



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 02:46 PM JST

PDB ID : 7XMA
Title : Crystal structure of Bovine heart cytochrome c oxidase, apo structure with DMSO
Authors : Nishida, Y.; Shinzawa-Itoh, K.; Mizuno, N.; Kumasaka, T.; Yoshikawa, S.; Tsukihara, T.; Takashima, S.; Shintani, Y.
Deposited on : 2022-04-25
Resolution : 2.20 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

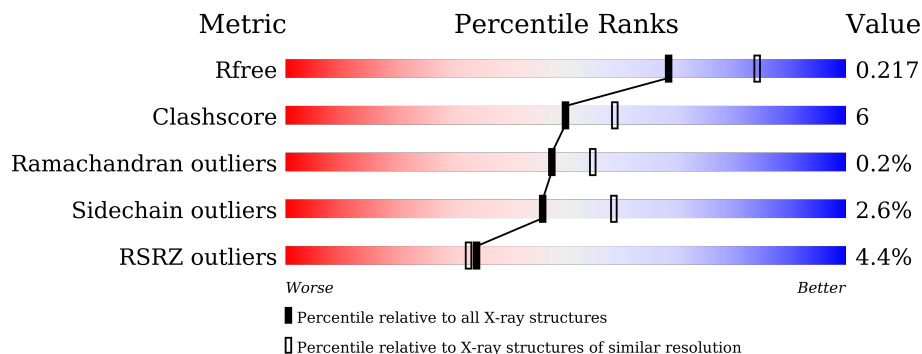
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.






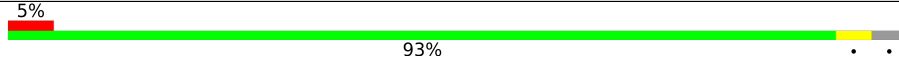
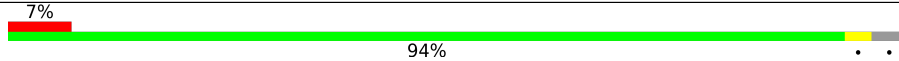
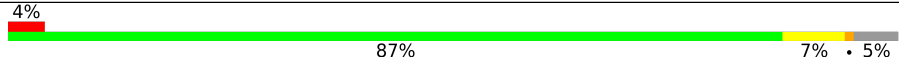
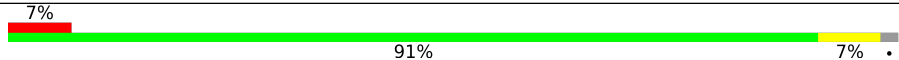
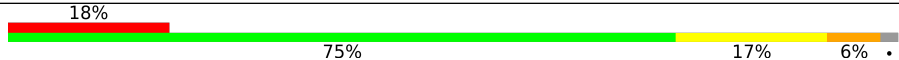
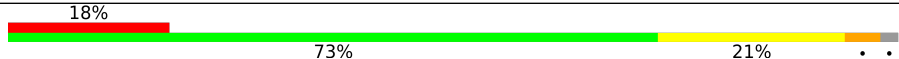
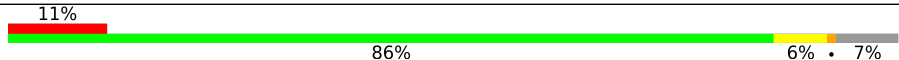

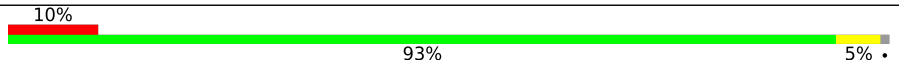
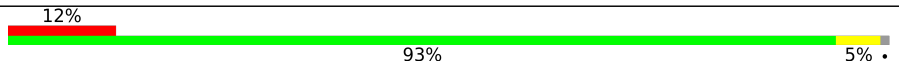
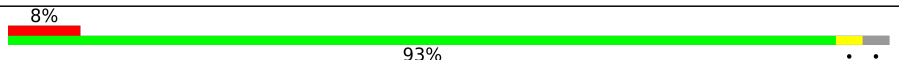
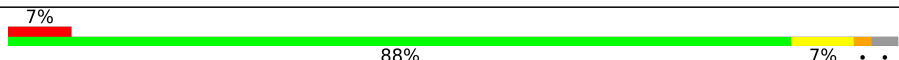
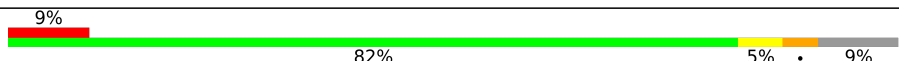
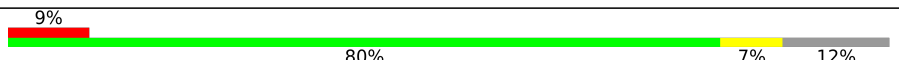
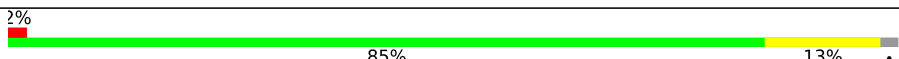
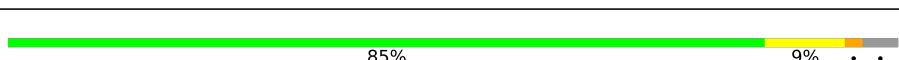
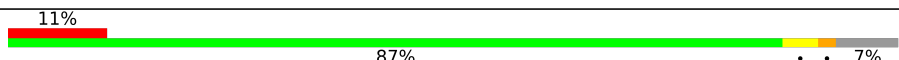
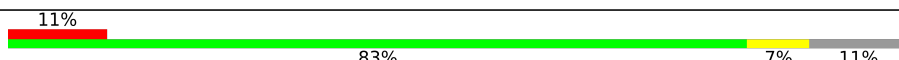
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	581	
2	O	581	
3	C	261	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	261	 % 89% 10%
4	D	147	 % 88% 10%
4	Q	147	 7% 85% 10% 5%
5	E	109	 5% 93% . .
5	R	109	 7% 94% . .
6	F	98	 4% 87% 7% 5%
6	S	98	 7% 91% 7% .
7	G	84	 18% 75% 17% 6% .
7	T	84	 18% 73% 21% . .
8	H	85	 11% 86% 6% 7%
8	U	85	 12% 81% 12% 7%
9	I	73	 10% 93% 5% .
9	V	73	 12% 93% 5% .
10	J	59	 8% 93% . .
10	W	59	 7% 88% 7% . .
11	K	56	 9% 82% 5% 9%
11	X	56	 9% 80% 7% 12%
12	L	47	 2% 85% 13% .
12	Y	47	 85% 9% . .
13	M	46	 11% 87% . . 7%
13	Z	46	 11% 83% 7% 11%

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
24	PEK	C	306	-	-	-	X
7	TPO	G	11	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	TPO	T	11	-	-	-	X

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 33571 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
			Total	C	N	O	S			
1	A	514	4115	2746	637	694	38	0	11	0
1	N	514	4115	2747	637	692	39	8	11	0

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2, Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	1869	1215	288	346	20	0	5	0
2	O	227	1877	1220	289	347	21	0	6	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	2181	1455	346	363	17	0	8	0
3	P	259	2184	1456	349	363	16	0	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	238	GLY	ALA	conflict	UNP P00415
P	238	GLY	ALA	conflict	UNP P00415

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	3	0
			1222	797	200	221	4			
4	Q	139	Total	C	N	O	S	0	2	0
			1182	770	195	213	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			
5	R	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	3	0
			737	456	132	144	5			
6	S	96	Total	C	N	O	S	0	1	0
			740	460	131	143	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	82	Total	C	N	O	P	S	0	1	0
			678	436	129	111	1	1			
7	T	82	Total	C	N	O	P	S	0	0	0
			664	425	127	110	1	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			
10	W	57	Total	C	N	O	S	0	1	0
			460	296	77	84	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	51	Total	C	N	O	S	0	0	0
			402	260	68	72	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

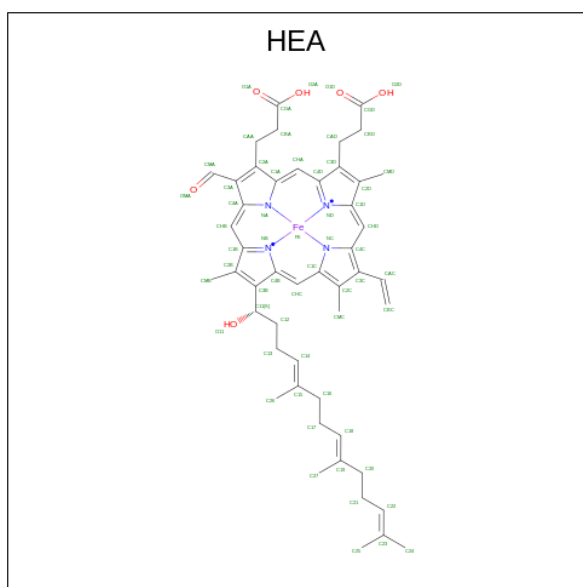
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	45	Total	C	N	O	S	0	1	0
			378	253	63	59	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	41	Total	C	N	O	0	0	0
			320	214	50	56			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

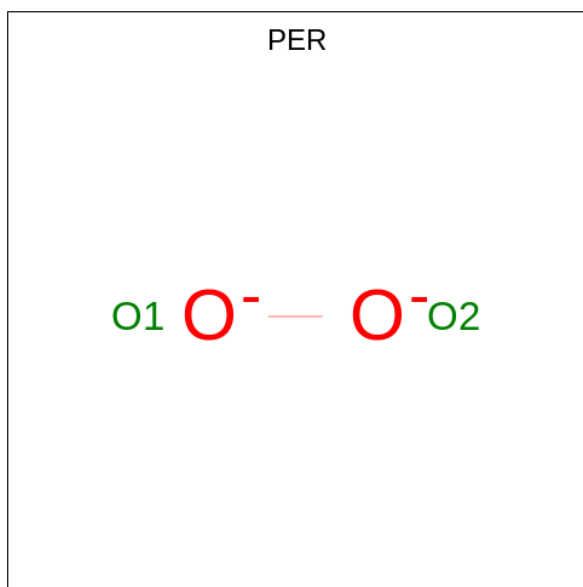
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

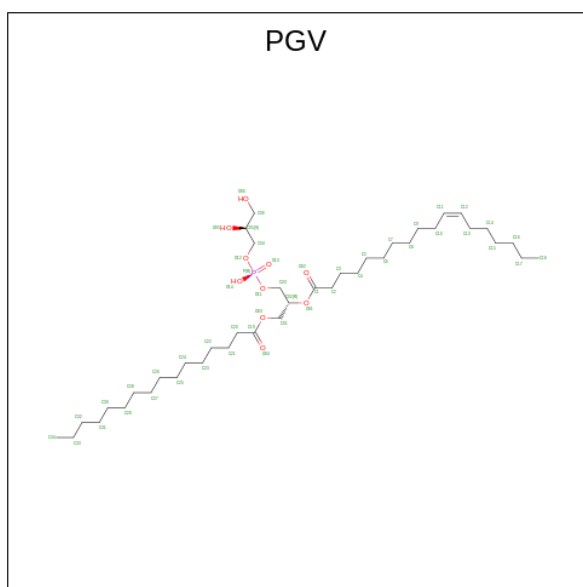
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



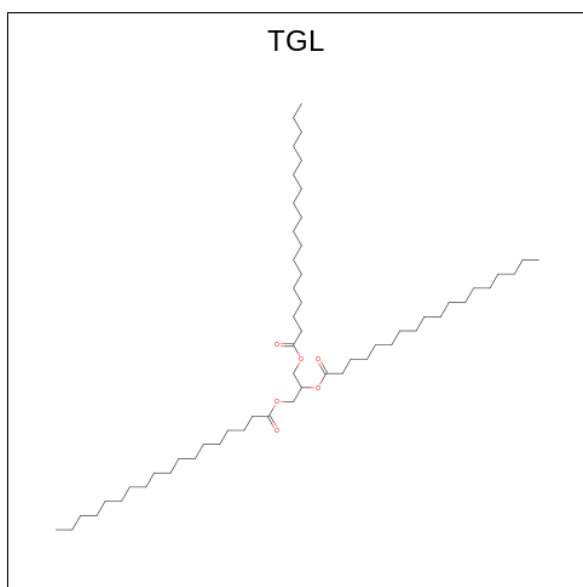
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 2 2	0	0
18	N	1	Total O 2 2	0	0

- Molecule 19 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



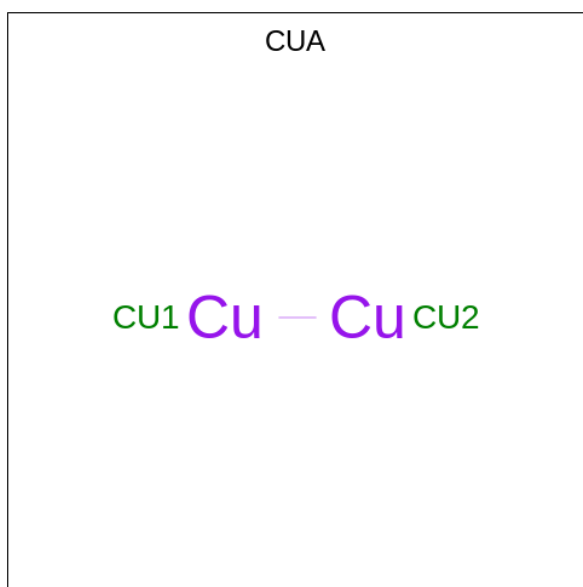
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
19	A	1	51	40	10	1	0	0
19	C	1	51	40	10	1	0	0
19	C	1	51	40	10	1	0	0
19	D	1	51	40	10	1	0	0
19	N	1	51	40	10	1	0	0
19	N	1	51	40	10	1	0	0
19	P	1	51	40	10	1	0	0
19	P	1	51	40	10	1	0	0

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



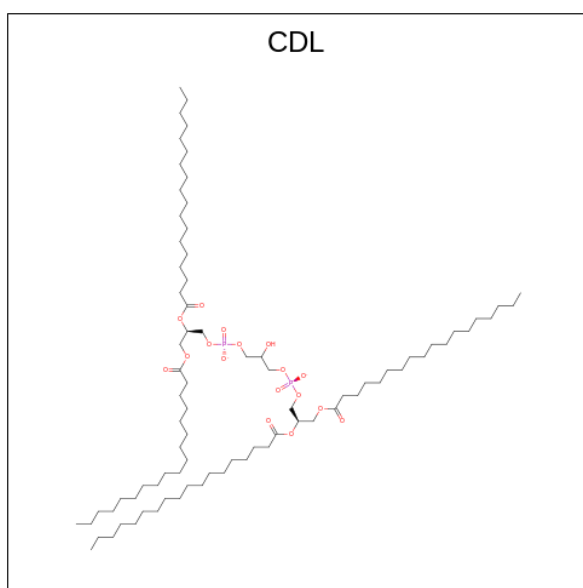
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	A	1	63	57	6	0	0
20	D	1	63	57	6	0	0
20	L	1	63	57	6	0	0
20	N	1	63	57	6	0	0
20	Q	1	63	57	6	0	0
20	Y	1	63	57	6	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



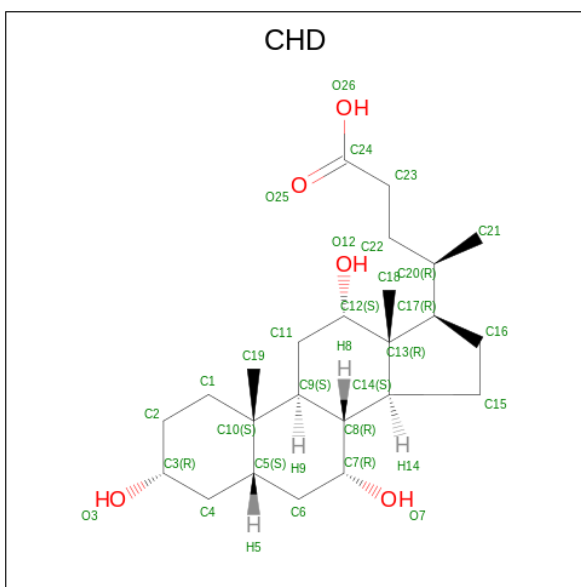
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O P 100 81 17 2	0	0
22	G	1	Total C O P 100 81 17 2	0	0

Continued on next page...

Continued from previous page...

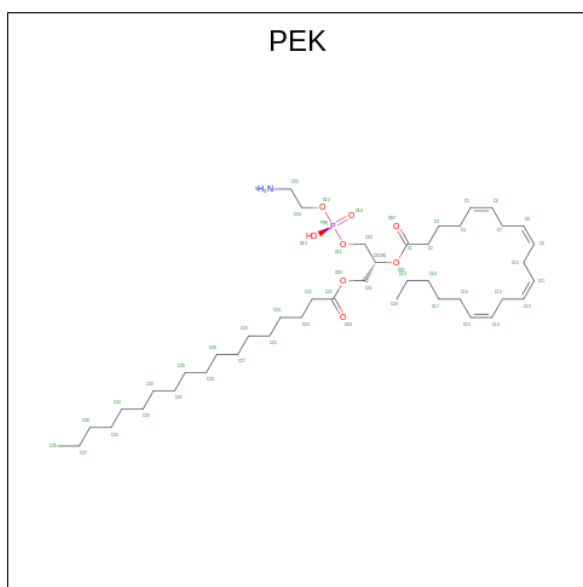
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
22	P	1	Total	C	O	P	0	0
			100	81	17	2		
22	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



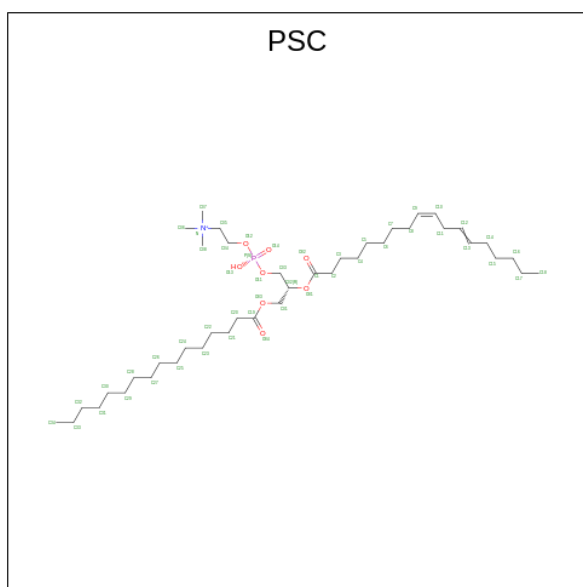
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	G	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	T	1	Total	C	O	0	0
			29	24	5		

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



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

- Molecule 25 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYL)OXY]METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).

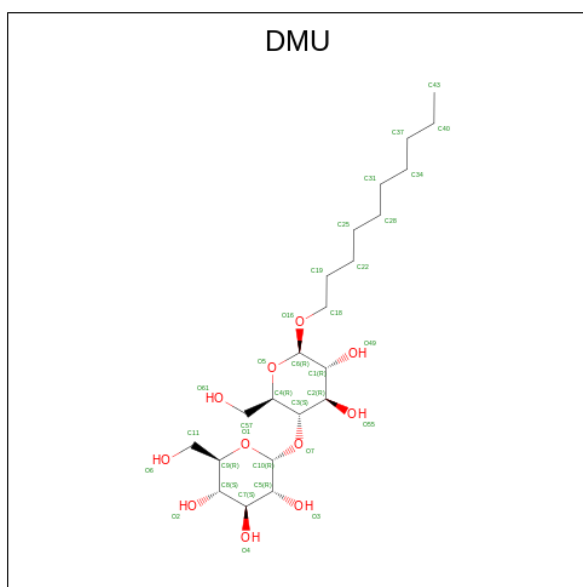


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	J	1	Total	C O	0	0
			33	22 11		
27	M	1	Total	C O	0	0
			33	22 11		
27	W	1	Total	C O	0	0
			33	22 11		
27	Z	1	Total	C O	0	0
			33	22 11		

- Molecule 28 is water.

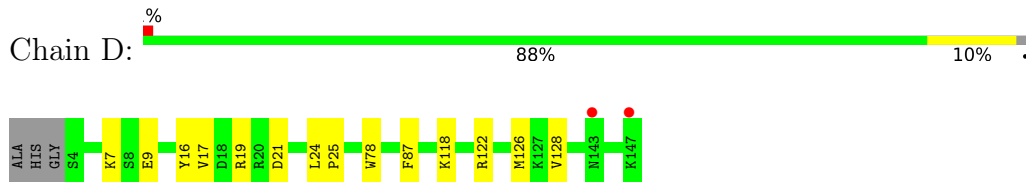
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	276	Total	O	0	0
			276	276		
28	B	180	Total	O	0	0
			180	180		
28	C	149	Total	O	0	0
			149	149		
28	D	179	Total	O	0	0
			179	179		
28	E	128	Total	O	0	0
			128	128		
28	F	119	Total	O	0	0
			119	119		
28	G	65	Total	O	0	0
			65	65		
28	H	76	Total	O	0	0
			76	76		

Continued on next page...

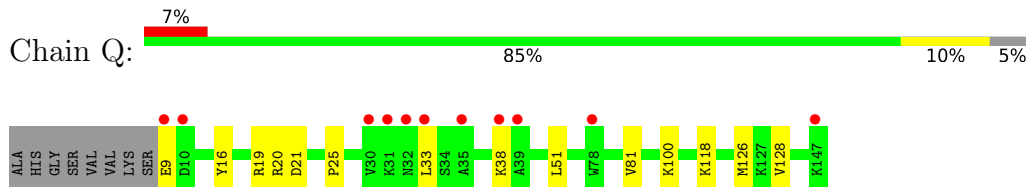
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	I	51	Total 51	O 51	0	0
28	J	41	Total 41	O 41	0	0
28	K	36	Total 36	O 36	0	0
28	L	40	Total 40	O 40	0	0
28	M	36	Total 36	O 36	0	0
28	N	289	Total 289	O 289	0	0
28	O	139	Total 139	O 139	0	0
28	P	144	Total 144	O 144	0	0
28	Q	69	Total 69	O 69	0	0
28	R	81	Total 81	O 81	0	0
28	S	118	Total 118	O 118	0	0
28	T	63	Total 63	O 63	0	0
28	U	61	Total 61	O 61	0	0
28	V	28	Total 28	O 28	0	0
28	W	35	Total 35	O 35	0	0
28	X	25	Total 25	O 25	0	0
28	Y	34	Total 34	O 34	0	0
28	Z	24	Total 24	O 24	0	0

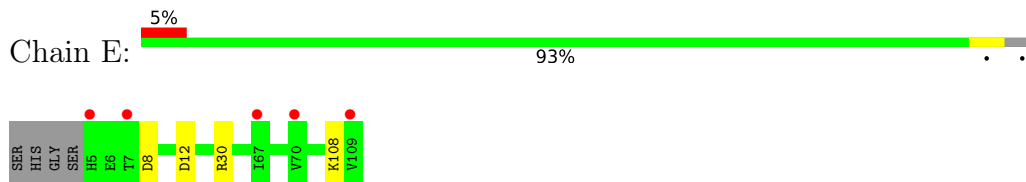
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



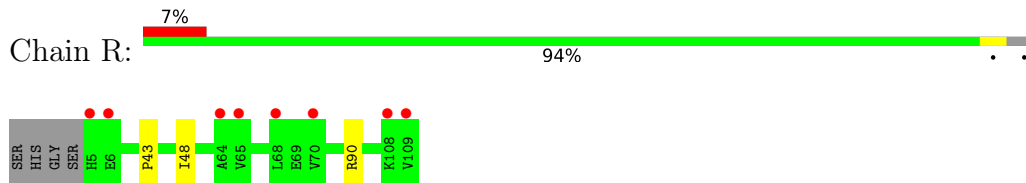
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



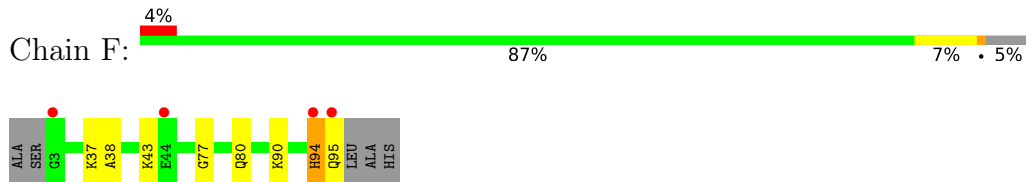
- Molecule 5: Cytochrome c oxidase subunit 5A



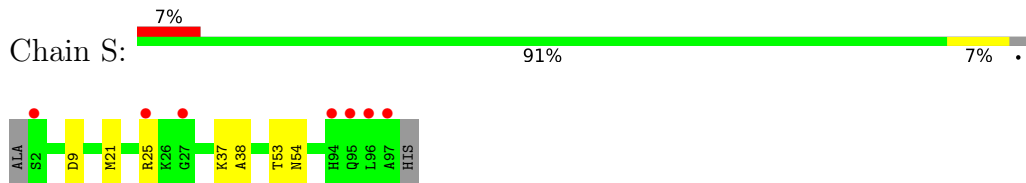
- Molecule 5: Cytochrome c oxidase subunit 5A



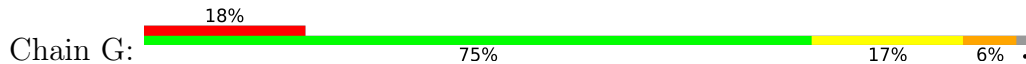
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

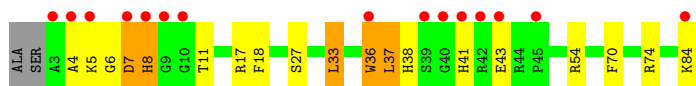


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

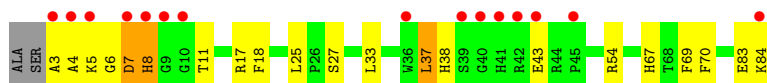
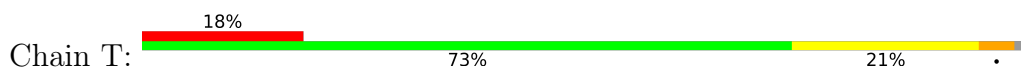


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

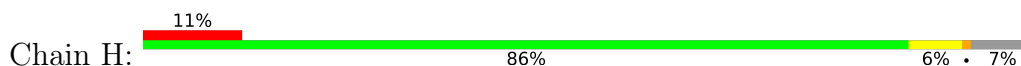




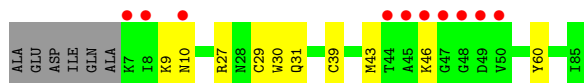
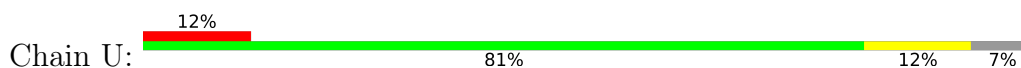
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



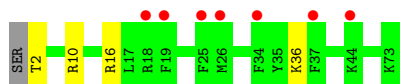
- Molecule 8: Cytochrome c oxidase subunit 6B1



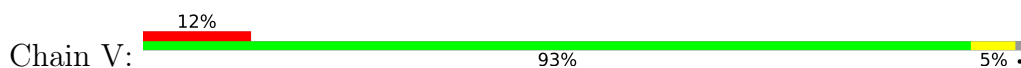
- Molecule 8: Cytochrome c oxidase subunit 6B1



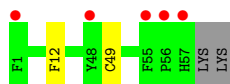
- Molecule 9: Cytochrome c oxidase subunit 6C



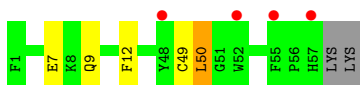
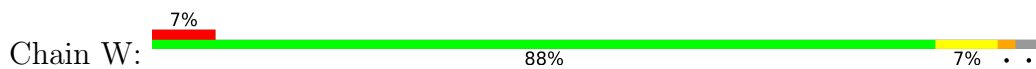
- Molecule 9: Cytochrome c oxidase subunit 6C



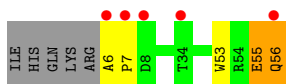
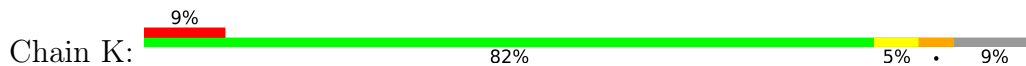
- Molecule 10: Cytochrome c oxidase subunit 7A1



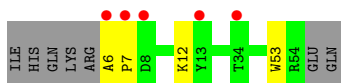
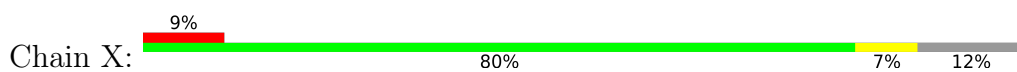
- Molecule 10: Cytochrome c oxidase subunit 7A1



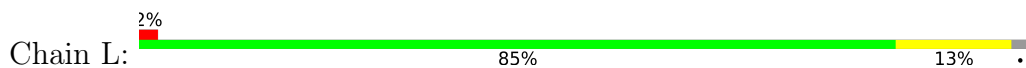
- Molecule 11: Cytochrome c oxidase subunit 7B



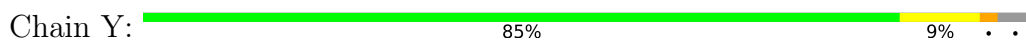
- Molecule 11: Cytochrome c oxidase subunit 7B



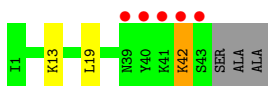
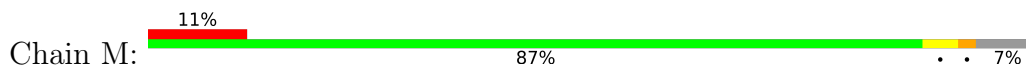
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



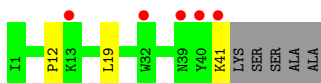
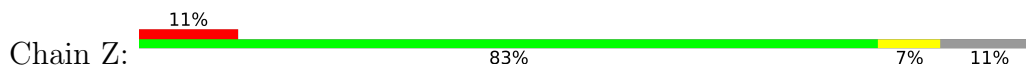
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.80Å 203.58Å 177.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.20 29.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.97-2.20) 99.9 (29.97-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.185 , 0.213 0.191 , 0.217	Depositor DCC
R_{free} test set	16583 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtrriage
Anisotropy	0.867	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.003 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33571	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, PSC, HEA, CUA, PER, TGL, CDL, CHD, NA, PGV, TPO, MG, PEK, FME, ZN, 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	0.25	0/4244	0.42	0/5795
1	N	0.25	0/4244	0.42	0/5794
2	B	0.26	0/1907	0.47	0/2597
2	O	0.25	0/1915	0.46	0/2607
3	C	0.25	0/2268	0.39	0/3096
3	P	0.26	0/2271	0.40	0/3100
4	D	0.24	0/1257	0.41	0/1695
4	Q	0.24	0/1217	0.42	0/1641
5	E	0.24	0/882	0.46	0/1196
5	R	0.25	0/882	0.47	0/1196
6	F	0.27	0/753	0.50	0/1023
6	S	0.25	0/756	0.49	0/1026
7	G	0.26	0/695	0.51	0/945
7	T	0.26	0/679	0.50	0/922
8	H	0.25	0/682	0.51	0/921
8	U	0.24	0/682	0.50	0/921
9	I	0.27	0/605	0.48	0/802
9	V	0.27	0/605	0.47	0/802
10	J	0.25	0/462	0.42	0/625
10	W	0.24	0/471	0.44	0/637
11	K	0.28	0/416	0.46	0/570
11	X	0.26	0/405	0.46	0/556
12	L	0.26	0/393	0.40	0/526
12	Y	0.26	0/391	0.41	0/525
13	M	0.25	0/345	0.39	0/470
13	Z	0.24	0/330	0.38	0/451
All	All	0.25	0/29757	0.44	0/40439

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4115	0	4087	45	0
1	N	4115	0	4092	45	0
2	B	1869	0	1868	24	0
2	O	1877	0	1876	27	0
3	C	2181	0	2092	31	0
3	P	2184	0	2095	26	0
4	D	1222	0	1211	17	0
4	Q	1182	0	1162	10	0
5	E	863	0	857	5	0
5	R	863	0	857	2	0
6	F	737	0	711	6	0
6	S	740	0	721	3	0
7	G	678	0	639	16	0
7	T	664	0	630	18	0
8	H	662	0	623	3	0
8	U	662	0	623	6	0
9	I	592	0	604	3	0
9	V	592	0	604	2	0
10	J	451	0	446	3	0
10	W	460	0	451	4	0
11	K	402	0	380	5	0
11	X	391	0	374	2	0
12	L	380	0	380	5	0
12	Y	378	0	375	7	0
13	M	335	0	352	2	0
13	Z	320	0	334	2	0
14	A	120	0	108	14	0
14	N	120	0	108	11	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	N	1	0	0	0	0
18	A	2	0	0	0	0
18	N	2	0	0	0	0
19	A	51	0	76	6	0
19	C	102	0	152	4	0
19	D	51	0	76	11	0
19	N	102	0	152	13	0
19	P	102	0	152	4	0
20	A	63	0	110	2	0
20	D	63	0	110	9	0
20	L	63	0	110	7	0
20	N	63	0	110	4	0
20	Q	63	0	110	5	0
20	Y	63	0	110	8	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	C	100	0	156	14	0
22	G	100	0	156	14	0
22	P	100	0	156	12	0
22	T	100	0	156	20	0
23	C	58	0	78	0	0
23	G	29	0	39	1	0
23	P	58	0	78	0	0
23	T	29	0	39	0	0
24	C	53	0	77	6	0
24	G	106	0	154	12	0
24	P	106	0	154	10	0
24	T	53	0	77	7	0
25	E	52	0	80	10	0
25	O	52	0	80	10	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	J	33	0	42	4	0
27	M	33	0	42	0	0
27	W	33	0	42	3	0
27	Z	33	0	42	0	0
28	A	276	0	0	1	0
28	B	180	0	0	0	0
28	C	149	0	0	1	0
28	D	179	0	0	1	0
28	E	128	0	0	0	0
28	F	119	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	G	65	0	0	2	0
28	H	76	0	0	1	0
28	I	51	0	0	0	0
28	J	41	0	0	0	0
28	K	36	0	0	2	0
28	L	40	0	0	0	0
28	M	36	0	0	0	0
28	N	289	0	0	4	0
28	O	139	0	0	0	0
28	P	144	0	0	0	0
28	Q	69	0	0	1	0
28	R	81	0	0	1	0
28	S	118	0	0	0	0
28	T	63	0	0	2	0
28	U	61	0	0	2	0
28	V	28	0	0	0	0
28	W	35	0	0	0	0
28	X	25	0	0	0	0
28	Y	34	0	0	0	0
28	Z	24	0	0	0	0
All	All	33571	0	31576	363	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 6.

