	a	606	TGL	CA6-CA7-CA8-CA9
22	B	302	PSC	C20-C21-C22-C23
26	c	307	DMU	O6-C11-C9-O1
18	C	303	PGV	C22-C23-C24-C25
26	c	307	DMU	C18-C19-C22-C25
19	D	201	TGL	CC5-CC6-CC7-CC8
19	l	101	TGL	CB5-CB6-CB7-CB8
24	G	102	PEK	C22-C23-C24-C25
24	G	102	PEK	C25-C26-C27-C28
24	g	102	PEK	C28-C29-C30-C31
25	g	103	CDL	C74-C75-C76-C77
26	c	307	DMU	C31-C34-C37-C40
19	L	101	TGL	CA6-CA7-CA8-CA9
24	C	309	PEK	C24-C25-C26-C27
25	g	103	CDL	C63-C64-C65-C66
18	C	304	PGV	C11-C10-C9-C8
22	B	302	PSC	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	C	308	PEK	C15-C16-C17-C18
18	A	607	PGV	C7-C8-C9-C10
24	C	308	PEK	C23-C24-C25-C26
25	G	101	CDL	C39-C40-C41-C42
25	G	101	CDL	C82-C83-C84-C85
25	G	101	CDL	C76-C77-C78-C79
25	c	305	CDL	C55-C56-C57-C58
24	g	102	PEK	C27-C28-C29-C30
25	c	305	CDL	C19-C20-C21-C22
25	c	305	CDL	C20-C21-C22-C23
22	B	302	PSC	O01-C02-C03-O11
18	A	606	PGV	C27-C28-C29-C30
19	A	608	TGL	C33-C34-C35-C36
19	a	606	TGL	CA9-C20-C21-C22
25	G	101	CDL	C81-C82-C83-C84
24	g	102	PEK	C24-C25-C26-C27
25	c	305	CDL	C15-C16-C17-C18
24	G	102	PEK	C26-C27-C28-C29
25	C	305	CDL	C77-C78-C79-C80
25	c	305	CDL	C38-C39-C40-C41
18	a	607	PGV	C13-C14-C15-C16
18	c	304	PGV	C25-C26-C27-C28
19	D	201	TGL	C14-C29-C30-C31
25	c	305	CDL	C33-C34-C35-C36
19	i	101	TGL	C29-C30-C31-C32
18	C	304	PGV	C13-C14-C15-C16
24	C	309	PEK	C30-C31-C32-C33
18	G	103	PGV	C15-C16-C17-C18
25	G	101	CDL	C44-C45-C46-C47
25	G	101	CDL	C12-C13-C14-C15
19	i	101	TGL	C21-C20-CA9-CA8
22	e	201	PSC	C25-C26-C27-C28
18	G	103	PGV	C11-C10-C9-C8
18	a	607	PGV	C24-C25-C26-C27
22	B	302	PSC	C15-C16-C17-C18
18	G	103	PGV	C20-C21-C22-C23
19	L	101	TGL	CC7-CC8-CC9-C15
24	G	102	PEK	C32-C33-C34-C35
18	C	304	PGV	C20-C19-O03-C01
19	L	101	TGL	CA5-CA6-CA7-CA8
19	a	606	TGL	C20-C21-C22-C23
18	c	304	PGV	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	a	606	TGL	C33-C34-C35-C36
22	e	201	PSC	C15-C16-C17-C18
19	A	608	TGL	C16-C17-C18-C19
25	G	101	CDL	C64-C65-C66-C67
25	G	101	CDL	C75-C76-C77-C78
18	c	304	PGV	O05-C05-C06-O06
18	c	301	PGV	C22-C23-C24-C25
19	D	201	TGL	C16-C15-CC9-CC8
19	L	101	TGL	C21-C20-CA9-CA8
19	L	101	TGL	C33-C34-C35-C36
26	C	307	DMU	O5-C4-C57-O61
18	c	301	PGV	C6-C7-C8-C9
24	c	303	PEK	C29-C30-C31-C32
19	D	201	TGL	C21-C20-CA9-CA8
22	B	302	PSC	C5-C6-C7-C8
18	A	606	PGV	C01-C02-C03-O11
18	C	304	PGV	C01-C02-C03-O11
25	G	101	CDL	OA5-CA3-CA4-CA6
25	c	305	CDL	OA5-CA3-CA4-CA6
25	g	103	CDL	OA5-CA3-CA4-CA6
18	A	606	PGV	C29-C30-C31-C32
22	B	302	PSC	C04-C05-N-C07
19	D	201	TGL	C25-C26-C27-C28
25	C	305	CDL	C84-C85-C86-C87
25	G	101	CDL	C24-C25-C26-C27
24	C	309	PEK	C25-C26-C27-C28
26	M	101	DMU	O6-C11-C9-C8
26	m	401	DMU	O6-C11-C9-O1
24	C	302	PEK	C31-C32-C33-C34
25	g	103	CDL	C76-C77-C78-C79
18	c	304	PGV	C20-C19-O03-C01
19	A	608	TGL	OG1-CG1-CG2-CG3
19	L	101	TGL	CA4-CA5-CA6-CA7
19	i	101	TGL	C25-C26-C27-C28
24	C	309	PEK	C17-C18-C19-C20
19	D	201	TGL	C11-C10-CB9-CB8
18	C	304	PGV	C24-C25-C26-C27
25	C	305	CDL	C31-C32-C33-C34
24	C	308	PEK	C35-C36-C37-C38
18	a	607	PGV	C11-C10-C9-C8
24	C	302	PEK	C15-C16-C17-C18
18	A	606	PGV	C02-C03-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	C	304	PGV	C02-C03-O11-P
24	C	308	PEK	C29-C30-C31-C32
24	G	102	PEK	C34-C35-C36-C37
25	g	103	CDL	C11-C12-C13-C14
24	c	303	PEK	O03-C01-C02-O01
25	G	101	CDL	OB6-CB4-CB6-OB8
24	C	302	PEK	C5-C6-C7-C8
24	C	302	PEK	C9-C10-C11-C12
24	C	308	PEK	C9-C10-C11-C12
24	C	309	PEK	C5-C6-C7-C8
24	C	309	PEK	C6-C7-C8-C9
24	C	309	PEK	C11-C12-C13-C14
24	C	309	PEK	C12-C13-C14-C15
24	G	102	PEK	C11-C10-C9-C8
24	c	303	PEK	C5-C6-C7-C8
24	c	303	PEK	C6-C7-C8-C9
24	c	303	PEK	C11-C12-C13-C14
24	g	102	PEK	C12-C13-C14-C15
18	A	606	PGV	C23-C24-C25-C26
25	G	101	CDL	C51-C52-C53-C54
18	c	304	PGV	C1-C2-C3-C4
18	c	301	PGV	C4-C5-C6-C7
19	D	201	TGL	C23-C24-C25-C26
24	c	303	PEK	C23-C24-C25-C26
25	g	103	CDL	C58-C59-C60-C61
25	C	305	CDL	C18-C19-C20-C21
25	g	103	CDL	C17-C18-C19-C20
19	L	101	TGL	C24-C25-C26-C27
19	A	608	TGL	C12-C13-C14-C29
25	G	101	CDL	C54-C55-C56-C57
25	g	103	CDL	C1-CA2-OA2-PA1
19	l	101	TGL	CB1-CB2-CB3-CB4
25	c	305	CDL	C79-C80-C81-C82
25	g	103	CDL	C21-C22-C23-C24
24	g	102	PEK	C16-C17-C18-C19
19	i	101	TGL	C17-C18-C19-C33
18	C	304	PGV	O04-C19-O03-C01
18	a	607	PGV	C20-C21-C22-C23
19	a	606	TGL	CG1-CG2-OG2-CB1
18	c	304	PGV	O04-C19-O03-C01
25	C	305	CDL	C42-C43-C44-C45
24	c	303	PEK	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	C	309	PEK	C29-C30-C31-C32
26	m	401	DMU	C31-C34-C37-C40
25	c	305	CDL	OA5-CA3-CA4-OA6
25	g	103	CDL	OA5-CA3-CA4-OA6
24	G	102	PEK	C16-C17-C18-C19
24	G	102	PEK	O03-C01-C02-C03
25	c	305	CDL	CB3-CB4-CB6-OB8
25	g	103	CDL	CB3-CB4-CB6-OB8
18	C	304	PGV	C4-C5-C6-C7
24	c	303	PEK	C24-C25-C26-C27
19	L	101	TGL	OG2-CG2-CG3-OG3
19	a	606	TGL	OG2-CG2-CG3-OG3
22	B	302	PSC	O03-C01-C02-O01
24	G	102	PEK	O03-C01-C02-O01
25	C	305	CDL	OB6-CB4-CB6-OB8
25	G	101	CDL	C61-C62-C63-C64
18	C	303	PGV	C26-C27-C28-C29
24	C	309	PEK	O04-C21-O03-C01
18	A	606	PGV	C6-C7-C8-C9
25	g	103	CDL	C41-C42-C43-C44
19	l	101	TGL	CC5-CC6-CC7-CC8
18	C	303	PGV	C02-C03-O11-P
18	G	103	PGV	C02-C03-O11-P
22	e	201	PSC	O12-C04-C05-N
19	i	101	TGL	CB6-CB7-CB8-CB9
24	c	303	PEK	C22-C23-C24-C25
25	g	103	CDL	C15-C16-C17-C18
24	g	102	PEK	C34-C35-C36-C37
19	l	101	TGL	C25-C26-C27-C28
18	A	607	PGV	C25-C26-C27-C28
18	C	304	PGV	C30-C31-C32-C33
19	l	101	TGL	CC2-CC1-OG3-CG3
18	c	301	PGV	C29-C30-C31-C32
25	C	305	CDL	C52-C53-C54-C55
24	g	102	PEK	C33-C34-C35-C36
22	B	302	PSC	C27-C28-C29-C30
18	A	606	PGV	C11-C12-C13-C14
19	l	101	TGL	C22-C23-C24-C25
25	c	305	CDL	C23-C24-C25-C26
18	A	606	PGV	O01-C02-C03-O11
25	G	101	CDL	OA5-CA3-CA4-OA6
22	e	201	PSC	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	C	304	PGV	C3-C4-C5-C6
25	C	305	CDL	C54-C55-C56-C57
19	A	608	TGL	CA3-CA4-CA5-CA6
19	l	101	TGL	OG2-CG2-CG3-OG3
25	c	305	CDL	OB6-CB4-CB6-OB8
19	L	101	TGL	CG1-CG2-CG3-OG3
19	a	606	TGL	CG1-CG2-CG3-OG3
22	B	302	PSC	O03-C01-C02-C03
24	C	302	PEK	C35-C36-C37-C38
18	c	301	PGV	C11-C10-C9-C8
18	A	607	PGV	C4-C5-C6-C7
18	A	606	PGV	C20-C19-O03-C01
24	C	309	PEK	C22-C21-O03-C01
18	A	606	PGV	C9-C10-C11-C12
18	A	606	PGV	C04-O12-P-O11
18	A	606	PGV	C04-O12-P-O13
18	A	606	PGV	C04-O12-P-O14
18	G	103	PGV	C03-O11-P-O14
22	e	201	PSC	C03-O11-P-O12
22	e	201	PSC	C03-O11-P-O14
24	C	309	PEK	C04-O12-P-O14
24	G	102	PEK	C04-O12-P-O14
25	C	305	CDL	CB3-OB5-PB2-OB2
25	C	305	CDL	CB3-OB5-PB2-OB4
25	G	101	CDL	CA2-OA2-PA1-OA3
25	c	305	CDL	CA3-OA5-PA1-OA3
25	g	103	CDL	CB2-OB2-PB2-OB3
19	l	101	TGL	OC1-CC1-OG3-CG3
22	e	201	PSC	C3-C4-C5-C6
19	l	101	TGL	OG2-CB1-CB2-CB3
24	g	102	PEK	C1-C2-C3-C4
18	c	304	PGV	C02-C03-O11-P
25	C	305	CDL	C37-C38-C39-C40
18	A	607	PGV	C21-C22-C23-C24
25	G	101	CDL	C21-C22-C23-C24
19	D	201	TGL	C21-C22-C23-C24
22	e	201	PSC	C26-C27-C28-C29
24	C	302	PEK	C23-C24-C25-C26
22	B	302	PSC	C01-C02-C03-O11
26	c	307	DMU	C19-C22-C25-C28
24	c	303	PEK	C22-C21-O03-C01
19	L	101	TGL	CC6-CC7-CC8-CC9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	C	309	PEK	C3-C4-C5-C6
25	g	103	CDL	CB5-C51-C52-C53
24	C	309	PEK	O01-C02-C03-O11
25	g	103	CDL	OB5-CB3-CB4-OB6
18	c	301	PGV	C30-C31-C32-C33
25	G	101	CDL	C36-C37-C38-C39
19	a	606	TGL	CC4-CC5-CC6-CC7
24	c	303	PEK	C33-C34-C35-C36
19	A	608	TGL	C14-C29-C30-C31
19	A	608	TGL	OG1-CG1-CG2-OG2
19	L	101	TGL	C25-C26-C27-C28
19	l	101	TGL	CB3-CB4-CB5-CB6
25	c	305	CDL	C72-C73-C74-C75
25	g	103	CDL	C81-C82-C83-C84
24	C	308	PEK	C2-C3-C4-C5
25	C	305	CDL	C24-C25-C26-C27
25	g	103	CDL	C83-C84-C85-C86
18	c	304	PGV	C9-C10-C11-C12
18	C	303	PGV	C1-C2-C3-C4
18	G	103	PGV	C26-C27-C28-C29
18	c	301	PGV	C21-C22-C23-C24
19	A	608	TGL	C21-C20-CA9-CA8
18	c	304	PGV	C05-C04-O12-P
18	c	304	PGV	C27-C28-C29-C30
19	i	101	TGL	CA5-CA6-CA7-CA8
24	c	303	PEK	O01-C02-C03-O11
18	c	301	PGV	C9-C10-C11-C12
25	c	305	CDL	C17-C18-C19-C20
22	B	302	PSC	C31-C32-C33-C34
24	C	308	PEK	C28-C29-C30-C31
25	C	305	CDL	C76-C77-C78-C79
18	A	606	PGV	O04-C19-O03-C01
24	g	102	PEK	O03-C01-C02-O01
18	C	303	PGV	C27-C28-C29-C30
19	i	101	TGL	CB4-CB5-CB6-CB7
25	c	305	CDL	C84-C85-C86-C87
19	A	608	TGL	CA6-CA7-CA8-CA9
18	C	303	PGV	C05-C04-O12-P
19	l	101	TGL	C11-C12-C13-C14
18	A	607	PGV	C24-C25-C26-C27
18	a	607	PGV	O12-C04-C05-C06
23	b	301	CHD	C22-C23-C24-O26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	305	CDL	CA3-CA4-CA6-OA8
25	G	101	CDL	C55-C56-C57-C58
25	c	305	CDL	C31-C32-C33-C34
18	A	606	PGV	C30-C31-C32-C33
18	c	301	PGV	C24-C25-C26-C27
25	c	305	CDL	C51-C52-C53-C54
23	b	301	CHD	C22-C23-C24-O25
22	B	302	PSC	C28-C29-C30-C31
14	A	602	HEA	CAD-CBD-CGD-O2D
19	l	101	TGL	CA1-CA2-CA3-CA4
19	a	606	TGL	C11-C12-C13-C14
25	G	101	CDL	C43-C44-C45-C46
24	G	102	PEK	C23-C24-C25-C26
18	A	607	PGV	C31-C32-C33-C34
25	g	103	CDL	C18-C19-C20-C21
22	e	201	PSC	C01-C02-C03-O11
25	g	103	CDL	C72-C73-C74-C75
26	M	101	DMU	O6-C11-C9-O1
24	c	303	PEK	O04-C21-O03-C01
26	C	307	DMU	C5-C10-O7-C3
22	e	201	PSC	C2-C3-C4-C5
24	C	302	PEK	C11-C12-C13-C14
24	C	308	PEK	C5-C6-C7-C8
24	C	308	PEK	C11-C12-C13-C14
24	G	102	PEK	C11-C12-C13-C14
24	G	102	PEK	C12-C13-C14-C15
24	c	303	PEK	C11-C10-C9-C8
24	g	102	PEK	C5-C6-C7-C8
24	C	309	PEK	C33-C34-C35-C36
26	M	101	DMU	C19-C22-C25-C28
26	C	307	DMU	O16-C18-C19-C22
19	a	606	TGL	CA1-CA2-CA3-CA4
14	A	601	HEA	CAD-CBD-CGD-O1D
25	g	103	CDL	C82-C83-C84-C85
14	a	601	HEA	CAD-CBD-CGD-O1D
23	B	303	CHD	C22-C23-C24-O25
25	G	101	CDL	C63-C64-C65-C66
25	C	305	CDL	CA4-CA3-OA5-PA1
23	c	302	CHD	C17-C20-C22-C23
24	G	102	PEK	C28-C29-C30-C31
14	A	601	HEA	C19-C20-C21-C22
19	A	608	TGL	CA5-CA6-CA7-CA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	G	101	CDL	C18-C19-C20-C21
24	G	102	PEK	C14-C15-C16-C17
25	C	305	CDL	C52-C51-CB5-OB6
25	G	101	CDL	C57-C58-C59-C60
25	C	305	CDL	C14-C15-C16-C17
18	A	606	PGV	O05-C05-C06-O06
14	a	602	HEA	C26-C15-C16-C17
24	G	102	PEK	C27-C28-C29-C30
18	G	103	PGV	C28-C29-C30-C31
24	c	303	PEK	C01-C02-C03-O11
19	D	201	TGL	OG2-CG2-CG3-OG3
19	l	101	TGL	OG1-CG1-CG2-OG2
22	B	302	PSC	C12-C13-C14-C15
18	G	103	PGV	C3-C4-C5-C6
14	a	602	HEA	CAD-CBD-CGD-O1D
19	A	608	TGL	CA2-CA3-CA4-CA5
25	c	305	CDL	C58-C59-C60-C61
24	C	302	PEK	C2-C3-C4-C5
24	c	303	PEK	C15-C16-C17-C18
24	C	302	PEK	C32-C33-C34-C35
25	G	101	CDL	C59-C60-C61-C62
14	a	602	HEA	CAD-CBD-CGD-O2D
18	a	607	PGV	O01-C1-C2-C3
24	C	309	PEK	C35-C36-C37-C38
19	a	606	TGL	OG2-CB1-CB2-CB3
25	C	305	CDL	C64-C65-C66-C67
19	a	606	TGL	CB1-CB2-CB3-CB4
18	a	607	PGV	C11-C12-C13-C14
24	g	102	PEK	C14-C15-C16-C17
25	c	305	CDL	C14-C15-C16-C17
18	C	303	PGV	C20-C19-O03-C01
19	a	606	TGL	CA5-CA6-CA7-CA8
19	l	101	TGL	CG1-CG2-CG3-OG3
24	c	303	PEK	O03-C01-C02-C03
18	a	607	PGV	C15-C16-C17-C18
18	A	607	PGV	C13-C14-C15-C16
14	A	602	HEA	CAD-CBD-CGD-O1D
19	D	201	TGL	CB2-CB3-CB4-CB5
18	c	304	PGV	C11-C12-C13-C14
22	B	302	PSC	C7-C8-C9-C10
25	g	103	CDL	C32-C33-C34-C35
23	B	303	CHD	C22-C23-C24-O26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	O01-C1-C2-C3
19	a	606	TGL	C29-C30-C31-C32
23	C	301	CHD	C21-C20-C22-C23
26	C	307	DMU	C19-C22-C25-C28
14	a	601	HEA	C2C-C3C-CAC-CBC
19	A	608	TGL	CC5-CC6-CC7-CC8
18	A	607	PGV	C9-C10-C11-C12
18	A	607	PGV	C6-C7-C8-C9
14	A	601	HEA	CAD-CBD-CGD-O2D
23	C	301	CHD	C16-C17-C20-C22
19	A	608	TGL	OG3-CC1-CC2-CC3
24	g	102	PEK	O01-C1-C2-C3
14	a	601	HEA	CAD-CBD-CGD-O2D
24	C	309	PEK	C14-C15-C16-C17
18	C	303	PGV	O04-C19-O03-C01
18	c	301	PGV	C2-C1-O01-C02
18	A	607	PGV	C14-C15-C16-C17
19	L	101	TGL	CC2-CC3-CC4-CC5
19	a	606	TGL	OG3-CC1-CC2-CC3
19	a	606	TGL	C23-C24-C25-C26
19	l	101	TGL	CA7-CA8-CA9-C20
25	c	305	CDL	C32-C31-CA7-OA8
19	A	608	TGL	C11-C12-C13-C14
22	B	302	PSC	C26-C27-C28-C29
19	A	608	TGL	CG1-CG2-CG3-OG3
19	D	201	TGL	CG1-CG2-CG3-OG3
19	l	101	TGL	OG1-CG1-CG2-CG3
22	e	201	PSC	C5-C6-C7-C8
14	a	602	HEA	CAA-CBA-CGA-O1A
19	L	101	TGL	OG2-CB1-CB2-CB3
23	C	301	CHD	C17-C20-C22-C23
19	A	608	TGL	OG2-CG2-CG3-OG3
14	A	602	HEA	CAA-CBA-CGA-O1A
18	a	607	PGV	C21-C22-C23-C24
18	A	607	PGV	O03-C19-C20-C21
25	g	103	CDL	C52-C51-CB5-OB6
25	c	305	CDL	C82-C83-C84-C85
19	D	201	TGL	C11-C12-C13-C14
18	G	103	PGV	C2-C3-C4-C5
24	G	102	PEK	C30-C31-C32-C33
19	A	608	TGL	CB4-CB5-CB6-CB7
19	l	101	TGL	C21-C20-CA9-CA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c	301	PGV	O03-C19-C20-C21
25	c	305	CDL	C32-C31-CA7-OA9
14	a	602	HEA	CAA-CBA-CGA-O2A
19	A	608	TGL	CB2-CB3-CB4-CB5
25	G	101	CDL	C53-C54-C55-C56
24	C	302	PEK	C3-C4-C5-C6
19	l	101	TGL	C11-C10-CB9-CB8
18	G	103	PGV	C6-C7-C8-C9
23	j	101	CHD	C22-C23-C24-O26
25	c	305	CDL	C81-C82-C83-C84
24	g	102	PEK	O02-C1-C2-C3
19	D	201	TGL	C15-C16-C17-C18
18	A	607	PGV	O04-C19-C20-C21
22	B	302	PSC	C30-C31-C32-C33
18	G	103	PGV	O03-C01-C02-C03
18	c	301	PGV	O04-C19-C20-C21
19	L	101	TGL	OB1-CB1-CB2-CB3
19	a	606	TGL	OC1-CC1-CC2-CC3
19	l	101	TGL	C15-C16-C17-C18
25	G	101	CDL	C84-C85-C86-C87
14	A	602	HEA	CAA-CBA-CGA-O2A
25	C	305	CDL	C72-C73-C74-C75
23	c	302	CHD	C22-C23-C24-O26
24	C	308	PEK	C25-C26-C27-C28
19	a	606	TGL	C14-C29-C30-C31
19	A	608	TGL	OC1-CC1-CC2-CC3
22	B	302	PSC	O03-C19-C20-C21
19	D	201	TGL	OG1-CA1-CA2-CA3
19	a	606	TGL	CA7-CA8-CA9-C20

There are no ring outliers.

