



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:09 PM UTC

PDB ID : 6NKN / pdb_00006nkn
Title : Time-resolved SFX structure of the PR intermediate of cytochrome c oxidase at room temperature
Authors : Rousseau, D.L.; Yeh, S.-R.; Ishigami, I.
Deposited on : 2019-01-07
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

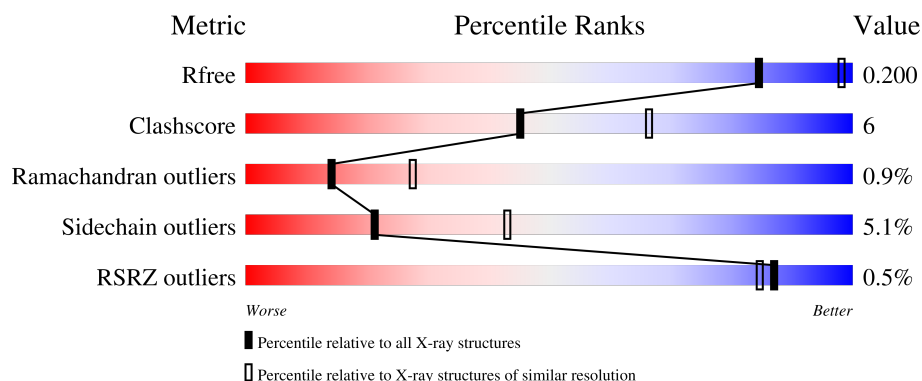
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



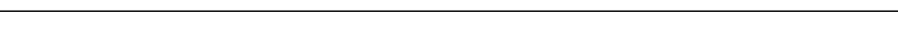
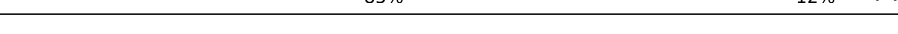
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	88% 11% .
1	N	514	81% 18% .
2	B	227	78% 21% .
2	O	227	77% 20% .
3	C	261	91% 7% .

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CDL	N	601	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 31419 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	139	Total	C	N	O	S	0	0	0
			1160	755	190	211	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	96	Total	C	N	O	S	0	0	0
			732	455	130	142	5			
6	S	94	Total	C	N	O	S	0	0	0
			721	449	128	139	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	78	Total	C	N	O	S	0	0	0
			653	411	119	118	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

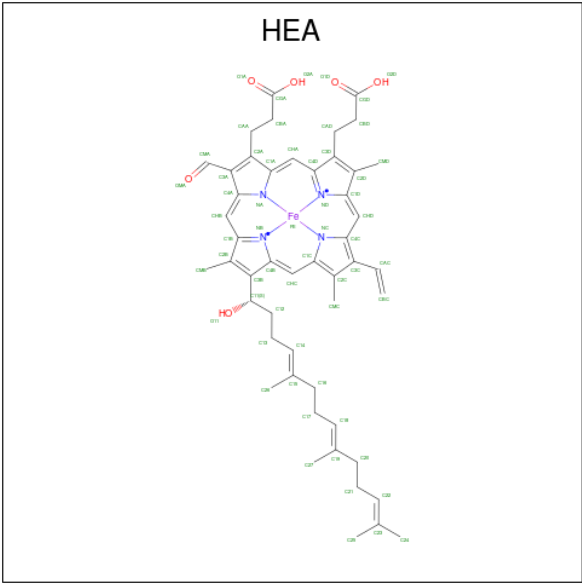
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

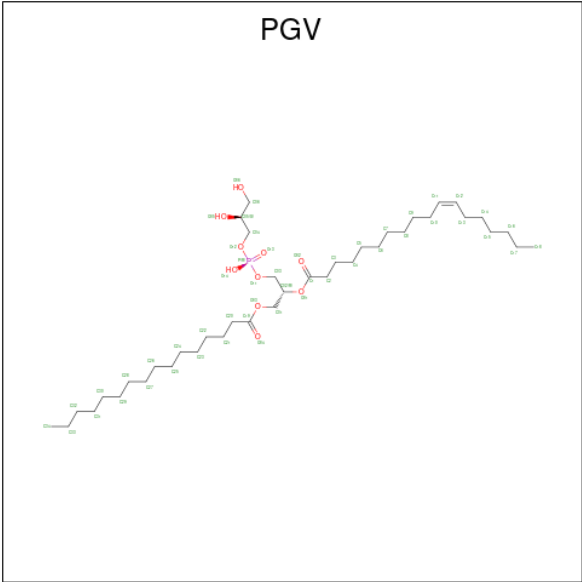
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



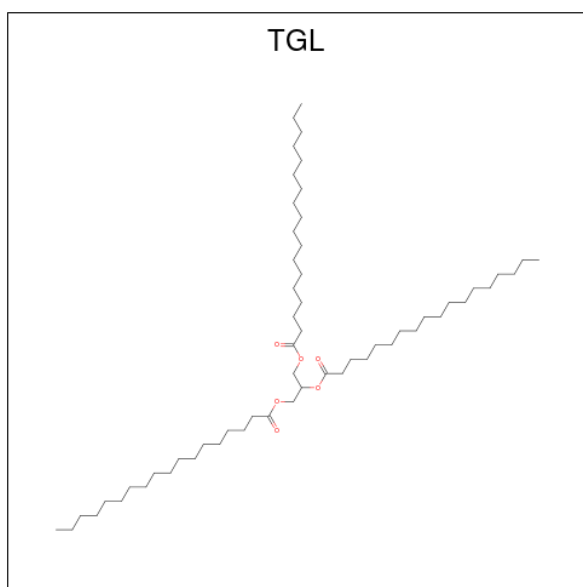
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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



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

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

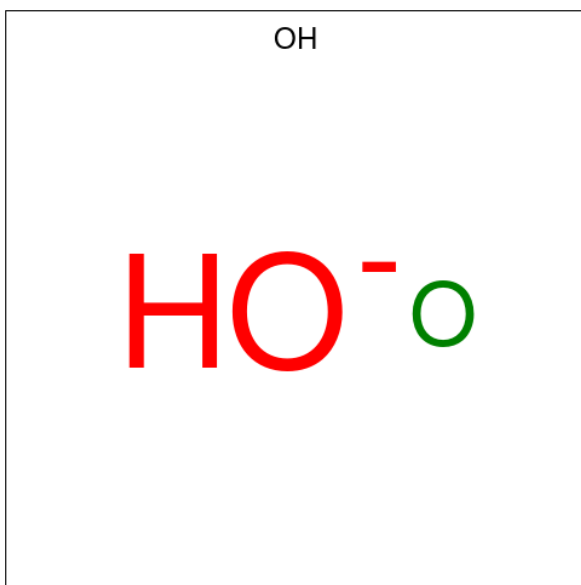


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	B	1	Total C O 63 57 6	0	0
19	L	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	Y	1	Total C O 63 57 6	0	0

- Molecule 20 is OXYGEN ATOM (CCD ID: O) (formula: O).

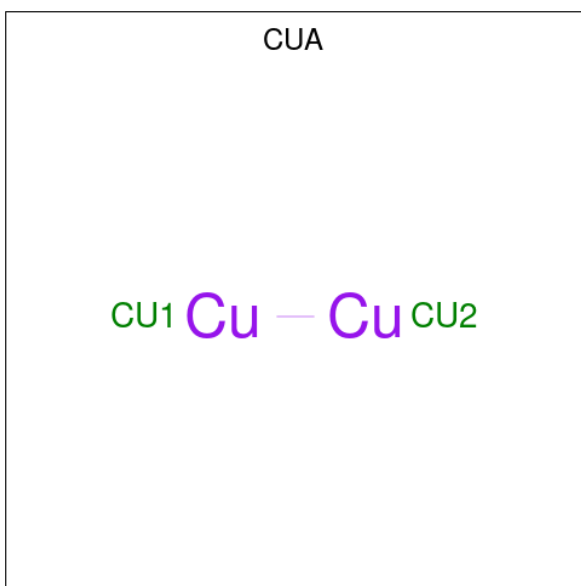
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total O 1 1	0	0
20	N	1	Total O 1 1	0	0

- Molecule 21 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



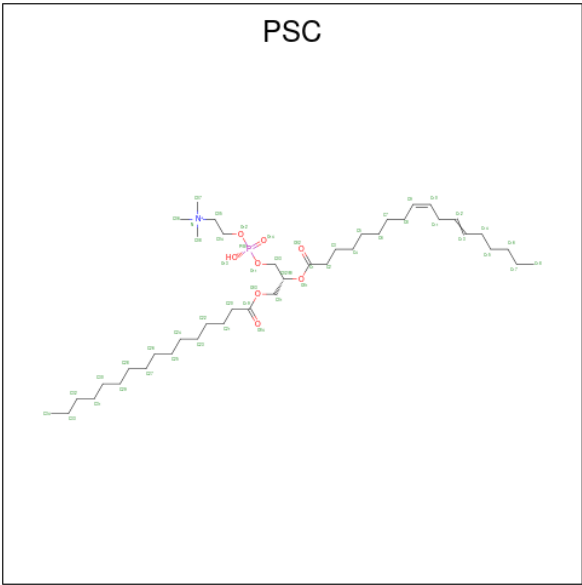
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total O 1 1	0	0
21	N	1	Total O 1 1	0	0

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



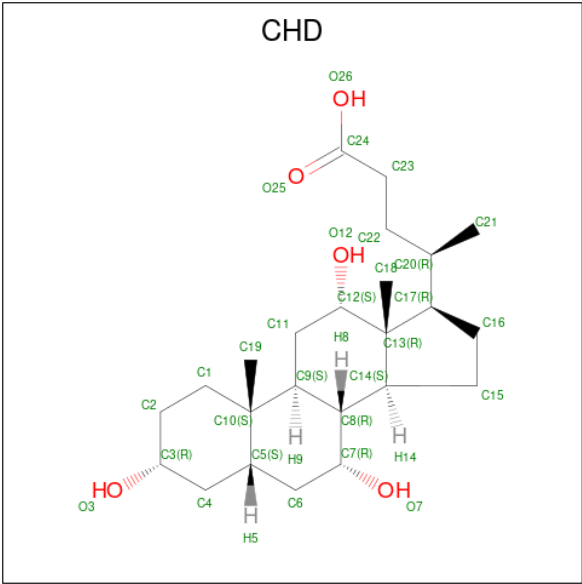
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



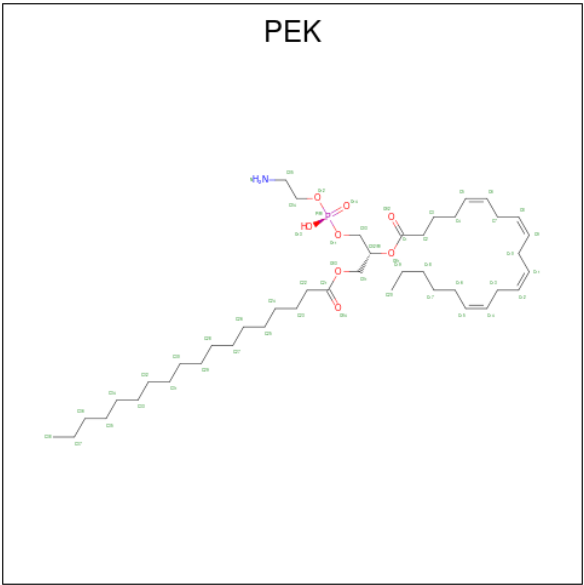
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 24 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



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

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



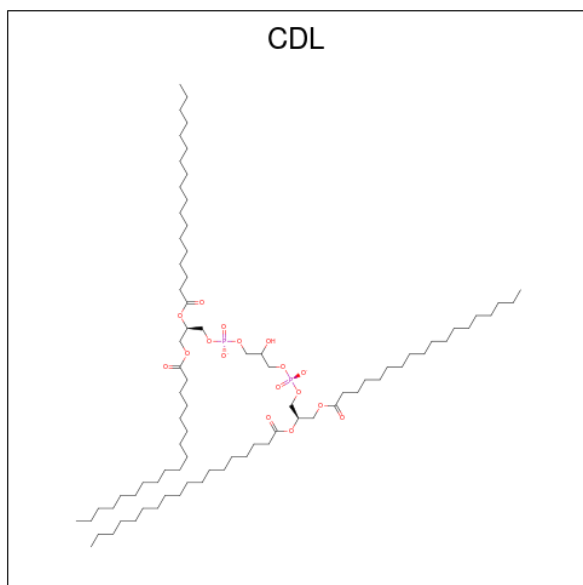
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

Continued on next page...

Continued from previous page...

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

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

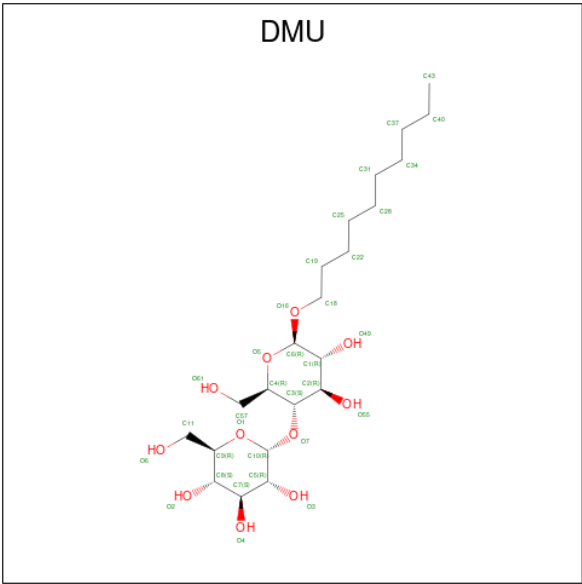


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	N	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

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

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

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	152	Total	O	0	0
			152	152		
29	B	102	Total	O	0	0
			102	102		
29	C	58	Total	O	0	0
			58	58		
29	D	45	Total	O	0	0
			45	45		
29	E	26	Total	O	0	0
			26	26		
29	F	36	Total	O	0	0
			36	36		

Continued on next page...

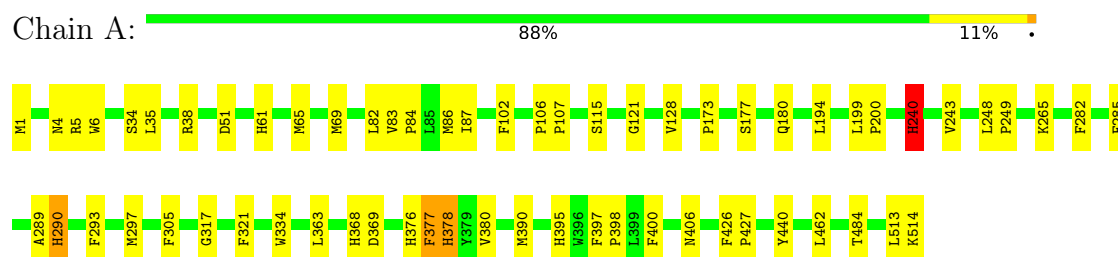
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	G	21	Total 21	O 21	0	0
29	H	21	Total 21	O 21	0	0
29	I	14	Total 14	O 14	0	0
29	J	10	Total 10	O 10	0	0
29	K	4	Total 4	O 4	0	0
29	L	9	Total 9	O 9	0	0
29	M	11	Total 11	O 11	0	0
29	N	84	Total 84	O 84	0	0
29	O	42	Total 42	O 42	0	0
29	P	36	Total 36	O 36	0	0
29	Q	18	Total 18	O 18	0	0
29	R	11	Total 11	O 11	0	0
29	S	22	Total 22	O 22	0	0
29	T	15	Total 15	O 15	0	0
29	U	7	Total 7	O 7	0	0
29	V	8	Total 8	O 8	0	0
29	W	7	Total 7	O 7	0	0
29	X	6	Total 6	O 6	0	0
29	Y	6	Total 6	O 6	0	0
29	Z	1	Total 1	O 1	0	0

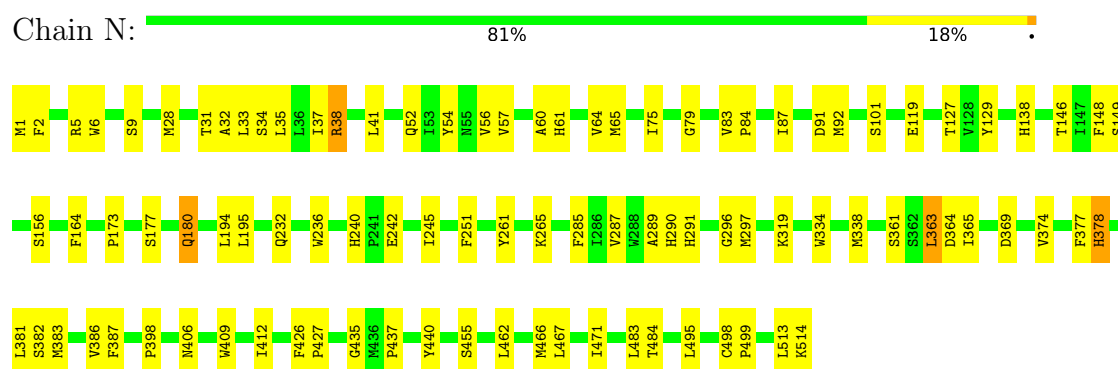
3 Residue-property plots

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

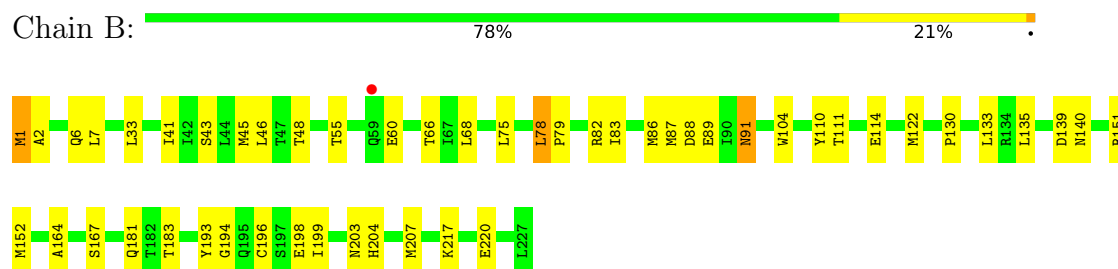
• Molecule 1: Cytochrome c oxidase subunit 1



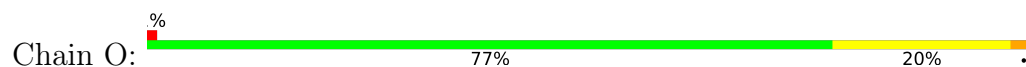
• Molecule 1: Cytochrome c oxidase subunit 1

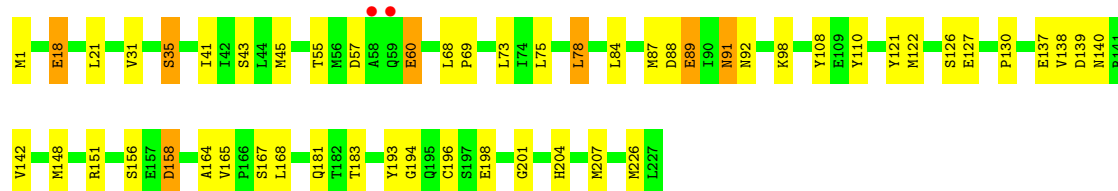


• Molecule 2: Cytochrome c oxidase subunit 2



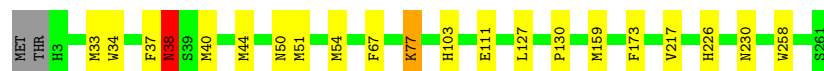
• Molecule 2: Cytochrome c oxidase subunit 2





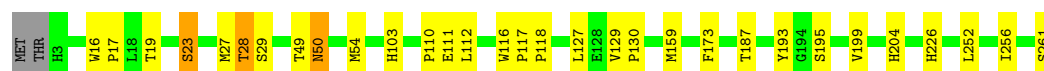
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 91% 7%



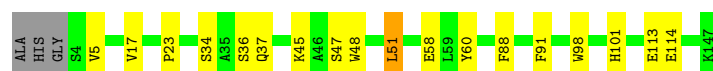
- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 87% 11%



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

Chain D: 86% 12%



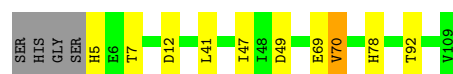
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 82% 12% 5%



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

Chain E: 87% 8%

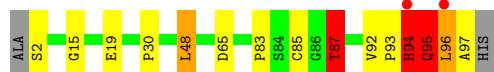
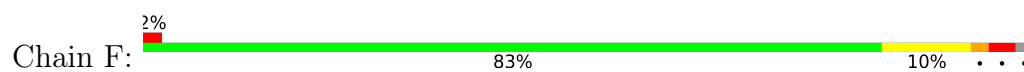


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

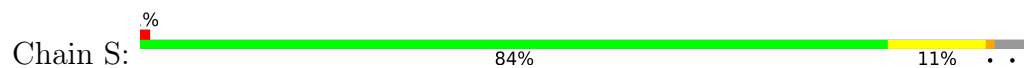
Chain R: 86% 9%



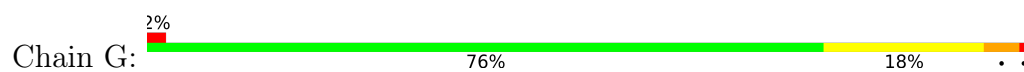
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



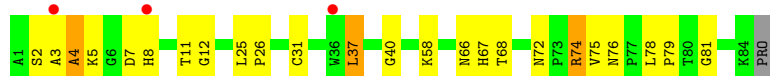
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



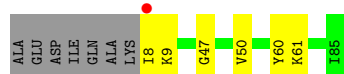
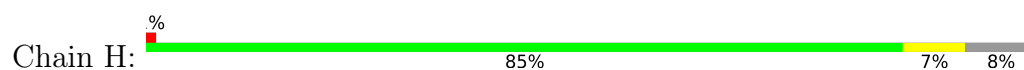
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



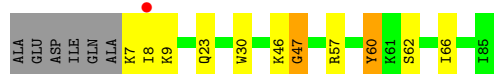
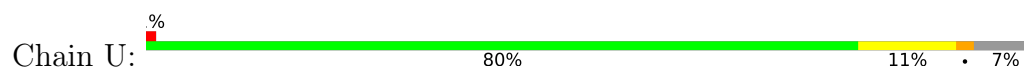
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



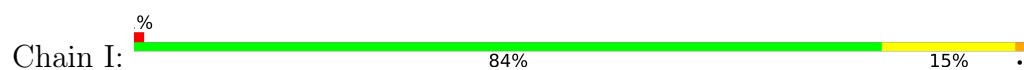
- Molecule 8: Cytochrome c oxidase subunit 6B1



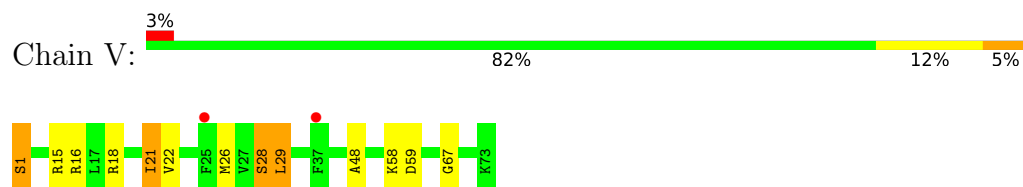
- Molecule 8: Cytochrome c oxidase subunit 6B1



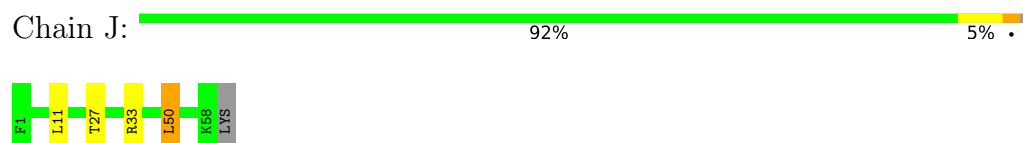
- Molecule 9: Cytochrome c oxidase subunit 6C



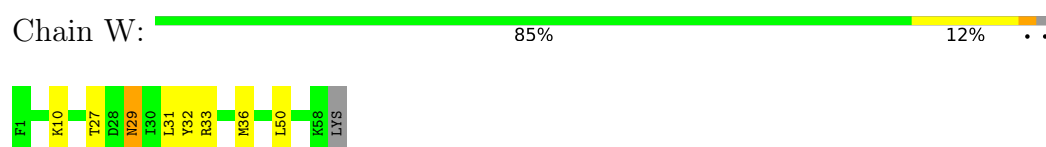
- Molecule 9: Cytochrome c oxidase subunit 6C



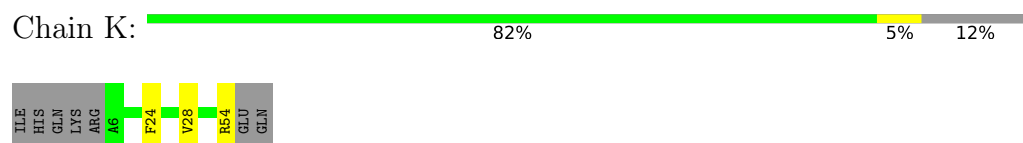
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



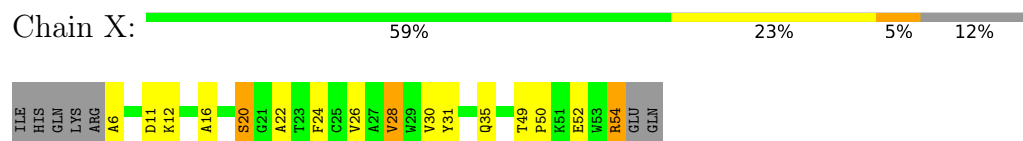
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



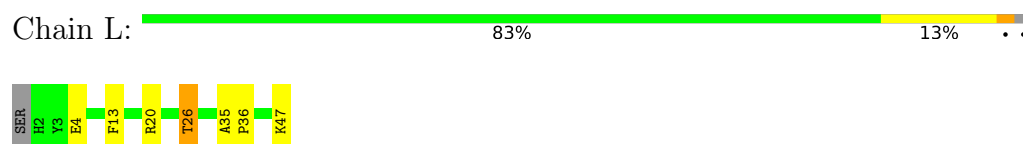
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



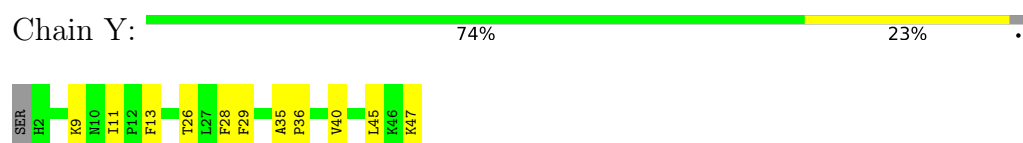
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

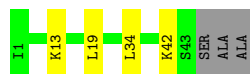


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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

Chain M:  85% 9% 7%



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

Chain Z:  72% 22% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.70Å 189.80Å 211.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.50 – 2.50 10.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (10.50-2.50) 98.5 (10.50-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.217 (Not available) , 0.200	Depositor DCC
R_{free} test set	12143 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31419	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, DMU, HEA, TPO, PEK, O, ZN, TGL, CDL, SAC, OH, MG, PSC, CHD, NA, FME, CUA, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.01	4/4156 (0.1%)	1.40	5/5678 (0.1%)
1	N	1.10	4/4156 (0.1%)	1.49	1/5678 (0.0%)
2	B	1.04	1/1860 (0.1%)	1.38	2/2534 (0.1%)
2	O	1.04	1/1860 (0.1%)	1.41	5/2534 (0.2%)
3	C	0.96	0/2197	1.40	0/3005
3	P	1.04	0/2197	1.47	9/3005 (0.3%)
4	D	1.00	0/1229	1.39	0/1658
4	Q	1.04	0/1194	1.43	4/1611 (0.2%)
5	E	1.00	0/871	1.47	0/1182
5	R	1.02	0/871	1.44	0/1182
6	F	1.02	0/748	1.45	4/1016 (0.4%)
6	S	1.03	0/737	1.43	2/1001 (0.2%)
7	G	1.04	0/690	1.41	0/937
7	T	1.05	1/690 (0.1%)	1.45	1/937 (0.1%)
8	H	1.00	0/673	1.48	0/910
8	U	1.01	1/682 (0.1%)	1.45	0/921
9	I	0.97	0/605	1.50	0/802
9	V	1.04	0/605	1.60	3/802 (0.4%)
10	J	1.04	0/471	1.49	0/636
10	W	1.07	0/471	1.57	0/636
11	K	1.05	0/398	1.37	0/546
11	X	1.12	0/398	1.44	0/546
12	L	1.01	0/393	1.45	1/526 (0.2%)
12	Y	1.06	0/393	1.47	0/526
13	M	0.98	0/345	1.44	0/470
13	Z	1.03	0/345	1.51	2/470 (0.4%)
All	All	1.03	12/29235 (0.0%)	1.44	39/39749 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	1
6	F	0	1
6	S	0	1
9	V	0	1
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	10.93	1.37	1.23
2	O	198	GLU	C-O	7.52	1.33	1.23
1	N	61	HIS	CE1-NE2	6.89	1.39	1.32
1	A	378	HIS	CE1-NE2	6.77	1.39	1.32
1	N	378	HIS	CE1-NE2	6.47	1.39	1.32
8	U	9	LYS	N-CA	5.71	1.49	1.46
1	A	376	HIS	CE1-NE2	5.54	1.38	1.32
1	N	240	HIS	CG-ND1	5.26	1.44	1.38
1	A	290	HIS	CE1-NE2	5.22	1.37	1.32
7	T	75	VAL	N-CA	5.17	1.50	1.46
1	N	290	HIS	CE1-NE2	5.16	1.37	1.32
1	A	240	HIS	CG-ND1	5.07	1.43	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	PHE	CA-CB-CG	6.26	120.06	113.80
4	Q	112	GLU	CA-C-N	6.25	128.94	120.38
4	Q	112	GLU	C-N-CA	6.25	128.94	120.38
6	F	87	THR	N-CA-CB	6.18	119.10	110.26
3	P	29	SER	CA-C-N	6.14	126.80	119.98
3	P	29	SER	C-N-CA	6.14	126.80	119.98
1	A	102	PHE	CA-CB-CG	-6.01	107.79	113.80
6	S	24	ALA	CA-C-N	5.84	128.03	120.44
6	S	24	ALA	C-N-CA	5.84	128.03	120.44
2	B	193	TYR	CA-C-N	5.79	127.61	121.48
2	B	193	TYR	C-N-CA	5.79	127.61	121.48
3	P	204	HIS	CA-CB-CG	-5.77	108.03	113.80
1	A	265	LYS	N-CA-C	-5.54	106.35	113.23
7	T	81	GLY	CA-C-O	-5.54	118.33	122.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	CA-CB-CG	-5.53	108.27	113.80
2	O	158	ASP	CA-CB-CG	5.49	118.09	112.60
6	F	94	HIS	CA-C-N	5.47	131.99	121.54
6	F	94	HIS	C-N-CA	5.47	131.99	121.54
9	V	48	ALA	CA-C-N	5.42	127.81	120.44
9	V	48	ALA	C-N-CA	5.42	127.81	120.44
6	F	83	PRO	CB-CA-C	-5.36	103.79	111.62
3	P	19	THR	CA-C-N	5.29	125.81	119.94
3	P	19	THR	C-N-CA	5.29	125.81	119.94
2	O	193	TYR	CA-C-N	5.27	126.25	121.82
2	O	193	TYR	C-N-CA	5.27	126.25	121.82
2	O	201	GLY	CA-C-N	5.25	127.27	120.44
2	O	201	GLY	C-N-CA	5.25	127.27	120.44
9	V	59	ASP	CA-CB-CG	5.22	117.82	112.60
3	P	173	PHE	CA-C-N	5.20	127.56	120.54
3	P	173	PHE	C-N-CA	5.20	127.56	120.54
4	Q	83	GLY	CA-C-N	5.20	127.24	120.28
4	Q	83	GLY	C-N-CA	5.20	127.24	120.28
13	Z	17	ILE	CA-C-N	5.18	125.84	119.99
13	Z	17	ILE	C-N-CA	5.18	125.84	119.99
12	L	26	THR	CA-CB-OG1	-5.16	101.86	109.60
1	N	287	VAL	CA-C-O	-5.13	114.92	119.38
3	P	103	HIS	CA-C-N	5.07	127.49	120.29
3	P	103	HIS	C-N-CA	5.07	127.49	120.29
1	A	395	HIS	O-C-N	5.05	127.27	122.07