All (363) 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)
19:N:609:PGV:H011	19:N:609:PGV:H31	1.57	0.87
22:P:304:CDL:H151	22:P:304:CDL:HA61	1.57	0.85
2:O:91:ASN:O	2:O:92:ASN:ND2	2.11	0.83
2:B:70:ALA:HB1	22:T:103:CDL:H451	1.62	0.82
6:F:94:HIS:CD2	28:F:206:HOH:O	2.36	0.79
22:T:103:CDL:H382	22:T:103:CDL:H161	1.65	0.78
22:G:103:CDL:H582	22:G:103:CDL:H781	1.65	0.78
3:P:80[B]:ARG:HH21	24:P:301:PEK:H031	1.46	0.78
4:D:87[B]:PHE:CE2	19:D:201:PGV:H151	2.20	0.77
4:D:87[A]:PHE:CD2	19:D:201:PGV:H131	2.21	0.75
6:F:94:HIS:HD2	28:F:206:HOH:O	1.69	0.75
2:O:57:ASP:H	25:O:602:PSC:H202	1.50	0.74
2:B:41:ILE:HG21	25:E:201:PSC:H332	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:TRP:HB3	20:D:202:TGL:HB21	1.72	0.70
2:O:92:ASN:ND2	2:O:92:ASN:O	2.24	0.70
7:T:6:GLY:O	7:T:8:HIS:N	2.24	0.69
7:G:38:HIS:CE1	22:G:103:CDL:H111	2.26	0.69
22:T:103:CDL:H1	22:T:103:CDL:H111	1.76	0.68
3:C:91:VAL:HG13	24:C:306:PEK:H14	1.76	0.68
22:C:302:CDL:H652	22:C:302:CDL:H242	1.76	0.68
7:G:6:GLY:O	7:G:8:HIS:N	2.27	0.67
24:P:307:PEK:H041	7:T:17:ARG:HH12	1.60	0.66
1:A:472:ILE:HG21	20:L:101:TGL:HA92	1.79	0.65
11:K:56:GLN:HG2	28:K:120:HOH:O	1.98	0.64
4:Q:9:GLU:N	4:Q:9:GLU:OE1	2.31	0.64
1:N:514:LYS:NZ	28:N:702:HOH:O	2.27	0.64
19:N:609:PGV:H142	19:N:609:PGV:H302	1.80	0.64
8:U:27:ARG:NH1	28:U:101:HOH:O	2.30	0.64
4:Q:100:LYS:NZ	28:Q:302:HOH:O	2.31	0.63
12:Y:20:ARG:NH1	12:Y:24[B]:MET:SD	2.71	0.63
1:N:472:ILE:HG21	20:Y:101:TGL:HA92	1.80	0.63
22:T:103:CDL:H782	22:T:103:CDL:H571	1.81	0.62
7:T:38:HIS:CE1	22:T:103:CDL:HA32	2.35	0.62
1:A:96:ARG:NE	19:A:607:PGV:O14	2.21	0.61
6:S:9:ASP:HB3	6:S:21[B]:MET:HE1	1.81	0.61
3:C:62:ILE:HD12	22:C:302:CDL:H522	1.81	0.61
1:A:278:MET:HB3	7:T:5:LYS:HG2	1.83	0.60
3:P:220:PHE:HB2	22:P:304:CDL:H711	1.83	0.60
3:P:51[B]:MET:HG2	22:P:304:CDL:H621	1.83	0.60
3:C:221:ARG:HH22	19:C:301:PGV:H041	1.67	0.60
20:D:202:TGL:HC32	20:D:202:TGL:HG12	1.83	0.60
1:N:24:ALA:HB2	14:N:601:HEA:H253	1.83	0.59
22:C:302:CDL:H382	22:C:302:CDL:H201	1.85	0.59
12:Y:13:PHE:HA	20:Y:101:TGL:HC41	1.85	0.59
19:C:305:PGV:H152	22:T:103:CDL:H621	1.85	0.59
10:W:50:LEU:HG	27:W:101:DMU:H23	1.84	0.59
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.83	0.58
24:G:101:PEK:H242	23:G:104:CHD:H12A	1.86	0.58
3:P:244:PHE:HA	24:P:301:PEK:H101	1.84	0.58
1:N:339:MET:HG2	20:Q:201:TGL:HA72	1.84	0.58
7:T:3:ALA:N	28:T:202:HOH:O	2.37	0.58
3:C:232:HIS:NE2	28:C:401:HOH:O	2.32	0.57
19:D:201:PGV:H322	13:M:19:LEU:HD23	1.85	0.57
20:D:202:TGL:H342	9:I:16:ARG:HE	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:37:LEU:HG	22:G:103:CDL:H372	1.87	0.56
19:N:609:PGV:H31	19:N:609:PGV:H202	1.87	0.56
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.88	0.56
5:R:90:ARG:NH2	28:R:201:HOH:O	2.37	0.56
2:B:56:MET:HA	25:E:201:PSC:H212	1.87	0.56
3:P:226:HIS:CE1	22:P:304:CDL:HB32	2.41	0.56
2:O:47:THR:HB	20:Q:201:TGL:H181	1.88	0.56
19:A:607:PGV:H182	3:C:28:THR:HG22	1.87	0.56
2:B:86:MET:HA	2:B:89:GLU:HG3	1.89	0.55
24:P:307:PEK:H041	7:T:17:ARG:NH1	2.21	0.55
3:C:51[C]:MET:HG2	22:C:302:CDL:H612	1.87	0.55
22:G:103:CDL:HB22	22:G:103:CDL:H112	1.90	0.55
3:P:184:ALA:HB3	24:T:102:PEK:H051	1.89	0.55
4:D:19:ARG:NH2	4:D:21:ASP:OD2	2.39	0.54
19:P:302:PGV:H011	19:P:302:PGV:O02	2.06	0.54
3:C:187:THR:HA	24:G:102:PEK:H042	1.88	0.54
22:C:302:CDL:HA61	22:C:302:CDL:H322	1.90	0.54
1:N:514:LYS:N	28:N:705:HOH:O	2.39	0.54
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.90	0.53
7:T:70:PHE:N	24:T:102:PEK:O14	2.33	0.53
2:B:78:LEU:HD12	22:T:103:CDL:H352	1.90	0.53
3:P:226:HIS:HE1	22:P:304:CDL:HB32	1.74	0.53
8:H:27:ARG:NH1	28:H:102:HOH:O	2.37	0.53
1:A:27:GLY:HA3	14:A:601:HEA:H273	1.91	0.52
7:G:70:PHE:N	24:G:102:PEK:O14	2.34	0.52
22:C:302:CDL:H752	22:C:302:CDL:H181	1.92	0.52
1:A:144:ASP:OD2	3:C:36:HIS:NE2	2.35	0.52
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.92	0.52
12:Y:20:ARG:HH22	20:Y:101:TGL:HC52	1.74	0.52
25:E:201:PSC:H011	25:E:201:PSC:H232	1.90	0.52
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.91	0.52
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.92	0.52
7:T:69:PHE:HB3	24:T:102:PEK:H011	1.90	0.52
3:C:184:ALA:HB3	24:G:102:PEK:H051	1.91	0.52
4:D:21:ASP:OD1	4:D:21:ASP:N	2.41	0.52
6:F:80[A]:GLN:NE2	28:F:204:HOH:O	2.42	0.52
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.45	0.52
4:Q:81:VAL:HG11	20:Q:201:TGL:HB52	1.92	0.51
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.51
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.91	0.51
1:A:311[A]:ILE:HD12	22:T:103:CDL:H221	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:103:CDL:H532	22:G:103:CDL:H222	1.91	0.51
1:A:377:PHE:HA	1:A:380:VAL:HG22	1.92	0.51
3:P:240:TRP:CG	24:P:301:PEK:H41	2.45	0.51
19:N:609:PGV:H312	13:Z:19:LEU:HD23	1.91	0.51
8:U:31:GLN:NE2	28:U:103:HOH:O	2.43	0.51
4:D:87[B]:PHE:CZ	19:D:201:PGV:H151	2.45	0.51
2:B:56:MET:HG2	25:E:201:PSC:H221	1.91	0.50
2:B:81:LEU:HD12	22:T:103:CDL:H351	1.93	0.50
4:D:87[A]:PHE:CZ	19:D:201:PGV:C15	2.95	0.50
24:G:102:PEK:H41	24:G:102:PEK:H222	1.93	0.50
12:L:25:MET:HG2	20:L:101:TGL:HA61	1.93	0.50
2:O:91:ASN:HB2	2:O:149:THR:HG21	1.93	0.50
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.94	0.50
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	1.94	0.50
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.50
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.11	0.50
4:D:126:MET:HG3	4:D:128:VAL:HG23	1.94	0.50
2:B:83:ILE:HA	2:B:86:MET:HG2	1.94	0.50
19:C:301:PGV:H183	22:C:302:CDL:H622	1.94	0.50
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.94	0.49
22:G:103:CDL:H241	22:G:103:CDL:H531	1.95	0.49
1:N:27:GLY:HA3	14:N:601:HEA:H273	1.95	0.49
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.12	0.49
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.95	0.49
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	1.95	0.49
2:O:41:ILE:HD13	25:O:602:PSC:H342	1.95	0.49
4:Q:33:LEU:O	4:Q:38:LYS:NZ	2.46	0.49
22:T:103:CDL:H382	22:T:103:CDL:C16	2.41	0.49
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.48	0.48
19:N:609:PGV:H241	13:Z:12:PRO:HG3	1.95	0.48
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.47	0.48
3:C:91:VAL:HG22	24:C:306:PEK:H12	1.95	0.48
14:N:602:HEA:H243	2:O:69:PRO:HB3	1.96	0.48
2:O:57:ASP:N	25:O:602:PSC:H202	2.24	0.48
1:A:18:LEU:HB3	1:A:102:PHE:CZ	2.48	0.48
4:D:24:LEU:HD12	5:E:30:ARG:HA	1.96	0.48
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.96	0.48
25:E:201:PSC:H322	25:E:201:PSC:H291	1.51	0.48
7:G:5:LYS:HG2	1:N:278[A]:MET:HB3	1.96	0.48
2:O:41:ILE:O	2:O:45:MET:HG2	2.14	0.48
20:Q:201:TGL:H352	9:V:16:ARG:HE	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:18:LEU:HB3	1:N:102:PHE:CZ	2.49	0.48
12:L:20:ARG:HH22	20:L:101:TGL:HC41	1.78	0.47
8:H:7:LYS:HD2	8:U:46:LYS:HA	1.96	0.47
24:P:307:PEK:H9	7:T:25:LEU:HD13	1.95	0.47
1:A:236:TRP:HH2	14:A:602:HEA:HBD1	1.79	0.47
4:D:87[A]:PHE:CZ	19:D:201:PGV:H152	2.49	0.47
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.96	0.47
1:A:374:VAL:HA	1:A:377:PHE:CE2	2.50	0.47
22:G:103:CDL:H442	1:N:311[B]:ILE:HG22	1.96	0.47
7:G:5:LYS:HG2	1:N:278[B]:MET:HB3	1.96	0.47
3:P:52:LEU:HD21	22:P:304:CDL:H432	1.96	0.47
7:T:38:HIS:HE1	22:T:103:CDL:HA32	1.75	0.47
3:P:187:THR:HA	24:T:102:PEK:H042	1.96	0.47
12:Y:20:ARG:NH2	20:Y:101:TGL:HC52	2.28	0.47
1:A:186:TRP:HH2	7:T:7:ASP:HB3	1.80	0.47
4:D:87[A]:PHE:CZ	19:D:201:PGV:H151	2.50	0.47
25:E:201:PSC:H082	25:E:201:PSC:O14	2.14	0.47
22:G:103:CDL:H382	2:O:81:LEU:HD12	1.97	0.47
12:L:14:SER:H	20:L:101:TGL:HC51	1.80	0.47
2:O:114:GLU:HG3	2:O:227:LEU:HD21	1.96	0.47
4:Q:21:ASP:OD1	4:Q:21:ASP:N	2.35	0.47
1:N:321:PHE:CD1	25:O:602:PSC:H341	2.49	0.47
19:N:609:PGV:H42	19:N:609:PGV:H231	1.97	0.47
1:A:20:LEU:HB3	20:L:101:TGL:H222	1.96	0.47
1:A:334:TRP:NE1	20:D:202:TGL:HC52	2.30	0.47
3:C:191:GLY:HA3	28:G:208:HOH:O	2.15	0.46
3:C:220:PHE:CB	22:C:302:CDL:H711	2.44	0.46
24:G:102:PEK:H131	24:G:102:PEK:H161	1.51	0.46
1:N:430:PHE:CE1	20:N:608:TGL:HB22	2.50	0.46
3:P:67:PHE:CE2	22:P:304:CDL:HB21	2.50	0.46
2:O:56:MET:HG2	25:O:602:PSC:H211	1.97	0.46
4:Q:16:TYR:CE1	4:Q:25:PRO:HG2	2.51	0.46
3:C:59:ARG:HB2	22:C:302:CDL:H511	1.97	0.46
19:N:607:PGV:H182	3:P:28:THR:HG22	1.97	0.46
2:B:139:ASP:OD1	2:B:140:ASN:N	2.49	0.46
7:G:5:LYS:NZ	28:G:203:HOH:O	2.33	0.46
22:T:103:CDL:H222	22:T:103:CDL:H512	1.96	0.46
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.51	0.46
2:O:83:ILE:HA	2:O:86:MET:HG2	1.98	0.46
3:P:67:PHE:HA	10:W:9:GLN:HG2	1.98	0.46
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:25:MET:HG2	20:Y:101:TGL:HA62	1.97	0.46
1:A:102:PHE:HZ	20:L:101:TGL:HB42	1.81	0.46
3:C:220:PHE:HB2	22:C:302:CDL:H711	1.98	0.46
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.51	0.46
3:P:67:PHE:CZ	22:P:304:CDL:HB21	2.51	0.46
3:P:191:GLY:HA3	28:T:211:HOH:O	2.16	0.46
22:P:304:CDL:H372	22:P:304:CDL:H401	1.60	0.46
1:A:202:LEU:HD22	1:A:238:PHE:CE2	2.51	0.45
2:B:41:ILE:O	2:B:45:MET:HG2	2.16	0.45
5:E:8:ASP:HA	25:E:201:PSC:H061	1.98	0.45
5:E:12:ASP:OD1	9:I:10:ARG:NH2	2.41	0.45
1:N:379:TYR:O	1:N:383:MET:HB2	2.17	0.45
20:Y:101:TGL:H352	20:Y:101:TGL:H191	1.78	0.45
24:C:306:PEK:H352	7:T:5:LYS:HD2	1.97	0.45
14:N:601:HEA:HHC	14:N:601:HEA:H122	1.97	0.45
25:O:602:PSC:H282	25:O:602:PSC:H311	1.64	0.45
14:A:602:HEA:HBD2	14:A:602:HEA:HMD1	1.99	0.45
4:D:87[A]:PHE:CE2	19:D:201:PGV:H131	2.51	0.45
1:N:240:HIS:O	1:N:243:VAL:HG22	2.15	0.45
22:G:103:CDL:H222	22:G:103:CDL:C53	2.47	0.45
1:N:430:PHE:HE1	20:N:608:TGL:HB22	1.82	0.45
19:A:607:PGV:H61	3:C:54[A]:MET:HG2	1.98	0.45
1:N:424:THR:HG21	14:N:601:HEA:HMB2	1.99	0.45
3:C:47:LEU:O	3:C:51[B]:MET:HG2	2.17	0.45
7:G:33:LEU:O	7:G:37:LEU:HD22	2.17	0.45
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.99	0.45
1:N:202:LEU:HD22	1:N:238:PHE:CE2	2.52	0.45
2:O:158:ASP:OD1	2:O:159:VAL:N	2.49	0.45
3:C:77:LYS:HZ1	24:C:306:PEK:H052	1.81	0.45
11:K:55:GLU:CD	28:K:105:HOH:O	2.54	0.45
2:O:139:ASP:OD1	2:O:140:ASN:N	2.50	0.45
1:A:240:HIS:O	1:A:243:VAL:HG22	2.16	0.44
2:B:41:ILE:HD13	25:E:201:PSC:H332	1.99	0.44
1:A:379:TYR:O	1:A:383:MET:HB2	2.17	0.44
3:P:233:PHE:HD2	19:P:303:PGV:H011	1.83	0.44
4:Q:19[B]:ARG:HG2	4:Q:21:ASP:OD1	2.17	0.44
7:T:37:LEU:HD23	22:T:103:CDL:H361	1.99	0.44
24:C:306:PEK:H312	7:T:5:LYS:O	2.15	0.44
5:E:12:ASP:CG	9:I:10:ARG:HH22	2.20	0.44
22:T:103:CDL:H571	22:T:103:CDL:C78	2.46	0.44
2:O:56:MET:CB	25:O:602:PSC:H211	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:43:PRO:HB2	5:R:48:ILE:HD11	2.00	0.44
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	2.00	0.44
14:A:602:HEA:H243	2:B:69:PRO:HB3	1.98	0.44
2:B:158:ASP:OD1	2:B:159:VAL:N	2.49	0.44
20:N:608:TGL:H281	20:N:608:TGL:HB91	2.00	0.44
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.53	0.44
3:P:240:TRP:CD2	24:P:301:PEK:H41	2.52	0.44
1:A:236:TRP:CH2	14:A:602:HEA:HBD1	2.52	0.44
24:C:306:PEK:H322	24:C:306:PEK:H351	1.60	0.44
4:D:87[A]:PHE:CE2	19:D:201:PGV:H152	2.53	0.44
7:G:17:ARG:NH1	24:G:101:PEK:H041	2.33	0.44
1:N:236:TRP:HH2	14:N:602:HEA:HBD1	1.83	0.44
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.52	0.44
22:P:304:CDL:H252	22:P:304:CDL:H222	1.65	0.44
14:A:601:HEA:HHC	14:A:601:HEA:H122	2.00	0.44
1:N:96:ARG:NE	19:N:607:PGV:O14	2.24	0.44
1:N:244:TYR:OH	1:N:312[B]:ILE:HD12	2.17	0.44
7:G:38:HIS:HE1	22:G:103:CDL:H111	1.79	0.44
19:A:607:PGV:H343	19:A:607:PGV:H311	1.77	0.43
7:G:7:ASP:HB3	1:N:278[B]:MET:HE3	2.00	0.43
13:M:42:LYS:HD2	13:M:42:LYS:HA	1.56	0.43
20:N:608:TGL:H283	20:N:608:TGL:H251	1.80	0.43
19:P:302:PGV:H272	19:P:302:PGV:H241	1.85	0.43
3:C:181:TYR:O	24:G:102:PEK:N	2.51	0.43
1:A:424:THR:HG21	14:A:601:HEA:HMB2	2.00	0.43
1:A:278:MET:SD	7:T:5:LYS:HB3	2.57	0.43
22:G:103:CDL:H211	1:N:311[B]:ILE:HD13	1.99	0.43
19:N:607:PGV:H132	19:N:607:PGV:H101	1.81	0.43
2:O:33:LEU:HD12	2:O:33:LEU:HA	1.85	0.43
3:P:33[A]:MET:HG3	27:W:101:DMU:H8	2.00	0.43
24:T:102:PEK:H301	24:T:102:PEK:H332	1.71	0.43
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	2.00	0.43
1:A:309:THR:HG22	14:A:602:HEA:HMB2	2.01	0.43
3:C:51[A]:MET:SD	22:C:302:CDL:H612	2.59	0.43
24:G:101:PEK:H15	24:G:101:PEK:H182	1.74	0.43
6:S:53:THR:OG1	6:S:54:ASN:N	2.52	0.43
1:A:101:SER:O	1:A:156:SER:OG	2.31	0.43
4:D:122:ARG:O	4:D:126:MET:HG2	2.19	0.43
1:N:87:ILE:O	1:N:173:PRO:HD3	2.19	0.43
2:O:56:MET:HA	25:O:602:PSC:H202	2.00	0.43
2:O:57:ASP:H	25:O:602:PSC:C20	2.28	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TRP:CD1	20:D:202:TGL:HC52	2.54	0.43
1:A:406:ASN:HD21	19:D:201:PGV:H31	1.83	0.43
10:J:49:CYS:HB3	27:J:101:DMU:C22	2.48	0.43
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	2.01	0.43
4:D:118:LYS:HB3	11:K:53:TRP:HB3	2.00	0.43
1:N:106:PRO:HB2	1:N:107:PRO:HD3	2.01	0.43
2:B:71:ILE:O	2:B:75:LEU:HD13	2.19	0.42
20:D:202:TGL:HB22	20:D:202:TGL:HB51	1.58	0.42
11:K:56:GLN:HG2	11:K:56:GLN:H	1.54	0.42
22:T:103:CDL:H552	22:T:103:CDL:H582	1.34	0.42
6:F:43:LYS:HB2	6:F:43:LYS:HE3	1.83	0.42
7:G:5:LYS:O	24:P:301:PEK:H342	2.18	0.42
1:N:55:ASN:ND2	28:N:707:HOH:O	2.40	0.42
19:N:607:PGV:H92	3:P:50:ASN:HD21	1.84	0.42
1:A:94:PHE:HB3	19:A:607:PGV:H032	2.01	0.42
1:A:296:GLY:O	2:B:178:ARG:NH2	2.53	0.42
19:A:607:PGV:O04	28:A:701:HOH:O	2.21	0.42
20:A:608:TGL:HB91	2:B:32[A]:PHE:CE1	2.55	0.42
20:L:101:TGL:H152	20:L:101:TGL:H182	1.40	0.42
25:O:602:PSC:H252	25:O:602:PSC:H221	1.62	0.42
22:C:302:CDL:O1	10:J:12:PHE:HE2	2.03	0.42
2:O:42:ILE:HG21	20:Q:201:TGL:H232	2.00	0.42
8:U:39:CYS:O	8:U:43:MET:HG2	2.20	0.42
7:G:27:SER:HB3	22:G:103:CDL:H562	2.01	0.42
22:G:103:CDL:H552	22:G:103:CDL:H581	1.78	0.42
7:T:27:SER:HB3	22:T:103:CDL:H561	2.01	0.42
1:A:334:TRP:HZ3	20:D:202:TGL:HA72	1.84	0.42
14:A:601:HEA:H271	14:A:601:HEA:H212	1.53	0.42
3:C:204:HIS:CE1	3:C:249:TRP:HB2	2.55	0.42
1:N:236:TRP:CH2	14:N:602:HEA:HBD1	2.54	0.42
1:A:87:ILE:O	1:A:173:PRO:HD3	2.20	0.42
2:B:146:MET:HA	2:B:213:LEU:HD12	2.02	0.42
24:G:102:PEK:H42	24:G:102:PEK:H72	1.36	0.42
1:N:406:ASN:HD21	19:N:609:PGV:H41	1.84	0.42
22:P:304:CDL:HB62	22:P:304:CDL:H521	2.01	0.42
3:C:86:PHE:HZ	19:C:301:PGV:H301	1.84	0.42
1:A:304:TYR:CD1	22:T:103:CDL:HB32	2.54	0.42
2:B:47:THR:HB	20:D:202:TGL:H181	2.02	0.42
12:Y:24[B]:MET:SD	20:Y:101:TGL:HC42	2.60	0.41
7:G:17:ARG:HH12	24:G:101:PEK:H041	1.84	0.41
7:G:36[A]:TRP:CE3	7:G:36[A]:TRP:HA	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:49:CYS:HB3	27:W:101:DMU:H10	2.01	0.41
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.02	0.41
7:G:41:HIS:HB3	7:G:74:ARG:NH1	2.34	0.41
19:P:303:PGV:H202	19:P:303:PGV:H012	1.36	0.41
1:A:334:TRP:CZ3	20:D:202:TGL:HA52	2.56	0.41
14:A:601:HEA:HMB1	14:A:601:HEA:H11	1.94	0.41
25:E:201:PSC:H082	25:E:201:PSC:H042	1.69	0.41
22:G:103:CDL:H381	22:G:103:CDL:H152	2.02	0.41
10:J:49:CYS:HB3	27:J:101:DMU:H11	2.03	0.41
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.84	0.41
11:X:6:ALA:HA	11:X:7:PRO:HD3	1.94	0.41
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.55	0.41
3:C:203:PHE:CE2	24:G:102:PEK:H8	2.56	0.41
14:N:601:HEA:HMB1	14:N:601:HEA:H11	1.94	0.41
2:B:1:FME:HE2	2:B:1:FME:HB3	1.86	0.41
22:C:302:CDL:H242	22:C:302:CDL:H271	1.90	0.41
1:N:309:THR:HG22	14:N:602:HEA:HMB2	2.02	0.41
2:O:91:ASN:C	2:O:92:ASN:HD22	2.16	0.41
22:T:103:CDL:H512	22:T:103:CDL:H202	2.03	0.41
20:Y:101:TGL:HC62	20:Y:101:TGL:HC32	1.86	0.41
6:F:77:GLY:O	6:F:90:LYS:NZ	2.52	0.41
11:K:6:ALA:HA	11:K:7:PRO:HD3	1.94	0.41
1:N:336:PRO:HG3	1:N:411:LYS:HG3	2.03	0.41
19:N:609:PGV:H042	28:N:946:HOH:O	2.20	0.41
3:P:172:TYR:CZ	24:P:307:PEK:H171	2.55	0.41
24:P:301:PEK:H312	24:P:301:PEK:H282	1.74	0.41
24:T:102:PEK:H71	24:T:102:PEK:H41	1.64	0.41
3:C:37:PHE:HB3	27:J:101:DMU:H29	2.03	0.41
22:C:302:CDL:OA6	22:C:302:CDL:H131	2.20	0.41
25:E:201:PSC:H011	25:E:201:PSC:C2	2.51	0.41
1:N:148:PHE:HB3	3:P:28:THR:HB	2.02	0.41
3:P:40:MET:O	3:P:44[A]:MET:HG2	2.21	0.41
1:A:274:VAL:O	1:A:278:MET:HG3	2.21	0.41
4:D:9:GLU:O	28:D:301:HOH:O	2.22	0.41
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.41
1:N:498:CYS:HA	1:N:499:PRO:HA	1.88	0.41
2:O:58:ALA:O	2:O:62:GLU:HG3	2.21	0.41
22:P:304:CDL:O1	10:W:12:PHE:HE2	2.04	0.41
1:A:217:THR:HG22	3:C:188:ILE:HG12	2.03	0.40
1:A:378:HIS:HE1	14:A:601:HEA:C1A	2.34	0.40
1:N:363:LEU:HD23	1:N:363:LEU:HA	1.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:607:PGV:H343	19:N:607:PGV:H311	1.87	0.40
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.47	0.40
1:A:422:ASN:OD1	20:A:608:TGL:H251	2.21	0.40
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.57	0.40
19:D:201:PGV:H011	19:D:201:PGV:H202	1.78	0.40
1:A:148:PHE:HB3	3:C:28:THR:HB	2.02	0.40
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.56	0.40
3:C:37:PHE:CE2	27:J:101:DMU:H13	2.56	0.40
1:N:151:HIS:CD2	24:T:102:PEK:H371	2.57	0.40
2:O:103:GLN:HA	2:O:104:TRP:HA	1.73	0.40
7:T:67:HIS:NE2	7:T:83:GLU:OE2	2.37	0.40
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.04	0.40
5:E:108:LYS:HB2	5:E:108:LYS:HE2	1.86	0.40
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.03	0.40
22:T:103:CDL:H712	22:T:103:CDL:H741	1.92	0.40
8:U:9:LYS:HB2	8:U:9:LYS:HE2	1.92	0.40
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.02	0.40
1:A:488:THR:HB	1:A:495:LEU:HD13	2.04	0.40
2:B:161:HIS:HB2	2:B:174:ALA:HB3	2.04	0.40
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.97	0.40
22:T:103:CDL:H311	22:T:103:CDL:HA62	1.94	0.40
9:V:21:ILE:HD13	9:V:21:ILE:HA	1.90	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	523/514 (102%)	509 (97%)	14 (3%)	0	100	100
1	N	523/514 (102%)	508 (97%)	15 (3%)	0	100	100
2	B	230/581 (40%)	225 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	231/581 (40%)	225 (97%)	5 (2%)	1 (0%)	34	37
3	C	266/261 (102%)	262 (98%)	4 (2%)	0	100	100
3	P	266/261 (102%)	262 (98%)	4 (2%)	0	100	100
4	D	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
4	Q	139/147 (95%)	136 (98%)	3 (2%)	0	100	100
5	E	104/109 (95%)	104 (100%)	0	0	100	100
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	94/98 (96%)	93 (99%)	1 (1%)	0	100	100
6	S	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
7	G	80/84 (95%)	73 (91%)	5 (6%)	2 (2%)	5	3
7	T	79/84 (94%)	74 (94%)	3 (4%)	2 (2%)	5	3
8	H	77/85 (91%)	73 (95%)	3 (4%)	1 (1%)	12	9
8	U	77/85 (91%)	73 (95%)	3 (4%)	1 (1%)	12	9
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
9	V	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
10	J	55/59 (93%)	55 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	44 (100%)	0	0	100	100
12	Y	44/47 (94%)	44 (100%)	0	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	39/46 (85%)	39 (100%)	0	0	100	100
All	All	3549/4320 (82%)	3467 (98%)	75 (2%)	7 (0%)	47	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	7	ASP
8	H	10	ASN
7	T	7	ASP
8	U	10	ASN
7	G	4	ALA
7	T	4	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	92	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	437/426 (103%)	428 (98%)	9 (2%)	53 67
1	N	437/426 (103%)	429 (98%)	8 (2%)	59 72
2	B	215/511 (42%)	208 (97%)	7 (3%)	38 49
2	O	216/511 (42%)	208 (96%)	8 (4%)	34 43
3	C	233/225 (104%)	229 (98%)	4 (2%)	60 74
3	P	233/225 (104%)	230 (99%)	3 (1%)	69 81
4	D	131/129 (102%)	128 (98%)	3 (2%)	50 63
4	Q	125/129 (97%)	124 (99%)	1 (1%)	81 90
5	E	93/95 (98%)	93 (100%)	0	100 100
5	R	93/95 (98%)	93 (100%)	0	100 100
6	F	81/81 (100%)	78 (96%)	3 (4%)	34 43
6	S	81/81 (100%)	79 (98%)	2 (2%)	47 60
7	G	67/67 (100%)	58 (87%)	9 (13%)	4 3
7	T	66/67 (98%)	59 (89%)	7 (11%)	6 6
8	H	71/75 (95%)	68 (96%)	3 (4%)	30 38
8	U	71/75 (95%)	69 (97%)	2 (3%)	43 56
9	I	57/58 (98%)	55 (96%)	2 (4%)	36 46
9	V	57/58 (98%)	55 (96%)	2 (4%)	36 46
10	J	48/50 (96%)	48 (100%)	0	100 100
10	W	49/50 (98%)	47 (96%)	2 (4%)	30 39
11	K	41/46 (89%)	39 (95%)	2 (5%)	25 31
11	X	40/46 (87%)	39 (98%)	1 (2%)	47 60
12	L	39/40 (98%)	38 (97%)	1 (3%)	46 58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	29
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	26
13	Z	35/38 (92%)	34 (97%)	1 (3%)	42	54
All	All	3092/3682 (84%)	3008 (97%)	84 (3%)	46	57

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	ARG
1	A	46	THR
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	369	ASP
1	A	486[A]	ASP
1	A	486[B]	ASP
2	B	59	GLN
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	94	SER
2	B	171	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	7	LYS
4	D	17[A]	VAL
4	D	17[B]	VAL
6	F	37	LYS
6	F	94	HIS
6	F	95	GLN
7	G	8	HIS
7	G	18	PHE
7	G	33	LEU
7	G	36[A]	TRP
7	G	36[B]	TRP
7	G	37	LEU
7	G	43	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	54	ARG
7	G	84	LYS
8	H	7	LYS
8	H	29	CYS
8	H	60	TYR
9	I	2	THR
9	I	36	LYS
11	K	55	GLU
11	K	56	GLN
12	L	47	LYS
13	M	13	LYS
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	138	HIS
1	N	180	GLN
1	N	311[A]	ILE
1	N	311[B]	ILE
1	N	363	LEU
1	N	369	ASP
2	O	32[A]	PHE
2	O	32[B]	PHE
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN
2	O	92	ASN
2	O	94	SER
2	O	171	LYS
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	51	LEU
6	S	25	ARG
6	S	37	LYS
7	T	8	HIS
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	43	GLU
7	T	54	ARG
7	T	84	LYS
8	U	29	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	U	60	TYR
9	V	2	THR
9	V	36	LYS
10	W	7	GLU
10	W	50	LEU
11	X	12	LYS
12	Y	24[A]	MET
12	Y	24[B]	MET
13	Z	41	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	52	HIS
4	D	101	HIS
11	K	56	GLN
7	T	38	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
2	FME	O	1	2	8,9,10	0.46	0	7,9,11	1.26	0
7	TPO	G	11	7	8,10,11	1.30	1 (12%)	10,14,16	0.99	1 (10%)
1	FME	N	1	1	8,9,10	0.46	0	7,9,11	1.30	0
7	TPO	T	11	7	8,10,11	1.29	1 (12%)	10,14,16	0.85	0
1	FME	A	1	1	8,9,10	0.48	0	7,9,11	1.34	0

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	0.47	0	7,9,11	1.34	0

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	2.77	1.59	1.50
7	T	11	TPO	P-O1P	2.76	1.59	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	11	TPO	CG2-CB-CA	2.31	117.71	113.16

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
2	B	1	FME	CB-CG-SD-CE
2	O	1	FME	CB-CG-SD-CE
1	A	1	FME	CB-CG-SD-CE
1	N	1	FME	CB-CG-SD-CE
7	G	11	TPO	CB-OG1-P-O1P
7	G	11	TPO	CB-OG1-P-O2P
7	T	11	TPO	CB-OG1-P-O2P
1	A	1	FME	CB-CA-N-CN
1	N	1	FME	CB-CA-N-CN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 8 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	PSC	O	602	-	51,51,51	1.13	3 (5%)	57,59,59	1.51	4 (7%)
23	CHD	C	304	-	32,32,32	0.83	1 (3%)	51,51,51	1.01	1 (1%)
24	PEK	P	301	-	52,52,52	0.98	2 (3%)	55,57,57	1.18	5 (9%)
22	CDL	C	302	-	99,99,99	1.33	12 (12%)	105,111,111	1.42	13 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CDL	P	304	-	99,99,99	1.31	12 (12%)	105,111,111	1.33	13 (12%)
24	PEK	C	306	-	52,52,52	0.94	2 (3%)	55,57,57	1.27	6 (10%)
22	CDL	G	103	-	99,99,99	1.32	12 (12%)	105,111,111	1.36	8 (7%)
14	HEA	A	601	1	57,67,67	1.48	9 (15%)	61,103,103	1.63	15 (24%)
23	CHD	T	101	-	32,32,32	0.82	1 (3%)	51,51,51	1.10	4 (7%)
22	CDL	T	103	-	99,99,99	1.31	12 (12%)	105,111,111	1.25	7 (6%)
24	PEK	G	101	-	52,52,52	0.89	2 (3%)	55,57,57	1.36	8 (14%)
19	PGV	N	607	-	50,50,50	0.94	2 (4%)	53,56,56	1.10	3 (5%)
14	HEA	N	601	1	57,67,67	1.48	9 (15%)	61,103,103	1.61	14 (22%)
18	PER	A	606	14,15	0,1,1	-	-	-	-	-
23	CHD	P	306	-	32,32,32	0.81	1 (3%)	51,51,51	0.95	1 (1%)
25	PSC	E	201	-	51,51,51	1.10	3 (5%)	57,59,59	1.41	5 (8%)
24	PEK	T	102	-	52,52,52	0.94	2 (3%)	55,57,57	1.22	4 (7%)
14	HEA	A	602	1,18	57,67,67	1.50	9 (15%)	61,103,103	1.65	19 (31%)
19	PGV	D	201	-	50,50,50	0.32	0	53,56,56	0.33	0
19	PGV	N	609	-	50,50,50	1.00	2 (4%)	53,56,56	1.31	7 (13%)
20	TGL	Y	101	-	62,62,62	1.00	3 (4%)	65,65,65	0.96	3 (4%)
23	CHD	P	305	-	32,32,32	0.78	0	51,51,51	1.76	8 (15%)
19	PGV	P	302	-	50,50,50	0.98	2 (4%)	53,56,56	1.35	8 (15%)
24	PEK	P	307	-	52,52,52	0.93	2 (3%)	55,57,57	1.41	9 (16%)
20	TGL	A	608	-	62,62,62	0.98	3 (4%)	65,65,65	1.15	5 (7%)
24	PEK	G	102	-	52,52,52	0.96	2 (3%)	55,57,57	1.21	5 (9%)
23	CHD	C	303	-	32,32,32	0.87	1 (3%)	51,51,51	1.35	7 (13%)
18	PER	N	606	14,15	0,1,1	-	-	-	-	-
19	PGV	A	607	-	50,50,50	0.94	2 (4%)	53,56,56	1.11	3 (5%)
19	PGV	P	303	-	50,50,50	0.33	0	53,56,56	0.53	0
27	DMU	Z	101	-	34,34,34	0.38	0	45,45,45	0.76	1 (2%)
20	TGL	D	202	-	62,62,62	0.97	3 (4%)	65,65,65	1.07	4 (6%)
27	DMU	W	101	-	34,34,34	0.34	0	45,45,45	0.85	1 (2%)
20	TGL	L	101	-	62,62,62	1.00	3 (4%)	65,65,65	1.13	5 (7%)
19	PGV	C	301	-	50,50,50	0.37	0	53,56,56	0.49	1 (1%)
20	TGL	N	608	-	62,62,62	0.99	3 (4%)	65,65,65	1.11	5 (7%)
21	CUA	B	601	2	0,1,1	-	-	-	-	-
14	HEA	N	602	1,18	57,67,67	1.49	10 (17%)	61,103,103	1.63	16 (26%)
23	CHD	G	104	-	32,32,32	0.81	1 (3%)	51,51,51	1.09	3 (5%)
27	DMU	J	101	-	34,34,34	0.48	1 (2%)	45,45,45	0.99	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	TGL	Q	201	-	62,62,62	0.99	3 (4%)	65,65,65	1.14	5 (7%)
27	DMU	M	101	-	34,34,34	0.36	0	45,45,45	0.76	1 (2%)
19	PGV	C	305	-	50,50,50	0.96	2 (4%)	53,56,56	1.37	8 (15%)
21	CUA	O	601	2	0,1,1	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSC	O	602	-	-	25/55/55/55	-
23	CHD	C	304	-	-	1/9/74/74	0/4/4/4
24	PEK	P	301	-	-	26/56/56/56	-
22	CDL	C	302	-	-	40/110/110/110	-
22	CDL	P	304	-	-	39/110/110/110	-
24	PEK	C	306	-	-	19/56/56/56	-
22	CDL	G	103	-	-	35/110/110/110	-
14	HEA	A	601	1	-	9/32/76/76	-
23	CHD	T	101	-	-	2/9/74/74	0/4/4/4
22	CDL	T	103	-	-	33/110/110/110	-
24	PEK	G	101	-	-	21/56/56/56	-
19	PGV	N	607	-	-	7/55/55/55	-
14	HEA	N	601	1	-	7/32/76/76	-
23	CHD	P	306	-	-	3/9/74/74	0/4/4/4
25	PSC	E	201	-	-	20/55/55/55	-
24	PEK	T	102	-	-	13/56/56/56	-
14	HEA	A	602	1,18	-	7/32/76/76	-
19	PGV	D	201	-	-	29/55/55/55	-
19	PGV	N	609	-	-	23/55/55/55	-
20	TGL	Y	101	-	-	34/65/65/65	-
23	CHD	P	305	-	-	5/9/74/74	1/4/4/4
19	PGV	P	302	-	-	19/55/55/55	-
24	PEK	P	307	-	-	20/56/56/56	-
20	TGL	A	608	-	-	26/65/65/65	-
24	PEK	G	102	-	-	20/56/56/56	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	C	303	-	-	5/9/74/74	0/4/4/4
19	PGV	A	607	-	-	11/55/55/55	-
19	PGV	P	303	-	-	22/55/55/55	-
27	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
20	TGL	D	202	-	-	27/65/65/65	-
27	DMU	W	101	-	-	8/19/59/59	0/2/2/2
20	TGL	L	101	-	-	28/65/65/65	-
19	PGV	C	301	-	-	21/55/55/55	-
20	TGL	N	608	-	-	27/65/65/65	-
23	CHD	G	104	-	-	2/9/74/74	0/4/4/4
14	HEA	N	602	1,18	-	6/32/76/76	-
27	DMU	J	101	-	-	8/19/59/59	0/2/2/2
20	TGL	Q	201	-	-	21/65/65/65	-
27	DMU	M	101	-	-	6/19/59/59	0/2/2/2
19	PGV	C	305	-	-	14/55/55/55	-

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	602	PSC	O01-C1	4.93	1.48	1.34
22	C	302	CDL	OA8-CA7	4.86	1.47	1.33
24	P	301	PEK	O03-C21	4.86	1.47	1.33
25	E	201	PSC	O01-C1	4.68	1.47	1.34
19	C	305	PGV	O03-C19	4.64	1.46	1.33
19	P	302	PGV	O03-C19	4.64	1.46	1.33
22	T	103	CDL	OA6-CA5	4.64	1.47	1.34
24	G	102	PEK	O03-C21	4.64	1.46	1.33
24	T	102	PEK	O03-C21	4.61	1.46	1.33
19	N	609	PGV	O01-C1	4.60	1.47	1.34
24	C	306	PEK	O03-C21	4.55	1.46	1.33
24	P	307	PEK	O03-C21	4.50	1.46	1.33
19	A	607	PGV	O03-C19	4.49	1.46	1.33
19	N	607	PGV	O03-C19	4.46	1.46	1.33
20	L	101	TGL	OG1-CA1	4.44	1.46	1.33
20	Y	101	TGL	OG1-CA1	4.38	1.46	1.33
20	N	608	TGL	OG1-CA1	4.35	1.46	1.33
22	C	302	CDL	OA6-CA5	4.35	1.46	1.34
22	G	103	CDL	OB6-CB5	4.35	1.46	1.34
20	L	101	TGL	OG3-CC1	4.34	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	608	TGL	OG1-CA1	4.33	1.46	1.33
20	D	202	TGL	OG1-CA1	4.30	1.45	1.33
20	Y	101	TGL	OG2-CB1	4.30	1.46	1.34
19	N	609	PGV	O03-C19	4.30	1.45	1.33
20	Q	201	TGL	OG1-CA1	4.29	1.45	1.33
19	P	302	PGV	O01-C1	4.29	1.46	1.34
22	G	103	CDL	OA8-CA7	4.28	1.45	1.33
22	T	103	CDL	OB8-CB7	4.27	1.45	1.33
20	Q	201	TGL	OG3-CC1	4.27	1.45	1.33
22	C	302	CDL	OB6-CB5	4.27	1.46	1.34
22	P	304	CDL	OA8-CA7	4.24	1.45	1.33
22	T	103	CDL	OA8-CA7	4.24	1.45	1.33
20	Y	101	TGL	OG3-CC1	4.24	1.45	1.33
22	G	103	CDL	OB8-CB7	4.24	1.45	1.33
20	N	608	TGL	OG3-CC1	4.23	1.45	1.33
20	A	608	TGL	OG3-CC1	4.23	1.45	1.33
24	C	306	PEK	O01-C1	4.20	1.46	1.34
24	P	301	PEK	O01-C1	4.20	1.46	1.34
22	G	103	CDL	OA6-CA5	4.17	1.46	1.34
24	G	101	PEK	O03-C21	4.16	1.45	1.33
20	D	202	TGL	OG3-CC1	4.16	1.45	1.33
22	P	304	CDL	OB6-CB5	4.16	1.46	1.34
22	P	304	CDL	OA6-CA5	4.15	1.46	1.34
24	G	101	PEK	O01-C1	4.14	1.46	1.34
24	G	102	PEK	O01-C1	4.13	1.46	1.34
19	C	305	PGV	O01-C1	4.13	1.45	1.34
20	L	101	TGL	OG2-CB1	4.10	1.45	1.34
20	N	608	TGL	OG2-CB1	4.04	1.45	1.34
19	N	607	PGV	O01-C1	4.03	1.45	1.34
20	A	608	TGL	OG2-CB1	4.01	1.45	1.34
20	Q	201	TGL	OG2-CB1	4.00	1.45	1.34
22	T	103	CDL	OB6-CB5	3.99	1.45	1.34
24	T	102	PEK	O01-C1	3.98	1.45	1.34
19	A	607	PGV	O01-C1	3.97	1.45	1.34
24	P	307	PEK	O01-C1	3.96	1.45	1.34
22	C	302	CDL	OB8-CB7	3.92	1.44	1.33
22	P	304	CDL	OB8-CB7	3.86	1.44	1.33
25	E	201	PSC	O03-C19	3.86	1.44	1.33
20	D	202	TGL	OG2-CB1	3.82	1.45	1.34
14	N	602	HEA	CHD-C1D	3.68	1.44	1.35
25	O	602	PSC	O03-C19	3.68	1.44	1.33
25	E	201	PSC	C13-C12	3.67	1.53	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	602	PSC	C13-C12	3.64	1.52	1.31
14	A	601	HEA	CHC-C4B	3.64	1.44	1.35
14	A	601	HEA	CHD-C1D	3.64	1.44	1.35
14	N	601	HEA	CHC-C4B	3.64	1.44	1.35
14	A	602	HEA	C4D-C3D	-3.63	1.38	1.45
14	N	601	HEA	CHD-C1D	3.63	1.44	1.35
14	A	602	HEA	CHD-C1D	3.61	1.44	1.35
14	N	602	HEA	C4D-C3D	-3.55	1.38	1.45
14	A	602	HEA	CHC-C4B	3.54	1.44	1.35
14	N	602	HEA	CHC-C4B	3.52	1.44	1.35
14	A	601	HEA	C4D-C3D	-3.51	1.39	1.45
14	N	601	HEA	C4D-C3D	-3.48	1.39	1.45
22	P	304	CDL	C19-C18	-3.43	1.32	1.51
22	G	103	CDL	C62-C61	-3.36	1.32	1.51
22	P	304	CDL	C62-C61	-3.36	1.32	1.51
22	P	304	CDL	C22-C21	-3.36	1.32	1.51
14	A	602	HEA	C4B-C3B	-3.35	1.38	1.44
22	T	103	CDL	C62-C61	-3.34	1.32	1.51
14	N	602	HEA	C4B-C3B	-3.34	1.39	1.44
22	P	304	CDL	C79-C78	-3.33	1.32	1.51
22	P	304	CDL	C82-C81	-3.33	1.32	1.51
22	C	302	CDL	C59-C58	-3.33	1.32	1.51
22	C	302	CDL	C19-C18	-3.32	1.32	1.51
22	G	103	CDL	C59-C58	-3.32	1.33	1.51
22	C	302	CDL	C82-C81	-3.32	1.33	1.51
22	P	304	CDL	C59-C58	-3.31	1.33	1.51
22	G	103	CDL	C79-C78	-3.31	1.33	1.51
22	T	103	CDL	C59-C58	-3.30	1.33	1.51
22	P	304	CDL	C42-C41	-3.30	1.33	1.51
22	G	103	CDL	C39-C38	-3.29	1.33	1.51
22	C	302	CDL	C22-C21	-3.28	1.33	1.51
22	G	103	CDL	C82-C81	-3.28	1.33	1.51
22	C	302	CDL	C62-C61	-3.28	1.33	1.51
22	C	302	CDL	C79-C78	-3.27	1.33	1.51
22	C	302	CDL	C39-C38	-3.27	1.33	1.51
22	G	103	CDL	C42-C41	-3.27	1.33	1.51
22	T	103	CDL	C22-C21	-3.25	1.33	1.51
22	T	103	CDL	C19-C18	-3.25	1.33	1.51
22	T	103	CDL	C39-C38	-3.24	1.33	1.51
22	P	304	CDL	C39-C38	-3.24	1.33	1.51
22	C	302	CDL	C42-C41	-3.24	1.33	1.51
22	T	103	CDL	C42-C41	-3.23	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601	HEA	C1D-ND	-3.22	1.34	1.40
22	G	103	CDL	C19-C18	-3.22	1.33	1.51
14	A	602	HEA	C1D-ND	-3.21	1.34	1.40
14	N	602	HEA	C1D-ND	-3.21	1.34	1.40
22	T	103	CDL	C82-C81	-3.19	1.33	1.51
14	A	601	HEA	C1D-ND	-3.18	1.34	1.40
14	N	602	HEA	C4B-NB	-3.17	1.34	1.40
22	G	103	CDL	C22-C21	-3.16	1.33	1.51
22	T	103	CDL	C79-C78	-3.16	1.33	1.51
14	A	602	HEA	C4B-NB	-3.14	1.34	1.40
14	N	601	HEA	C4B-C3B	-3.12	1.39	1.44
14	A	601	HEA	C4B-C3B	-3.05	1.39	1.44
14	N	601	HEA	C4B-NB	-3.00	1.35	1.40
14	A	602	HEA	C1B-C2B	-2.98	1.38	1.44
14	A	601	HEA	C4B-NB	-2.97	1.35	1.40
14	A	601	HEA	C1B-C2B	-2.92	1.38	1.44
14	A	601	HEA	C1D-C2D	-2.89	1.39	1.44
14	N	601	HEA	C1B-C2B	-2.89	1.39	1.44
14	N	601	HEA	C1D-C2D	-2.88	1.39	1.44
14	N	602	HEA	C1B-C2B	-2.86	1.39	1.44
14	N	602	HEA	C1D-C2D	-2.82	1.39	1.44
14	A	602	HEA	C1D-C2D	-2.80	1.39	1.44
23	C	303	CHD	C13-C14	-2.29	1.51	1.55
23	T	101	CHD	C13-C14	-2.10	1.51	1.55
14	A	602	HEA	C4D-ND	-2.10	1.34	1.38
27	J	101	DMU	O16-C6	2.10	1.43	1.40
23	G	104	CHD	C13-C14	-2.10	1.51	1.55
14	N	602	HEA	C4D-ND	-2.06	1.34	1.38
14	N	601	HEA	C1B-NB	-2.05	1.34	1.38
23	C	304	CHD	C13-C14	-2.05	1.52	1.55
23	P	306	CHD	C13-C14	-2.04	1.52	1.55
14	A	601	HEA	C1B-NB	-2.03	1.34	1.38
14	N	602	HEA	C1B-NB	-2.01	1.34	1.38