18 monomers are involved in 24 short contacts:

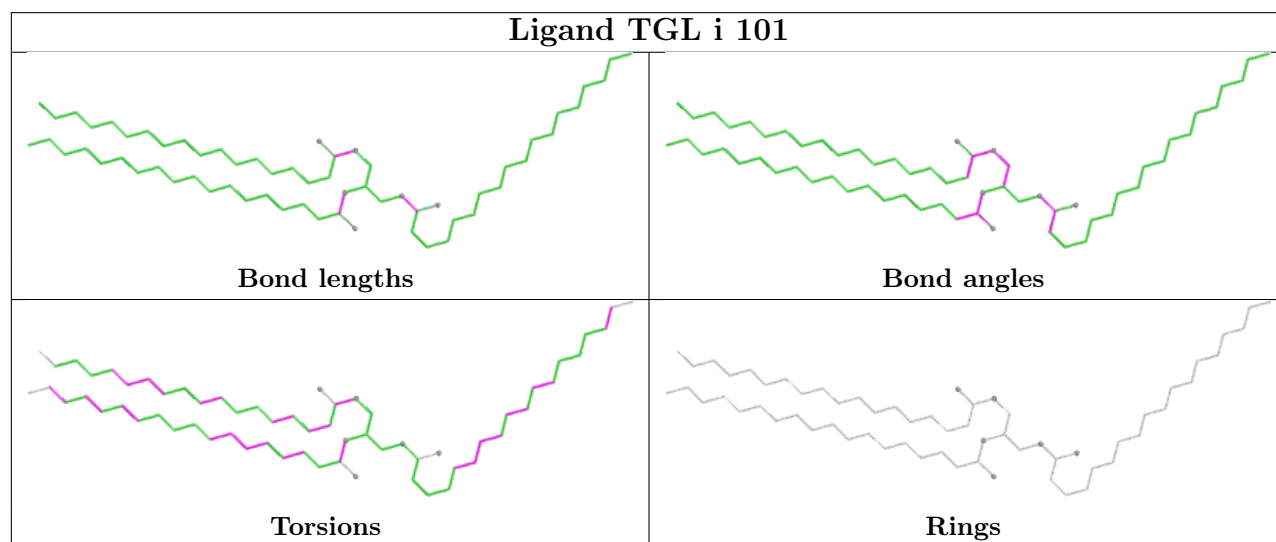
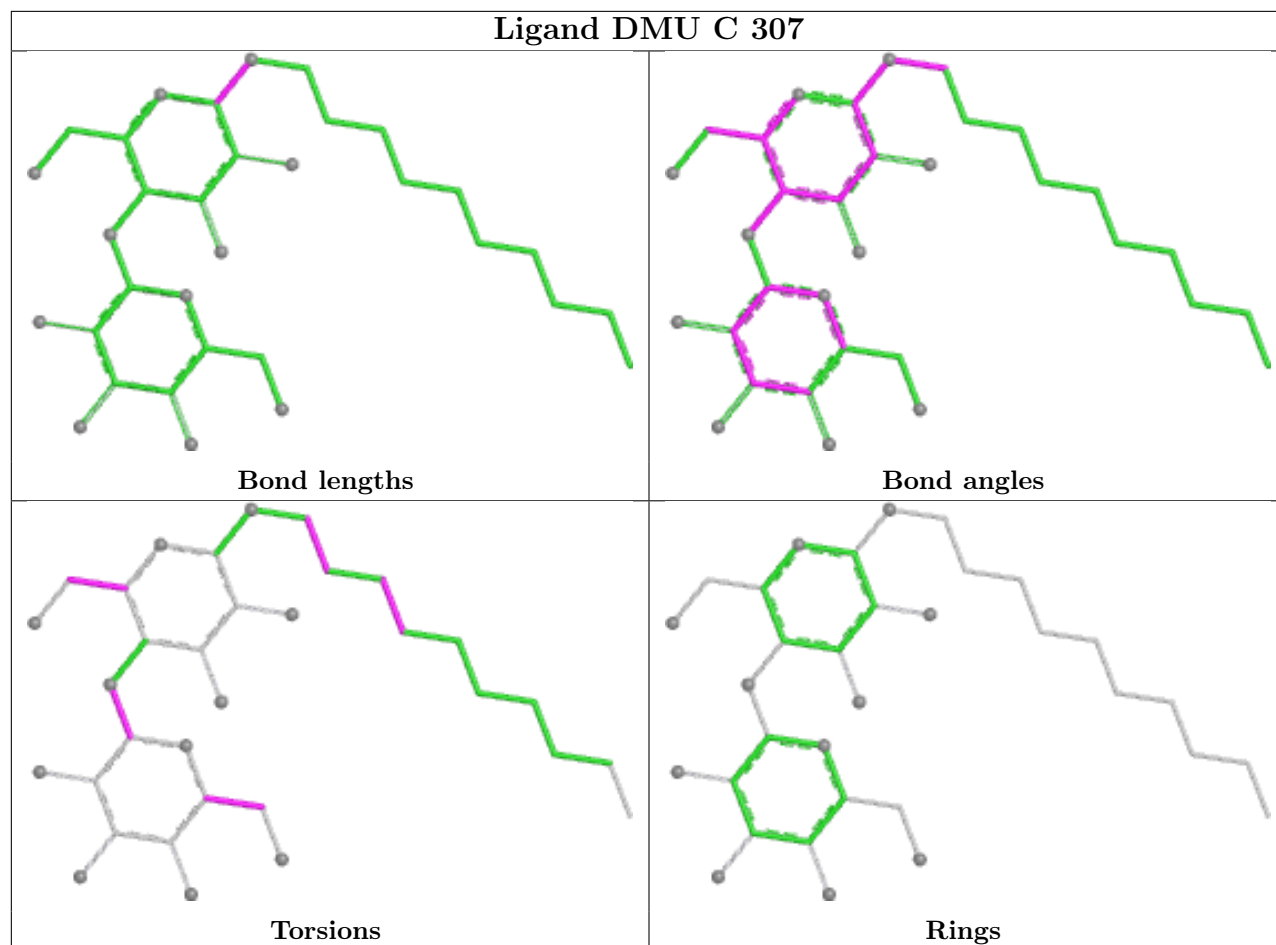
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	307	DMU	1	0
23	c	306	CHD	1	0
23	C	306	CHD	1	0
18	A	606	PGV	1	0
18	C	303	PGV	1	0
14	a	601	HEA	1	0
25	g	103	CDL	1	0
23	c	302	CHD	1	0

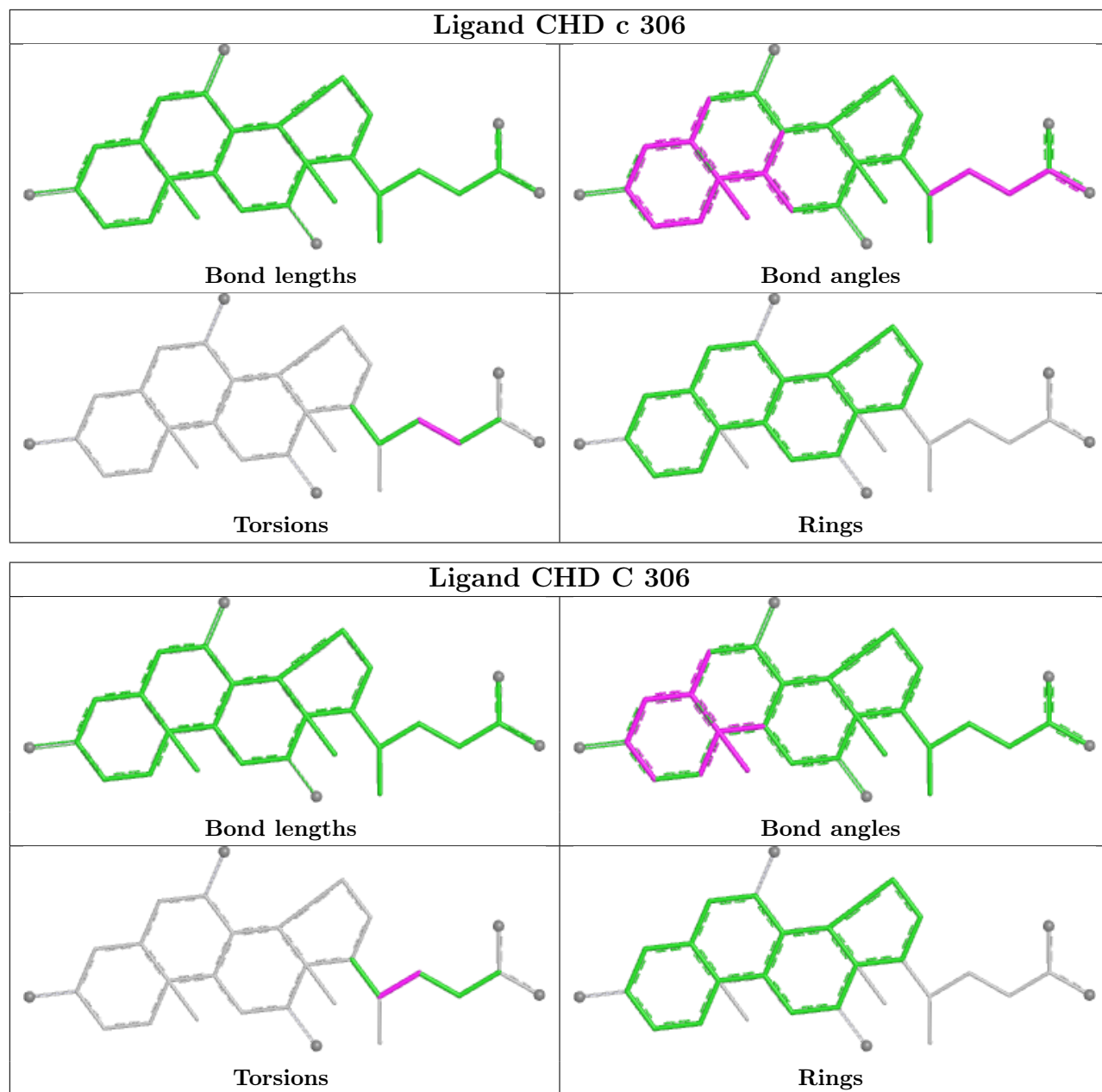
Continued on next page...

Continued from previous page...

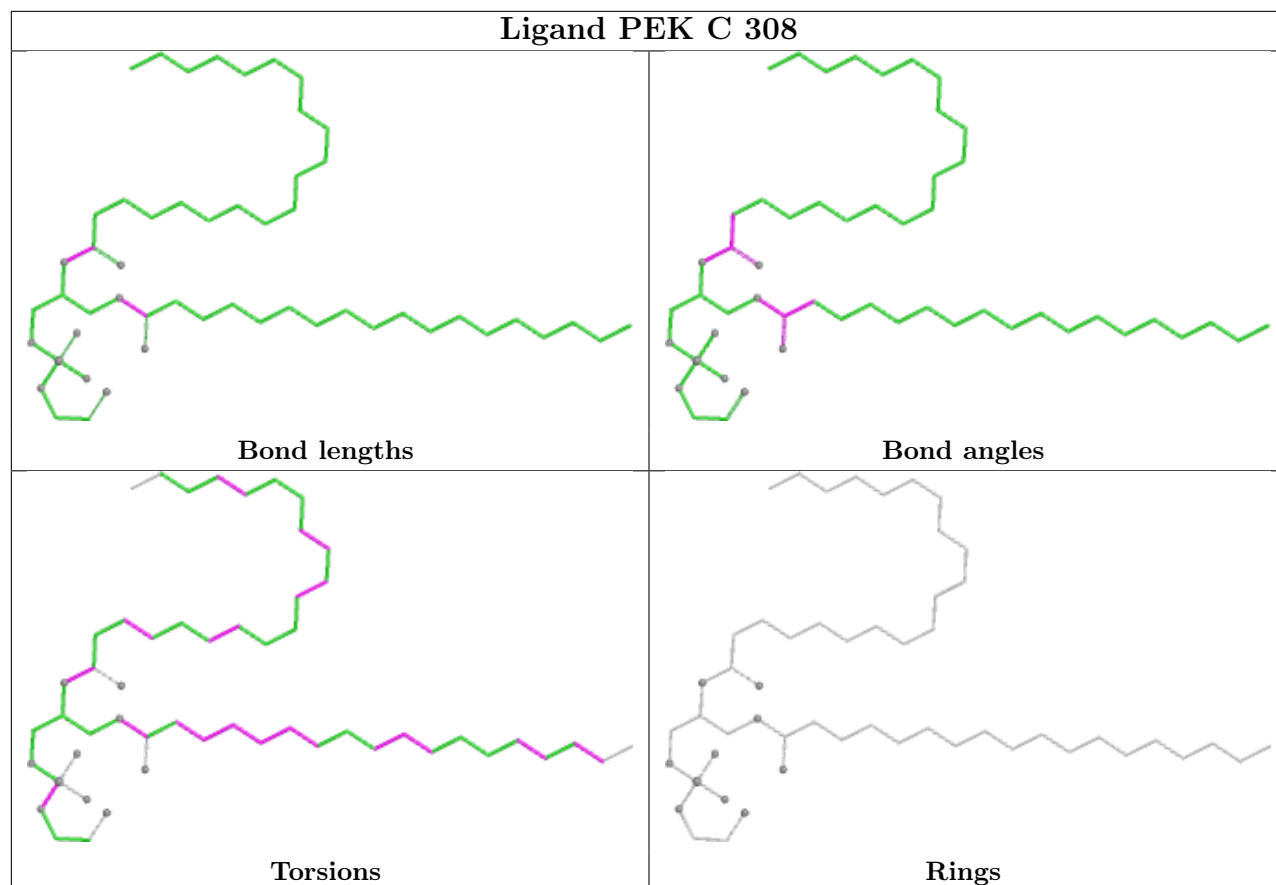
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	302	PEK	2	0
23	b	301	CHD	1	0
14	A	602	HEA	3	0
18	A	607	PGV	1	0
14	a	602	HEA	4	0
26	m	401	DMU	1	0
14	A	601	HEA	2	0
20	a	608	CMO	2	0
23	B	303	CHD	1	0
24	C	309	PEK	1	0

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.

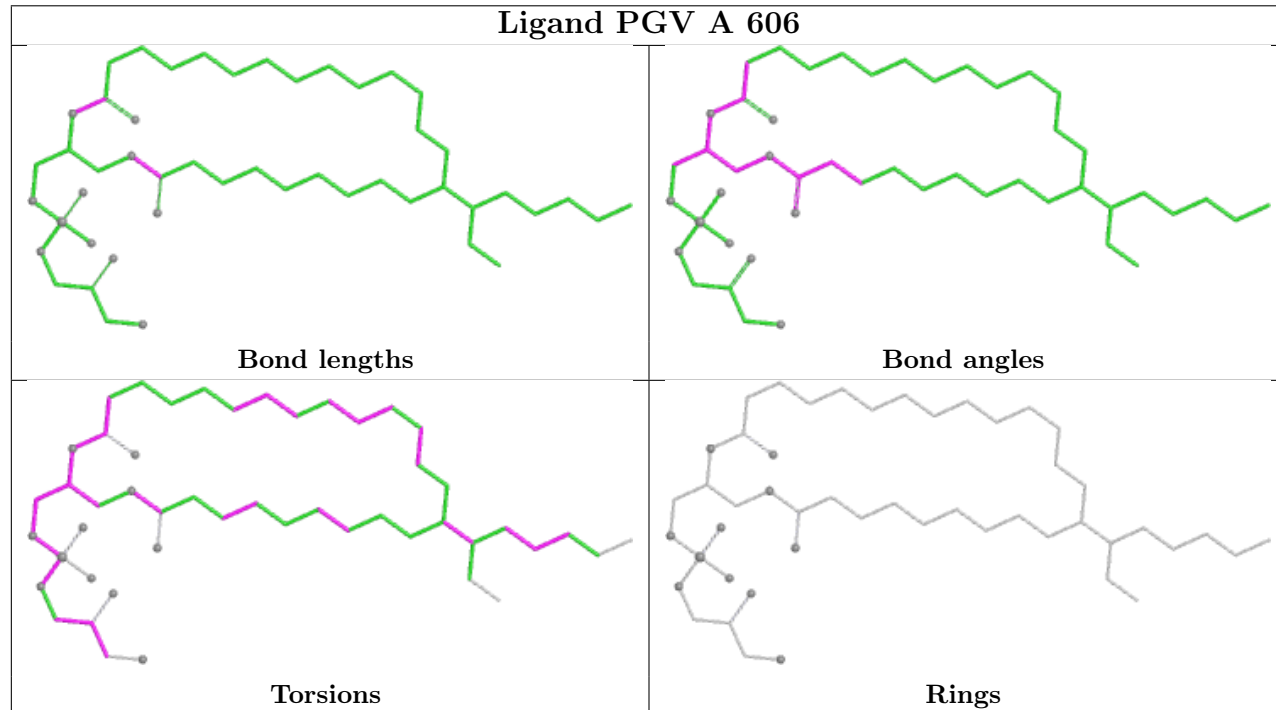


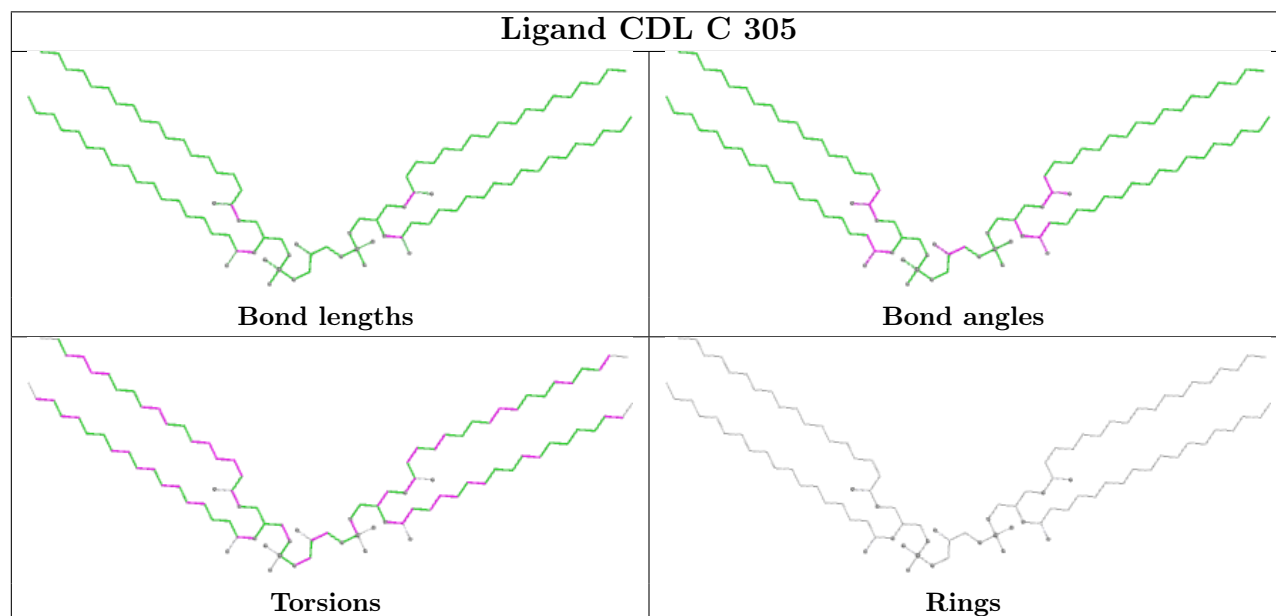
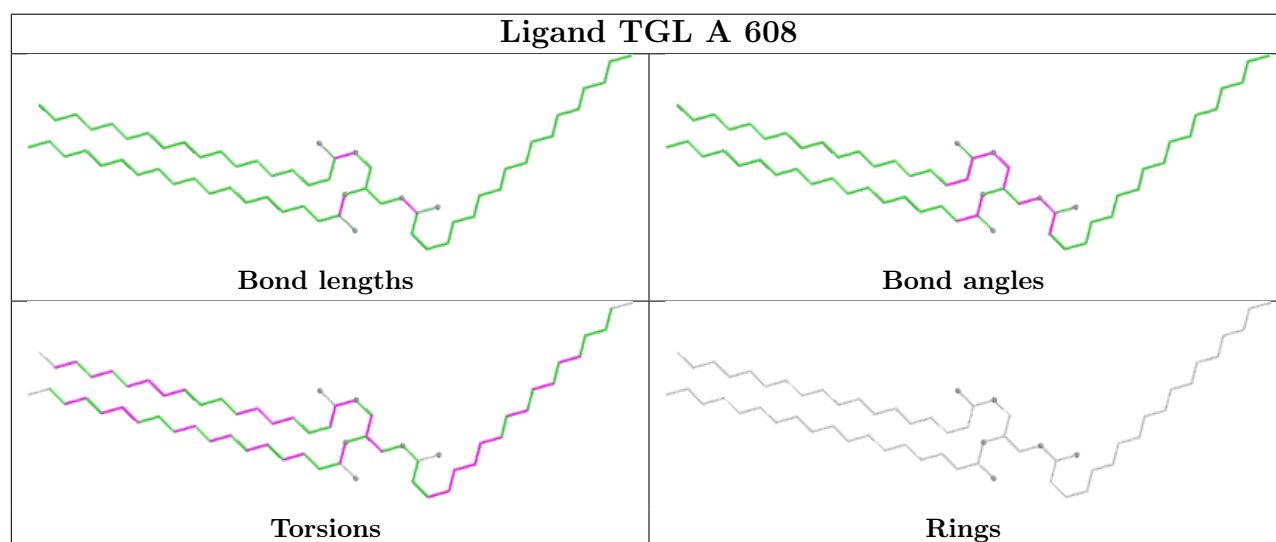
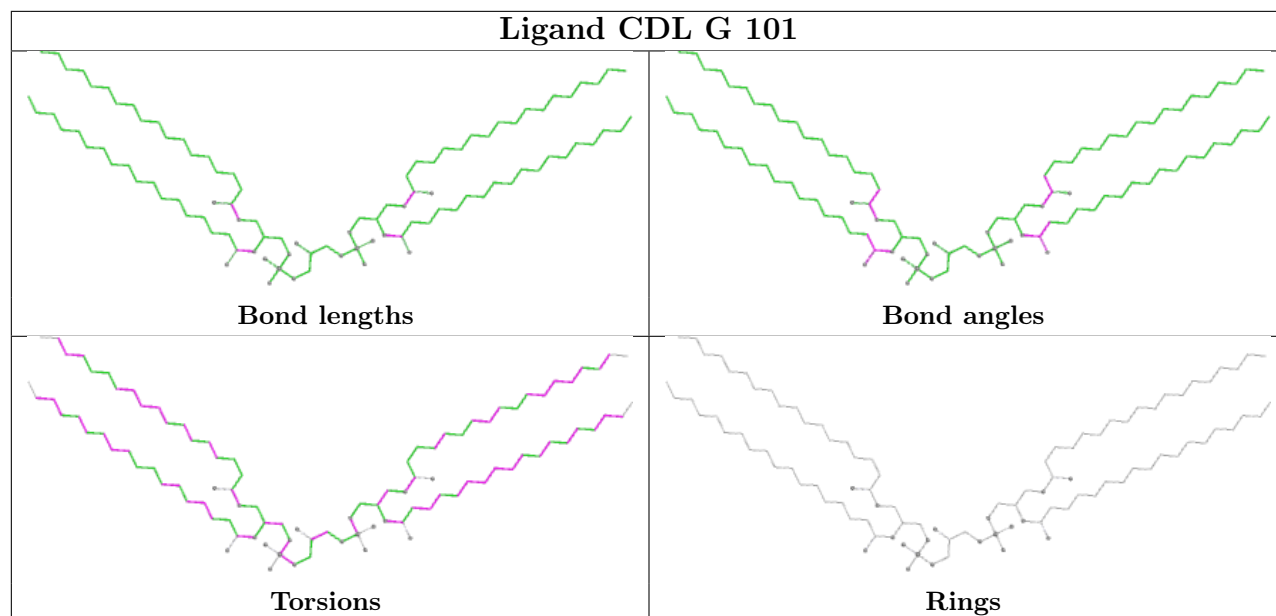


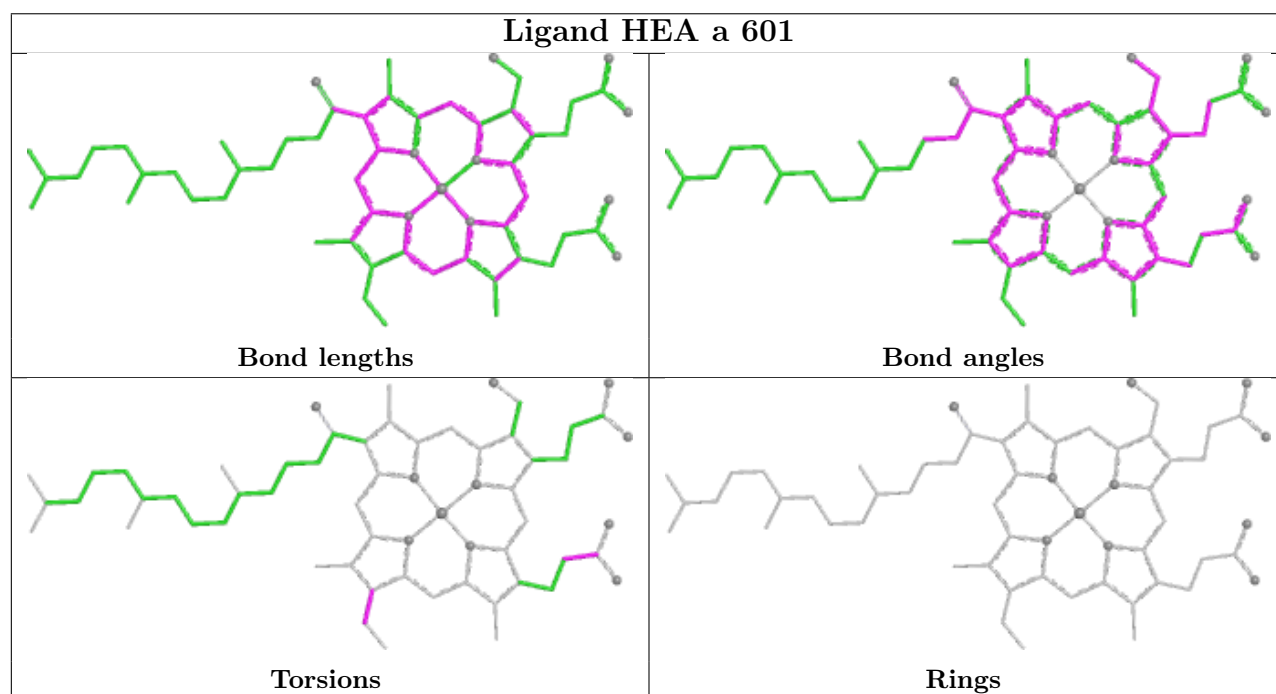
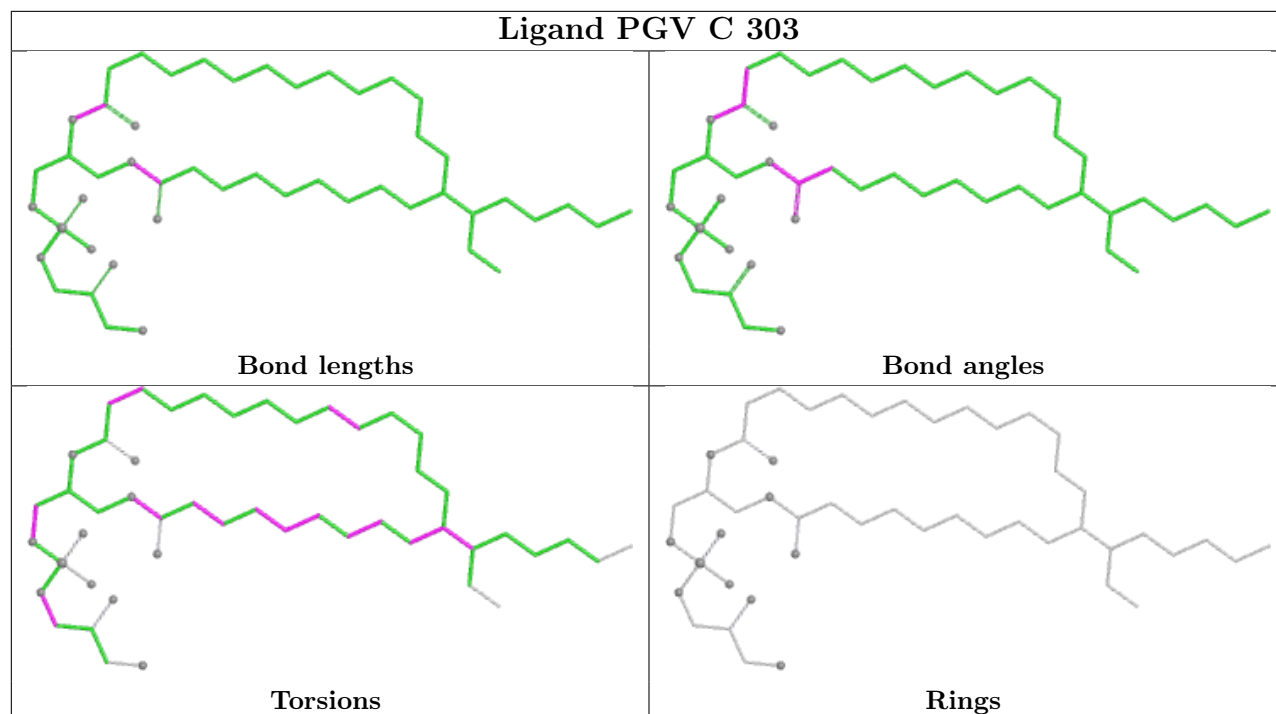
Ligand PEK C 308