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	368	HIS	Sidechain
6	F	93	PRO	Peptide
1	N	291	HIS	Sidechain
6	S	93	PRO	Peptide
9	V	1	SAC	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	34	0
1	N	4027	0	4001	56	0
2	B	1824	0	1833	24	0
2	O	1824	0	1833	27	0
3	C	2110	0	2027	13	0
3	P	2110	0	2027	16	0
4	D	1195	0	1183	7	0
4	Q	1160	0	1142	14	0
5	E	852	0	845	6	0
5	R	852	0	845	2	0
6	F	732	0	713	8	0
6	S	721	0	703	4	0
7	G	675	0	643	10	0
7	T	675	0	643	17	0
8	H	653	0	610	1	0
8	U	662	0	623	5	0
9	I	601	0	612	5	0
9	V	601	0	613	9	0
10	J	460	0	459	4	0
10	W	460	0	459	5	0
11	K	384	0	366	1	0
11	X	384	0	366	9	0
12	L	380	0	380	7	0
12	Y	380	0	380	7	0
13	M	335	0	352	0	0
13	Z	335	0	352	4	0
14	A	1	0	0	0	0
14	N	1	0	0	0	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	120	0	108	4	0
17	N	120	0	108	6	0
18	A	153	0	228	5	0
18	C	51	0	76	0	0
18	N	102	0	152	1	0
18	P	51	0	76	0	0
18	U	51	0	76	0	0
19	A	63	0	109	1	0
19	B	63	0	110	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	63	0	110	12	0
19	N	126	0	220	20	0
19	Y	63	0	110	2	0
20	A	1	0	0	1	0
20	N	1	0	0	0	0
21	A	1	0	0	1	0
21	N	1	0	0	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	6	0
23	O	52	0	80	3	0
24	B	29	0	39	0	0
24	C	29	0	39	1	0
24	G	29	0	39	0	0
24	J	58	0	78	4	0
24	P	29	0	39	1	0
24	W	58	0	78	2	0
25	C	53	0	77	3	0
25	G	106	0	154	2	0
25	P	106	0	154	2	0
25	T	53	0	77	2	0
26	C	100	0	156	14	0
26	N	100	0	156	23	0
26	P	100	0	156	9	0
26	T	100	0	156	1	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	42	3	0
28	M	33	0	42	2	0
28	Q	33	0	42	0	0
28	T	33	0	42	0	0
29	A	152	0	0	3	0
29	B	102	0	0	5	0
29	C	58	0	0	2	0
29	D	45	0	0	1	0
29	E	26	0	0	0	0
29	F	36	0	0	2	0
29	G	21	0	0	4	0
29	H	21	0	0	1	0
29	I	14	0	0	0	0
29	J	10	0	0	3	0
29	K	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	L	9	0	0	0	0
29	M	11	0	0	1	0
29	N	84	0	0	3	0
29	O	42	0	0	1	0
29	P	36	0	0	0	0
29	Q	18	0	0	8	0
29	R	11	0	0	0	0
29	S	22	0	0	2	0
29	T	15	0	0	4	0
29	U	7	0	0	2	0
29	V	8	0	0	6	0
29	W	7	0	0	1	0
29	X	6	0	0	2	0
29	Y	6	0	0	1	0
29	Z	1	0	0	0	0
All	All	31419	0	31220	365	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 (365) 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:607:TGL:OG1	29:N:701:HOH:O	1.67	1.11
12:L:20:ARG:HH22	19:L:101:TGL:HC52	1.12	1.06
4:Q:19:ARG:CD	29:Q:301:HOH:O	2.03	1.04
6:F:19:GLU:HG2	29:F:235:HOH:O	1.62	0.98
4:Q:19:ARG:HD3	29:Q:301:HOH:O	1.63	0.91
19:N:607:TGL:H272	19:N:607:TGL:H222	1.51	0.90
1:A:1:FME:HCN	1:A:4:ASN:HD22	1.40	0.86
19:A:609:TGL:H281	29:B:500:HOH:O	1.75	0.86
1:N:180:GLN:CD	29:N:708:HOH:O	2.19	0.85
12:L:20:ARG:HH22	19:L:101:TGL:CC5	1.88	0.85
19:L:101:TGL:HC61	19:L:101:TGL:HC22	1.60	0.83
19:N:609:TGL:H192	19:N:609:TGL:H362	1.61	0.82
7:G:76:ASN:HD21	25:G:102:PEK:HN2	1.28	0.81
12:Y:9:LYS:HG3	29:Y:204:HOH:O	1.79	0.80
12:L:20:ARG:NH2	19:L:101:TGL:HC52	1.93	0.80
1:A:35:LEU:HG	29:A:849:HOH:O	1.83	0.78
26:C:304:CDL:HB21	26:C:304:CDL:HB32	1.66	0.77
2:B:82:ARG:NH1	29:B:401:HOH:O	2.16	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:607:TGL:H301	19:N:607:TGL:H122	1.66	0.77
4:Q:9:GLU:HA	29:Q:317:HOH:O	1.84	0.76
25:P:302:PEK:HN2	7:T:76:ASN:HD21	1.34	0.76
26:N:601:CDL:H511	26:N:601:CDL:H231	1.66	0.75
10:W:32:TYR:CE2	29:W:201:HOH:O	2.40	0.74
1:N:334:TRP:CE3	19:N:609:TGL:HA31	2.23	0.74
7:G:72:ASN:H	7:G:76:ASN:HD22	1.32	0.73
12:L:13:PHE:HA	19:L:101:TGL:HC32	1.69	0.73
19:N:609:TGL:H231	19:N:609:TGL:HA71	1.73	0.71
19:N:607:TGL:HC61	29:Q:318:HOH:O	1.91	0.70
6:F:85:CYS:SG	6:F:87:THR:HG23	2.32	0.69
7:G:12:GLY:HA3	29:G:215:HOH:O	1.92	0.69
3:C:111:GLU:HB3	29:H:120:HOH:O	1.93	0.67
26:N:601:CDL:H782	26:N:601:CDL:C56	2.25	0.67
26:N:601:CDL:H782	26:N:601:CDL:C55	2.24	0.67
19:L:101:TGL:H202	19:L:101:TGL:C24	2.24	0.67
1:N:462:LEU:HG	1:N:466:MET:HE2	1.77	0.66
2:B:89:GLU:O	2:B:91:ASN:OD1	2.13	0.66
26:P:305:CDL:HB32	26:P:305:CDL:HB21	1.76	0.66
26:N:601:CDL:H181	26:N:601:CDL:HB32	1.79	0.65
26:N:601:CDL:H231	26:N:601:CDL:C51	2.26	0.65
17:A:605:HEA:HBC1	17:A:605:HEA:HMC1	1.79	0.65
7:T:5:LYS:HD2	25:T:102:PEK:H383	1.79	0.65
26:N:601:CDL:H782	26:N:601:CDL:C54	2.27	0.64
4:Q:109:HIS:HD2	29:Q:314:HOH:O	1.79	0.64
19:B:303:TGL:H212	19:B:303:TGL:H272	1.79	0.64
3:P:226:HIS:CE1	26:P:305:CDL:HB31	2.33	0.64
3:P:226:HIS:HE1	26:P:305:CDL:HB31	1.64	0.63
26:C:304:CDL:HA4	26:C:304:CDL:H122	1.80	0.62
1:N:60:ALA:O	1:N:64:VAL:HG23	1.99	0.62
26:C:304:CDL:OA3	26:C:304:CDL:O1	2.16	0.62
24:W:102:CHD:H183	24:W:102:CHD:H222	1.80	0.62
19:L:101:TGL:HC61	19:L:101:TGL:CC2	2.28	0.62
20:A:610:O:O	21:A:611:OH:O	2.18	0.62
7:T:72:ASN:H	7:T:76:ASN:HD22	1.46	0.62
1:N:398:PRO:O	1:N:498:CYS:HB3	2.01	0.61
19:N:607:TGL:HA41	19:N:607:TGL:OA1	2.00	0.61
10:W:32:TYR:HE1	10:W:36:MET:HE2	1.66	0.61
26:P:305:CDL:HA4	26:P:305:CDL:H122	1.83	0.60
23:B:302:PSC:O12	23:B:302:PSC:H072	2.02	0.60
26:C:304:CDL:H432	26:C:304:CDL:C38	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:601:CDL:H511	26:N:601:CDL:C23	2.31	0.60
3:C:67:PHE:HE2	26:C:304:CDL:H1	1.67	0.59
26:N:601:CDL:H372	2:O:78:LEU:HD12	1.83	0.59
6:S:92:VAL:C	29:S:201:HOH:O	2.44	0.59
26:N:601:CDL:H372	2:O:78:LEU:CD1	2.32	0.59
9:V:29:LEU:HD13	29:V:106:HOH:O	2.02	0.59
25:C:302:PEK:H383	26:N:601:CDL:H272	1.84	0.59
2:O:41:ILE:O	2:O:45:MET:HG2	2.02	0.59
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.83	0.59
26:N:601:CDL:H351	26:N:601:CDL:OA7	2.03	0.59
23:O:302:PSC:O12	29:O:401:HOH:O	2.17	0.58
19:N:607:TGL:H272	19:N:607:TGL:C22	2.27	0.58
2:O:164:ALA:O	2:O:194:GLY:HA3	2.03	0.58
10:W:32:TYR:CE1	10:W:36:MET:HE2	2.38	0.58
1:A:289:ALA:HB1	1:A:297:MET:HE1	1.85	0.57
2:B:7:LEU:HD11	19:B:303:TGL:H161	1.85	0.57
6:F:94:HIS:O	6:F:96:LEU:HD12	2.04	0.57
7:T:5:LYS:NZ	29:T:202:HOH:O	2.38	0.57
10:W:29:ASN:HD22	10:W:29:ASN:H	1.53	0.57
11:X:16:ALA:O	11:X:20:SER:OG	2.23	0.57
1:N:54:TYR:O	1:N:57:VAL:HB	2.05	0.57
19:B:303:TGL:H212	19:B:303:TGL:C26	2.33	0.57
2:O:130:PRO:HA	4:Q:115:TRP:CZ2	2.40	0.56
1:A:321:PHE:CD1	23:B:302:PSC:H341	2.40	0.56
24:P:301:CHD:H183	24:P:301:CHD:H212	1.86	0.56
19:N:607:TGL:HA21	19:N:607:TGL:HB21	1.86	0.56
4:Q:109:HIS:CD2	29:Q:314:HOH:O	2.54	0.56
18:A:606:PGV:H341	29:M:211:HOH:O	2.06	0.56
26:N:601:CDL:H752	26:N:601:CDL:H562	1.87	0.55
19:B:303:TGL:H212	19:B:303:TGL:C27	2.36	0.55
26:C:304:CDL:H192	26:C:304:CDL:H621	1.88	0.55
26:P:305:CDL:H391	26:P:305:CDL:H221	1.88	0.55
26:C:304:CDL:HB32	26:C:304:CDL:CB2	2.34	0.55
6:F:30:PRO:O	6:F:96:LEU:HD23	2.06	0.55
19:B:303:TGL:H212	19:B:303:TGL:C25	2.37	0.55
7:G:62:TRP:HB3	28:G:101:DMU:O61	2.07	0.55
6:F:48:LEU:HG	6:F:92:VAL:HG11	1.89	0.54
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.42	0.54
11:X:54:ARG:C	29:X:105:HOH:O	2.50	0.54
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.89	0.54
29:A:803:HOH:O	3:C:77:LYS:HD2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:SER:H	4:D:37:GLN:NE2	2.05	0.54
1:N:261:TYR:HB2	1:N:338:MET:HE2	1.89	0.54
1:A:1:FME:HE2	1:A:1:FME:HA	1.89	0.54
7:T:31:CYS:SG	26:T:103:CDL:H532	2.49	0.53
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.08	0.53
24:J:101:CHD:H221	29:J:210:HOH:O	2.09	0.53
2:O:31:VAL:O	2:O:35:SER:OG	2.26	0.53
3:P:111:GLU:CG	29:U:206:HOH:O	2.57	0.53
1:A:87:ILE:O	1:A:173:PRO:HD3	2.08	0.53
2:B:41:ILE:HD13	23:B:302:PSC:H342	1.90	0.53
26:N:601:CDL:OA7	26:N:601:CDL:H321	2.08	0.53
2:O:41:ILE:HD13	23:O:302:PSC:H342	1.90	0.53
19:B:303:TGL:H272	19:B:303:TGL:C21	2.39	0.53
1:N:28:MET:HE3	12:Y:29:PHE:CD1	2.44	0.53
1:A:289:ALA:HB3	1:A:305:PHE:CD2	2.45	0.52
1:A:400:PHE:HB3	19:L:101:TGL:H272	1.90	0.52
2:B:41:ILE:O	2:B:45:MET:HG2	2.09	0.52
18:A:608:PGV:H032	29:C:451:HOH:O	2.08	0.52
26:C:304:CDL:H432	26:C:304:CDL:H382	1.91	0.52
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.44	0.52
3:P:187:THR:HB	7:T:68:THR:HG21	1.91	0.52
7:T:66:ASN:HD22	7:T:78:LEU:HD13	1.75	0.52
26:N:601:CDL:HB32	26:N:601:CDL:C18	2.41	0.52
9:V:29:LEU:HB2	29:V:106:HOH:O	2.10	0.51
1:N:261:TYR:CB	1:N:338:MET:HE2	2.40	0.51
17:A:604:HEA:HBC1	17:A:604:HEA:HMC1	1.91	0.51
1:N:146:THR:O	1:N:149:SER:HB3	2.10	0.51
19:N:609:TGL:H362	19:N:609:TGL:C19	2.38	0.51
12:Y:13:PHE:CE2	19:Y:101:TGL:HA72	2.45	0.51
1:A:406:ASN:HD21	18:A:606:PGV:H22	1.75	0.51
4:Q:109:HIS:CE1	4:Q:115:TRP:CZ3	2.99	0.51
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.26	0.50
1:N:334:TRP:CZ3	19:N:609:TGL:HA31	2.46	0.50
19:L:101:TGL:H202	19:L:101:TGL:H242	1.92	0.50
2:O:151:ARG:CD	2:O:181:GLN:HE21	2.25	0.50
5:E:78:HIS:CD2	9:I:12:LEU:HD22	2.46	0.50
1:N:127:THR:HB	1:N:129:TYR:CE1	2.47	0.50
12:L:20:ARG:HH22	19:L:101:TGL:CC4	2.23	0.50
1:N:31:THR:O	1:N:34:SER:OG	2.27	0.50
3:C:50:ASN:HD22	3:C:54:MET:HE2	1.75	0.50
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:MET:SD	1:A:69:MET:HE3	2.52	0.49
1:A:115:SER:O	1:A:121:GLY:HA2	2.12	0.49
1:A:177:SER:H	1:A:180:GLN:NE2	2.10	0.49
1:N:87:ILE:O	1:N:173:PRO:HD3	2.11	0.49
9:V:29:LEU:CB	29:V:106:HOH:O	2.60	0.49
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.94	0.49
19:Y:101:TGL:HA92	19:Y:101:TGL:H231	1.94	0.49
3:C:103:HIS:ND1	24:C:301:CHD:O26	2.37	0.49
7:G:61:SER:CB	29:G:201:HOH:O	2.59	0.49
1:N:2:PHE:CD1	1:N:2:PHE:C	2.91	0.49
11:X:22:ALA:O	11:X:26:VAL:HG23	2.12	0.49
3:C:44:MET:HE2	3:C:44:MET:HA	1.95	0.48
26:N:601:CDL:H771	26:N:601:CDL:H571	1.94	0.48
2:O:98:LYS:HE2	8:U:62:SER:O	2.13	0.48
24:W:102:CHD:H183	24:W:102:CHD:C22	2.43	0.48
19:N:609:TGL:C36	9:V:16:ARG:HE	2.27	0.48
3:P:129:VAL:N	3:P:130:PRO:CD	2.77	0.48
17:N:605:HEA:HHC	17:N:605:HEA:H122	1.95	0.48
9:I:36:LYS:HA	9:I:40:ALA:HB3	1.96	0.48
24:J:102:CHD:C18	24:J:102:CHD:H222	2.43	0.48
28:M:101:DMU:H30	28:M:101:DMU:O1	2.13	0.48
1:N:180:GLN:CG	29:N:708:HOH:O	2.57	0.48
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.48	0.48
19:N:607:TGL:CB9	19:N:607:TGL:H283	2.42	0.48
2:O:126:SER:O	2:O:126:SER:OG	2.27	0.48
1:N:378:HIS:CE1	17:N:605:HEA:NA	2.82	0.48
26:N:601:CDL:C37	2:O:78:LEU:HD12	2.44	0.48
19:N:607:TGL:H283	19:N:607:TGL:HB92	1.95	0.47
3:P:111:GLU:HG3	29:U:206:HOH:O	2.12	0.47
4:D:60:TYR:OH	5:E:69:GLU:OE1	2.29	0.47
1:N:251:PHE:HB3	1:N:319:LYS:HE2	1.96	0.47
1:N:467:LEU:O	1:N:471:ILE:HG13	2.15	0.47
1:A:440:TYR:HE1	2:B:204:HIS:CE1	2.33	0.47
1:N:52:GLN:O	1:N:56:VAL:HG23	2.13	0.47
4:Q:109:HIS:HE1	4:Q:115:TRP:CZ3	2.32	0.47
4:D:23:PRO:HG3	5:E:70:VAL:HG21	1.97	0.47
4:D:98:TRP:CE2	28:M:101:DMU:H11	2.49	0.47
1:A:240:HIS:O	1:A:243:VAL:HG22	2.14	0.47
10:J:50:LEU:HD22	10:J:50:LEU:O	2.14	0.47
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.79	0.47
17:A:605:HEA:HBC1	17:A:605:HEA:CMC	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:61:SER:HB2	29:G:201:HOH:O	2.15	0.47
19:N:607:TGL:CC6	29:Q:318:HOH:O	2.55	0.47
11:X:6:ALA:N	29:X:101:HOH:O	2.47	0.47
19:B:303:TGL:H272	19:B:303:TGL:HA92	1.97	0.47
19:B:303:TGL:H302	19:B:303:TGL:H132	1.76	0.47
5:E:49:ASP:OD1	5:E:92:THR:OG1	2.23	0.47
1:N:386:VAL:HG11	17:N:605:HEA:H261	1.97	0.47
4:D:34:SER:H	4:D:37:GLN:HE21	1.61	0.47
1:N:409:TRP:HA	1:N:412:ILE:HD12	1.97	0.47
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.97	0.46
4:D:88:PHE:O	4:D:91:PHE:HB3	2.15	0.46
1:N:177:SER:H	1:N:180:GLN:NE2	2.14	0.46
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.51	0.46
2:B:41:ILE:HD13	23:B:302:PSC:C34	2.45	0.46
2:O:18:GLU:O	2:O:21:LEU:HB2	2.16	0.46
1:N:92:MET:HE1	1:N:164:PHE:CD1	2.51	0.46
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.98	0.46
1:A:35:LEU:HD11	1:A:462:LEU:HD13	1.98	0.46
3:C:37:PHE:O	3:C:38:ASN:C	2.59	0.46
4:Q:19:ARG:NE	29:Q:301:HOH:O	2.35	0.46
13:Z:1:ILE:HG23	13:Z:1:ILE:O	2.16	0.46
7:G:3:ALA:O	7:G:4:ALA:HB2	2.15	0.46
23:O:302:PSC:H343	23:O:302:PSC:H142	1.96	0.46
10:J:33:ARG:HD2	29:J:206:HOH:O	2.15	0.46
2:B:139:ASP:OD1	2:B:140:ASN:N	2.49	0.45
12:L:20:ARG:NH2	19:L:101:TGL:CC4	2.78	0.45
2:O:91:ASN:O	2:O:91:ASN:ND2	2.47	0.45
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.81	0.45
26:P:305:CDL:H241	26:P:305:CDL:H392	1.97	0.45
9:V:22:VAL:O	9:V:26:MET:HG2	2.17	0.45
1:N:426:PHE:N	1:N:427:PRO:CD	2.79	0.45
11:X:24:PHE:CE1	11:X:28:VAL:HG11	2.50	0.45
17:A:604:HEA:HBC1	17:A:604:HEA:CMC	2.47	0.45
18:A:608:PGV:C03	29:C:451:HOH:O	2.64	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.17	0.45
19:B:303:TGL:H323	19:B:303:TGL:H121	1.97	0.45
3:C:226:HIS:HE1	26:C:304:CDL:HB31	1.82	0.45
1:N:101:SER:O	1:N:156:SER:OG	2.31	0.45
1:N:383:MET:HA	1:N:387:PHE:CD1	2.50	0.45
26:N:601:CDL:H782	26:N:601:CDL:H562	1.97	0.45
3:P:112:LEU:HD22	3:P:118:PRO:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:601:CDL:H571	26:N:601:CDL:C78	2.46	0.45
1:A:199:LEU:N	1:A:200:PRO:CD	2.79	0.45
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.46	0.45
3:C:217:VAL:HG21	26:C:304:CDL:H561	1.99	0.45
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.99	0.45
2:O:126:SER:O	2:O:127:GLU:HG3	2.16	0.45
5:E:12:ASP:HA	5:E:47:ILE:HD11	1.97	0.45
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.99	0.45
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.99	0.45
1:N:148:PHE:CD1	3:P:28:THR:HG22	2.52	0.45
7:T:58:LYS:HG2	29:T:204:HOH:O	2.17	0.45
12:Y:36:PRO:O	12:Y:40:VAL:HG23	2.17	0.45
2:O:151:ARG:HE	2:O:181:GLN:NE2	2.15	0.45
1:N:38:ARG:HD2	17:N:605:HEA:OMA	2.17	0.45
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.99	0.44
28:G:101:DMU:C57	28:G:101:DMU:H36	2.47	0.44
1:N:75:ILE:O	1:N:79:GLY:HA3	2.17	0.44
9:V:29:LEU:HD22	29:V:106:HOH:O	2.16	0.44
6:F:65:ASP:HB2	29:F:224:HOH:O	2.17	0.44
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.99	0.44
2:O:108:TYR:CE2	2:O:142:VAL:HG21	2.52	0.44
7:T:66:ASN:HD21	7:T:79:PRO:HD2	1.82	0.44
1:A:5:ARG:HG2	1:A:6:TRP:NE1	2.32	0.44
1:N:435:GLY:O	1:N:437:PRO:HD3	2.18	0.44
1:N:498:CYS:HA	1:N:499:PRO:HA	1.87	0.44
5:R:67:ILE:O	5:R:70:VAL:HG12	2.16	0.44
19:B:303:TGL:HC52	19:B:303:TGL:HC82	1.74	0.44
25:C:302:PEK:H383	26:N:601:CDL:C27	2.48	0.44
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.82	0.44
19:N:609:TGL:H363	9:V:16:ARG:HE	1.82	0.44
1:A:397:PHE:N	1:A:398:PRO:CD	2.81	0.44
28:G:101:DMU:H36	28:G:101:DMU:H30	1.99	0.44
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.18	0.43
25:C:302:PEK:H032	29:G:213:HOH:O	2.18	0.43
26:C:304:CDL:HB21	26:C:304:CDL:CB3	2.43	0.43
1:N:195:LEU:HD23	1:N:245:ILE:HD13	1.99	0.43
2:B:86:MET:HE1	29:B:401:HOH:O	2.18	0.43
1:A:363:LEU:HD23	1:A:363:LEU:HA	1.86	0.43
26:N:601:CDL:H231	26:N:601:CDL:C52	2.48	0.43
12:Y:45:LEU:HD21	13:Z:40:TYR:CD1	2.54	0.43
26:N:601:CDL:H231	26:N:601:CDL:H531	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:88:ASP:O	2:O:89:GLU:O	2.36	0.43
3:P:16:TRP:N	3:P:17:PRO:CD	2.81	0.43
26:P:305:CDL:HB32	26:P:305:CDL:CB2	2.45	0.43
2:B:83:ILE:O	2:B:87:MET:HG3	2.18	0.43
26:C:304:CDL:H432	26:C:304:CDL:H381	2.00	0.43
7:G:5:LYS:HG3	25:G:103:PEK:H383	2.00	0.43
2:O:121:TYR:O	2:O:138:VAL:HA	2.18	0.43
25:P:302:PEK:C05	7:T:76:ASN:HD21	2.30	0.43
1:A:426:PHE:N	1:A:427:PRO:CD	2.81	0.43
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.43
9:V:21:ILE:HD13	9:V:21:ILE:HA	1.90	0.43
9:V:67:GLY:HA2	29:V:103:HOH:O	2.19	0.43
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.54	0.43
3:C:173:PHE:CD1	3:C:173:PHE:C	2.97	0.43
1:N:83:VAL:HB	1:N:84:PRO:HD3	2.00	0.43
1:N:129:TYR:CZ	1:N:232:GLN:HG2	2.54	0.43
4:Q:138:TRP:CH2	11:X:50:PRO:CG	3.02	0.43
1:A:240:HIS:CD2	1:A:240:HIS:C	2.97	0.42
6:F:95:GLN:O	6:F:97:ALA:N	2.52	0.42
7:T:12:GLY:HA3	29:T:208:HOH:O	2.19	0.42
1:N:365:ILE:HG13	2:O:87:MET:HE1	2.01	0.42
1:A:83:VAL:N	1:A:84:PRO:CD	2.82	0.42
19:L:101:TGL:H101	19:L:101:TGL:H131	1.89	0.42
1:N:381:LEU:O	1:N:386:VAL:HG23	2.19	0.42
1:N:495:LEU:HD12	1:N:495:LEU:HA	1.90	0.42
19:N:607:TGL:H283	19:N:607:TGL:H111	2.02	0.42
3:P:195:SER:O	3:P:199:VAL:HG23	2.19	0.42
2:B:33:LEU:HD12	9:I:28:SER:HB3	2.00	0.42
2:B:48:THR:HB	9:I:16:ARG:CZ	2.49	0.42
1:N:236:TRP:HA	1:N:236:TRP:CE3	2.54	0.42
4:Q:76:ASN:ND2	11:X:11:ASP:OD1	2.53	0.42
24:J:101:CHD:H231	29:J:205:HOH:O	2.18	0.42
8:U:46:LYS:O	8:U:47:GLY:C	2.62	0.42
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.01	0.42
1:N:361:SER:OG	2:O:84:LEU:HD13	2.19	0.42
26:P:305:CDL:H241	26:P:305:CDL:C39	2.50	0.42
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.55	0.42
1:N:33:LEU:O	1:N:37:ILE:HG13	2.20	0.42
7:T:67:HIS:NE2	7:T:78:LEU:HD11	2.35	0.42
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.72	0.42
10:J:11:LEU:HD12	10:J:11:LEU:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:33:ARG:HG2	24:J:102:CHD:H151	2.01	0.42
1:A:390:MET:HE3	1:A:390:MET:HA	2.01	0.42
11:X:26:VAL:O	11:X:30:VAL:HG23	2.20	0.42
2:B:111:THR:HA	2:B:114:GLU:O	2.20	0.41
4:Q:16:TYR:OH	4:Q:18:ASP:OD1	2.21	0.41
6:S:93:PRO:N	29:S:201:HOH:O	2.52	0.41
1:A:248:LEU:HB2	1:A:249:PRO:HD3	2.02	0.41
2:B:217:LYS:HG2	29:B:483:HOH:O	2.20	0.41
3:C:226:HIS:CE1	26:C:304:CDL:HB31	2.54	0.41
1:N:5:ARG:HG2	1:N:6:TRP:CE2	2.54	0.41
1:N:41:LEU:HD11	1:N:54:TYR:OH	2.21	0.41
1:N:289:ALA:HB1	1:N:297:MET:HE1	2.01	0.41
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.19	0.41
3:P:23:SER:O	3:P:27:MET:HG3	2.20	0.41
26:P:305:CDL:H401	26:P:305:CDL:H432	1.81	0.41
7:T:12:GLY:CA	29:T:208:HOH:O	2.67	0.41
1:A:377:PHE:HA	1:A:380:VAL:HG22	2.02	0.41
2:B:151:ARG:HE	2:B:181:GLN:NE2	2.18	0.41
7:G:11:TPO:O	7:G:11:TPO:CG2	2.68	0.41
8:H:8:ILE:O	8:H:8:ILE:HG22	2.20	0.41
1:N:65:MET:HE3	17:N:605:HEA:HMC2	2.01	0.41
4:Q:91:PHE:CD2	4:Q:91:PHE:C	2.96	0.41
1:A:82:LEU:O	1:A:86:MET:HG3	2.20	0.41
19:N:607:TGL:HC61	29:V:107:HOH:O	2.20	0.41
7:T:72:ASN:OD1	7:T:74:ARG:HB2	2.20	0.41
1:A:290:HIS:HA	1:A:293:PHE:CZ	2.56	0.41
26:N:601:CDL:OB4	26:N:601:CDL:H1	2.18	0.41
1:A:106:PRO:HD2	1:A:107:PRO:HD2	2.03	0.41
18:A:606:PGV:H331	29:D:245:HOH:O	2.20	0.41
1:N:440:TYR:HE1	2:O:204:HIS:CE1	2.39	0.41
19:N:607:TGL:H111	19:N:607:TGL:C28	2.51	0.41
3:P:50:ASN:HD22	3:P:54:MET:HE2	1.84	0.41
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.56	0.41
2:O:139:ASP:OD1	2:O:140:ASN:N	2.52	0.41
11:X:31:TYR:CD1	11:X:35:GLN:HG3	2.56	0.41
2:B:78:LEU:CB	2:B:79:PRO:CD	2.98	0.41
23:B:302:PSC:H063	23:B:302:PSC:P	2.61	0.41
3:P:193:TYR:CD1	3:P:193:TYR:C	2.99	0.41
10:W:29:ASN:H	10:W:29:ASN:ND2	2.19	0.41
1:A:317:GLY:HA3	29:A:754:HOH:O	2.21	0.41
1:A:377:PHE:CE1	1:A:378:HIS:CE1	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:601:CDL:H252	26:N:601:CDL:H222	1.79	0.41
3:P:252:LEU:CD2	3:P:256:ILE:HD12	2.51	0.41
13:Z:32:TRP:CD1	13:Z:36:HIS:CE1	3.09	0.41
2:O:122:MET:HA	2:O:137:GLU:O	2.21	0.40
2:B:122:MET:SD	2:B:135:LEU:HA	2.61	0.40
5:E:41:LEU:C	5:E:41:LEU:HD12	2.46	0.40
7:G:64:ASP:OD1	7:G:67:HIS:ND1	2.45	0.40
1:N:363:LEU:HD23	1:N:363:LEU:HA	1.88	0.40
1:N:364:ASP:OD1	17:N:606:HEA:O1A	2.38	0.40
1:N:406:ASN:HD21	18:N:610:PGV:H22	1.85	0.40
2:O:69:PRO:O	2:O:73:LEU:HG	2.21	0.40
2:O:165:VAL:HG11	2:O:168:LEU:HD12	2.02	0.40
7:T:5:LYS:CD	25:T:102:PEK:H383	2.49	0.40
23:B:302:PSC:H011	23:B:302:PSC:H222	2.03	0.40
26:C:304:CDL:H831	26:C:304:CDL:H861	1.94	0.40
3:P:116:TRP:HA	3:P:117:PRO:C	2.45	0.40
7:T:25:LEU:N	7:T:26:PRO:CD	2.84	0.40
11:K:24:PHE:O	11:K:28:VAL:HG12	2.21	0.40
2:B:220:GLU:CG	29:B:458:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	512/514 (100%)	492 (96%)	19 (4%)	1 (0%)	43 63
1	N	512/514 (100%)	488 (95%)	23 (4%)	1 (0%)	43 63
2	B	225/227 (99%)	213 (95%)	12 (5%)	0	100 100
2	O	225/227 (99%)	210 (93%)	13 (6%)	2 (1%)	14 27
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	30 49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
4	D	142/147 (97%)	135 (95%)	6 (4%)	1 (1%)	18	34
4	Q	137/147 (93%)	123 (90%)	13 (10%)	1 (1%)	18	34
5	E	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	94/98 (96%)	87 (93%)	3 (3%)	4 (4%)	2	2
6	S	92/98 (94%)	87 (95%)	3 (3%)	2 (2%)	5	9
7	G	81/85 (95%)	66 (82%)	9 (11%)	6 (7%)	1	1
7	T	81/85 (95%)	64 (79%)	12 (15%)	5 (6%)	1	1
8	H	76/85 (89%)	73 (96%)	1 (1%)	2 (3%)	4	7
8	U	77/85 (91%)	72 (94%)	3 (4%)	2 (3%)	4	7
9	I	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	9	17
9	V	71/73 (97%)	64 (90%)	6 (8%)	1 (1%)	9	17
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	39 (83%)	7 (15%)	1 (2%)	5	9
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	40 (91%)	3 (7%)	1 (2%)	5	8
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	36 (88%)	5 (12%)	0	100	100
All	All	3492/3614 (97%)	3293 (94%)	167 (5%)	32 (1%)	14	27