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	O	602	PSC	O01-C1-C2	6.98	126.54	111.50
23	P	305	CHD	C6-C5-C4	-6.64	103.54	111.19
25	E	201	PSC	O01-C1-C2	5.81	124.02	111.50
22	G	103	CDL	OA6-CA5-C11	5.55	123.45	111.50
24	P	301	PEK	O01-C1-C2	5.36	123.06	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C13-C12-C11	-5.10	106.69	114.35
22	C	302	CDL	OA8-CA7-C31	4.96	127.48	111.91
14	N	601	HEA	C13-C12-C11	-4.80	107.14	114.35
24	C	306	PEK	O01-C1-C2	4.78	121.79	111.50
24	G	101	PEK	O01-C1-C2	4.76	121.77	111.50
19	C	305	PGV	O01-C1-C2	4.75	121.74	111.50
22	P	304	CDL	OB6-CB5-C51	4.68	121.58	111.50
19	N	609	PGV	O01-C1-C2	4.66	121.55	111.50
19	P	302	PGV	O03-C19-C20	4.65	126.49	111.91
20	Q	201	TGL	OG2-CB1-CB2	4.55	121.31	111.50
22	C	302	CDL	OB6-CB5-C51	4.54	121.29	111.50
20	A	608	TGL	OG2-CB1-CB2	4.46	121.12	111.50
20	L	101	TGL	OG2-CB1-CB2	4.42	121.02	111.50
22	G	103	CDL	OB6-CB5-C51	4.22	120.59	111.50
22	G	103	CDL	CA4-OA6-CA5	-4.08	107.74	117.79
25	O	602	PSC	C03-C02-C01	-4.06	102.18	111.79
25	O	602	PSC	O01-C1-O02	-4.04	113.94	123.70
19	N	607	PGV	O03-C19-C20	4.03	124.54	111.91
19	C	305	PGV	O03-C19-C20	3.96	124.32	111.91
19	A	607	PGV	O03-C19-C20	3.95	124.29	111.91
24	P	307	PEK	O03-C21-C22	3.89	124.11	111.91
20	N	608	TGL	OG2-CB1-CB2	3.89	119.88	111.50
23	P	305	CHD	C5-C6-C7	3.84	118.70	114.46
22	C	302	CDL	OA6-CA5-C11	3.83	119.75	111.50
22	T	103	CDL	OA6-CA5-C11	3.78	119.64	111.50
24	P	307	PEK	C02-O01-C1	-3.71	108.66	117.79
22	P	304	CDL	OA6-CA5-C11	3.69	119.46	111.50
20	D	202	TGL	OG2-CB1-CB2	3.64	119.36	111.50
22	T	103	CDL	OB6-CB5-C51	3.63	119.31	111.50
19	N	609	PGV	O03-C19-C20	3.60	123.21	111.91
24	T	102	PEK	C2-C3-C4	-3.60	106.82	113.23
24	P	307	PEK	O01-C1-C2	3.55	119.15	111.50
19	N	609	PGV	C02-O01-C1	-3.54	109.06	117.79
22	C	302	CDL	CB4-OB6-CB5	-3.53	109.11	117.79
20	Y	101	TGL	OG2-CB1-CB2	3.51	119.06	111.50
23	C	303	CHD	C23-C22-C20	-3.50	108.12	114.52
20	D	202	TGL	CG2-OG2-CB1	-3.50	109.18	117.79
23	P	305	CHD	C11-C9-C10	-3.48	110.14	113.73
24	G	102	PEK	O03-C21-C22	3.48	122.82	111.91
22	T	103	CDL	CB4-OB6-CB5	-3.47	109.24	117.79
20	Q	201	TGL	CG2-OG2-CB1	-3.40	109.43	117.79
24	T	102	PEK	O01-C1-C2	3.38	118.79	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	103	CDL	CB4-OB6-CB5	-3.37	109.49	117.79
25	E	201	PSC	C03-C02-C01	-3.30	103.97	111.79
24	G	102	PEK	C02-O01-C1	-3.29	109.68	117.79
14	A	601	HEA	CAA-CBA-CGA	-3.27	104.60	113.76
22	P	304	CDL	CB4-OB6-CB5	-3.25	109.78	117.79
24	T	102	PEK	O03-C21-C22	3.23	122.06	111.91
19	N	607	PGV	O03-C19-O04	-3.19	115.55	123.59
23	C	303	CHD	C14-C13-C12	3.17	110.36	107.40
24	G	101	PEK	O03-C21-C22	3.13	121.72	111.91
14	N	601	HEA	CAA-CBA-CGA	-3.12	105.02	113.76
19	A	607	PGV	O03-C19-O04	-3.10	115.77	123.59
24	C	306	PEK	C02-O01-C1	-3.10	110.17	117.79
22	T	103	CDL	CB6-CB4-CB3	-3.09	104.47	111.79
24	G	102	PEK	O01-C1-C2	3.08	118.14	111.50
24	C	306	PEK	O03-C01-C02	3.06	117.33	108.43
20	A	608	TGL	CG2-OG2-CB1	-3.03	110.32	117.79
19	C	305	PGV	C02-O01-C1	-3.02	110.36	117.79
19	P	302	PGV	C01-O03-C19	3.02	128.29	117.12
14	N	602	HEA	C27-C19-C20	2.99	120.31	115.27
14	N	602	HEA	C26-C15-C16	2.99	120.30	115.27
24	P	301	PEK	O03-C21-C22	2.98	121.26	111.91
22	C	302	CDL	OA8-CA7-OA9	-2.97	116.09	123.59
14	N	602	HEA	CAA-CBA-CGA	-2.97	105.44	113.76
27	J	101	DMU	O5-C6-C1	-2.95	104.10	110.35
24	G	102	PEK	O03-C01-C02	2.91	116.92	108.43
24	P	307	PEK	O01-C1-O02	-2.90	116.69	123.70
14	N	602	HEA	C13-C14-C15	-2.90	120.68	127.66
22	G	103	CDL	CB6-CB4-CB3	-2.90	104.94	111.79
19	P	302	PGV	O01-C1-C2	2.90	117.74	111.50
23	P	305	CHD	C14-C8-C7	2.89	115.65	111.81
22	P	304	CDL	OB8-CB7-C71	2.89	120.99	111.91
22	P	304	CDL	CA4-OA6-CA5	-2.88	110.69	117.79
20	Q	201	TGL	OG1-CA1-CA2	2.87	120.91	111.91
22	P	304	CDL	CA6-CA4-CA3	-2.86	105.01	111.79
22	C	302	CDL	CB6-CB4-CB3	-2.86	105.02	111.79
20	N	608	TGL	OG1-CA1-CA2	2.83	120.78	111.91
22	T	103	CDL	OB8-CB7-C71	2.83	120.78	111.91
20	A	608	TGL	OG1-CA1-CA2	2.81	120.74	111.91
27	W	101	DMU	C18-O16-C6	-2.81	109.18	113.84
20	L	101	TGL	OG3-CC1-CC2	2.80	120.70	111.91
14	A	602	HEA	C27-C19-C20	2.79	119.97	115.27
19	P	302	PGV	O03-C19-O04	-2.79	116.55	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	302	CDL	CA6-CA4-CA3	-2.78	105.22	111.79
20	L	101	TGL	OG1-CA1-CA2	2.77	120.61	111.91
19	P	302	PGV	C21-C20-C19	-2.76	103.57	113.62
14	N	601	HEA	C26-C15-C16	2.73	119.87	115.27
23	P	305	CHD	C6-C7-C8	2.73	114.40	111.48
24	C	306	PEK	C2-C3-C4	-2.73	108.36	113.23
14	A	602	HEA	C26-C15-C16	2.73	119.86	115.27
24	G	101	PEK	C02-O01-C1	-2.72	111.09	117.79
25	E	201	PSC	O01-C1-O02	-2.70	117.17	123.70
23	C	303	CHD	C21-C20-C17	-2.68	108.82	112.92
22	C	302	CDL	OB8-CB7-C71	2.68	120.31	111.91
14	A	602	HEA	C13-C14-C15	-2.67	121.22	127.66
14	A	602	HEA	CMC-C2C-C1C	-2.64	124.41	128.46
14	A	602	HEA	CAA-CBA-CGA	-2.62	106.41	113.76
20	N	608	TGL	OG3-CC1-CC2	2.61	120.11	111.91
20	D	202	TGL	OG1-CA1-CA2	2.61	120.10	111.91
19	N	609	PGV	O03-C19-O04	-2.60	117.03	123.59
23	C	303	CHD	C22-C20-C17	2.57	115.59	110.28
14	A	602	HEA	CMB-C2B-C3B	-2.57	125.45	130.34
24	G	101	PEK	C01-O03-C21	2.56	126.59	117.12
20	N	608	TGL	CG2-OG2-CB1	-2.55	111.50	117.79
23	T	101	CHD	C13-C17-C20	-2.55	116.45	119.50
19	A	607	PGV	O01-C1-C2	2.55	117.00	111.50
22	G	103	CDL	OA6-CA5-OA7	-2.54	117.56	123.70
19	N	609	PGV	O01-C02-C03	2.54	117.59	108.40
20	A	608	TGL	OG3-CC1-CC2	2.53	119.86	111.91
14	N	601	HEA	C3C-C4C-NC	2.53	112.48	109.21
19	C	305	PGV	C01-O03-C19	2.52	126.47	117.12
23	G	104	CHD	C13-C17-C20	-2.52	116.49	119.50
19	C	305	PGV	O03-C19-O04	-2.51	117.27	123.59
23	C	303	CHD	C13-C17-C20	-2.50	116.51	119.50
24	G	101	PEK	O03-C01-C02	-2.50	101.15	108.43
23	T	101	CHD	C17-C13-C14	2.49	102.61	100.09
14	N	602	HEA	CMB-C2B-C3B	-2.48	125.61	130.34
14	A	602	HEA	CMC-C2C-C3C	2.48	129.32	124.68
14	A	602	HEA	CHA-C4D-C3D	-2.48	121.19	124.84
14	A	601	HEA	C25-C23-C24	2.48	120.07	114.60
24	P	307	PEK	C3-C2-C1	-2.48	104.61	113.62
20	Q	201	TGL	OG2-CB1-OB1	-2.47	117.72	123.70
14	N	602	HEA	CBA-CAA-C2A	2.47	116.76	112.60
14	A	602	HEA	C3C-C4C-NC	2.46	112.39	109.21
14	N	601	HEA	CMC-C2C-C1C	-2.46	124.68	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	101	TGL	OG1-CA1-CA2	2.46	119.62	111.91
24	C	306	PEK	C03-C02-C01	-2.45	105.99	111.79
24	P	301	PEK	O01-C1-O02	-2.44	117.80	123.70
14	N	602	HEA	CHA-C4D-C3D	-2.44	121.26	124.84
14	A	601	HEA	C26-C15-C16	2.43	119.36	115.27
14	N	602	HEA	C13-C12-C11	-2.43	110.70	114.35
24	P	307	PEK	C2-C3-C4	-2.41	108.92	113.23
14	A	601	HEA	C3C-C4C-NC	2.41	112.33	109.21
23	G	104	CHD	C17-C13-C14	2.41	102.53	100.09
14	A	601	HEA	C13-C14-C15	-2.41	121.86	127.66
14	N	601	HEA	C13-C14-C15	-2.40	121.89	127.66
24	G	101	PEK	C03-C02-C01	2.39	117.45	111.79
22	C	302	CDL	C58-C57-C56	-2.39	102.29	114.42
20	L	101	TGL	CG3-CG2-CG1	-2.38	106.16	111.79
23	C	303	CHD	C13-C14-C8	-2.37	111.71	114.74
20	Y	101	TGL	OG3-CC1-CC2	2.37	119.34	111.91
22	P	304	CDL	C72-C71-CB7	-2.36	105.03	113.62
14	A	602	HEA	C25-C23-C24	2.36	119.82	114.60
19	N	607	PGV	O01-C1-C2	2.36	116.59	111.50
22	P	304	CDL	C21-C20-C19	-2.36	102.44	114.42
24	P	307	PEK	O03-C21-O04	-2.36	117.64	123.59
19	P	302	PGV	O01-C02-C01	2.36	116.93	108.40
19	P	302	PGV	C02-O01-C1	2.35	123.58	117.79
14	N	602	HEA	C25-C23-C24	2.35	119.80	114.60
22	T	103	CDL	OA8-CA7-C31	2.35	119.28	111.91
22	C	302	CDL	CA4-OA6-CA5	-2.33	112.06	117.79
27	M	101	DMU	C10-O7-C3	-2.32	112.23	117.96
22	P	304	CDL	OA8-CA7-C31	2.31	119.16	111.91
14	A	601	HEA	CMC-C2C-C1C	-2.31	124.92	128.46
23	T	101	CHD	C13-C14-C8	-2.31	111.79	114.74
24	G	101	PEK	O01-C1-O02	-2.30	118.14	123.70
14	A	602	HEA	C2D-C1D-ND	2.30	112.56	109.84
14	A	601	HEA	CHA-C4D-C3D	-2.30	121.46	124.84
20	N	608	TGL	CG3-CG2-CG1	-2.29	106.36	111.79
24	T	102	PEK	C02-O01-C1	-2.29	112.14	117.79
14	N	602	HEA	C3B-C4B-NB	2.29	112.55	109.84
14	A	601	HEA	CHB-C1B-C2B	-2.28	121.41	124.98
14	N	601	HEA	CHB-C1B-C2B	-2.28	121.42	124.98
14	N	601	HEA	CBA-CAA-C2A	2.28	116.44	112.60
24	C	306	PEK	O01-C1-O02	-2.27	118.21	123.70
23	P	305	CHD	O7-C7-C6	-2.26	104.34	109.94
14	N	601	HEA	CHA-C4D-C3D	-2.26	121.52	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	CBA-CAA-C2A	2.25	116.39	112.60
23	P	305	CHD	C17-C13-C14	2.25	102.36	100.09
14	N	601	HEA	C25-C23-C24	2.24	119.56	114.60
22	P	304	CDL	OA6-CA4-CA3	2.24	116.53	108.40
23	P	305	CHD	C16-C17-C20	-2.24	108.67	112.15
14	A	602	HEA	CHB-C1B-NB	2.24	126.87	124.43
14	N	601	HEA	CHB-C1B-NB	2.24	126.87	124.43
14	N	601	HEA	CMB-C2B-C3B	-2.23	126.08	130.34
24	P	307	PEK	C01-O03-C21	2.23	125.37	117.12
14	N	602	HEA	CAD-CBD-CGD	-2.23	108.81	113.60
14	A	601	HEA	CMC-C2C-C3C	2.22	128.82	124.68
19	C	305	PGV	O01-C1-O02	-2.21	118.36	123.70
14	N	602	HEA	CMC-C2C-C3C	2.21	128.80	124.68
20	A	608	TGL	OG2-CB1-OB1	-2.20	118.38	123.70
27	Z	101	DMU	C10-O7-C3	-2.18	112.58	117.96
14	A	602	HEA	C3B-C4B-NB	2.17	112.42	109.84
14	A	602	HEA	CHA-C4D-ND	2.16	126.78	124.43
24	G	101	PEK	O03-C21-O04	-2.16	118.13	123.59
22	G	103	CDL	C61-C60-C59	-2.16	103.45	114.42
20	Q	201	TGL	OG3-CC1-CC2	2.16	118.69	111.91
14	A	601	HEA	CHB-C1B-NB	2.16	126.78	124.43
20	L	101	TGL	CG2-OG2-CB1	-2.16	112.48	117.79
23	T	101	CHD	C11-C9-C10	-2.14	111.52	113.73
20	D	202	TGL	OG3-CC1-CC2	2.14	118.63	111.91
24	P	301	PEK	C02-O01-C1	-2.14	112.52	117.79
14	A	601	HEA	C27-C19-C20	2.14	118.87	115.27
22	G	103	CDL	OB6-CB5-OB7	-2.12	118.58	123.70
22	P	304	CDL	OB6-CB5-OB7	-2.12	118.58	123.70
22	P	304	CDL	OB8-CB7-OB9	-2.12	118.24	123.59
24	G	102	PEK	O03-C21-O04	-2.12	118.25	123.59
22	T	103	CDL	CA6-CA4-CA3	2.10	116.76	111.79
19	P	302	PGV	O14-P-O13	2.10	122.62	112.24
24	P	307	PEK	C23-C22-C21	-2.10	105.99	113.62
14	A	601	HEA	C21-C22-C23	-2.10	120.59	127.75
23	C	303	CHD	C16-C17-C20	2.09	115.39	112.15
22	C	302	CDL	OA8-CA6-CA4	2.09	114.52	108.43
14	A	602	HEA	CBA-CAA-C2A	2.08	116.11	112.60
23	C	304	CHD	C9-C11-C12	-2.08	111.56	114.30
25	O	602	PSC	C14-C13-C12	-2.08	108.77	124.73
14	N	602	HEA	C3C-C4C-NC	2.07	111.89	109.21
14	A	602	HEA	CAD-CBD-CGD	-2.07	109.14	113.60
14	A	602	HEA	CHB-C1B-C2B	-2.07	121.74	124.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	CMC-C2C-C1C	-2.07	125.28	128.46
14	N	602	HEA	CHA-C4D-ND	2.06	126.67	124.43
22	C	302	CDL	OB6-CB5-OB7	-2.06	118.72	123.70
23	G	104	CHD	C13-C14-C8	-2.06	112.11	114.74
14	N	602	HEA	CHB-C1B-NB	2.05	126.66	124.43
14	A	601	HEA	CMB-C2B-C3B	-2.05	126.43	130.34
22	P	304	CDL	C81-C80-C79	-2.05	104.00	114.42
14	N	601	HEA	C3B-C4B-NB	2.05	112.27	109.84
19	N	609	PGV	O01-C1-O02	-2.05	118.75	123.70
19	C	305	PGV	C21-C20-C19	-2.05	106.17	113.62
19	C	305	PGV	O14-P-O13	2.04	122.32	112.24
14	N	601	HEA	CMC-C2C-C3C	2.04	128.49	124.68
24	P	301	PEK	C2-C3-C4	-2.04	109.60	113.23
25	E	201	PSC	C01-O03-C19	-2.03	109.60	117.12
22	C	302	CDL	OB8-CB7-OB9	-2.03	118.47	123.59
25	E	201	PSC	O13-P-O14	2.02	122.23	112.24
23	P	306	CHD	C9-C11-C12	-2.02	111.64	114.30
14	A	602	HEA	C1D-C2D-C3D	-2.01	104.84	106.96
19	N	609	PGV	O14-P-O13	2.01	122.18	112.24
19	C	301	PGV	O14-P-O12	-2.00	98.44	107.75
14	A	602	HEA	C13-C12-C11	-2.00	111.34	114.35

There are no chirality outliers.

All (693) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C18-C19-C20-C21
14	A	601	HEA	C27-C19-C20-C21
19	C	301	PGV	C04-O12-P-O13
19	C	305	PGV	C04-C05-C06-O06
19	C	305	PGV	O04-C19-O03-C01
19	C	305	PGV	C20-C19-O03-C01
19	C	305	PGV	C10-C11-C12-C13
19	D	201	PGV	C2-C1-O01-C02
19	N	609	PGV	C03-O11-P-O13
19	N	609	PGV	O04-C19-O03-C01
19	N	609	PGV	C20-C19-O03-C01
19	N	609	PGV	C10-C11-C12-C13
19	P	302	PGV	C04-O12-P-O13
19	P	302	PGV	C04-O12-P-O14
19	P	302	PGV	C01-C02-O01-C1
19	P	302	PGV	O04-C19-O03-C01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	P	302	PGV	C20-C19-O03-C01
19	P	303	PGV	C03-O11-P-O12
19	P	303	PGV	C04-O12-P-O13
19	P	303	PGV	C04-O12-P-O14
19	P	303	PGV	O12-C04-C05-C06
19	P	303	PGV	O04-C19-O03-C01
19	P	303	PGV	C20-C19-O03-C01
19	P	303	PGV	C12-C13-C14-C15
20	D	202	TGL	CB2-CB1-OG2-CG2
20	D	202	TGL	OB1-CB1-OG2-CG2
20	L	101	TGL	CB2-CB1-OG2-CG2
22	C	302	CDL	CA2-OA2-PA1-OA5
22	C	302	CDL	C11-CA5-OA6-CA4
22	C	302	CDL	OA9-CA7-OA8-CA6
22	C	302	CDL	C31-CA7-OA8-CA6
22	G	103	CDL	CA2-C1-CB2-OB2
22	G	103	CDL	CA2-OA2-PA1-OA4
22	G	103	CDL	OA9-CA7-OA8-CA6
22	G	103	CDL	C31-CA7-OA8-CA6
22	G	103	CDL	CB2-OB2-PB2-OB4
22	G	103	CDL	CB3-OB5-PB2-OB4
22	G	103	CDL	OB6-CB4-CB6-OB8
22	P	304	CDL	CA2-OA2-PA1-OA3
22	P	304	CDL	CA2-OA2-PA1-OA4
22	P	304	CDL	CA2-OA2-PA1-OA5
22	P	304	CDL	CA3-OA5-PA1-OA2
22	P	304	CDL	CA3-OA5-PA1-OA3
22	P	304	CDL	C11-CA5-OA6-CA4
22	P	304	CDL	OA9-CA7-OA8-CA6
22	P	304	CDL	C31-CA7-OA8-CA6
22	P	304	CDL	CB3-OB5-PB2-OB4
22	P	304	CDL	C51-CB5-OB6-CB4
22	T	103	CDL	CA3-OA5-PA1-OA4
22	T	103	CDL	OA9-CA7-OA8-CA6
22	T	103	CDL	C31-CA7-OA8-CA6
22	T	103	CDL	CB2-OB2-PB2-OB4
22	T	103	CDL	CB3-OB5-PB2-OB4
22	T	103	CDL	OB6-CB4-CB6-OB8
24	C	306	PEK	O04-C21-O03-C01
24	C	306	PEK	C22-C21-O03-C01
24	C	306	PEK	C5-C6-C7-C8
24	G	101	PEK	C03-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	G	101	PEK	C03-O11-P-O13
24	G	101	PEK	C03-O11-P-O14
24	G	101	PEK	O04-C21-O03-C01
24	G	101	PEK	C22-C21-O03-C01
24	P	301	PEK	O03-C01-C02-O01
24	P	301	PEK	O04-C21-O03-C01
24	P	301	PEK	C22-C21-O03-C01
24	P	307	PEK	O04-C21-O03-C01
24	P	307	PEK	C22-C21-O03-C01
24	T	102	PEK	C03-O11-P-O13
24	T	102	PEK	O04-C21-O03-C01
24	T	102	PEK	C22-C21-O03-C01
24	T	102	PEK	C13-C14-C15-C16
25	E	201	PSC	C03-O11-P-O13
25	E	201	PSC	C04-O12-P-O13
25	E	201	PSC	C04-O12-P-O14
25	E	201	PSC	C01-C02-O01-C1
25	E	201	PSC	O02-C1-O01-C02
25	E	201	PSC	C2-C1-O01-C02
25	O	602	PSC	O02-C1-O01-C02
25	O	602	PSC	C2-C1-O01-C02
27	J	101	DMU	C1-C6-O16-C18
27	J	101	DMU	O5-C6-O16-C18
27	J	101	DMU	C19-C18-O16-C6
27	W	101	DMU	C19-C18-O16-C6
24	G	102	PEK	O04-C21-O03-C01
24	G	102	PEK	C22-C21-O03-C01
25	E	201	PSC	C20-C19-O03-C01
19	A	607	PGV	O04-C19-O03-C01
19	D	201	PGV	O04-C19-O03-C01
19	N	607	PGV	O04-C19-O03-C01
25	E	201	PSC	O04-C19-O03-C01
19	D	201	PGV	O02-C1-O01-C02
20	L	101	TGL	OB1-CB1-OG2-CG2
22	C	302	CDL	OA7-CA5-OA6-CA4
22	P	304	CDL	OA7-CA5-OA6-CA4
19	N	607	PGV	C20-C19-O03-C01
14	A	602	HEA	C2D-C3D-CAD-CBD
19	A	607	PGV	C20-C19-O03-C01
19	D	201	PGV	C20-C19-O03-C01
19	A	607	PGV	C10-C11-C12-C13
19	C	301	PGV	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	D	201	PGV	C10-C11-C12-C13
19	P	303	PGV	C10-C11-C12-C13
24	G	101	PEK	C4-C5-C6-C7
24	G	101	PEK	C7-C8-C9-C10
24	P	307	PEK	C10-C11-C12-C13
24	P	307	PEK	C13-C14-C15-C16
24	T	102	PEK	C7-C8-C9-C10
24	T	102	PEK	C10-C11-C12-C13
14	A	602	HEA	C4D-C3D-CAD-CBD
22	P	304	CDL	OB7-CB5-OB6-CB4
24	C	306	PEK	O02-C1-O01-C02
23	C	303	CHD	C16-C17-C20-C21
19	P	302	PGV	O12-C04-C05-O05
19	P	303	PGV	O12-C04-C05-O05
22	G	103	CDL	O1-C1-CA2-OA2
22	G	103	CDL	O1-C1-CB2-OB2
22	T	103	CDL	O1-C1-CA2-OA2
22	P	304	CDL	C71-CB7-OB8-CB6
22	P	304	CDL	OB9-CB7-OB8-CB6
24	C	306	PEK	C2-C1-O01-C02
27	W	101	DMU	O6-C11-C9-O1
19	P	303	PGV	C28-C29-C30-C31
22	P	304	CDL	C20-C21-C22-C23
27	J	101	DMU	O6-C11-C9-C8
23	P	305	CHD	C17-C20-C22-C23
27	M	101	DMU	O6-C11-C9-O1
20	Y	101	TGL	C21-C22-C23-C24
20	L	101	TGL	OA1-CA1-OG1-CG1
14	A	601	HEA	C19-C20-C21-C22
14	N	601	HEA	C19-C20-C21-C22
20	L	101	TGL	CA2-CA1-OG1-CG1
23	C	303	CHD	C13-C17-C20-C22
19	P	302	PGV	O12-C04-C05-C06
22	C	302	CDL	CB2-C1-CA2-OA2
22	G	103	CDL	CB2-C1-CA2-OA2
23	P	306	CHD	C21-C20-C22-C23
22	T	103	CDL	C55-C56-C57-C58
25	O	602	PSC	C04-C05-N-C06
20	D	202	TGL	CC2-CC1-OG3-CG3
20	Q	201	TGL	CC2-CC1-OG3-CG3
22	T	103	CDL	C60-C61-C62-C63
20	L	101	TGL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	T	103	CDL	C40-C41-C42-C43
27	M	101	DMU	O6-C11-C9-C8
27	J	101	DMU	O6-C11-C9-O1
20	D	202	TGL	OC1-CC1-OG3-CG3
23	C	303	CHD	C13-C17-C20-C21
19	C	305	PGV	C2-C1-O01-C02
23	C	303	CHD	C16-C17-C20-C22
20	A	608	TGL	CC1-CC2-CC3-CC4
23	P	305	CHD	C21-C20-C22-C23
24	C	306	PEK	C7-C8-C9-C10
19	C	301	PGV	C19-C20-C21-C22
19	D	201	PGV	C1-C2-C3-C4
19	P	303	PGV	C19-C20-C21-C22
20	Q	201	TGL	CC1-CC2-CC3-CC4
14	N	602	HEA	C2D-C3D-CAD-CBD
27	J	101	DMU	O5-C4-C57-O61
20	Q	201	TGL	CB1-CB2-CB3-CB4
23	P	305	CHD	C20-C22-C23-C24
20	Q	201	TGL	OC1-CC1-OG3-CG3
14	A	601	HEA	C15-C16-C17-C18
14	N	601	HEA	C15-C16-C17-C18
27	Z	101	DMU	O16-C18-C19-C22
22	C	302	CDL	O1-C1-CA2-OA2
19	C	305	PGV	O02-C1-O01-C02
24	P	307	PEK	O02-C1-O01-C02
27	W	101	DMU	O16-C18-C19-C22
24	C	306	PEK	C4-C5-C6-C7
24	G	101	PEK	C13-C14-C15-C16
24	P	301	PEK	C4-C5-C6-C7
24	P	307	PEK	C7-C8-C9-C10
14	N	602	HEA	C4D-C3D-CAD-CBD
24	P	307	PEK	C2-C1-O01-C02
20	D	202	TGL	CB2-CB3-CB4-CB5
19	C	301	PGV	C04-O12-P-O11
19	P	302	PGV	C04-O12-P-O11
22	C	302	CDL	CA3-OA5-PA1-OA2
22	C	302	CDL	CB2-OB2-PB2-OB5
22	G	103	CDL	CA3-OA5-PA1-OA2
22	G	103	CDL	CB2-OB2-PB2-OB5
22	G	103	CDL	CB3-OB5-PB2-OB2
22	P	304	CDL	CB3-OB5-PB2-OB2
22	T	103	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	T	103	CDL	CB3-OB5-PB2-OB2
25	E	201	PSC	C04-O12-P-O11
25	O	602	PSC	C03-O11-P-O12
22	P	304	CDL	CA2-C1-CB2-OB2
25	O	602	PSC	C04-C05-N-C07
19	C	305	PGV	C13-C14-C15-C16
20	L	101	TGL	CB4-CB5-CB6-CB7
19	N	609	PGV	C2-C1-O01-C02
20	N	608	TGL	CB2-CB1-OG2-CG2
19	D	201	PGV	C27-C28-C29-C30
22	G	103	CDL	C57-C58-C59-C60
20	L	101	TGL	C10-C11-C12-C13
20	N	608	TGL	C11-C12-C13-C14
20	Q	201	TGL	CB2-CB3-CB4-CB5
19	N	609	PGV	O02-C1-O01-C02
20	N	608	TGL	OB1-CB1-OG2-CG2
20	A	608	TGL	CC7-CC8-CC9-C15
20	L	101	TGL	C21-C20-CA9-CA8
20	Y	101	TGL	CB3-CB4-CB5-CB6
24	P	301	PEK	C28-C29-C30-C31
19	P	302	PGV	C10-C11-C12-C13
24	C	306	PEK	C13-C14-C15-C16
24	G	102	PEK	C10-C11-C12-C13
24	P	301	PEK	C7-C8-C9-C10
20	A	608	TGL	CA5-CA6-CA7-CA8
20	D	202	TGL	CC7-CC8-CC9-C15
20	N	608	TGL	CA3-CA4-CA5-CA6
20	N	608	TGL	C22-C23-C24-C25
22	P	304	CDL	C60-C61-C62-C63
22	P	304	CDL	O1-C1-CB2-OB2
19	D	201	PGV	C7-C8-C9-C10
19	N	609	PGV	C29-C30-C31-C32
27	W	101	DMU	O6-C11-C9-C8
20	D	202	TGL	C10-C11-C12-C13
20	L	101	TGL	CB5-CB6-CB7-CB8
20	Q	201	TGL	C11-C10-CB9-CB8
20	D	202	TGL	C20-C21-C22-C23
22	C	302	CDL	C77-C78-C79-C80
22	G	103	CDL	C80-C81-C82-C83
19	C	301	PGV	C20-C21-C22-C23
20	D	202	TGL	CA3-CA4-CA5-CA6
20	Y	101	TGL	CA4-CA5-CA6-CA7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	P	304	CDL	C57-C58-C59-C60
24	C	306	PEK	C24-C25-C26-C27
24	G	101	PEK	C33-C34-C35-C36
20	L	101	TGL	CB6-CB7-CB8-CB9
20	N	608	TGL	C13-C14-C29-C30
19	D	201	PGV	C04-C05-C06-O06
19	D	201	PGV	C29-C30-C31-C32
22	T	103	CDL	C37-C38-C39-C40
19	P	302	PGV	C1-C2-C3-C4
19	P	303	PGV	C22-C23-C24-C25
22	P	304	CDL	C17-C18-C19-C20
27	Z	101	DMU	C31-C34-C37-C40
25	O	602	PSC	C04-C05-N-C08
20	D	202	TGL	CA7-CA8-CA9-C20
20	N	608	TGL	CC7-CC8-CC9-C15
22	C	302	CDL	C57-C58-C59-C60
25	E	201	PSC	C23-C24-C25-C26
19	D	201	PGV	C28-C29-C30-C31
20	Y	101	TGL	CA5-CA6-CA7-CA8
20	Y	101	TGL	C10-C11-C12-C13
25	O	602	PSC	C11-C10-C9-C8
20	A	608	TGL	CC3-CC4-CC5-CC6
20	N	608	TGL	CB5-CB6-CB7-CB8
25	O	602	PSC	C20-C19-O03-C01
22	P	304	CDL	C37-C38-C39-C40
19	C	301	PGV	C12-C13-C14-C15
19	N	609	PGV	C19-C20-C21-C22
20	A	608	TGL	C21-C22-C23-C24
19	D	201	PGV	C19-C20-C21-C22
19	P	302	PGV	O02-C1-O01-C02
20	D	202	TGL	C16-C15-CC9-CC8
20	L	101	TGL	CC9-C15-C16-C17
20	Y	101	TGL	C24-C25-C26-C27
20	Q	201	TGL	C19-C33-C34-C35
24	G	102	PEK	C24-C25-C26-C27
27	W	101	DMU	C25-C28-C31-C34
20	A	608	TGL	CB1-CB2-CB3-CB4
20	N	608	TGL	C12-C13-C14-C29
19	N	609	PGV	C20-C21-C22-C23
24	C	306	PEK	C10-C11-C12-C13
24	T	102	PEK	C4-C5-C6-C7
25	O	602	PSC	O04-C19-O03-C01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	D	201	PGV	C25-C26-C27-C28
19	C	301	PGV	C15-C16-C17-C18
19	N	609	PGV	C1-C2-C3-C4
20	N	608	TGL	CB1-CB2-CB3-CB4
20	L	101	TGL	C12-C13-C14-C29
20	Q	201	TGL	CA9-C20-C21-C22
20	L	101	TGL	CC6-CC7-CC8-CC9
24	G	101	PEK	C30-C31-C32-C33
24	G	102	PEK	C31-C32-C33-C34
20	D	202	TGL	C24-C25-C26-C27
22	T	103	CDL	C17-C18-C19-C20
24	G	102	PEK	C1-C2-C3-C4
19	P	302	PGV	C2-C1-O01-C02
20	A	608	TGL	CB2-CB1-OG2-CG2
20	Q	201	TGL	CB2-CB1-OG2-CG2
20	Y	101	TGL	CB2-CB1-OG2-CG2
22	T	103	CDL	C51-CB5-OB6-CB4
24	G	102	PEK	C2-C1-O01-C02
20	D	202	TGL	CA9-C20-C21-C22
19	P	302	PGV	C23-C24-C25-C26
25	E	201	PSC	C22-C23-C24-C25
20	Q	201	TGL	OB1-CB1-OG2-CG2
20	Y	101	TGL	OB1-CB1-OG2-CG2
22	T	103	CDL	OB7-CB5-OB6-CB4
24	G	102	PEK	O02-C1-O01-C02
20	Q	201	TGL	CC6-CC7-CC8-CC9
22	T	103	CDL	C54-C55-C56-C57
20	D	202	TGL	C12-C13-C14-C29
20	L	101	TGL	CA9-C20-C21-C22
20	A	608	TGL	OB1-CB1-OG2-CG2
22	G	103	CDL	OB7-CB5-OB6-CB4
22	G	103	CDL	C51-CB5-OB6-CB4
19	P	303	PGV	C04-O12-P-O11
22	C	302	CDL	CB3-OB5-PB2-OB2
24	T	102	PEK	C03-O11-P-O12
22	C	302	CDL	C72-C73-C74-C75
22	C	302	CDL	OA5-CA3-CA4-CA6
19	P	303	PGV	C24-C25-C26-C27
20	L	101	TGL	C20-C21-C22-C23
20	D	202	TGL	C11-C10-CB9-CB8
24	P	301	PEK	C31-C32-C33-C34
20	L	101	TGL	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	608	TGL	CC2-CC1-OG3-CG3
22	C	302	CDL	C18-C19-C20-C21
20	L	101	TGL	CC1-CC2-CC3-CC4
19	P	303	PGV	C30-C31-C32-C33
20	A	608	TGL	C20-C21-C22-C23
20	D	202	TGL	C19-C33-C34-C35
19	P	302	PGV	O03-C01-C02-C03
20	L	101	TGL	OG1-CG1-CG2-CG3
22	G	103	CDL	CB3-CB4-CB6-OB8
24	P	301	PEK	O03-C01-C02-C03
24	G	102	PEK	C7-C8-C9-C10
20	Y	101	TGL	C17-C18-C19-C33
20	L	101	TGL	C16-C17-C18-C19
19	D	201	PGV	C14-C15-C16-C17
22	C	302	CDL	C80-C81-C82-C83
22	C	302	CDL	C82-C83-C84-C85
20	Y	101	TGL	CC9-C15-C16-C17
22	G	103	CDL	C60-C61-C62-C63
22	P	304	CDL	C18-C19-C20-C21
19	C	305	PGV	O05-C05-C06-O06
19	N	607	PGV	C19-C20-C21-C22
24	P	301	PEK	O01-C1-C2-C3
20	Q	201	TGL	C25-C26-C27-C28
22	C	302	CDL	C55-C56-C57-C58
20	D	202	TGL	C11-C12-C13-C14
20	A	608	TGL	C25-C26-C27-C28
22	P	304	CDL	C19-C20-C21-C22
22	C	302	CDL	C60-C61-C62-C63
20	Q	201	TGL	CA2-CA1-OG1-CG1
25	E	201	PSC	C11-C10-C9-C8
20	Q	201	TGL	CC5-CC6-CC7-CC8
22	G	103	CDL	OA7-CA5-OA6-CA4
19	P	302	PGV	C3-C4-C5-C6
20	L	101	TGL	CC7-CC8-CC9-C15
22	T	103	CDL	C32-C33-C34-C35
19	D	201	PGV	C30-C31-C32-C33
22	T	103	CDL	C77-C78-C79-C80
20	Y	101	TGL	C18-C19-C33-C34
19	N	607	PGV	C10-C11-C12-C13
24	G	101	PEK	C10-C11-C12-C13
19	A	607	PGV	C19-C20-C21-C22
24	C	306	PEK	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	P	307	PEK	C01-C02-C03-O11
25	E	201	PSC	C01-C02-C03-O11
25	O	602	PSC	C01-C02-C03-O11
22	P	304	CDL	C77-C78-C79-C80
19	D	201	PGV	C24-C25-C26-C27
25	O	602	PSC	C19-C20-C21-C22
19	P	303	PGV	C02-C03-O11-P
22	G	103	CDL	C1-CB2-OB2-PB2
20	N	608	TGL	CA7-CA8-CA9-C20
20	Q	201	TGL	C23-C24-C25-C26
20	Y	101	TGL	C22-C23-C24-C25
24	T	102	PEK	C16-C17-C18-C19
20	Y	101	TGL	OG1-CG1-CG2-CG3
22	T	103	CDL	CA3-CA4-CA6-OA8
24	P	301	PEK	C10-C11-C12-C13
22	G	103	CDL	C12-C13-C14-C15
20	D	202	TGL	CC9-C15-C16-C17
22	G	103	CDL	C41-C42-C43-C44
20	Y	101	TGL	CA2-CA3-CA4-CA5
22	C	302	CDL	C56-C57-C58-C59
20	Q	201	TGL	OA1-CA1-OG1-CG1
24	C	306	PEK	C6-C7-C8-C9
24	C	306	PEK	C11-C10-C9-C8
24	C	306	PEK	C9-C10-C11-C12
24	C	306	PEK	C11-C12-C13-C14
24	C	306	PEK	C12-C13-C14-C15
24	G	101	PEK	C5-C6-C7-C8
24	G	101	PEK	C11-C10-C9-C8
24	G	101	PEK	C9-C10-C11-C12
24	G	101	PEK	C11-C12-C13-C14
24	G	101	PEK	C12-C13-C14-C15
24	G	102	PEK	C6-C7-C8-C9
24	G	102	PEK	C11-C10-C9-C8
24	P	301	PEK	C5-C6-C7-C8
24	P	301	PEK	C6-C7-C8-C9
24	P	301	PEK	C11-C10-C9-C8
24	P	301	PEK	C9-C10-C11-C12
24	P	301	PEK	C11-C12-C13-C14
24	P	301	PEK	C12-C13-C14-C15
24	P	307	PEK	C6-C7-C8-C9
24	P	307	PEK	C11-C10-C9-C8
24	P	307	PEK	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	P	307	PEK	C11-C12-C13-C14
24	P	307	PEK	C12-C13-C14-C15
24	T	102	PEK	C9-C10-C11-C12
25	E	201	PSC	C9-C10-C11-C12
25	O	602	PSC	C9-C10-C11-C12
25	O	602	PSC	C10-C11-C12-C13
19	D	201	PGV	C31-C32-C33-C34
19	D	201	PGV	O05-C05-C06-O06
20	A	608	TGL	C19-C33-C34-C35
22	C	302	CDL	OA5-CA3-CA4-OA6
20	A	608	TGL	OC1-CC1-OG3-CG3
19	C	301	PGV	C30-C31-C32-C33
19	N	609	PGV	C2-C3-C4-C5
24	G	101	PEK	C32-C33-C34-C35
22	G	103	CDL	C19-C20-C21-C22
20	Q	201	TGL	CA6-CA7-CA8-CA9
19	N	609	PGV	O12-C04-C05-C06
22	T	103	CDL	CB2-C1-CA2-OA2
20	Y	101	TGL	C16-C15-CC9-CC8
22	C	302	CDL	C38-C39-C40-C41
19	D	201	PGV	C05-C04-O12-P
22	T	103	CDL	CB4-CB3-OB5-PB2
20	D	202	TGL	C17-C18-C19-C33
19	D	201	PGV	C6-C7-C8-C9
20	Y	101	TGL	CA9-C20-C21-C22
22	G	103	CDL	C11-CA5-OA6-CA4
19	C	301	PGV	C22-C23-C24-C25
19	C	305	PGV	C2-C3-C4-C5
22	T	103	CDL	C74-C75-C76-C77
19	D	201	PGV	C15-C16-C17-C18
19	N	609	PGV	O12-C04-C05-O05
20	N	608	TGL	CA2-CA1-OG1-CG1
20	A	608	TGL	CA9-C20-C21-C22
22	P	304	CDL	C41-C42-C43-C44
19	A	607	PGV	C30-C31-C32-C33
20	D	202	TGL	CA2-CA3-CA4-CA5
20	D	202	TGL	CB6-CB7-CB8-CB9
20	N	608	TGL	CC2-CC1-OG3-CG3
20	A	608	TGL	CA7-CA8-CA9-C20
20	Y	101	TGL	CB7-CB8-CB9-C10
20	Y	101	TGL	CG1-CG2-OG2-CB1
19	C	301	PGV	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	N	608	TGL	C21-C22-C23-C24
22	P	304	CDL	C1-CA2-OA2-PA1
22	T	103	CDL	CB3-CB4-CB6-OB8
24	P	307	PEK	O03-C01-C02-C03
20	N	608	TGL	OA1-CA1-OG1-CG1
19	D	201	PGV	O01-C02-C03-O11
25	E	201	PSC	O01-C02-C03-O11
20	Y	101	TGL	CC2-CC1-OG3-CG3
22	G	103	CDL	C61-C62-C63-C64
22	G	103	CDL	C71-C72-C73-C74
19	A	607	PGV	O03-C01-C02-O01
19	N	607	PGV	O03-C01-C02-O01
20	D	202	TGL	OG2-CG2-CG3-OG3
20	N	608	TGL	OG1-CG1-CG2-OG2
22	P	304	CDL	C14-C15-C16-C17
20	Q	201	TGL	CB3-CB4-CB5-CB6
22	P	304	CDL	C33-C34-C35-C36
22	P	304	CDL	C21-C22-C23-C24
19	D	201	PGV	C23-C24-C25-C26
22	T	103	CDL	C56-C57-C58-C59
19	N	609	PGV	C03-O11-P-O12
25	O	602	PSC	C04-O12-P-O11
27	J	101	DMU	C34-C37-C40-C43
19	C	301	PGV	C13-C14-C15-C16
19	C	301	PGV	C04-O12-P-O14
19	P	303	PGV	C03-O11-P-O13
22	C	302	CDL	CA2-OA2-PA1-OA3
22	C	302	CDL	CA3-OA5-PA1-OA3
22	C	302	CDL	CB2-OB2-PB2-OB3
22	C	302	CDL	CB3-OB5-PB2-OB3
22	G	103	CDL	CA3-OA5-PA1-OA3
22	P	304	CDL	CA3-OA5-PA1-OA4
25	O	602	PSC	C03-O11-P-O13
25	O	602	PSC	C03-O11-P-O14
24	C	306	PEK	C01-C02-C03-O11
20	Y	101	TGL	CC6-CC7-CC8-CC9
14	A	601	HEA	O11-C11-C12-C13
14	N	601	HEA	O11-C11-C12-C13
20	A	608	TGL	C18-C19-C33-C34
20	Y	101	TGL	C20-C21-C22-C23
19	C	305	PGV	C19-C20-C21-C22
20	N	608	TGL	CC3-CC4-CC5-CC6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	P	304	CDL	OA5-CA3-CA4-OA6
24	P	307	PEK	O01-C02-C03-O11
25	O	602	PSC	O01-C02-C03-O11
22	P	304	CDL	C76-C77-C78-C79
20	Y	101	TGL	C16-C17-C18-C19
20	N	608	TGL	OC1-CC1-OG3-CG3
20	A	608	TGL	CC5-CC6-CC7-CC8
20	D	202	TGL	CG1-CG2-CG3-OG3
20	Y	101	TGL	CG1-CG2-CG3-OG3
25	O	602	PSC	O12-C04-C05-N
19	D	201	PGV	O03-C01-C02-O01
19	P	302	PGV	O03-C01-C02-O01
20	L	101	TGL	OG1-CG1-CG2-OG2
20	L	101	TGL	OG2-CG2-CG3-OG3
20	Y	101	TGL	OG2-CG2-CG3-OG3
24	P	307	PEK	O03-C01-C02-O01
19	P	302	PGV	C02-C03-O11-P
19	A	607	PGV	C27-C28-C29-C30
25	O	602	PSC	C29-C30-C31-C32
19	N	609	PGV	C22-C23-C24-C25
20	Y	101	TGL	CC5-CC6-CC7-CC8
22	T	103	CDL	C82-C83-C84-C85
20	L	101	TGL	OG2-CB1-CB2-CB3
27	M	101	DMU	C19-C22-C25-C28
24	G	102	PEK	C03-C02-O01-C1
22	C	302	CDL	OB7-CB5-OB6-CB4
22	C	302	CDL	C51-CB5-OB6-CB4
20	Y	101	TGL	OC1-CC1-OG3-CG3
19	C	301	PGV	C05-C04-O12-P
19	C	301	PGV	C1-C2-C3-C4
22	P	304	CDL	C39-C40-C41-C42
22	C	302	CDL	C21-C22-C23-C24
24	G	102	PEK	C22-C23-C24-C25
19	C	305	PGV	C04-O12-P-O11
19	D	201	PGV	C04-O12-P-O11
22	T	103	CDL	CA2-OA2-PA1-OA5
20	N	608	TGL	CC5-CC6-CC7-CC8
22	C	302	CDL	C83-C84-C85-C86
19	A	607	PGV	O03-C01-C02-C03
19	C	305	PGV	O03-C01-C02-C03
20	N	608	TGL	OG1-CG1-CG2-CG3
19	N	607	PGV	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	C	301	PGV	C14-C15-C16-C17
20	A	608	TGL	CB4-CB5-CB6-CB7
20	Y	101	TGL	C14-C29-C30-C31
22	C	302	CDL	C22-C23-C24-C25
22	G	103	CDL	C75-C76-C77-C78
14	N	601	HEA	CAD-CBD-CGD-O1D
27	M	101	DMU	C22-C25-C28-C31
20	Q	201	TGL	C15-C16-C17-C18
24	P	301	PEK	C32-C33-C34-C35
20	N	608	TGL	CA1-CA2-CA3-CA4
20	N	608	TGL	C20-C21-C22-C23
20	Y	101	TGL	CC2-CC3-CC4-CC5
27	J	101	DMU	C28-C31-C34-C37
24	G	102	PEK	C4-C5-C6-C7
14	A	602	HEA	CAA-CBA-CGA-O1A
19	C	301	PGV	C02-C03-O11-P
24	P	301	PEK	O02-C1-C2-C3
23	G	104	CHD	C22-C23-C24-O26
23	T	101	CHD	C22-C23-C24-O26
24	T	102	PEK	C2-C3-C4-C5
25	E	201	PSC	C29-C30-C31-C32
27	W	101	DMU	C18-C19-C22-C25
19	D	201	PGV	C2-C3-C4-C5
20	D	202	TGL	C15-C16-C17-C18
19	N	607	PGV	O03-C01-C02-C03
25	O	602	PSC	O03-C01-C02-C03
24	P	301	PEK	C34-C35-C36-C37
27	M	101	DMU	C28-C31-C34-C37
20	N	608	TGL	CB4-CB5-CB6-CB7
22	T	103	CDL	C76-C77-C78-C79
20	A	608	TGL	CC2-CC3-CC4-CC5
22	G	103	CDL	C56-C57-C58-C59
23	G	104	CHD	C22-C23-C24-O25
22	T	103	CDL	CA6-CA4-OA6-CA5
24	G	102	PEK	C01-C02-O01-C1
25	O	602	PSC	C12-C13-C14-C15
23	P	306	CHD	C22-C23-C24-O25
19	P	303	PGV	C23-C24-C25-C26
20	N	608	TGL	CA9-C20-C21-C22
24	G	101	PEK	C6-C7-C8-C9
24	G	102	PEK	C9-C10-C11-C12
14	N	601	HEA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	G	102	PEK	C16-C17-C18-C19
24	G	102	PEK	C13-C14-C15-C16
22	G	103	CDL	C20-C21-C22-C23
19	D	201	PGV	C01-C02-C03-O11
23	T	101	CHD	C22-C23-C24-O25
24	P	307	PEK	C28-C29-C30-C31
14	A	602	HEA	CAA-CBA-CGA-O2A
20	N	608	TGL	C23-C24-C25-C26
20	D	202	TGL	CB3-CB4-CB5-CB6
23	P	306	CHD	C22-C23-C24-O26
20	A	608	TGL	OG1-CG1-CG2-OG2
23	C	303	CHD	C22-C23-C24-O26
20	A	608	TGL	CC4-CC5-CC6-CC7
20	L	101	TGL	C14-C29-C30-C31
22	C	302	CDL	C42-C43-C44-C45
20	D	202	TGL	CB7-CB8-CB9-C10
14	N	602	HEA	CAA-CBA-CGA-O1A
23	P	305	CHD	C22-C23-C24-O25
22	P	304	CDL	C52-C51-CB5-OB6
27	M	101	DMU	O16-C18-C19-C22
20	L	101	TGL	OG1-CA1-CA2-CA3
25	E	201	PSC	C12-C13-C14-C15
25	O	602	PSC	O03-C19-C20-C21
14	N	602	HEA	CAD-CBD-CGD-O2D
19	C	305	PGV	O01-C1-C2-C3
19	D	201	PGV	C4-C5-C6-C7
19	A	607	PGV	C26-C27-C28-C29
22	C	302	CDL	C36-C37-C38-C39
22	C	302	CDL	C39-C40-C41-C42
22	C	302	CDL	C16-C17-C18-C19
20	Y	101	TGL	OG1-CG1-CG2-OG2
22	C	302	CDL	OA6-CA4-CA6-OA8
20	Y	101	TGL	C11-C12-C13-C14
19	N	609	PGV	C24-C25-C26-C27
27	W	101	DMU	C22-C25-C28-C31
24	P	307	PEK	C14-C15-C16-C17
19	P	303	PGV	C7-C8-C9-C10
27	Z	101	DMU	C22-C25-C28-C31
19	A	607	PGV	C9-C10-C11-C12
19	C	305	PGV	C9-C10-C11-C12
19	P	303	PGV	C9-C10-C11-C12
14	A	602	HEA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	C	301	PGV	C7-C8-C9-C10
22	G	103	CDL	C43-C44-C45-C46
22	G	103	CDL	C39-C40-C41-C42
22	C	302	CDL	C20-C21-C22-C23
14	A	601	HEA	CAD-CBD-CGD-O1D
19	N	609	PGV	O01-C1-C2-C3
19	C	301	PGV	C9-C10-C11-C12
19	N	609	PGV	C11-C12-C13-C14
19	P	302	PGV	C9-C10-C11-C12
24	C	306	PEK	C14-C15-C16-C17
24	P	301	PEK	C14-C15-C16-C17
25	E	201	PSC	C7-C8-C9-C10
22	P	304	CDL	C59-C60-C61-C62
24	P	307	PEK	C4-C5-C6-C7
20	Y	101	TGL	C12-C13-C14-C29
22	P	304	CDL	C11-C12-C13-C14
23	P	305	CHD	C22-C23-C24-O26
20	A	608	TGL	C22-C23-C24-C25
14	N	601	HEA	CAA-CBA-CGA-O1A
14	N	602	HEA	CAD-CBD-CGD-O1D
19	A	607	PGV	C11-C12-C13-C14
25	O	602	PSC	C7-C8-C9-C10
24	P	301	PEK	C29-C30-C31-C32
27	Z	101	DMU	C34-C37-C40-C43
14	A	601	HEA	CAD-CBD-CGD-O2D
14	A	602	HEA	CAD-CBD-CGD-O1D
24	P	301	PEK	C2-C3-C4-C5
20	A	608	TGL	C13-C14-C29-C30
22	P	304	CDL	OA5-CA3-CA4-CA6
24	G	102	PEK	C01-C02-C03-O11
23	C	304	CHD	C22-C23-C24-O25
25	O	602	PSC	O03-C01-C02-O01
20	Q	201	TGL	CC7-CC8-CC9-C15
14	A	601	HEA	CAA-CBA-CGA-O1A
19	C	301	PGV	C31-C32-C33-C34
20	D	202	TGL	CC2-CC3-CC4-CC5
25	O	602	PSC	C26-C27-C28-C29
14	N	602	HEA	CAA-CBA-CGA-O2A
19	P	303	PGV	C1-C2-C3-C4
24	G	101	PEK	C1-C2-C3-C4
20	A	608	TGL	OG1-CA1-CA2-CA3
22	P	304	CDL	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	N	609	PGV	O02-C1-C2-C3
19	N	609	PGV	O03-C19-C20-C21
22	C	302	CDL	C41-C42-C43-C44
24	P	301	PEK	C3-C4-C5-C6
20	Q	201	TGL	CA2-CA3-CA4-CA5
19	D	201	PGV	O03-C01-C02-C03
20	L	101	TGL	CG1-CG2-CG3-OG3
22	C	302	CDL	CA3-CA4-CA6-OA8
20	N	608	TGL	OG3-CC1-CC2-CC3
19	C	301	PGV	C03-O11-P-O12
25	E	201	PSC	C03-O11-P-O12
20	Y	101	TGL	CB6-CB7-CB8-CB9
22	T	103	CDL	C32-C31-CA7-OA8
22	T	103	CDL	OA7-CA5-OA6-CA4
19	P	303	PGV	C05-C04-O12-P
19	N	609	PGV	C25-C26-C27-C28
19	N	609	PGV	C9-C10-C11-C12
24	P	307	PEK	C3-C4-C5-C6
22	G	103	CDL	CA2-OA2-PA1-OA3
24	T	102	PEK	C03-O11-P-O14
25	E	201	PSC	C03-O11-P-O14
24	P	301	PEK	O03-C21-C22-C23
14	N	601	HEA	CAA-CBA-CGA-O2A
20	L	101	TGL	CA5-CA6-CA7-CA8
24	G	102	PEK	O12-C04-C05-N
24	P	301	PEK	O12-C04-C05-N
24	T	102	PEK	O12-C04-C05-N
14	A	602	HEA	C26-C15-C16-C17
22	T	103	CDL	C32-C31-CA7-OA9
24	P	301	PEK	O04-C21-C22-C23
14	A	601	HEA	CAA-CBA-CGA-O2A
24	G	101	PEK	C3-C4-C5-C6
19	P	302	PGV	O01-C1-C2-C3
24	G	101	PEK	O01-C1-C2-C3
20	A	608	TGL	CB5-CB6-CB7-CB8
22	T	103	CDL	C57-C58-C59-C60
24	C	306	PEK	C33-C34-C35-C36
20	Y	101	TGL	CA7-CA8-CA9-C20
20	Y	101	TGL	C19-C33-C34-C35
22	G	103	CDL	CB7-C71-C72-C73
20	N	608	TGL	OC1-CC1-CC2-CC3
20	L	101	TGL	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	C	301	PGV	C27-C28-C29-C30
22	C	302	CDL	C32-C31-CA7-OA8
20	A	608	TGL	OA1-CA1-CA2-CA3
27	W	101	DMU	C19-C22-C25-C28
19	N	609	PGV	O04-C19-C20-C21