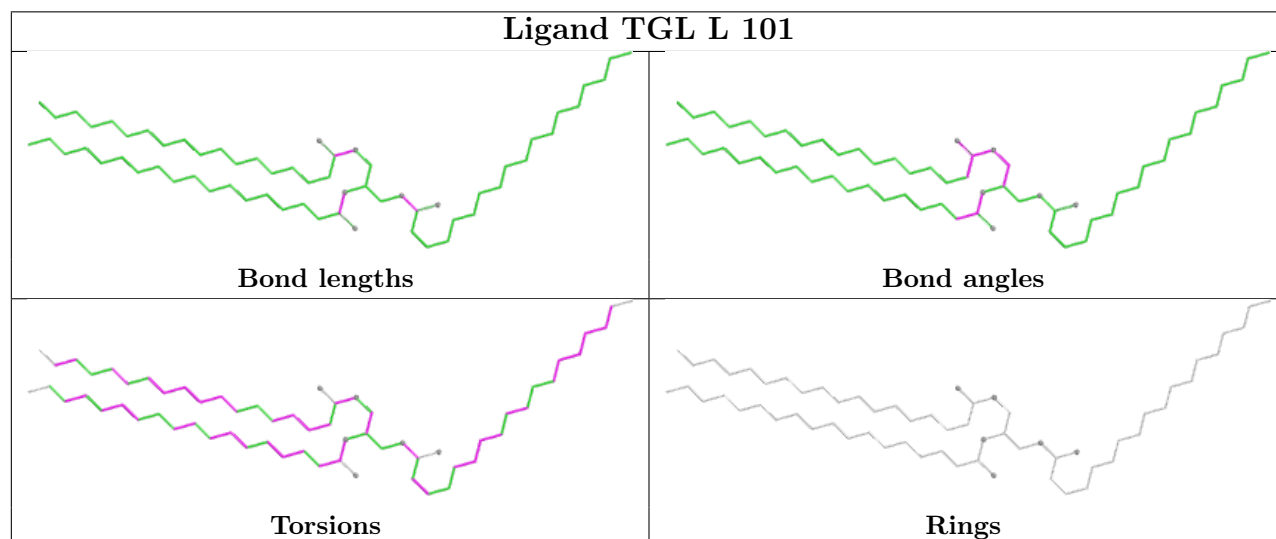
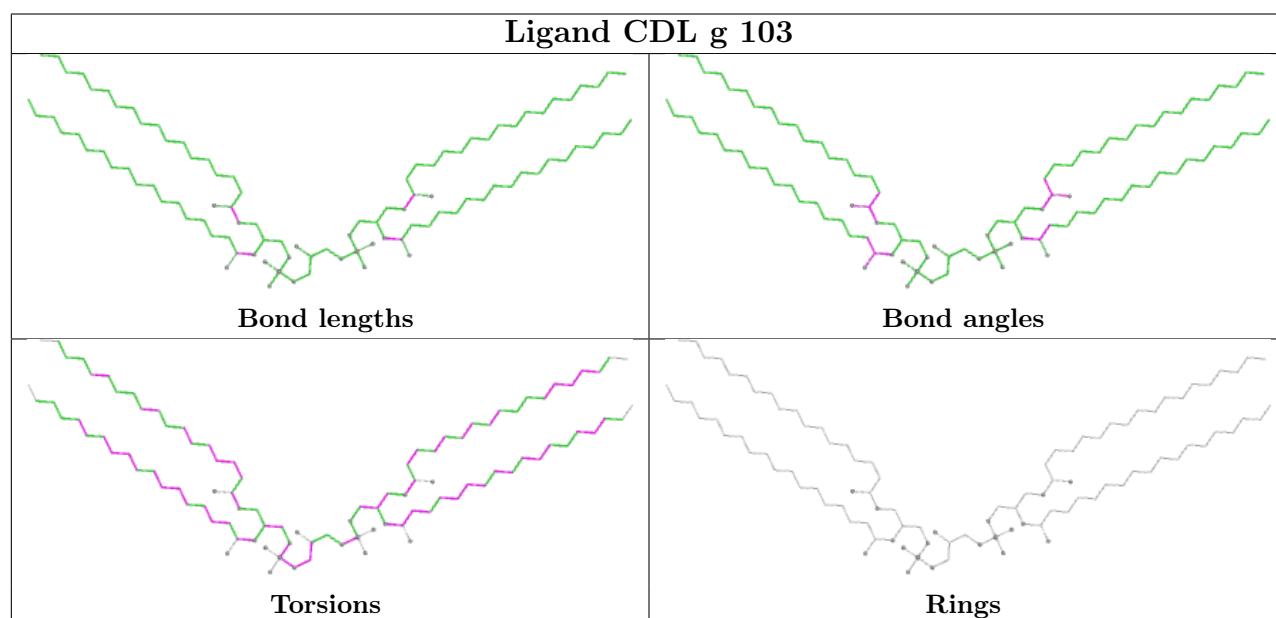
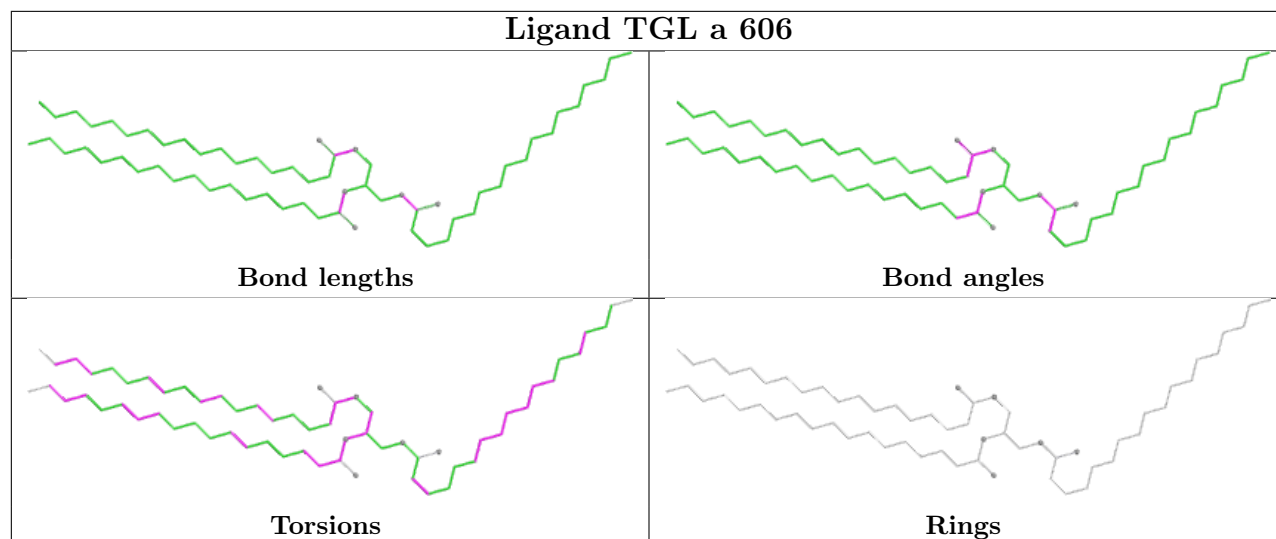