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	5	LYS
7	G	7	ASP
7	G	37	LEU
2	O	89	GLU
6	S	94	HIS
7	T	4	ALA
7	T	7	ASP
7	T	37	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	38	ASN
4	D	5	VAL
6	F	96	LEU
8	H	47	GLY
9	I	37	PHE
6	S	95	GLN
7	T	3	ALA
7	T	40	GLY
9	V	28	SER
6	F	15	GLY
7	G	41	HIS
11	X	12	LYS
12	Y	28	PHE
1	A	51	ASP
8	H	9	LYS
1	N	119	GLU
2	O	60	GLU
8	U	8	ILE
6	F	94	HIS
6	F	95	GLN
7	G	6	GLY
4	Q	103	VAL
8	U	47	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	420 (99%)	6 (1%)	59	81
1	N	426/426 (100%)	413 (97%)	13 (3%)	35	62
2	B	210/210 (100%)	195 (93%)	15 (7%)	13	29
2	O	210/210 (100%)	192 (91%)	18 (9%)	10	21
3	C	224/226 (99%)	215 (96%)	9 (4%)	28	54
3	P	224/226 (99%)	217 (97%)	7 (3%)	35	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	128/129 (99%)	119 (93%)	9 (7%)	14	29
4	Q	123/129 (95%)	118 (96%)	5 (4%)	27	53
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	61
5	R	92/95 (97%)	84 (91%)	8 (9%)	9	21
6	F	80/81 (99%)	76 (95%)	4 (5%)	22	44
6	S	79/81 (98%)	74 (94%)	5 (6%)	16	34
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	19
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	36
8	H	70/75 (93%)	67 (96%)	3 (4%)	26	51
8	U	71/75 (95%)	68 (96%)	3 (4%)	26	52
9	I	57/57 (100%)	52 (91%)	5 (9%)	9	20
9	V	57/57 (100%)	51 (90%)	6 (10%)	6	14
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	53
10	W	49/50 (98%)	43 (88%)	6 (12%)	5	10
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	68
11	X	39/46 (85%)	34 (87%)	5 (13%)	4	9
12	L	39/40 (98%)	36 (92%)	3 (8%)	12	25
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	25
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	13
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	23
All	All	3031/3082 (98%)	2875 (95%)	156 (5%)	21	43

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	128	VAL
1	A	369	ASP
1	A	484	THR
1	A	513	LEU
1	A	514	LYS
2	B	43	SER
2	B	55	THR
2	B	60	GLU
2	B	66	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	88	ASP
2	B	91	ASN
2	B	110	TYR
2	B	130	PRO
2	B	152	MET
2	B	167	SER
2	B	183	THR
2	B	199	ILE
3	C	33	MET
3	C	38	ASN
3	C	51	MET
3	C	77	LYS
3	C	127	LEU
3	C	130	PRO
3	C	159	MET
3	C	230	ASN
3	C	258	TRP
4	D	17	VAL
4	D	36	SER
4	D	45	LYS
4	D	47	SER
4	D	51	LEU
4	D	58	GLU
4	D	101	HIS
4	D	113	GLU
4	D	114	GLU
5	E	5	HIS
5	E	7	THR
5	E	70	VAL
6	F	2	SER
6	F	48	LEU
6	F	87	THR
6	F	95	GLN
7	G	5	LYS
7	G	8	HIS
7	G	33	LEU
7	G	34	ASN
7	G	61	SER
7	G	84	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	50	VAL
8	H	60	TYR
8	H	61	LYS
9	I	8	GLN
9	I	15	ARG
9	I	18	ARG
9	I	21	ILE
9	I	29	LEU
10	J	27	THR
10	J	50	LEU
11	K	54	ARG
12	L	4	GLU
12	L	26	THR
12	L	47	LYS
13	M	13	LYS
13	M	19	LEU
13	M	34	LEU
13	M	42	LYS
1	N	9	SER
1	N	38	ARG
1	N	91	ASP
1	N	138	HIS
1	N	180	GLN
1	N	265	LYS
1	N	363	LEU
1	N	369	ASP
1	N	382	SER
1	N	455	SER
1	N	483	LEU
1	N	484	THR
1	N	513	LEU
2	O	18	GLU
2	O	35	SER
2	O	43	SER
2	O	55	THR
2	O	57	ASP
2	O	60	GLU
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	92	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	110	TYR
2	O	148	MET
2	O	156	SER
2	O	158	ASP
2	O	167	SER
2	O	183	THR
2	O	226	MET
3	P	23	SER
3	P	28	THR
3	P	49	THR
3	P	50	ASN
3	P	127	LEU
3	P	159	MET
3	P	261	SER
4	Q	38	LYS
4	Q	47	SER
4	Q	110	THR
4	Q	123	MET
4	Q	143	ASN
5	R	7	THR
5	R	9	GLU
5	R	14	ARG
5	R	46	LYS
5	R	70	VAL
5	R	80	GLU
5	R	81	ILE
5	R	109	VAL
6	S	48	LEU
6	S	52	ILE
6	S	53	THR
6	S	54	ASN
6	S	96	LEU
7	T	2	SER
7	T	8	HIS
7	T	37	LEU
7	T	74	ARG
8	U	7	LYS
8	U	60	TYR
8	U	66	ILE
9	V	15	ARG
9	V	18	ARG
9	V	21	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	V	28	SER
9	V	29	LEU
9	V	58	LYS
10	W	10	LYS
10	W	27	THR
10	W	29	ASN
10	W	31	LEU
10	W	33	ARG
10	W	50	LEU
11	X	20	SER
11	X	28	VAL
11	X	49	THR
11	X	52	GLU
11	X	54	ARG
12	Y	11	ILE
12	Y	26	THR
12	Y	47	LYS
13	Z	13	LYS
13	Z	42	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	43	GLN
1	A	180	GLN
1	A	422	ASN
1	A	512	ASN
2	B	10	GLN
2	B	140	ASN
2	B	181	GLN
3	C	38	ASN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
3	C	161	GLN
4	D	32	ASN
4	D	37	GLN
4	D	109	HIS
4	D	119	GLN
5	E	78	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	94	ASN
6	F	80	GLN
7	G	76	ASN
8	H	31	GLN
8	H	32	ASN
1	N	512	ASN
2	O	10	GLN
2	O	24	HIS
2	O	59	GLN
2	O	181	GLN
2	O	203	ASN
3	P	50	ASN
3	P	161	GLN
4	Q	37	GLN
4	Q	76	ASN
4	Q	101	HIS
4	Q	109	HIS
5	R	78	HIS
5	R	94	ASN
6	S	88	HIS
7	T	34	ASN
7	T	66	ASN
7	T	76	ASN
8	U	31	GLN
8	U	32	ASN
8	U	37	HIS
9	V	8	GLN
10	W	13	GLN
10	W	29	ASN
11	X	15	ASN
13	Z	36	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	N	1	1	8,9,10	0.50	0	8,9,11	1.26	1 (12%)
2	FME	O	1	2	8,9,10	0.48	0	8,9,11	1.50	2 (25%)
1	FME	A	1	1	8,9,10	0.52	0	8,9,11	1.01	0
9	SAC	I	1	9	7,8,9	0.71	0	7,9,11	1.10	1 (14%)
2	FME	B	1	2	8,9,10	0.60	0	8,9,11	1.91	2 (25%)
7	TPO	G	11	7	8,10,11	1.36	1 (12%)	10,14,16	0.82	0
7	TPO	T	11	7	8,10,11	0.94	1 (12%)	10,14,16	0.82	0
9	SAC	V	1	9	7,8,9	0.66	0	7,9,11	1.59	1 (14%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.43	1.65	1.59
7	T	11	TPO	P-OG1	2.02	1.63	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-4.15	116.43	122.82
9	V	1	SAC	O-C-CA	-4.08	114.27	124.77
2	B	1	FME	C-CA-N	3.04	115.37	109.50
2	O	1	FME	CA-N-CN	-2.95	118.28	122.82
2	O	1	FME	C-CA-N	2.81	114.92	109.50
9	I	1	SAC	O-C-CA	-2.70	117.83	124.77
1	N	1	FME	CB-CA-N	2.51	115.08	110.52

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	C-CA-N-C1A
9	I	1	SAC	CB-CA-N-C1A
9	I	1	SAC	O-C-CA-CB
1	N	1	FME	O1-CN-N-CA
2	O	1	FME	O1-CN-N-CA
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	V	1	SAC	C-CA-N-C1A
9	V	1	SAC	CB-CA-N-C1A
9	V	1	SAC	O-C-CA-CB
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	CA-CB-CG-SD
7	T	11	TPO	CB-OG1-P-O3P
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	C2A-C1A-N-CA
7	T	11	TPO	CB-OG1-P-O1P
1	N	1	FME	CB-CA-N-CN
7	T	11	TPO	CB-OG1-P-O2P
7	G	11	TPO	O-C-CA-CB
9	I	1	SAC	C-CA-CB-OG
7	T	11	TPO	CG2-CB-OG1-P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	2	0
2	B	1	FME	1	0
7	G	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 10 are monoatomic and 2 are modelled with single atom - 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	$\# Z > 2$
23	PSC	O	302	-	51,51,51	0.32	0	57,59,59	0.40	0
25	PEK	T	102	-	52,52,52	0.33	0	55,57,57	0.50	0
19	TGL	B	303	-	62,62,62	1.02	4 (6%)	65,65,65	1.08	7 (10%)
28	DMU	Q	201	-	34,34,34	1.07	2 (5%)	45,45,45	1.30	5 (11%)
18	PGV	A	607	-	50,50,50	0.85	2 (4%)	53,56,56	1.36	5 (9%)
18	PGV	C	303	-	50,50,50	0.86	2 (4%)	53,56,56	1.15	6 (11%)
26	CDL	P	305	-	99,99,99	0.99	4 (4%)	105,111,111	0.87	6 (5%)
18	PGV	P	304	-	50,50,50	0.94	2 (4%)	53,56,56	1.03	4 (7%)
28	DMU	M	101	-	34,34,34	1.09	3 (8%)	45,45,45	1.50	8 (17%)
17	HEA	A	604	1	67,67,67	2.31	25 (37%)	81,103,103	2.34	30 (37%)
24	CHD	J	101	-	32,32,32	0.65	0	51,51,51	1.12	5 (9%)
24	CHD	W	101	-	32,32,32	0.57	0	51,51,51	0.71	0
17	HEA	N	605	1	67,67,67	2.32	25 (37%)	81,103,103	2.57	35 (43%)
18	PGV	A	608	-	50,50,50	1.18	2 (4%)	53,56,56	1.35	4 (7%)
18	PGV	U	101	-	50,50,50	1.12	2 (4%)	53,56,56	1.23	5 (9%)
28	DMU	T	101	-	34,34,34	1.84	6 (17%)	45,45,45	1.61	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHD	B	304	-	32,32,32	0.48	0	51,51,51	0.70	0
17	HEA	A	605	20,1	67,67,67	2.40	26 (38%)	81,103,103	2.42	28 (34%)
25	PEK	P	303	-	52,52,52	0.38	0	55,57,57	0.57	0
19	TGL	L	101	-	62,62,62	1.13	5 (8%)	65,65,65	1.10	4 (6%)
19	TGL	Y	101	-	62,62,62	1.10	4 (6%)	65,65,65	0.98	5 (7%)
19	TGL	N	609	-	62,62,62	1.14	3 (4%)	65,65,65	1.05	5 (7%)
23	PSC	B	302	-	51,51,51	0.35	0	57,59,59	0.48	0
25	PEK	C	302	-	52,52,52	0.35	0	55,57,57	0.47	0
24	CHD	J	102	-	32,32,32	0.79	0	51,51,51	1.26	4 (7%)
25	PEK	P	302	-	52,52,52	0.31	0	55,57,57	0.55	0
18	PGV	A	606	-	50,50,50	1.10	2 (4%)	53,56,56	1.15	5 (9%)
24	CHD	G	104	-	32,32,32	0.59	0	51,51,51	0.85	0
24	CHD	P	301	-	32,32,32	0.64	0	51,51,51	0.75	0
26	CDL	C	304	-	99,99,99	0.98	4 (4%)	105,111,111	0.82	4 (3%)
19	TGL	N	607	-	62,62,62	1.08	4 (6%)	65,65,65	1.10	5 (7%)
24	CHD	C	301	-	32,32,32	0.66	1 (3%)	51,51,51	0.73	0
18	PGV	N	608	-	50,50,50	0.88	2 (4%)	53,56,56	1.10	4 (7%)
26	CDL	T	103	-	99,99,99	1.02	4 (4%)	105,111,111	0.70	5 (4%)
26	CDL	N	601	-	99,99,99	0.96	4 (4%)	105,111,111	0.71	3 (2%)
22	CUA	O	301	2	0,1,1	-	-	-	-	-
18	PGV	N	610	-	50,50,50	1.06	2 (4%)	53,56,56	0.96	3 (5%)
25	PEK	G	102	-	52,52,52	0.34	0	55,57,57	0.57	0
17	HEA	N	606	1	67,67,67	2.32	25 (37%)	81,103,103	2.43	29 (35%)
28	DMU	G	101	-	34,34,34	1.38	5 (14%)	45,45,45	1.74	9 (20%)
24	CHD	W	102	-	32,32,32	0.70	0	51,51,51	1.04	4 (7%)
19	TGL	A	609	-	62,62,62	1.14	4 (6%)	65,65,65	1.06	7 (10%)
22	CUA	B	301	2	0,1,1	-	-	-	-	-
25	PEK	G	103	-	52,52,52	0.37	0	55,57,57	0.54	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
23	PSC	O	302	-	-	31/55/55/55	-
25	PEK	T	102	-	-	30/56/56/56	-
19	TGL	B	303	-	-	40/65/65/65	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DMU	Q	201	-	-	10/19/59/59	0/2/2/2
18	PGV	A	607	-	-	16/55/55/55	-
18	PGV	C	303	-	-	13/55/55/55	-
26	CDL	P	305	-	-	70/110/110/110	-
18	PGV	P	304	-	-	14/55/55/55	-
28	DMU	M	101	-	-	10/19/59/59	0/2/2/2
17	HEA	A	604	1	-	7/36/76/76	-
24	CHD	J	101	-	-	4/9/74/74	0/4/4/4
24	CHD	W	101	-	-	0/9/74/74	0/4/4/4
17	HEA	N	605	1	-	4/36/76/76	-
18	PGV	A	608	-	-	25/55/55/55	-
18	PGV	U	101	-	-	28/55/55/55	-
28	DMU	T	101	-	-	10/19/59/59	0/2/2/2
24	CHD	B	304	-	-	4/9/74/74	0/4/4/4
17	HEA	A	605	20,1	-	7/36/76/76	-
25	PEK	P	303	-	-	21/56/56/56	-
19	TGL	L	101	-	-	36/65/65/65	-
19	TGL	Y	101	-	-	33/65/65/65	-
19	TGL	N	609	-	-	42/65/65/65	-
23	PSC	B	302	-	-	27/55/55/55	-
25	PEK	C	302	-	-	23/56/56/56	-
24	CHD	J	102	-	-	6/9/74/74	0/4/4/4
25	PEK	P	302	-	-	22/56/56/56	-
18	PGV	A	606	-	-	31/55/55/55	-
24	CHD	G	104	-	-	4/9/74/74	0/4/4/4
24	CHD	P	301	-	-	3/9/74/74	0/4/4/4
26	CDL	C	304	-	-	59/110/110/110	-
19	TGL	N	607	-	-	38/65/65/65	-
24	CHD	C	301	-	-	0/9/74/74	0/4/4/4
18	PGV	N	608	-	-	15/55/55/55	-
26	CDL	T	103	-	-	65/110/110/110	-
26	CDL	N	601	-	-	57/110/110/110	-
18	PGV	N	610	-	-	33/55/55/55	-
25	PEK	G	102	-	-	21/56/56/56	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEA	N	606	1	-	5/36/76/76	-
28	DMU	G	101	-	-	12/19/59/59	0/2/2/2
24	CHD	W	102	-	-	6/9/74/74	0/4/4/4
19	TGL	A	609	-	-	40/65/65/65	-
25	PEK	G	103	-	-	26/56/56/56	-

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	101	DMU	O16-C6	6.63	1.51	1.40
17	N	606	HEA	C3B-C2B	5.93	1.48	1.34
17	N	605	HEA	C3B-C2B	5.61	1.47	1.34
18	A	608	PGV	O01-C1	5.48	1.49	1.34
17	N	606	HEA	FE-ND	5.18	2.10	1.94
18	A	606	PGV	O03-C19	5.16	1.48	1.33
18	U	101	PGV	O01-C1	5.07	1.48	1.34
19	N	609	TGL	OG2-CB1	5.05	1.48	1.34
17	A	605	HEA	FE-NA	5.02	2.11	1.95
17	A	605	HEA	C3B-C2B	4.98	1.46	1.34
17	A	605	HEA	CHB-C4A	4.94	1.48	1.38
17	N	605	HEA	FE-ND	4.93	2.10	1.94
17	N	606	HEA	CHB-C4A	4.91	1.48	1.38
19	B	303	TGL	OG2-CB1	4.83	1.47	1.34
19	L	101	TGL	OG1-CA1	4.77	1.47	1.33
19	N	609	TGL	OG3-CC1	4.76	1.47	1.33
17	A	604	HEA	C3B-C2B	4.75	1.45	1.34
17	A	605	HEA	FE-NC	4.73	2.10	1.95
17	A	605	HEA	FE-NB	4.73	2.09	1.94
17	A	604	HEA	FE-NB	4.71	2.09	1.94
17	A	604	HEA	CHB-C4A	4.70	1.47	1.38
17	A	604	HEA	FE-NA	4.69	2.10	1.95
17	N	605	HEA	FE-NB	4.67	2.09	1.94
18	U	101	PGV	O03-C19	4.66	1.46	1.33
19	L	101	TGL	OG2-CB1	4.66	1.47	1.34
17	A	605	HEA	CHA-C1A	4.64	1.47	1.38
17	A	604	HEA	C3D-C2D	4.62	1.46	1.36
19	A	609	TGL	OG2-CB1	4.62	1.47	1.34
17	A	604	HEA	FE-NC	4.62	2.10	1.95
18	A	608	PGV	O03-C19	4.61	1.46	1.33
17	A	605	HEA	CHC-C4B	4.55	1.47	1.38
28	Q	201	DMU	O16-C6	4.55	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	P	304	PGV	O01-C1	4.55	1.47	1.34
18	A	606	PGV	O01-C1	4.54	1.47	1.34
18	N	610	PGV	O03-C19	4.53	1.46	1.33
19	A	609	TGL	OG3-CC1	4.52	1.46	1.33
17	N	605	HEA	CHA-C1A	4.50	1.47	1.38
26	T	103	CDL	OB8-CB7	4.46	1.46	1.33
26	T	103	CDL	OA8-CA7	4.45	1.46	1.33
17	A	605	HEA	C3D-C2D	4.42	1.46	1.36
17	N	606	HEA	FE-NB	4.41	2.08	1.94
26	P	305	CDL	OA6-CA5	4.40	1.46	1.34
26	C	304	CDL	OA6-CA5	4.40	1.46	1.34
26	C	304	CDL	OA8-CA7	4.40	1.46	1.33
17	A	604	HEA	CHD-C1D	4.39	1.47	1.38
26	T	103	CDL	OA6-CA5	4.39	1.46	1.34
19	Y	101	TGL	OG3-CC1	4.38	1.46	1.33
26	P	305	CDL	OA8-CA7	4.38	1.46	1.33
26	N	601	CDL	OB6-CB5	4.35	1.46	1.34
17	A	605	HEA	C1D-ND	-4.35	1.32	1.40
26	P	305	CDL	OB6-CB5	4.31	1.46	1.34
26	C	304	CDL	OB6-CB5	4.31	1.46	1.34
17	N	605	HEA	C11-C3B	-4.30	1.46	1.51
28	M	101	DMU	O16-C6	4.30	1.47	1.40
26	N	601	CDL	OA8-CA7	4.28	1.45	1.33
18	N	610	PGV	O01-C1	4.27	1.46	1.34
19	A	609	TGL	OG1-CA1	4.27	1.45	1.33
26	N	601	CDL	OA6-CA5	4.22	1.46	1.34
26	N	601	CDL	OB8-CB7	4.19	1.45	1.33
17	A	605	HEA	C4C-NC	-4.19	1.31	1.39
17	N	605	HEA	CHB-C4A	4.15	1.46	1.38
19	Y	101	TGL	OG2-CB1	4.15	1.46	1.34
26	P	305	CDL	OB8-CB7	4.13	1.45	1.33
17	A	605	HEA	CHC-C1C	4.12	1.48	1.39
26	T	103	CDL	OB6-CB5	4.12	1.45	1.34
17	A	604	HEA	FE-ND	4.08	2.07	1.94
17	A	604	HEA	CHC-C4B	4.06	1.46	1.38
19	Y	101	TGL	OG1-CA1	4.05	1.45	1.33
19	N	607	TGL	OG3-CC1	4.03	1.45	1.33
17	N	605	HEA	FE-NA	4.02	2.08	1.95
17	N	606	HEA	C3A-C2A	4.02	1.46	1.37
26	C	304	CDL	OB8-CB7	4.00	1.45	1.33
17	N	605	HEA	CHD-C1D	3.97	1.46	1.38
17	N	606	HEA	C3D-C2D	3.96	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	606	HEA	CHA-C1A	3.96	1.46	1.38
28	T	101	DMU	O7-C10	3.94	1.52	1.41
19	N	607	TGL	OG2-CB1	3.90	1.45	1.34
19	N	609	TGL	OG1-CA1	3.88	1.44	1.33
17	N	605	HEA	C3D-C2D	3.78	1.44	1.36
17	A	605	HEA	FE-ND	3.75	2.06	1.94
18	N	608	PGV	O01-C1	3.74	1.44	1.34
17	N	606	HEA	FE-NC	3.74	2.07	1.95
17	A	604	HEA	CHA-C1A	3.73	1.45	1.38
18	P	304	PGV	O03-C19	3.72	1.44	1.33
17	A	604	HEA	C3A-C2A	3.71	1.45	1.37
17	A	605	HEA	CHA-C4D	3.69	1.47	1.39
17	N	605	HEA	C3A-C2A	3.69	1.45	1.37
19	N	607	TGL	OG2-CG2	-3.67	1.38	1.46
18	N	608	PGV	O03-C19	3.65	1.44	1.33
19	N	607	TGL	OG1-CA1	3.62	1.43	1.33
28	G	101	DMU	O1-C10	3.62	1.51	1.41
17	N	606	HEA	C4B-NB	-3.58	1.34	1.40
17	A	604	HEA	C4B-C3B	3.57	1.51	1.44
17	N	606	HEA	CHC-C1C	3.57	1.47	1.39
17	N	605	HEA	CHC-C1C	3.56	1.47	1.39
17	N	605	HEA	C1D-ND	-3.56	1.34	1.40
18	A	607	PGV	O01-C1	3.56	1.44	1.34
18	C	303	PGV	O01-C1	3.55	1.44	1.34
17	N	606	HEA	FE-NA	3.52	2.06	1.95
17	A	605	HEA	C3A-C2A	3.51	1.45	1.37
17	N	606	HEA	CHB-C1B	3.48	1.47	1.39
19	B	303	TGL	OG1-CA1	3.47	1.43	1.33
17	N	605	HEA	C4D-ND	-3.46	1.32	1.38
17	N	606	HEA	C1D-ND	-3.46	1.34	1.40
17	N	605	HEA	C1C-NC	-3.45	1.33	1.39
17	N	605	HEA	C4B-NB	-3.42	1.34	1.40
17	A	604	HEA	CHB-C1B	3.39	1.46	1.39
28	T	101	DMU	O1-C10	3.36	1.50	1.41
19	Y	101	TGL	OG2-CG2	-3.34	1.38	1.46
28	G	101	DMU	O7-C10	3.33	1.51	1.41
17	A	604	HEA	CHD-C4C	3.33	1.46	1.39
18	A	607	PGV	O03-C19	3.28	1.42	1.33
17	N	605	HEA	FE-NC	3.25	2.05	1.95
17	N	606	HEA	C4C-NC	-3.24	1.33	1.39
17	N	605	HEA	CHD-C4C	3.24	1.46	1.39
17	A	605	HEA	CHB-C1B	3.23	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	605	HEA	C4B-NB	-3.21	1.34	1.40
18	C	303	PGV	O03-C19	3.21	1.42	1.33
28	T	101	DMU	O7-C3	3.21	1.52	1.43
17	N	606	HEA	CHC-C4B	3.20	1.44	1.38
17	A	604	HEA	C1D-ND	-3.17	1.34	1.40
17	A	604	HEA	C4B-NB	-3.14	1.34	1.40
19	L	101	TGL	OG3-CC1	3.14	1.42	1.33
28	G	101	DMU	O16-C6	3.12	1.45	1.40
17	A	605	HEA	C4A-NA	-3.11	1.33	1.39
17	N	606	HEA	CHA-C4D	3.09	1.46	1.39
17	A	604	HEA	CHC-C1C	3.07	1.46	1.39
17	N	606	HEA	CHD-C4C	3.05	1.46	1.39
17	N	605	HEA	CHC-C4B	3.05	1.44	1.38
17	N	605	HEA	CHB-C1B	3.03	1.46	1.39
17	A	604	HEA	C4A-NA	-3.02	1.33	1.39
17	N	606	HEA	C4A-NA	-2.97	1.34	1.39
17	A	605	HEA	CHD-C1D	2.96	1.44	1.38
28	G	101	DMU	C10-C5	2.96	1.61	1.52
19	L	101	TGL	OG2-CG2	-2.94	1.39	1.46
19	A	609	TGL	OG2-CG2	-2.88	1.39	1.46
17	N	606	HEA	CHD-C1D	2.85	1.44	1.38
17	N	606	HEA	C4D-ND	-2.81	1.33	1.38
17	A	605	HEA	CHD-C4C	2.80	1.45	1.39
17	N	606	HEA	C11-C3B	-2.79	1.48	1.51
17	N	605	HEA	C1A-C2A	2.78	1.50	1.45
17	A	604	HEA	CHA-C4D	2.78	1.45	1.39
17	N	606	HEA	C1A-NA	-2.74	1.34	1.39
17	A	605	HEA	C1A-NA	-2.66	1.34	1.39
17	N	605	HEA	CHA-C4D	2.61	1.45	1.39
28	T	101	DMU	C2-C1	2.59	1.59	1.52
17	A	605	HEA	C1C-C2C	2.59	1.49	1.43
17	N	605	HEA	C4A-NA	-2.58	1.34	1.39
17	A	604	HEA	C11-C3B	-2.58	1.48	1.51
17	A	604	HEA	C1A-NA	-2.57	1.34	1.39
17	A	604	HEA	C4D-ND	-2.56	1.33	1.38
17	N	605	HEA	C4C-NC	-2.54	1.34	1.39
17	N	605	HEA	C1A-NA	-2.50	1.34	1.39
17	N	606	HEA	C1C-NC	-2.46	1.35	1.39
19	B	303	TGL	OC1-CC1	-2.45	1.15	1.22
28	G	101	DMU	O7-C3	2.45	1.50	1.43
17	A	605	HEA	C1B-NB	-2.34	1.34	1.38
19	L	101	TGL	OG3-CG3	-2.31	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	605	HEA	C1C-C2C	2.29	1.48	1.43
28	M	101	DMU	O1-C9	2.28	1.49	1.44
17	N	606	HEA	C1C-C2C	2.26	1.48	1.43
24	C	301	CHD	O26-C24	-2.23	1.23	1.30
28	T	101	DMU	C2-C3	2.22	1.58	1.52
17	A	604	HEA	C1B-NB	-2.21	1.34	1.38
19	B	303	TGL	OG3-CC1	2.21	1.39	1.33
17	A	605	HEA	C11-C3B	-2.19	1.48	1.51
17	A	604	HEA	C1B-C2B	2.17	1.48	1.44
17	N	606	HEA	C1B-NB	-2.15	1.34	1.38
17	A	604	HEA	C1C-NC	-2.14	1.35	1.39
17	A	605	HEA	C1C-NC	-2.10	1.35	1.39
17	A	605	HEA	C4D-C3D	2.07	1.48	1.45
28	M	101	DMU	O1-C10	2.06	1.47	1.41
17	A	605	HEA	C4D-ND	-2.05	1.34	1.38
28	Q	201	DMU	O7-C10	2.01	1.47	1.41