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	P	305	CHD	C1-C10-C2-C3-C4-C5

33 monomers are involved in 218 short contacts:

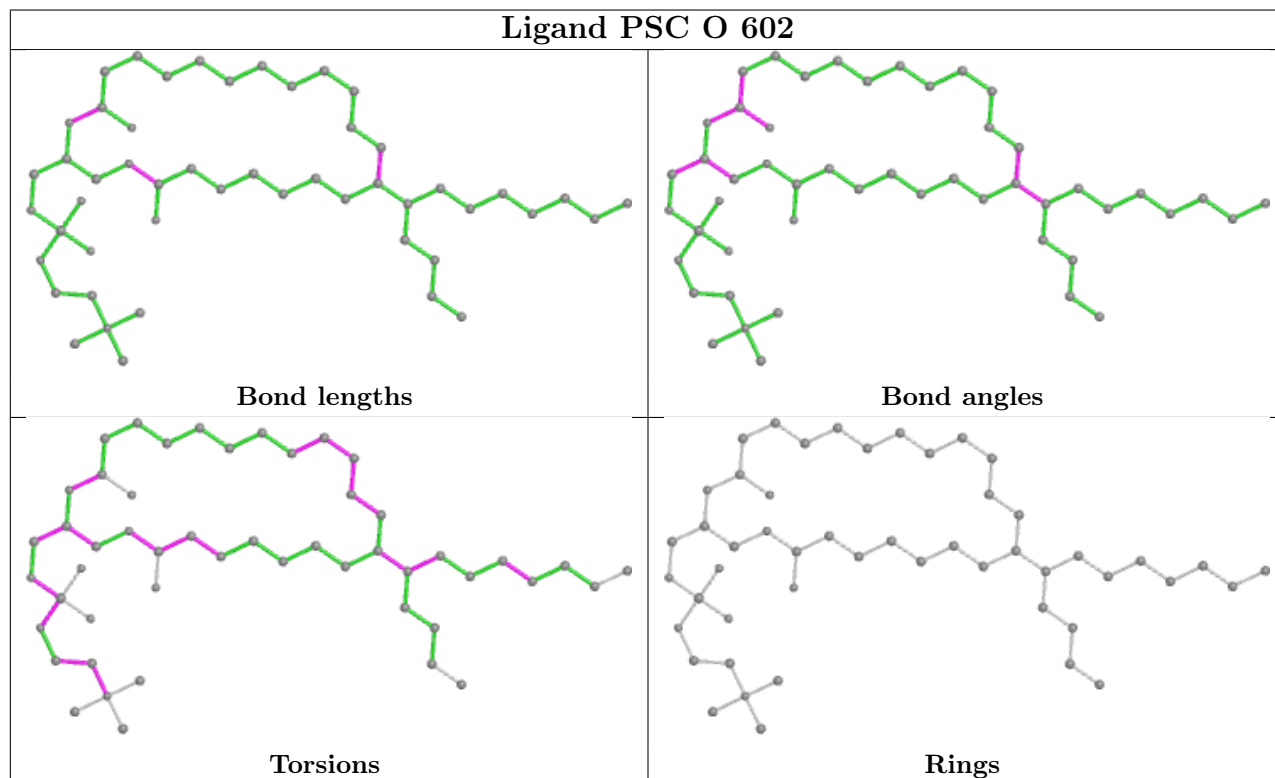
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	O	602	PSC	10	0
24	P	301	PEK	6	0
22	C	302	CDL	14	0
22	P	304	CDL	12	0
24	C	306	PEK	6	0
22	G	103	CDL	14	0
14	A	601	HEA	8	0
22	T	103	CDL	20	0
24	G	101	PEK	4	0
19	N	607	PGV	5	0
14	N	601	HEA	7	0
25	E	201	PSC	10	0
24	T	102	PEK	7	0
14	A	602	HEA	6	0
19	D	201	PGV	11	0
19	N	609	PGV	8	0
20	Y	101	TGL	8	0
19	P	302	PGV	2	0
24	P	307	PEK	4	0
20	A	608	TGL	2	0
24	G	102	PEK	8	0
19	A	607	PGV	6	0
19	P	303	PGV	2	0
20	D	202	TGL	9	0
27	W	101	DMU	3	0
20	L	101	TGL	7	0
19	C	301	PGV	3	0
20	N	608	TGL	4	0

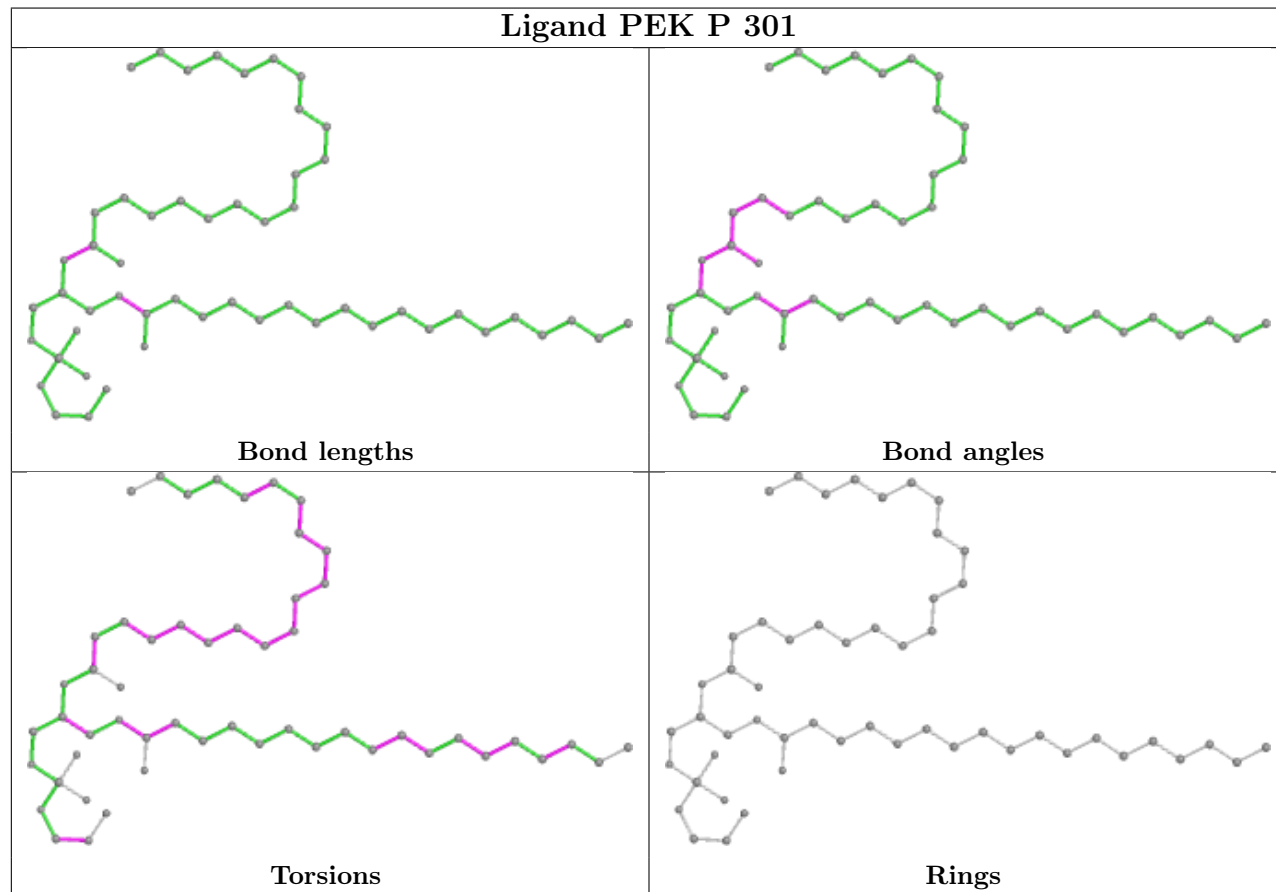
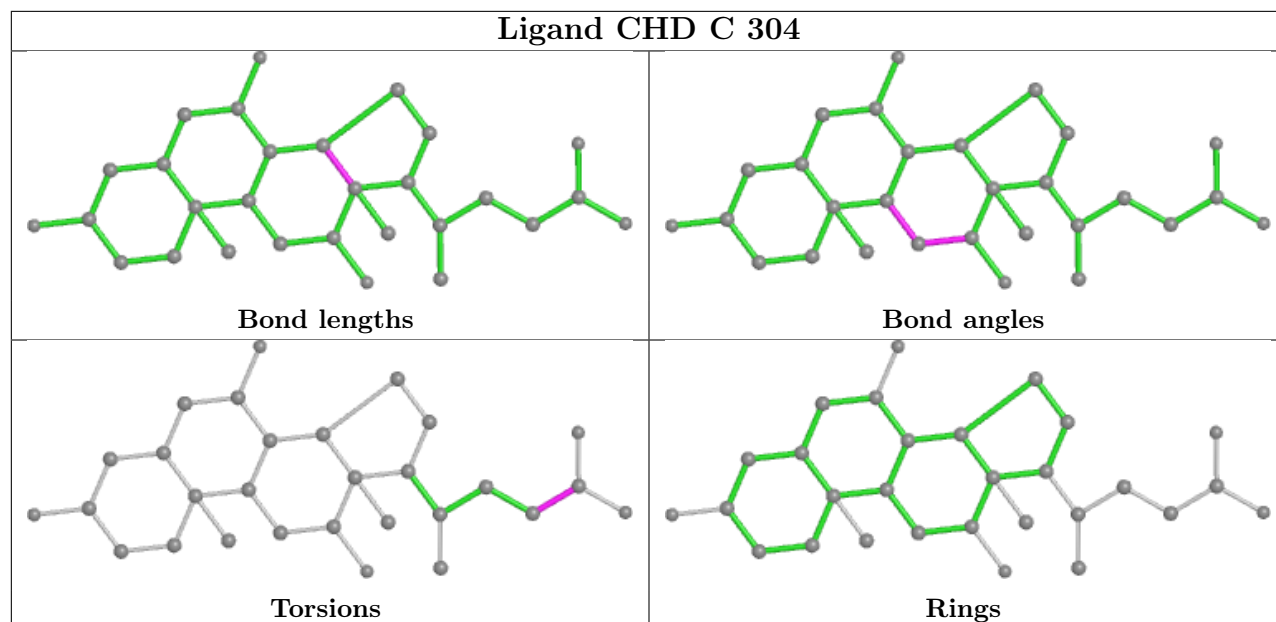
Continued on next page...

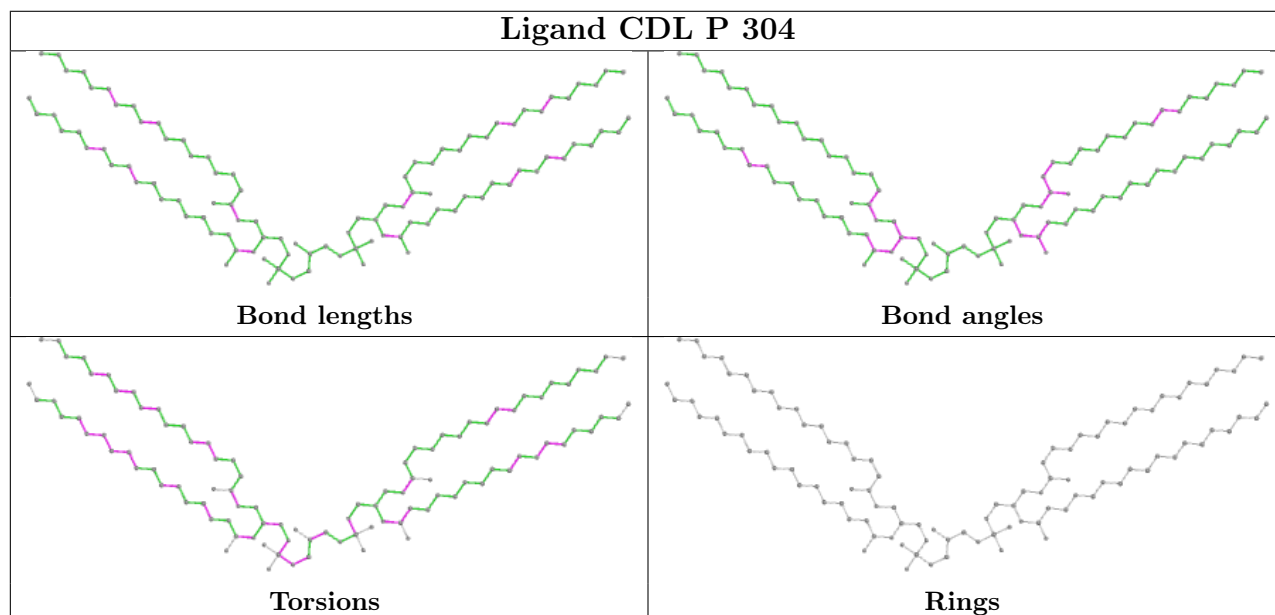
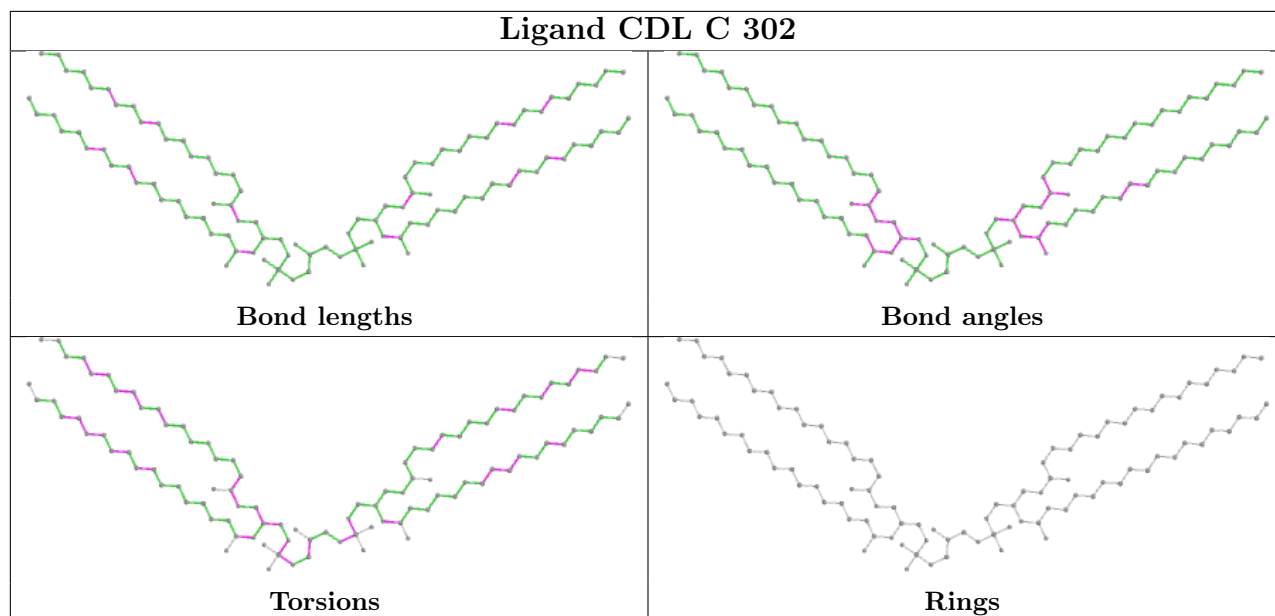
Continued from previous page...

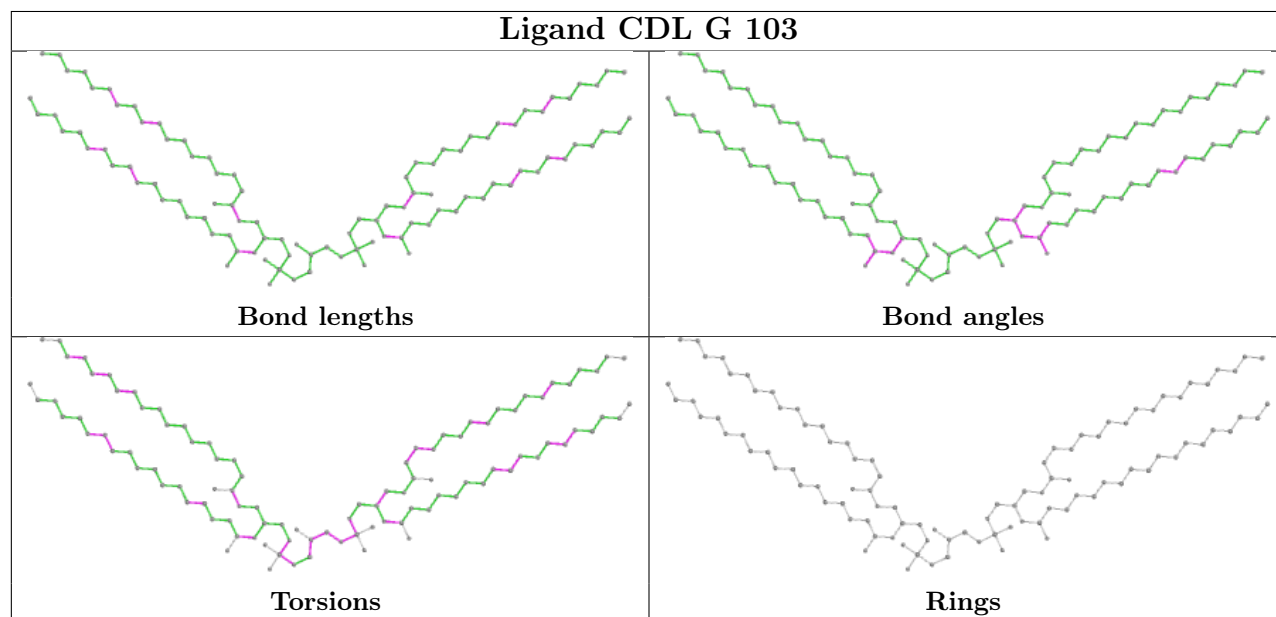
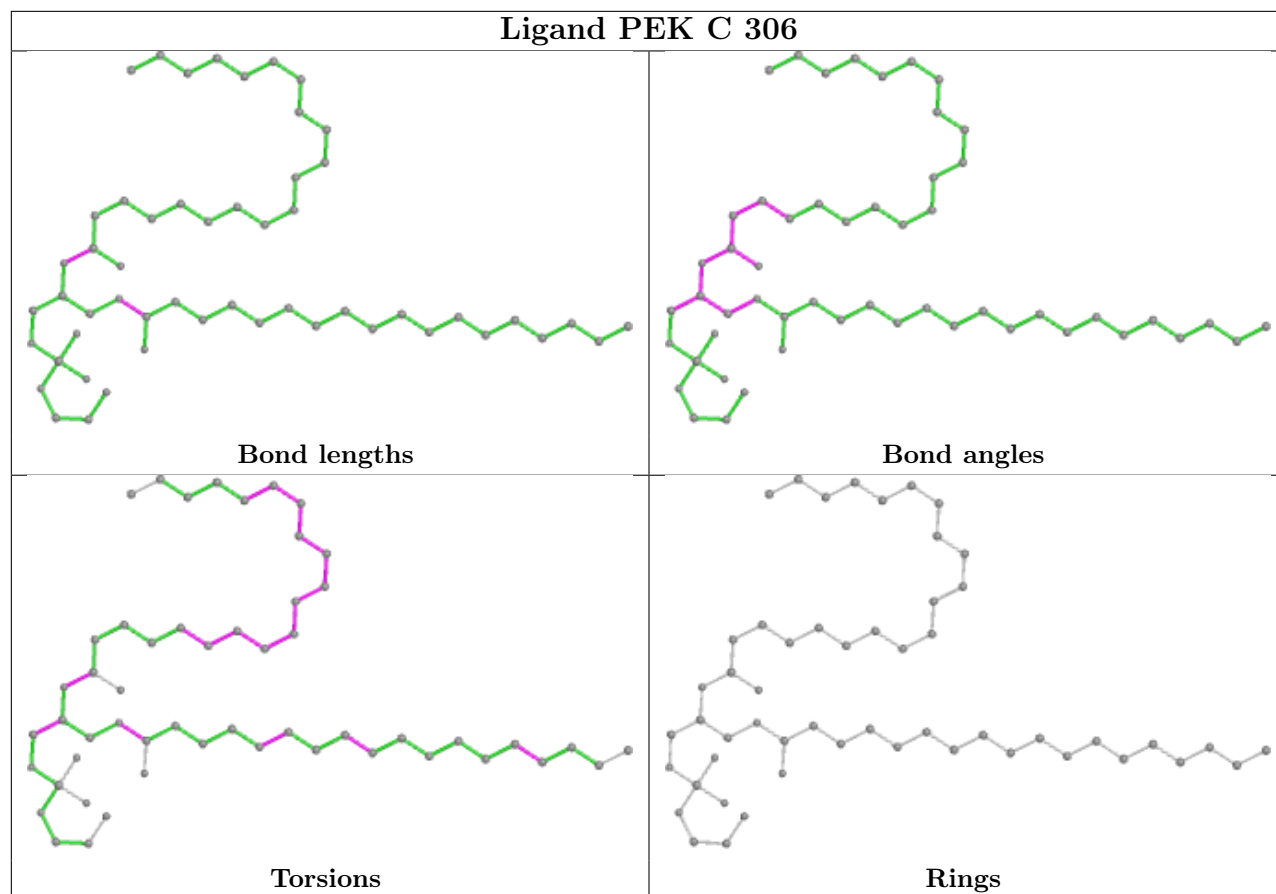
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	602	HEA	4	0
23	G	104	CHD	1	0
27	J	101	DMU	4	0
20	Q	201	TGL	5	0
19	C	305	PGV	1	0

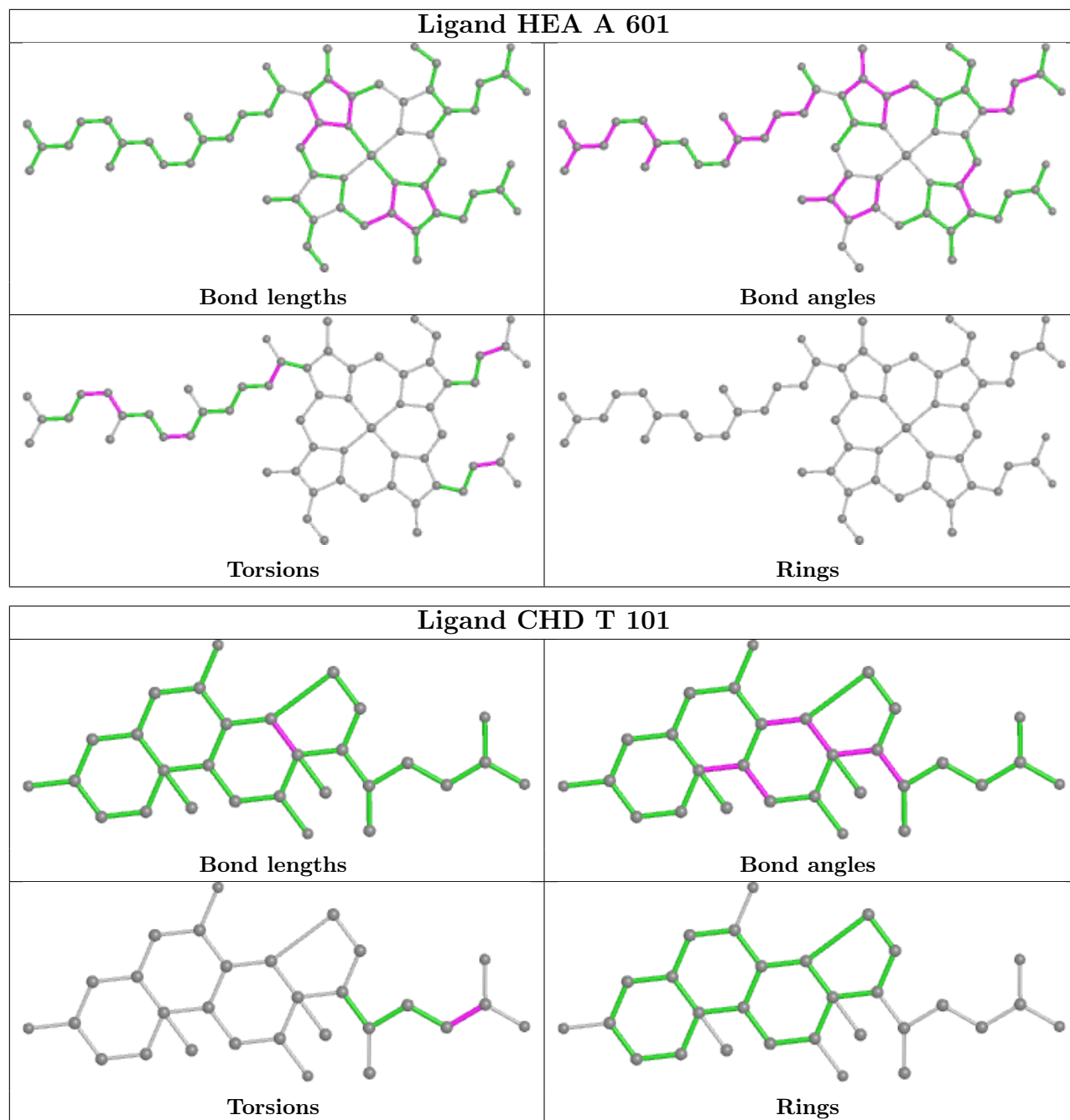
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

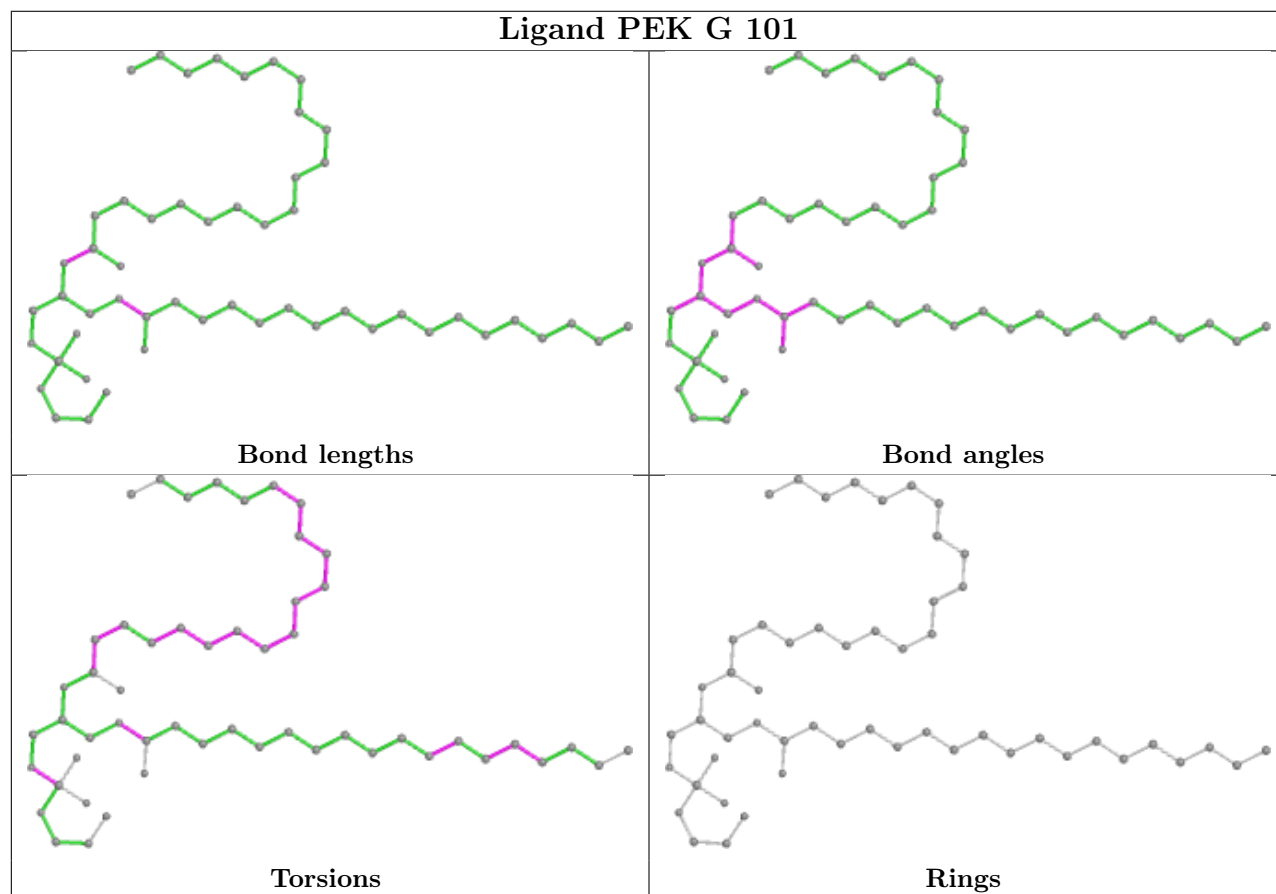
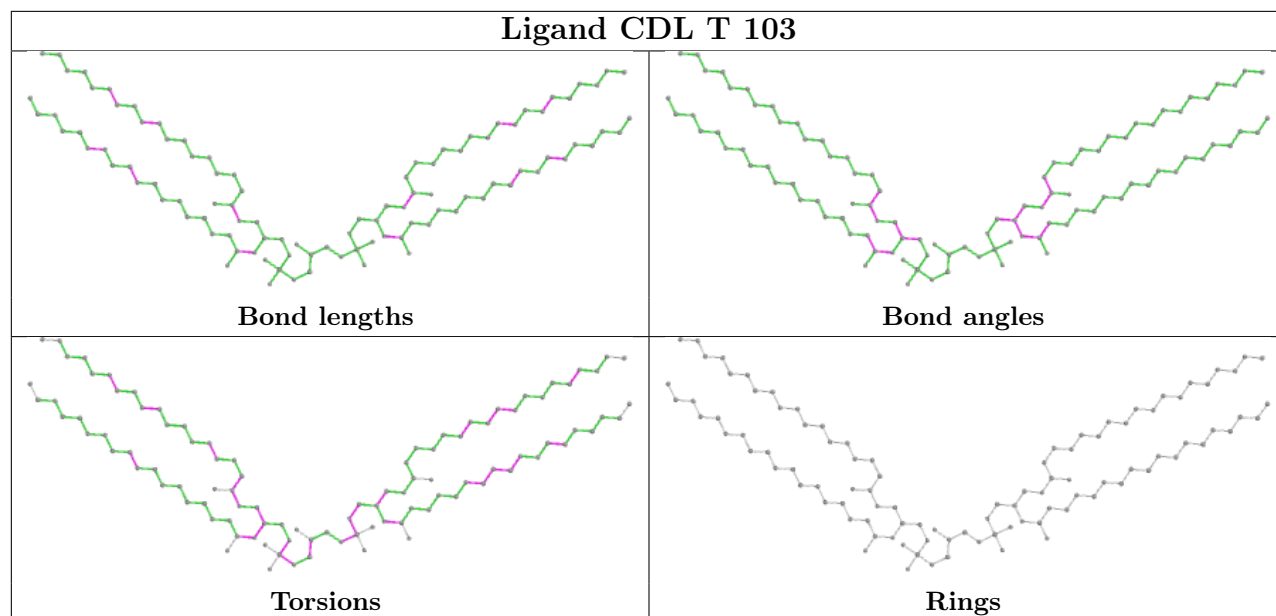