Ligand PGV A 606

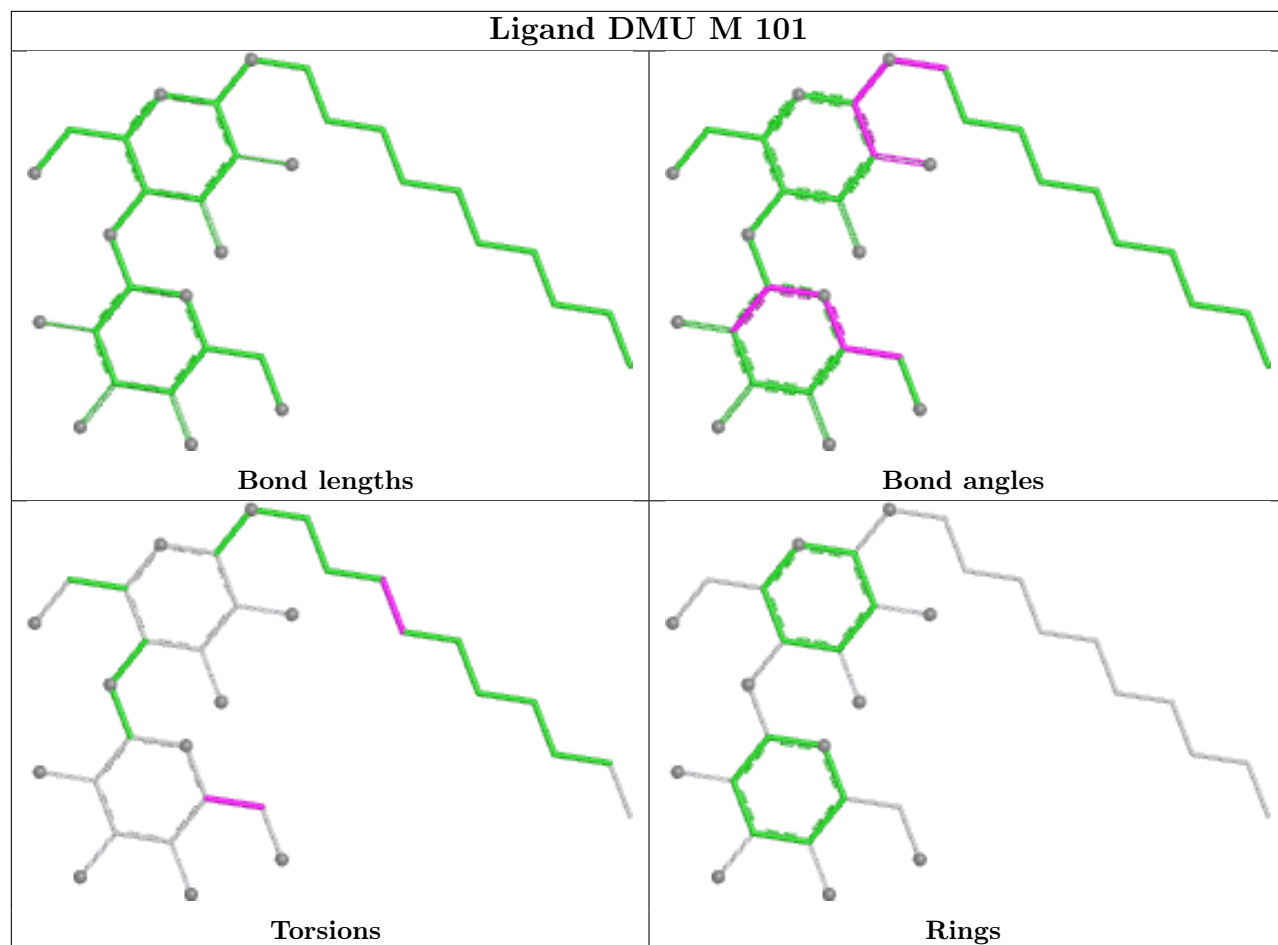




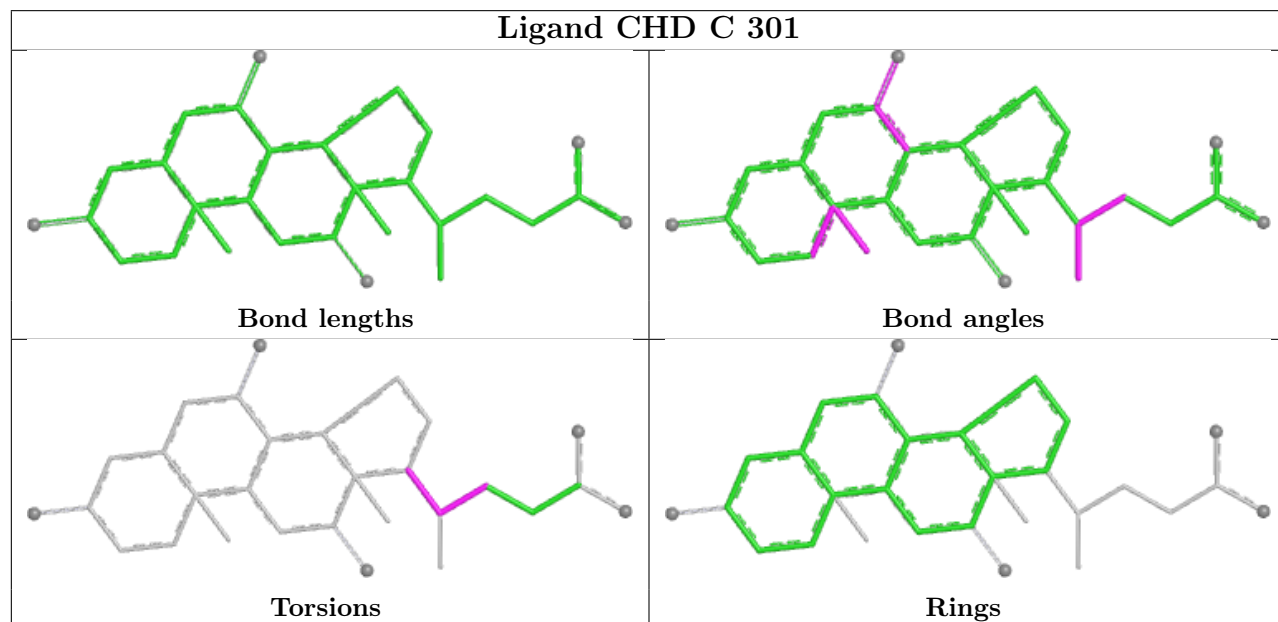


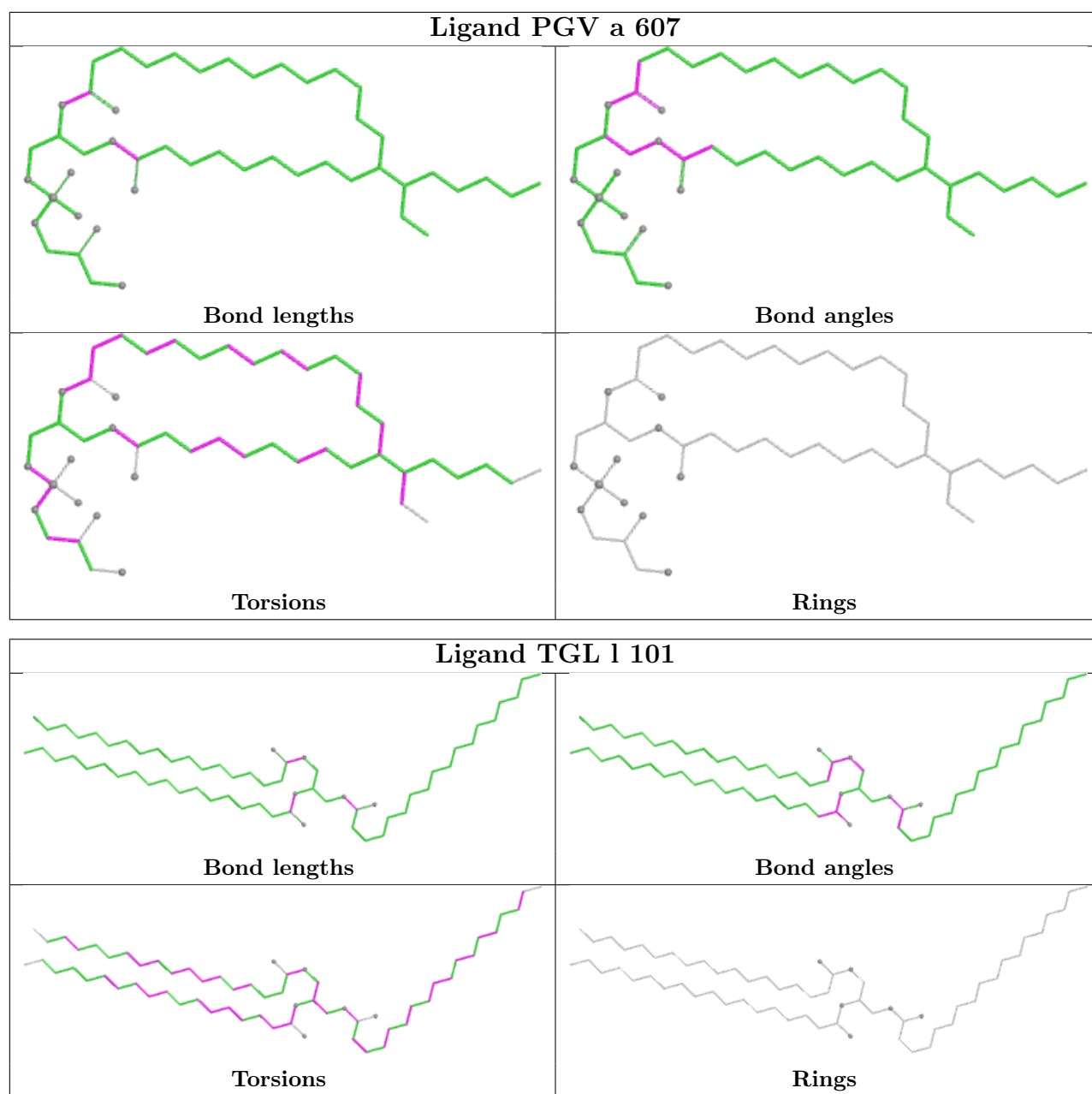


Ligand DMU M 101

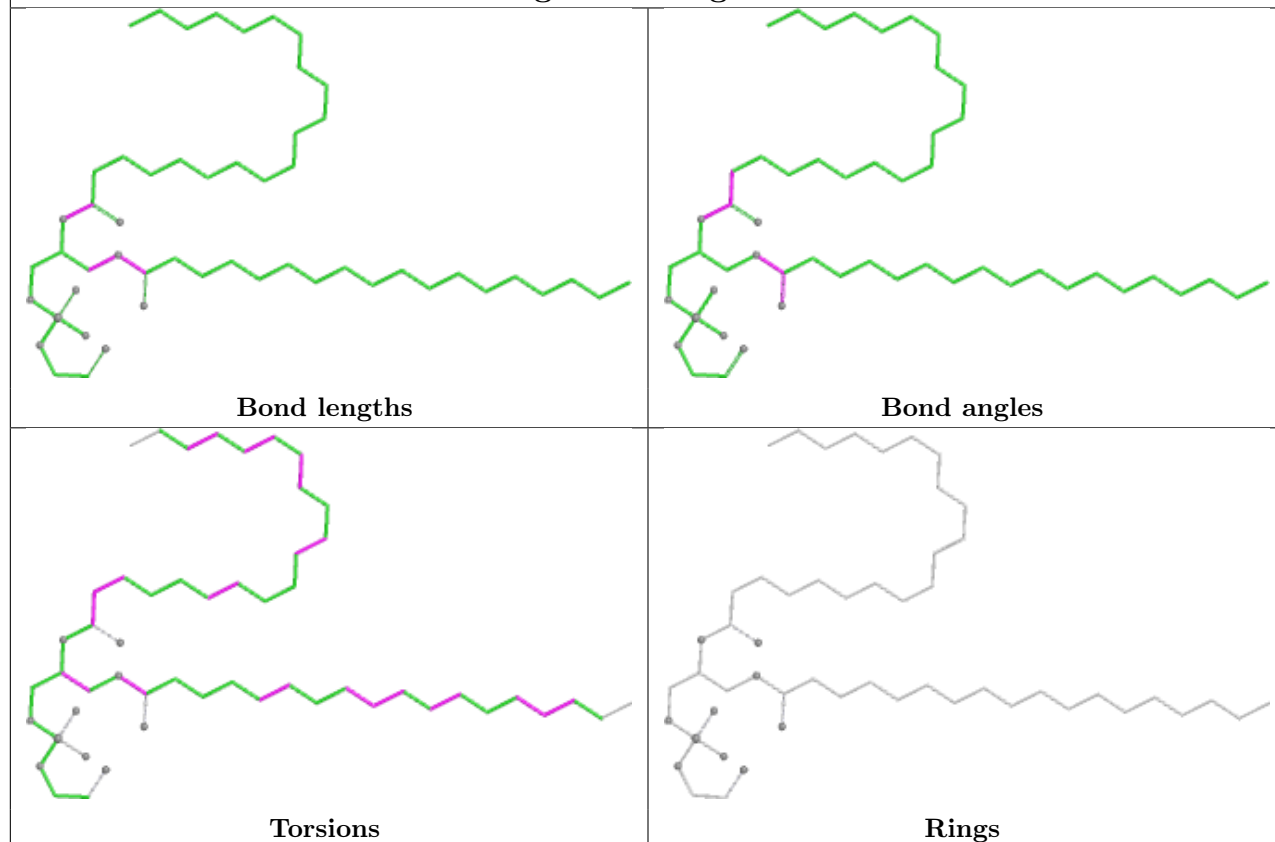


Ligand CHD C 301

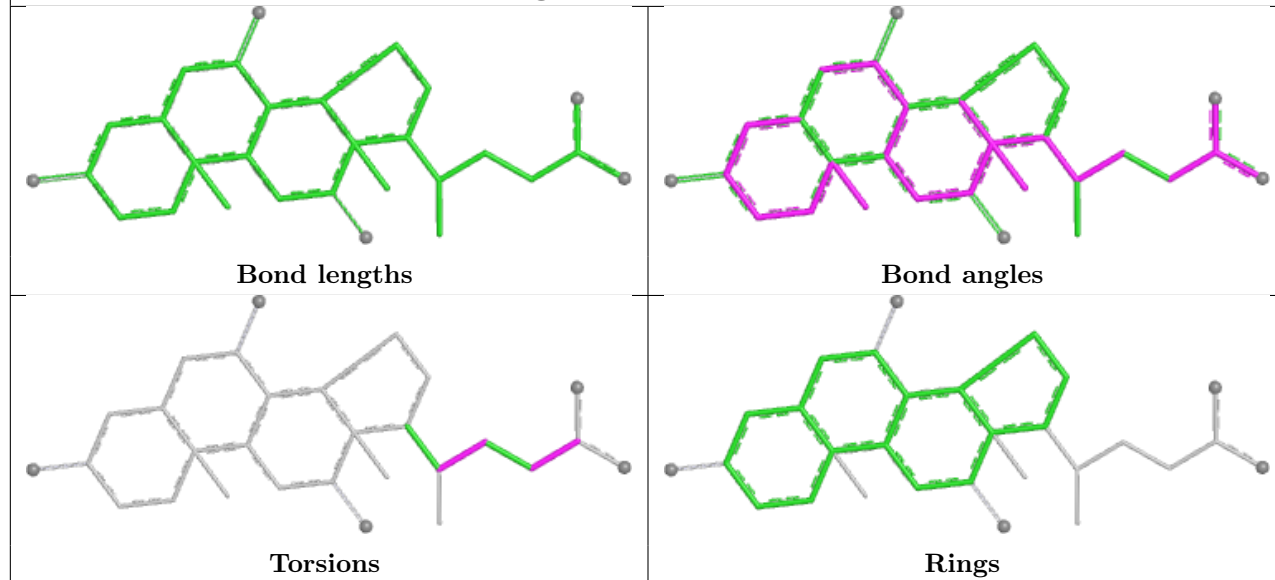




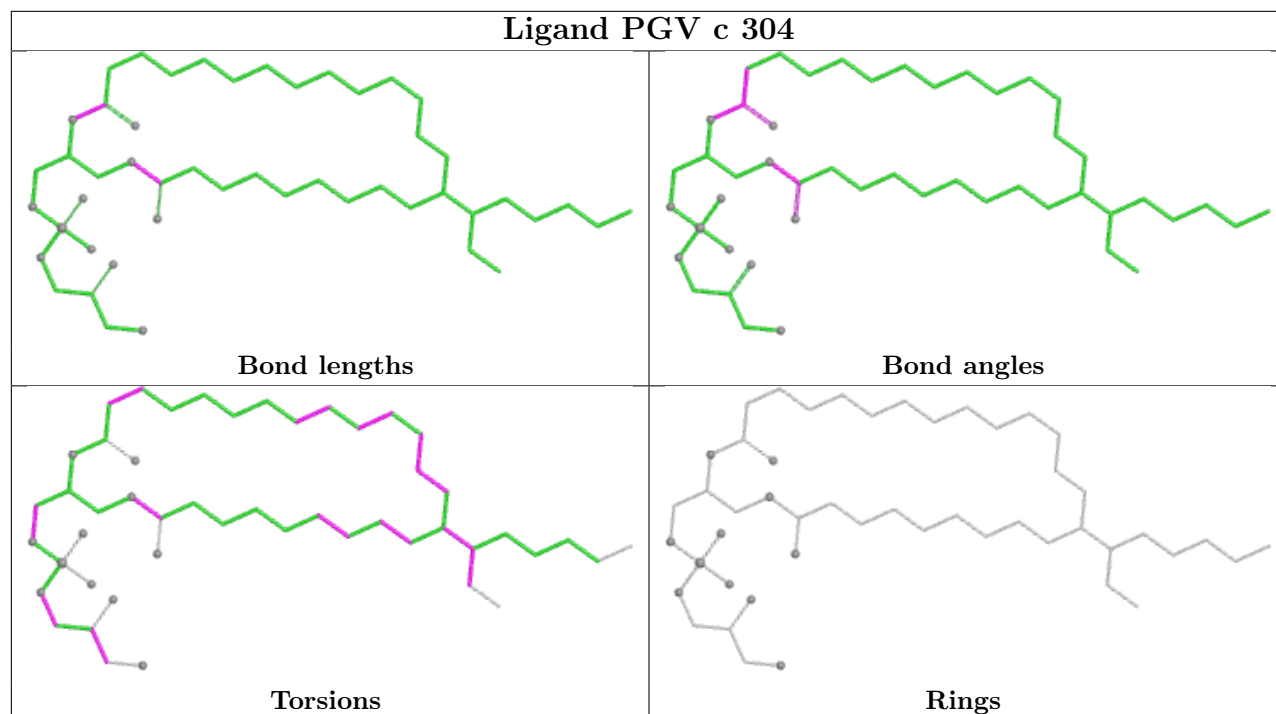
Ligand PEK g 102



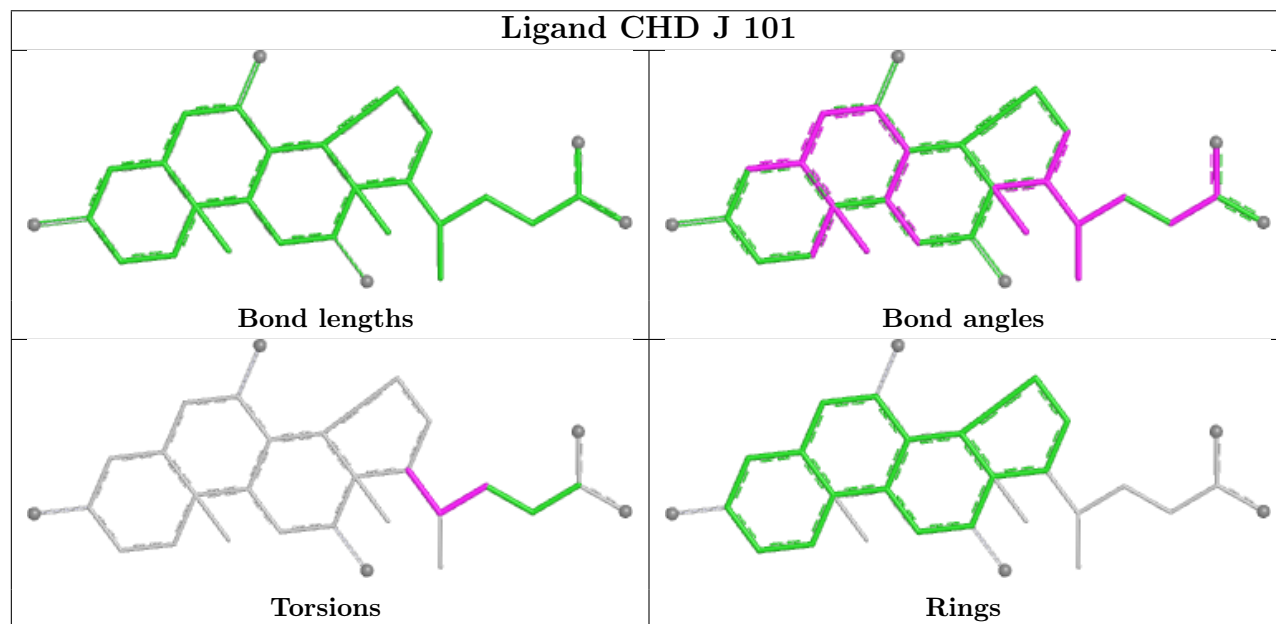
Ligand CHD c 302



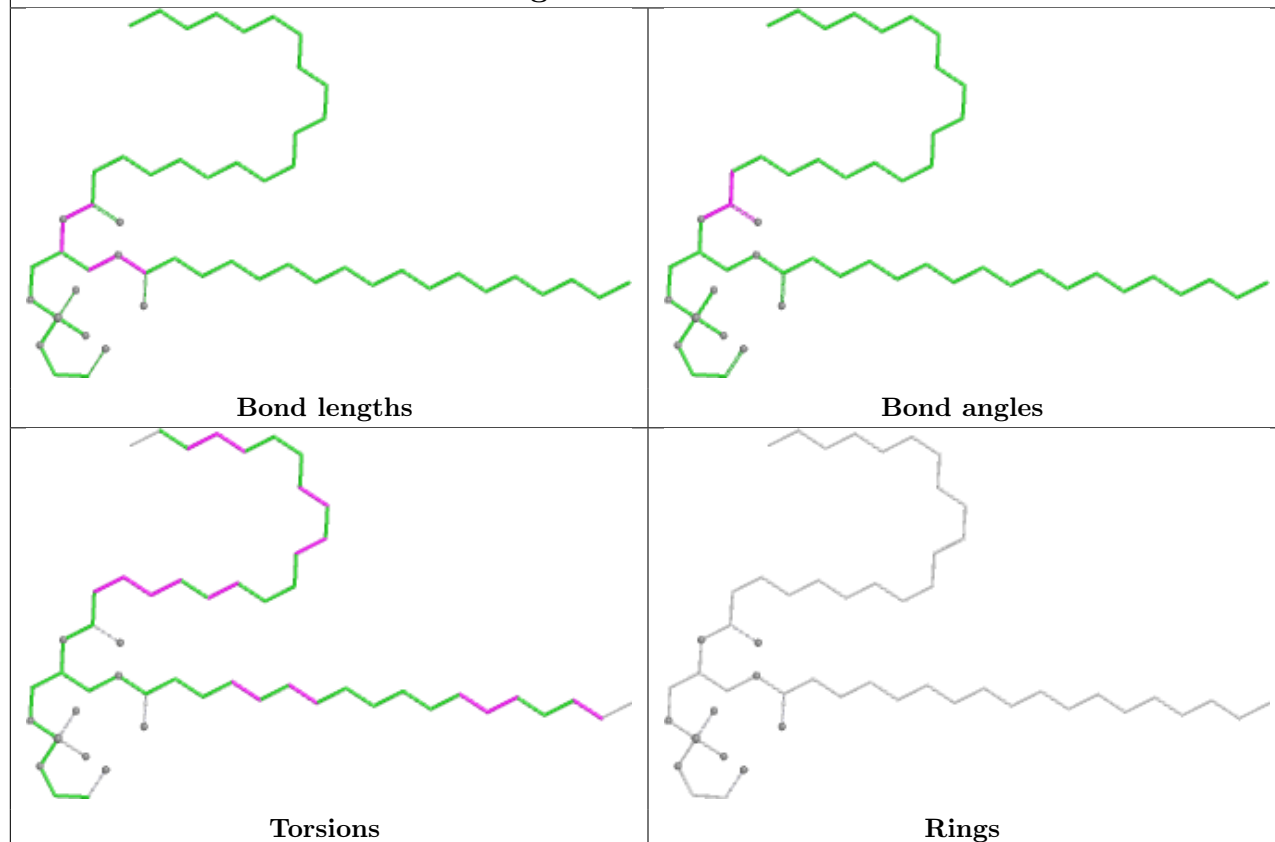
Ligand PGV c 304



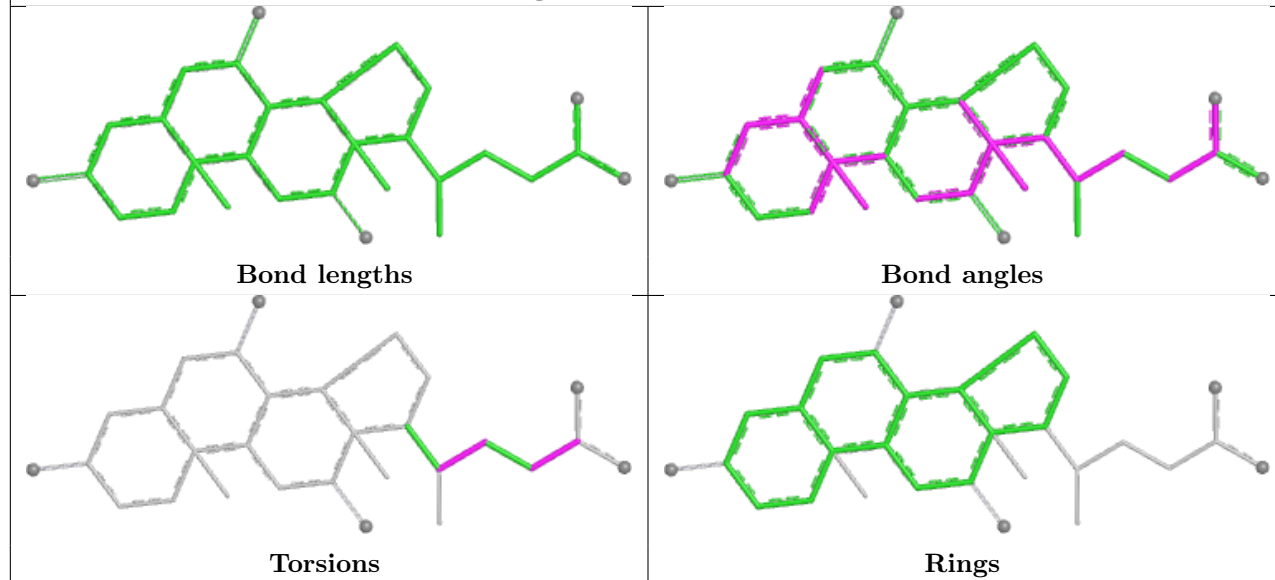
Ligand CHD J 101

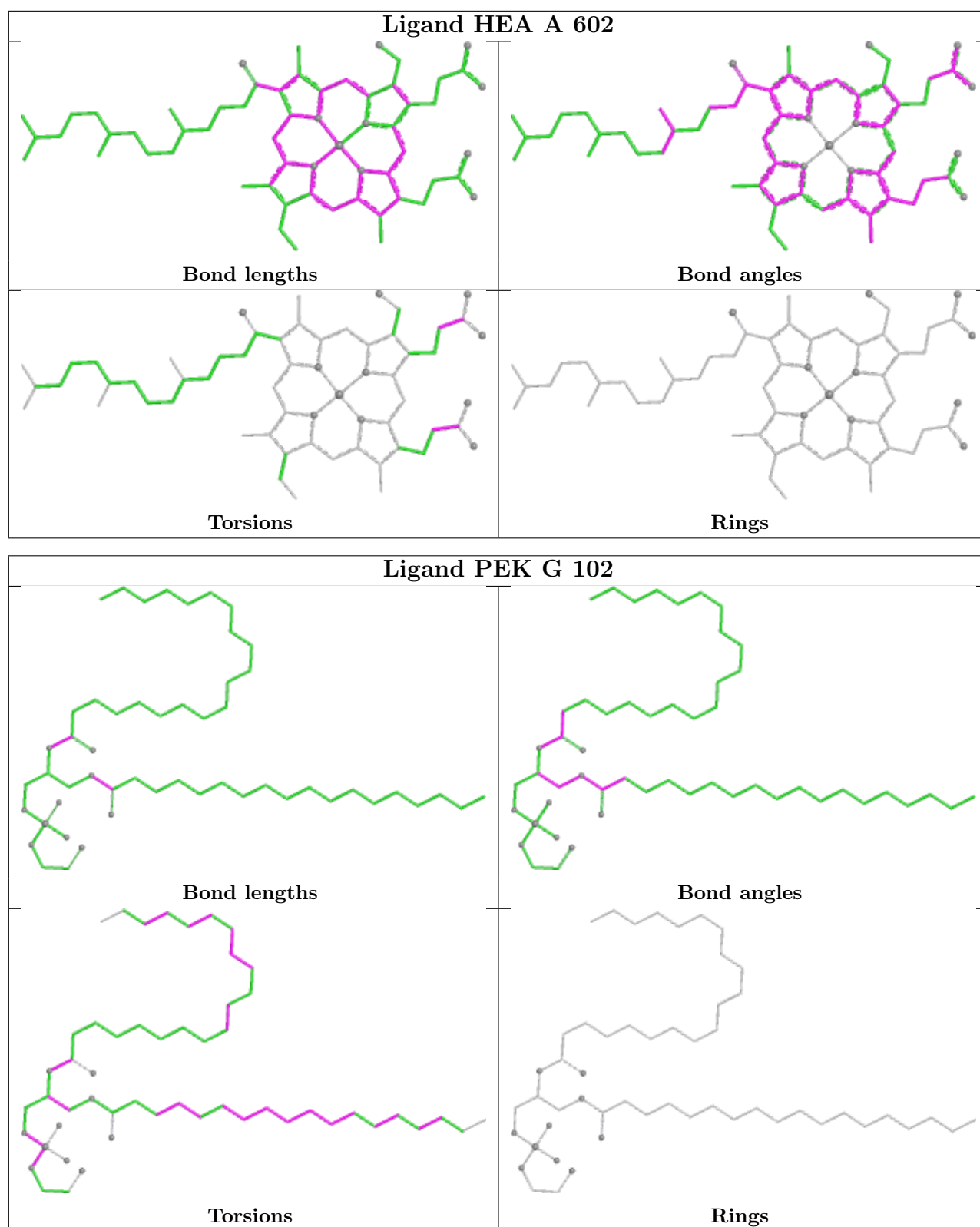


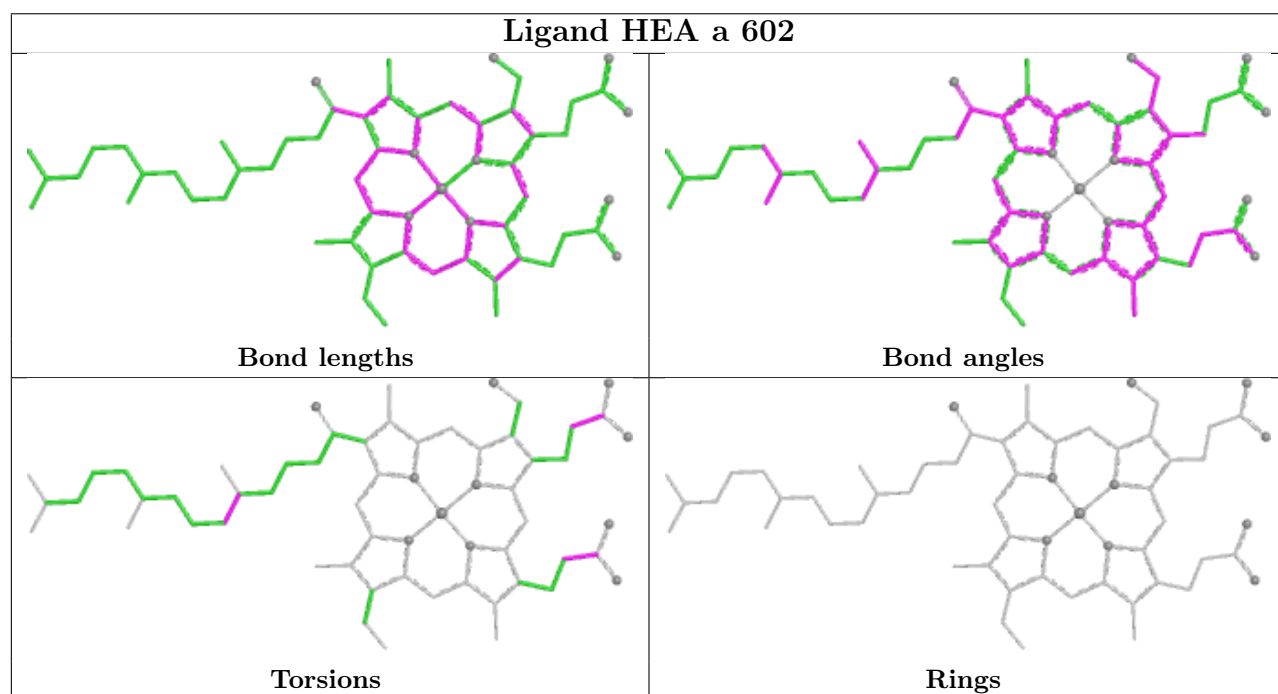
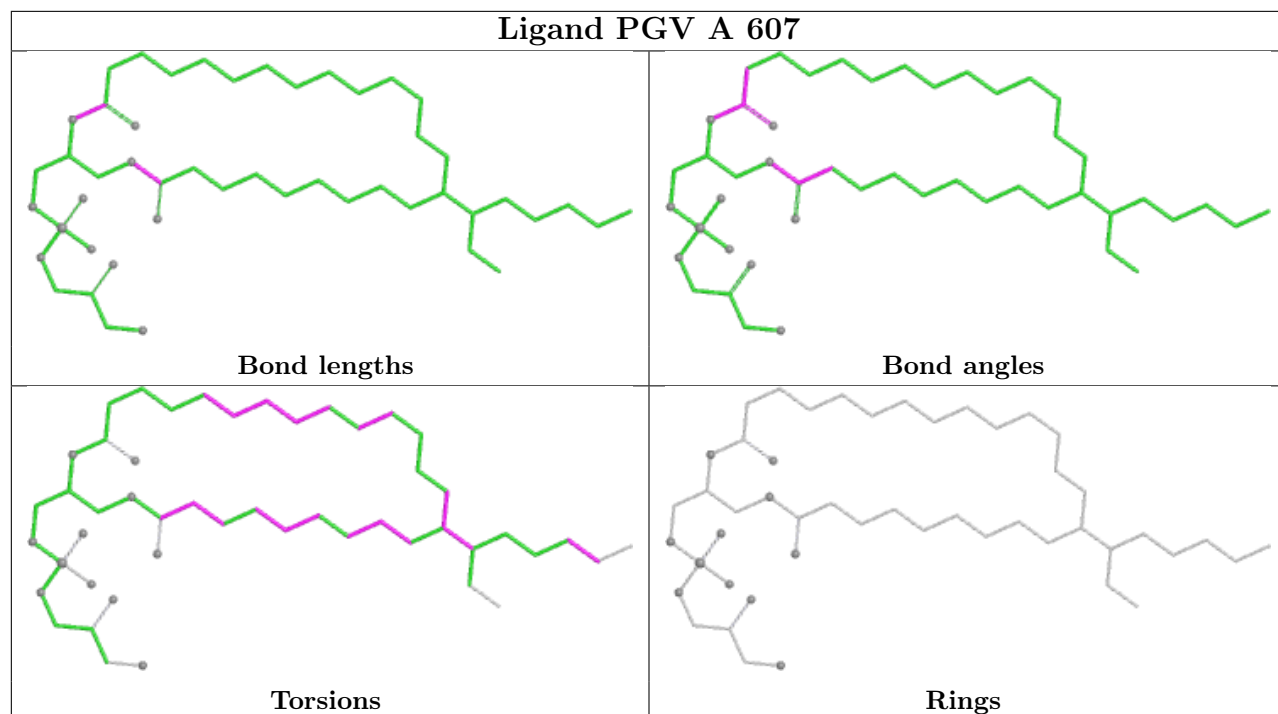
Ligand PEK C 302



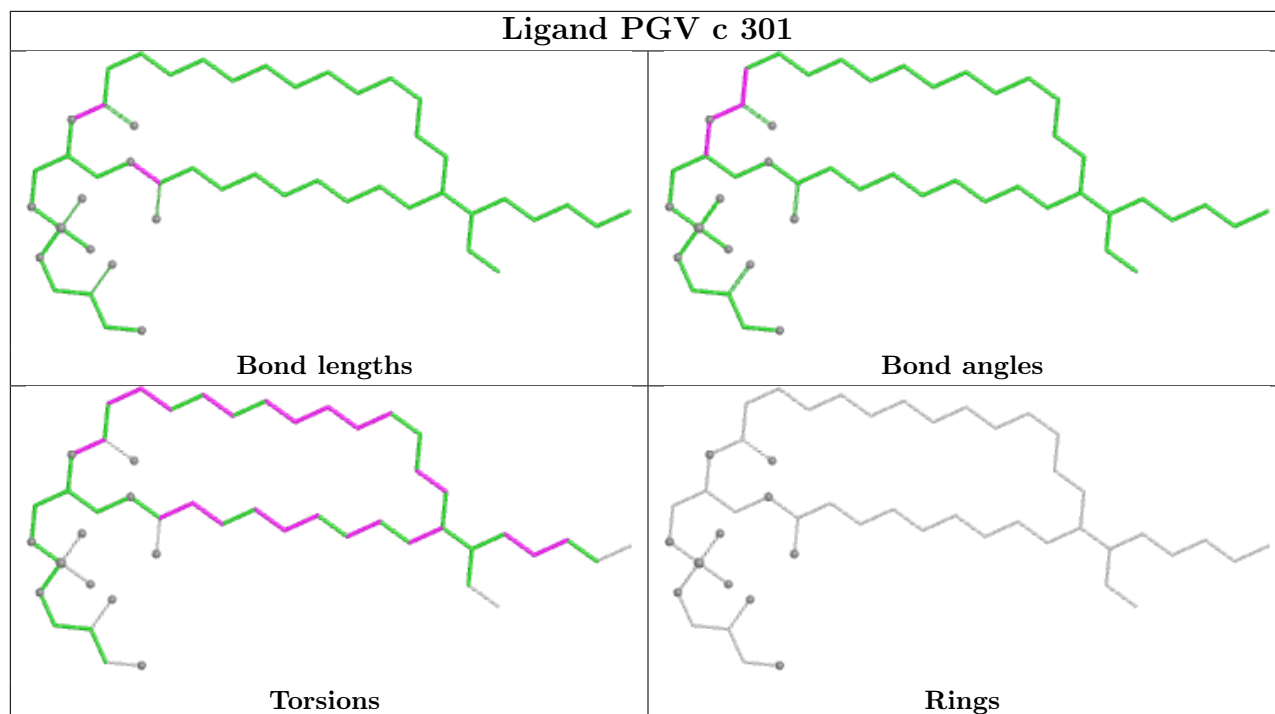
Ligand CHD b 301



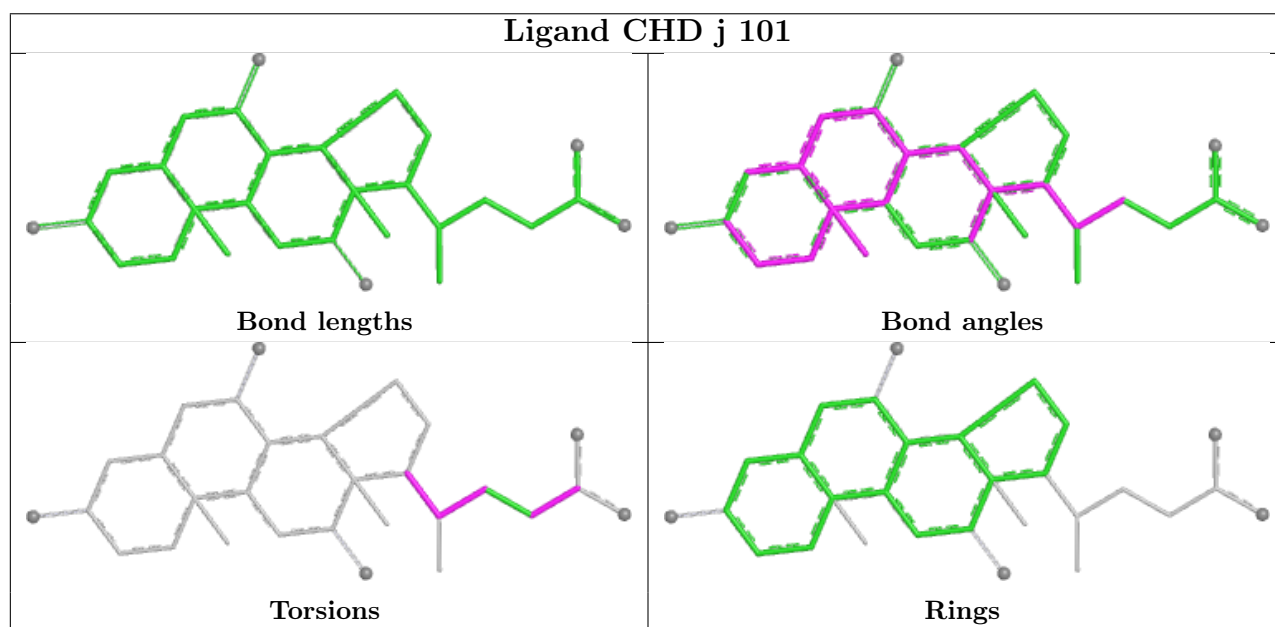


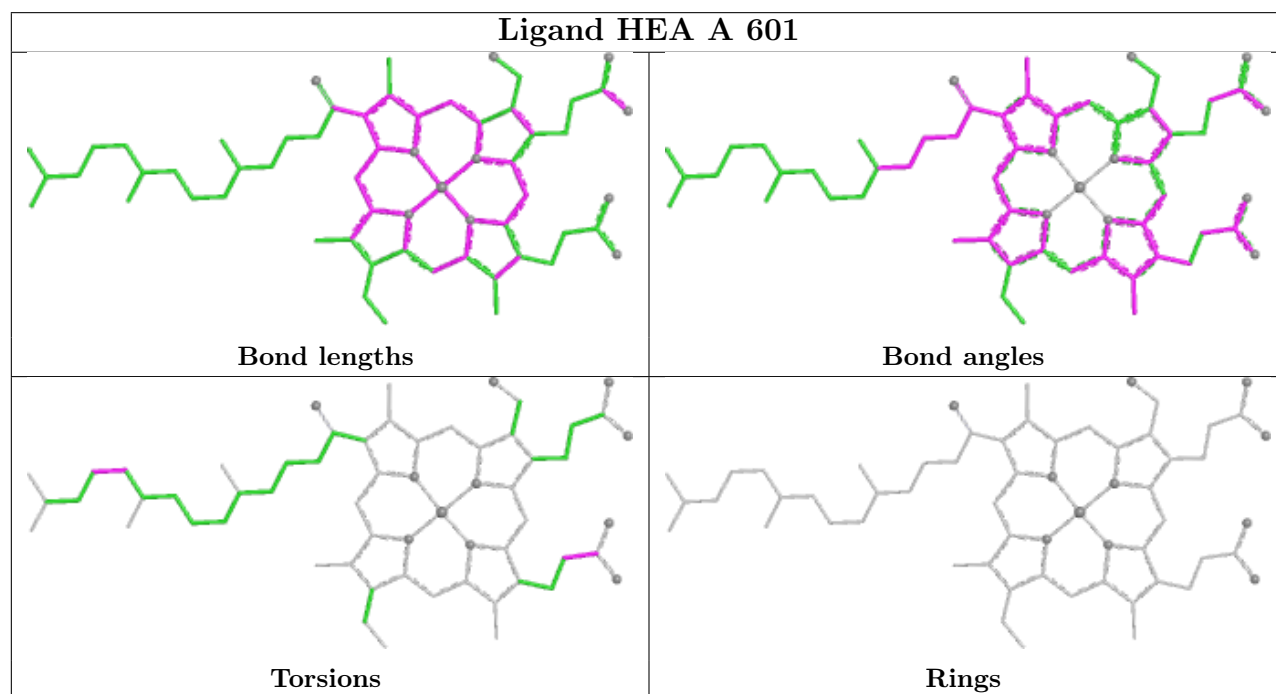
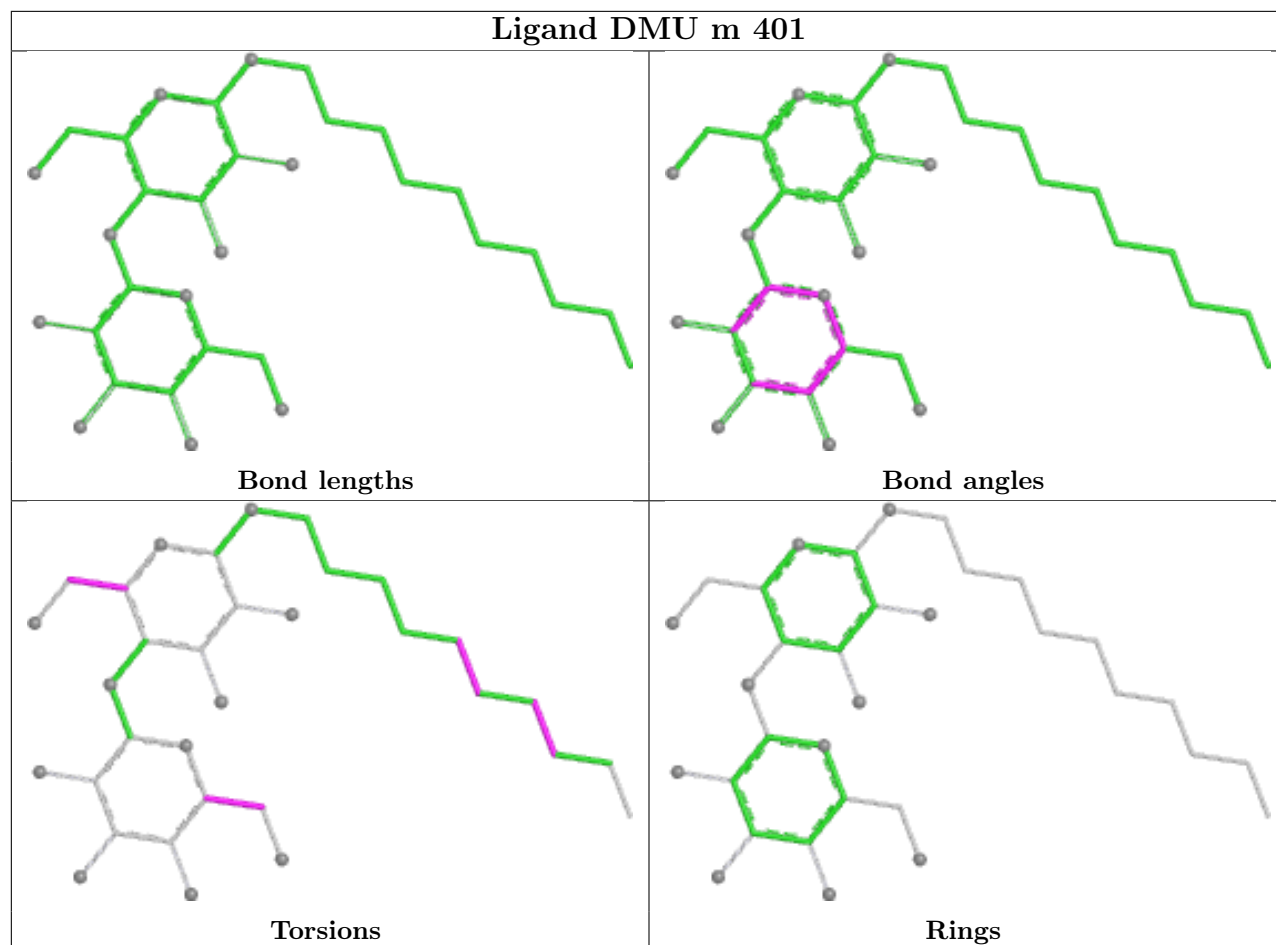