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	605	HEA	C3A-C2A-C1A	-7.92	99.55	107.05
17	A	604	HEA	C3A-C2A-C1A	-7.30	100.14	107.05
17	A	605	HEA	C3C-C4C-NC	6.84	115.56	109.80
17	N	605	HEA	C2A-C1A-NA	6.68	116.77	110.32
17	N	606	HEA	C3A-C2A-C1A	-6.53	100.87	107.05
17	N	606	HEA	C2D-C1D-ND	6.46	117.27	109.84
17	A	605	HEA	C3A-C2A-C1A	-6.46	100.93	107.05
17	A	604	HEA	C2A-C1A-NA	6.42	116.51	110.32
18	A	608	PGV	O01-C1-C2	6.27	125.04	111.48
17	N	606	HEA	C3D-C4D-ND	6.04	116.19	110.35
17	N	605	HEA	C3D-C4D-ND	6.02	116.17	110.35
28	T	101	DMU	O16-C6-C1	6.02	117.41	108.27
17	N	606	HEA	C2A-C1A-NA	5.89	116.00	110.32
17	A	605	HEA	C2D-C1D-ND	5.77	116.48	109.84
17	A	605	HEA	C2A-C1A-NA	5.76	115.88	110.32
17	N	606	HEA	C1D-C2D-C3D	-5.72	100.96	106.98
28	G	101	DMU	C10-O1-C9	5.56	124.57	113.72
17	N	606	HEA	C3C-C4C-NC	5.48	114.41	109.80
17	A	605	HEA	C3C-C2C-C1C	-5.40	100.80	107.17
17	A	604	HEA	C2B-C1B-NB	5.28	116.01	109.90
17	N	605	HEA	C2D-C1D-ND	5.27	115.90	109.84
17	A	604	HEA	C3B-C4B-NB	5.08	115.68	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	605	HEA	CAD-CBD-CGD	-4.96	100.50	113.67
18	A	606	PGV	O01-C1-C2	4.93	122.15	111.48
18	U	101	PGV	O01-C1-C2	4.86	121.99	111.48
17	A	605	HEA	C1D-C2D-C3D	-4.85	101.88	106.98
17	N	605	HEA	C3C-C4C-NC	4.85	113.89	109.80
17	N	605	HEA	C1D-C2D-C3D	-4.80	101.93	106.98
17	A	604	HEA	C3C-C2C-C1C	-4.76	101.56	107.17
17	A	605	HEA	C2B-C1B-NB	4.73	115.38	109.90
18	A	607	PGV	O03-C19-C20	4.70	126.17	111.83
26	P	305	CDL	OA6-CA5-C11	4.62	121.48	111.48
18	A	607	PGV	O03-C19-O04	-4.62	112.07	123.63
18	U	101	PGV	O03-C19-C20	4.62	125.92	111.83
17	N	606	HEA	C2B-C1B-NB	4.58	115.20	109.90
24	J	102	CHD	C13-C17-C20	4.58	125.03	119.48
17	A	605	HEA	C3B-C4B-NB	4.57	115.10	109.84
26	C	304	CDL	OA6-CA5-C11	4.53	121.28	111.48
17	N	606	HEA	C3B-C4B-NB	4.45	114.95	109.84
17	N	606	HEA	C3C-C2C-C1C	-4.39	101.99	107.17
17	A	604	HEA	C3D-C4D-ND	4.38	114.59	110.35
19	N	607	TGL	CG2-OG2-CB1	4.36	128.22	117.80
18	A	608	PGV	O03-C19-C20	4.30	124.95	111.83
17	N	605	HEA	OMA-CMA-C3A	-4.29	115.93	125.62
28	G	101	DMU	C10-O7-C3	4.23	128.00	117.98
17	A	604	HEA	C1D-C2D-C3D	-4.23	102.53	106.98
17	N	605	HEA	C3C-C2C-C1C	-4.22	102.19	107.17
17	N	605	HEA	C3B-C4B-NB	4.18	114.64	109.84
28	T	101	DMU	C18-O16-C6	4.13	120.74	113.68
17	A	605	HEA	C3D-C4D-ND	4.11	114.33	110.35
18	C	303	PGV	O01-C1-C2	4.10	120.34	111.48
19	N	607	TGL	CG3-CG2-CG1	4.09	121.33	111.78
17	N	605	HEA	C2B-C1B-NB	4.08	114.61	109.90
19	L	101	TGL	OG2-CG2-CG1	4.02	122.75	108.34
18	A	607	PGV	O01-C1-C2	4.01	120.16	111.48
19	N	609	TGL	OG2-CB1-CB2	3.98	120.08	111.48
24	W	102	CHD	C13-C17-C20	3.86	124.16	119.48
17	A	604	HEA	C2D-C1D-ND	3.86	114.28	109.84
17	A	604	HEA	CHA-C4D-C3D	-3.77	119.27	124.77
18	N	610	PGV	O01-C1-C2	3.72	119.53	111.48
19	B	303	TGL	OG2-CB1-CB2	3.72	119.53	111.48
24	J	101	CHD	C10-C9-C8	3.69	115.96	111.84
28	M	101	DMU	C18-O16-C6	3.67	119.94	113.68
17	N	606	HEA	CMD-C2D-C1D	3.61	130.68	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	606	HEA	CAD-CBD-CGD	-3.61	104.09	113.67
17	N	605	HEA	CHB-C1B-C2B	-3.57	119.39	125.03
17	N	606	HEA	C1B-C2B-C3B	-3.49	102.75	106.80
19	A	609	TGL	CG2-OG2-CB1	-3.49	109.44	117.80
17	A	605	HEA	CMD-C2D-C1D	3.47	130.46	125.03
19	A	609	TGL	OG2-CG2-CG1	3.47	120.79	108.34
17	N	606	HEA	OMA-CMA-C3A	-3.39	117.98	125.62
18	A	608	PGV	O03-C19-O04	-3.38	115.17	123.63
18	A	607	PGV	O01-C1-O02	-3.31	115.96	123.70
17	A	605	HEA	C2C-C1C-NC	3.31	115.45	110.14
19	N	607	TGL	OG2-CB1-CB2	3.28	118.58	111.48
17	N	605	HEA	C17-C18-C19	-3.28	120.12	127.62
17	A	604	HEA	C4B-C3B-C2B	-3.27	101.95	107.44
28	M	101	DMU	C10-O1-C9	3.26	120.08	113.72
28	G	101	DMU	O7-C10-C5	3.22	116.01	108.09
17	A	604	HEA	CMB-C2B-C1B	3.21	130.04	125.03
19	N	609	TGL	OG2-CG2-CG1	3.19	119.77	108.34
17	N	605	HEA	CHA-C4D-C3D	-3.17	120.15	124.77
18	N	608	PGV	O01-C1-C2	3.16	118.32	111.48
17	N	605	HEA	CHA-C1A-C2A	-3.14	119.91	124.86
18	P	304	PGV	O01-C1-C2	3.10	118.18	111.48
17	A	605	HEA	C4B-C3B-C2B	-3.09	102.24	107.44
19	L	101	TGL	OG2-CB1-CB2	3.09	118.17	111.48
19	A	609	TGL	CG3-CG2-CG1	3.09	118.98	111.78
19	A	609	TGL	OG3-CC1-CC2	3.08	121.23	111.83
17	A	604	HEA	C1B-C2B-C3B	-3.08	103.23	106.80
17	A	604	HEA	CMD-C2D-C1D	3.06	129.82	125.03
18	N	610	PGV	O03-C19-C20	3.06	121.16	111.83
17	N	605	HEA	O11-C11-C3B	-3.04	105.69	111.26
17	N	605	HEA	CAA-C2A-C1A	3.04	131.03	124.85
17	N	606	HEA	CHB-C1B-C2B	-3.02	120.27	125.03
17	N	605	HEA	CMD-C2D-C1D	3.01	129.74	125.03
17	A	604	HEA	CHB-C1B-C2B	-3.00	120.29	125.03
18	N	608	PGV	O03-C19-C20	3.00	120.97	111.83
26	P	305	CDL	OB6-CB5-C51	2.99	117.96	111.48
17	A	605	HEA	CHB-C1B-C2B	-2.99	120.31	125.03
17	N	606	HEA	C2C-C1C-NC	2.99	114.93	110.14
28	M	101	DMU	O1-C9-C11	2.98	113.84	106.44
18	A	607	PGV	O03-C01-C02	2.98	116.97	108.40
17	N	606	HEA	CHA-C4D-C3D	-2.97	120.45	124.77
24	J	102	CHD	C22-C23-C24	2.96	120.39	112.49
17	N	606	HEA	C4B-C3B-C2B	-2.96	102.46	107.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	609	TGL	CG2-OG2-CB1	-2.95	110.73	117.80
18	A	606	PGV	C02-O01-C1	2.95	124.86	117.80
28	M	101	DMU	C8-C7-C5	-2.94	105.67	110.83
17	N	605	HEA	C4C-C3C-C2C	-2.94	103.65	107.30
28	T	101	DMU	C10-O7-C3	2.94	124.94	117.98
17	N	605	HEA	C26-C15-C16	2.93	120.31	115.23
19	Y	101	TGL	OG2-CG2-CG1	2.92	118.83	108.34
17	N	605	HEA	C1B-C2B-C3B	-2.91	103.43	106.80
26	N	601	CDL	OA6-CA5-C11	2.90	117.76	111.48
17	N	605	HEA	C13-C12-C11	-2.90	109.76	114.39
18	N	608	PGV	O03-C01-C02	2.90	116.76	108.40
28	M	101	DMU	C11-C9-C8	-2.90	105.90	113.02
19	B	303	TGL	OG2-CG2-CG3	2.89	118.71	108.34
17	N	606	HEA	CHA-C1A-C2A	-2.88	120.32	124.86
26	T	103	CDL	OA6-CA5-C11	2.86	117.68	111.48
17	N	605	HEA	C4B-C3B-C2B	-2.86	102.63	107.44
26	T	103	CDL	OB6-CB5-C51	2.86	117.67	111.48
17	A	604	HEA	CHC-C4B-NB	-2.86	120.83	124.37
17	A	605	HEA	C1B-C2B-C3B	-2.85	103.49	106.80
17	A	605	HEA	CMC-C2C-C1C	2.85	129.75	125.42
17	A	604	HEA	C3C-C4C-NC	2.84	112.19	109.80
18	C	303	PGV	O01-C1-O02	-2.82	117.10	123.70
28	G	101	DMU	O16-C6-C1	2.82	112.56	108.27
17	N	605	HEA	C2C-C1C-NC	2.81	114.64	110.14
18	C	303	PGV	O12-P-O13	-2.79	97.86	108.94
17	A	604	HEA	C13-C14-C15	-2.79	121.24	127.62
17	N	606	HEA	C4C-C3C-C2C	-2.78	103.85	107.30
17	A	604	HEA	C2C-C1C-NC	2.75	114.54	110.14
17	N	605	HEA	C4D-C3D-C2D	-2.74	102.90	106.89
28	G	101	DMU	C2-C3-C4	-2.71	104.92	110.93
28	Q	201	DMU	O5-C6-O16	2.71	116.45	110.04
19	N	609	TGL	OG2-CG2-CG3	2.70	118.03	108.34
19	Y	101	TGL	CG2-OG2-CB1	2.70	124.25	117.80
17	N	606	HEA	C1D-ND-C4D	-2.69	102.02	105.21
17	A	604	HEA	C17-C18-C19	-2.69	121.47	127.62
19	Y	101	TGL	CG3-CG2-CG1	2.69	118.05	111.78
17	A	605	HEA	C13-C12-C11	-2.69	110.10	114.39
17	A	605	HEA	CHA-C4D-C3D	-2.68	120.87	124.77
17	A	604	HEA	OMA-CMA-C3A	-2.68	119.57	125.62
24	J	101	CHD	C14-C8-C9	-2.68	106.01	109.75
28	Q	201	DMU	C18-O16-C6	-2.66	109.13	113.68
17	N	605	HEA	O2D-CGD-CBD	2.65	122.39	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	604	HEA	CBD-CAD-C3D	-2.65	105.20	112.53
18	U	101	PGV	O03-C19-O04	-2.65	117.00	123.63
17	A	604	HEA	CHA-C1A-C2A	-2.65	120.68	124.86
19	B	303	TGL	CG2-OG2-CB1	-2.64	111.49	117.80
17	A	605	HEA	CAD-C3D-C4D	2.64	129.29	124.70
17	N	606	HEA	CAA-C2A-C1A	2.62	130.18	124.85
26	C	304	CDL	OA6-CA5-OA7	-2.60	117.64	123.70
28	Q	201	DMU	C7-C8-C9	2.59	114.93	110.23
28	T	101	DMU	C10-O1-C9	2.59	118.78	113.72
26	P	305	CDL	CB4-OB6-CB5	-2.58	111.62	117.80
17	N	605	HEA	C12-C13-C14	-2.57	105.40	112.16
17	A	604	HEA	C26-C15-C16	2.55	119.65	115.23
24	W	102	CHD	C16-C17-C13	-2.51	101.11	103.54
28	G	101	DMU	O7-C3-C4	2.51	116.05	109.48
17	A	605	HEA	C4D-C3D-C2D	-2.51	103.25	106.89
19	Y	101	TGL	OG2-CB1-CB2	2.50	116.89	111.48
17	N	605	HEA	O2A-CGA-CBA	2.49	121.85	114.00
17	A	605	HEA	CHD-C1D-C2D	-2.48	119.89	126.95
26	P	305	CDL	OA8-CA7-OA9	-2.48	117.42	123.63
17	N	605	HEA	O2A-CGA-O1A	-2.48	116.96	123.33
17	A	605	HEA	C20-C19-C18	-2.47	115.63	121.17
19	L	101	TGL	OG3-CG3-CG2	2.45	115.47	108.40
18	A	606	PGV	O03-C19-C20	2.44	119.28	111.83
28	Q	201	DMU	O1-C9-C8	2.43	114.08	109.70
17	A	604	HEA	C13-C12-C11	-2.43	110.51	114.39
28	M	101	DMU	O1-C9-C8	2.42	114.06	109.70
28	G	101	DMU	C6-O5-C4	-2.41	109.02	113.72
18	U	101	PGV	O01-C1-O02	-2.39	118.11	123.70
18	P	304	PGV	C03-C02-C01	-2.39	106.22	111.78
26	T	103	CDL	OA8-CA7-C31	2.38	119.09	111.83
17	N	606	HEA	CHC-C1C-C2C	-2.37	120.55	127.43
19	N	607	TGL	OG3-CC1-CC2	2.36	119.03	111.83
18	P	304	PGV	O03-C19-O04	-2.36	117.73	123.63
17	N	606	HEA	O1D-CGD-CBD	-2.35	115.65	123.09
18	N	610	PGV	O03-C19-O04	-2.34	117.78	123.63
17	A	605	HEA	C27-C19-C20	2.33	119.27	115.23
26	N	601	CDL	CA4-OA6-CA5	-2.33	112.22	117.80
17	A	605	HEA	C4C-C3C-C2C	-2.33	104.41	107.30
19	B	303	TGL	OG3-CG3-CG2	2.32	115.10	108.40
28	T	101	DMU	C1-C2-C3	2.32	114.95	109.68
24	W	102	CHD	C22-C20-C17	2.31	115.13	110.33
17	A	604	HEA	CHD-C1D-C2D	-2.31	120.38	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	T	101	DMU	O1-C9-C11	2.30	112.15	106.44
19	B	303	TGL	OG3-CC1-CC2	2.30	118.85	111.83
17	N	606	HEA	C4D-C3D-C2D	-2.29	103.55	106.89
24	J	102	CHD	C22-C20-C17	2.29	115.09	110.33
18	C	303	PGV	O03-C19-O04	-2.29	117.89	123.63
26	C	304	CDL	OA8-CA7-OA9	-2.28	117.92	123.63
26	P	305	CDL	OA6-CA5-OA7	-2.28	118.37	123.70
17	N	605	HEA	CHC-C1C-C2C	-2.28	120.81	127.43
17	N	606	HEA	CHD-C1D-C2D	-2.28	120.47	126.95
17	A	604	HEA	C4D-C3D-C2D	-2.28	103.58	106.89
17	N	605	HEA	C21-C20-C19	-2.25	105.71	113.19
17	A	605	HEA	CHA-C1A-C2A	-2.24	121.32	124.86
26	C	304	CDL	OA8-CA7-C31	2.23	118.63	111.83
28	M	101	DMU	C6-O5-C4	2.22	118.06	113.72
19	Y	101	TGL	OG1-CG1-CG2	-2.22	102.00	108.40
18	P	304	PGV	O14-P-O13	2.20	122.67	112.44
17	A	605	HEA	CMB-C2B-C1B	2.20	128.47	125.03
18	N	608	PGV	C02-O01-C1	-2.19	112.54	117.80
24	W	102	CHD	C22-C23-C24	2.19	118.33	112.49
17	A	605	HEA	OMA-CMA-C3A	-2.18	120.69	125.62
18	U	101	PGV	O03-C01-C02	2.18	114.68	108.40
28	G	101	DMU	C34-C31-C28	-2.18	103.35	114.37
24	J	102	CHD	C5-C6-C7	2.18	116.99	114.40
18	A	606	PGV	O03-C01-C02	2.18	114.67	108.40
17	N	605	HEA	CAA-CBA-CGA	-2.17	107.90	113.67
17	A	605	HEA	O11-C11-C3B	-2.16	107.31	111.26
17	N	606	HEA	CAA-CBA-CGA	-2.15	107.96	113.67
17	N	606	HEA	O2D-CGD-CBD	2.14	120.77	114.00
19	N	607	TGL	CG3-OG3-CC1	2.14	124.95	117.12
18	C	303	PGV	C27-C26-C25	-2.13	103.60	114.37
17	N	605	HEA	CBD-CAD-C3D	-2.13	106.66	112.53
19	B	303	TGL	OB1-CB1-CB2	-2.12	115.49	123.78
17	A	604	HEA	CAD-C3D-C4D	2.12	128.39	124.70
19	A	609	TGL	OG1-CG1-CG2	2.11	114.49	108.40
19	N	609	TGL	OG3-CC1-CC2	2.11	118.28	111.83
19	B	303	TGL	OG3-CC1-OC1	-2.11	118.35	123.63
28	Q	201	DMU	C6-O5-C4	-2.11	109.61	113.72
17	A	604	HEA	CHC-C1C-C2C	-2.09	121.35	127.43
24	J	101	CHD	C9-C8-C7	2.09	114.49	111.86
28	M	101	DMU	O49-C1-C6	-2.09	105.10	110.08
26	T	103	CDL	OA8-CA7-OA9	-2.08	118.42	123.63
18	A	608	PGV	O01-C1-O02	-2.08	118.84	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	101	DMU	O1-C10-C5	2.08	114.64	110.37
19	L	101	TGL	OG2-CG2-CG3	2.08	115.80	108.34
18	C	303	PGV	C03-C02-C01	-2.08	106.94	111.78
17	N	605	HEA	CHD-C1D-C2D	-2.07	121.07	126.95
17	A	604	HEA	CMC-C2C-C1C	2.07	128.57	125.42
25	G	103	PEK	O01-C1-C2	2.07	115.95	111.48
17	N	605	HEA	CAD-C3D-C4D	2.06	128.29	124.70
17	N	605	HEA	CHC-C4B-NB	-2.05	121.83	124.37
24	J	101	CHD	C1-C2-C3	2.05	113.20	110.48
26	T	103	CDL	OA6-CA5-OA7	-2.04	118.94	123.70
26	N	601	CDL	OA6-CA5-OA7	-2.04	118.94	123.70
26	P	305	CDL	OA8-CA7-C31	2.03	118.03	111.83
19	A	609	TGL	OG2-CG2-CG3	2.03	115.62	108.34
17	N	606	HEA	O11-C11-C3B	-2.02	107.55	111.26
17	N	606	HEA	C21-C22-C23	-2.01	120.95	127.64
19	A	609	TGL	OG3-CC1-OC1	-2.01	118.61	123.63
17	A	604	HEA	CAA-C2A-C1A	2.01	128.93	124.85
18	A	606	PGV	O03-C19-O04	-2.00	118.61	123.63
24	J	101	CHD	C11-C9-C8	-2.00	107.93	110.89

There are no chirality outliers.