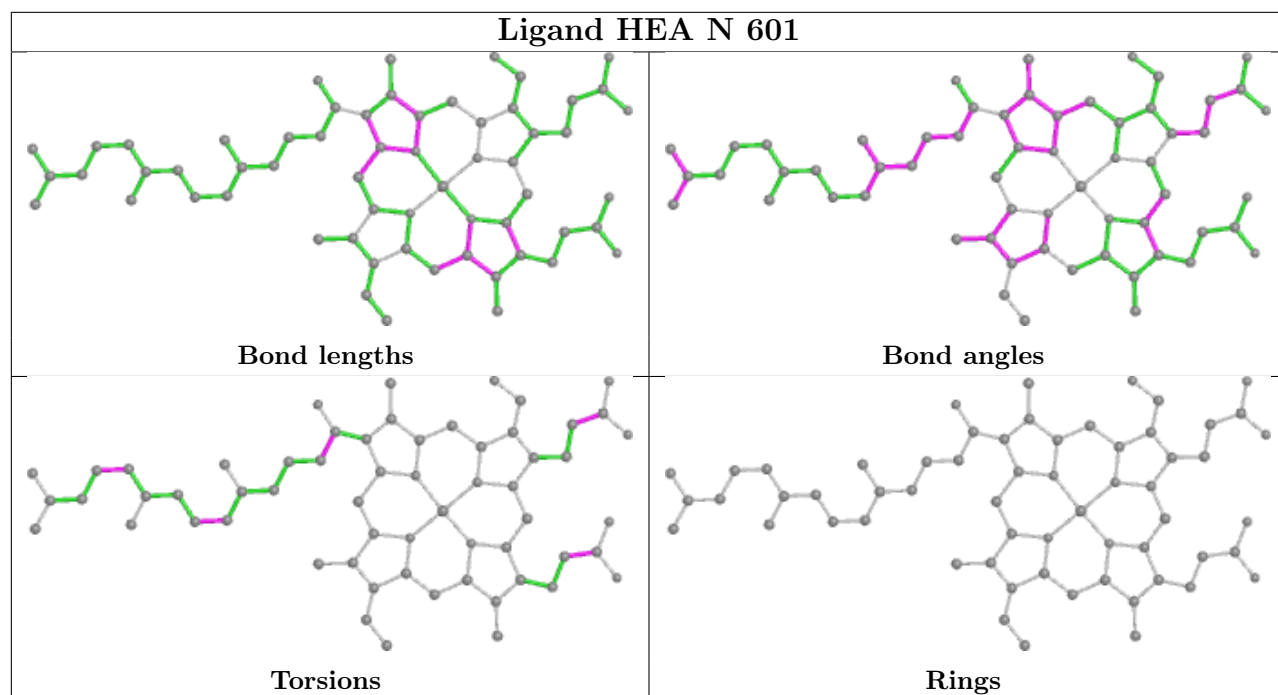
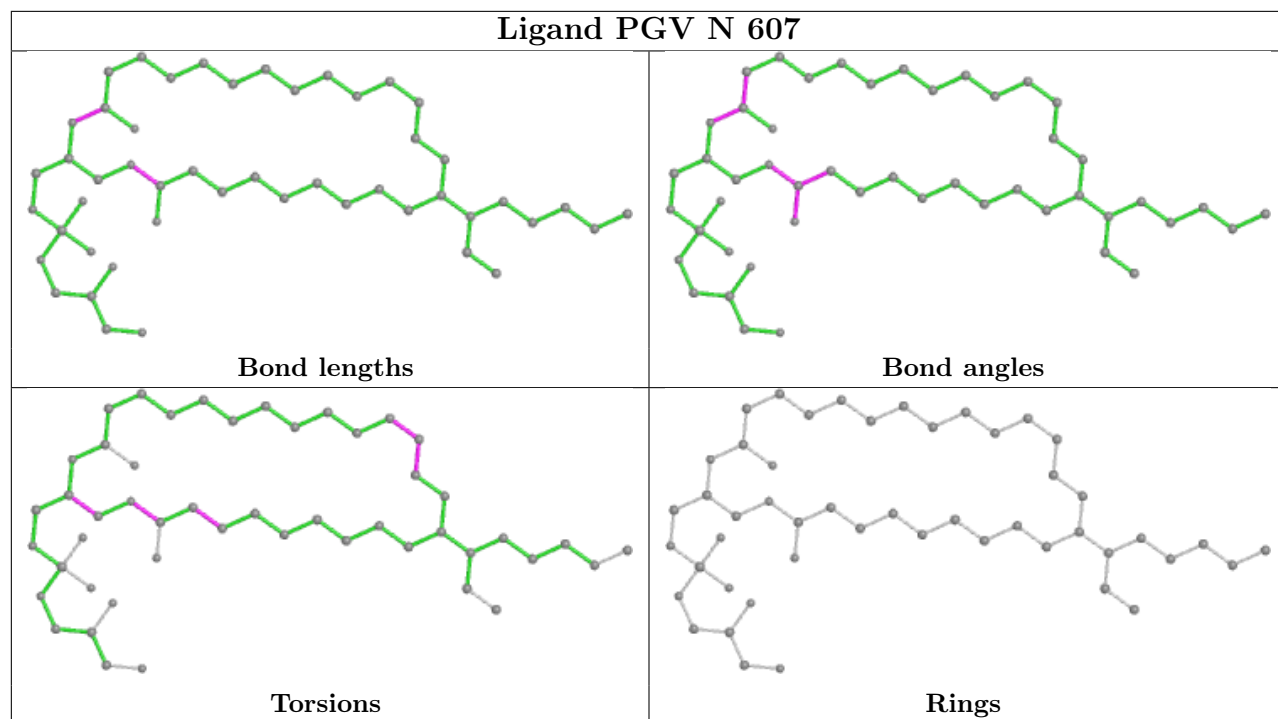


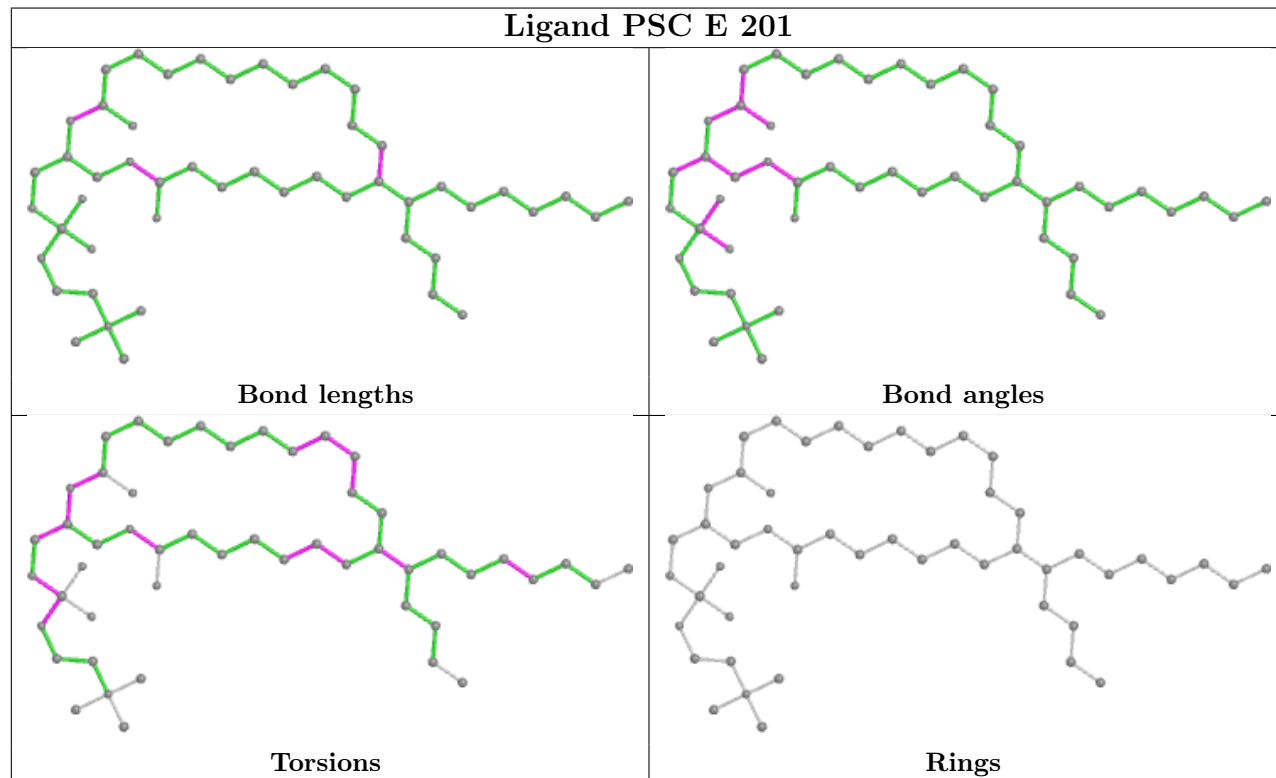
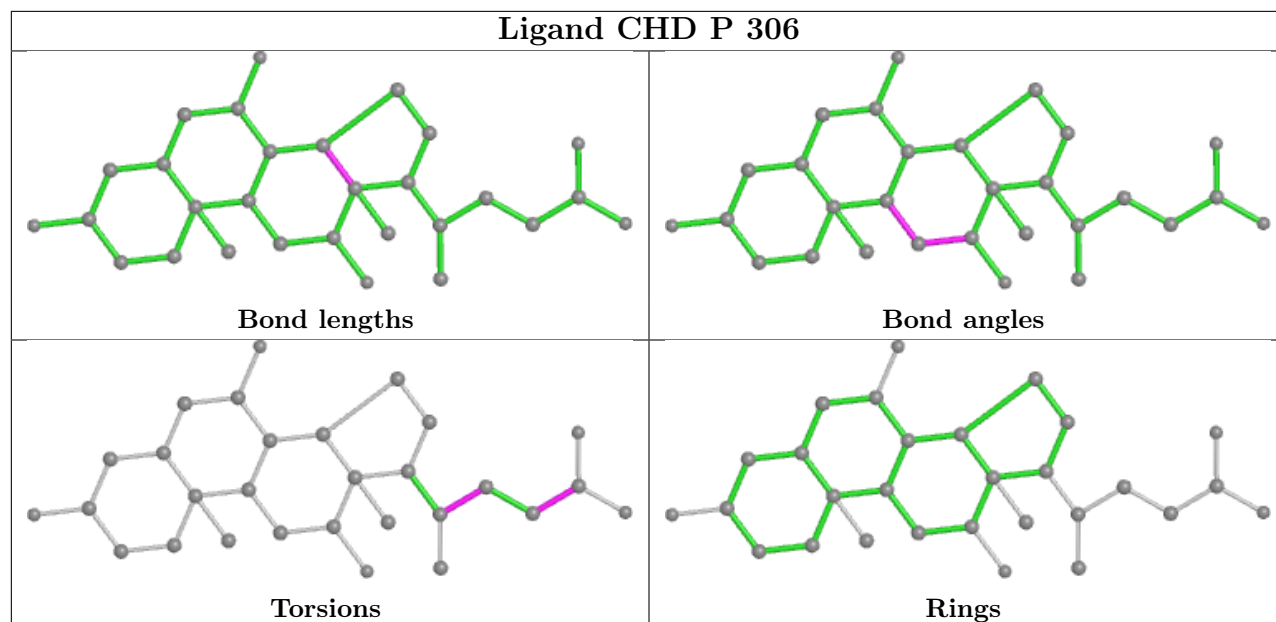


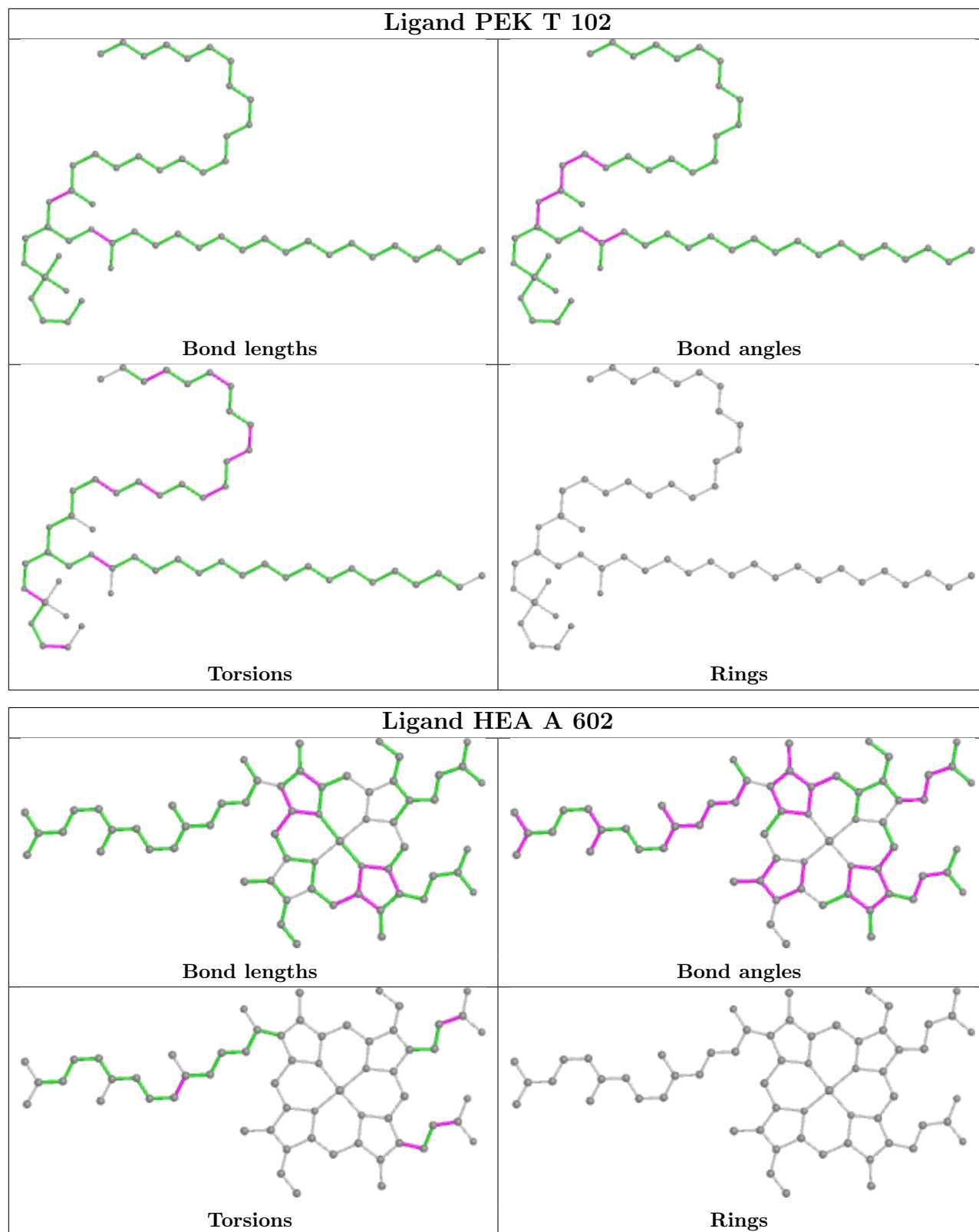


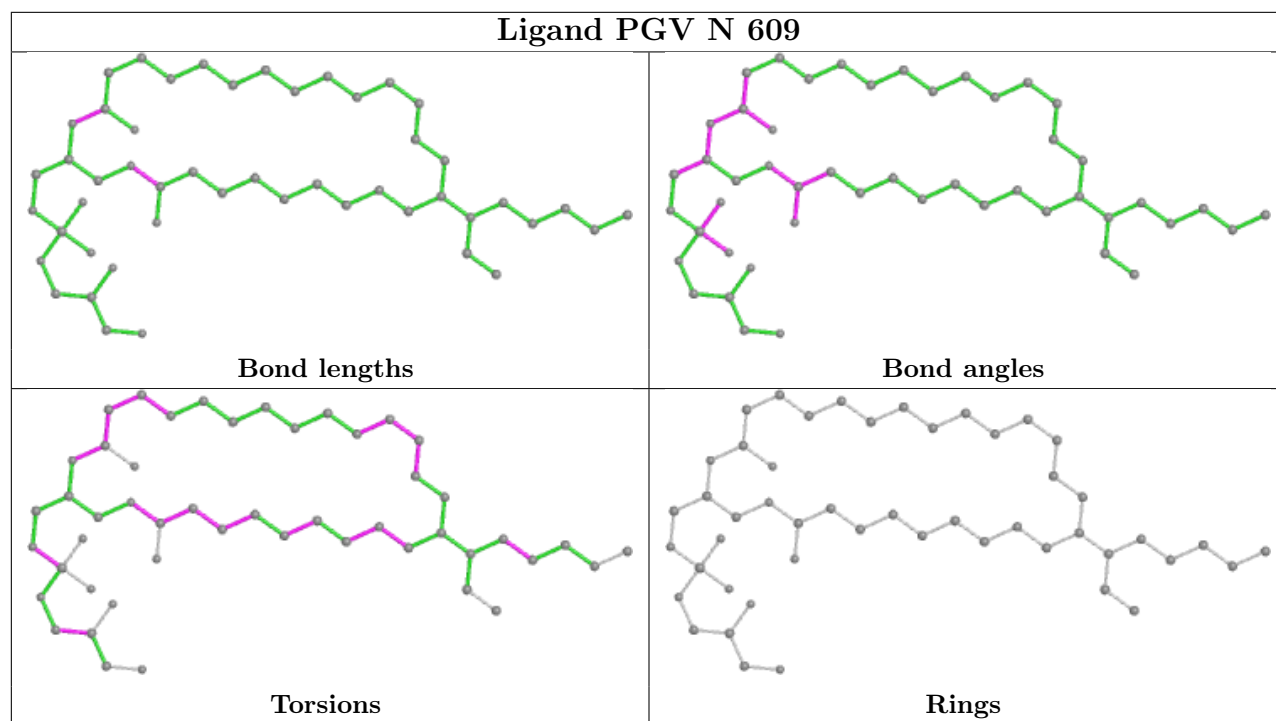
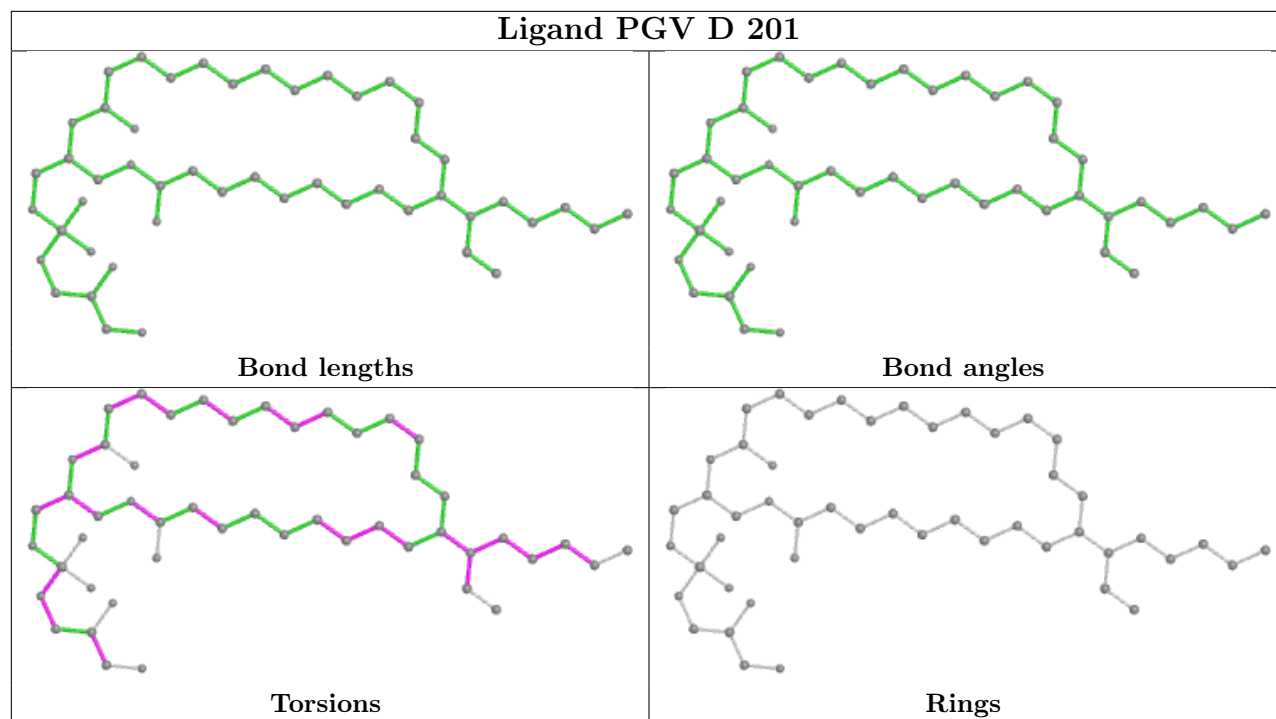


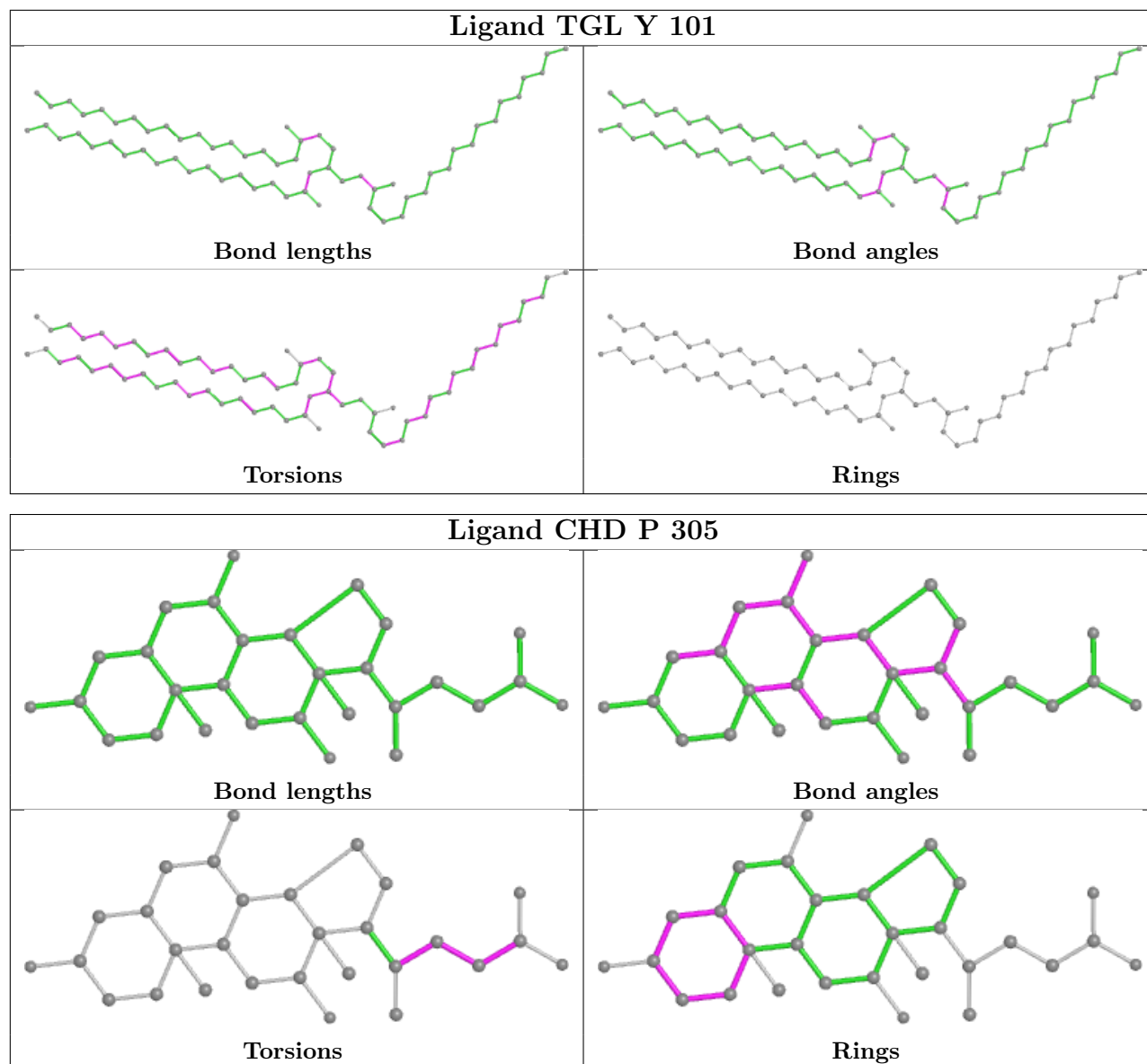


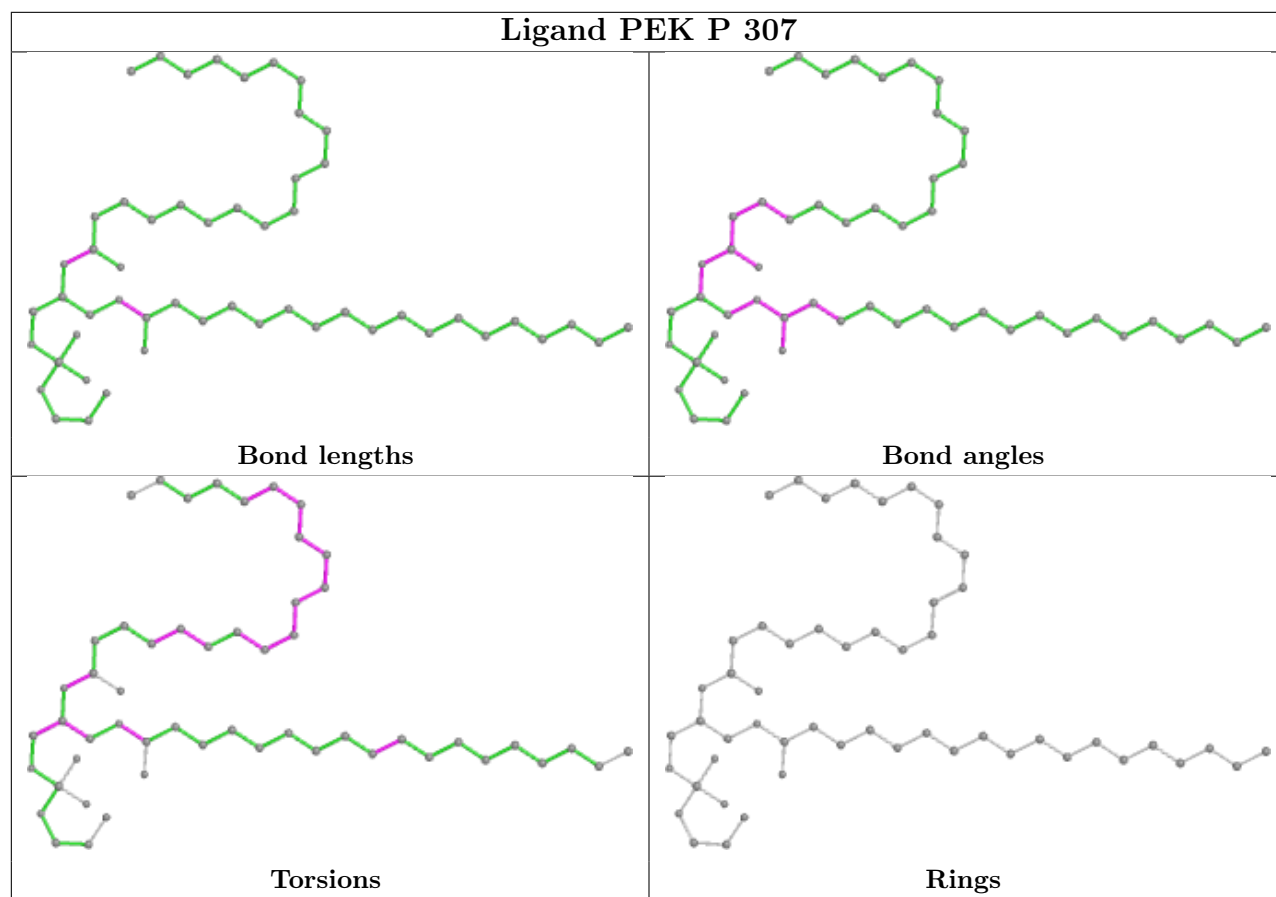
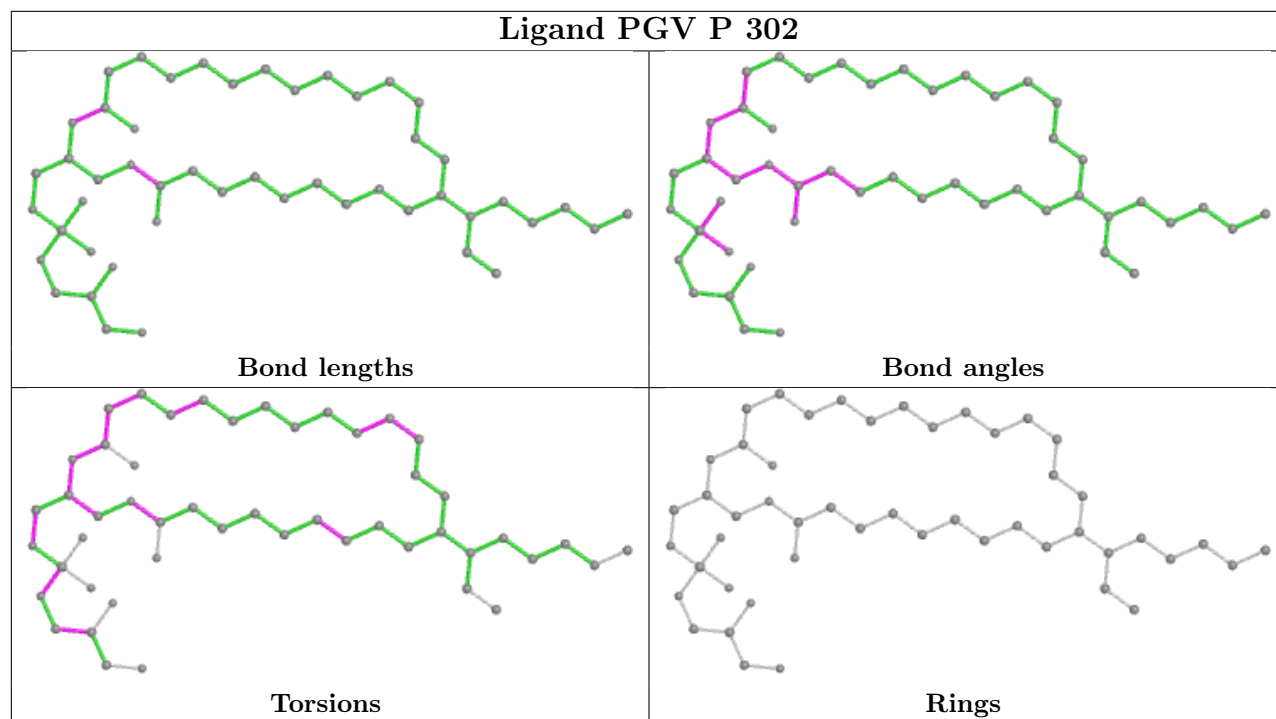


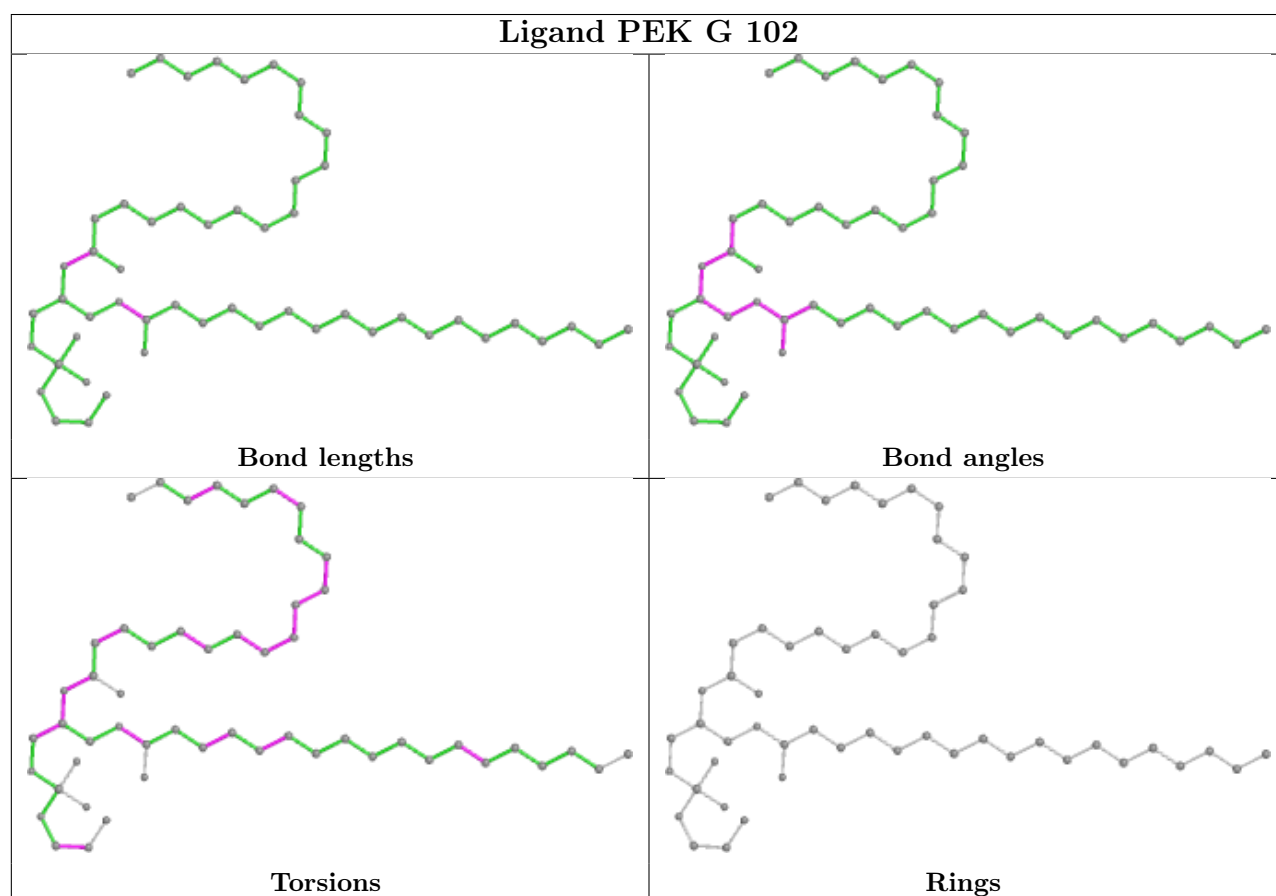
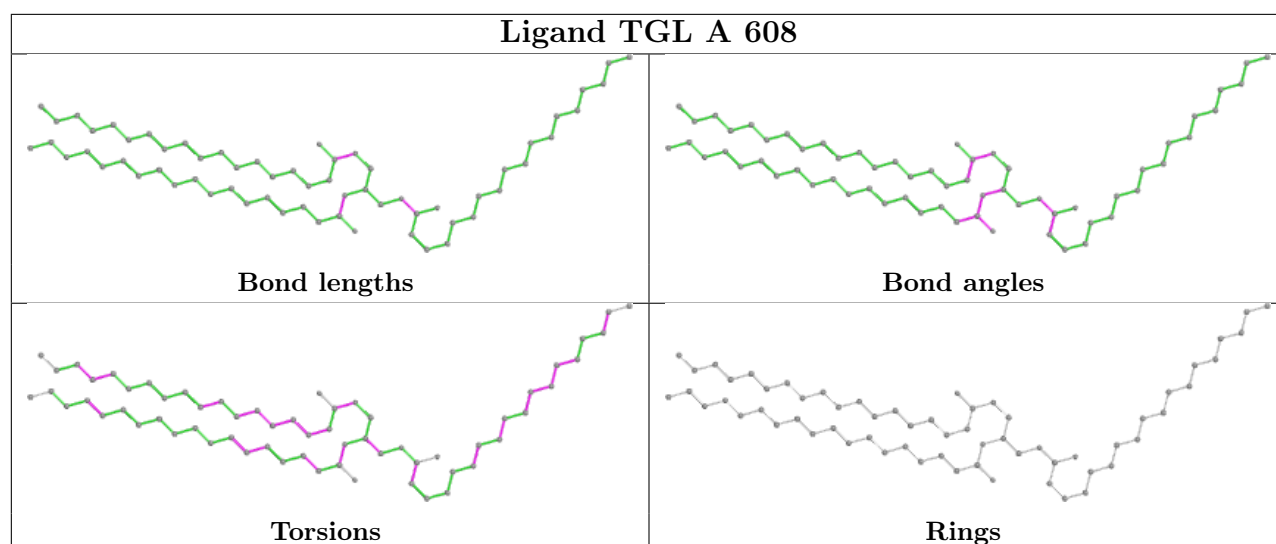


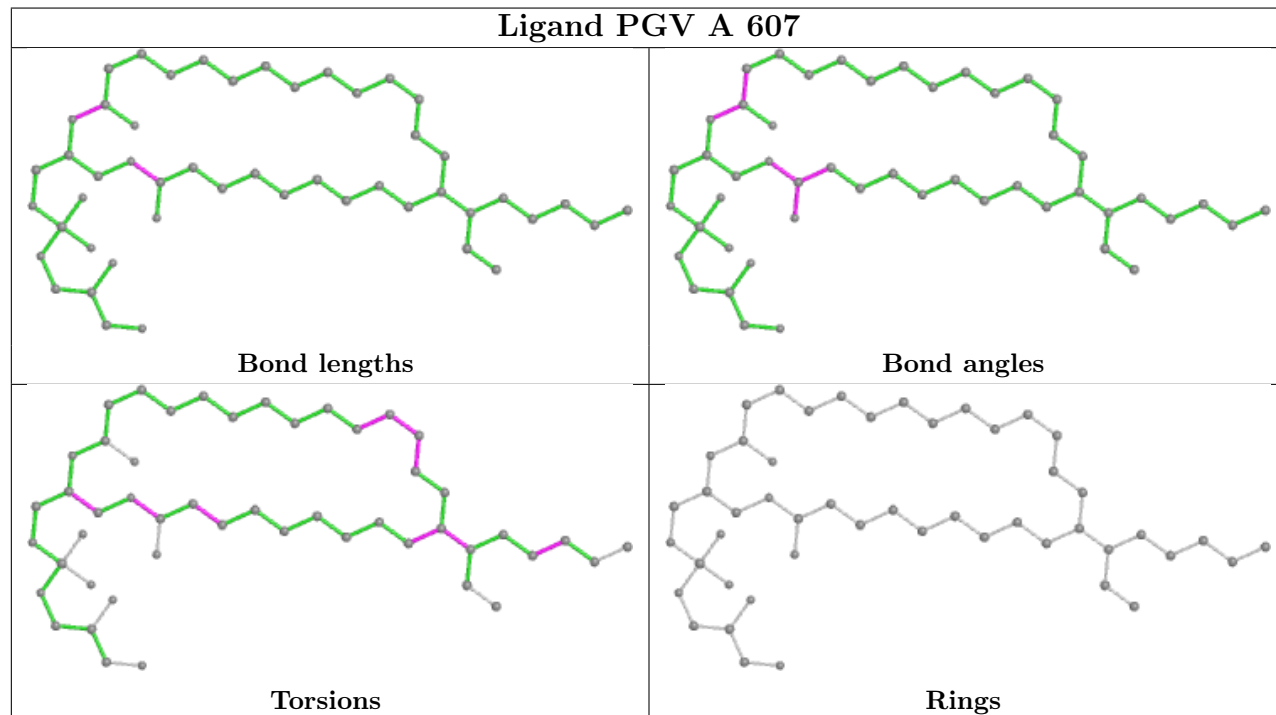
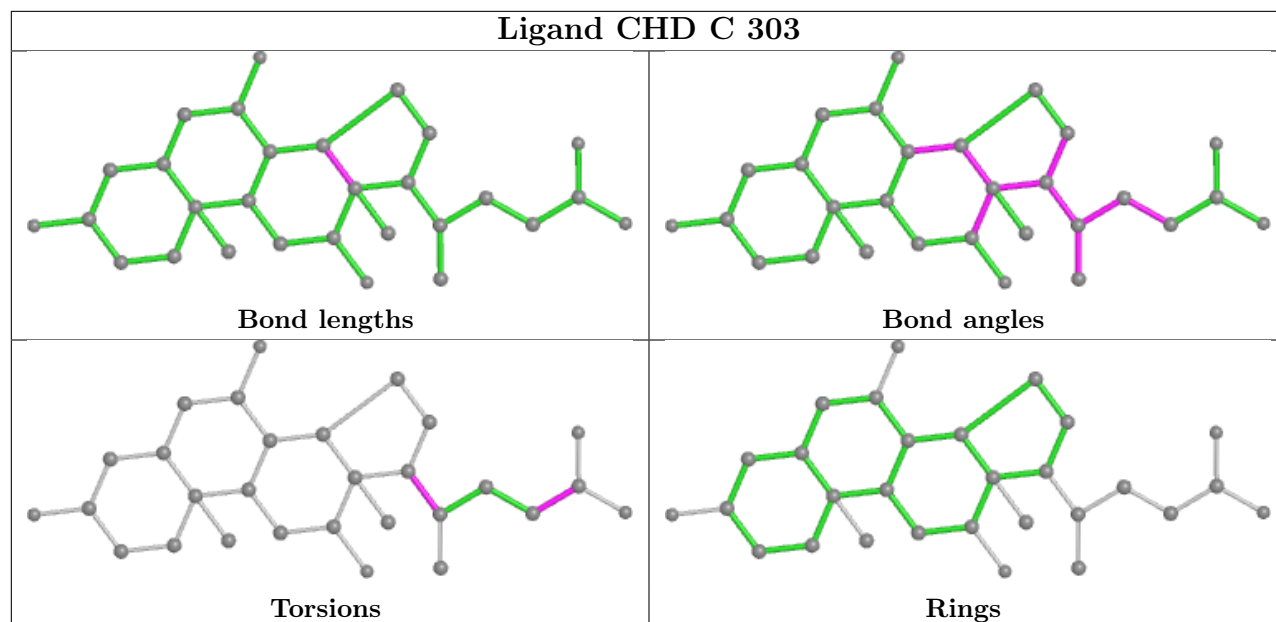