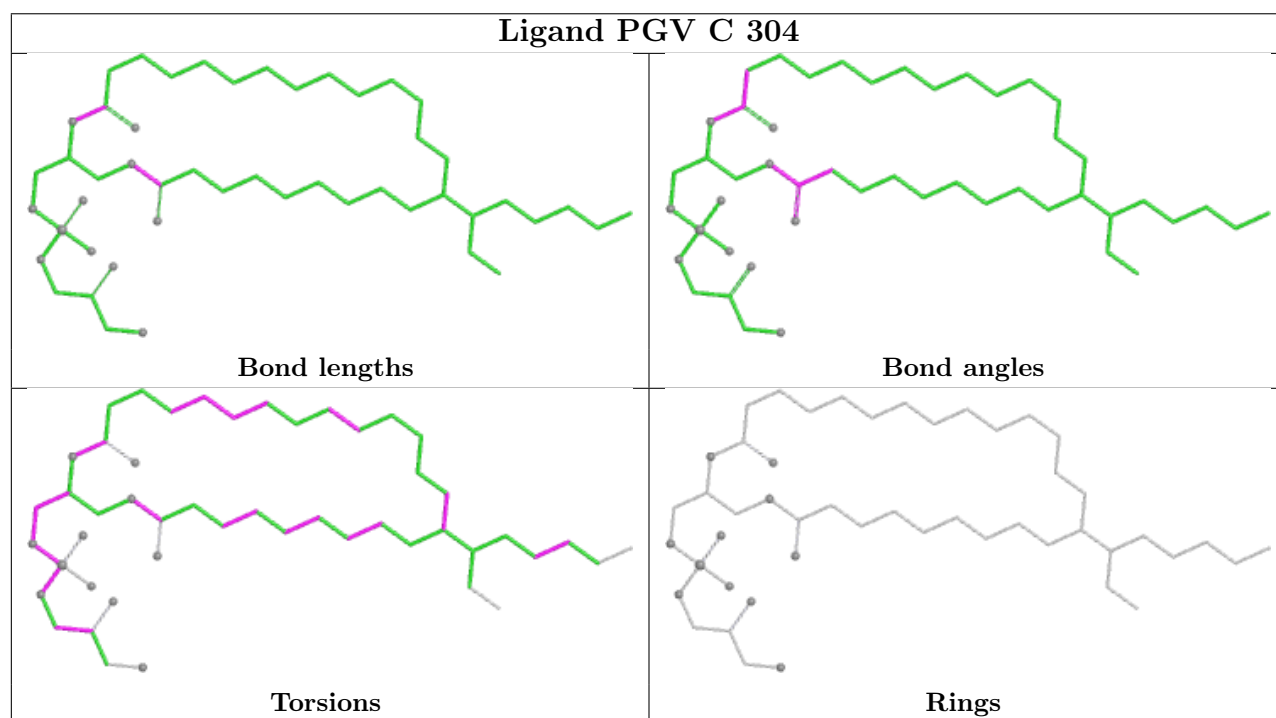
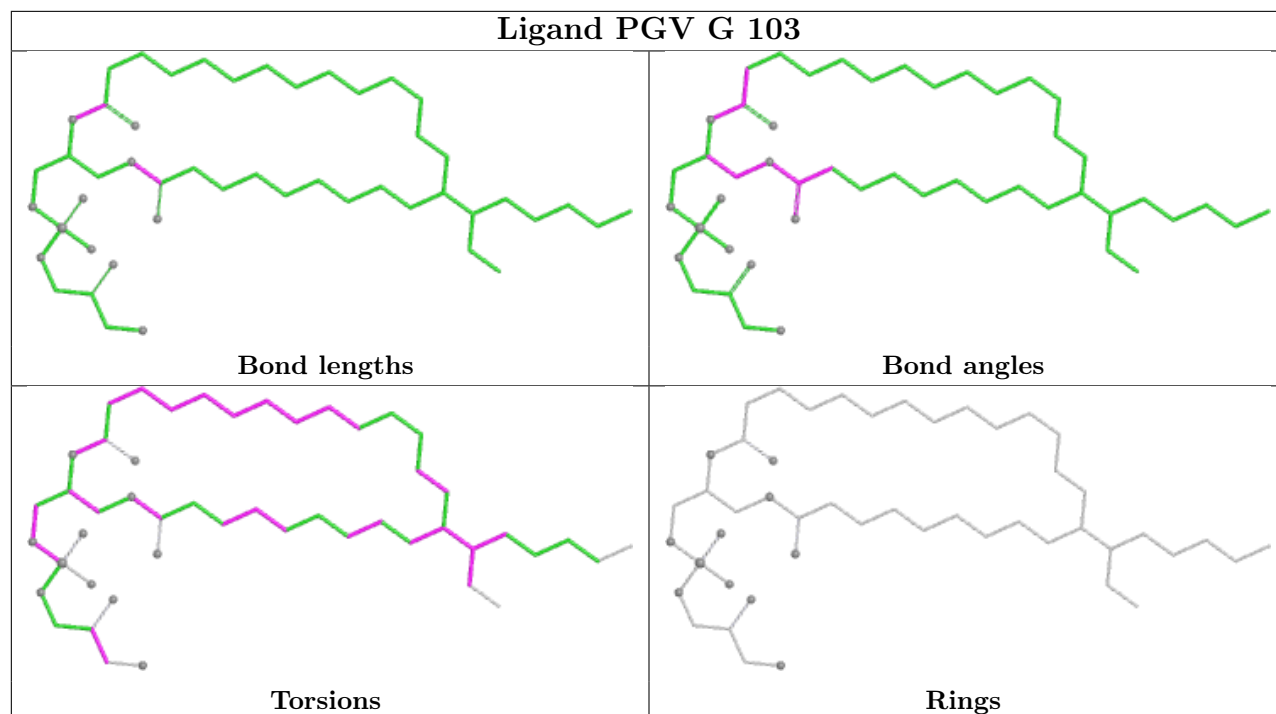
Ligand PGV c 301

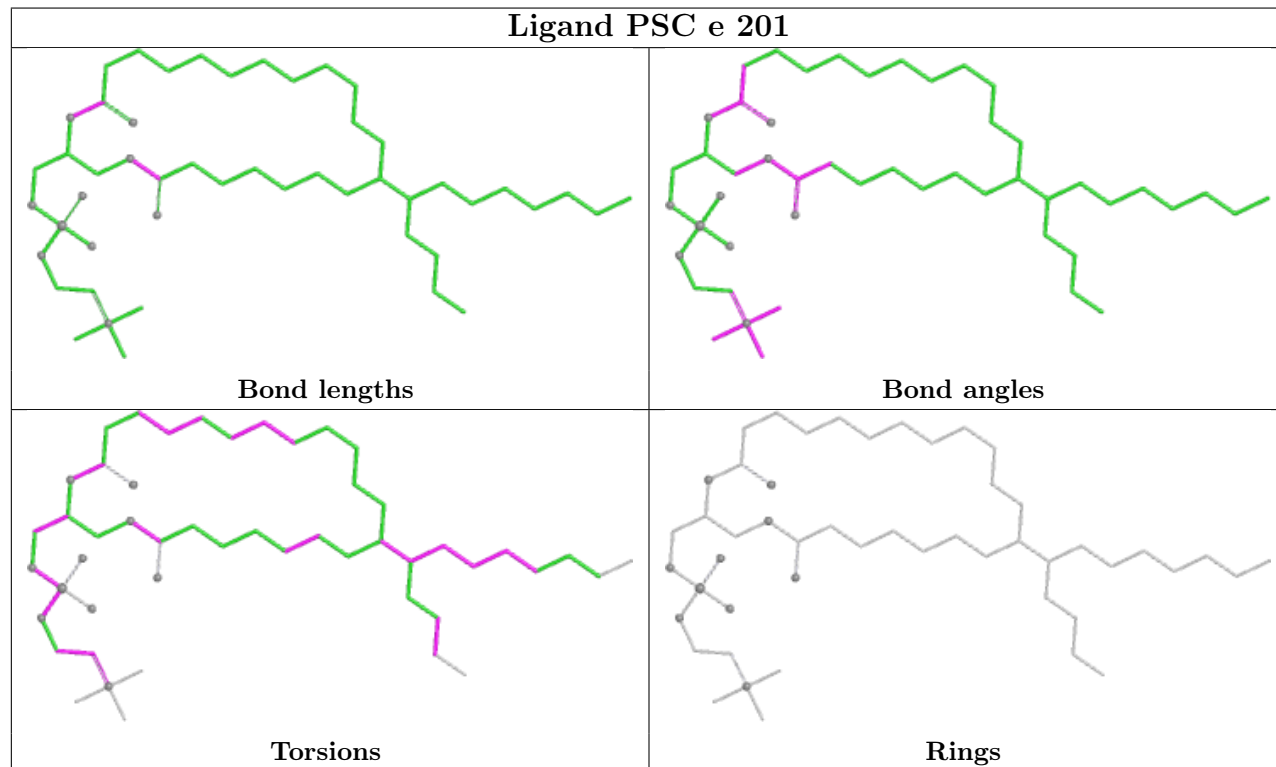
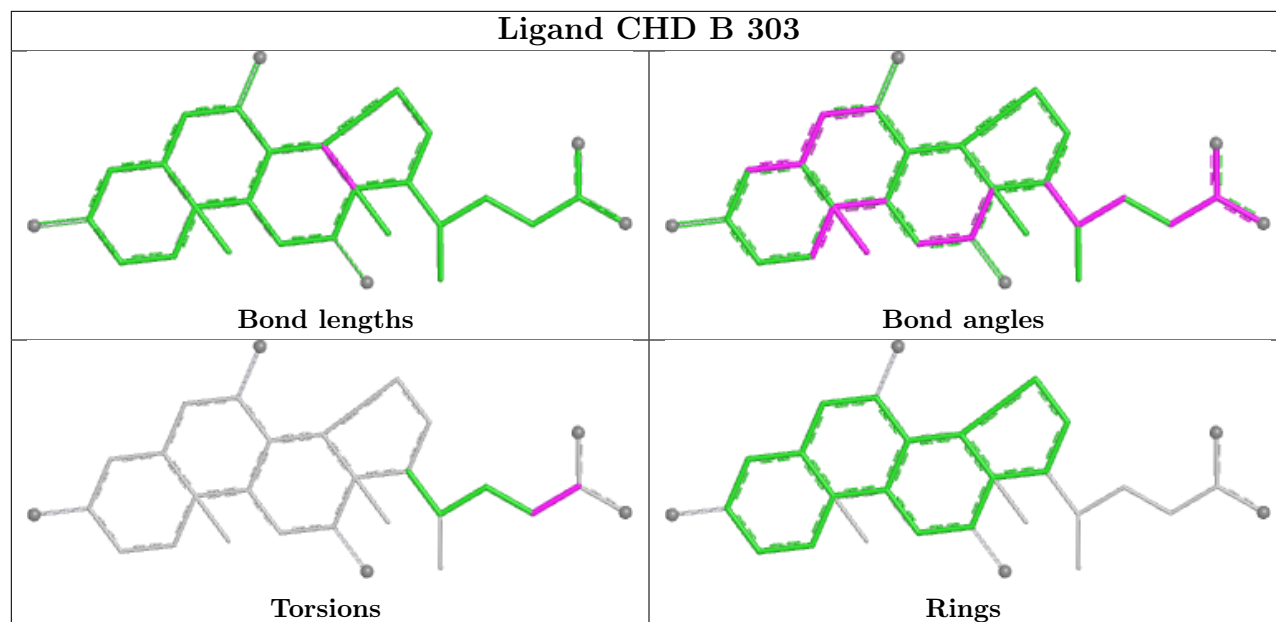


Ligand CHD j 101

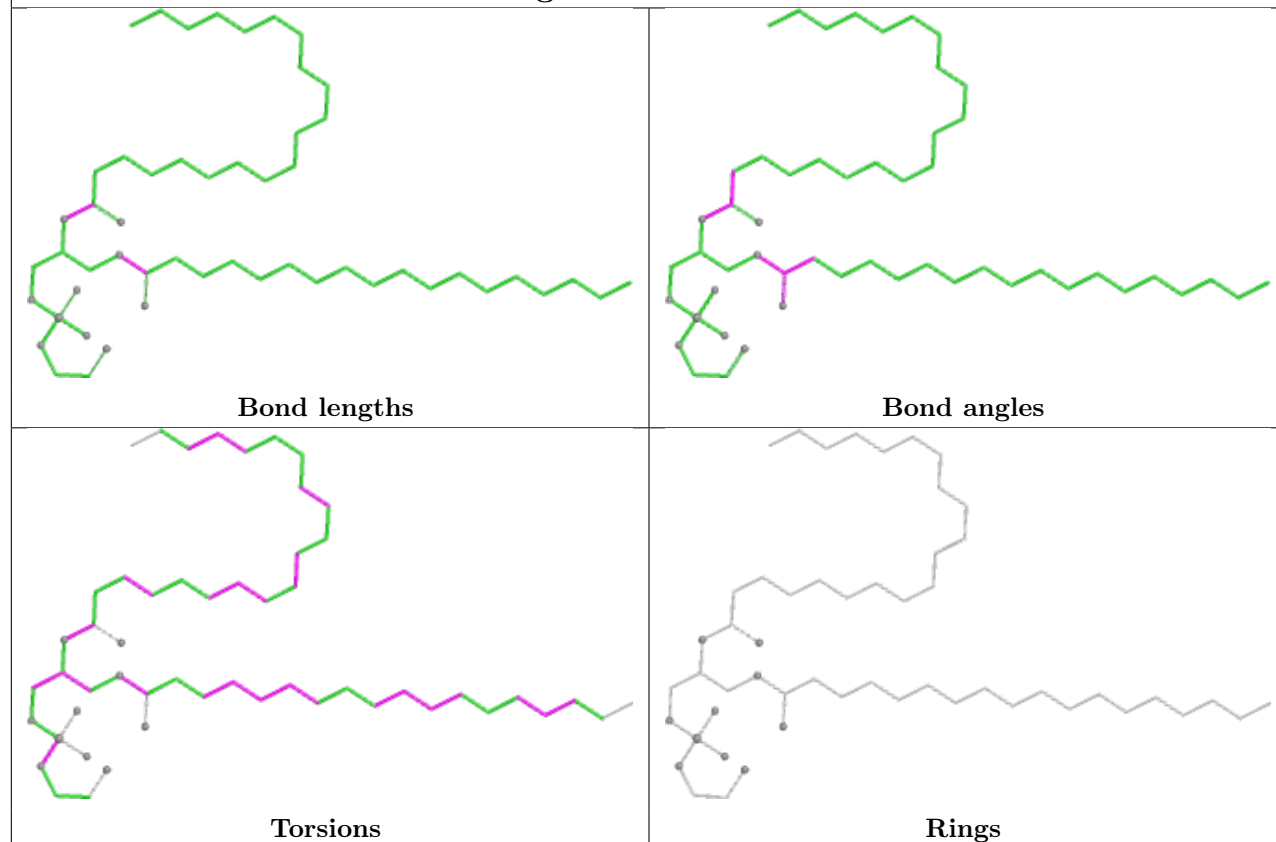




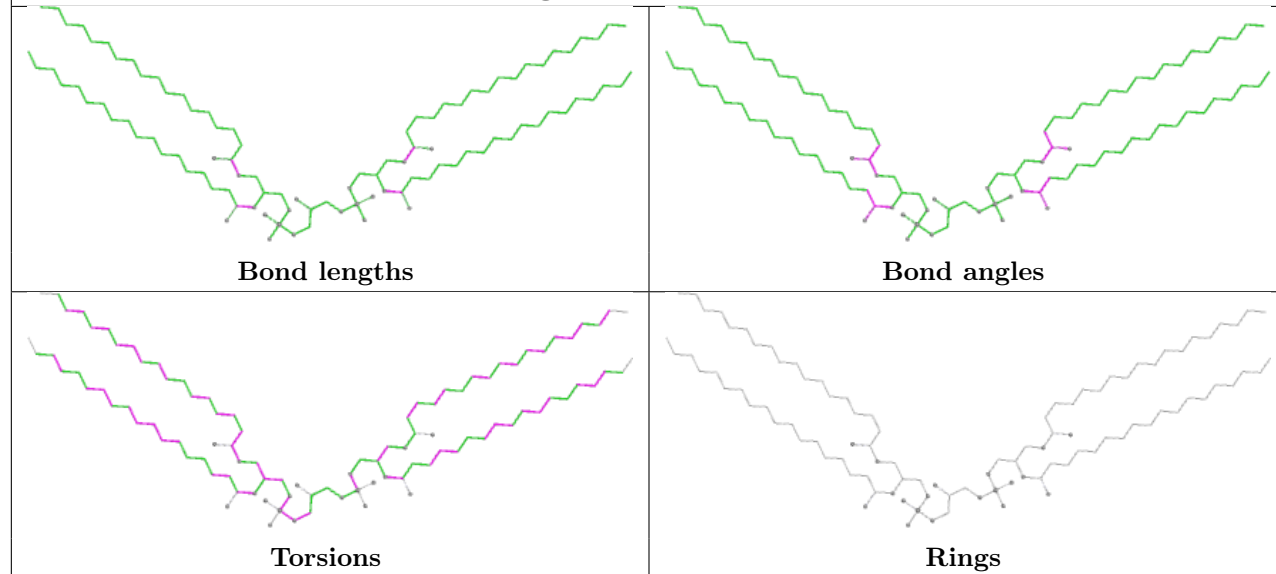


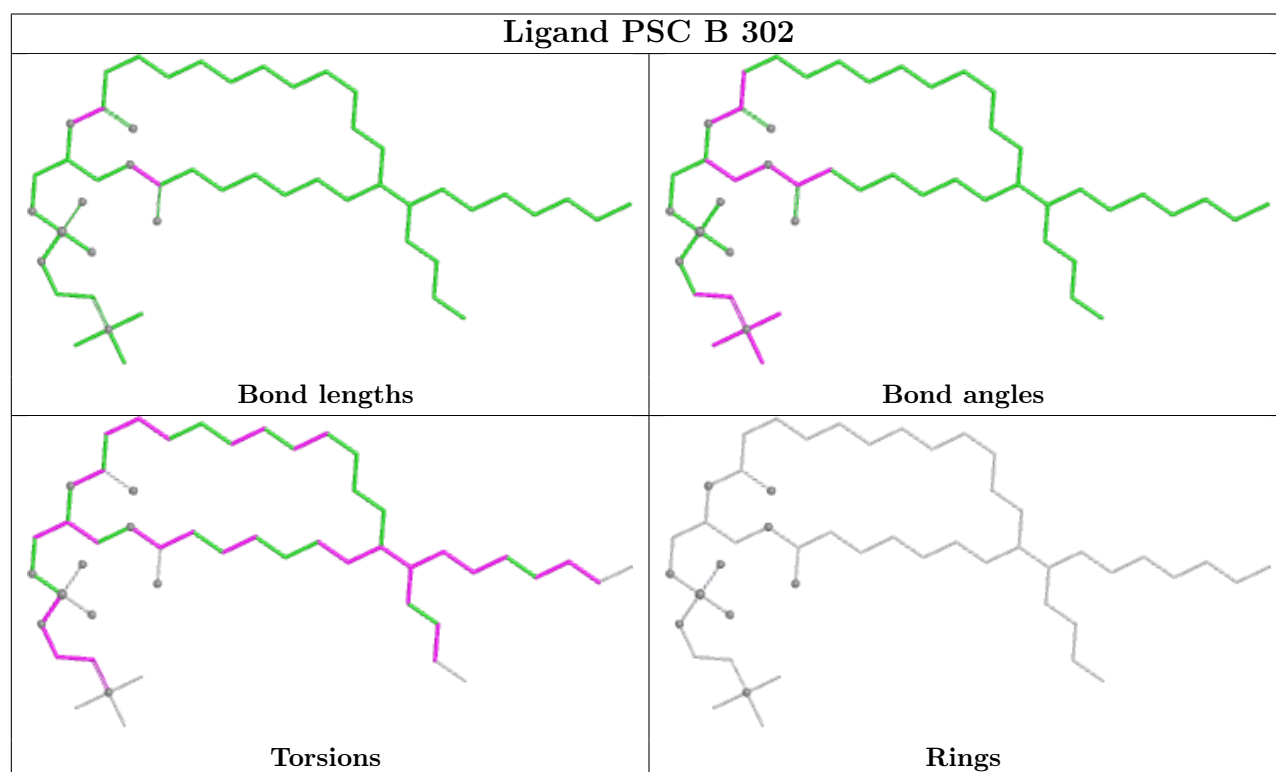
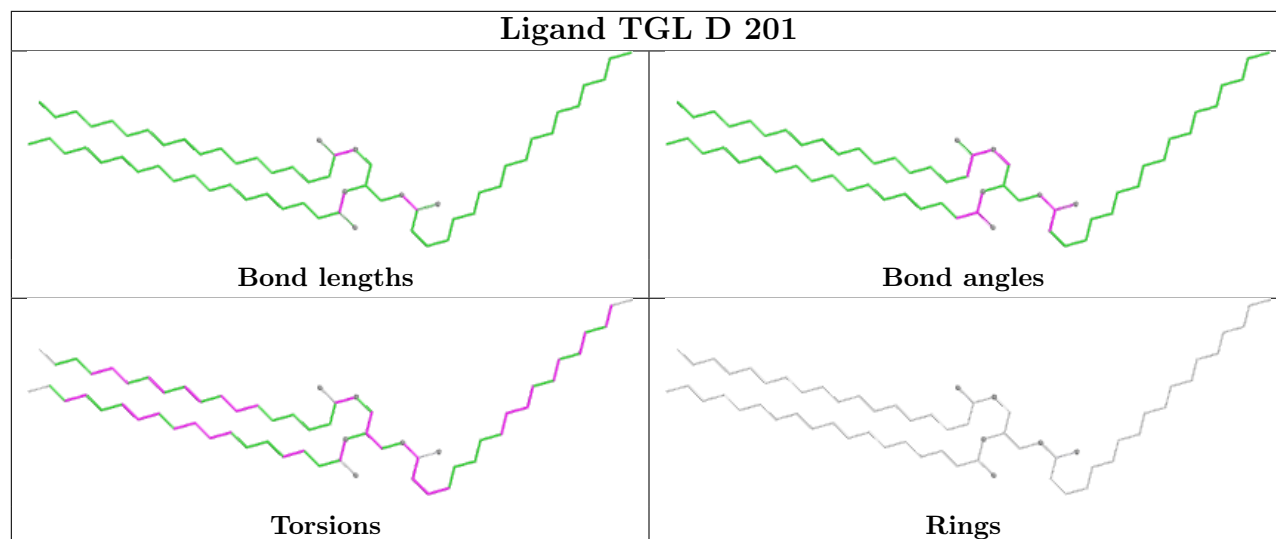