All (948) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	HEA	C2A-C3A-CMA-OMA
17	N	605	HEA	C2A-C3A-CMA-OMA
18	A	606	PGV	C03-O11-P-O12
18	A	606	PGV	C03-O11-P-O14
18	A	606	PGV	C04-O12-P-O11
18	A	606	PGV	C04-O12-P-O13
18	A	606	PGV	C04-O12-P-O14
18	A	606	PGV	C02-C03-O11-P
18	A	606	PGV	C04-C05-C06-O06
18	A	606	PGV	O05-C05-C06-O06
18	A	606	PGV	O02-C1-O01-C02
18	A	606	PGV	C2-C1-O01-C02
18	A	606	PGV	O04-C19-O03-C01
18	A	606	PGV	C20-C19-O03-C01
18	A	607	PGV	C04-O12-P-O11
18	A	607	PGV	C04-O12-P-O13
18	A	608	PGV	C05-C04-O12-P
18	N	610	PGV	C03-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	N	610	PGV	C03-O11-P-O13
18	N	610	PGV	C04-O12-P-O11
18	N	610	PGV	C04-C05-C06-O06
18	N	610	PGV	O02-C1-O01-C02
18	N	610	PGV	C20-C19-O03-C01
18	U	101	PGV	C03-O11-P-O12
18	U	101	PGV	C03-O11-P-O13
18	U	101	PGV	O01-C02-C03-O11
18	U	101	PGV	O02-C1-O01-C02
18	U	101	PGV	C2-C1-O01-C02
19	L	101	TGL	CB2-CB1-OG2-CG2
19	N	607	TGL	OB1-CB1-OG2-CG2
23	B	302	PSC	C04-O12-P-O13
23	B	302	PSC	O12-C04-C05-N
23	B	302	PSC	C9-C10-C11-C12
23	O	302	PSC	C03-O11-P-O12
23	O	302	PSC	C03-O11-P-O13
23	O	302	PSC	C04-O12-P-O11
23	O	302	PSC	C04-O12-P-O14
23	O	302	PSC	O12-C04-C05-N
24	W	102	CHD	C13-C17-C20-C22
24	W	102	CHD	C16-C17-C20-C22
25	C	302	PEK	C03-O11-P-O12
25	C	302	PEK	C03-O11-P-O13
25	C	302	PEK	C03-O11-P-O14
25	C	302	PEK	C2-C1-O01-C02
25	G	103	PEK	C03-O11-P-O14
25	G	103	PEK	C04-O12-P-O11
25	G	103	PEK	C04-O12-P-O13
25	G	103	PEK	C04-O12-P-O14
25	G	103	PEK	O12-C04-C05-N
25	P	303	PEK	C03-O11-P-O12
25	P	303	PEK	C03-O11-P-O13
25	P	303	PEK	C03-O11-P-O14
25	P	303	PEK	O02-C1-O01-C02
25	T	102	PEK	C03-O11-P-O12
25	T	102	PEK	C03-O11-P-O13
25	T	102	PEK	C03-O11-P-O14
25	T	102	PEK	C04-O12-P-O11
25	T	102	PEK	C04-O12-P-O13
25	T	102	PEK	O12-C04-C05-N
26	C	304	CDL	C1-CA2-OA2-PA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	304	CDL	CA2-OA2-PA1-OA3
26	C	304	CDL	CA2-OA2-PA1-OA5
26	C	304	CDL	C11-CA5-OA6-CA4
26	C	304	CDL	CB3-OB5-PB2-OB2
26	C	304	CDL	CB3-OB5-PB2-OB3
26	N	601	CDL	CA2-OA2-PA1-OA5
26	N	601	CDL	CA3-OA5-PA1-OA2
26	N	601	CDL	CA3-OA5-PA1-OA3
26	N	601	CDL	C11-CA5-OA6-CA4
26	N	601	CDL	C1-CB2-OB2-PB2
26	P	305	CDL	CA2-C1-CB2-OB2
26	P	305	CDL	C1-CA2-OA2-PA1
26	P	305	CDL	CA2-OA2-PA1-OA4
26	P	305	CDL	CA2-OA2-PA1-OA5
26	P	305	CDL	CA3-OA5-PA1-OA2
26	P	305	CDL	CA3-OA5-PA1-OA4
26	P	305	CDL	OA7-CA5-OA6-CA4
26	P	305	CDL	C11-CA5-OA6-CA4
26	P	305	CDL	CB3-OB5-PB2-OB3
26	P	305	CDL	C51-CB5-OB6-CB4
26	T	103	CDL	CA2-OA2-PA1-OA3
26	T	103	CDL	CA3-OA5-PA1-OA2
26	T	103	CDL	CA3-OA5-PA1-OA3
26	T	103	CDL	CA3-OA5-PA1-OA4
26	T	103	CDL	C11-CA5-OA6-CA4
26	T	103	CDL	C1-CB2-OB2-PB2
26	T	103	CDL	CB2-OB2-PB2-OB5
26	T	103	CDL	CB3-OB5-PB2-OB2
26	T	103	CDL	CB3-OB5-PB2-OB3
26	T	103	CDL	CB3-OB5-PB2-OB4
28	T	101	DMU	C1-C6-O16-C18
28	T	101	DMU	O5-C6-O16-C18
18	N	610	PGV	O04-C19-O03-C01
23	O	302	PSC	O04-C19-O03-C01
19	N	607	TGL	OA1-CA1-OG1-CG1
25	T	102	PEK	O04-C21-O03-C01
19	L	101	TGL	OB1-CB1-OG2-CG2
25	C	302	PEK	O02-C1-O01-C02
26	C	304	CDL	OA7-CA5-OA6-CA4
26	N	601	CDL	OA7-CA5-OA6-CA4
26	P	305	CDL	OB7-CB5-OB6-CB4
26	T	103	CDL	OA7-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	N	607	TGL	CA2-CA1-OG1-CG1
23	B	302	PSC	C20-C19-O03-C01
25	T	102	PEK	C22-C21-O03-C01
18	N	610	PGV	C2-C1-O01-C02
19	N	607	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	OA1-CA1-OG1-CG1
24	W	102	CHD	C16-C17-C20-C21
28	G	101	DMU	C5-C10-O7-C3
19	Y	101	TGL	CA2-CA1-OG1-CG1
23	O	302	PSC	C20-C19-O03-C01
26	C	304	CDL	C31-CA7-OA8-CA6
28	G	101	DMU	O6-C11-C9-O1
28	Q	201	DMU	O6-C11-C9-O1
23	B	302	PSC	O04-C19-O03-C01
26	C	304	CDL	OA9-CA7-OA8-CA6
18	A	606	PGV	O12-C04-C05-O05
18	U	101	PGV	O12-C04-C05-O05
19	L	101	TGL	CA2-CA1-OG1-CG1
25	P	303	PEK	C2-C1-O01-C02
19	Y	101	TGL	OA1-CA1-OG1-CG1
28	T	101	DMU	O5-C4-C57-O61
28	Q	201	DMU	O6-C11-C9-C8
17	A	604	HEA	C15-C16-C17-C18
17	N	605	HEA	C15-C16-C17-C18
28	M	101	DMU	O5-C6-O16-C18
28	Q	201	DMU	O5-C6-O16-C18
28	G	101	DMU	O5-C4-C57-O61
28	G	101	DMU	O6-C11-C9-C8
24	J	102	CHD	C13-C17-C20-C22
24	B	304	CHD	C17-C20-C22-C23
24	G	104	CHD	C17-C20-C22-C23
26	N	601	CDL	C80-C81-C82-C83
18	A	608	PGV	O12-C04-C05-C06
18	N	610	PGV	O12-C04-C05-C06
18	A	608	PGV	C20-C19-O03-C01
19	A	609	TGL	CC2-CC1-OG3-CG3
26	T	103	CDL	C31-CA7-OA8-CA6
19	N	607	TGL	CA3-CA4-CA5-CA6
28	G	101	DMU	C3-C4-C57-O61
28	M	101	DMU	C1-C6-O16-C18
19	N	607	TGL	CA9-C20-C21-C22
18	A	608	PGV	O12-C04-C05-O05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	N	610	PGV	O12-C04-C05-O05
26	N	601	CDL	O1-C1-CB2-OB2
26	P	305	CDL	O1-C1-CB2-OB2
19	N	609	TGL	CB9-C10-C11-C12
19	B	303	TGL	CC5-CC6-CC7-CC8
19	A	609	TGL	OC1-CC1-OG3-CG3
26	T	103	CDL	OA9-CA7-OA8-CA6
24	J	101	CHD	C17-C20-C22-C23
24	J	102	CHD	C17-C20-C22-C23
28	Q	201	DMU	C3-C4-C57-O61
23	O	302	PSC	C2-C1-O01-C02
19	N	609	TGL	CC2-CC1-OG3-CG3
26	P	305	CDL	C31-CA7-OA8-CA6
24	B	304	CHD	C21-C20-C22-C23
24	J	101	CHD	C21-C20-C22-C23
26	N	601	CDL	C71-C72-C73-C74
28	T	101	DMU	C3-C4-C57-O61
19	A	609	TGL	CA2-CA1-OG1-CG1
28	G	101	DMU	O1-C10-O7-C3
26	N	601	CDL	CA5-C11-C12-C13
19	Y	101	TGL	OB1-CB1-OG2-CG2
23	O	302	PSC	O02-C1-O01-C02
19	N	607	TGL	CA5-CA6-CA7-CA8
19	N	607	TGL	C13-C14-C29-C30
26	P	305	CDL	C40-C41-C42-C43
19	B	303	TGL	CA1-CA2-CA3-CA4
19	B	303	TGL	CB1-CB2-CB3-CB4
18	A	608	PGV	O04-C19-O03-C01
19	Y	101	TGL	CB2-CB1-OG2-CG2
28	G	101	DMU	C4-C3-O7-C10
28	T	101	DMU	C2-C3-O7-C10
24	J	102	CHD	C21-C20-C22-C23
18	A	608	PGV	C1-C2-C3-C4
25	T	102	PEK	C1-C2-C3-C4
26	C	304	CDL	CA5-C11-C12-C13
26	C	304	CDL	CB7-C71-C72-C73
26	N	601	CDL	CA7-C31-C32-C33
28	G	101	DMU	C2-C3-O7-C10
19	N	609	TGL	C19-C33-C34-C35
26	C	304	CDL	O1-C1-CB2-OB2
28	Q	201	DMU	O16-C18-C19-C22
19	Y	101	TGL	CC1-CC2-CC3-CC4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	305	CDL	C61-C62-C63-C64
23	O	302	PSC	C19-C20-C21-C22
25	G	103	PEK	C1-C2-C3-C4
25	P	302	PEK	C1-C2-C3-C4
26	P	305	CDL	CA5-C11-C12-C13
26	P	305	CDL	CB5-C51-C52-C53
26	T	103	CDL	CB7-C71-C72-C73
19	N	609	TGL	C20-C21-C22-C23
18	P	304	PGV	C20-C19-O03-C01
19	N	609	TGL	OC1-CC1-OG3-CG3
26	P	305	CDL	OA9-CA7-OA8-CA6
28	Q	201	DMU	O5-C4-C57-O61
26	P	305	CDL	C42-C43-C44-C45
18	A	606	PGV	O12-C04-C05-C06
26	C	304	CDL	CA2-C1-CB2-OB2
26	N	601	CDL	CA2-C1-CB2-OB2
25	G	102	PEK	C22-C21-O03-C01
25	P	302	PEK	C22-C21-O03-C01
24	W	102	CHD	C13-C17-C20-C21
19	B	303	TGL	CC2-CC1-OG3-CG3
25	T	102	PEK	C2-C1-O01-C02
25	T	102	PEK	O02-C1-O01-C02
26	T	103	CDL	O1-C1-CA2-OA2
26	C	304	CDL	C55-C56-C57-C58
26	N	601	CDL	C22-C23-C24-C25
28	T	101	DMU	C4-C3-O7-C10
18	P	304	PGV	O04-C19-O03-C01
19	L	101	TGL	CB3-CB4-CB5-CB6
19	L	101	TGL	CC9-C15-C16-C17
18	U	101	PGV	C04-C05-C06-O06
19	N	609	TGL	CC2-CC3-CC4-CC5
19	A	609	TGL	OA1-CA1-OG1-CG1
19	N	607	TGL	CC5-CC6-CC7-CC8
26	P	305	CDL	C43-C44-C45-C46
26	T	103	CDL	C71-CB7-OB8-CB6
19	A	609	TGL	C18-C19-C33-C34
19	N	607	TGL	CB6-CB7-CB8-CB9
26	C	304	CDL	C74-C75-C76-C77
26	P	305	CDL	C73-C74-C75-C76
18	N	610	PGV	C14-C15-C16-C17
19	A	609	TGL	CC9-C15-C16-C17
19	A	609	TGL	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	303	TGL	CA3-CA4-CA5-CA6
19	B	303	TGL	CB5-CB6-CB7-CB8
19	L	101	TGL	CA3-CA4-CA5-CA6
19	N	607	TGL	C11-C10-CB9-CB8
19	N	609	TGL	CC5-CC6-CC7-CC8
19	N	609	TGL	C23-C24-C25-C26
19	Y	101	TGL	CB6-CB7-CB8-CB9
19	Y	101	TGL	C16-C15-CC9-CC8
26	C	304	CDL	C15-C16-C17-C18
26	C	304	CDL	C71-C72-C73-C74
18	P	304	PGV	C25-C26-C27-C28
19	B	303	TGL	C20-C21-C22-C23
19	N	607	TGL	CB4-CB5-CB6-CB7
26	C	304	CDL	C11-C12-C13-C14
26	T	103	CDL	C78-C79-C80-C81
25	P	302	PEK	O04-C21-O03-C01
19	L	101	TGL	C11-C12-C13-C14
19	Y	101	TGL	CC3-CC4-CC5-CC6
19	Y	101	TGL	C21-C22-C23-C24
23	B	302	PSC	C26-C27-C28-C29
25	G	103	PEK	C29-C30-C31-C32
25	P	303	PEK	C25-C26-C27-C28
25	T	102	PEK	C25-C26-C27-C28
26	C	304	CDL	C39-C40-C41-C42
26	P	305	CDL	C22-C23-C24-C25
26	T	103	CDL	C59-C60-C61-C62
18	N	610	PGV	O05-C05-C06-O06
18	U	101	PGV	O05-C05-C06-O06
28	M	101	DMU	C19-C18-O16-C6
19	N	607	TGL	C23-C24-C25-C26
26	N	601	CDL	C20-C21-C22-C23
26	N	601	CDL	C23-C24-C25-C26
26	P	305	CDL	C14-C15-C16-C17
26	C	304	CDL	C59-C60-C61-C62
26	N	601	CDL	C79-C80-C81-C82
26	P	305	CDL	C31-C32-C33-C34
26	P	305	CDL	C51-C52-C53-C54
26	T	103	CDL	C21-C22-C23-C24
26	N	601	CDL	C58-C59-C60-C61
26	P	305	CDL	C63-C64-C65-C66
18	A	608	PGV	C2-C1-O01-C02
28	T	101	DMU	O6-C11-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	N	607	TGL	C16-C15-CC9-CC8
25	G	102	PEK	C29-C30-C31-C32
26	N	601	CDL	C16-C17-C18-C19
26	N	601	CDL	C77-C78-C79-C80
23	B	302	PSC	C1-C2-C3-C4
25	P	303	PEK	C1-C2-C3-C4
26	P	305	CDL	CB7-C71-C72-C73
18	A	606	PGV	C2-C3-C4-C5
18	N	608	PGV	C3-C4-C5-C6
18	N	608	PGV	C25-C26-C27-C28
19	L	101	TGL	CA2-CA3-CA4-CA5
26	N	601	CDL	C41-C42-C43-C44
26	T	103	CDL	C20-C21-C22-C23
26	T	103	CDL	C41-C42-C43-C44
28	G	101	DMU	C22-C25-C28-C31
18	A	607	PGV	C5-C6-C7-C8
25	T	102	PEK	C29-C30-C31-C32
26	N	601	CDL	C39-C40-C41-C42
19	N	607	TGL	C20-C21-C22-C23
25	G	103	PEK	C31-C32-C33-C34
19	N	609	TGL	CB1-CB2-CB3-CB4
19	A	609	TGL	C15-C16-C17-C18
19	B	303	TGL	C13-C14-C29-C30
19	Y	101	TGL	CA2-CA3-CA4-CA5
25	T	102	PEK	C16-C17-C18-C19
26	T	103	CDL	C72-C73-C74-C75
19	A	609	TGL	CC2-CC3-CC4-CC5
23	O	302	PSC	C29-C30-C31-C32
25	P	302	PEK	C25-C26-C27-C28
26	P	305	CDL	C82-C83-C84-C85
19	B	303	TGL	CA2-CA1-OG1-CG1
26	N	601	CDL	C71-CB7-OB8-CB6
19	A	609	TGL	CG1-CG2-CG3-OG3
19	N	609	TGL	CB4-CB5-CB6-CB7
25	G	102	PEK	C24-C25-C26-C27
26	C	304	CDL	C20-C21-C22-C23
18	A	607	PGV	C19-C20-C21-C22
19	L	101	TGL	C23-C24-C25-C26
19	N	607	TGL	CB3-CB4-CB5-CB6
19	N	609	TGL	CB6-CB7-CB8-CB9
19	Y	101	TGL	C13-C14-C29-C30
26	P	305	CDL	C62-C63-C64-C65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	305	CDL	C76-C77-C78-C79
26	T	103	CDL	C76-C77-C78-C79
25	G	102	PEK	O04-C21-O03-C01
18	U	101	PGV	C29-C30-C31-C32
23	B	302	PSC	C29-C30-C31-C32
26	N	601	CDL	C53-C54-C55-C56
26	P	305	CDL	C72-C73-C74-C75
19	B	303	TGL	CB7-CB8-CB9-C10
19	Y	101	TGL	CB9-C10-C11-C12
18	C	303	PGV	C7-C8-C9-C10
19	B	303	TGL	CB9-C10-C11-C12
19	Y	101	TGL	C22-C23-C24-C25
26	C	304	CDL	C80-C81-C82-C83
28	M	101	DMU	C19-C22-C25-C28
18	P	304	PGV	C1-C2-C3-C4
19	L	101	TGL	CB1-CB2-CB3-CB4
18	A	607	PGV	C6-C7-C8-C9
18	A	608	PGV	C29-C30-C31-C32
19	A	609	TGL	C13-C14-C29-C30
19	L	101	TGL	CC7-CC8-CC9-C15
19	N	609	TGL	CA5-CA6-CA7-CA8
26	C	304	CDL	C33-C34-C35-C36
26	N	601	CDL	C15-C16-C17-C18
26	N	601	CDL	C35-C36-C37-C38
26	P	305	CDL	C15-C16-C17-C18
19	A	609	TGL	CB2-CB1-OG2-CG2
25	G	102	PEK	C2-C1-O01-C02
18	A	607	PGV	C7-C8-C9-C10
19	A	609	TGL	C17-C18-C19-C33
19	L	101	TGL	CC1-CC2-CC3-CC4
19	N	609	TGL	C15-C16-C17-C18
19	B	303	TGL	OC1-CC1-OG3-CG3
26	T	103	CDL	OB9-CB7-OB8-CB6
28	M	101	DMU	O16-C18-C19-C22
23	B	302	PSC	C3-C4-C5-C6
18	A	608	PGV	O02-C1-O01-C02
19	A	609	TGL	OB1-CB1-OG2-CG2
18	A	607	PGV	C22-C23-C24-C25
18	P	304	PGV	C24-C25-C26-C27
24	J	102	CHD	C13-C17-C20-C21
24	P	301	CHD	C13-C17-C20-C21
19	Y	101	TGL	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	P	302	PEK	C24-C25-C26-C27
26	N	601	CDL	C73-C74-C75-C76
25	P	303	PEK	C28-C29-C30-C31
18	A	606	PGV	C28-C29-C30-C31
19	A	609	TGL	C11-C10-CB9-CB8
19	N	607	TGL	CC6-CC7-CC8-CC9
19	N	609	TGL	CA6-CA7-CA8-CA9
26	N	601	CDL	C21-C22-C23-C24
26	P	305	CDL	C71-C72-C73-C74
18	N	610	PGV	C20-C21-C22-C23
19	A	609	TGL	CA3-CA4-CA5-CA6
19	B	303	TGL	CB3-CB4-CB5-CB6
19	B	303	TGL	C23-C24-C25-C26
19	N	607	TGL	CC7-CC8-CC9-C15
18	A	606	PGV	C4-C5-C6-C7
18	A	606	PGV	C20-C21-C22-C23
26	P	305	CDL	C23-C24-C25-C26
19	A	609	TGL	CA7-CA8-CA9-C20
19	B	303	TGL	CA4-CA5-CA6-CA7
19	L	101	TGL	CB5-CB6-CB7-CB8
26	P	305	CDL	C36-C37-C38-C39
28	Q	201	DMU	C19-C22-C25-C28
26	C	304	CDL	C71-CB7-OB8-CB6
19	N	609	TGL	CC6-CC7-CC8-CC9
25	G	103	PEK	C2-C1-O01-C02
26	T	103	CDL	C51-CB5-OB6-CB4
19	L	101	TGL	CC3-CC4-CC5-CC6
25	C	302	PEK	C25-C26-C27-C28
24	P	301	CHD	C16-C17-C20-C22
18	N	610	PGV	C12-C13-C14-C15
19	B	303	TGL	C16-C15-CC9-CC8
25	G	103	PEK	C24-C25-C26-C27
26	N	601	CDL	C32-C33-C34-C35
26	P	305	CDL	C41-C42-C43-C44
18	A	608	PGV	C26-C27-C28-C29
26	N	601	CDL	C42-C43-C44-C45
24	G	104	CHD	C21-C20-C22-C23
18	N	608	PGV	C6-C7-C8-C9
18	C	303	PGV	C22-C23-C24-C25
18	P	304	PGV	C7-C8-C9-C10
26	C	304	CDL	C14-C15-C16-C17
26	P	305	CDL	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	305	CDL	C38-C39-C40-C41
26	P	305	CDL	C58-C59-C60-C61
25	P	303	PEK	C24-C25-C26-C27
28	G	101	DMU	C18-C19-C22-C25
18	A	608	PGV	C22-C23-C24-C25
19	B	303	TGL	CC4-CC5-CC6-CC7
18	A	608	PGV	O01-C02-C03-O11
18	A	607	PGV	C25-C26-C27-C28
19	B	303	TGL	OA1-CA1-OG1-CG1
26	P	305	CDL	C37-C38-C39-C40
28	M	101	DMU	C18-C19-C22-C25
18	A	607	PGV	C24-C25-C26-C27
26	T	103	CDL	C13-C14-C15-C16
19	B	303	TGL	OG1-CG1-CG2-OG2
18	A	607	PGV	C26-C27-C28-C29
18	C	303	PGV	C23-C24-C25-C26
26	N	601	CDL	OB9-CB7-OB8-CB6
18	A	608	PGV	C3-C4-C5-C6
19	N	609	TGL	CC7-CC8-CC9-C15
26	C	304	CDL	C17-C18-C19-C20
26	T	103	CDL	C31-C32-C33-C34
19	L	101	TGL	C24-C25-C26-C27
19	N	607	TGL	CB2-CB3-CB4-CB5
19	A	609	TGL	CA9-C20-C21-C22
19	L	101	TGL	C22-C23-C24-C25
26	N	601	CDL	C74-C75-C76-C77
26	T	103	CDL	C73-C74-C75-C76
26	T	103	CDL	C35-C36-C37-C38
25	G	103	PEK	O02-C1-O01-C02
19	N	607	TGL	C16-C17-C18-C19
26	C	304	CDL	C60-C61-C62-C63
26	C	304	CDL	C76-C77-C78-C79
19	B	303	TGL	C16-C17-C18-C19
19	N	609	TGL	CB3-CB4-CB5-CB6
28	G	101	DMU	C19-C22-C25-C28
25	G	103	PEK	C4-C5-C6-C7
19	Y	101	TGL	CA9-C20-C21-C22
19	N	609	TGL	C11-C10-CB9-CB8
25	G	102	PEK	C33-C34-C35-C36
24	J	102	CHD	C16-C17-C20-C21
19	N	607	TGL	CC4-CC5-CC6-CC7
26	T	103	CDL	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	303	TGL	C24-C25-C26-C27
19	A	609	TGL	C16-C15-CC9-CC8
23	B	302	PSC	C6-C7-C8-C9
25	T	102	PEK	C2-C3-C4-C5
18	A	608	PGV	C27-C28-C29-C30
19	L	101	TGL	C11-C10-CB9-CB8
25	P	302	PEK	C26-C27-C28-C29
26	C	304	CDL	C52-C53-C54-C55
18	N	610	PGV	C01-C02-C03-O11
26	N	601	CDL	OB5-CB3-CB4-CB6
26	T	103	CDL	OB7-CB5-OB6-CB4
23	O	302	PSC	C21-C22-C23-C24
25	G	103	PEK	C27-C28-C29-C30
26	N	601	CDL	C82-C83-C84-C85
18	N	608	PGV	C19-C20-C21-C22
26	N	601	CDL	CB5-C51-C52-C53
19	N	607	TGL	C21-C22-C23-C24
25	P	302	PEK	C27-C28-C29-C30
26	P	305	CDL	C21-C22-C23-C24
18	A	606	PGV	C30-C31-C32-C33
19	L	101	TGL	C21-C22-C23-C24
19	N	609	TGL	CA4-CA5-CA6-CA7
25	G	102	PEK	C31-C32-C33-C34
26	N	601	CDL	C54-C55-C56-C57
19	B	303	TGL	C19-C33-C34-C35
25	G	102	PEK	O02-C1-O01-C02
19	N	609	TGL	CA1-CA2-CA3-CA4
18	A	606	PGV	O03-C01-C02-C03
18	N	610	PGV	O03-C01-C02-C03
19	A	609	TGL	OG1-CG1-CG2-CG3
25	P	302	PEK	O03-C01-C02-C03
28	T	101	DMU	C34-C37-C40-C43
18	C	303	PGV	C28-C29-C30-C31
19	N	607	TGL	CC2-CC3-CC4-CC5
25	T	102	PEK	C33-C34-C35-C36
18	N	608	PGV	C29-C30-C31-C32
19	L	101	TGL	C16-C17-C18-C19
25	P	303	PEK	C22-C21-O03-C01
18	A	606	PGV	C19-C20-C21-C22
18	N	608	PGV	C13-C14-C15-C16
19	A	609	TGL	C19-C33-C34-C35
26	P	305	CDL	C74-C75-C76-C77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	N	608	PGV	C4-C5-C6-C7
25	P	303	PEK	O04-C21-O03-C01
19	B	303	TGL	CB4-CB5-CB6-CB7
23	B	302	PSC	C21-C22-C23-C24
25	T	102	PEK	C27-C28-C29-C30
26	T	103	CDL	C82-C83-C84-C85
18	A	608	PGV	C2-C3-C4-C5
18	N	610	PGV	C3-C4-C5-C6
19	N	609	TGL	CC4-CC5-CC6-CC7
26	C	304	CDL	OB9-CB7-OB8-CB6
18	A	608	PGV	C14-C15-C16-C17
19	N	607	TGL	C10-C11-C12-C13
26	N	601	CDL	C34-C35-C36-C37
18	A	608	PGV	C6-C7-C8-C9
18	A	606	PGV	C11-C10-C9-C8
18	A	608	PGV	C7-C8-C9-C10
19	A	609	TGL	CA5-CA6-CA7-CA8
19	B	303	TGL	C18-C19-C33-C34
25	G	102	PEK	C27-C28-C29-C30
25	P	303	PEK	C23-C24-C25-C26
26	N	601	CDL	C60-C61-C62-C63
18	N	608	PGV	C7-C8-C9-C10
19	Y	101	TGL	C11-C10-CB9-CB8
26	C	304	CDL	C16-C17-C18-C19
26	C	304	CDL	C79-C80-C81-C82
18	A	606	PGV	C22-C23-C24-C25
19	N	609	TGL	C24-C25-C26-C27
26	P	305	CDL	C34-C35-C36-C37
26	C	304	CDL	C63-C64-C65-C66
25	C	302	PEK	C28-C29-C30-C31
18	A	606	PGV	C25-C26-C27-C28
19	B	303	TGL	C12-C13-C14-C29
25	T	102	PEK	C22-C23-C24-C25
19	B	303	TGL	CC6-CC7-CC8-CC9
25	T	102	PEK	C31-C32-C33-C34
26	T	103	CDL	C38-C39-C40-C41
18	A	607	PGV	C30-C31-C32-C33
18	A	608	PGV	C20-C21-C22-C23
19	L	101	TGL	C18-C19-C33-C34
23	O	302	PSC	C2-C3-C4-C5
26	T	103	CDL	C56-C57-C58-C59
25	T	102	PEK	O03-C01-C02-O01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	N	601	CDL	OB6-CB4-CB6-OB8
26	T	103	CDL	OB6-CB4-CB6-OB8
23	O	302	PSC	C15-C16-C17-C18
26	T	103	CDL	O1-C1-CB2-OB2
19	B	303	TGL	C29-C30-C31-C32
18	A	608	PGV	C30-C31-C32-C33
18	N	610	PGV	C6-C7-C8-C9
19	L	101	TGL	C29-C30-C31-C32
19	L	101	TGL	C21-C20-CA9-CA8
19	N	607	TGL	C15-C16-C17-C18
25	P	303	PEK	C29-C30-C31-C32
26	T	103	CDL	C34-C35-C36-C37
23	B	302	PSC	C15-C16-C17-C18
26	T	103	CDL	C44-C45-C46-C47
26	C	304	CDL	C84-C85-C86-C87
18	U	101	PGV	C15-C16-C17-C18
19	B	303	TGL	CC2-CC3-CC4-CC5
26	N	601	CDL	C55-C56-C57-C58
18	N	610	PGV	C31-C32-C33-C34
26	N	601	CDL	C13-C14-C15-C16
19	Y	101	TGL	C25-C26-C27-C28
25	T	102	PEK	C35-C36-C37-C38
26	N	601	CDL	C56-C57-C58-C59
28	M	101	DMU	C34-C37-C40-C43
28	M	101	DMU	C28-C31-C34-C37
18	U	101	PGV	C02-C03-O11-P
26	T	103	CDL	CB4-CB3-OB5-PB2
25	C	302	PEK	C16-C17-C18-C19
19	N	609	TGL	CB2-CB3-CB4-CB5
26	N	601	CDL	C24-C25-C26-C27
19	B	303	TGL	CA7-CA8-CA9-C20
26	T	103	CDL	C37-C38-C39-C40
18	A	608	PGV	C01-C02-C03-O11
18	U	101	PGV	C01-C02-C03-O11
26	T	103	CDL	OB5-CB3-CB4-CB6
26	N	601	CDL	C59-C60-C61-C62
26	T	103	CDL	C54-C55-C56-C57
18	N	608	PGV	C15-C16-C17-C18
19	N	609	TGL	C25-C26-C27-C28
23	O	302	PSC	C31-C32-C33-C34
23	O	302	PSC	C14-C15-C16-C17
23	B	302	PSC	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	304	CDL	C64-C65-C66-C67
19	L	101	TGL	C12-C13-C14-C29
26	N	601	CDL	C31-C32-C33-C34
18	P	304	PGV	C27-C28-C29-C30
19	N	607	TGL	C12-C13-C14-C29
26	T	103	CDL	C11-C12-C13-C14
26	N	601	CDL	C33-C34-C35-C36
26	P	305	CDL	C75-C76-C77-C78
18	P	304	PGV	C13-C14-C15-C16
26	T	103	CDL	C77-C78-C79-C80
26	T	103	CDL	CA2-C1-CB2-OB2
28	T	101	DMU	O6-C11-C9-O1
26	C	304	CDL	C81-C82-C83-C84
23	B	302	PSC	O03-C01-C02-C03
23	O	302	PSC	O03-C01-C02-C03
25	C	302	PEK	O03-C01-C02-C03
25	G	102	PEK	O03-C01-C02-C03
26	C	304	CDL	CB3-CB4-CB6-OB8
19	B	303	TGL	C10-C11-C12-C13
18	U	101	PGV	C30-C31-C32-C33
25	C	302	PEK	C29-C30-C31-C32
19	L	101	TGL	CB2-CB3-CB4-CB5
25	G	103	PEK	C33-C34-C35-C36
19	A	609	TGL	C10-C11-C12-C13
25	C	302	PEK	O01-C02-C03-O11
25	T	102	PEK	O01-C02-C03-O11
19	N	609	TGL	CA7-CA8-CA9-C20
25	C	302	PEK	C35-C36-C37-C38
18	N	610	PGV	C02-C03-O11-P
19	B	303	TGL	C25-C26-C27-C28
18	N	610	PGV	C15-C16-C17-C18
18	U	101	PGV	C23-C24-C25-C26
23	O	302	PSC	C27-C28-C29-C30
19	N	607	TGL	OG2-CG2-CG3-OG3
25	C	302	PEK	O03-C01-C02-O01
26	P	305	CDL	OB6-CB4-CB6-OB8
23	O	302	PSC	C9-C10-C11-C12
25	C	302	PEK	C6-C7-C8-C9
25	G	103	PEK	C6-C7-C8-C9
25	P	302	PEK	C11-C10-C9-C8
25	P	303	PEK	C6-C7-C8-C9
25	P	303	PEK	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	T	102	PEK	C6-C7-C8-C9
18	N	610	PGV	C30-C31-C32-C33
26	P	305	CDL	C54-C55-C56-C57
19	L	101	TGL	CB6-CB7-CB8-CB9
19	L	101	TGL	CA9-C20-C21-C22
26	N	601	CDL	C11-C12-C13-C14
23	B	302	PSC	C13-C14-C15-C16
26	C	304	CDL	C35-C36-C37-C38
19	A	609	TGL	CC7-CC8-CC9-C15
19	L	101	TGL	CA4-CA5-CA6-CA7
18	C	303	PGV	C1-C2-C3-C4
25	C	302	PEK	C34-C35-C36-C37
25	T	102	PEK	C30-C31-C32-C33
19	N	607	TGL	C18-C19-C33-C34
18	N	608	PGV	O03-C19-C20-C21
26	P	305	CDL	C52-C51-CB5-OB6
19	A	609	TGL	C33-C34-C35-C36
25	T	102	PEK	C01-C02-C03-O11
19	B	303	TGL	CA6-CA7-CA8-CA9
19	Y	101	TGL	C16-C17-C18-C19
25	T	102	PEK	C26-C27-C28-C29
18	U	101	PGV	C31-C32-C33-C34
19	B	303	TGL	CB2-CB1-OG2-CG2
26	P	305	CDL	C11-C12-C13-C14
26	T	103	CDL	C24-C25-C26-C27
26	T	103	CDL	C64-C65-C66-C67
25	P	302	PEK	C22-C23-C24-C25
19	N	609	TGL	CG1-CG2-OG2-CB1
26	P	305	CDL	C59-C60-C61-C62
18	N	610	PGV	O01-C02-C03-O11
26	T	103	CDL	OB5-CB3-CB4-OB6
26	C	304	CDL	C44-C45-C46-C47
19	B	303	TGL	OG1-CG1-CG2-CG3
19	N	607	TGL	CG1-CG2-CG3-OG3
25	T	102	PEK	O03-C01-C02-C03
26	P	305	CDL	CB3-CB4-CB6-OB8
23	O	302	PSC	C05-C04-O12-P
18	C	303	PGV	C30-C31-C32-C33
19	A	609	TGL	C21-C20-CA9-CA8
19	L	101	TGL	CC4-CC5-CC6-CC7
18	A	606	PGV	O03-C01-C02-O01
23	O	302	PSC	O03-C01-C02-O01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	G	102	PEK	O03-C01-C02-O01
28	Q	201	DMU	C25-C28-C31-C34
18	U	101	PGV	C7-C8-C9-C10
26	C	304	CDL	C12-C13-C14-C15
19	Y	101	TGL	CB1-CB2-CB3-CB4
25	G	102	PEK	C34-C35-C36-C37
19	N	609	TGL	CB2-CB1-OG2-CG2
19	A	609	TGL	CA2-CA3-CA4-CA5
26	C	304	CDL	C73-C74-C75-C76
26	P	305	CDL	C18-C19-C20-C21
19	L	101	TGL	C10-C11-C12-C13
26	C	304	CDL	C83-C84-C85-C86
19	N	609	TGL	CA3-CA4-CA5-CA6
26	N	601	CDL	C18-C19-C20-C21
24	P	301	CHD	C16-C17-C20-C21
25	P	303	PEK	C35-C36-C37-C38
19	B	303	TGL	OB1-CB1-OG2-CG2
28	M	101	DMU	C22-C25-C28-C31
18	C	303	PGV	C14-C15-C16-C17
18	N	610	PGV	C11-C10-C9-C8
18	A	608	PGV	C13-C14-C15-C16
25	G	103	PEK	C35-C36-C37-C38
19	N	609	TGL	OB1-CB1-OG2-CG2
25	G	102	PEK	C28-C29-C30-C31
19	N	609	TGL	C11-C12-C13-C14
23	B	302	PSC	C2-C3-C4-C5
19	L	101	TGL	CC2-CC3-CC4-CC5
26	N	601	CDL	C64-C65-C66-C67
26	C	304	CDL	C42-C43-C44-C45
26	C	304	CDL	C75-C76-C77-C78
19	N	607	TGL	CC3-CC4-CC5-CC6
18	N	610	PGV	C05-C04-O12-P
26	N	601	CDL	C75-C76-C77-C78
26	C	304	CDL	OA5-CA3-CA4-OA6
26	P	305	CDL	OB5-CB3-CB4-OB6
19	N	609	TGL	C33-C34-C35-C36
18	P	304	PGV	C31-C32-C33-C34
18	U	101	PGV	C24-C25-C26-C27
26	N	601	CDL	C62-C63-C64-C65
26	T	103	CDL	C43-C44-C45-C46
17	A	604	HEA	C4A-C3A-CMA-OMA
19	N	609	TGL	C14-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	L	101	TGL	CC6-CC7-CC8-CC9
18	N	610	PGV	O03-C01-C02-O01
19	N	609	TGL	OG2-CG2-CG3-OG3
25	P	302	PEK	O03-C01-C02-O01
26	C	304	CDL	OB6-CB4-CB6-OB8
25	C	302	PEK	C10-C11-C12-C13
25	P	302	PEK	C10-C11-C12-C13
18	N	610	PGV	C2-C3-C4-C5
19	L	101	TGL	CG1-CG2-CG3-OG3
19	N	607	TGL	OG1-CG1-CG2-CG3
26	N	601	CDL	CB3-CB4-CB6-OB8
26	T	103	CDL	CB3-CB4-CB6-OB8
18	A	607	PGV	C23-C24-C25-C26
19	B	303	TGL	C11-C12-C13-C14
26	T	103	CDL	C57-C58-C59-C60
25	P	303	PEK	C30-C31-C32-C33
26	C	304	CDL	C36-C37-C38-C39
25	P	302	PEK	C33-C34-C35-C36
18	A	608	PGV	C03-O11-P-O13
18	N	610	PGV	C03-O11-P-O14
18	N	610	PGV	C04-O12-P-O13
18	U	101	PGV	C03-O11-P-O14
18	U	101	PGV	C04-O12-P-O13
23	B	302	PSC	C04-O12-P-O11
23	B	302	PSC	C04-O12-P-O14
23	O	302	PSC	C04-O12-P-O13
25	C	302	PEK	C04-O12-P-O11
25	G	103	PEK	C03-O11-P-O12
25	G	103	PEK	C03-O11-P-O13
26	C	304	CDL	CA2-OA2-PA1-OA4
26	C	304	CDL	CB3-OB5-PB2-OB4
26	N	601	CDL	CA3-OA5-PA1-OA4
26	P	305	CDL	CB3-OB5-PB2-OB2
26	T	103	CDL	CA2-OA2-PA1-OA5
19	Y	101	TGL	C21-C20-CA9-CA8
19	L	101	TGL	CA7-CA8-CA9-C20
25	P	302	PEK	C16-C17-C18-C19
18	A	606	PGV	C05-C04-O12-P
18	C	303	PGV	C02-C03-O11-P
23	O	302	PSC	C02-C03-O11-P
28	Q	201	DMU	C34-C37-C40-C43
19	Y	101	TGL	CB2-CB3-CB4-CB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	609	TGL	C24-C25-C26-C27
23	B	302	PSC	C28-C29-C30-C31
18	N	610	PGV	C26-C27-C28-C29
19	N	609	TGL	C16-C15-CC9-CC8
19	A	609	TGL	C14-C29-C30-C31
19	B	303	TGL	C21-C20-CA9-CA8
18	N	610	PGV	C03-C02-O01-C1
19	A	609	TGL	CG1-CG2-OG2-CB1
19	N	609	TGL	C29-C30-C31-C32
18	N	610	PGV	C11-C12-C13-C14
18	U	101	PGV	O12-C04-C05-C06
26	N	601	CDL	OB5-CB3-CB4-OB6
26	P	305	CDL	C35-C36-C37-C38
18	U	101	PGV	C3-C4-C5-C6
23	B	302	PSC	O03-C01-C02-O01
26	P	305	CDL	C24-C25-C26-C27
26	P	305	CDL	C13-C14-C15-C16
19	L	101	TGL	C33-C34-C35-C36
23	O	302	PSC	C13-C14-C15-C16
18	A	607	PGV	O03-C19-C20-C21
23	O	302	PSC	C3-C4-C5-C6
23	O	302	PSC	C12-C13-C14-C15
18	N	608	PGV	C31-C32-C33-C34
25	G	102	PEK	C2-C3-C4-C5
19	N	609	TGL	C13-C14-C29-C30
28	M	101	DMU	C25-C28-C31-C34
18	U	101	PGV	C11-C10-C9-C8
19	N	607	TGL	C22-C23-C24-C25
18	P	304	PGV	C9-C10-C11-C12
23	O	302	PSC	C7-C8-C9-C10
26	P	305	CDL	OB5-CB3-CB4-CB6
26	P	305	CDL	C33-C34-C35-C36
19	N	607	TGL	C33-C34-C35-C36
19	A	609	TGL	OG3-CC1-CC2-CC3
23	B	302	PSC	C22-C23-C24-C25
18	U	101	PGV	C25-C26-C27-C28
18	A	606	PGV	C27-C28-C29-C30
19	Y	101	TGL	C15-C16-C17-C18
23	O	302	PSC	C4-C5-C6-C7
17	N	606	HEA	CAD-CBD-CGD-O2D
19	B	303	TGL	CC7-CC8-CC9-C15
19	B	303	TGL	CA9-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	P	304	PGV	C02-C03-O11-P
23	O	302	PSC	C24-C25-C26-C27
26	C	304	CDL	C41-C42-C43-C44
24	W	102	CHD	C22-C23-C24-O25
26	P	305	CDL	C20-C21-C22-C23
17	A	605	HEA	CAD-CBD-CGD-O2D
25	C	302	PEK	C24-C25-C26-C27
18	A	606	PGV	C03-C02-O01-C1
23	B	302	PSC	C01-C02-O01-C1
23	O	302	PSC	C03-C02-O01-C1
26	C	304	CDL	CA3-CA4-OA6-CA5
26	C	304	CDL	CA6-CA4-OA6-CA5
26	P	305	CDL	CA3-CA4-OA6-CA5
17	N	606	HEA	CAD-CBD-CGD-O1D
24	B	304	CHD	C22-C23-C24-O26
24	G	104	CHD	C22-C23-C24-O26
24	W	102	CHD	C22-C23-C24-O26
26	T	103	CDL	C75-C76-C77-C78
25	P	303	PEK	C22-C23-C24-C25
26	C	304	CDL	CA4-CA3-OA5-PA1
25	C	302	PEK	C33-C34-C35-C36
26	P	305	CDL	C56-C57-C58-C59
25	C	302	PEK	C01-C02-C03-O11
19	A	609	TGL	CC1-CC2-CC3-CC4
25	P	302	PEK	C34-C35-C36-C37
25	G	103	PEK	O03-C01-C02-O01
17	N	605	HEA	CAA-CBA-CGA-O1A
19	N	609	TGL	C21-C20-CA9-CA8
23	B	302	PSC	C10-C11-C12-C13
25	C	302	PEK	C11-C12-C13-C14
25	G	103	PEK	C11-C10-C9-C8
25	P	302	PEK	C5-C6-C7-C8
25	T	102	PEK	C12-C13-C14-C15
19	Y	101	TGL	CC5-CC6-CC7-CC8
26	P	305	CDL	C19-C20-C21-C22
25	P	302	PEK	C15-C16-C17-C18
17	N	606	HEA	CAA-CBA-CGA-O1A
26	P	305	CDL	C60-C61-C62-C63
25	G	102	PEK	C17-C18-C19-C20
19	N	609	TGL	CC9-C15-C16-C17
18	N	608	PGV	C2-C3-C4-C5
28	G	101	DMU	C25-C28-C31-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	G	104	CHD	C22-C23-C24-O25
17	N	606	HEA	C26-C15-C16-C17
26	T	103	CDL	C1-CA2-OA2-PA1
17	A	605	HEA	CAA-CBA-CGA-O1A
17	A	605	HEA	CAA-CBA-CGA-O2A
17	N	605	HEA	CAA-CBA-CGA-O2A
18	U	101	PGV	C20-C21-C22-C23
18	A	607	PGV	C4-C5-C6-C7
26	P	305	CDL	C39-C40-C41-C42
25	T	102	PEK	C24-C25-C26-C27
25	G	102	PEK	C16-C17-C18-C19
17	N	606	HEA	CAA-CBA-CGA-O2A
24	B	304	CHD	C22-C23-C24-O25
19	N	607	TGL	CB9-C10-C11-C12
18	C	303	PGV	C11-C12-C13-C14
25	C	302	PEK	C3-C4-C5-C6
18	C	303	PGV	C21-C22-C23-C24
19	N	607	TGL	C24-C25-C26-C27
18	U	101	PGV	C1-C2-C3-C4
26	C	304	CDL	OB7-CB5-OB6-CB4
18	U	101	PGV	C22-C23-C24-C25
26	T	103	CDL	C79-C80-C81-C82
26	C	304	CDL	OA5-CA3-CA4-CA6
19	B	303	TGL	CC1-CC2-CC3-CC4
19	N	607	TGL	CB1-CB2-CB3-CB4
18	N	608	PGV	C9-C10-C11-C12
24	J	102	CHD	C16-C17-C20-C22
17	A	605	HEA	CAD-CBD-CGD-O1D
25	G	103	PEK	C16-C17-C18-C19
18	U	101	PGV	C4-C5-C6-C7
26	T	103	CDL	C58-C59-C60-C61
18	N	608	PGV	C11-C12-C13-C14
25	G	103	PEK	C3-C4-C5-C6
25	T	102	PEK	C3-C4-C5-C6
18	A	608	PGV	C31-C32-C33-C34
24	J	101	CHD	C22-C23-C24-O26
19	Y	101	TGL	CB7-CB8-CB9-C10
25	P	302	PEK	C21-C22-C23-C24
26	P	305	CDL	CA6-CA4-OA6-CA5
26	P	305	CDL	C52-C53-C54-C55
18	N	608	PGV	C11-C10-C9-C8
19	A	609	TGL	CB2-CB3-CB4-CB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	605	HEA	C2A-C3A-CMA-OMA
19	Y	101	TGL	CC7-CC8-CC9-C15
26	T	103	CDL	C60-C61-C62-C63
24	J	101	CHD	C22-C23-C24-O25
19	N	609	TGL	CA2-CA3-CA4-CA5
26	T	103	CDL	C36-C37-C38-C39
18	P	304	PGV	C11-C12-C13-C14
26	P	305	CDL	OA5-CA3-CA4-OA6
19	Y	101	TGL	C12-C13-C14-C29
26	T	103	CDL	C84-C85-C86-C87
18	A	606	PGV	C7-C8-C9-C10
18	P	304	PGV	C28-C29-C30-C31
18	A	606	PGV	O01-C1-C2-C3
19	A	609	TGL	C16-C17-C18-C19
25	G	102	PEK	C21-C22-C23-C24
26	C	304	CDL	C37-C38-C39-C40
25	P	302	PEK	C3-C4-C5-C6
19	N	609	TGL	OG3-CC1-CC2-CC3
26	P	305	CDL	OA5-CA3-CA4-CA6
26	T	103	CDL	CA5-C11-C12-C13
19	Y	101	TGL	CB4-CB5-CB6-CB7
18	A	608	PGV	C23-C24-C25-C26
25	G	102	PEK	O01-C1-C2-C3
26	T	103	CDL	C32-C31-CA7-OA8
17	A	605	HEA	C2C-C3C-CAC-CBC
25	P	303	PEK	C33-C34-C35-C36
26	P	305	CDL	C52-C51-CB5-OB7
18	A	607	PGV	C9-C10-C11-C12
25	P	303	PEK	C3-C4-C5-C6
26	C	304	CDL	C51-CB5-OB6-CB4
19	N	609	TGL	OG1-CA1-CA2-CA3
19	Y	101	TGL	OG3-CC1-CC2-CC3
26	C	304	CDL	C54-C55-C56-C57
23	B	302	PSC	C14-C15-C16-C17
25	P	302	PEK	O01-C1-C2-C3
26	T	103	CDL	C74-C75-C76-C77
18	A	607	PGV	C15-C16-C17-C18
18	C	303	PGV	C9-C10-C11-C12
17	A	605	HEA	C26-C15-C16-C17
28	Q	201	DMU	C31-C34-C37-C40
19	L	101	TGL	C14-C29-C30-C31
28	T	101	DMU	C25-C28-C31-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	609	TGL	CA6-CA7-CA8-CA9
25	G	102	PEK	C14-C15-C16-C17
17	A	604	HEA	CAA-CBA-CGA-O1A
17	A	604	HEA	CAD-CBD-CGD-O1D
18	C	303	PGV	O03-C19-C20-C21
26	N	601	CDL	C32-C31-CA7-OA8
19	Y	101	TGL	CG1-CG2-CG3-OG3
17	A	604	HEA	CAD-CBD-CGD-O2D
18	P	304	PGV	C14-C15-C16-C17
26	N	601	CDL	OB7-CB5-OB6-CB4
26	N	601	CDL	C72-C73-C74-C75
26	C	304	CDL	OB5-CB3-CB4-CB6
25	G	103	PEK	O03-C21-C22-C23
26	T	103	CDL	C52-C53-C54-C55
25	G	103	PEK	C25-C26-C27-C28
19	A	609	TGL	C20-C21-C22-C23
23	B	302	PSC	C23-C24-C25-C26
17	A	604	HEA	CAA-CBA-CGA-O2A
25	G	102	PEK	O02-C1-C2-C3
19	A	609	TGL	CB6-CB7-CB8-CB9
19	Y	101	TGL	CA5-CA6-CA7-CA8
25	P	302	PEK	O02-C1-C2-C3
19	A	609	TGL	C23-C24-C25-C26
18	A	606	PGV	O02-C1-C2-C3
18	C	303	PGV	O04-C19-C20-C21
19	Y	101	TGL	OC1-CC1-CC2-CC3
19	A	609	TGL	OG2-CB1-CB2-CB3
19	Y	101	TGL	CC4-CC5-CC6-CC7
19	N	609	TGL	OC1-CC1-CC2-CC3
25	G	103	PEK	O04-C21-C22-C23
26	T	103	CDL	C32-C31-CA7-OA9
23	B	302	PSC	O03-C19-C20-C21
25	P	303	PEK	O01-C1-C2-C3
26	N	601	CDL	C52-C51-CB5-OB6
18	U	101	PGV	C28-C29-C30-C31
26	T	103	CDL	C22-C23-C24-C25
19	N	607	TGL	CA6-CA7-CA8-CA9
25	G	103	PEK	O03-C01-C02-C03
25	G	102	PEK	C02-C03-O11-P
26	P	305	CDL	C44-C45-C46-C47
19	Y	101	TGL	C17-C18-C19-C33
18	N	610	PGV	O01-C1-C2-C3

Continued on next page...