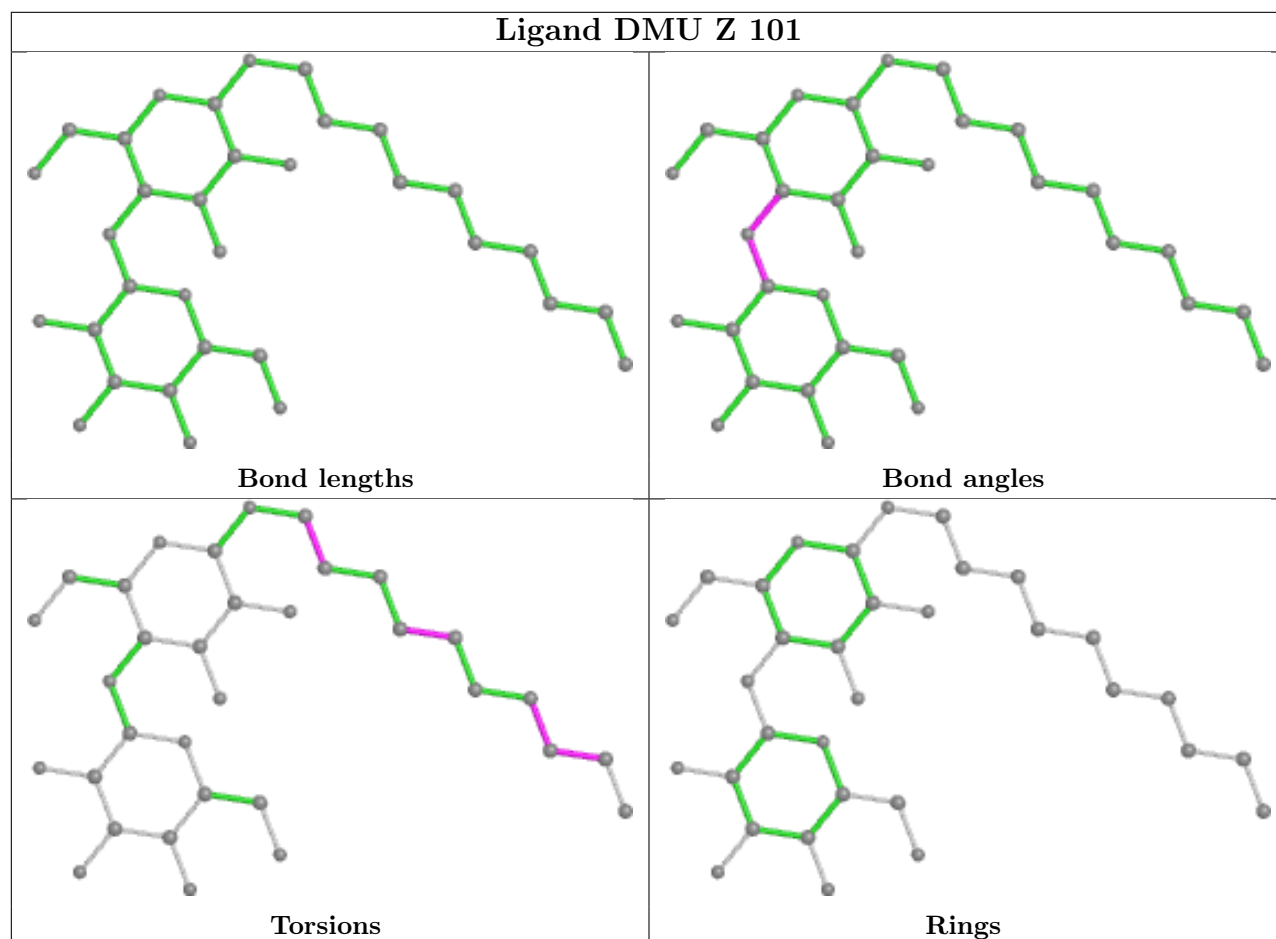
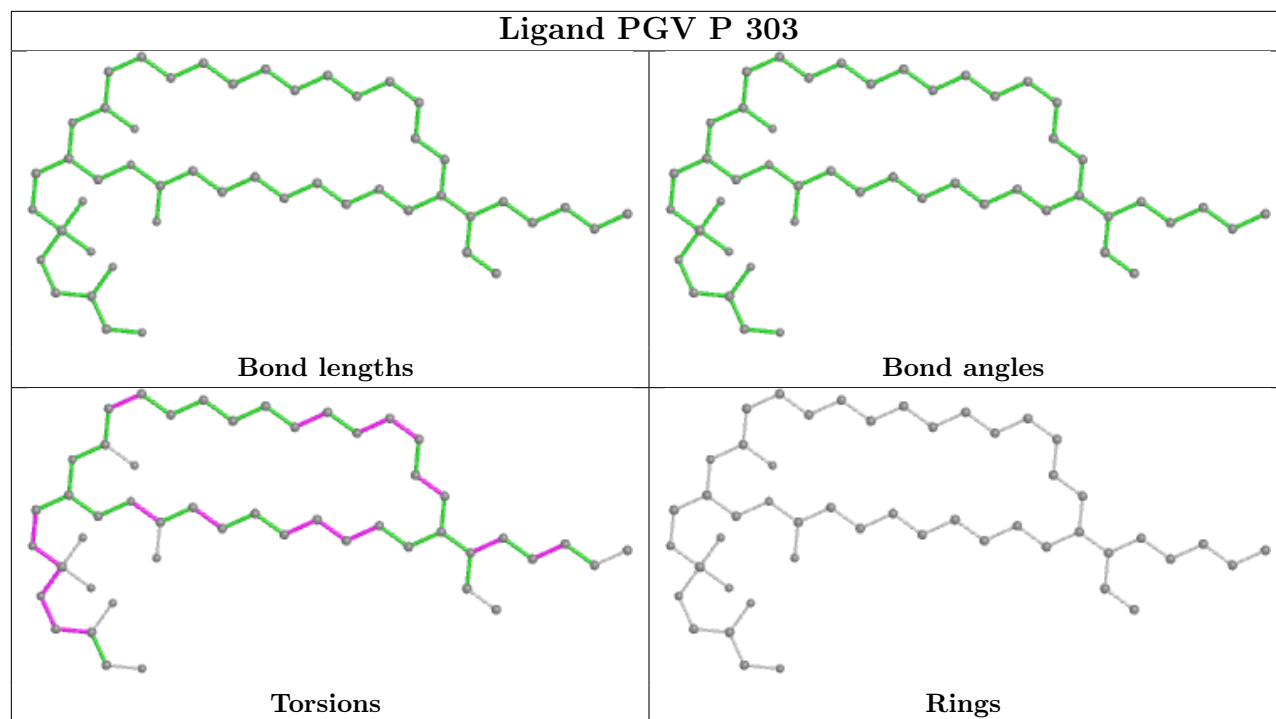


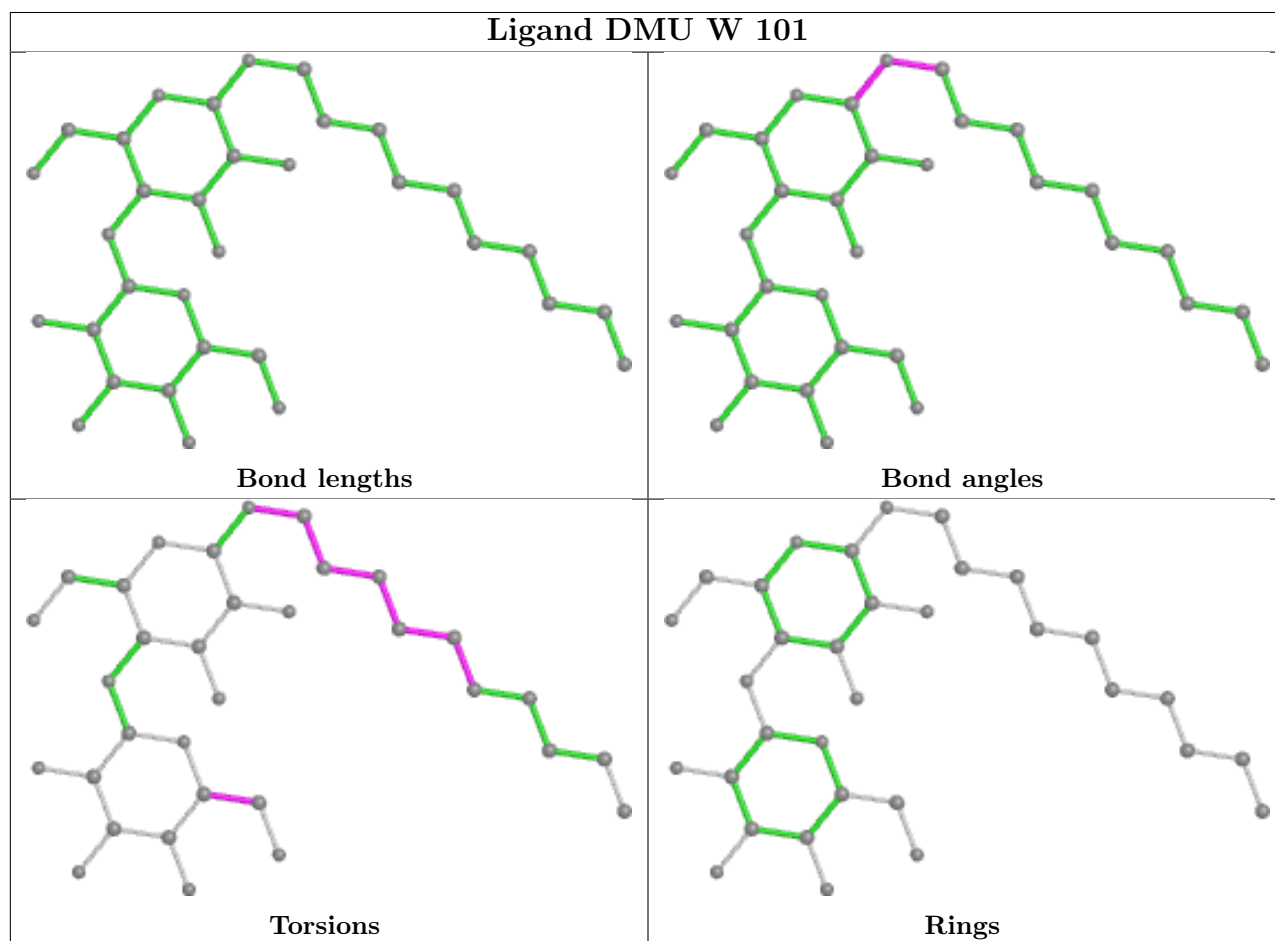
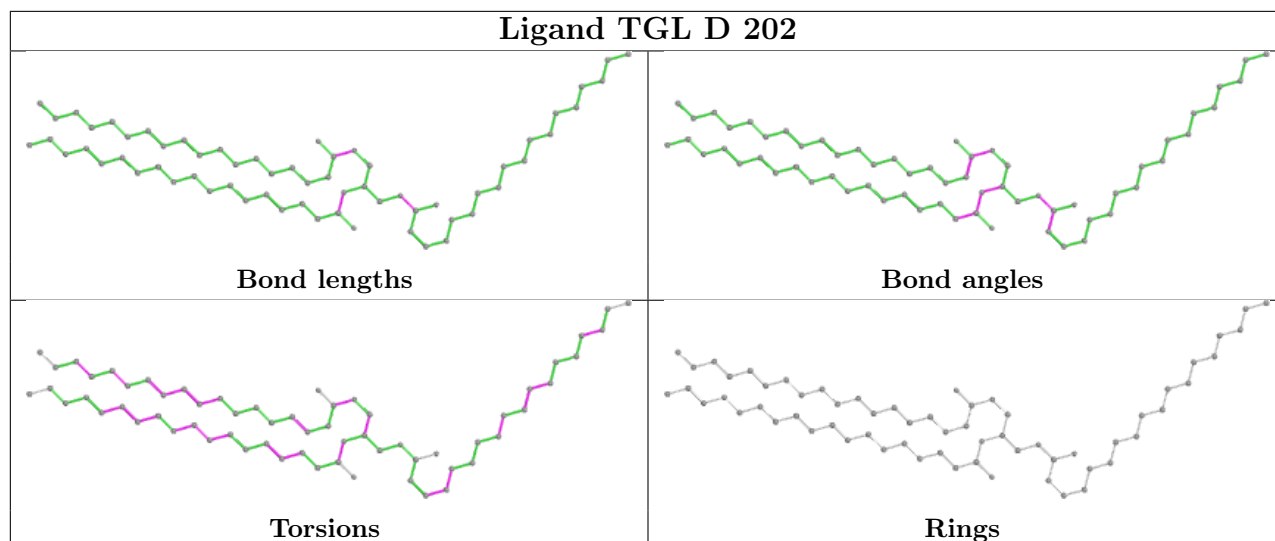


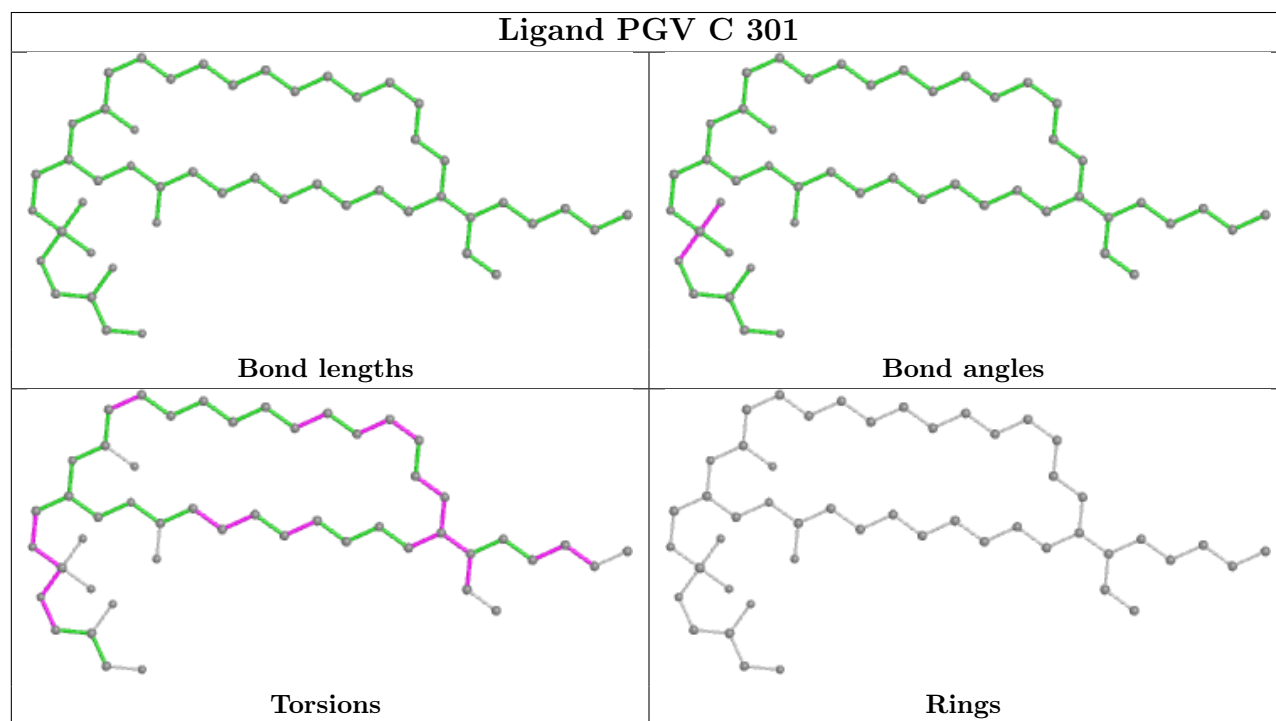
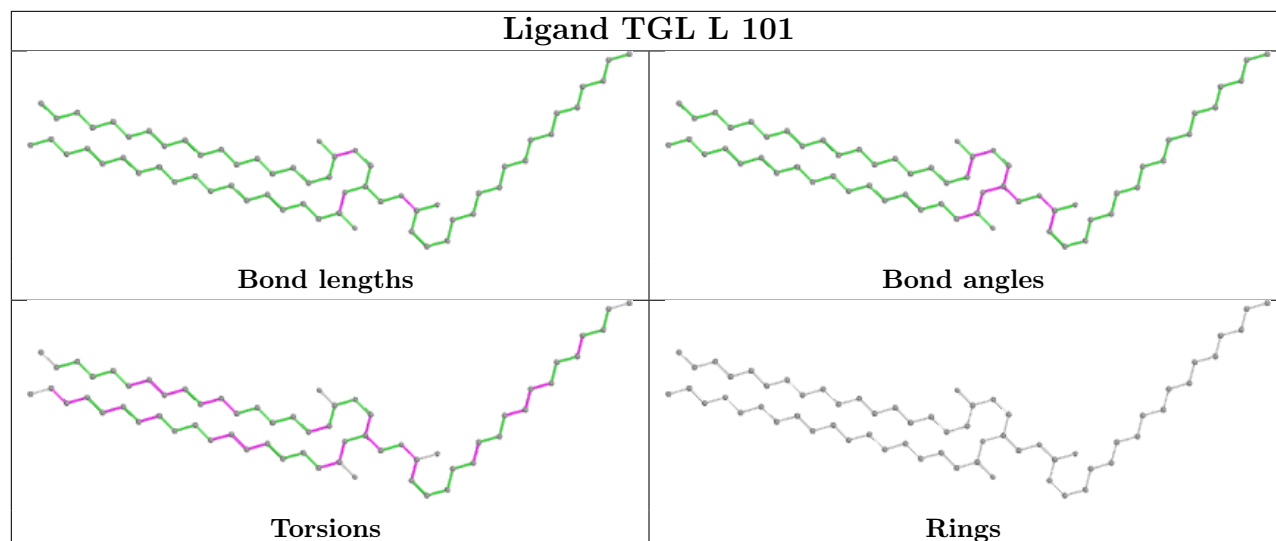


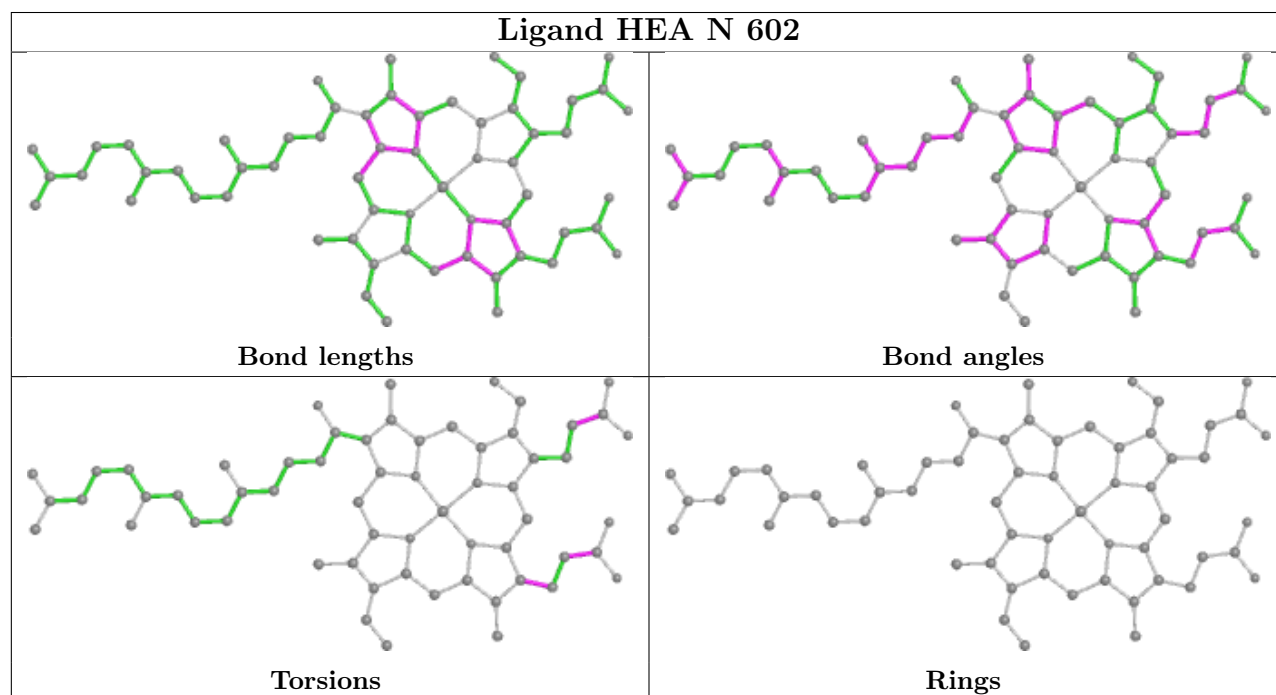
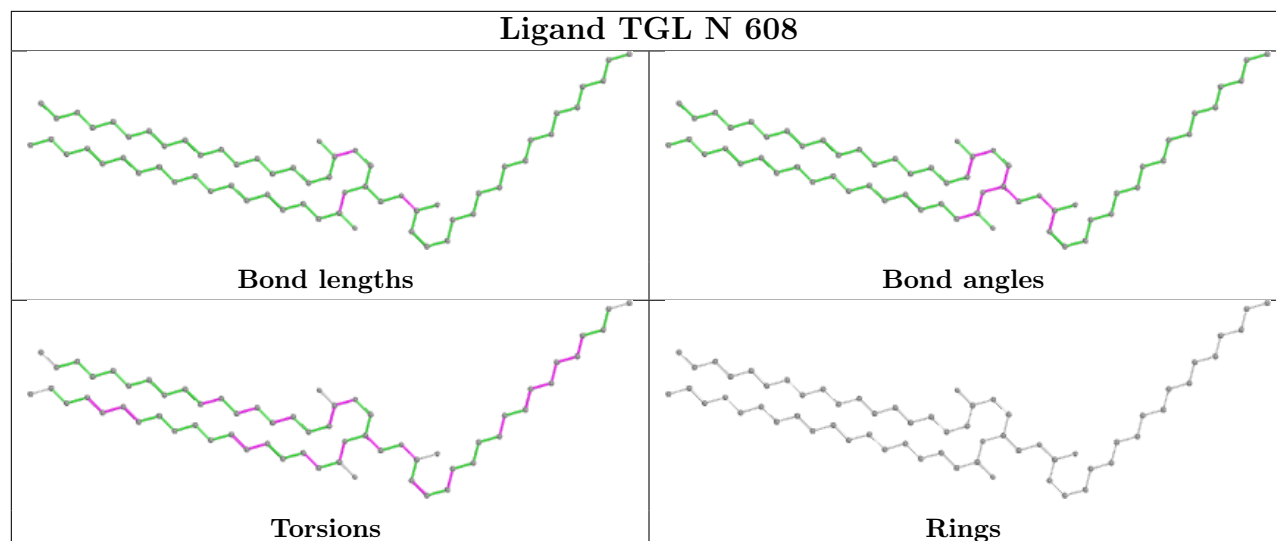


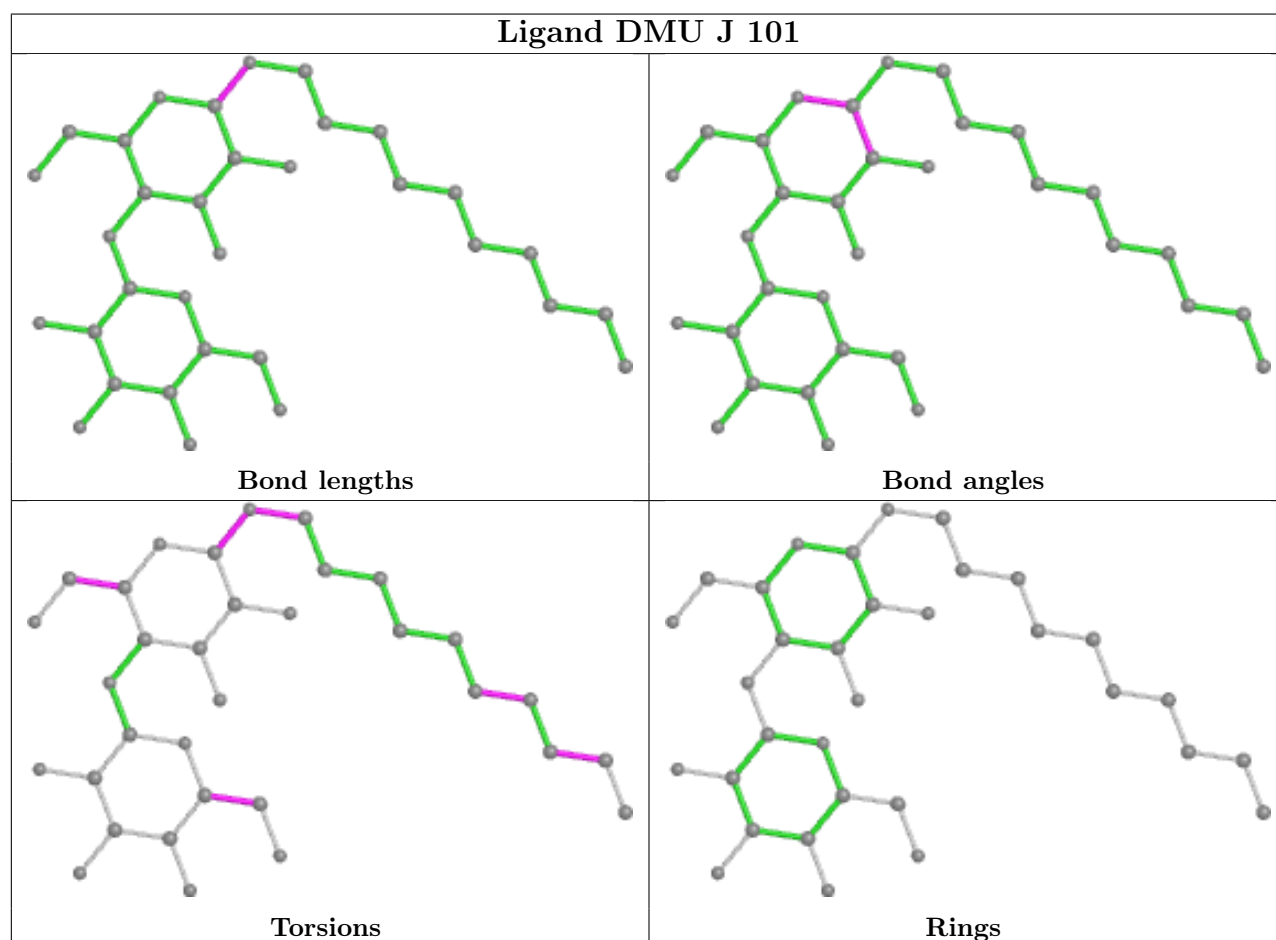
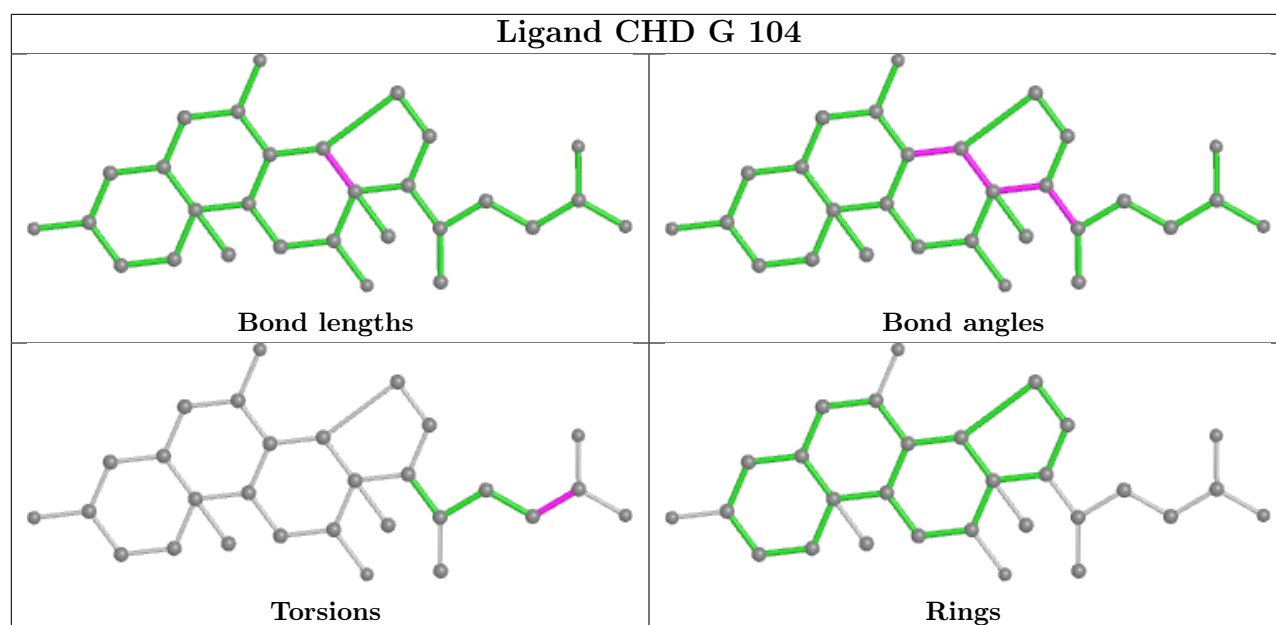


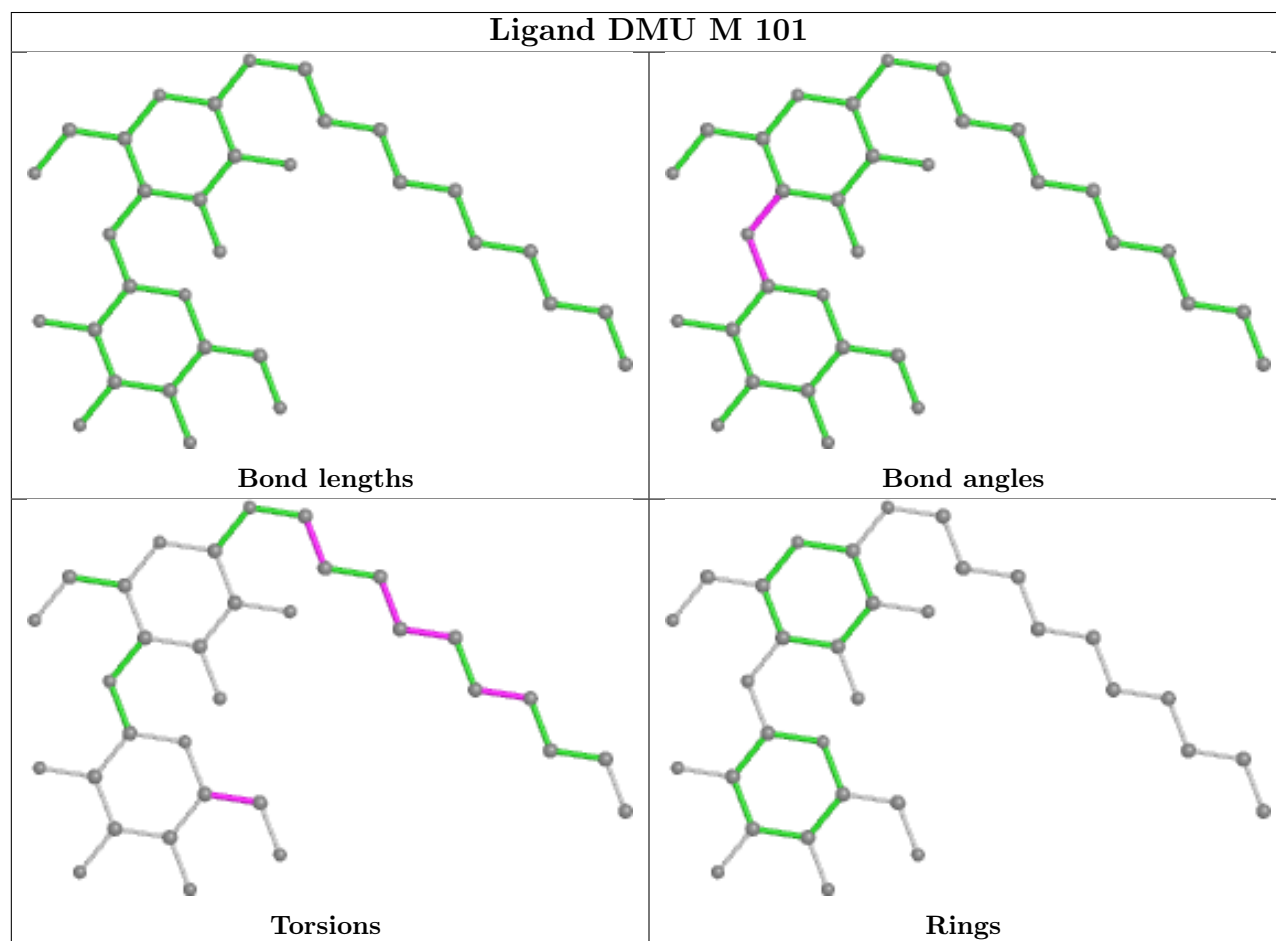
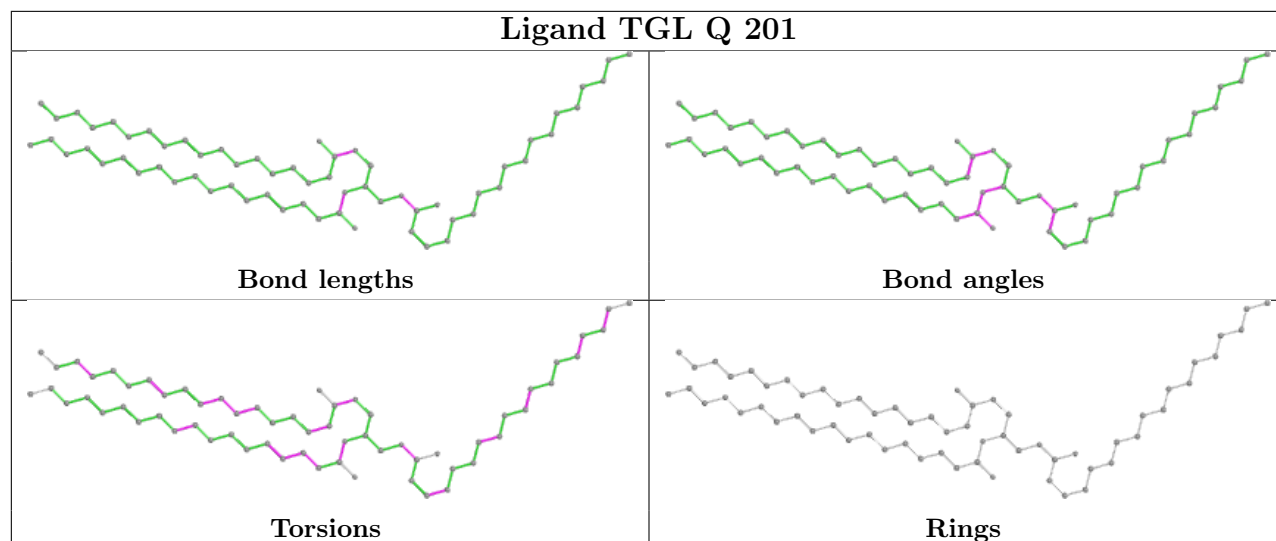


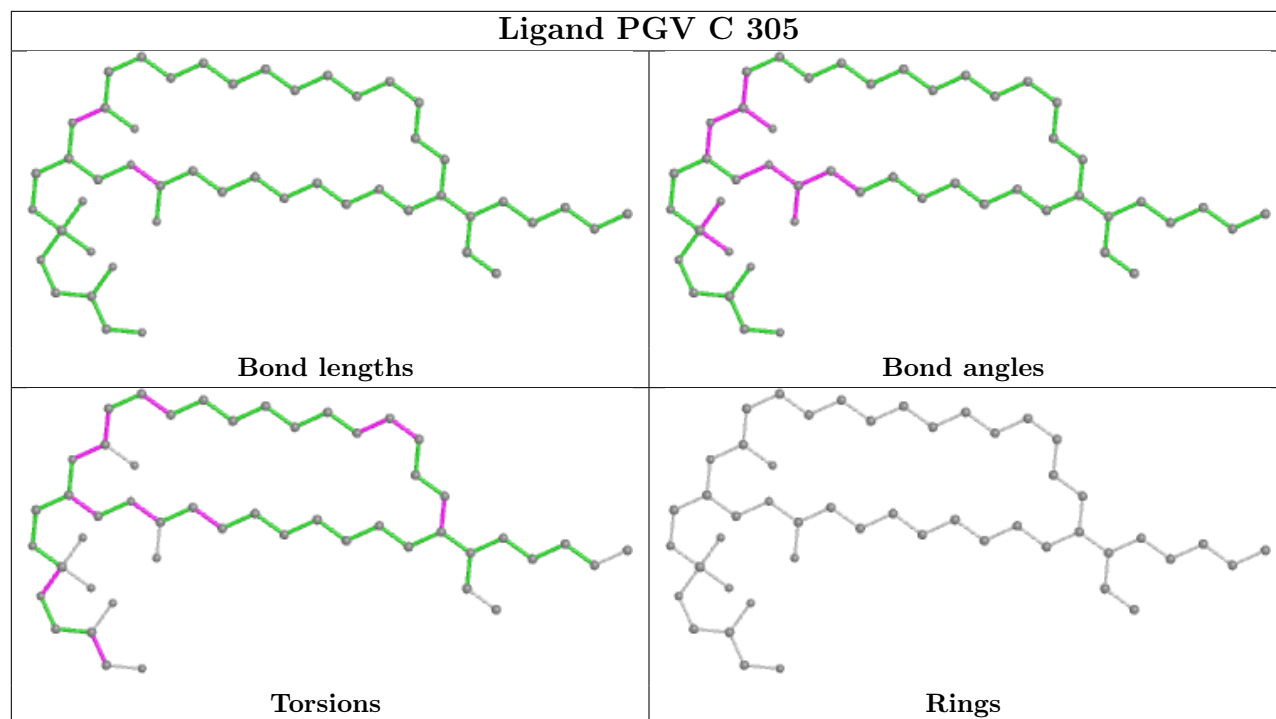












5.7 Other polymers [i](#)

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 i

6.1 Protein, DNA and RNA chains i

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%)	-0.42	1 (0%) 95 94	22, 29, 39, 92	0
1	N	513/514 (99%)	-0.39	1 (0%) 95 94	24, 32, 44, 79	0
2	B	226/581 (38%)	-0.15	7 (3%) 49 47	24, 38, 70, 123	0
2	O	226/581 (38%)	-0.05	11 (4%) 29 28	28, 42, 79, 167	0
3	C	259/261 (99%)	-0.43	3 (1%) 79 77	24, 33, 49, 95	0
3	P	259/261 (99%)	-0.35	2 (0%) 86 85	26, 33, 51, 97	0
4	D	144/147 (97%)	-0.33	2 (1%) 75 73	30, 39, 61, 99	0
4	Q	139/147 (94%)	0.25	11 (7%) 12 11	34, 52, 86, 150	0
5	E	105/109 (96%)	-0.14	5 (4%) 30 29	31, 40, 69, 146	0
5	R	105/109 (96%)	0.21	8 (7%) 13 12	36, 49, 79, 144	0
6	F	93/98 (94%)	0.02	4 (4%) 35 33	26, 39, 67, 139	0
6	S	96/98 (97%)	0.01	7 (7%) 15 14	26, 38, 76, 113	0
7	G	81/84 (96%)	0.63	15 (18%) 1 1	30, 41, 124, 185	0
7	T	81/84 (96%)	0.74	15 (18%) 1 1	30, 43, 124, 198	0
8	H	79/85 (92%)	0.18	9 (11%) 5 4	29, 42, 124, 143	0
8	U	79/85 (92%)	0.38	10 (12%) 3 3	34, 47, 138, 151	0
9	I	72/73 (98%)	0.32	7 (9%) 7 6	35, 52, 81, 101	0
9	V	72/73 (98%)	0.65	9 (12%) 3 3	37, 58, 94, 139	0
10	J	57/59 (96%)	0.06	5 (8%) 10 8	32, 44, 79, 96	0
10	W	57/59 (96%)	0.15	4 (7%) 16 15	34, 47, 84, 109	0
11	K	51/56 (91%)	0.37	5 (9%) 7 6	34, 45, 71, 97	0
11	X	49/56 (87%)	0.60	5 (10%) 6 6	44, 52, 77, 89	0
12	L	46/47 (97%)	-0.40	1 (2%) 62 59	28, 36, 62, 111	0
12	Y	45/47 (95%)	-0.27	0 100 100	32, 43, 78, 91	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%)	-0.01	5 (11%) 4 4	30, 35, 95, 136	0
13	Z	41/46 (89%)	0.14	5 (12%) 4 3	36, 44, 84, 109	0
All	All	3531/4320 (81%)	-0.11	157 (4%) 34 32	22, 37, 76, 198	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	8	HIS	9.0
8	U	45	ALA	8.5
7	G	7	ASP	8.0
8	H	45	ALA	7.6
5	R	109	VAL	7.5
5	R	5	HIS	7.1
9	V	37	PHE	6.6
7	G	8	HIS	6.4
11	X	6	ALA	6.4
7	T	4	ALA	6.4
2	O	90	ILE	6.3
7	G	36[A]	TRP	6.2
9	I	37	PHE	6.1
8	U	7	LYS	5.8
8	U	47	GLY	5.5
7	T	3	ALA	5.5
9	V	2	THR	5.4
13	M	43	SER	5.4
4	Q	9	GLU	5.2
7	G	4	ALA	5.2
13	M	42	LYS	5.1
10	J	1	PHE	4.7
7	G	41	HIS	4.7
12	L	2	HIS	4.6
2	B	90	ILE	4.6
7	G	42	ARG	4.6
6	S	95	GLN	4.5
2	B	60	GLU	4.5
7	T	40	GLY	4.5
4	Q	10	ASP	4.5
7	G	84	LYS	4.5
7	T	41	HIS	4.4
10	J	57	HIS	4.4
11	X	7	PRO	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	94	HIS	4.4
7	T	7	ASP	4.4
8	H	8	ILE	4.4
8	U	8	ILE	4.4
11	K	7	PRO	4.3
10	W	57	HIS	4.2
7	G	9	GLY	4.2
5	E	5	HIS	4.2
8	H	46	LYS	4.2
7	T	5	LYS	4.2
13	Z	40	TYR	4.1
7	T	42	ARG	4.1
7	G	40	GLY	4.1
13	Z	39	ASN	4.0
2	O	227	LEU	4.0
6	S	96	LEU	3.9
7	T	36	TRP	3.9
9	V	33	THR	3.8
8	U	10	ASN	3.8
8	H	7	LYS	3.7
6	S	94	HIS	3.7
13	M	40	TYR	3.7
8	H	44	THR	3.7
6	F	95	GLN	3.7
10	J	56	PRO	3.6
7	T	84	LYS	3.6
4	Q	39	ALA	3.6
7	T	9	GLY	3.6
6	S	97	ALA	3.6
13	M	39	ASN	3.6
7	G	5	LYS	3.6
7	T	39	SER	3.6
2	O	113	TYR	3.6
7	G	43	GLU	3.5
11	K	6	ALA	3.5
9	V	25	PHE	3.4
7	T	10	GLY	3.4
2	B	57	ASP	3.4
8	H	47	GLY	3.4
9	V	34	PHE	3.4
9	V	26	MET	3.3
7	G	3	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	Q	147	LYS	3.2
9	I	26	MET	3.2
7	G	39	SER	3.2
4	Q	31	LYS	3.2
10	W	48	TYR	3.2
8	U	44	THR	3.1
4	Q	32	ASN	3.0
2	B	59	GLN	3.0
5	E	109	VAL	3.0
9	V	19	PHE	3.0
7	G	10	GLY	2.9
4	Q	30	VAL	2.9
8	U	48	GLY	2.9
11	X	13	TYR	2.9
8	U	49	ASP	2.8
4	Q	33	LEU	2.8
8	H	48	GLY	2.8
10	J	48	TYR	2.8
2	O	59	GLN	2.8
5	R	108	LYS	2.8
6	F	3	GLY	2.7
7	T	45	PRO	2.7
11	K	56	GLN	2.7
8	H	49	ASP	2.7
3	C	61	VAL	2.7
3	P	38	ASN	2.6
9	I	19	PHE	2.6
9	I	18	ARG	2.6
4	Q	35	ALA	2.6
2	B	56	MET	2.6
5	E	67	ILE	2.5
10	W	52	TRP	2.5
4	D	147	LYS	2.5
9	I	34	PHE	2.5
2	B	61	VAL	2.5
11	K	34	THR	2.5
1	N	312[A]	ILE	2.5
2	O	192	TYR	2.4
5	R	70	VAL	2.4
6	S	25	ARG	2.4
1	A	514	LYS	2.4
2	O	167	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	143	ASN	2.4
6	F	44	GLU	2.4
6	S	2	SER	2.4
2	O	165	VAL	2.4
2	O	223	SER	2.4
7	T	43	GLU	2.3
5	E	7	THR	2.3
10	J	55	PHE	2.3
7	G	45	PRO	2.3
3	P	62	ILE	2.3
11	K	8	ASP	2.3
9	V	29	LEU	2.2
2	O	226	MET	2.2
8	H	10	ASN	2.2
9	I	44	LYS	2.2
9	V	5	ALA	2.2
11	X	34	THR	2.2
11	X	8	ASP	2.2
13	Z	32	TRP	2.2
3	C	38	ASN	2.2
4	Q	38	LYS	2.2
5	E	70	VAL	2.1
5	R	68	LEU	2.1
4	Q	78	TRP	2.1
13	Z	13	LYS	2.1
13	Z	41	LYS	2.1
2	B	55	THR	2.1
9	I	25	PHE	2.1
8	U	50	VAL	2.1
5	R	6	GLU	2.1
5	R	64	ALA	2.1
2	O	217	LYS	2.1
6	S	27	GLY	2.1
3	C	62	ILE	2.1
2	O	221	LYS	2.1
13	M	41	LYS	2.1
5	R	65	VAL	2.1
10	W	55	PHE	2.1
8	U	46	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.65	0.43	97,139,209,217	0
7	TPO	T	11	11/12	0.70	0.41	86,138,197,210	0
1	FME	N	1	10/11	0.92	0.28	43,50,90,92	0
1	FME	A	1	10/11	0.95	0.29	38,51,75,118	0
2	FME	O	1	10/11	0.97	0.17	35,40,60,89	0
2	FME	B	1	10/11	0.97	0.16	32,36,49,94	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