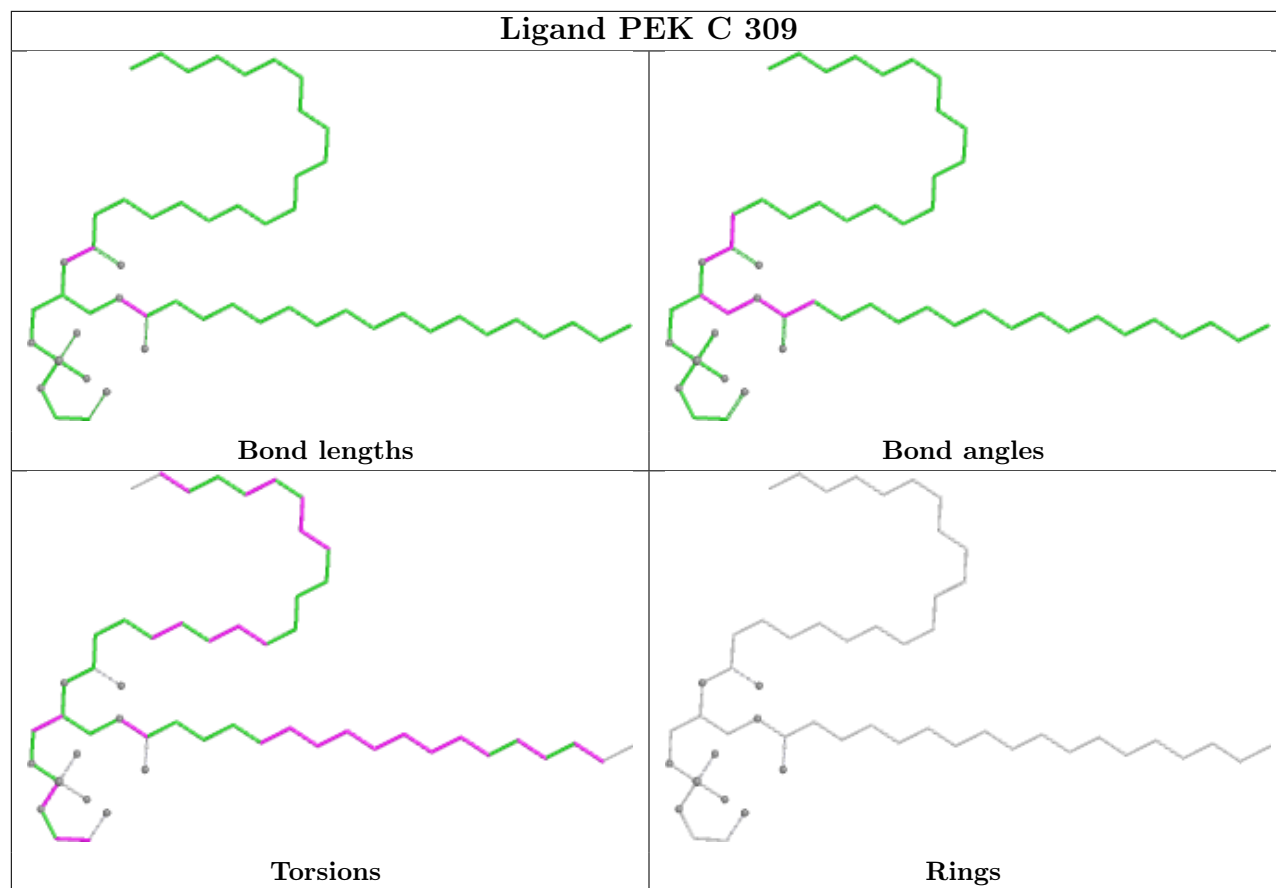
Ligand PEK c 303

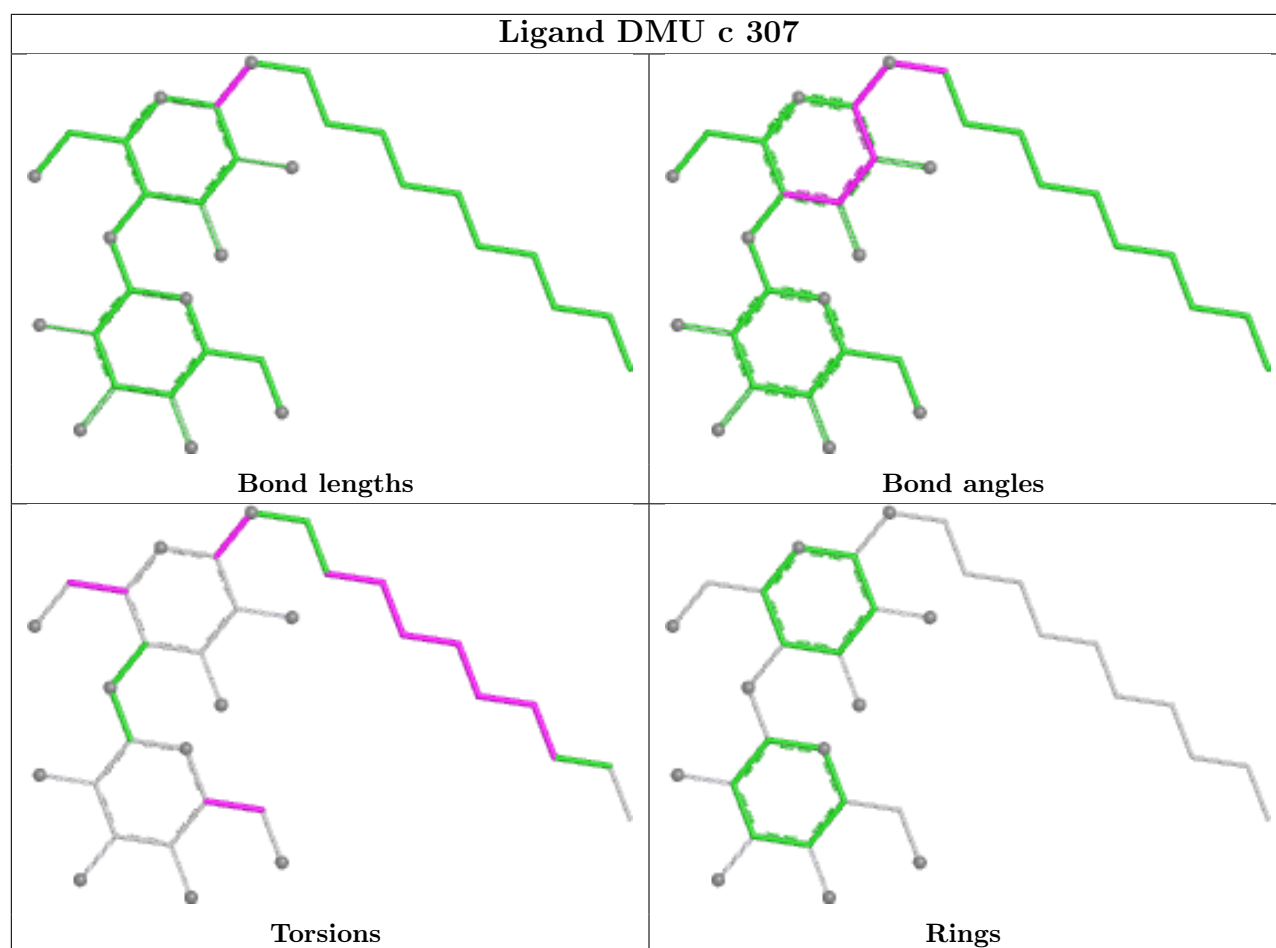


Ligand CDL c 305









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.66	2 (0%) 88 89	22, 28, 39, 85	0
1	a	513/514 (99%)	-0.14	3 (0%) 85 86	27, 41, 58, 93	0
2	B	226/227 (99%)	-0.32	3 (1%) 75 76	23, 35, 62, 123	0
2	b	226/227 (99%)	0.31	10 (4%) 39 41	36, 52, 90, 134	0
3	C	259/261 (99%)	-0.48	1 (0%) 88 89	25, 33, 52, 87	0
3	c	259/261 (99%)	-0.09	5 (1%) 66 68	31, 41, 64, 92	0
4	D	144/147 (97%)	-0.36	1 (0%) 84 85	29, 39, 65, 108	0
4	d	144/147 (97%)	0.74	10 (6%) 23 25	49, 67, 109, 200	0
5	E	105/109 (96%)	-0.31	1 (0%) 79 80	29, 40, 77, 124	0
5	e	105/109 (96%)	0.20	1 (0%) 79 80	37, 56, 79, 118	0
6	F	98/98 (100%)	0.09	8 (8%) 17 19	28, 43, 118, 148	0
6	f	98/98 (100%)	0.36	8 (8%) 17 19	37, 53, 130, 160	0
7	G	83/85 (97%)	0.52	15 (18%) 3 4	31, 43, 128, 140	0
7	g	83/85 (97%)	0.77	15 (18%) 3 4	33, 55, 133, 156	0
8	H	79/85 (92%)	0.25	6 (7%) 20 21	30, 46, 113, 133	0
8	h	79/85 (92%)	0.61	9 (11%) 10 11	40, 62, 133, 154	0
9	I	72/73 (98%)	-0.04	1 (1%) 73 75	33, 47, 73, 76	0
9	i	72/73 (98%)	0.59	6 (8%) 17 19	38, 65, 90, 129	0
10	J	58/59 (98%)	0.13	3 (5%) 33 34	36, 48, 82, 130	0
10	j	58/59 (98%)	0.98	6 (10%) 12 13	49, 62, 106, 176	0
11	K	49/56 (87%)	0.27	4 (8%) 17 19	30, 46, 76, 107	0
11	k	49/56 (87%)	0.83	3 (6%) 27 29	53, 68, 91, 111	0
12	L	46/47 (97%)	-0.30	2 (4%) 40 41	28, 36, 58, 118	0
12	l	46/47 (97%)	0.55	2 (4%) 40 41	42, 59, 89, 140	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.15	1 (2%) 61 63	33, 38, 69, 116	0
13	m	43/46 (93%)	0.76	4 (9%) 14 16	51, 60, 97, 163	0
All	All	3550/3614 (98%)	-0.03	130 (3%) 45 48	22, 42, 87, 200	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	d	6	VAL	8.7
4	d	5	VAL	8.5
11	K	42	PRO	7.4
6	F	1	ALA	6.9
7	G	9	GLY	6.6
7	G	3	ALA	6.6
7	G	4	ALA	6.4
6	f	1	ALA	6.2
7	G	10	GLY	6.0
6	f	2	SER	5.8
8	h	48	GLY	5.8
8	h	8	ILE	5.5
10	j	58	LYS	5.5
7	g	5	LYS	5.2
7	g	7	ASP	5.1
10	j	52	TRP	5.1
7	G	5	LYS	5.1
6	f	97	ALA	5.0
6	f	96	LEU	4.8
7	g	1	ALA	4.8
12	l	2	HIS	4.8
10	j	56	PRO	4.7
11	k	6	ALA	4.6
11	K	41	ASN	4.6
8	H	8	ILE	4.6
6	f	95	GLN	4.5
7	G	6	GLY	4.4
7	g	10	GLY	4.4
7	g	3	ALA	4.4
2	B	90	ILE	4.3
7	g	9	GLY	4.3
8	H	48	GLY	4.3
7	G	1	ALA	4.2
6	F	95	GLN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	K	6	ALA	4.0
7	g	2	SER	4.0
7	g	42	ARG	4.0
6	F	97	ALA	4.0
8	H	45	ALA	4.0
3	c	37	PHE	4.0
6	f	94	HIS	3.9
2	b	59	GLN	3.8
4	D	4	SER	3.8
6	F	94	HIS	3.7
10	j	1	PHE	3.6
7	g	36	TRP	3.6
4	d	7	LYS	3.6
2	b	90	ILE	3.6
7	G	2	SER	3.5
7	g	84	LYS	3.5
7	G	41	HIS	3.5
4	d	4	SER	3.4
13	m	41	LYS	3.4
10	j	57	HIS	3.3
7	G	7	ASP	3.3
8	H	7	LYS	3.3
8	h	47	GLY	3.3
7	G	8	HIS	3.3
7	g	39	SER	3.3
6	F	96	LEU	3.2
2	b	227	LEU	3.2
4	d	8	SER	3.2
2	b	131	GLY	3.1
2	b	113	TYR	3.1
3	c	38	ASN	3.0
8	h	50	VAL	3.0
7	G	42	ARG	3.0
2	B	113	TYR	2.9
8	h	46	LYS	2.9
12	L	2	HIS	2.9
6	F	93	PRO	2.9
3	c	3	HIS	2.9
8	H	9	LYS	2.8
13	m	32	TRP	2.8
5	E	5	HIS	2.8
7	g	6	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	d	102	TYR	2.8
6	f	98	HIS	2.7
2	B	59	GLN	2.7
9	i	73	LYS	2.7
7	g	41	HIS	2.7
10	J	57	HIS	2.6
8	H	47	GLY	2.6
6	F	2	SER	2.6
13	m	43	SER	2.6
1	A	514	LYS	2.6
9	i	3	ALA	2.6
12	l	20	ARG	2.6
2	b	130	PRO	2.6
1	a	514	LYS	2.6
4	d	53	ILE	2.5
7	G	39	SER	2.5
13	m	1	ILE	2.5
10	J	58	LYS	2.5
6	F	3	GLY	2.5
3	c	39	SER	2.4
10	j	50	LEU	2.4
10	J	1	PHE	2.4
8	h	7	LYS	2.4
8	h	9	LYS	2.4
4	d	101	HIS	2.4
6	f	3	GLY	2.3
1	a	48	LEU	2.3
1	a	483	LEU	2.3
12	L	47	LYS	2.3
2	b	224	ALA	2.3
2	b	217	LYS	2.3
3	c	33	MET	2.2
11	k	54	ARG	2.2
11	K	46	GLY	2.2
7	G	36	TRP	2.2
4	d	10	ASP	2.2
3	C	3	HIS	2.2
2	b	120	SER	2.2
9	i	2	THR	2.2
8	h	49	ASP	2.1
9	i	19	PHE	2.1
7	g	40	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	d	140	TYR	2.1
11	k	53	TRP	2.1
13	M	43	SER	2.1
7	G	84	LYS	2.1
1	A	513	LEU	2.1
8	h	10	ASN	2.1
9	I	37	PHE	2.1
7	g	12	GLY	2.1
5	e	108	LYS	2.1
2	b	136	LEU	2.1
9	i	31	PHE	2.1
9	i	72	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	i	1	9/10	0.39	0.19	117,152,162,171	0
9	SAC	I	1	9/10	0.59	0.20	86,107,126,130	0
7	TPO	g	11	11/12	0.60	0.22	93,121,137,145	0
7	TPO	G	11	11/12	0.64	0.24	92,134,145,151	0
1	FME	a	1	10/11	0.77	0.21	80,89,130,142	0
1	FME	A	1	10/11	0.87	0.13	53,62,98,100	0
2	FME	b	1	10/11	0.92	0.13	48,55,57,58	0
2	FME	B	1	10/11	0.97	0.08	29,35,42,44	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

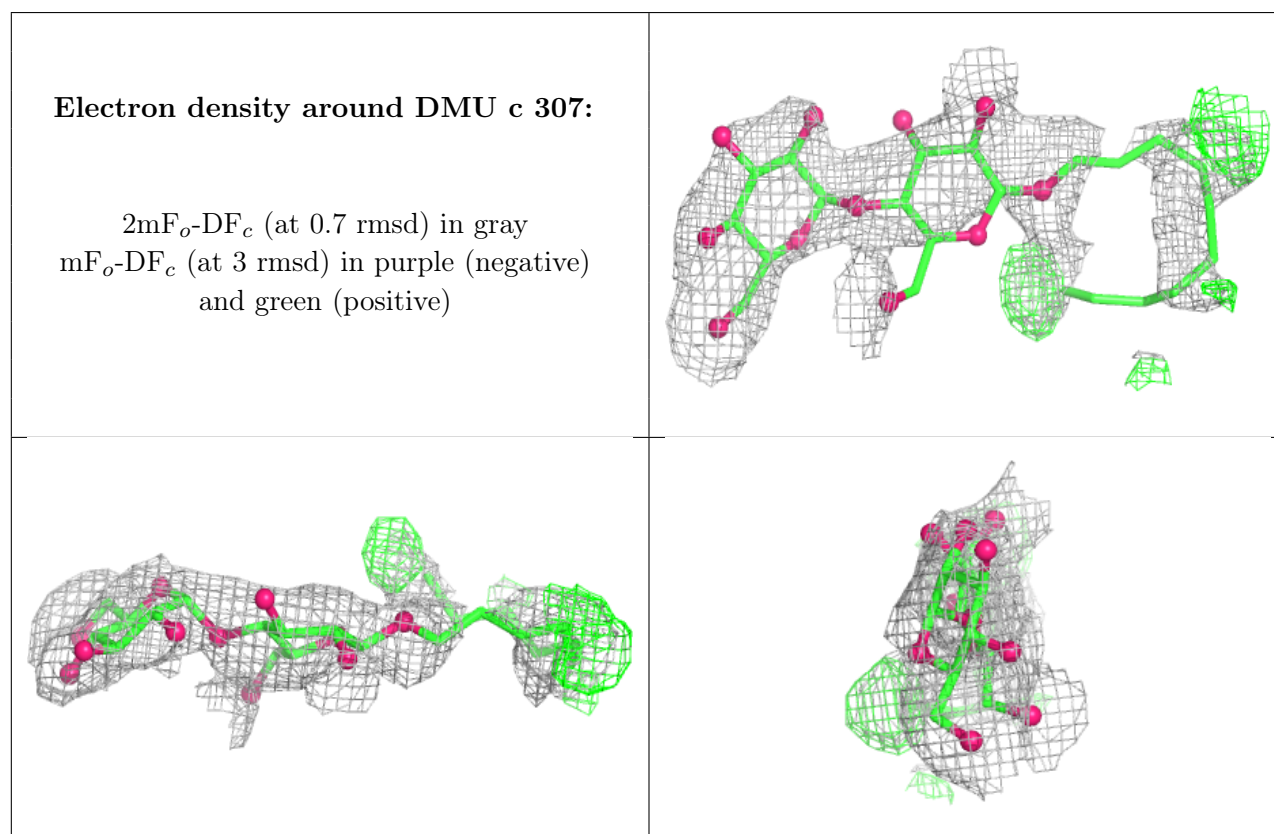
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	DMU	c	307	33/33	0.58	0.21	90,138,163,171	0
24	PEK	G	102	53/53	0.74	0.25	64,117,204,226	0
26	DMU	C	307	33/33	0.75	0.18	66,126,146,150	0
24	PEK	C	309	53/53	0.75	0.23	66,98,168,173	0
19	TGL	D	201	63/63	0.76	0.27	66,92,121,126	0
22	PSC	e	201	52/52	0.77	0.25	56,121,231,239	0
23	CHD	j	101	29/29	0.77	0.21	104,119,130,134	0
18	PGV	C	304	51/51	0.78	0.23	61,95,132,142	0
18	PGV	G	103	51/51	0.79	0.24	54,108,130,139	0
25	CDL	c	305	100/100	0.79	0.23	49,107,143,157	0
17	NA	a	605	1/1	0.80	0.15	50,50,50,50	0
25	CDL	g	103	100/100	0.80	0.27	63,112,158,182	0
19	TGL	a	606	63/63	0.81	0.23	74,95,131,133	0
25	CDL	G	101	100/100	0.81	0.26	71,112,154,164	0
18	PGV	A	606	51/51	0.81	0.23	53,89,136,151	0
18	PGV	a	607	51/51	0.82	0.23	58,96,149,171	0
19	TGL	l	101	63/63	0.82	0.24	55,100,146,161	0
24	PEK	c	303	53/53	0.82	0.22	59,104,133,143	0
24	PEK	C	308	53/53	0.82	0.23	67,103,158,173	0
22	PSC	B	302	52/52	0.83	0.25	57,118,223,244	0
19	TGL	L	101	63/63	0.83	0.22	43,88,128,130	0
25	CDL	C	305	100/100	0.83	0.21	46,102,140,147	0
23	CHD	J	101	29/29	0.83	0.19	76,89,111,117	0
19	TGL	A	608	63/63	0.84	0.22	37,87,127,146	0
19	TGL	i	101	63/63	0.85	0.23	46,99,142,151	0
26	DMU	m	401	33/33	0.85	0.13	67,94,108,112	0
23	CHD	C	306	29/29	0.89	0.15	72,84,88,90	0
23	CHD	c	306	29/29	0.91	0.13	78,83,100,101	0
24	PEK	g	102	53/53	0.94	0.14	41,65,100,105	0
26	DMU	M	101	33/33	0.94	0.09	42,54,66,67	0
23	CHD	c	302	29/29	0.95	0.07	34,38,40,44	0
18	PGV	C	303	51/51	0.96	0.10	27,39,95,97	0
24	PEK	C	302	53/53	0.96	0.12	28,56,114,116	0
23	CHD	b	301	29/29	0.96	0.07	32,39,46,51	0
18	PGV	c	301	51/51	0.96	0.11	29,56,75,82	0
18	PGV	c	304	51/51	0.96	0.11	31,44,93,100	0
14	HEA	a	601	60/60	0.97	0.09	34,41,52,53	0
16	MG	a	604	1/1	0.97	0.07	42,42,42,42	0
23	CHD	B	303	29/29	0.97	0.06	32,36,45,49	0
23	CHD	C	301	29/29	0.97	0.05	29,32,37,41	0
14	HEA	A	601	60/60	0.98	0.06	20,25,42,54	0
14	HEA	a	602	60/60	0.98	0.06	27,31,41,45	0
16	MG	A	604	1/1	0.98	0.03	26,26,26,26	0

Continued on next page...

Continued from previous page...

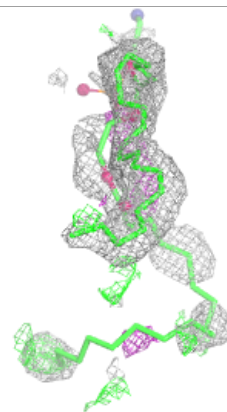
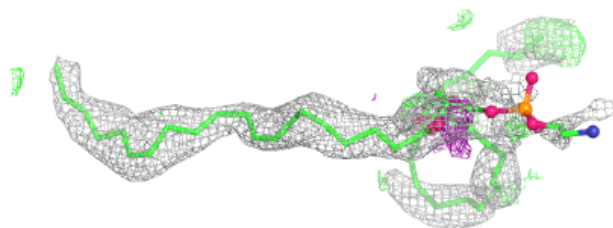
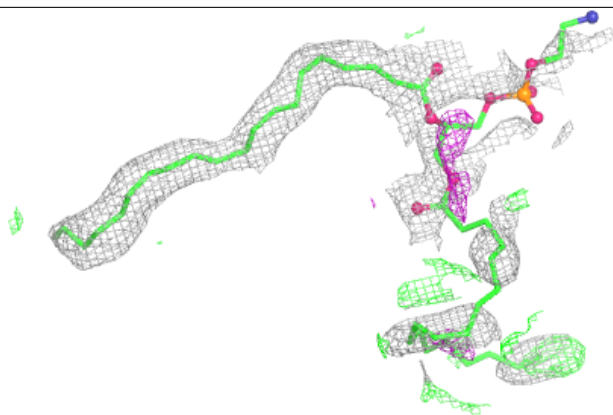
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	PGV	A	607	51/51	0.98	0.08	24,46,64,72	0
20	CMO	a	608	2/2	0.98	0.07	33,33,33,36	0
21	CUA	b	302	2/2	0.98	0.04	46,46,46,47	0
20	CMO	A	609	2/2	0.99	0.08	23,23,23,24	0
17	NA	A	605	1/1	0.99	0.03	31,31,31,31	0
21	CUA	B	301	2/2	0.99	0.02	29,29,29,31	0
14	HEA	A	602	60/60	0.99	0.05	20,23,36,43	0
15	CU	A	603	1/1	1.00	0.04	28,28,28,28	0
15	CU	a	603	1/1	1.00	0.05	39,39,39,39	0
27	ZN	F	101	1/1	1.00	0.04	45,45,45,45	0
27	ZN	f	101	1/1	1.00	0.05	52,52,52,52	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.

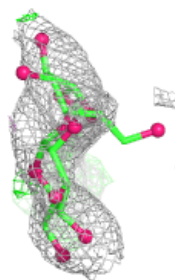
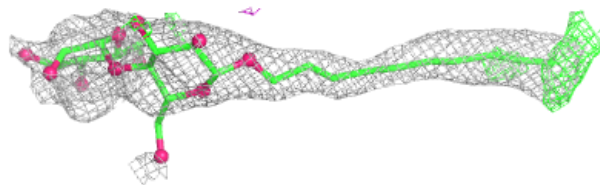
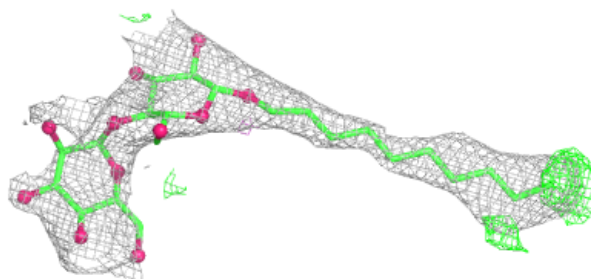


Electron density around PEK G 102:

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

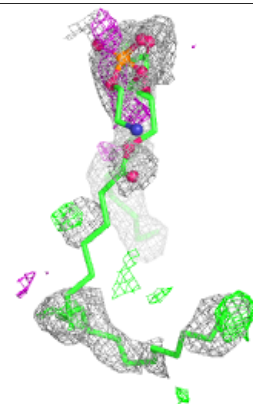
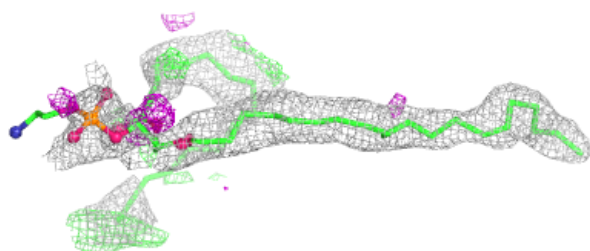
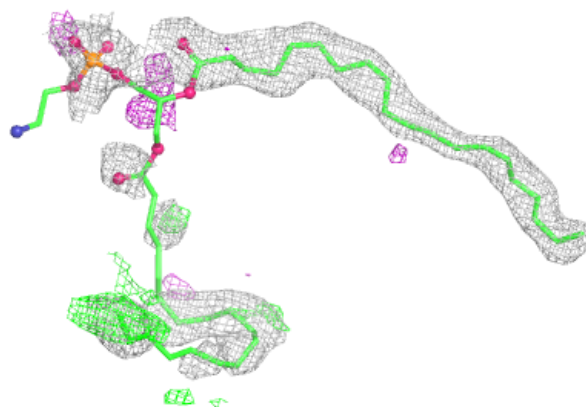
**Electron density around DMU C 307:**

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

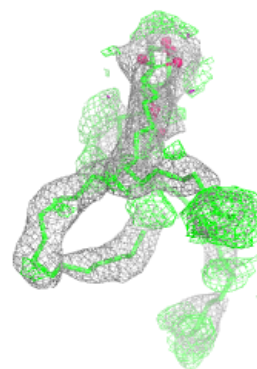
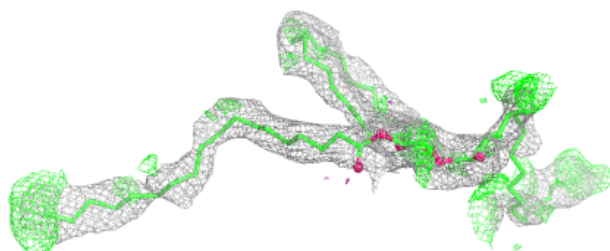
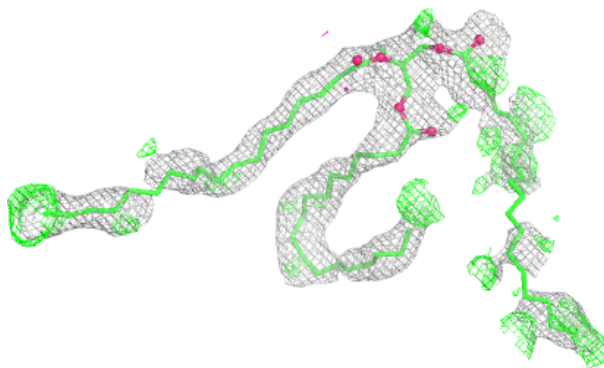


Electron density around PEK C 309:

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

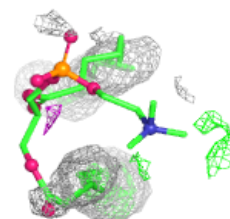
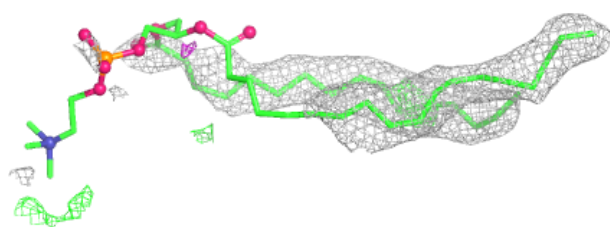
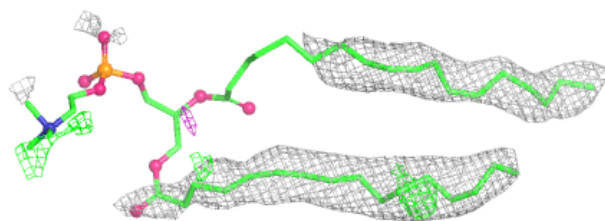
**Electron density around TGL D 201:**