Continued from previous page...

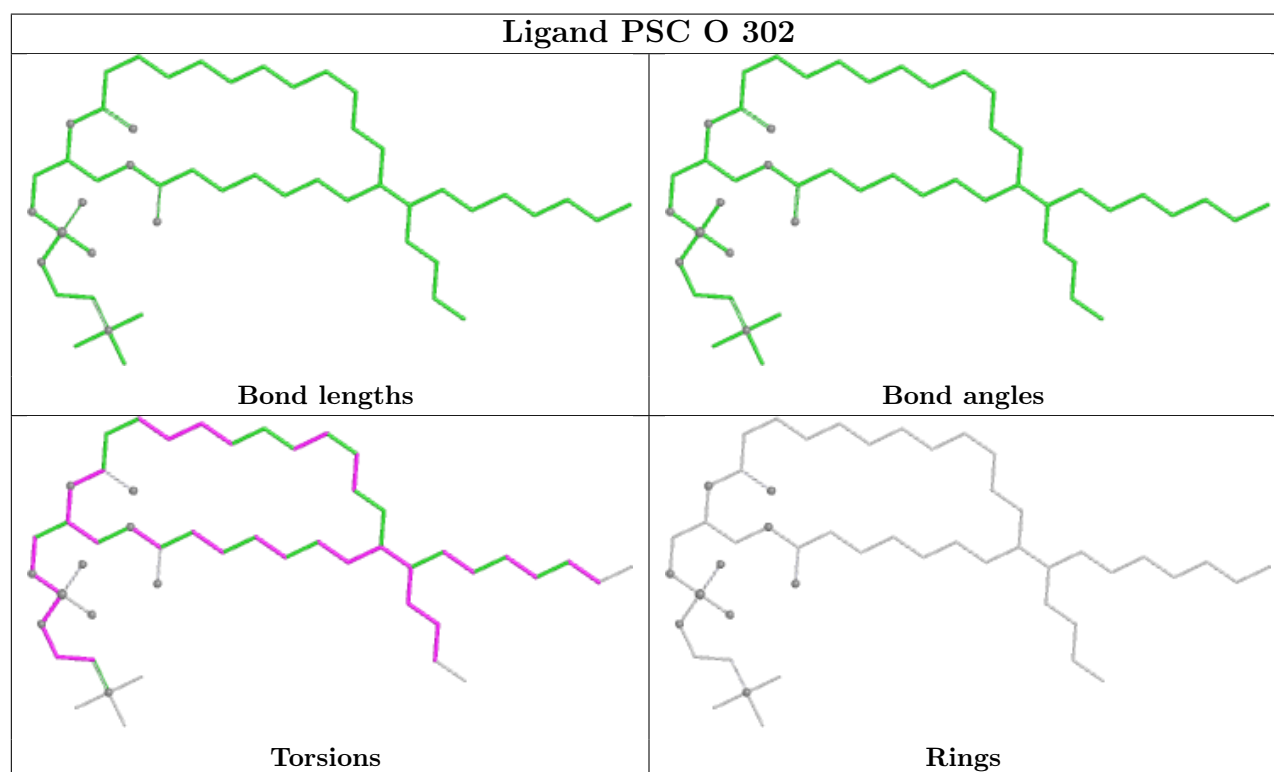
Mol	Chain	Res	Type	Atoms
19	N	607	TGL	OG2-CB1-CB2-CB3
25	P	302	PEK	C2-C1-O01-C02
25	C	302	PEK	O01-C1-C2-C3
19	A	609	TGL	OB1-CB1-CB2-CB3
23	B	302	PSC	C27-C28-C29-C30
23	O	302	PSC	C23-C24-C25-C26

There are no ring outliers.

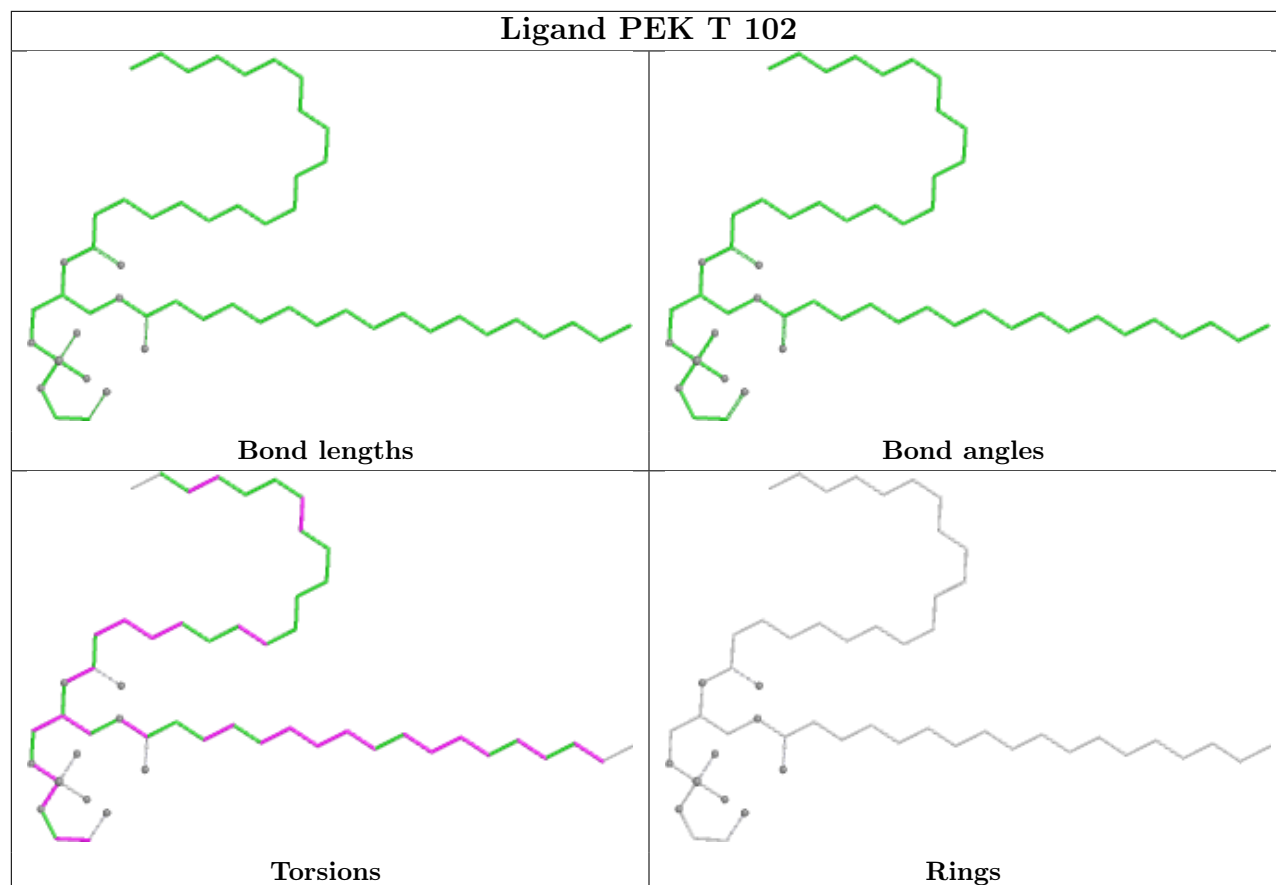
31 monomers are involved in 137 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	O	302	PSC	3	0
25	T	102	PEK	2	0
19	B	303	TGL	10	0
26	P	305	CDL	9	0
28	M	101	DMU	2	0
17	A	604	HEA	2	0
24	J	101	CHD	2	0
17	N	605	HEA	5	0
18	A	608	PGV	2	0
17	A	605	HEA	2	0
19	L	101	TGL	12	0
19	Y	101	TGL	2	0
19	N	609	TGL	7	0
23	B	302	PSC	6	0
25	C	302	PEK	3	0
24	J	102	CHD	2	0
25	P	302	PEK	2	0
18	A	606	PGV	3	0
24	P	301	CHD	1	0
26	C	304	CDL	14	0
19	N	607	TGL	13	0
24	C	301	CHD	1	0
26	T	103	CDL	1	0
26	N	601	CDL	23	0
18	N	610	PGV	1	0
25	G	102	PEK	1	0
17	N	606	HEA	1	0
28	G	101	DMU	3	0
24	W	102	CHD	2	0
19	A	609	TGL	1	0
25	G	103	PEK	1	0

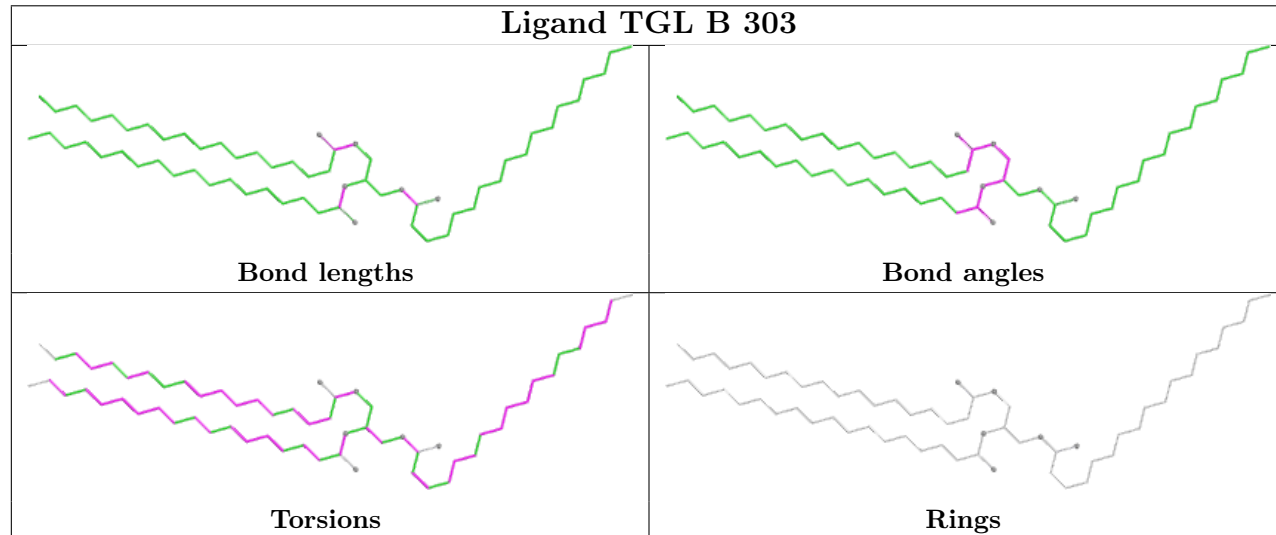
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

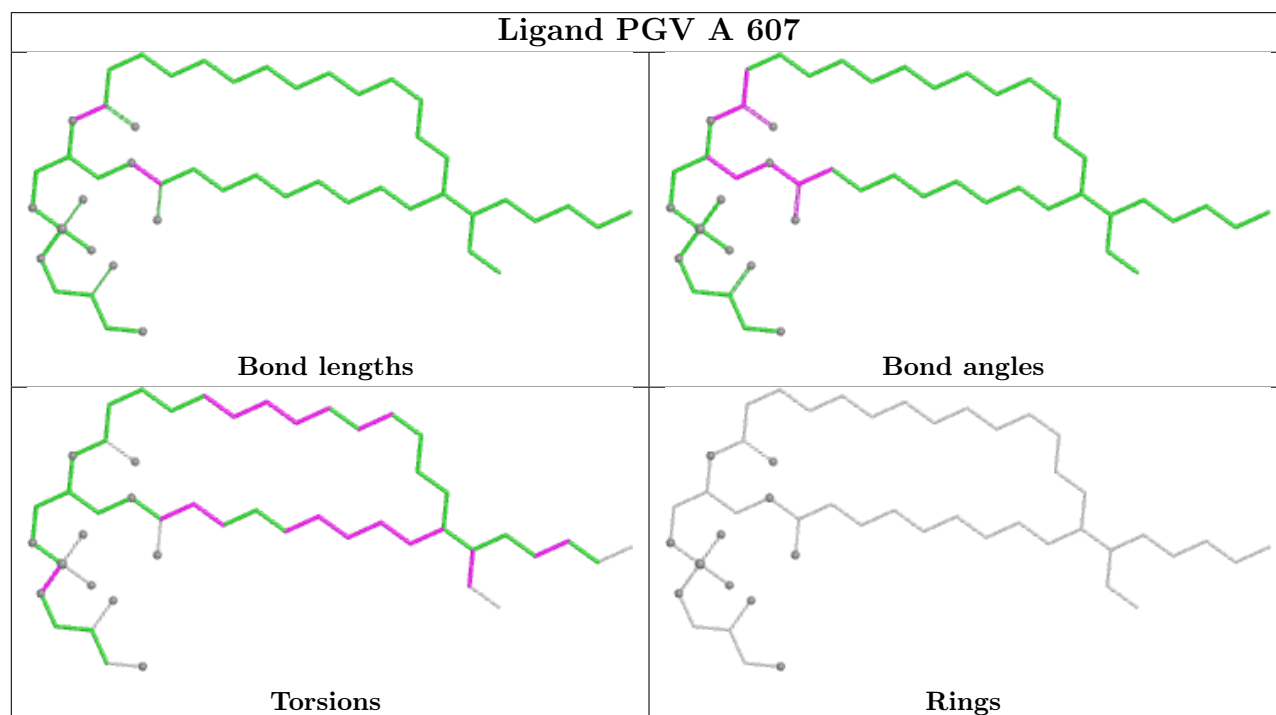
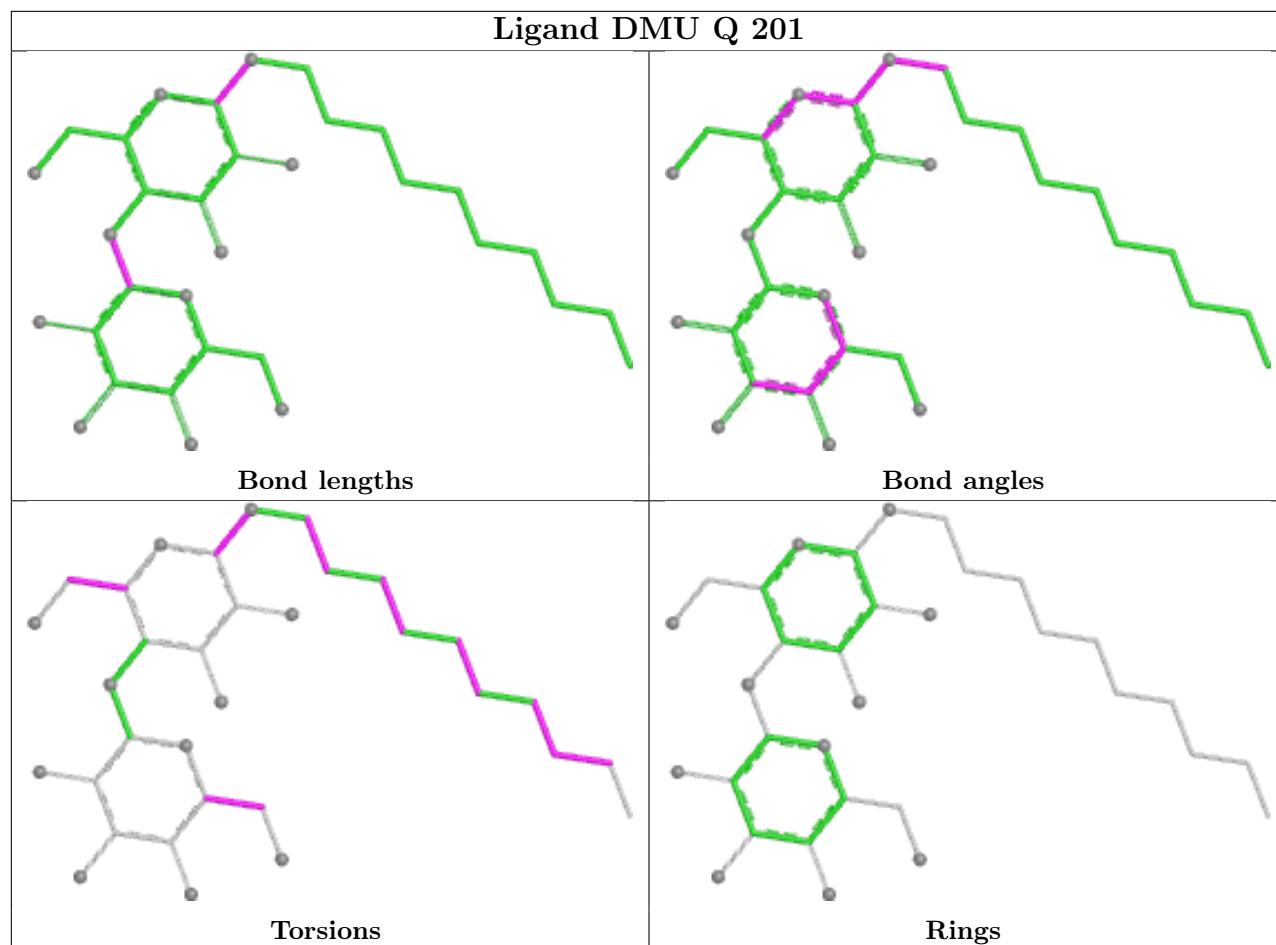


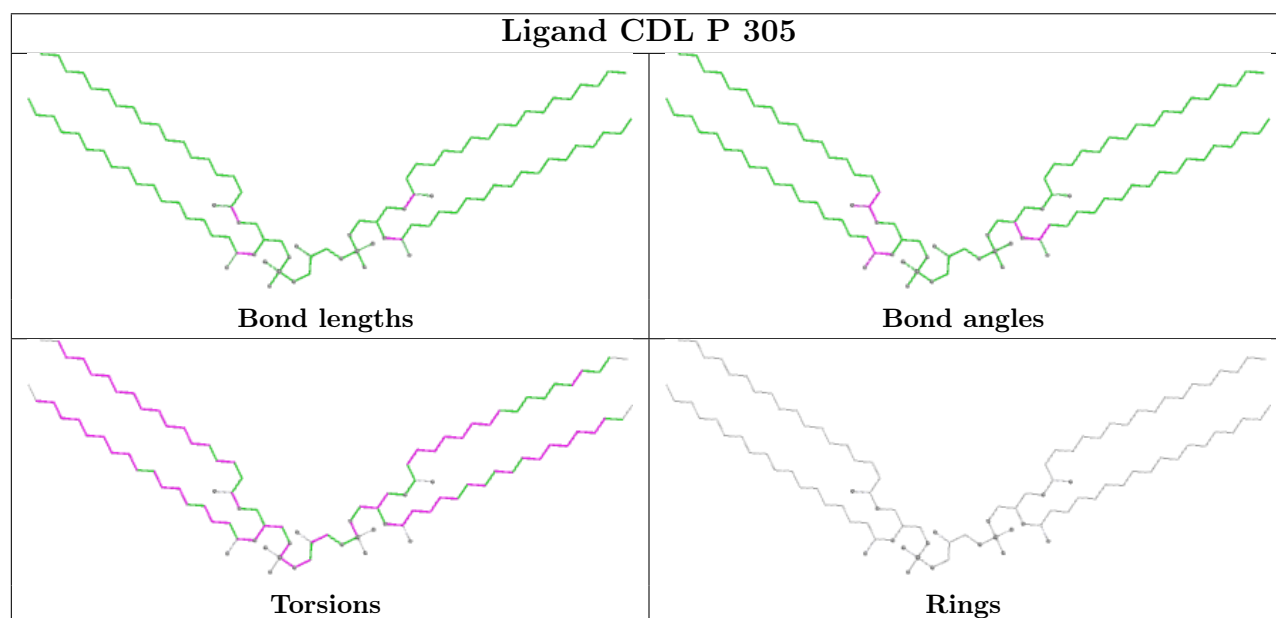
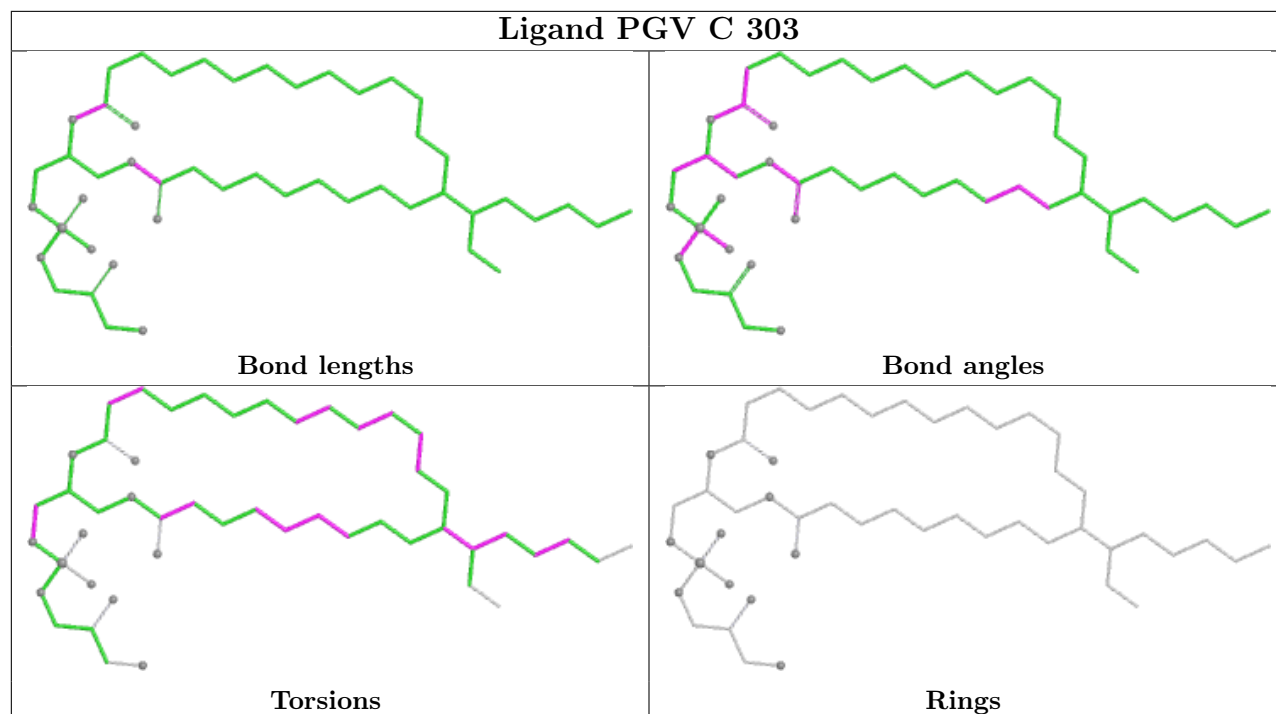
Ligand PEK T 102

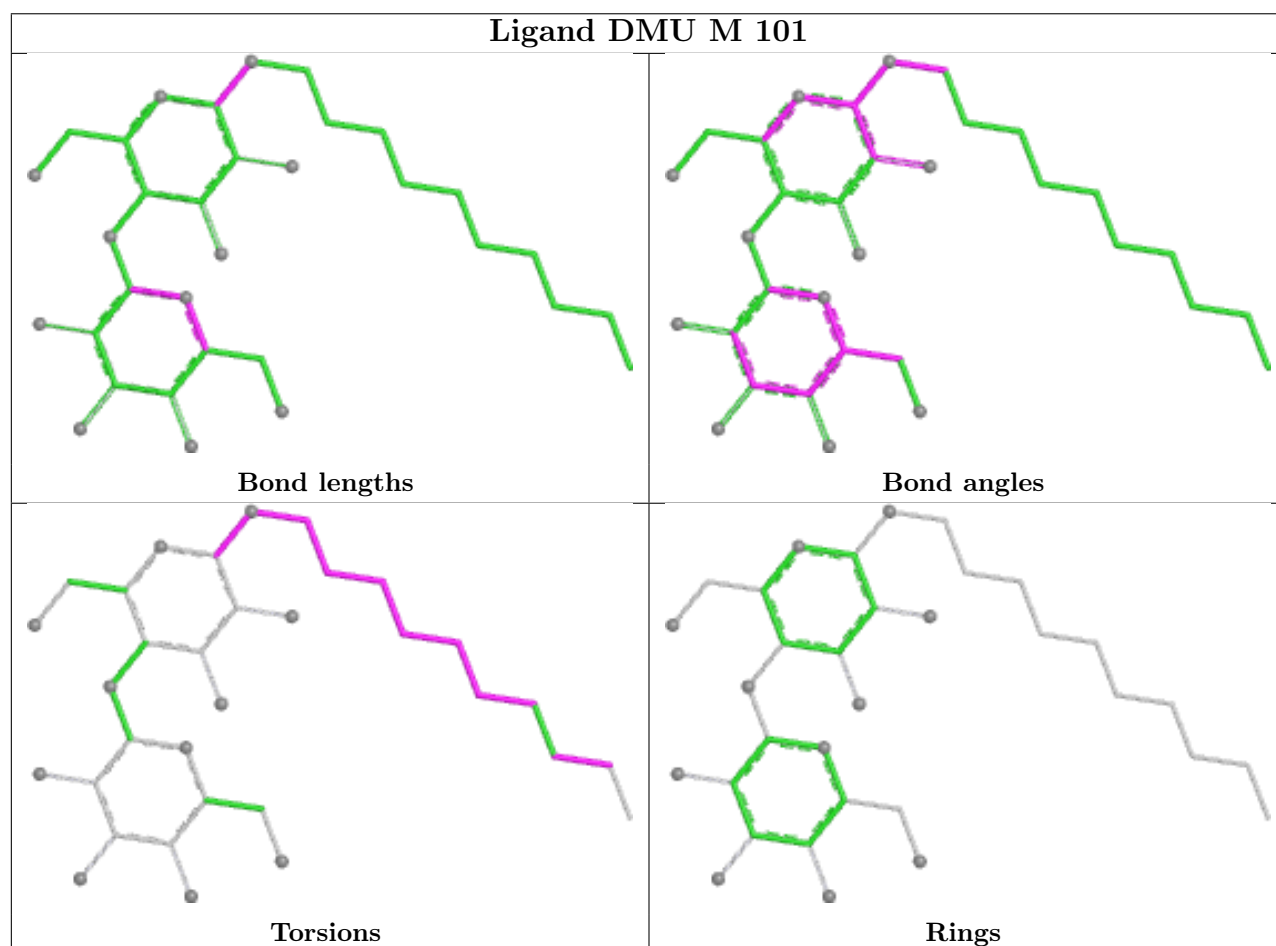
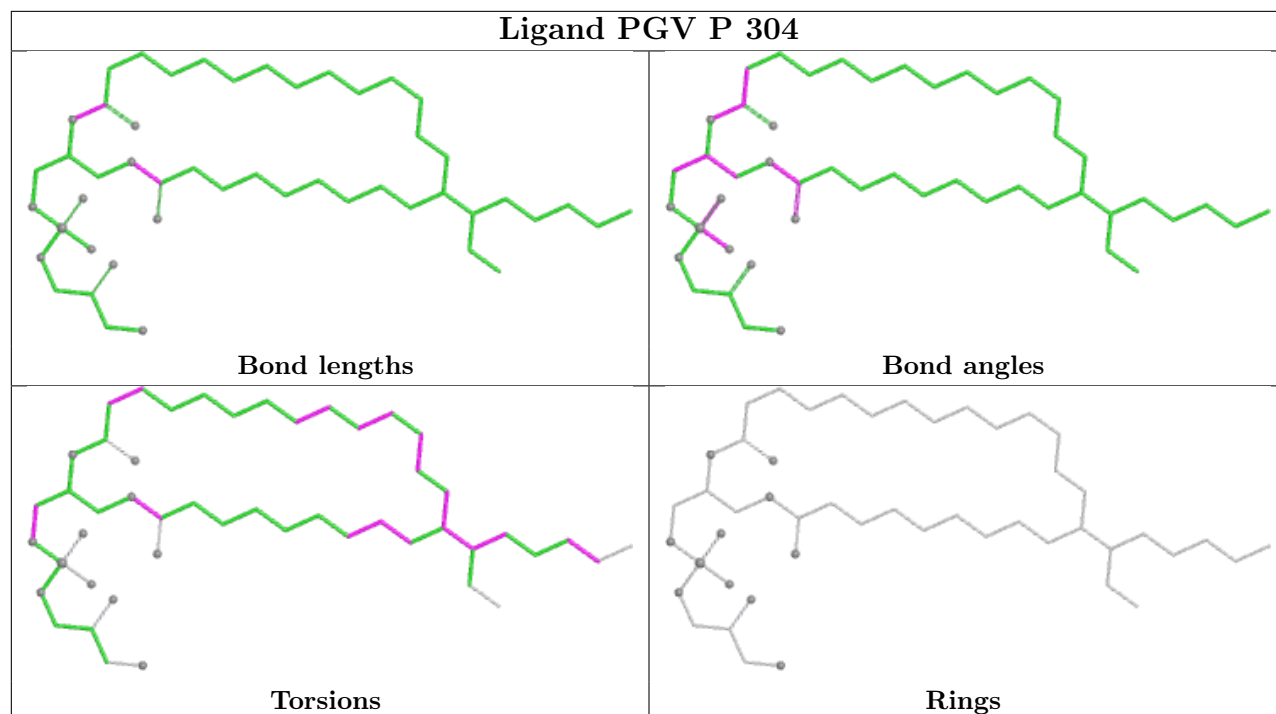