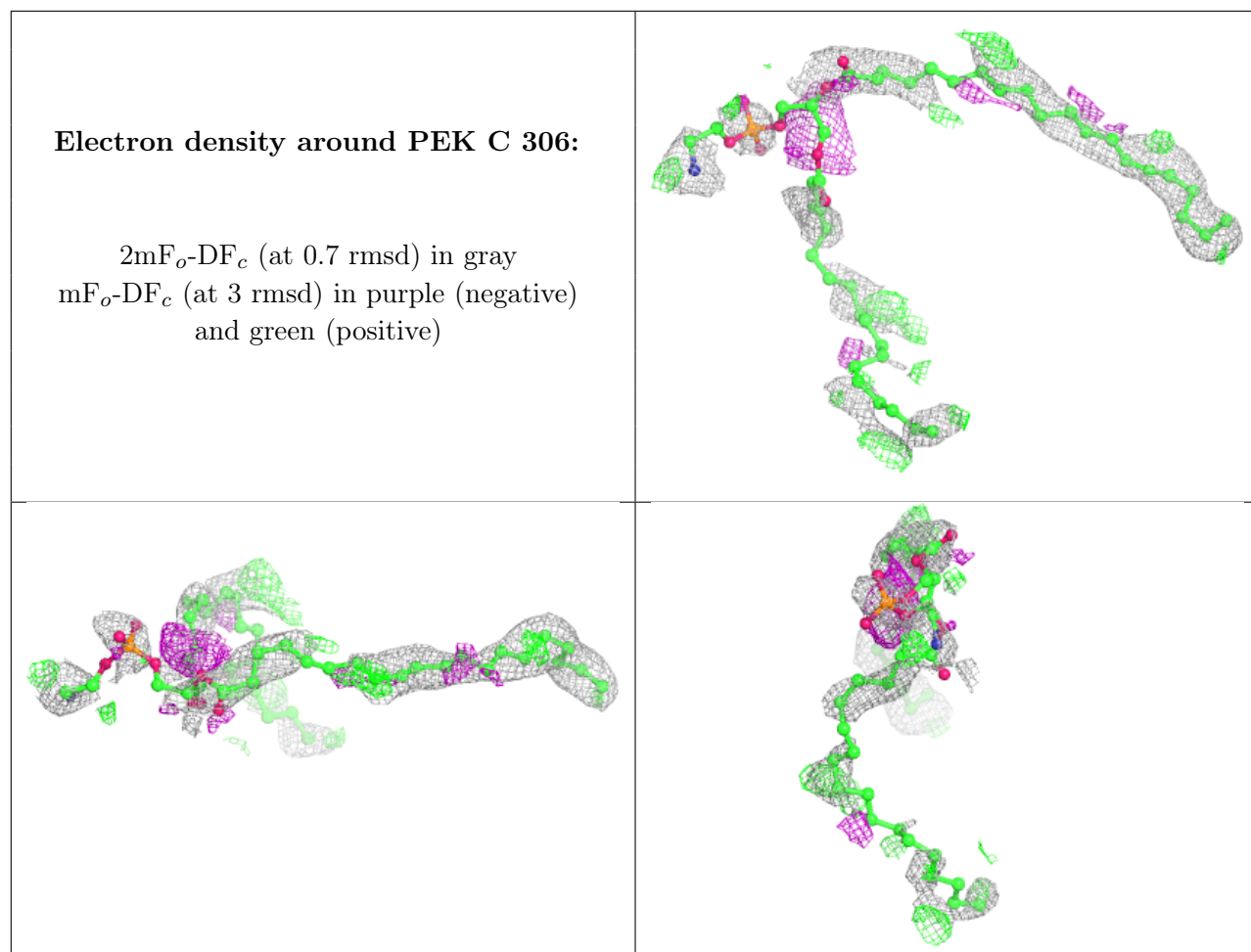
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	PEK	C	306	53/53	0.51	0.50	41,97,176,196	0
24	PEK	G	101	53/53	0.52	0.36	41,88,171,203	0
24	PEK	P	301	53/53	0.61	0.36	39,89,173,197	0
27	DMU	J	101	33/33	0.61	0.37	43,89,113,124	0
22	CDL	G	103	100/100	0.63	0.40	51,107,157,207	0
25	PSC	O	602	52/52	0.64	0.36	41,94,202,234	0
24	PEK	P	307	53/53	0.64	0.36	43,91,163,188	0
22	CDL	T	103	100/100	0.65	0.37	46,97,179,209	0
25	PSC	E	201	52/52	0.65	0.35	40,114,206,225	0
19	PGV	P	302	51/51	0.66	0.32	52,93,171,178	0
22	CDL	C	302	100/100	0.68	0.34	38,88,143,153	0
23	CHD	P	305	29/29	0.70	0.35	63,100,124,132	0
20	TGL	Q	201	63/63	0.70	0.24	44,79,121,133	0
27	DMU	W	101	33/33	0.70	0.40	41,89,119,122	0
20	TGL	Y	101	63/63	0.71	0.27	35,70,121,169	0
22	CDL	P	304	100/100	0.71	0.33	38,95,140,162	0

Continued on next page...

Continued from previous page...

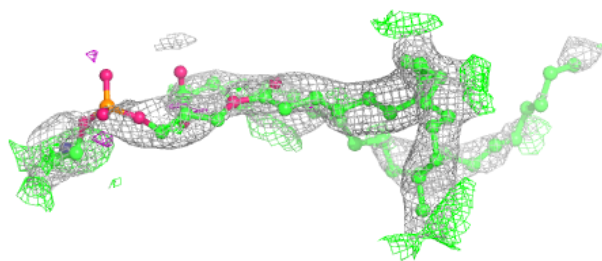
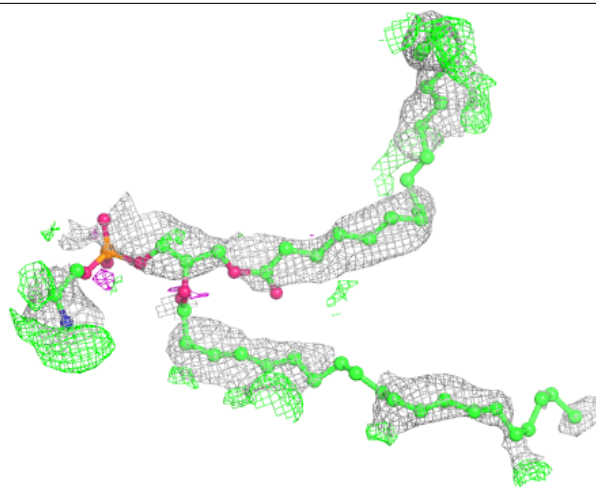
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CHD	C	303	29/29	0.72	0.39	75,97,118,124	0
19	PGV	N	609	51/51	0.74	0.36	39,91,166,187	0
27	DMU	M	101	33/33	0.77	0.24	34,49,62,87	0
19	PGV	D	201	51/51	0.77	0.30	34,83,159,180	0
20	TGL	L	101	63/63	0.80	0.21	32,61,108,130	0
19	PGV	C	305	51/51	0.80	0.30	34,83,144,188	0
27	DMU	Z	101	33/33	0.80	0.29	40,56,76,89	0
20	TGL	D	202	63/63	0.81	0.20	39,74,102,128	0
20	TGL	A	608	63/63	0.81	0.20	33,76,105,138	0
20	TGL	N	608	63/63	0.83	0.21	33,75,107,121	0
24	PEK	T	102	53/53	0.87	0.24	29,54,103,123	0
24	PEK	G	102	53/53	0.88	0.26	31,54,111,129	0
19	PGV	A	607	51/51	0.88	0.26	21,44,73,90	0
19	PGV	C	301	51/51	0.89	0.31	22,46,88,101	0
19	PGV	N	607	51/51	0.90	0.23	17,49,75,89	0
23	CHD	C	304	29/29	0.90	0.11	25,35,44,47	0
19	PGV	P	303	51/51	0.90	0.29	28,46,107,120	0
23	CHD	P	306	29/29	0.92	0.11	24,37,45,53	0
23	CHD	G	104	29/29	0.94	0.10	21,29,38,49	0
14	HEA	N	602	60/60	0.95	0.12	18,30,45,54	0
14	HEA	N	601	60/60	0.95	0.16	18,34,62,79	0
23	CHD	T	101	29/29	0.95	0.09	20,28,43,56	0
14	HEA	A	601	60/60	0.96	0.14	11,29,56,88	0
14	HEA	A	602	60/60	0.96	0.12	18,28,46,49	0
16	MG	A	604	1/1	0.97	0.07	13,13,13,13	0
18	PER	N	606	2/2	0.97	0.19	38,38,38,46	0
26	ZN	F	101	1/1	0.97	0.14	21,21,21,21	0
26	ZN	S	101	1/1	0.97	0.11	21,21,21,21	0
18	PER	A	606	2/2	0.98	0.20	36,36,36,42	0
15	CU	N	603	1/1	0.98	0.03	18,18,18,18	0
15	CU	A	603	1/1	0.98	0.04	18,18,18,18	0
17	NA	A	605	1/1	0.98	0.10	15,15,15,15	0
17	NA	N	605	1/1	0.98	0.07	17,17,17,17	0
16	MG	N	604	1/1	0.99	0.11	13,13,13,13	0
21	CUA	B	601	2/2	0.99	0.04	17,17,17,20	0
21	CUA	O	601	2/2	0.99	0.08	20,20,20,20	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.



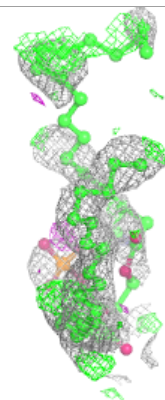
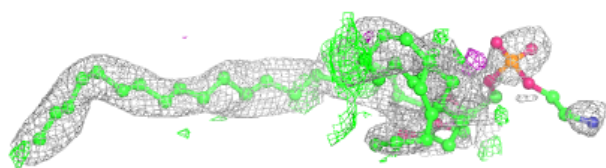
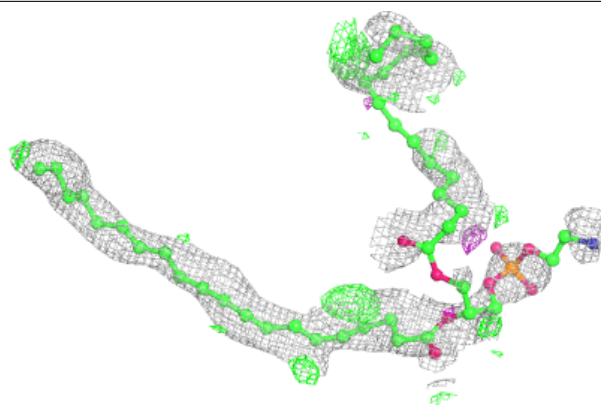
Electron density around PEK G 101:

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

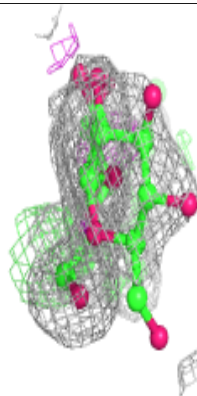
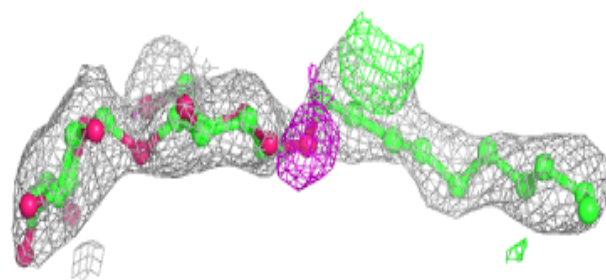
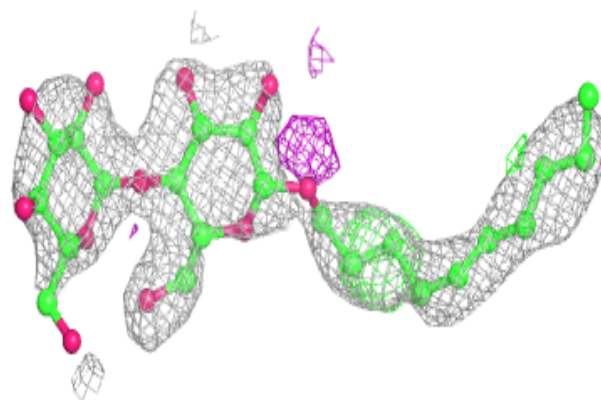


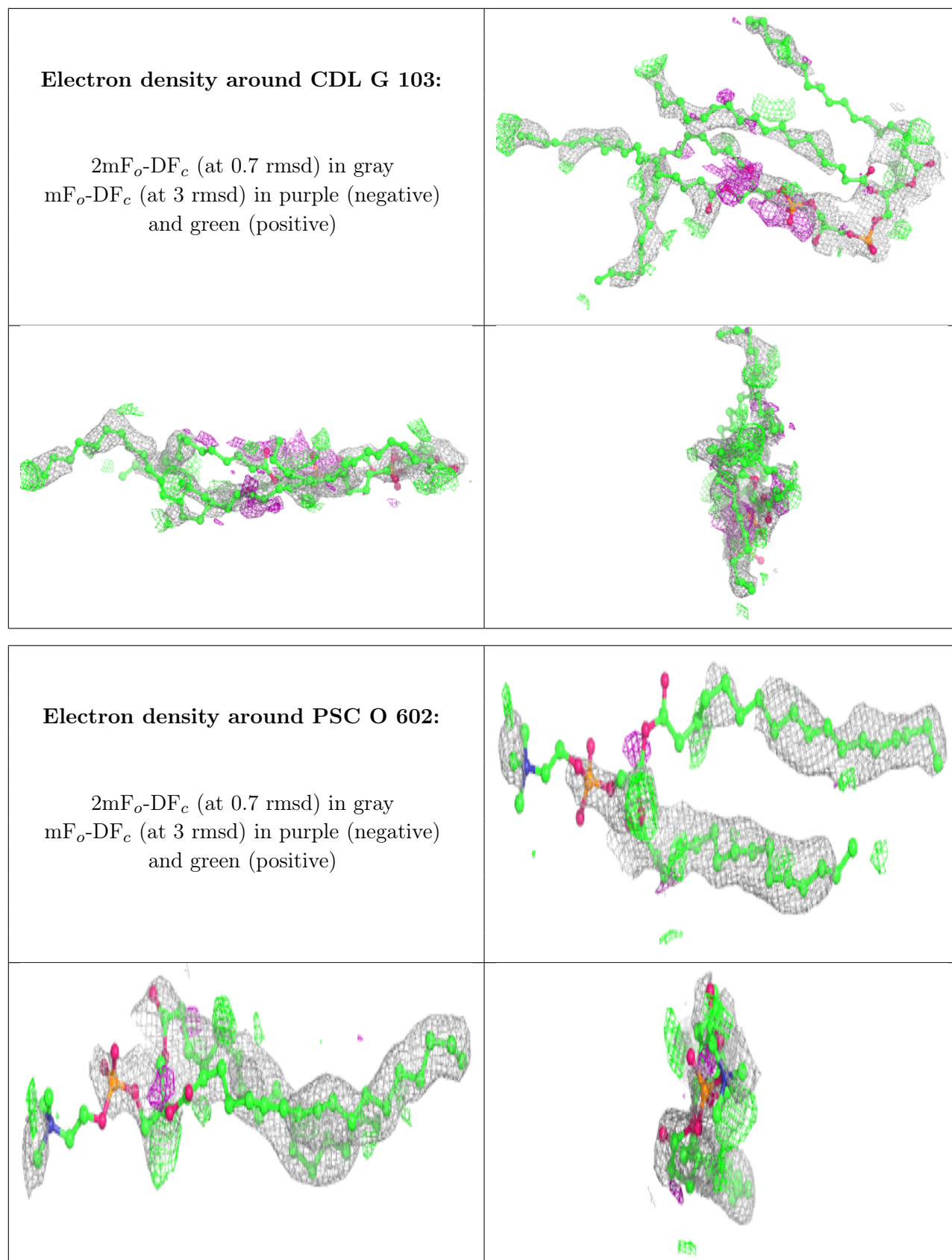
Electron density around PEK P 301:

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

**Electron density around DMU J 101:**

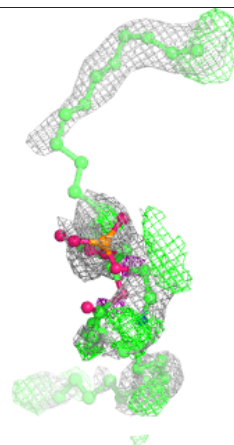
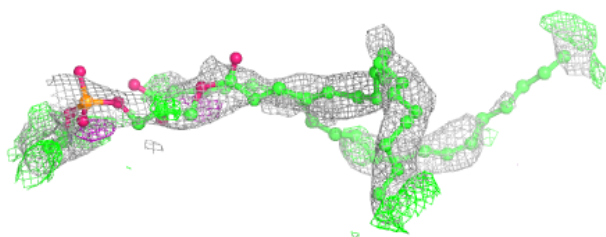
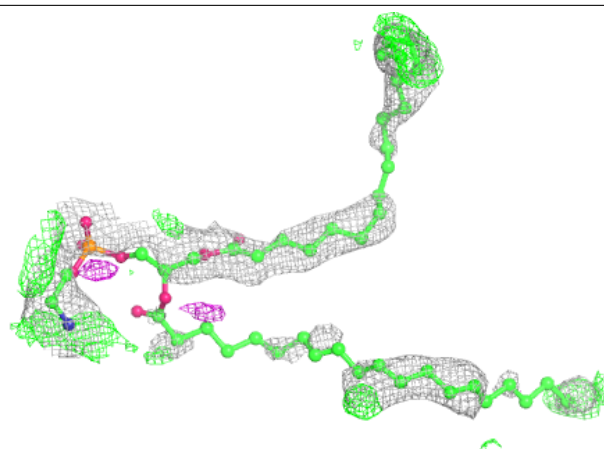
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



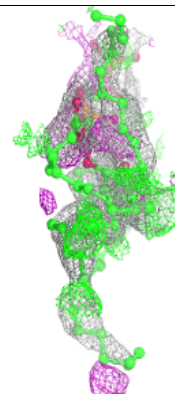
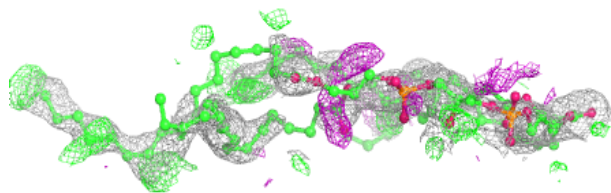
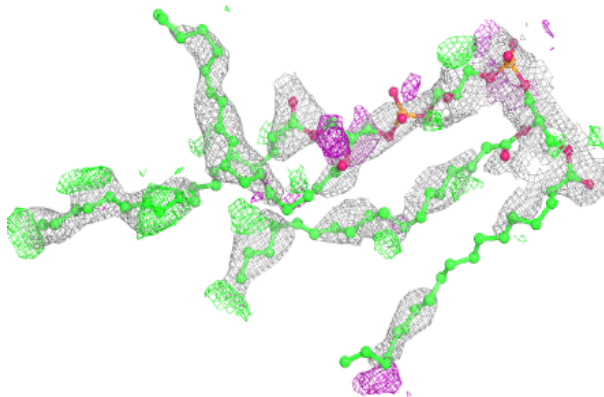


Electron density around PEK P 307:

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

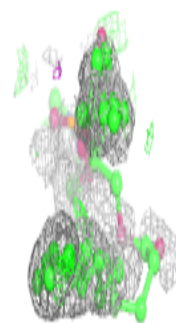
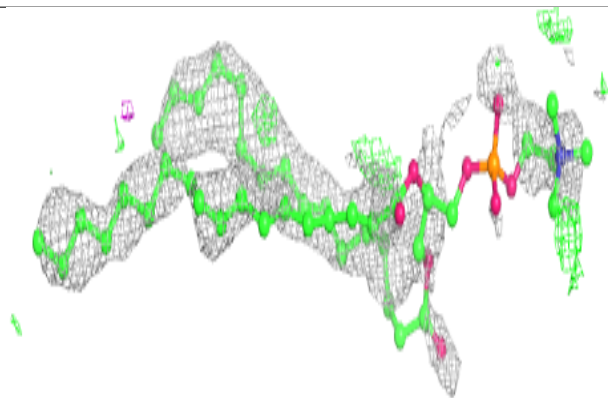
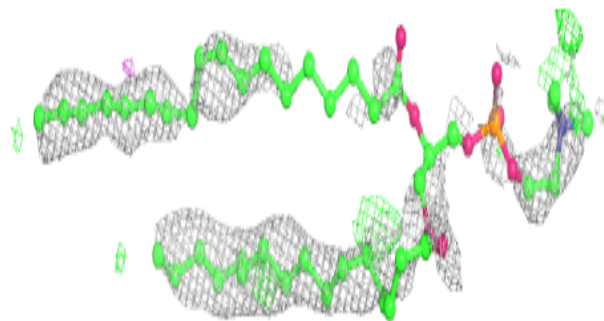
**Electron density around CDL T 103:**

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

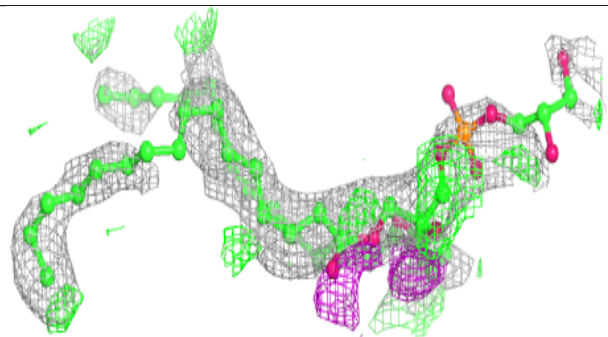
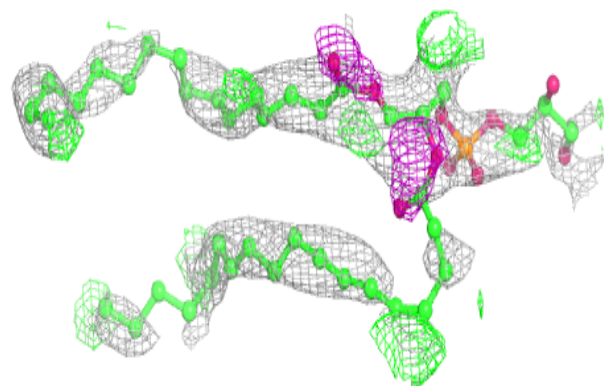


Electron density around PSC E 201:

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

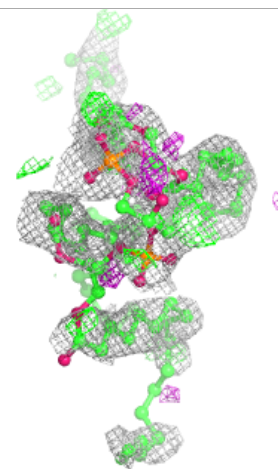
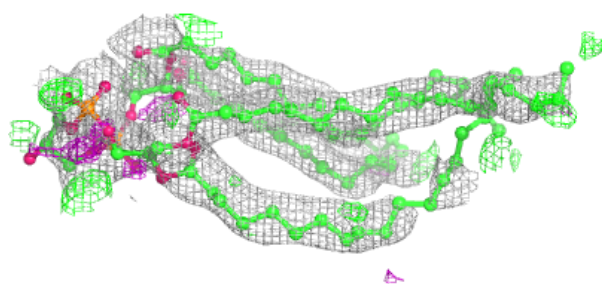
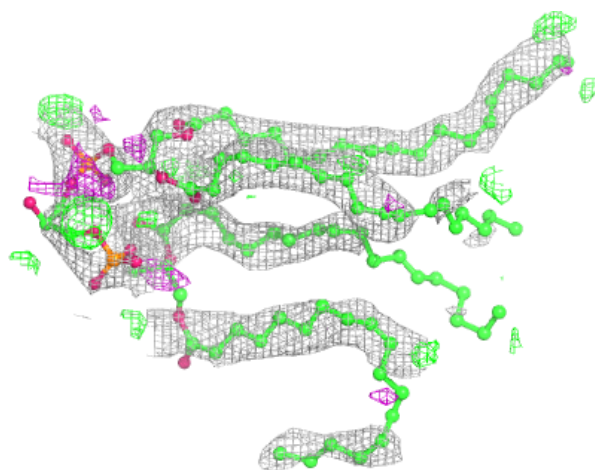
**Electron density around PGV P 302:**

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



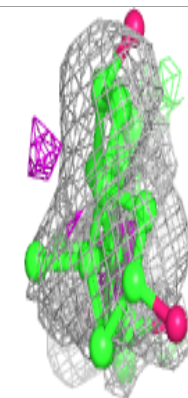
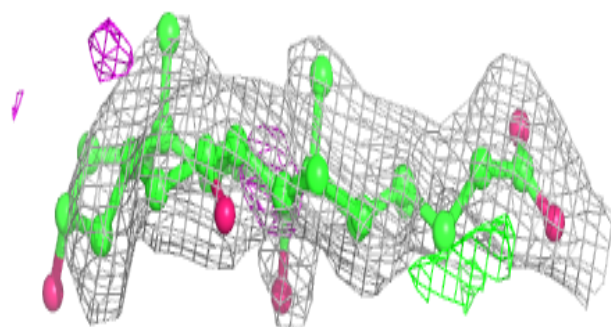
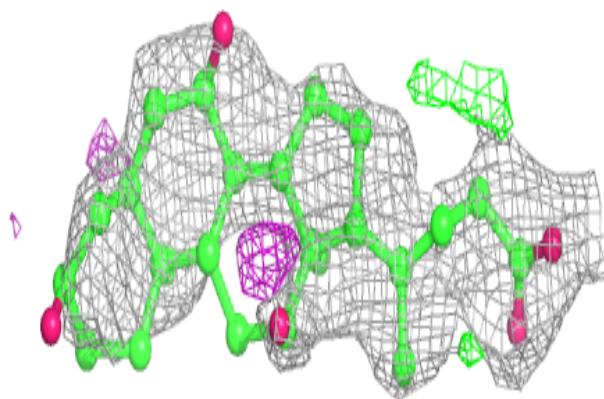
Electron density around CDL C 302:

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

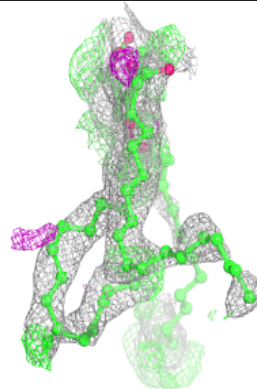
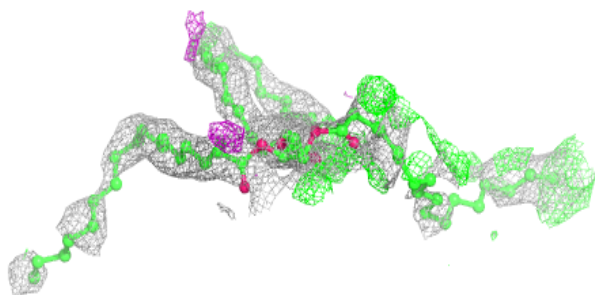
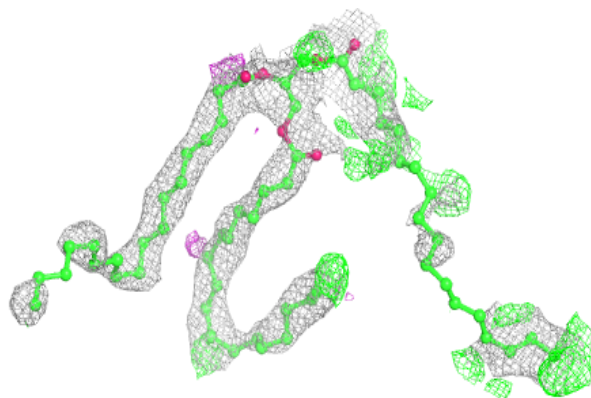


Electron density around CHD P 305:

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

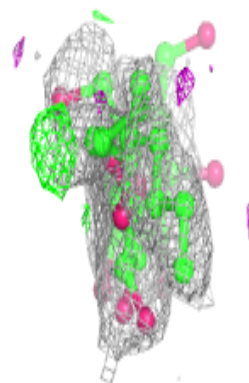
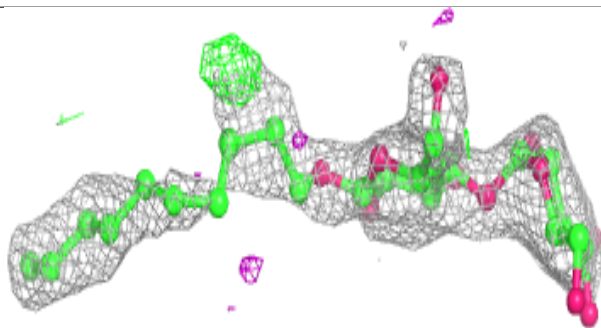
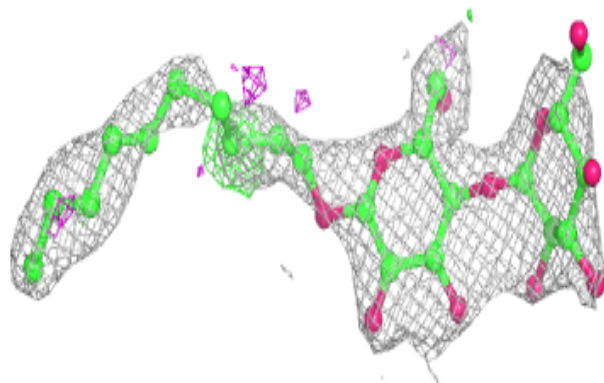
**Electron density around TGL Q 201:**

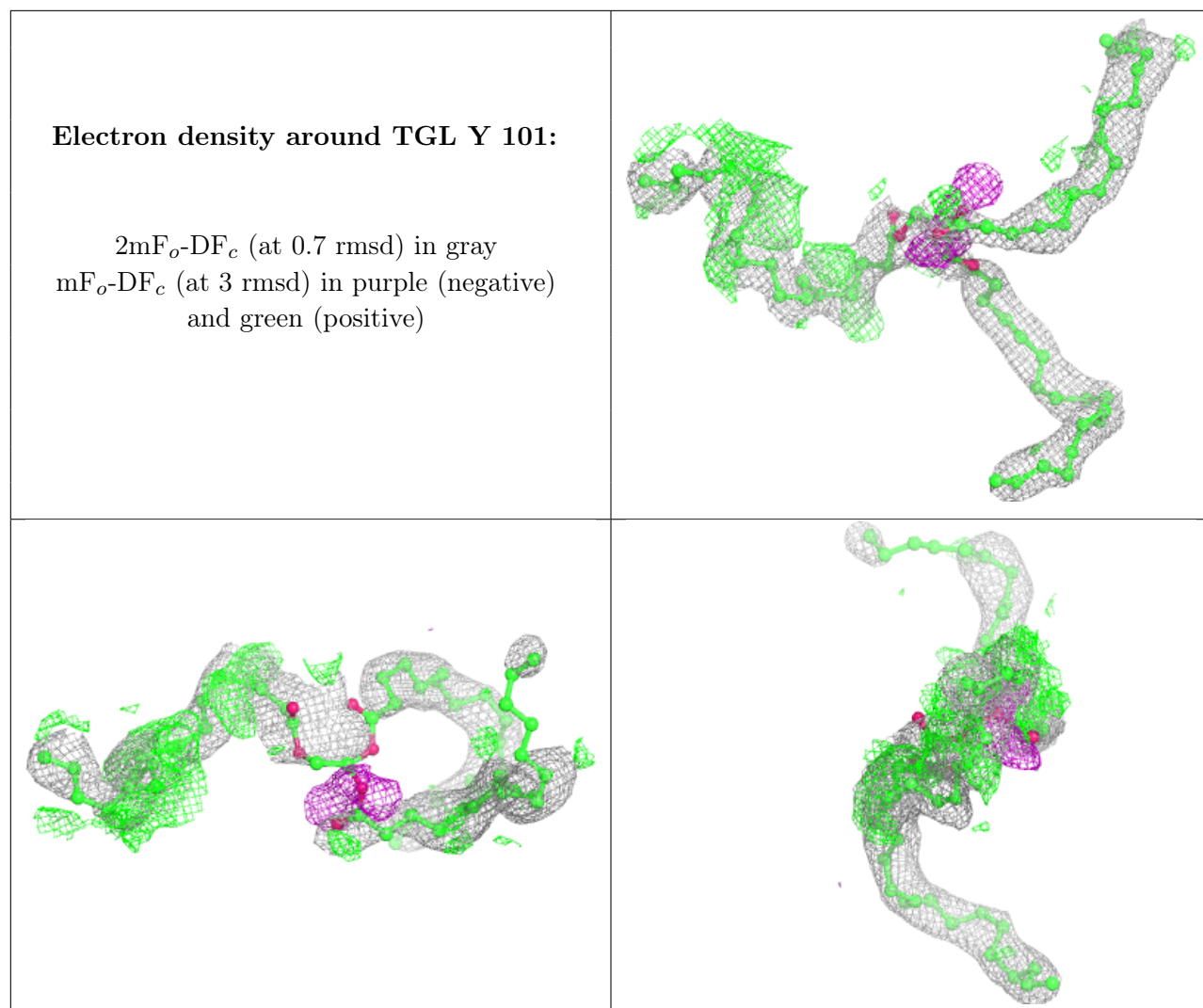
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DMU W 101:

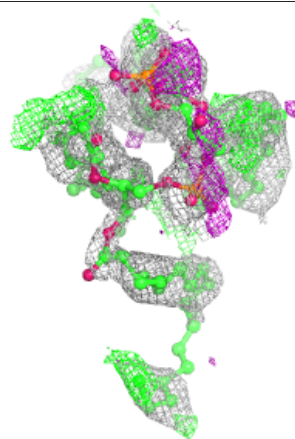
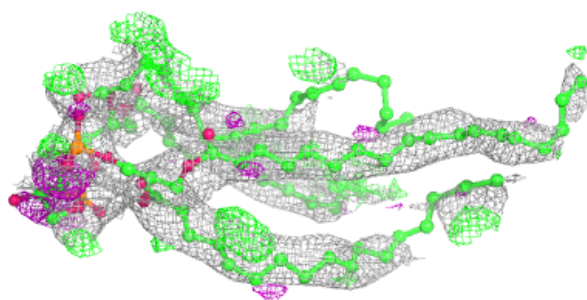
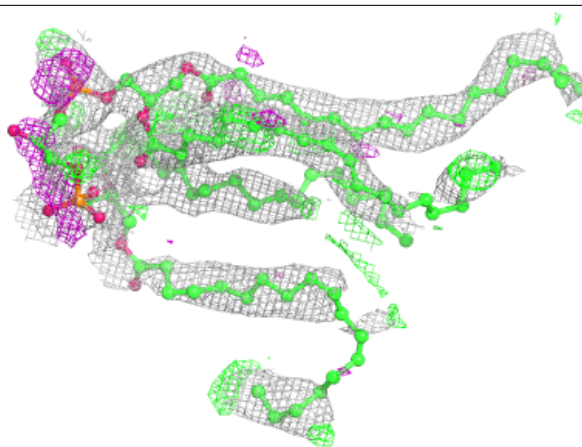
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



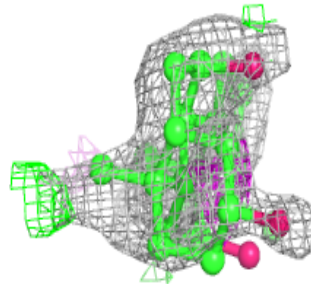
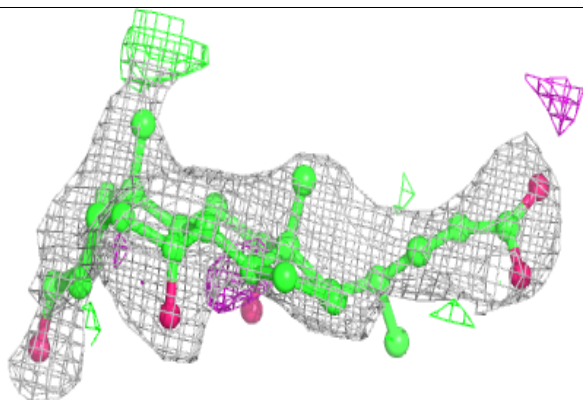
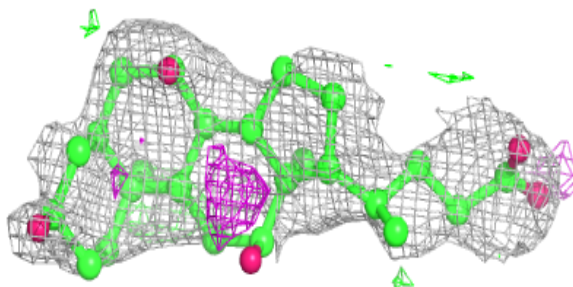


Electron density around CDL P 304:

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

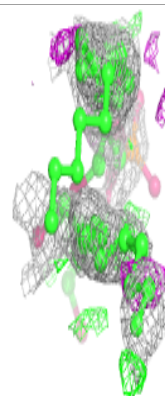
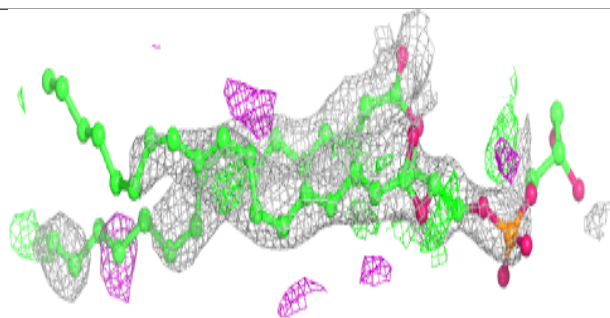
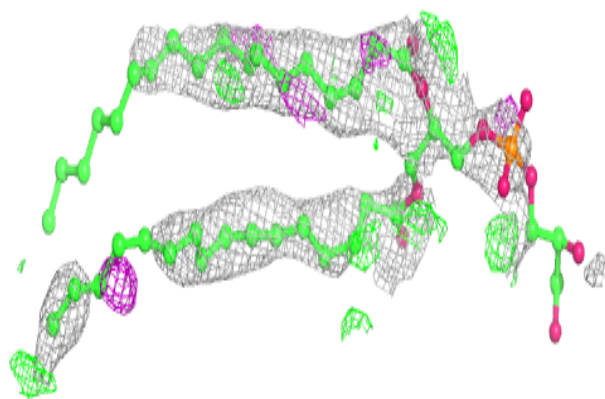
**Electron density around CHD C 303:**