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

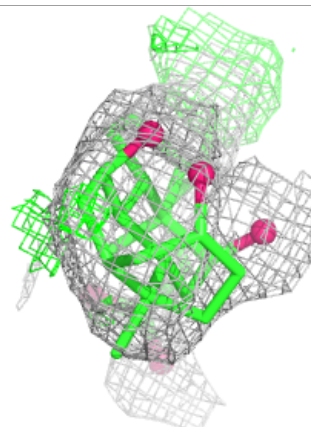
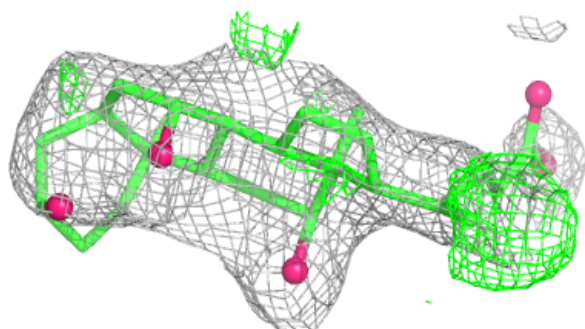
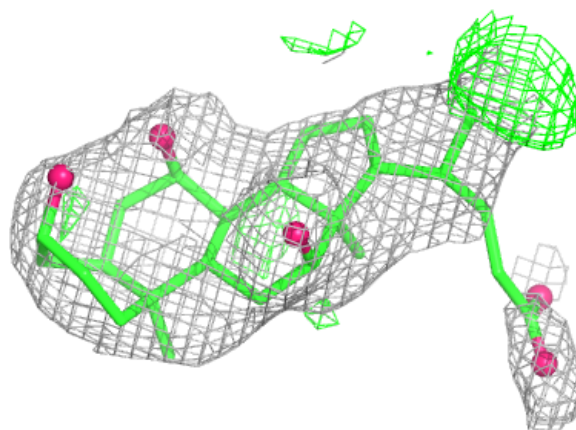


Electron density around PSC e 201:

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

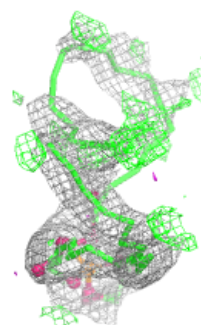
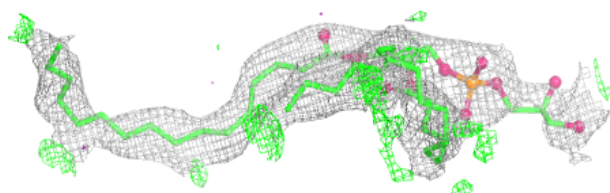
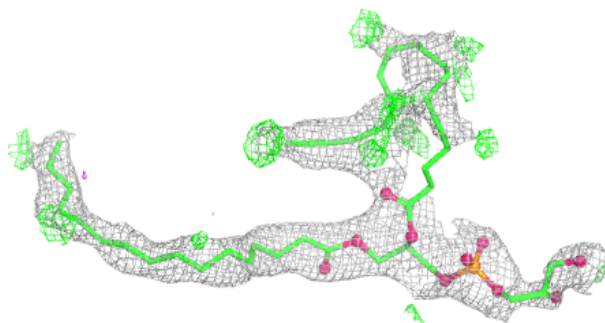
**Electron density around CHD j 101:**

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

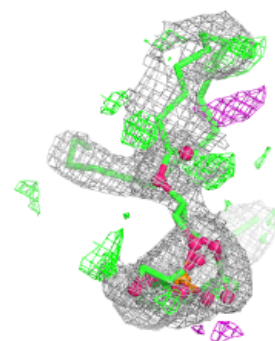
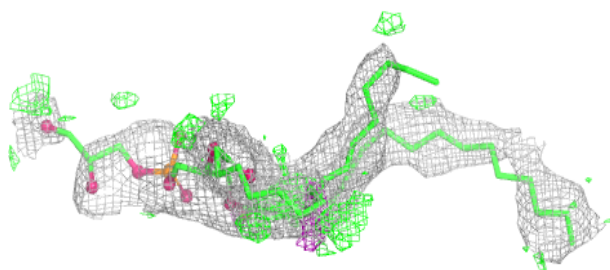
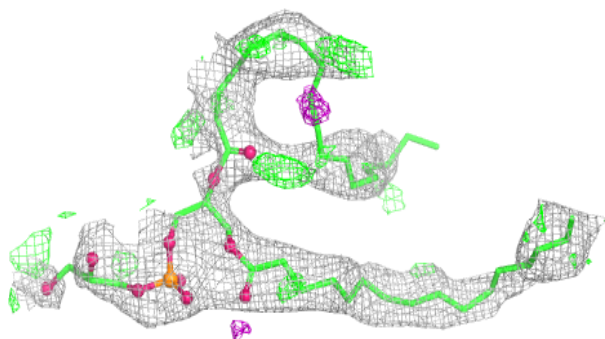


Electron density around PGV C 304:

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

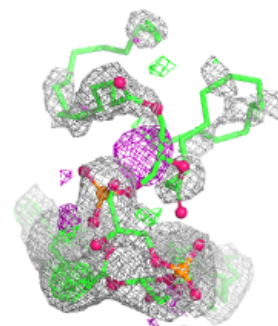
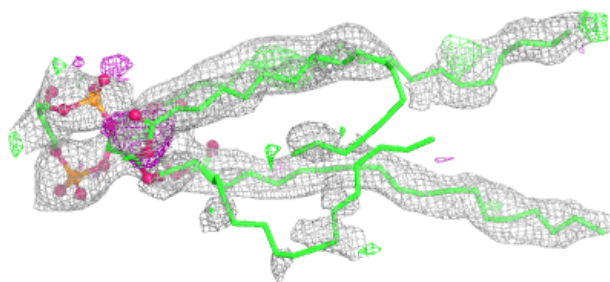
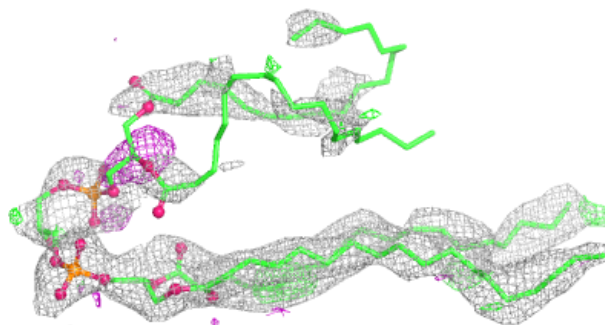
**Electron density around PGV G 103:**

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

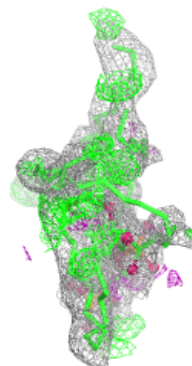
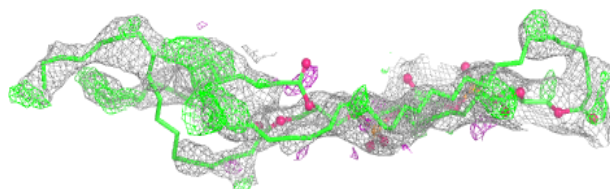
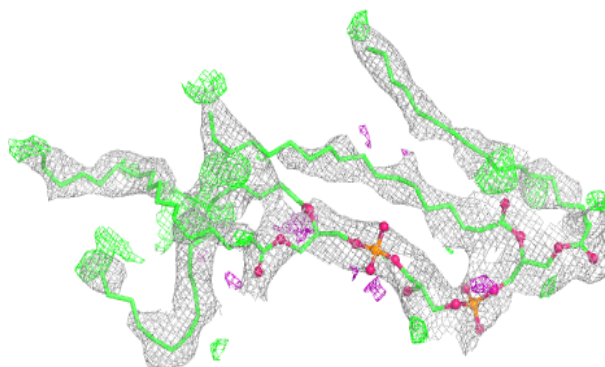


Electron density around CDL c 305:

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

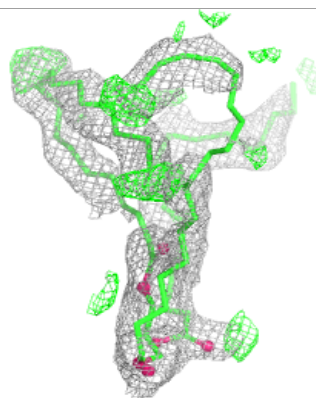
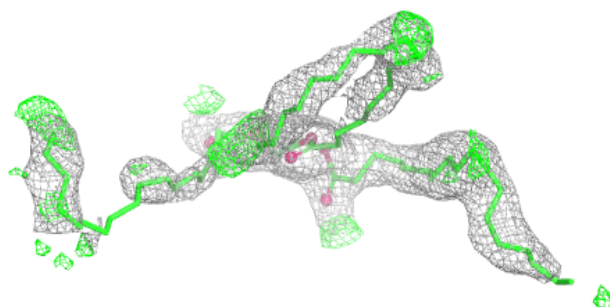
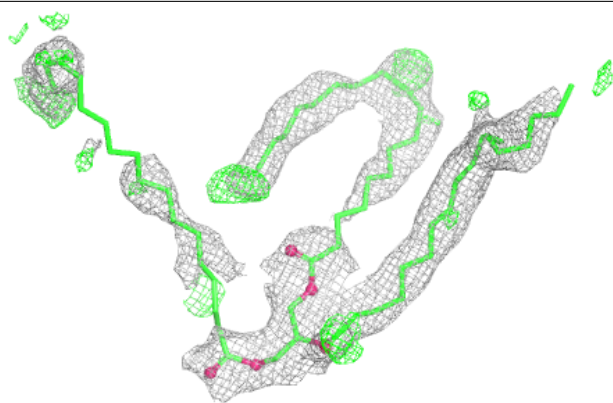
**Electron density around CDL g 103:**

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

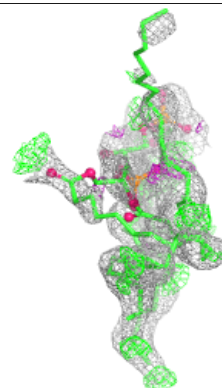
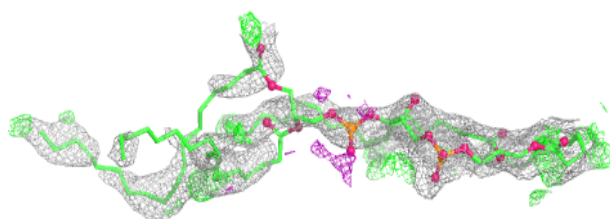
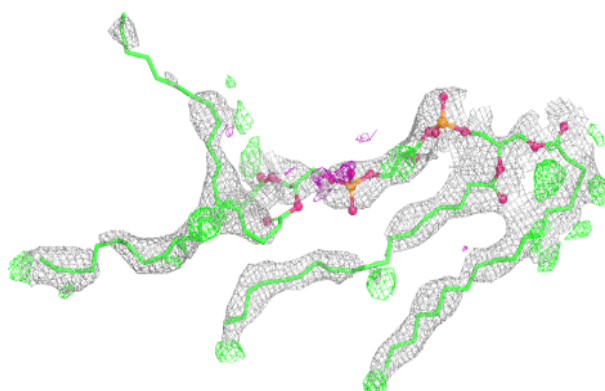


Electron density around TGL a 606:

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

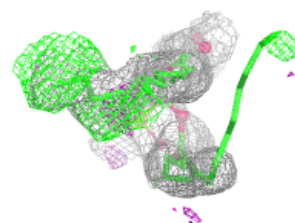
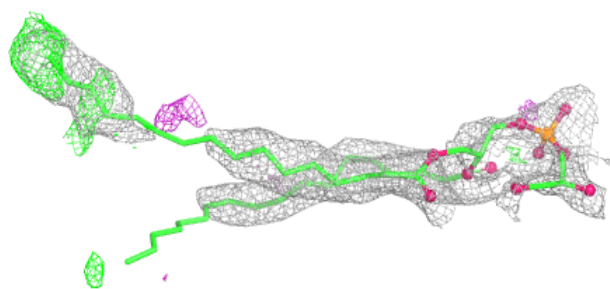
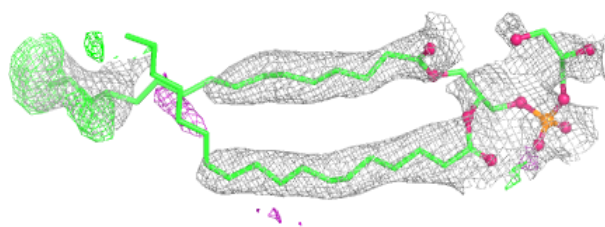
**Electron density around CDL G 101:**

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

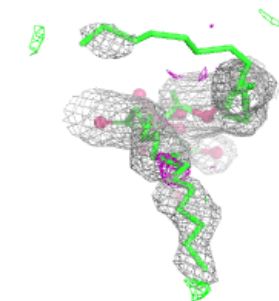
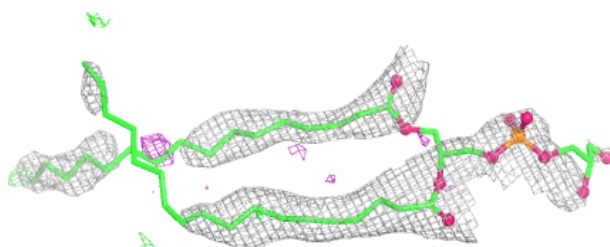
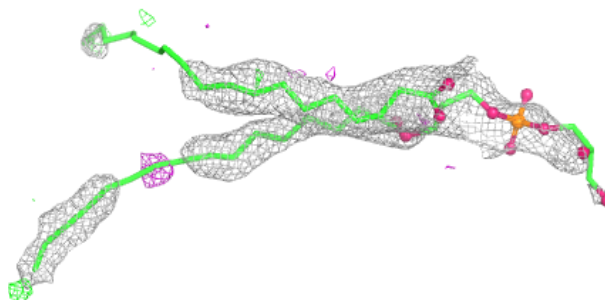


Electron density around PGV A 606:

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

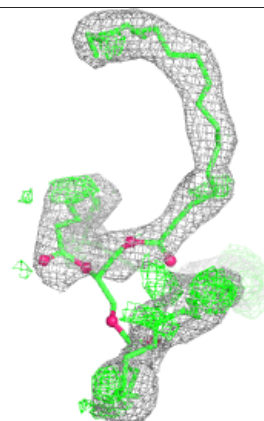
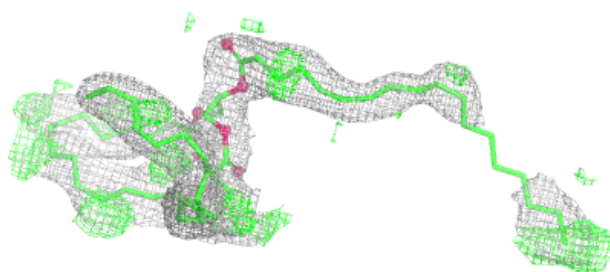
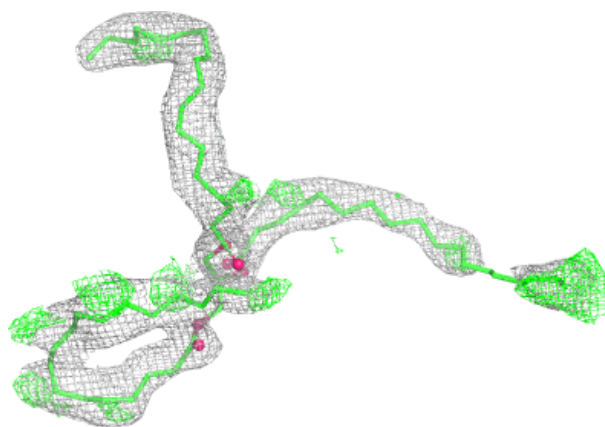
**Electron density around PGV a 607:**

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



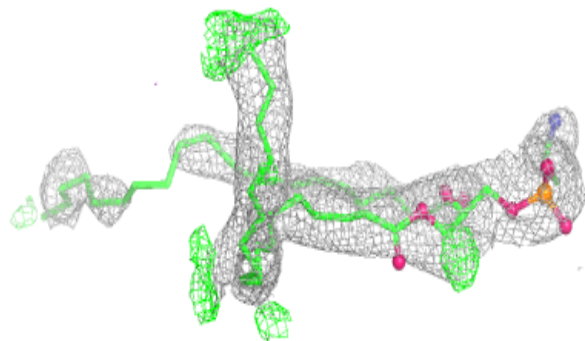
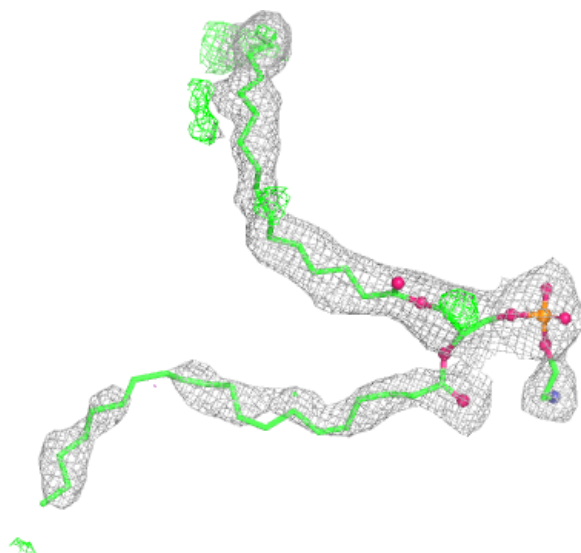
Electron density around TGL 1 101:

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



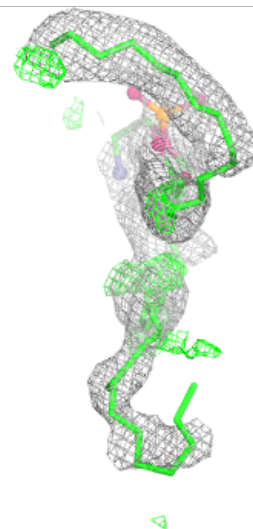
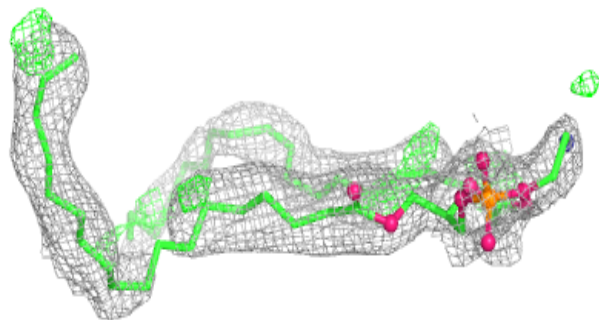
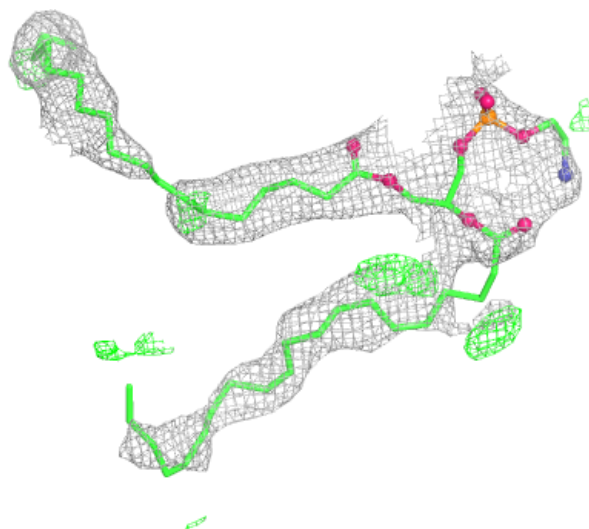
Electron density around PEK c 303:

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



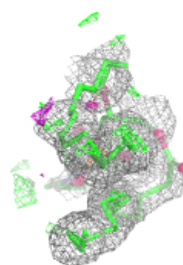
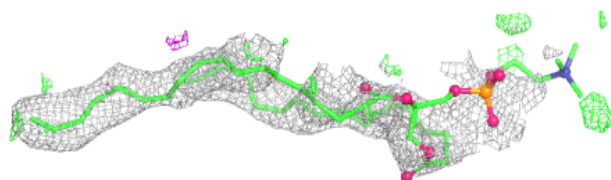
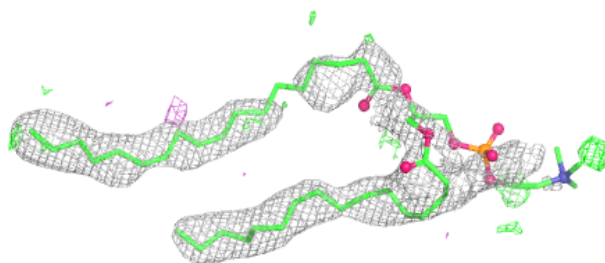
Electron density around PEK C 308:

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



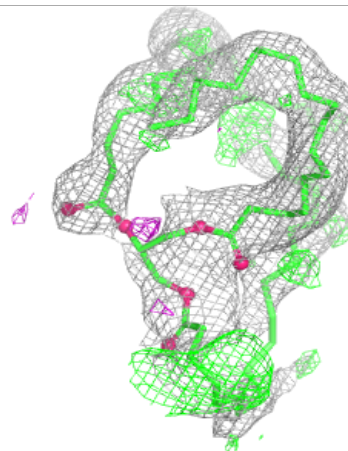
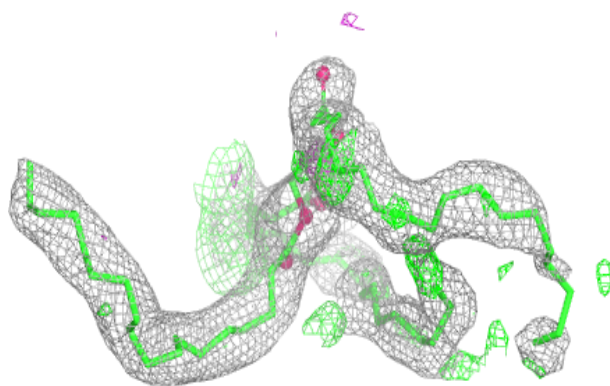
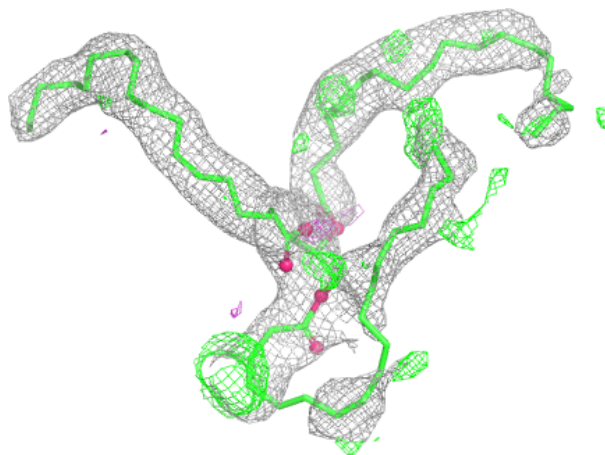
Electron density around PSC B 302:

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



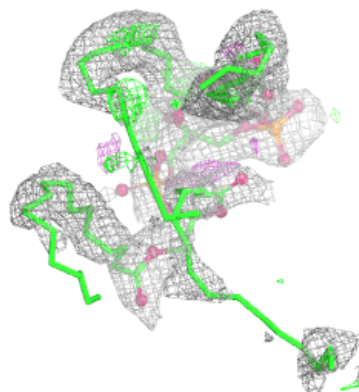
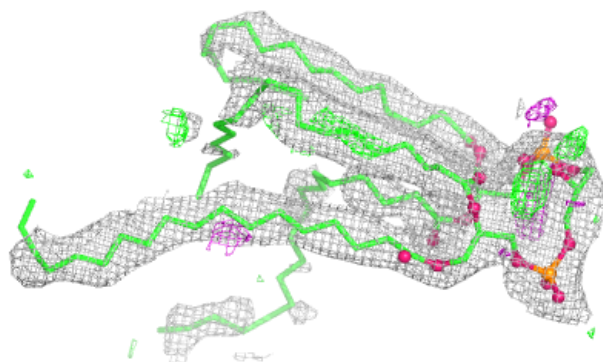
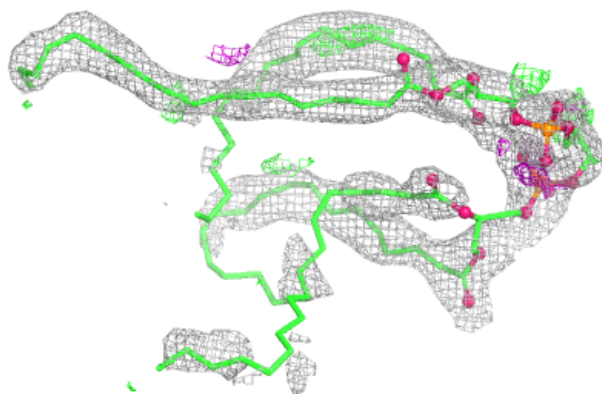
Electron density around TGL L 101:

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

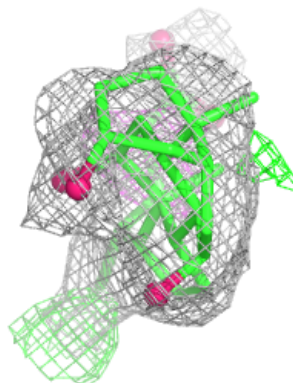
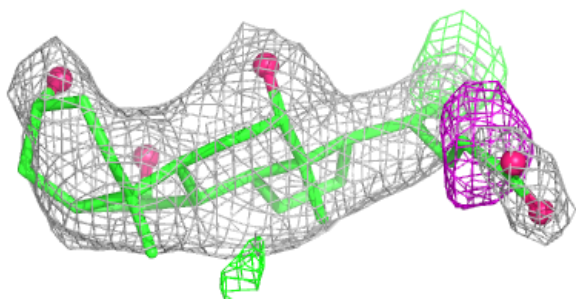
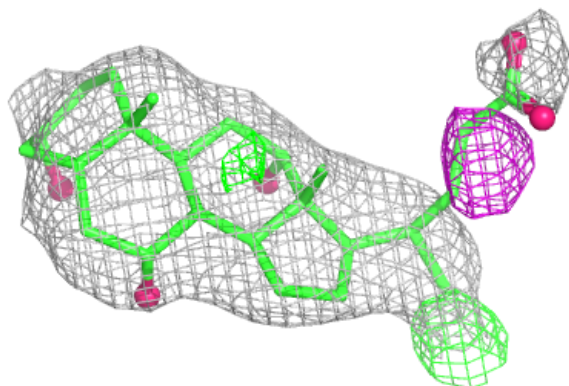


Electron density around CDL C 305:

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

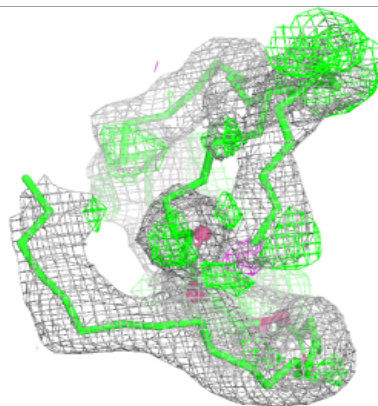
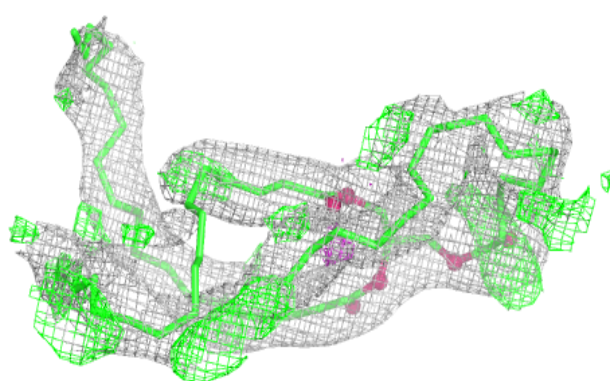
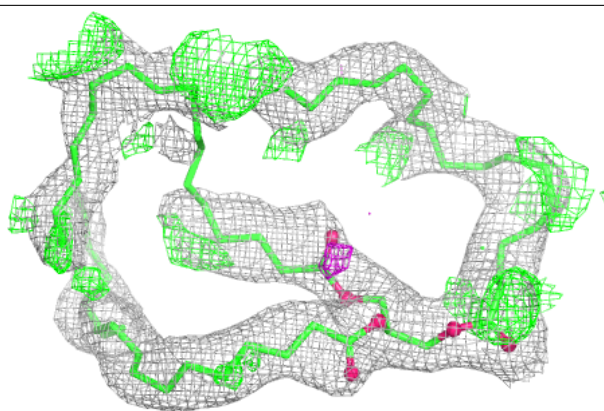
**Electron density around CHD J 101:**

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

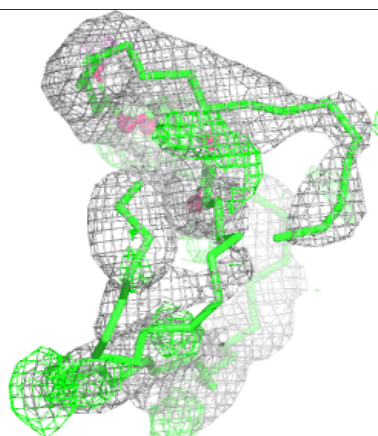
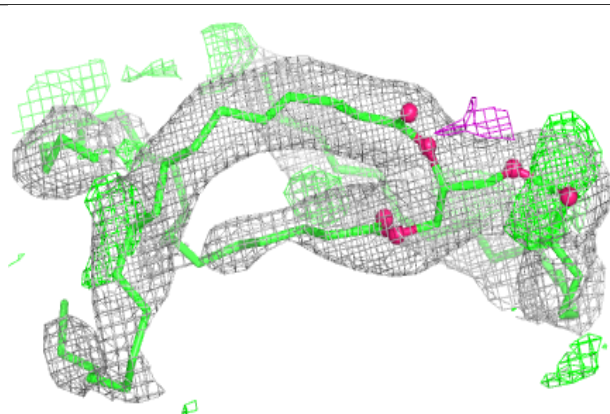
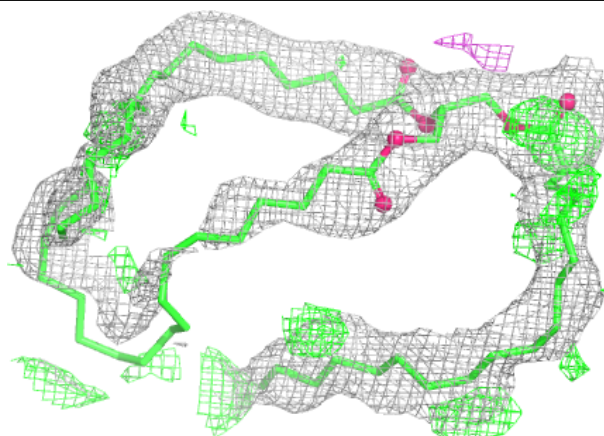


Electron density around TGL A 608:

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

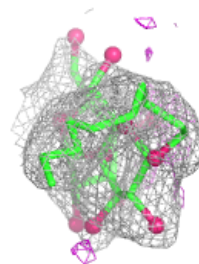
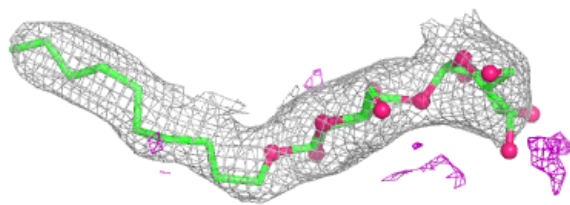
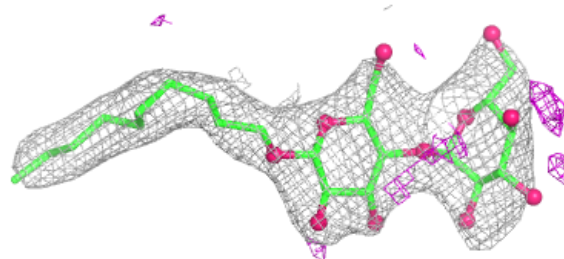
**Electron density around TGL i 101:**

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

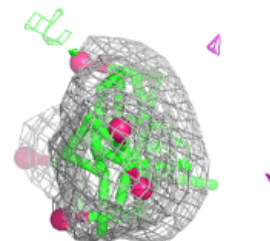
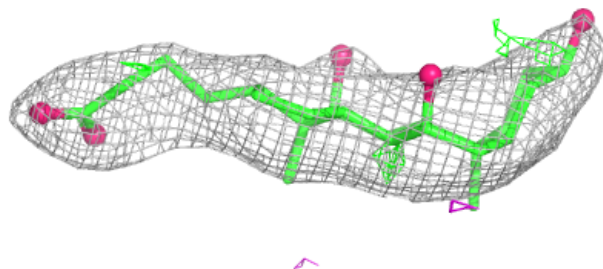
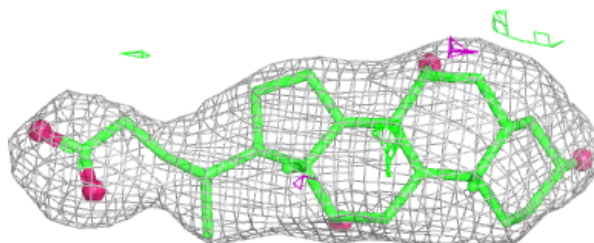


Electron density around DMU m 401:

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

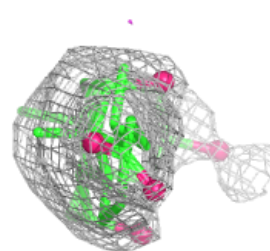
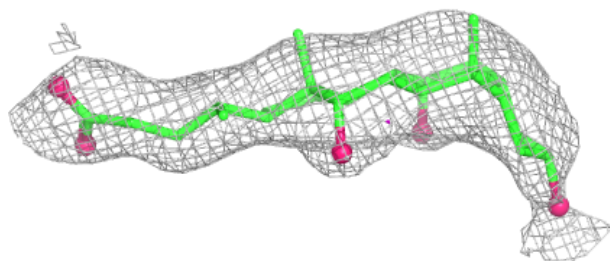
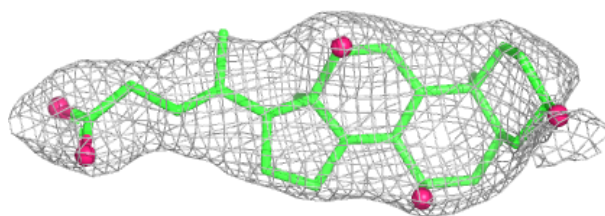
**Electron density around CHD C 306:**

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

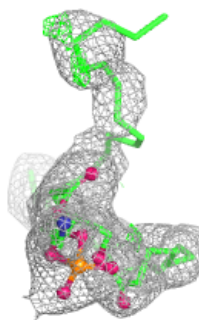
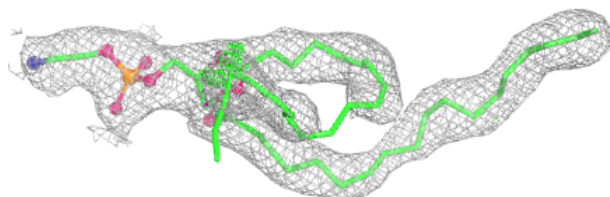
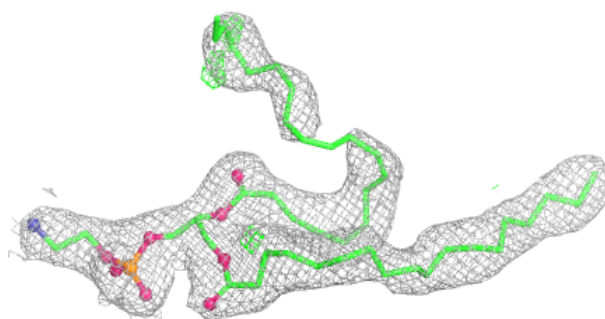


Electron density around CHD c 306:

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

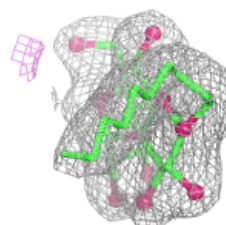
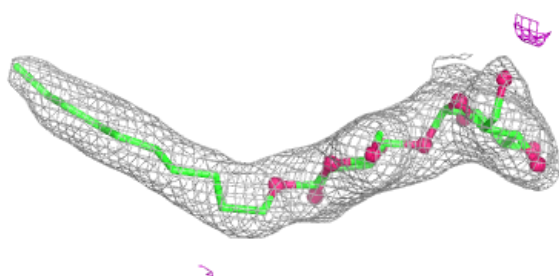
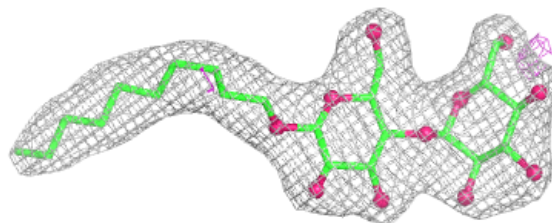
**Electron density around PEK g 102:**

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

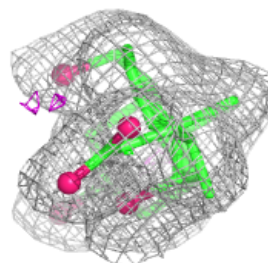
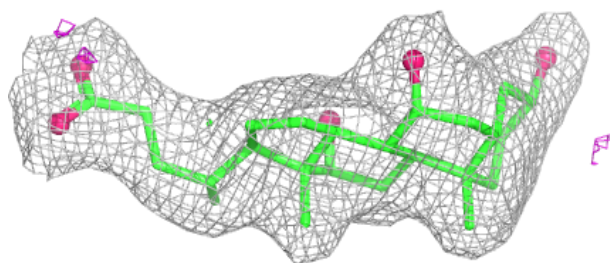
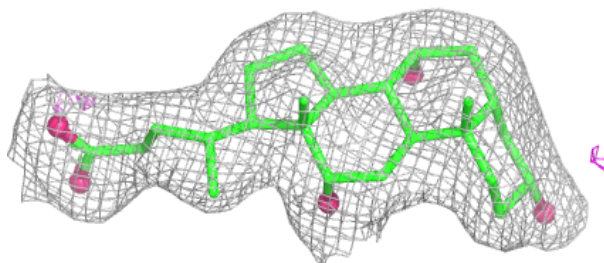


Electron density around DMU M 101:

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

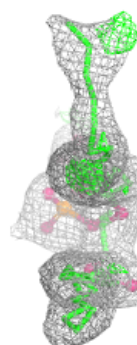
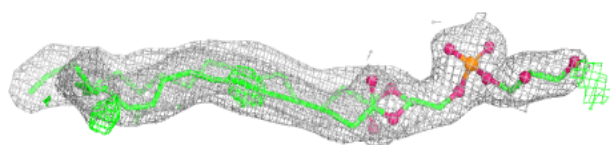
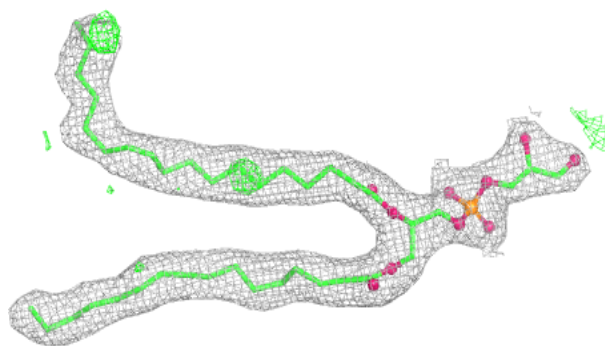
**Electron density around CHD c 302:**

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

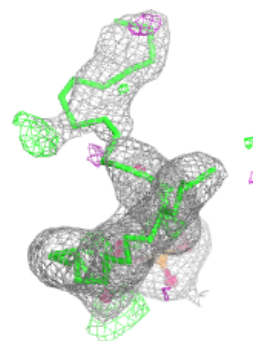
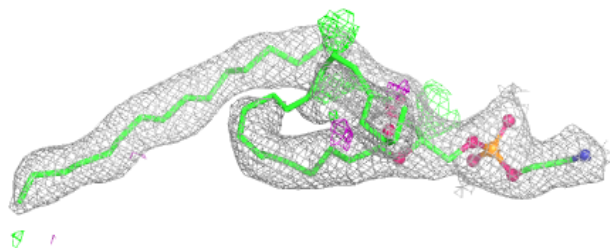
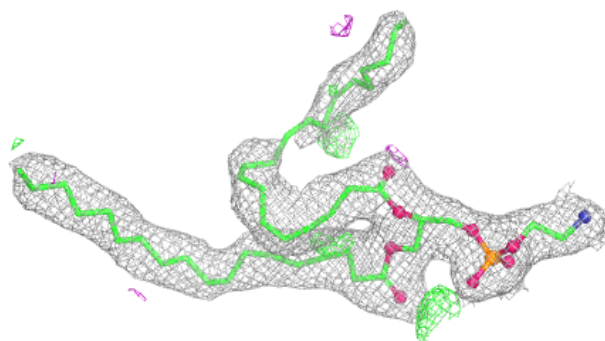


Electron density around PGV C 303:

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

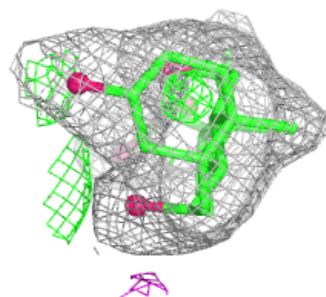
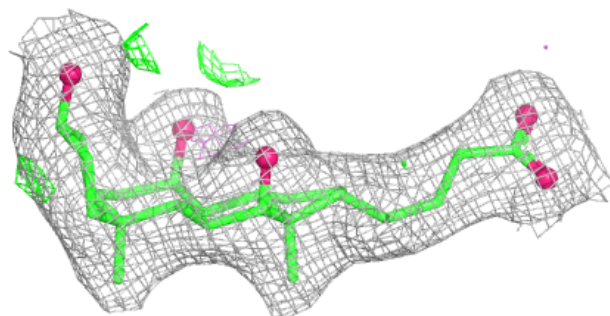
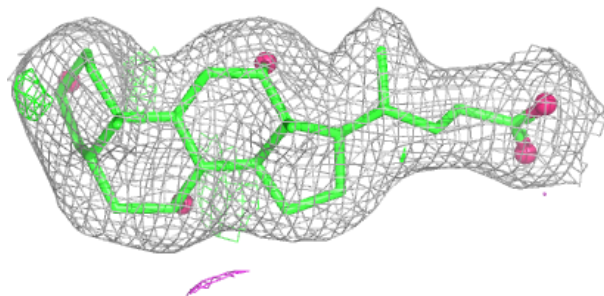
**Electron density around PEK C 302:**

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

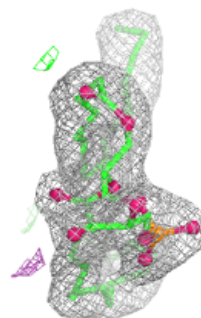
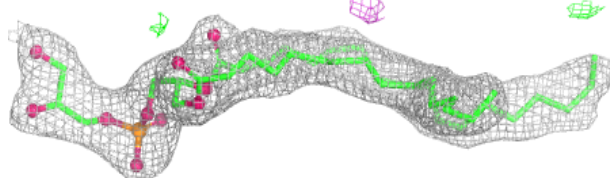
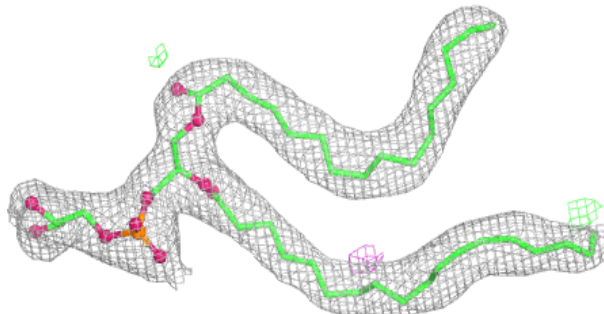


Electron density around CHD b 301:

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

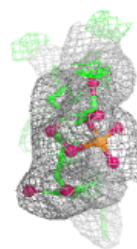
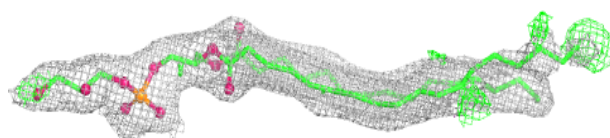
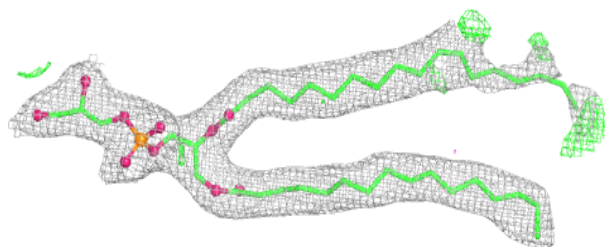
**Electron density around PGV c 301:**

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

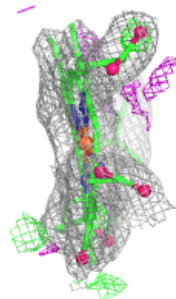
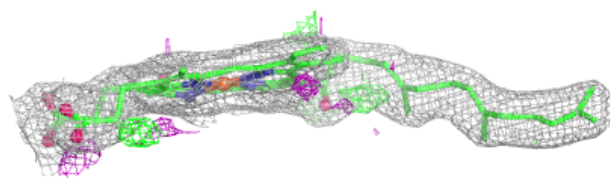
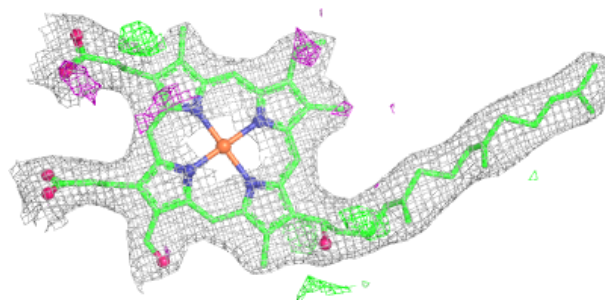


Electron density around PGV c 304:

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

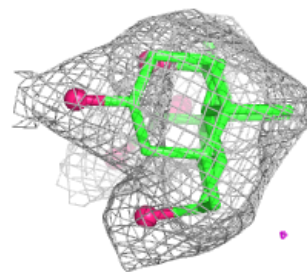
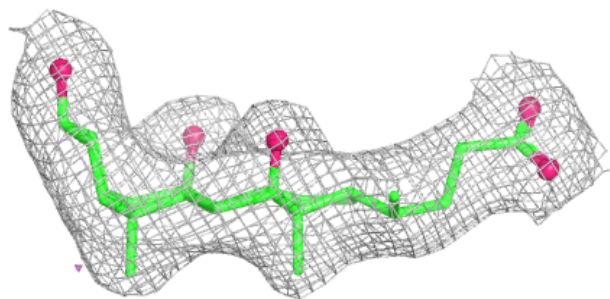
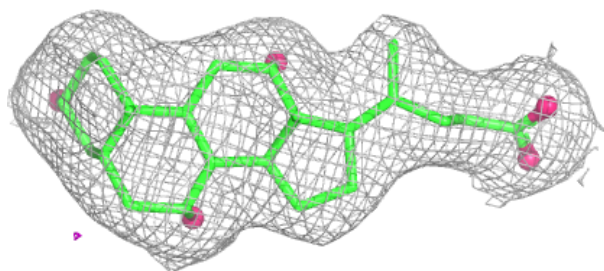
**Electron density around HEA a 601:**

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

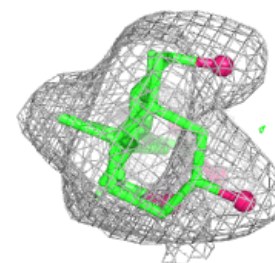
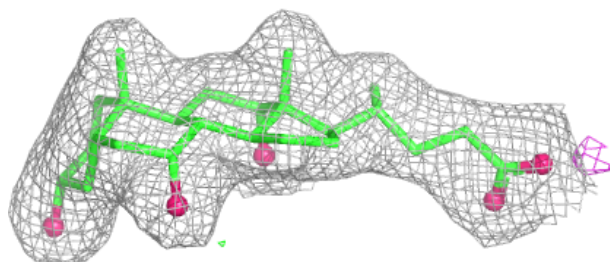
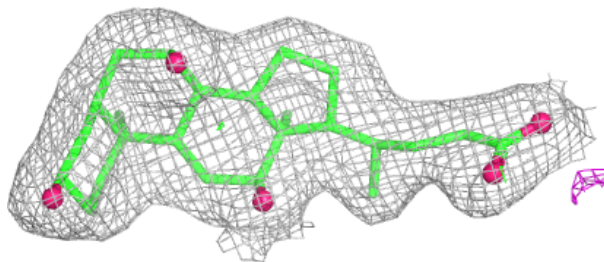


Electron density around CHD B 303:

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

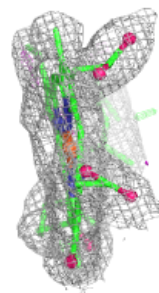
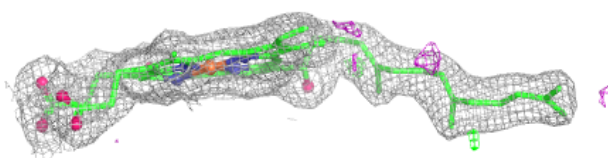
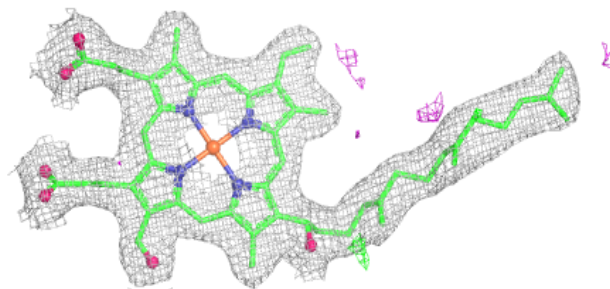
**Electron density around CHD C 301:**

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

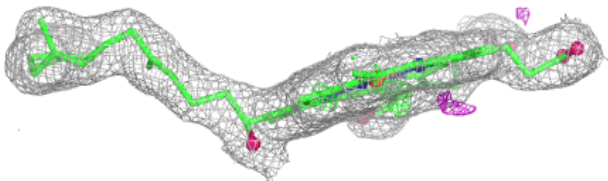
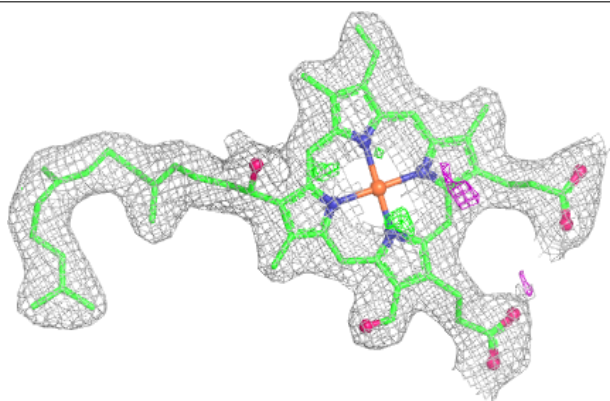


Electron density around HEA A 601:

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

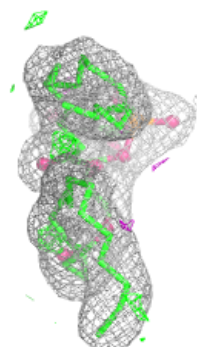
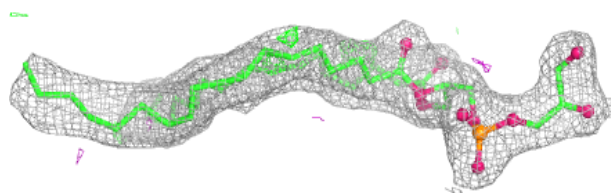
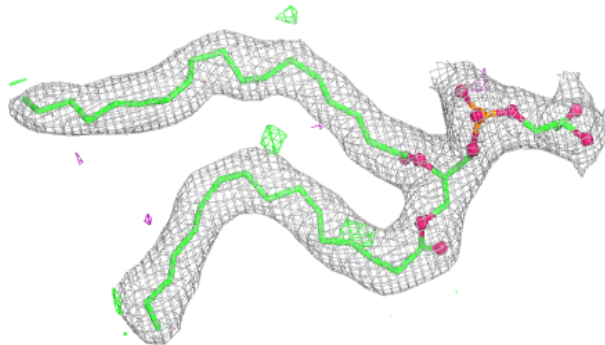
**Electron density around HEA a 602:**

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

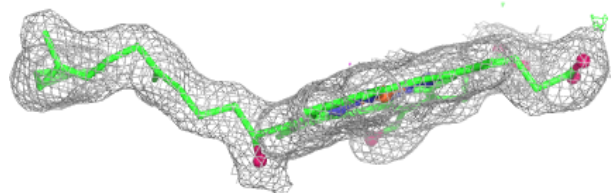
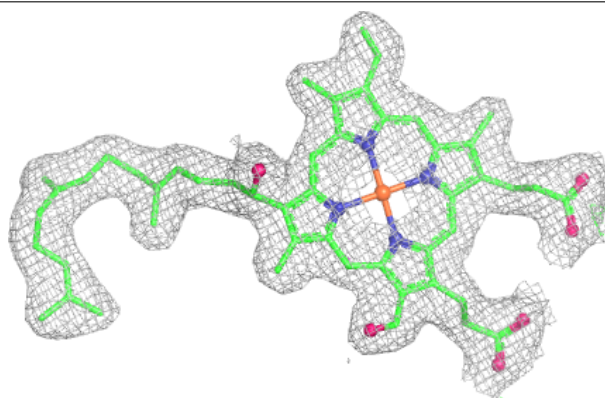


Electron density around PGV A 607:

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

**Electron density around 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.