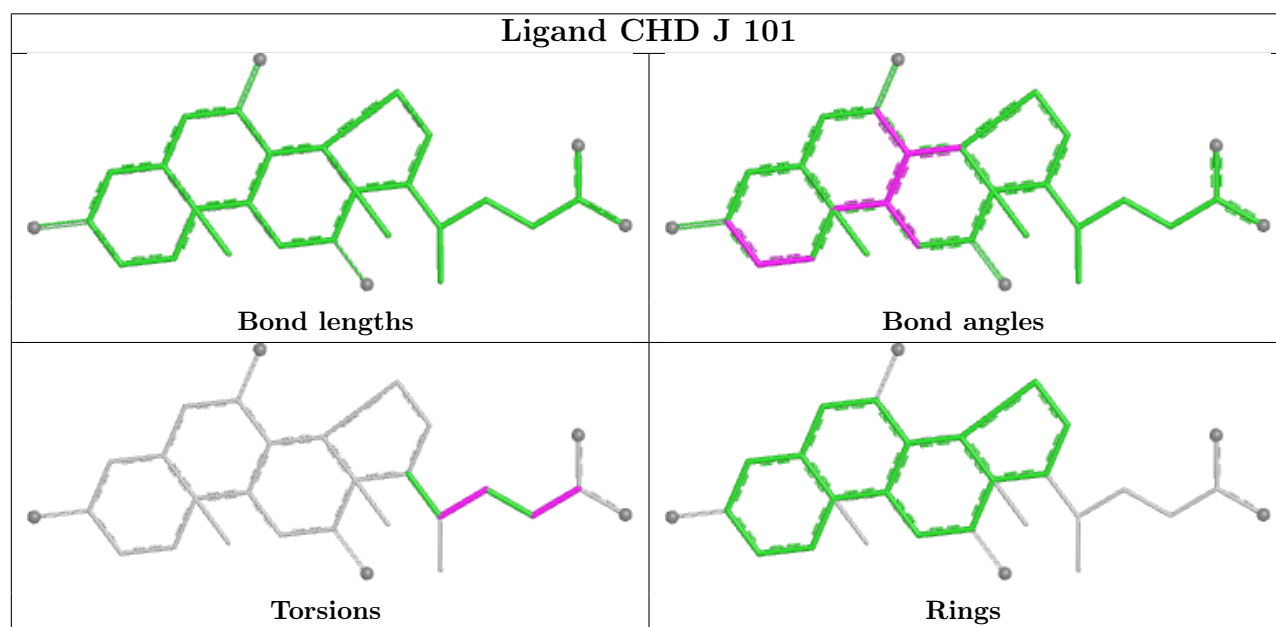
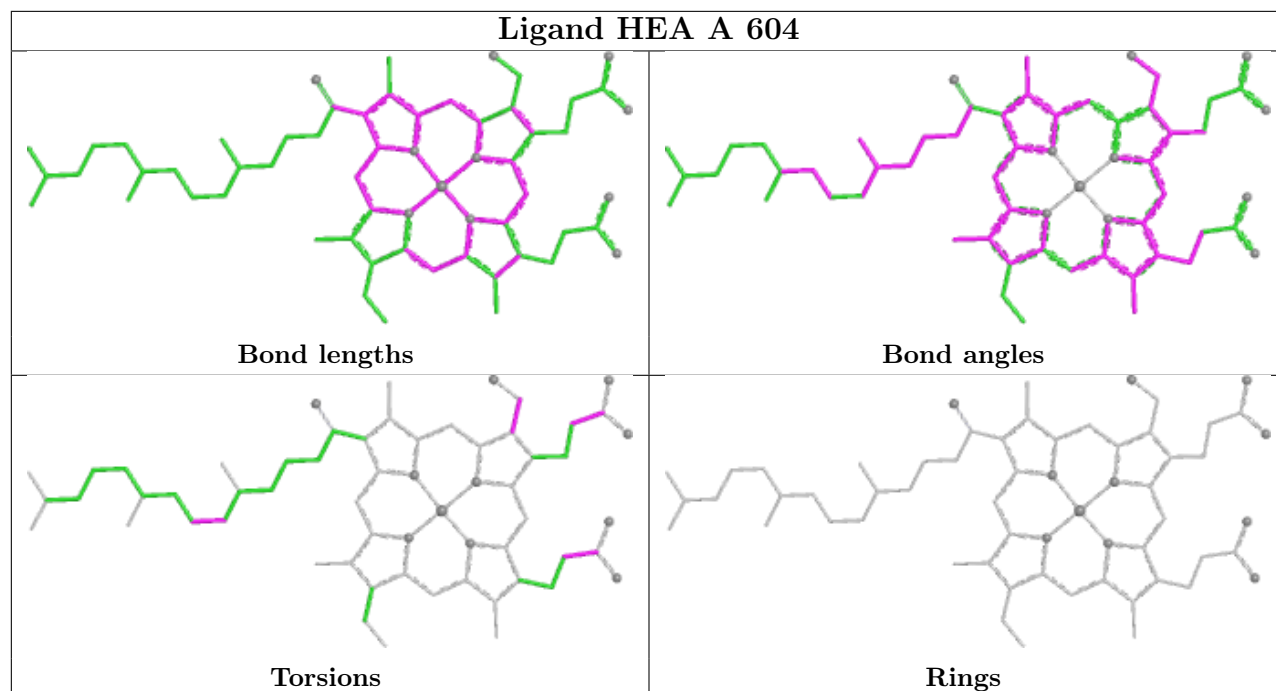
Ligand TGL B 303

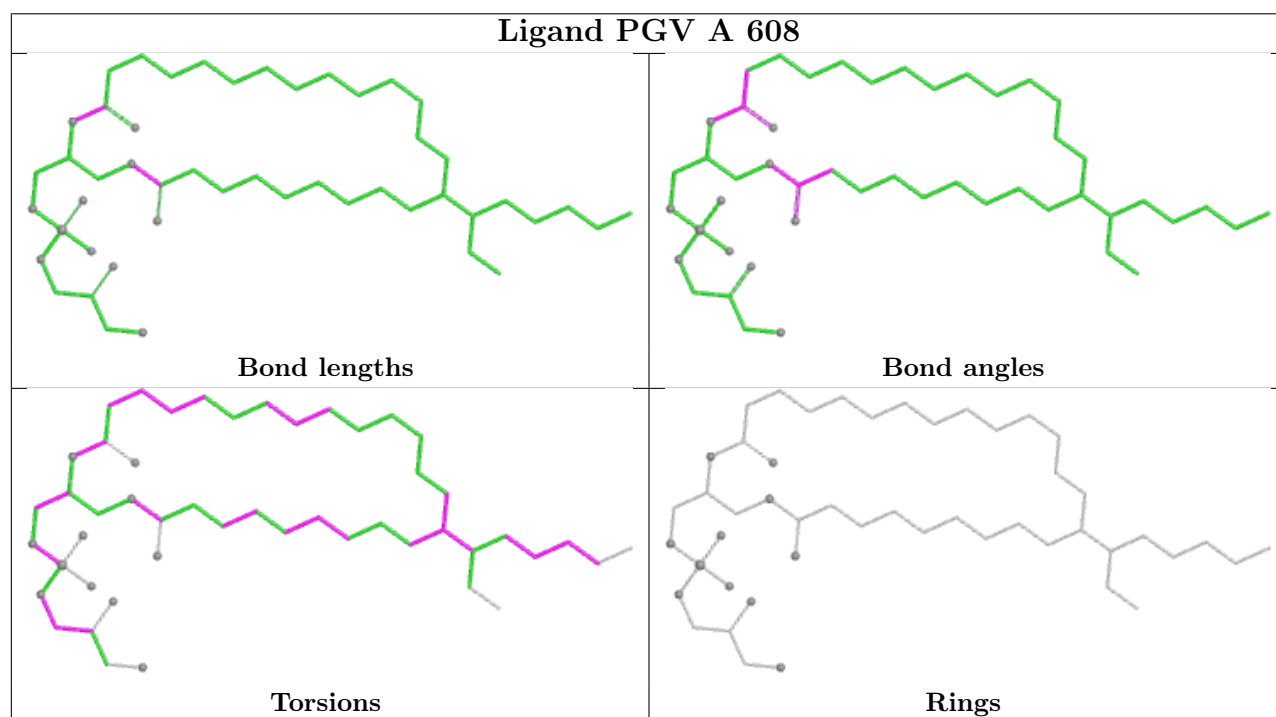
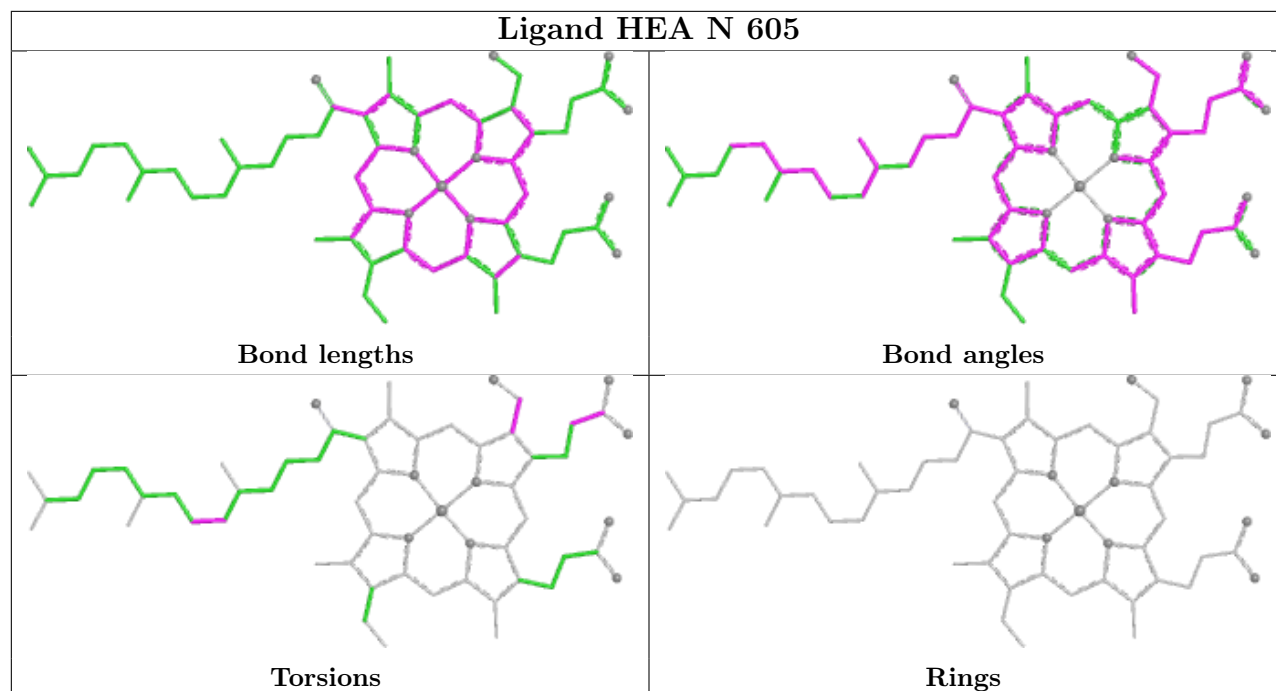


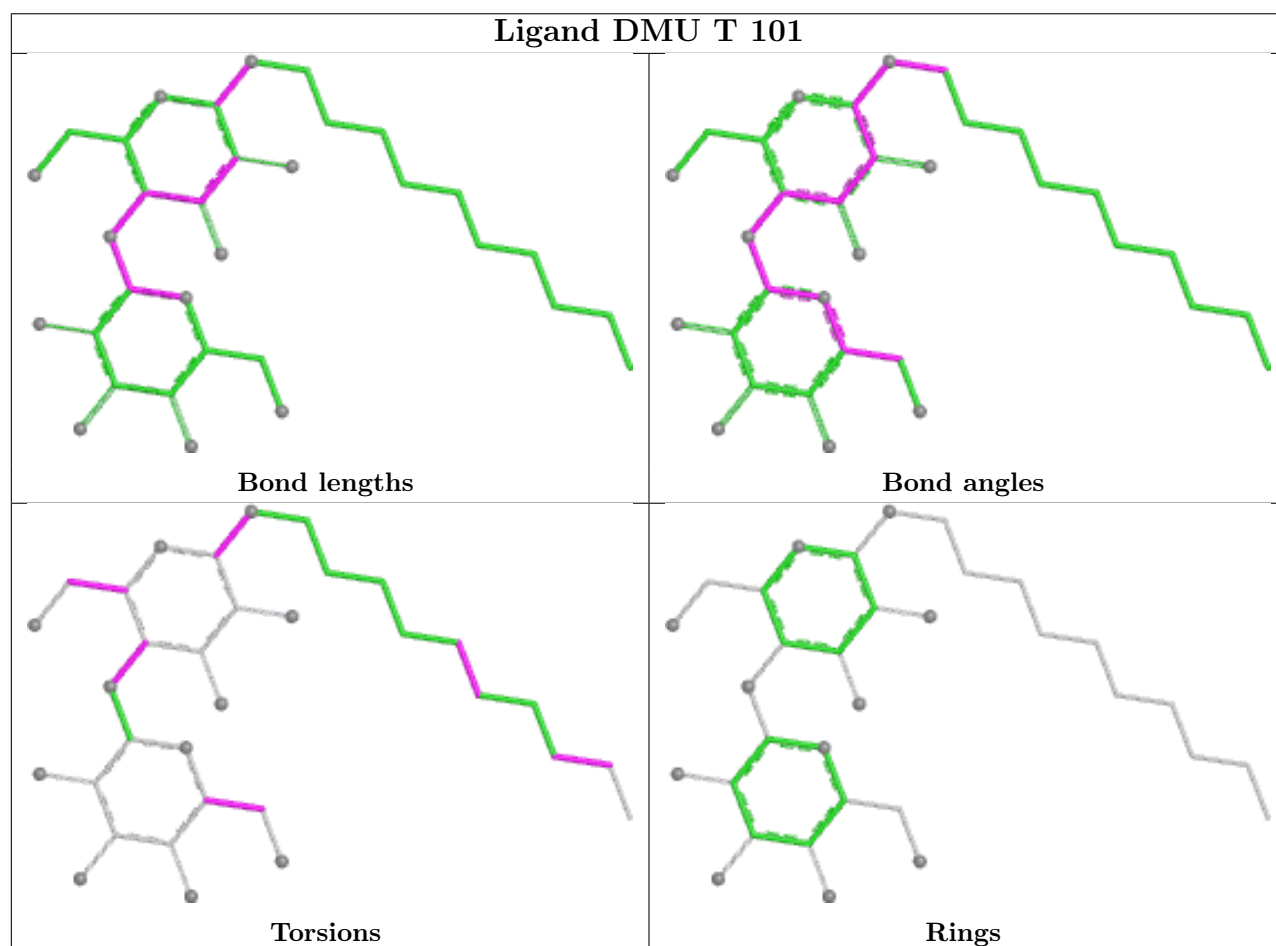
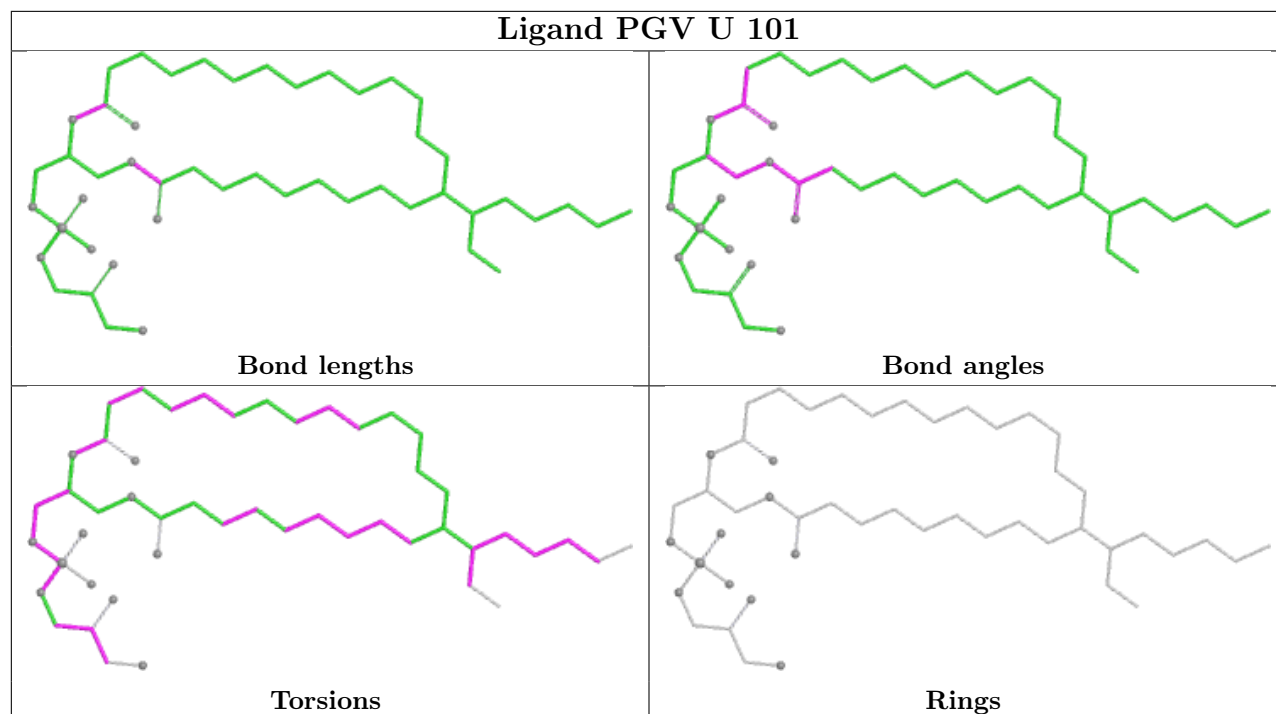


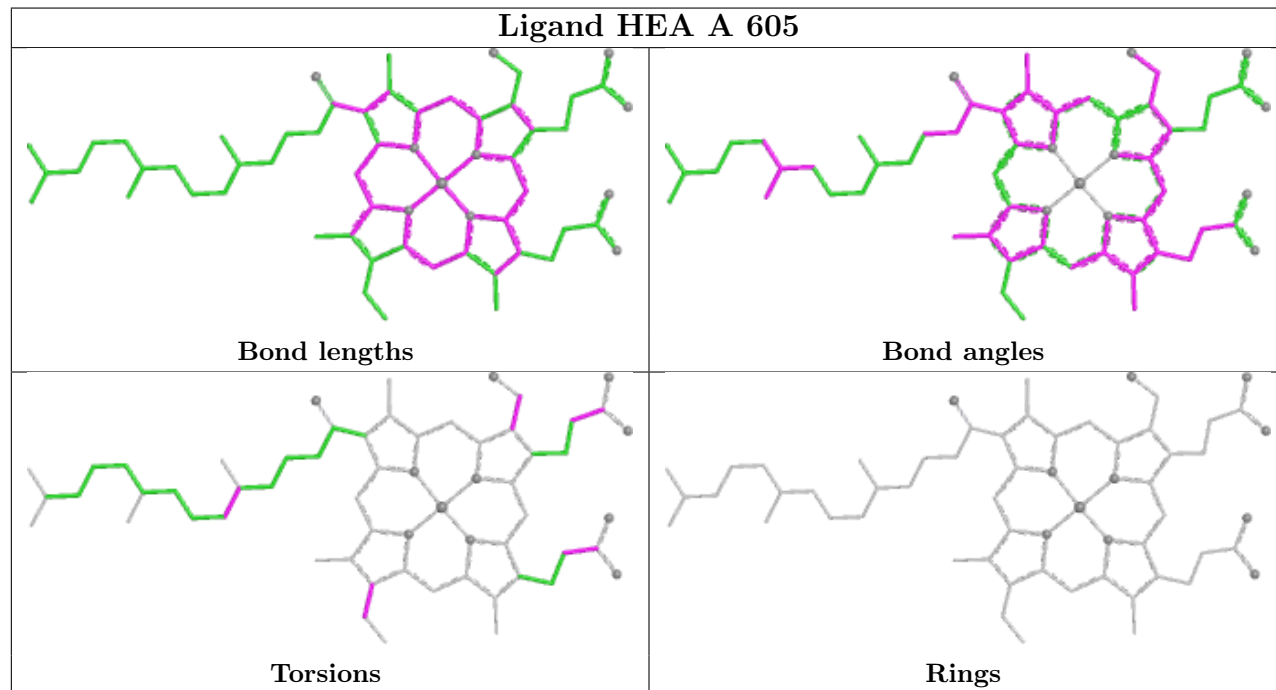
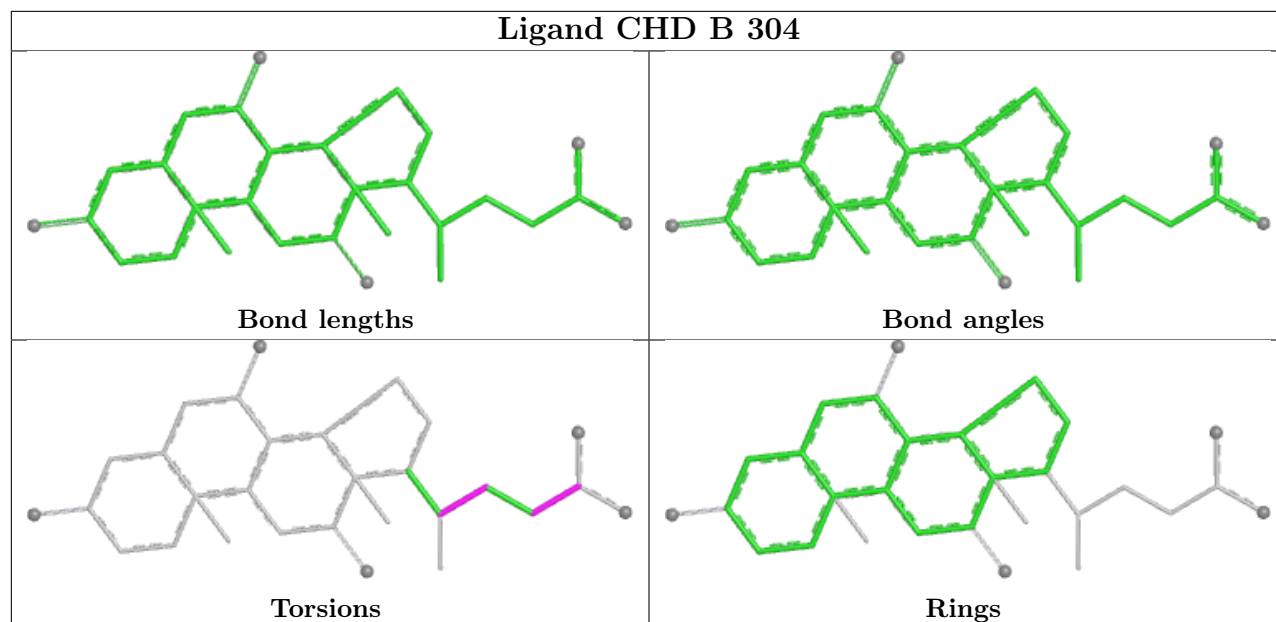




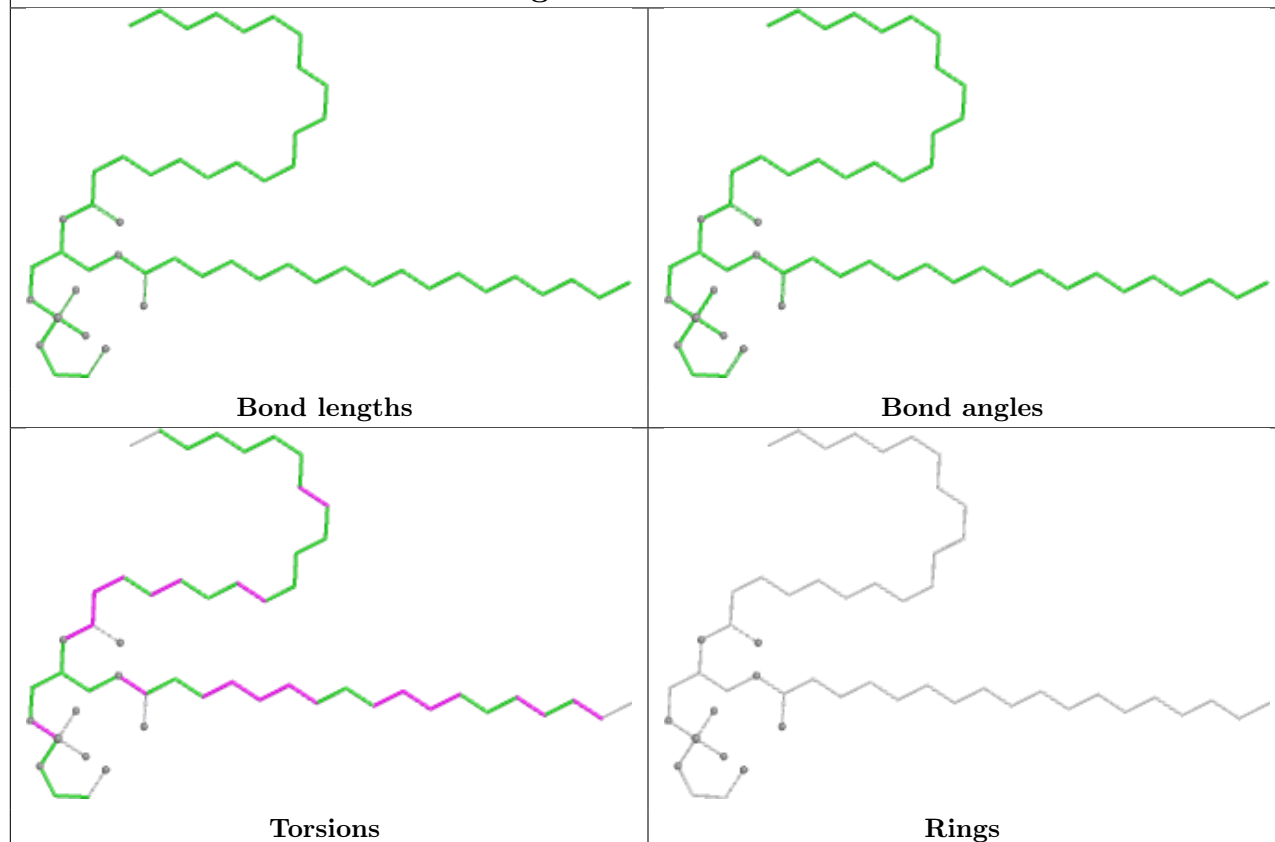




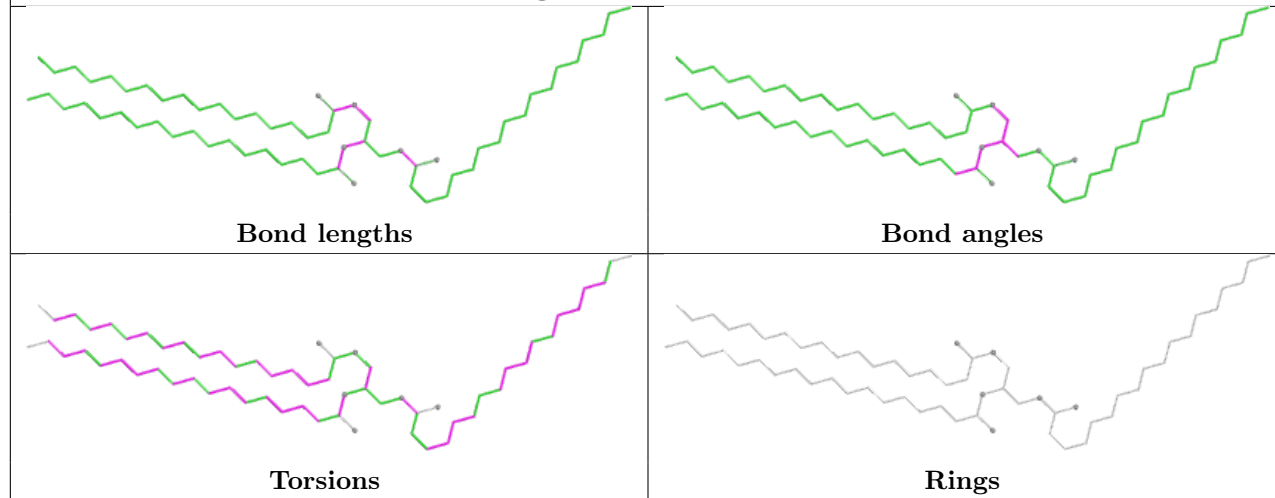


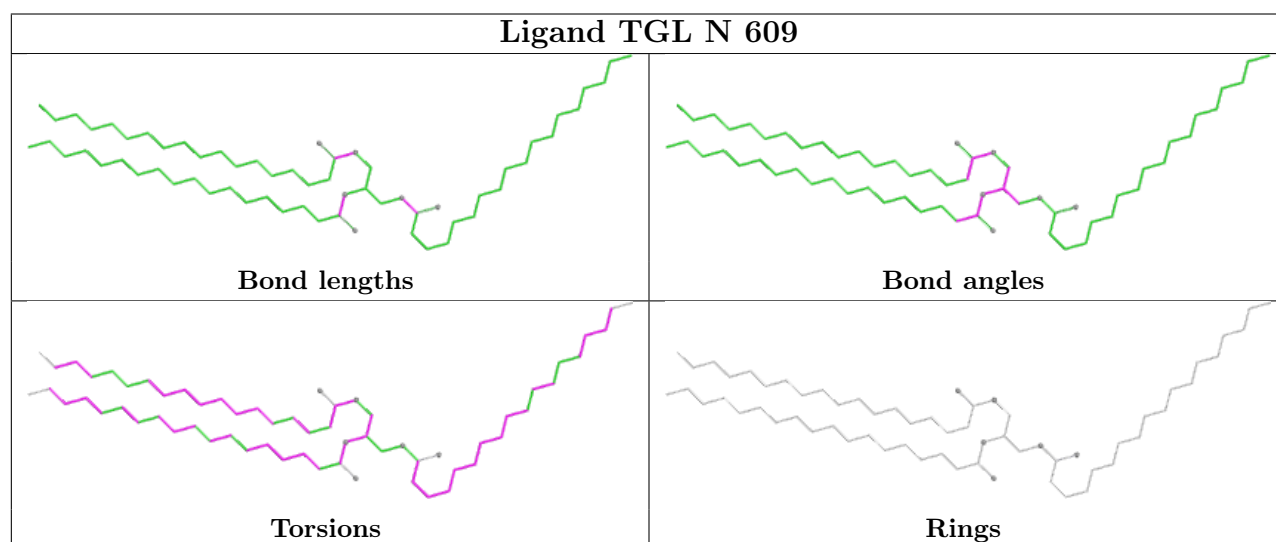
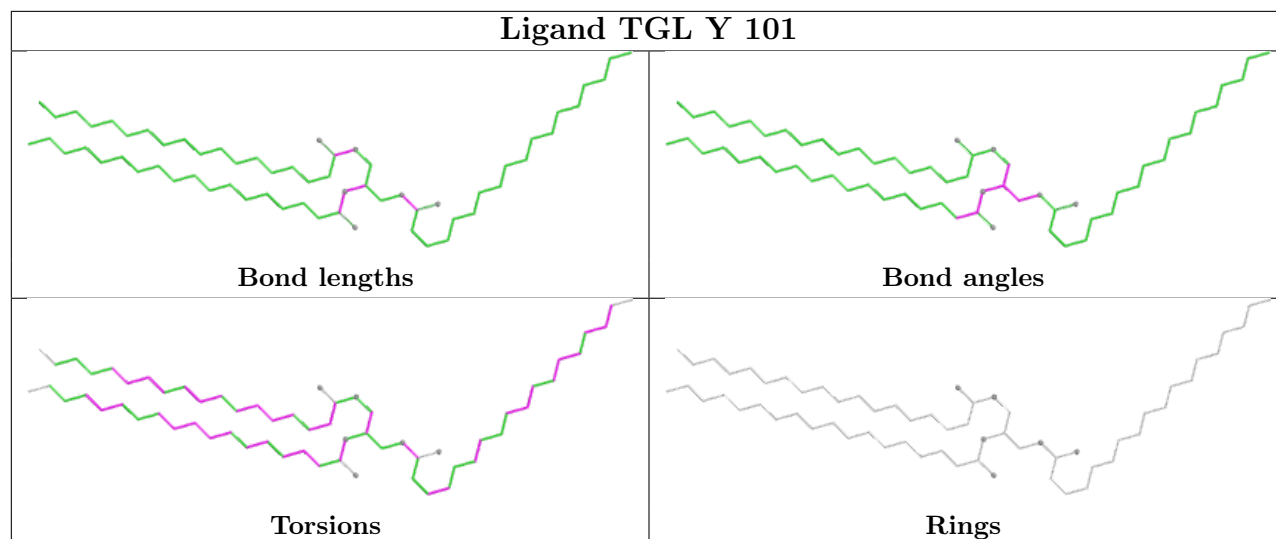