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

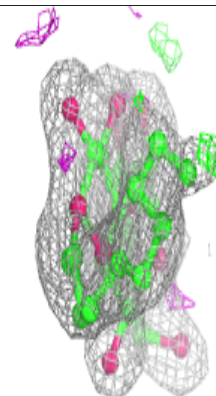
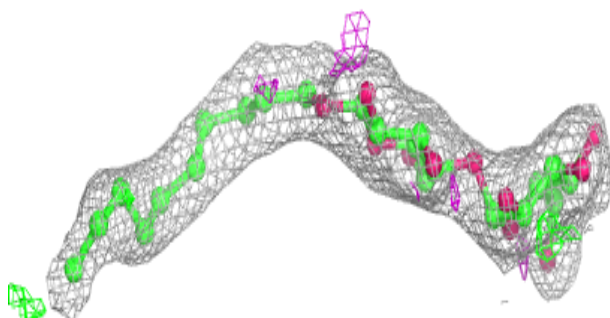
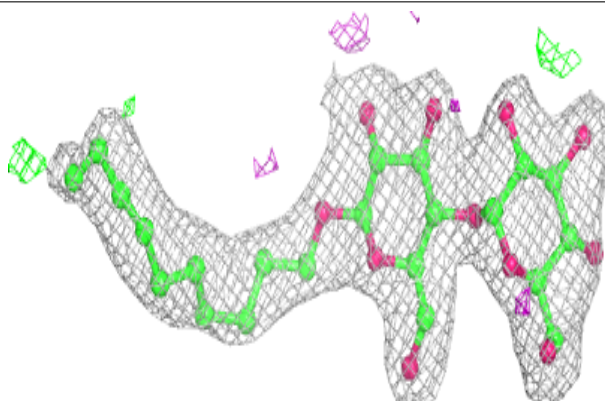


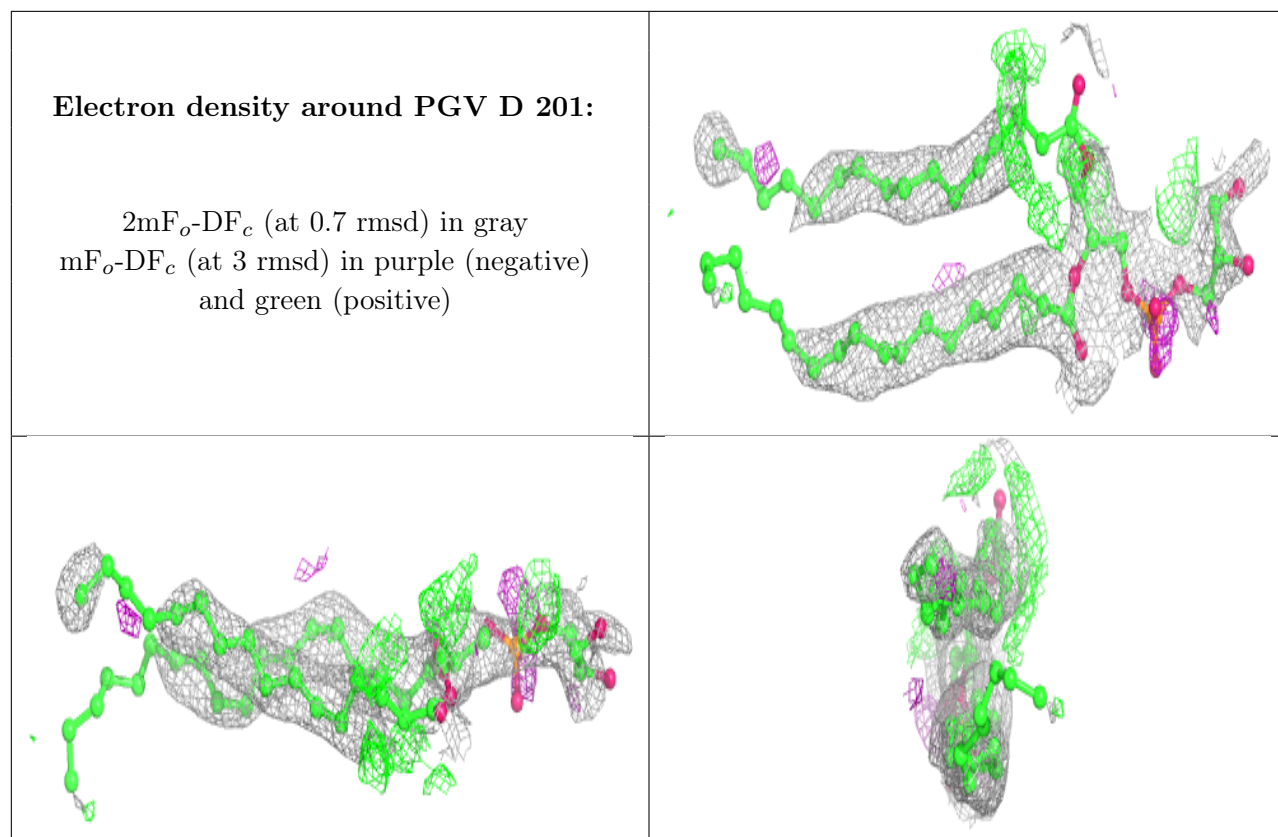
Electron density around PGV N 609:

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

**Electron density around DMU M 101:**

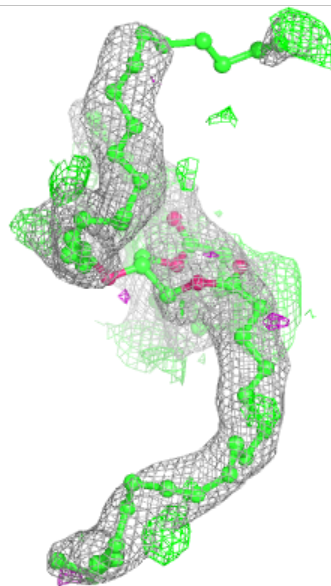
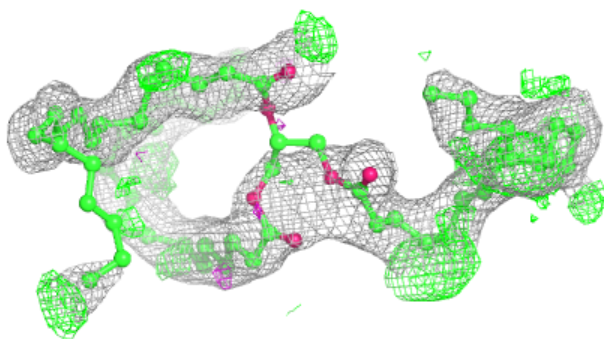
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





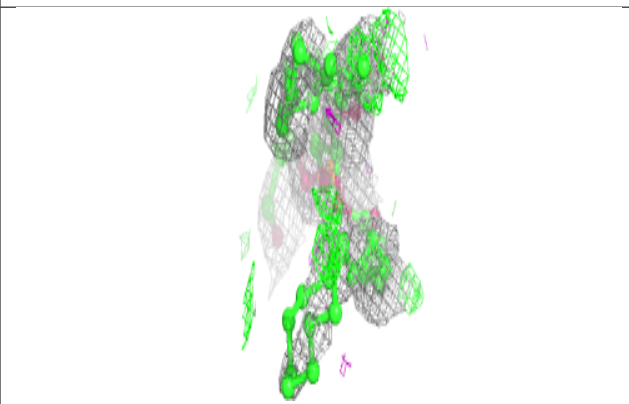
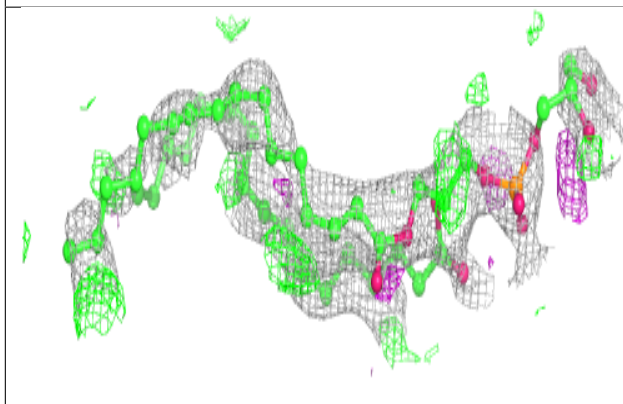
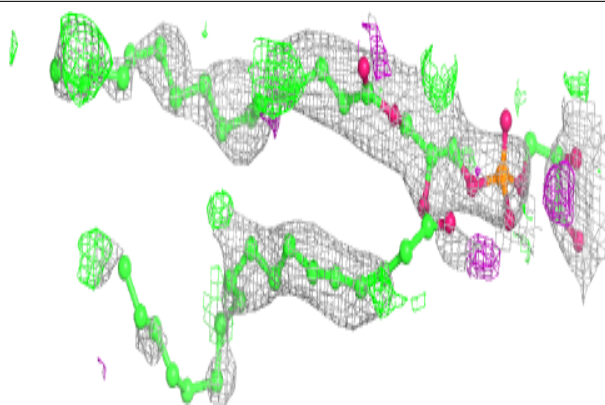
Electron density around TGL L 101:

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

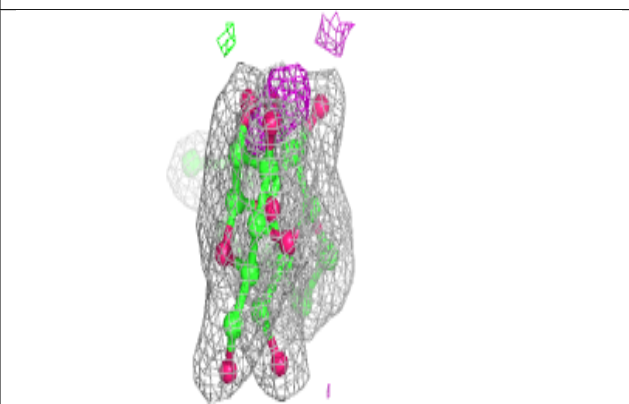
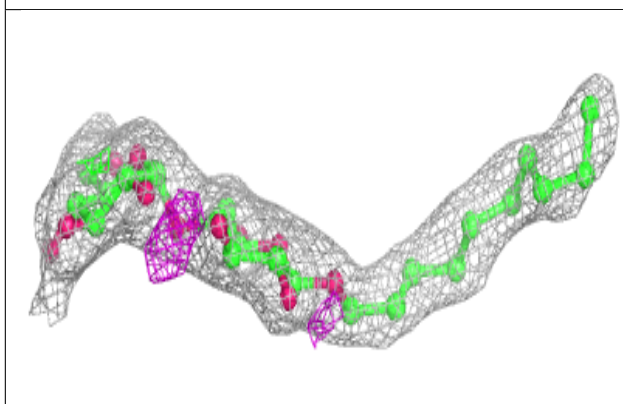
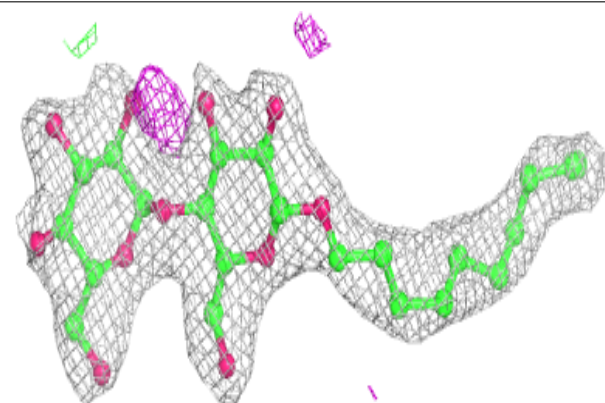


Electron density around PGV C 305:

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

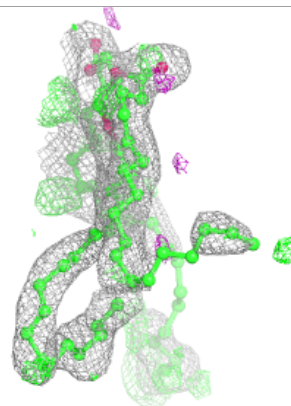
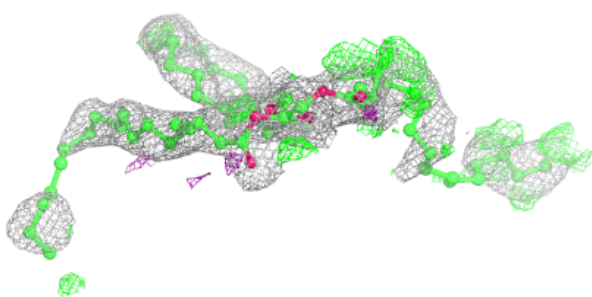
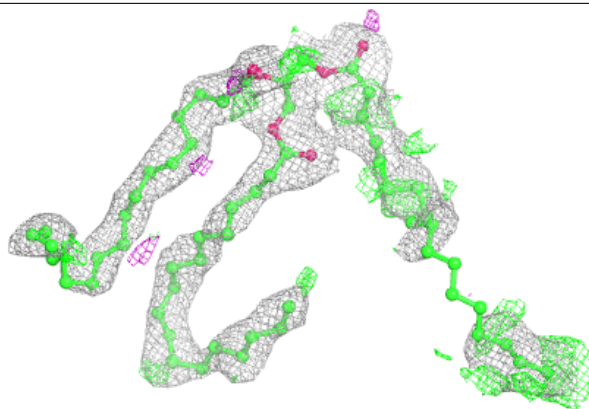
**Electron density around DMU Z 101:**

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

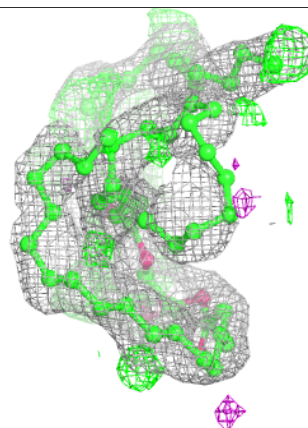
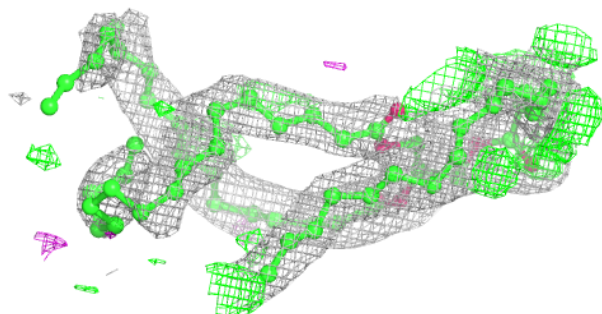
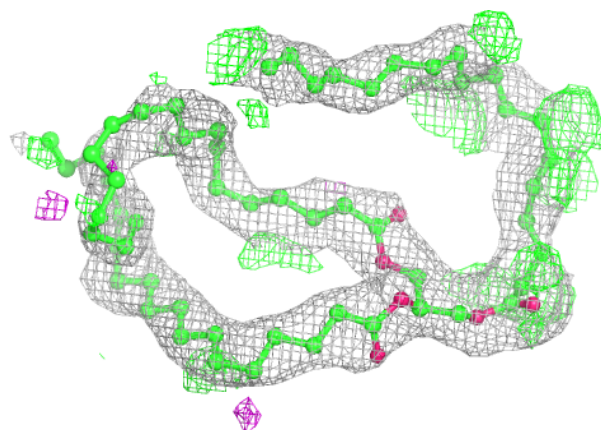


Electron density around TGL D 202:

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

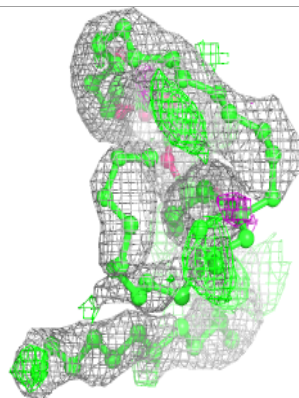
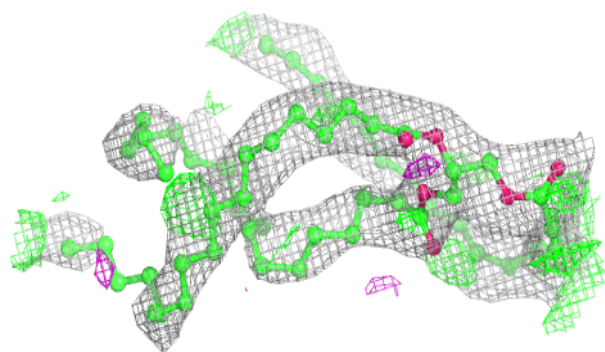
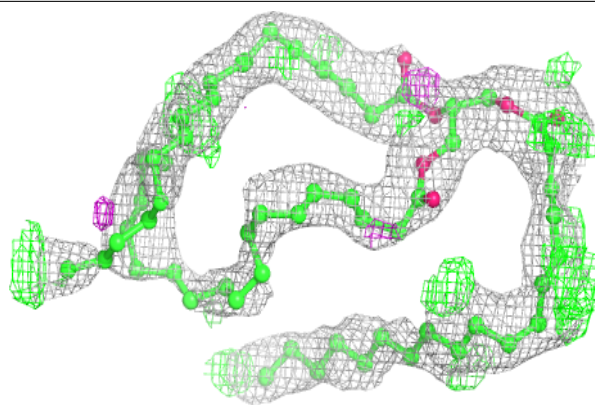
**Electron density around TGL A 608:**

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

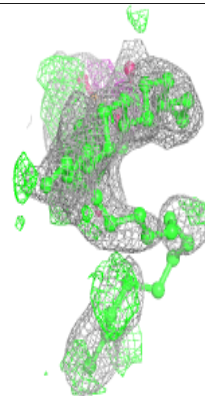
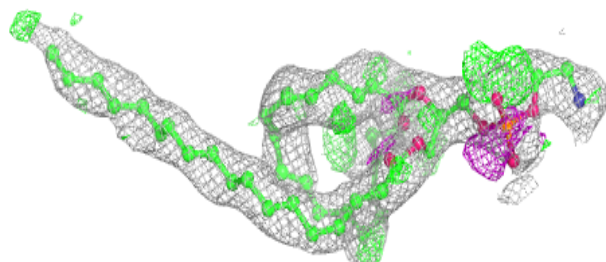
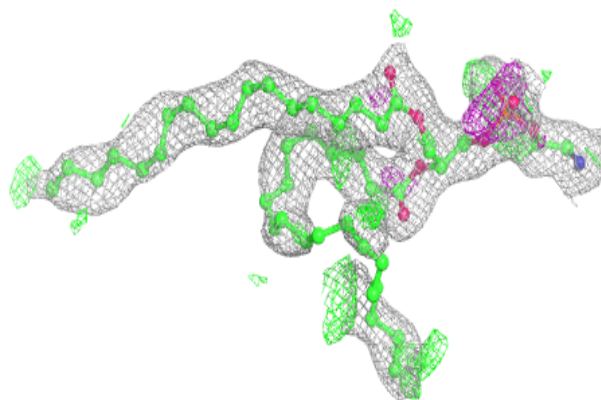


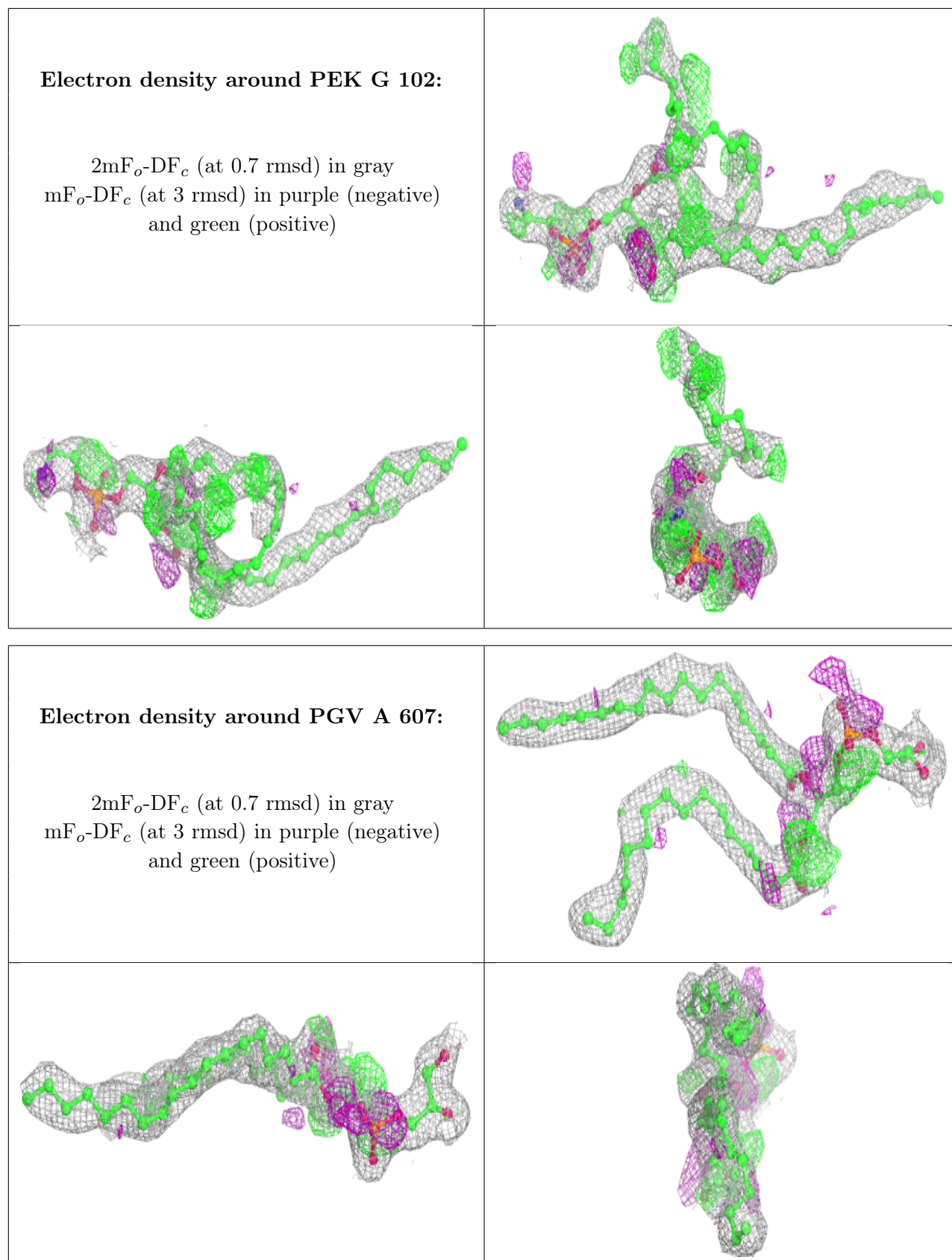
Electron density around TGL N 608:

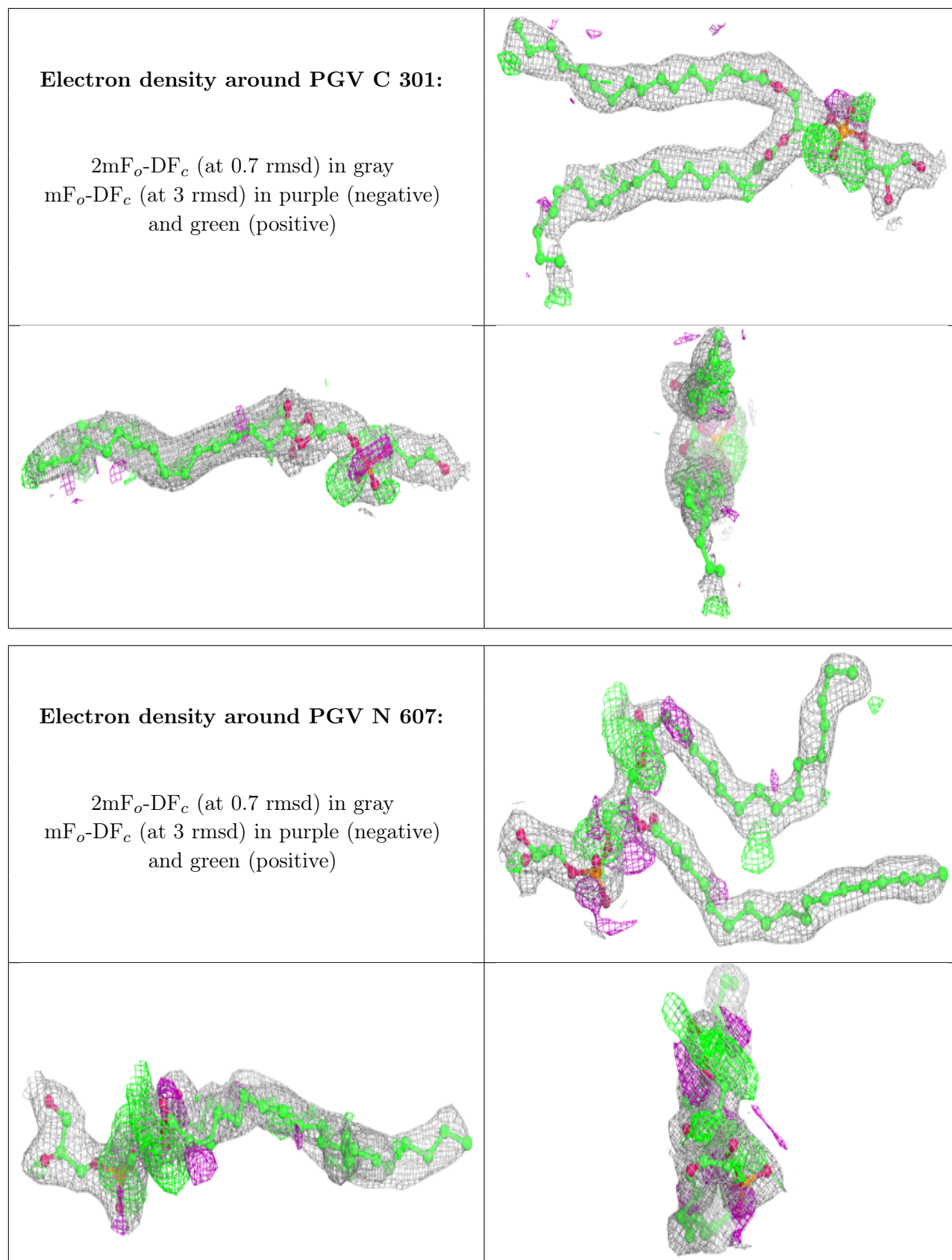
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

**Electron density around PEK T 102:**

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

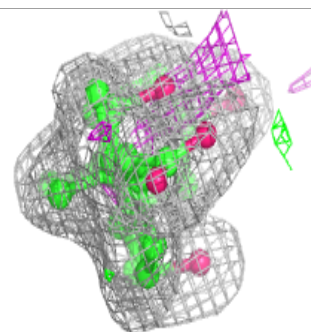
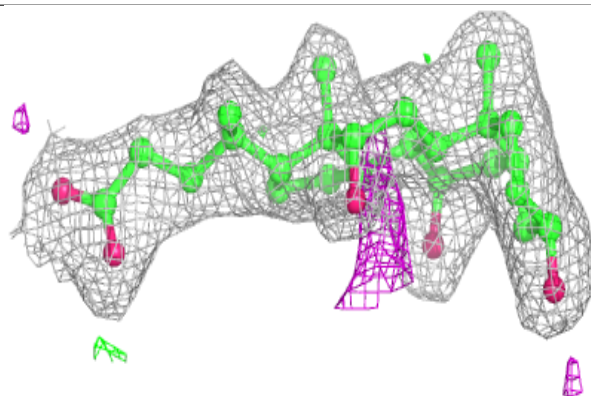
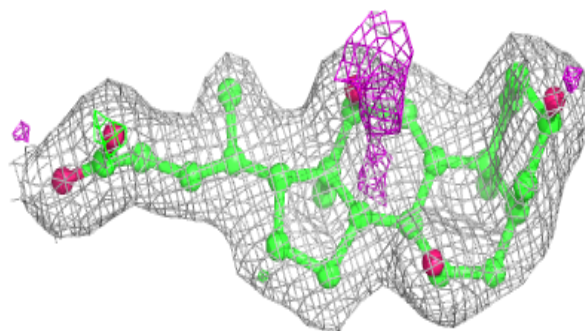




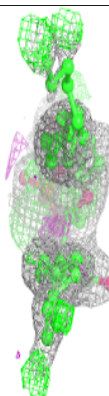
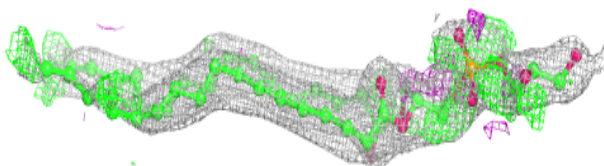
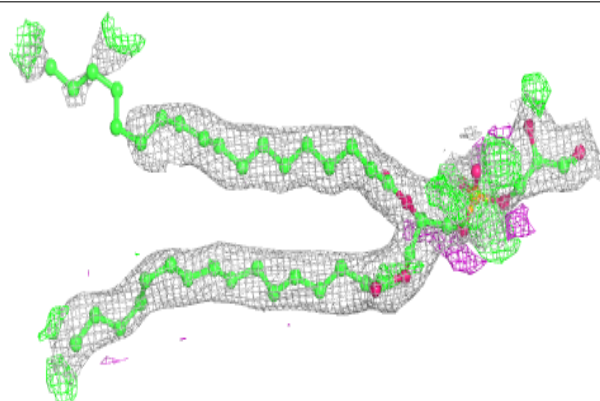


Electron density around CHD C 304:

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

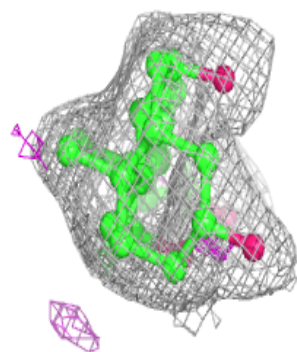
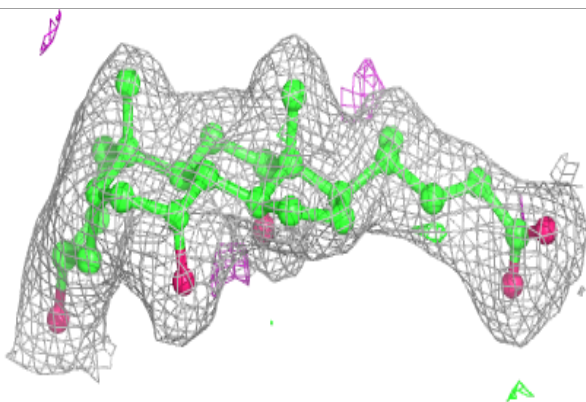
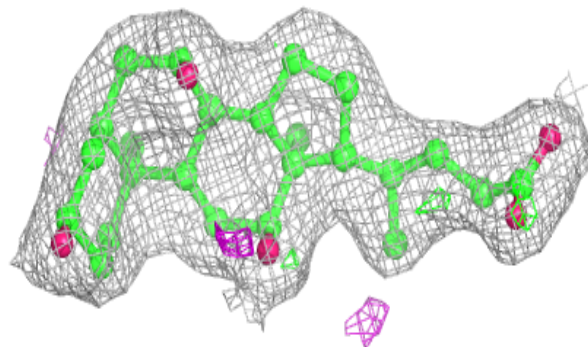
**Electron density around PGV P 303:**

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

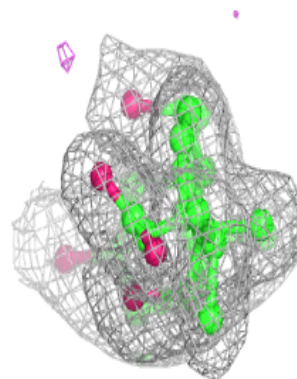
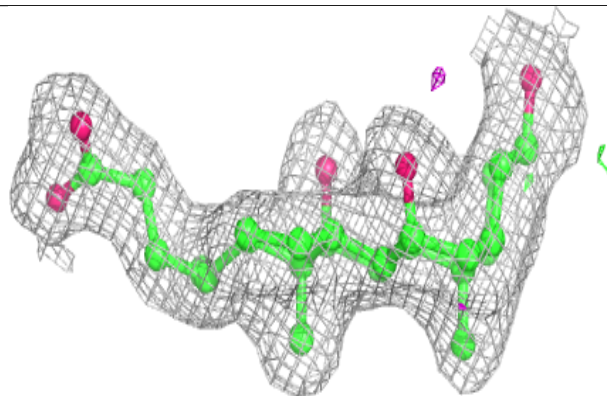
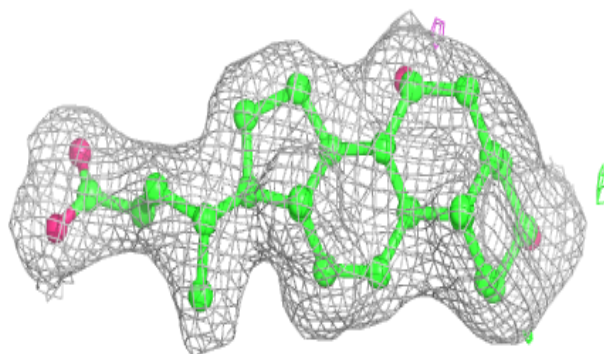


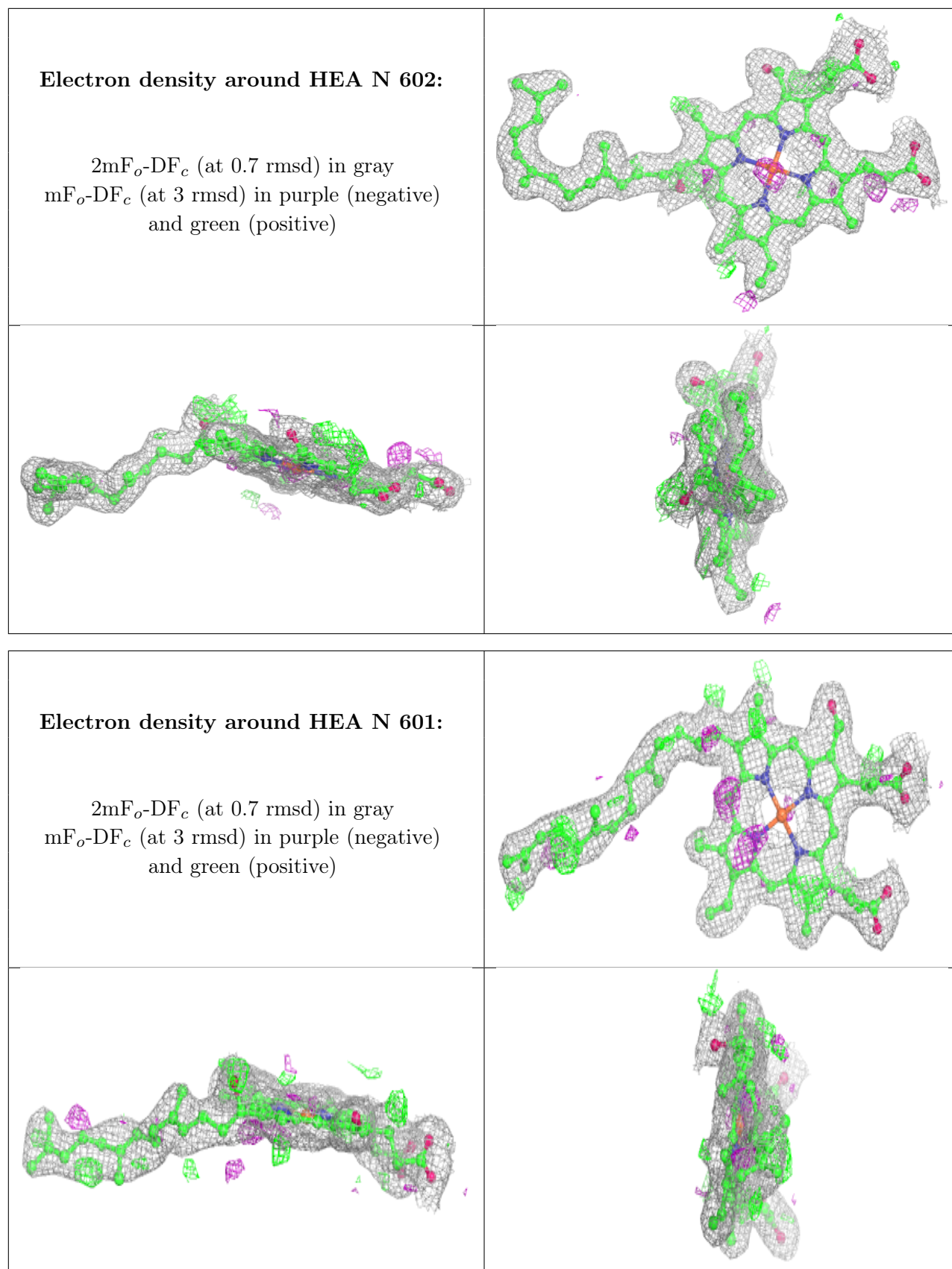
Electron density around CHD P 306:

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

**Electron density around CHD G 104:**

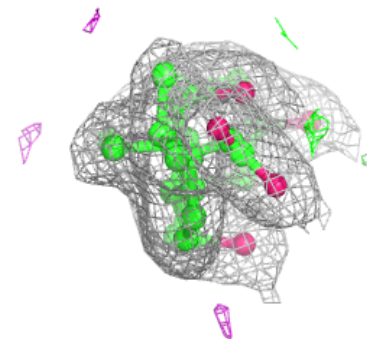
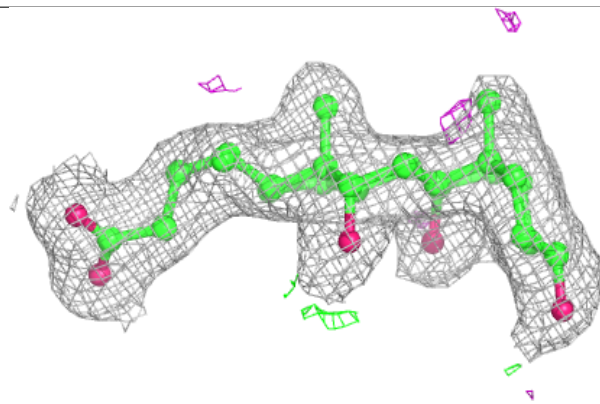
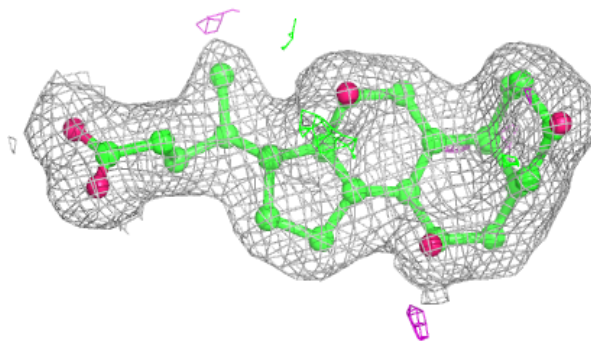
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



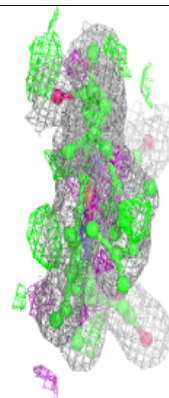
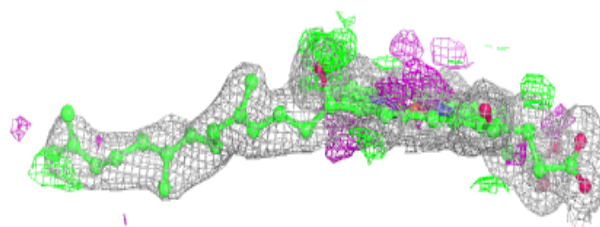
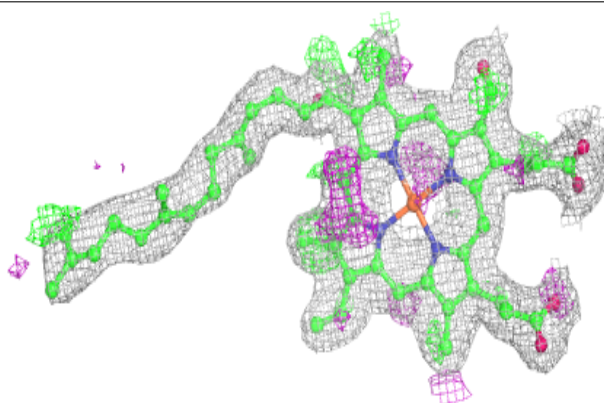


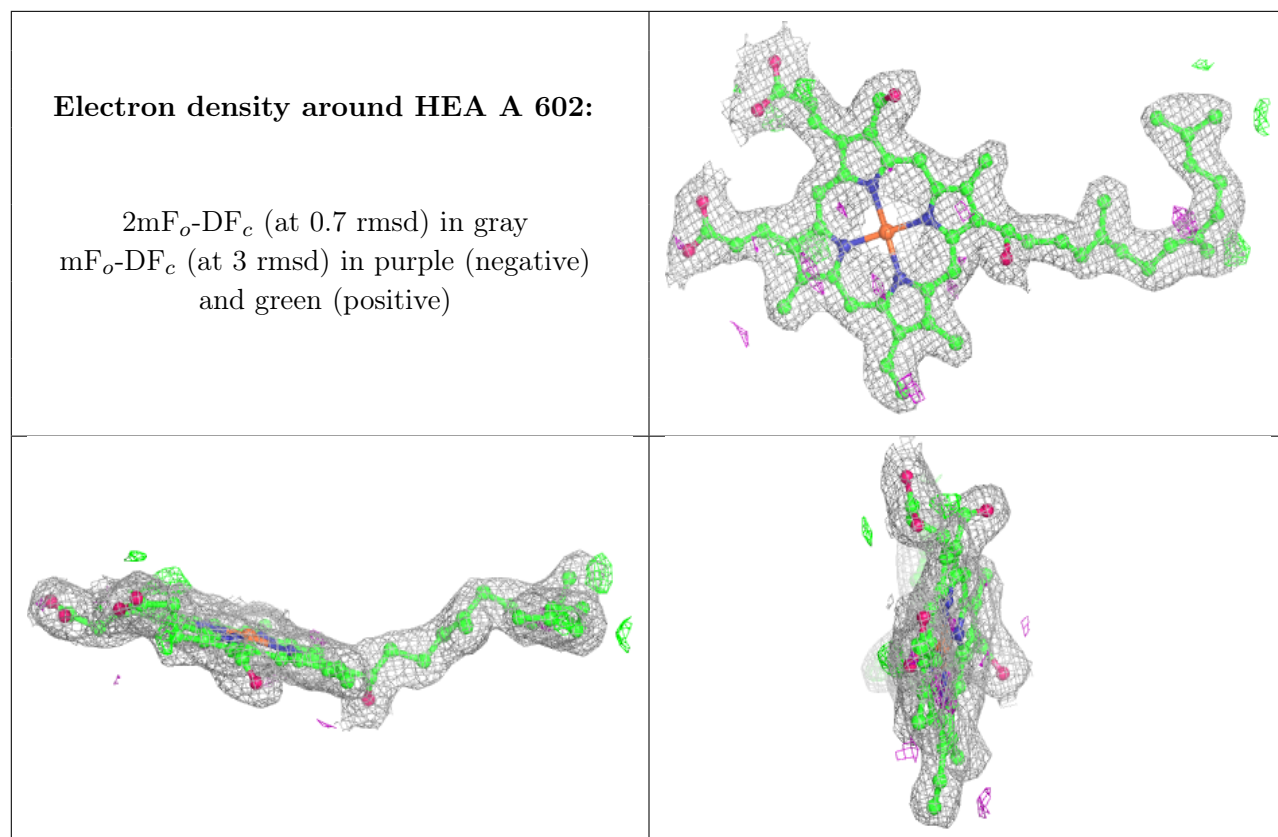
Electron density around CHD T 101:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.