Ligand PEK P 303

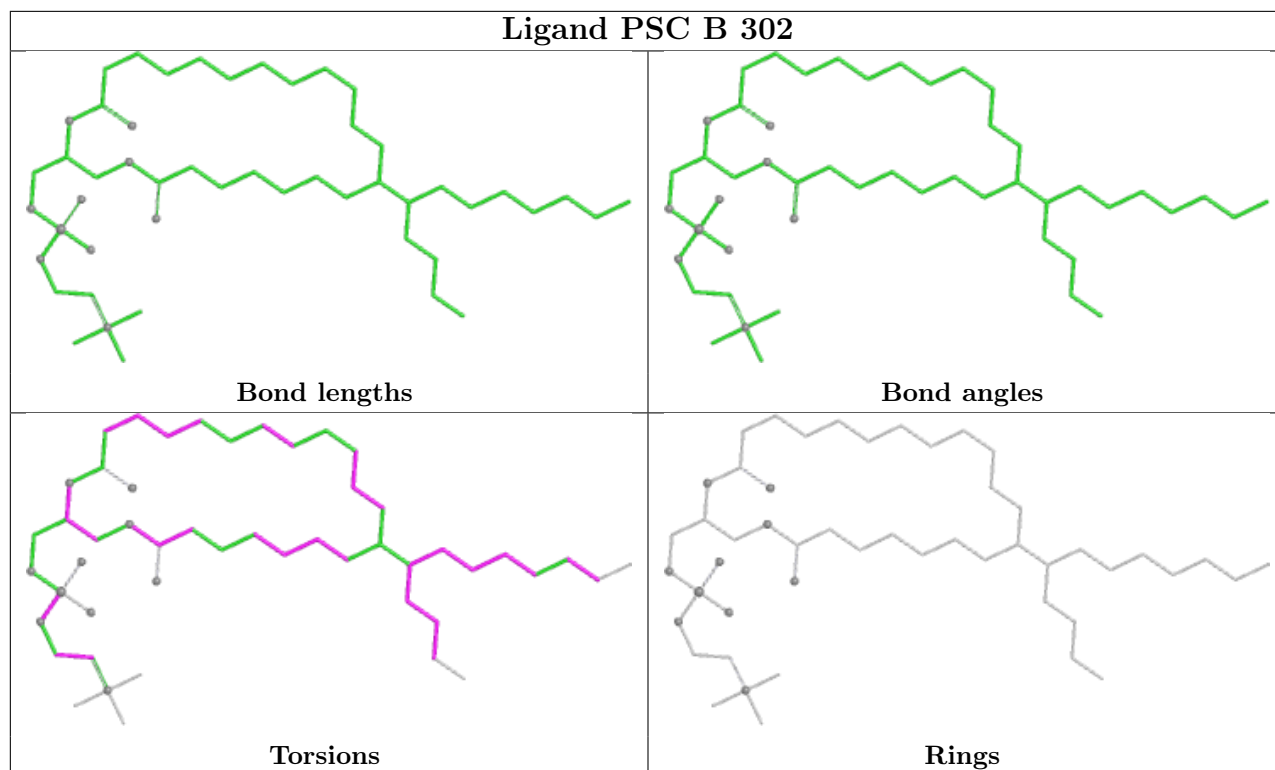


Ligand TGL L 101

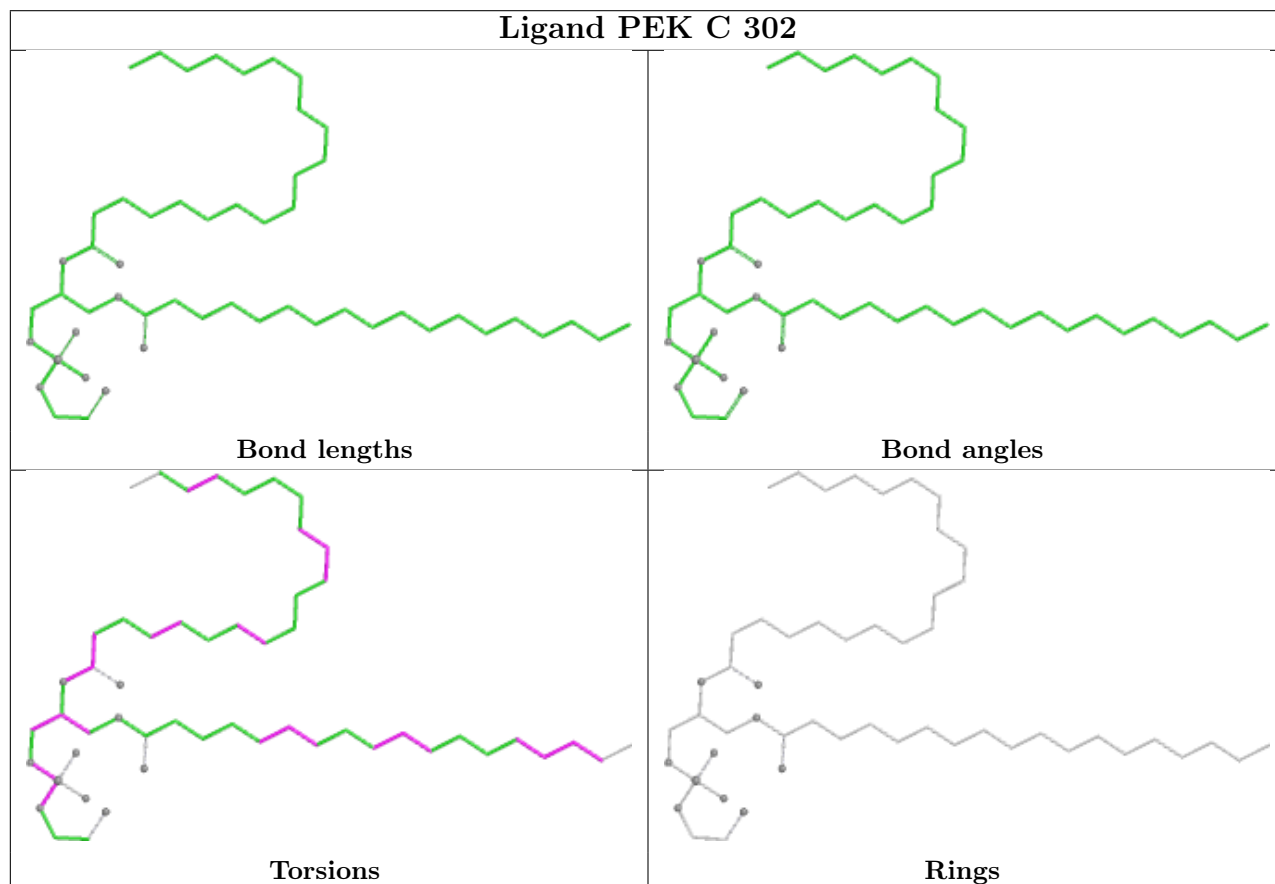




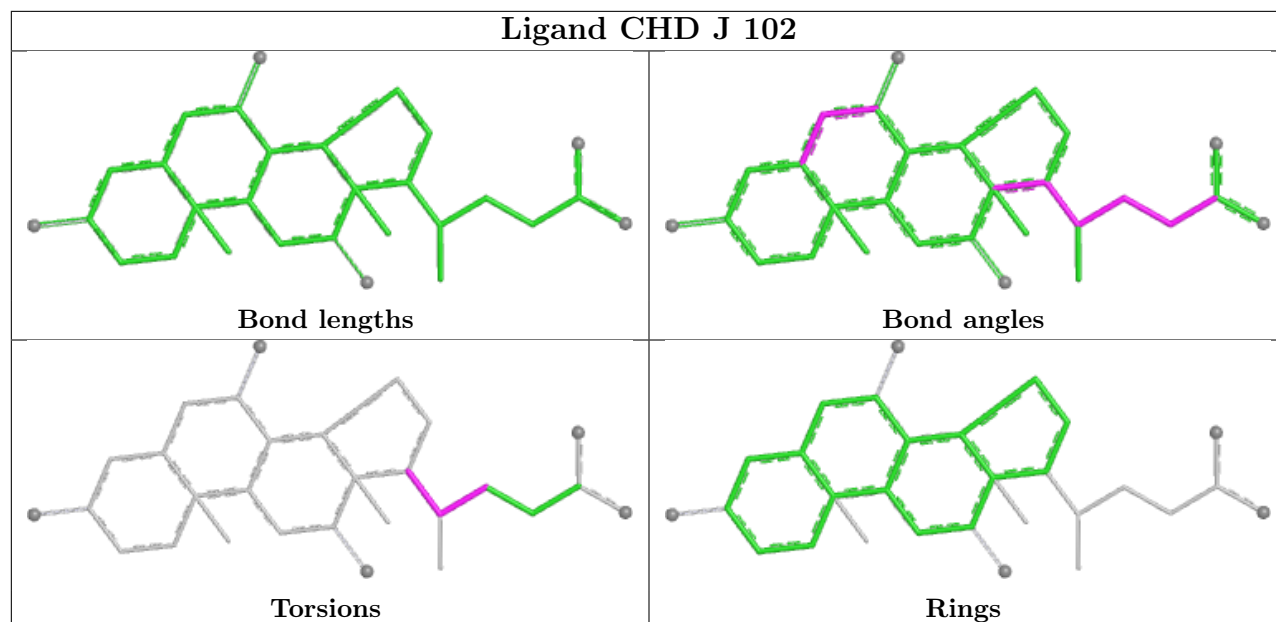
Ligand PSC B 302



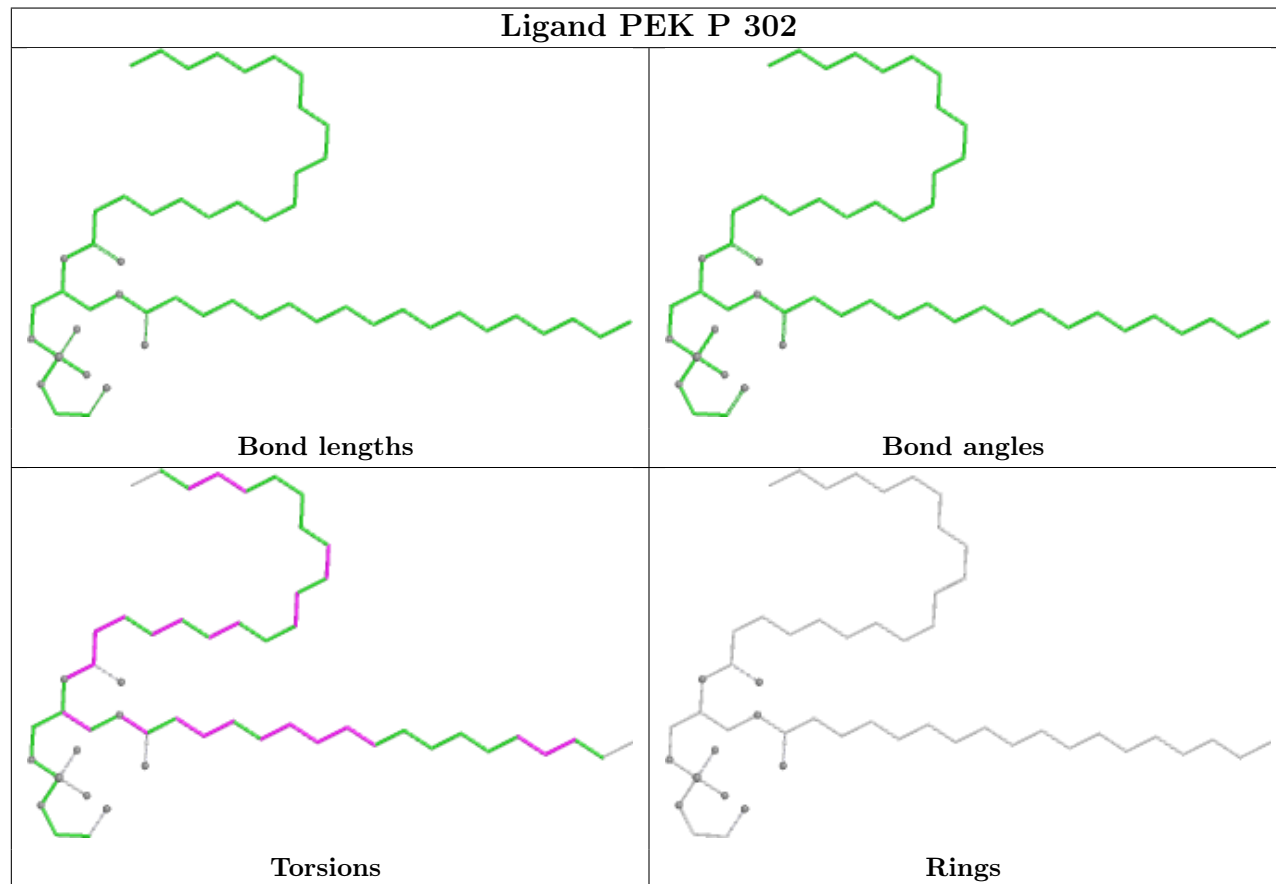
Ligand PEK C 302

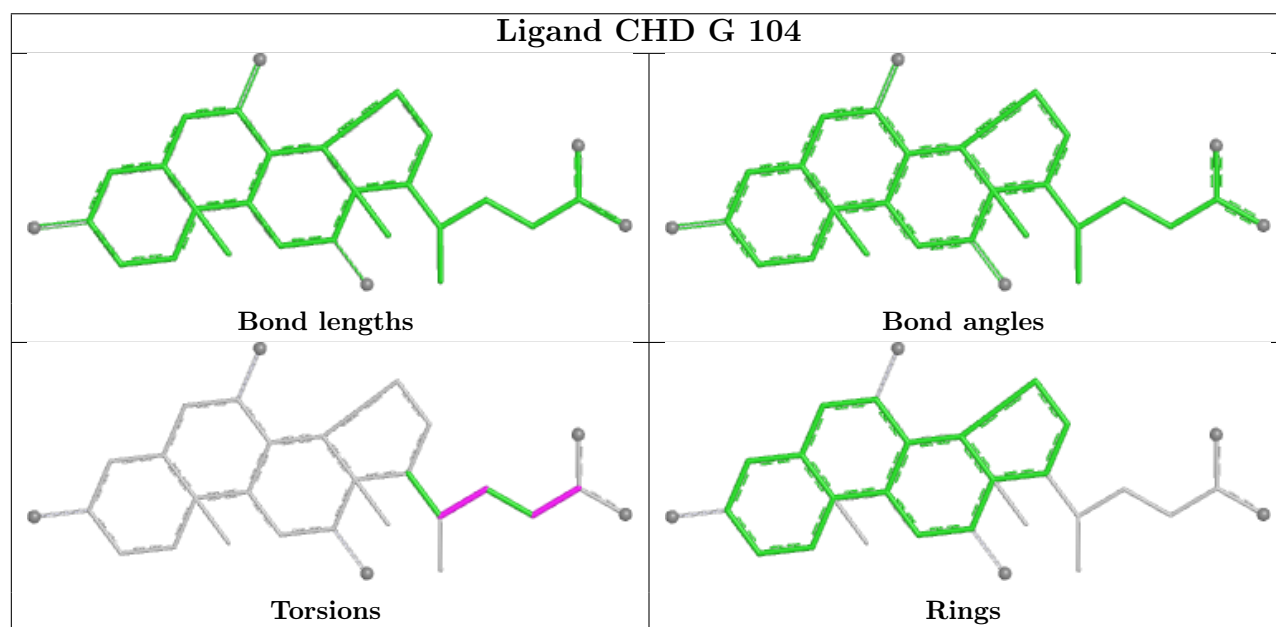
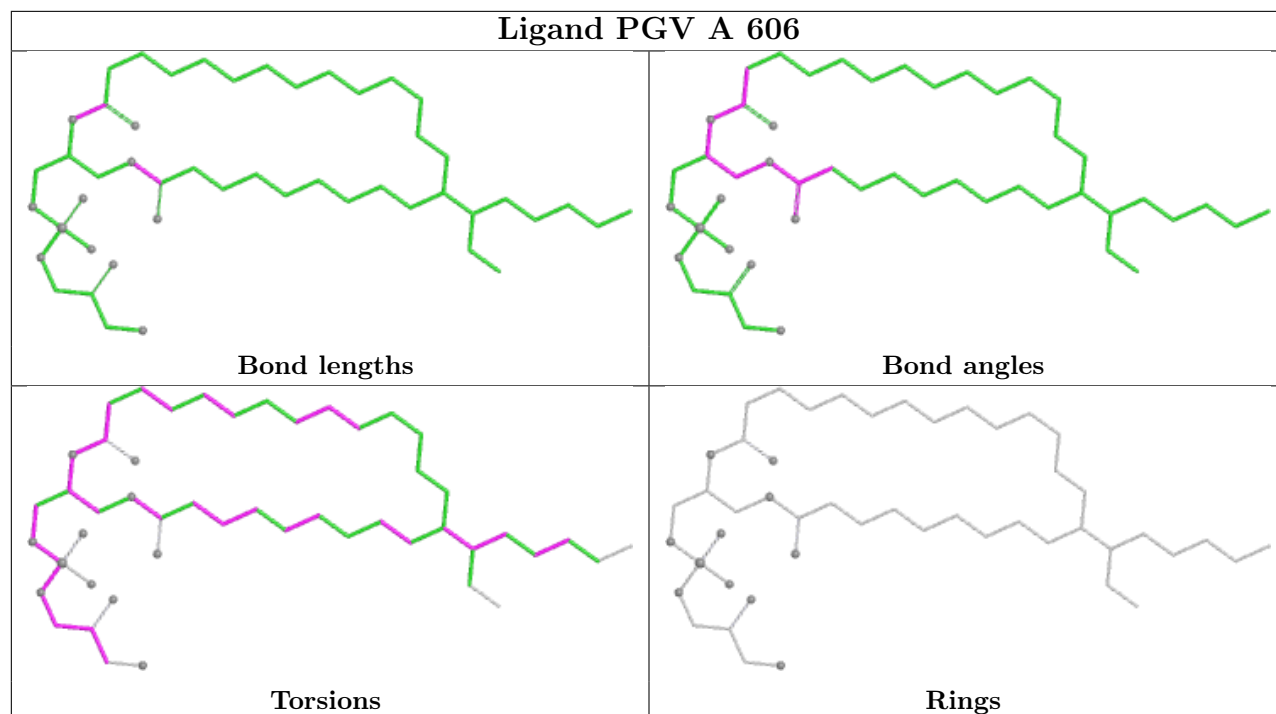


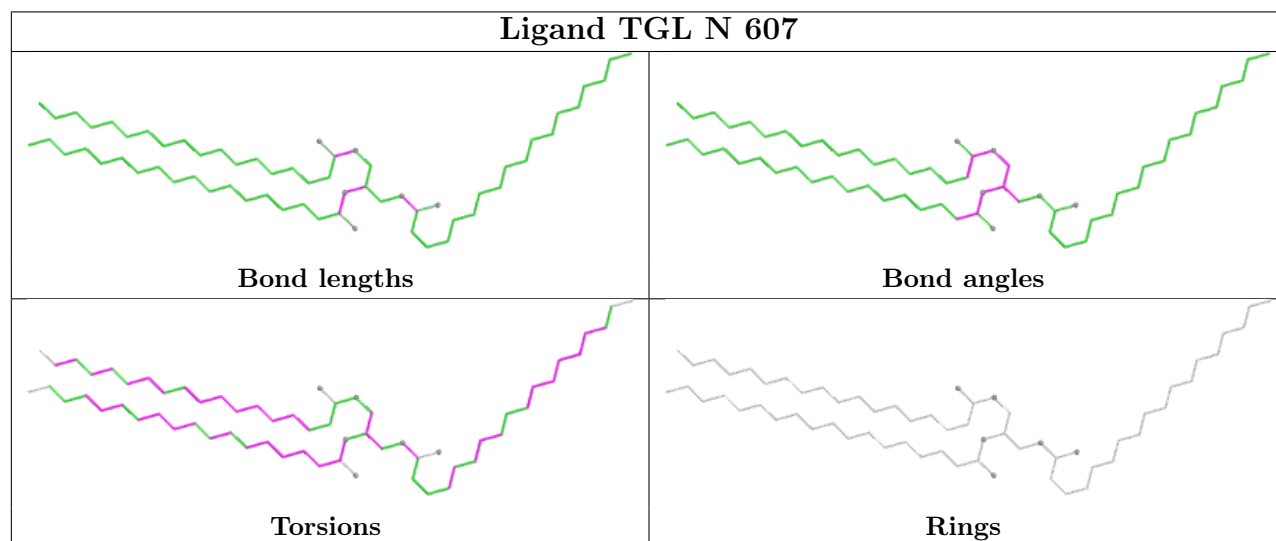
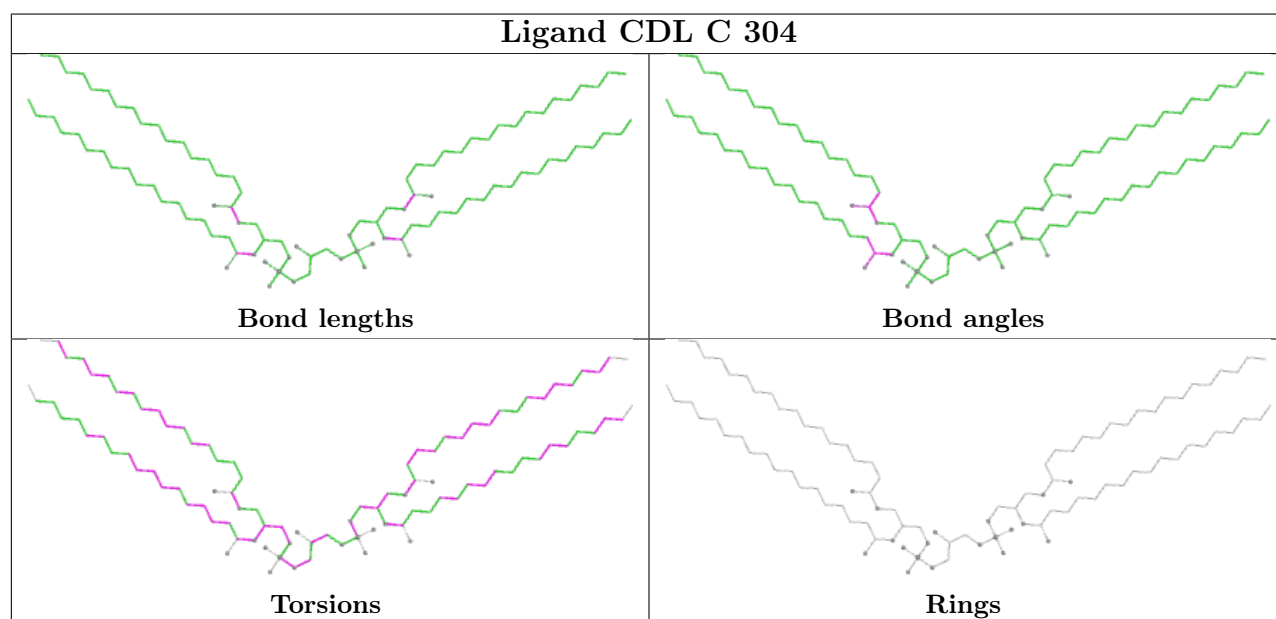
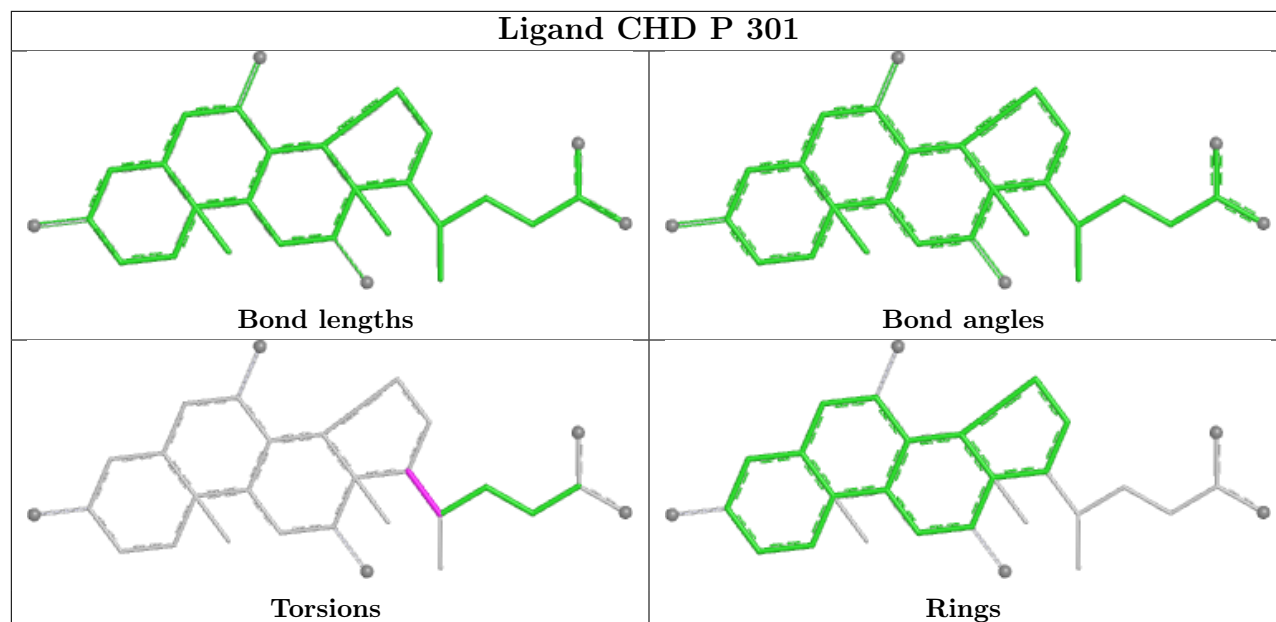
Ligand CHD J 102

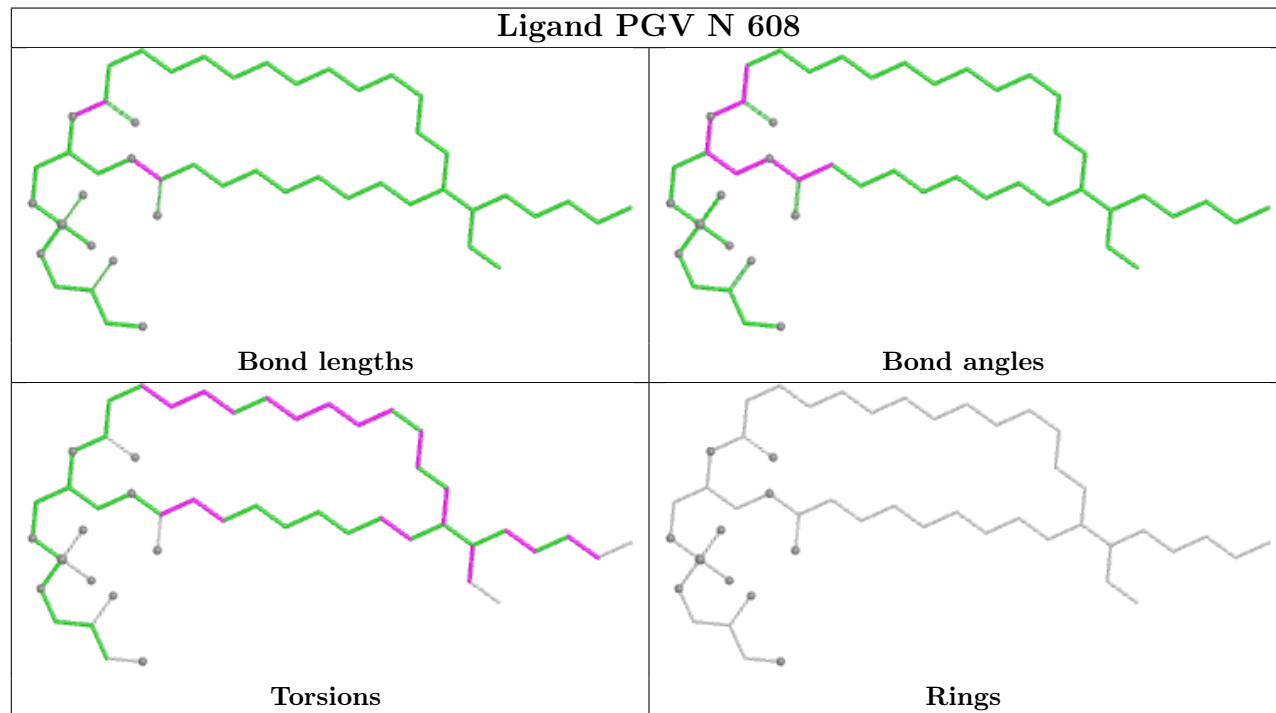
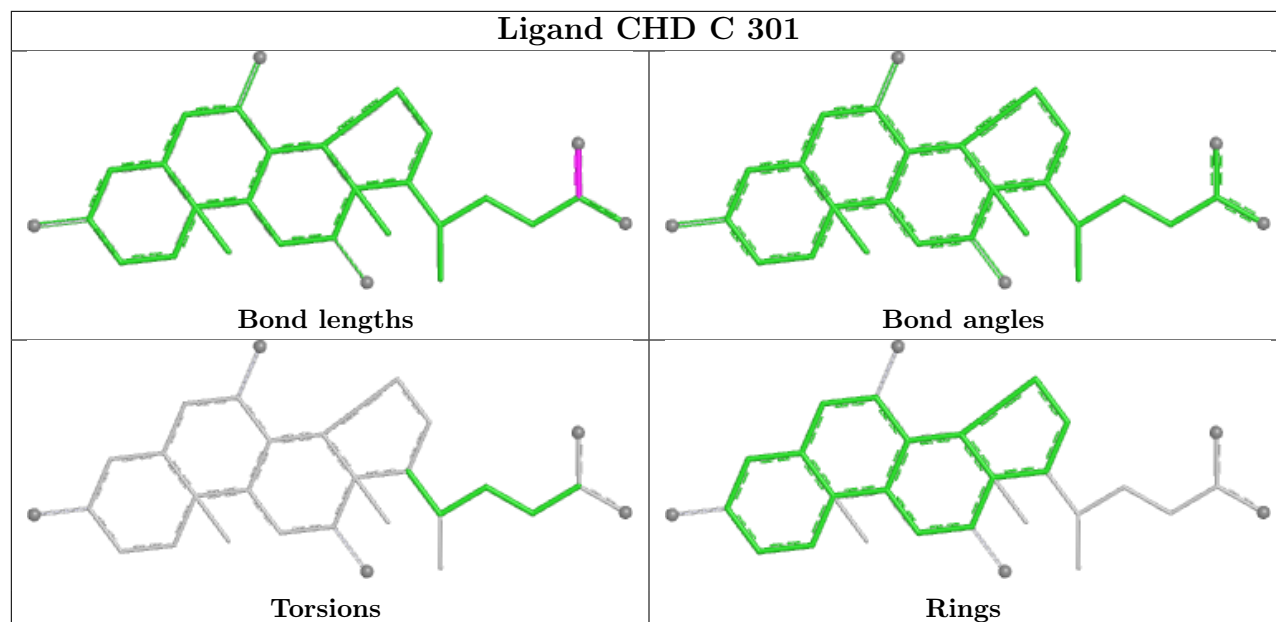


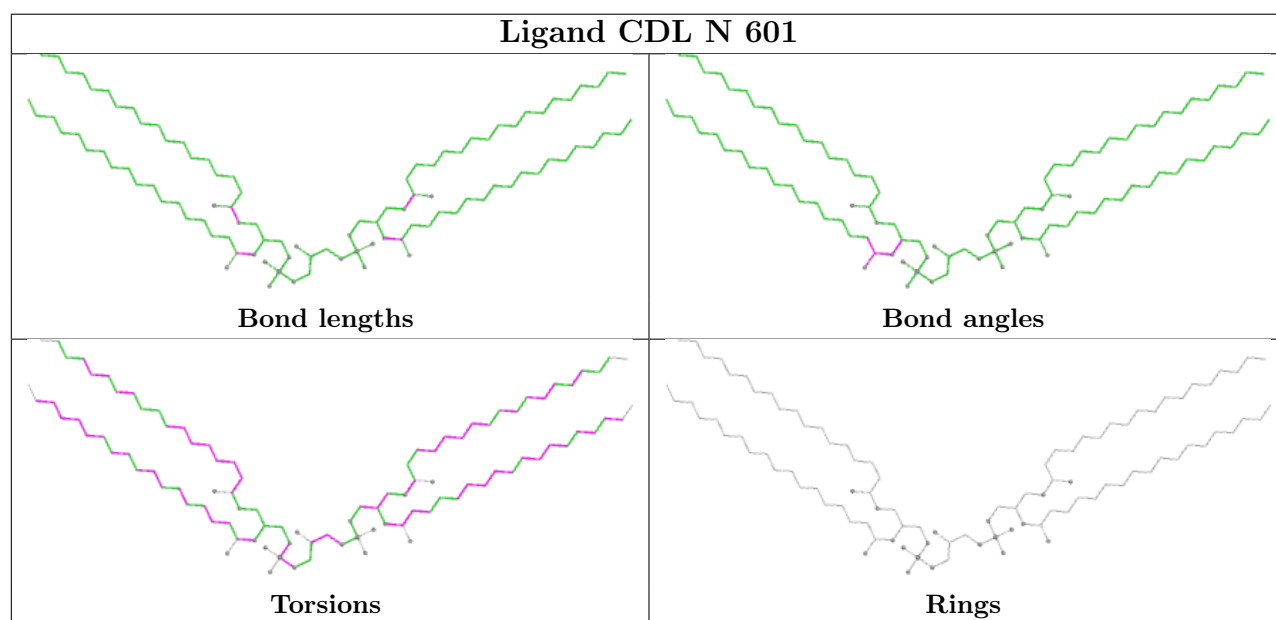
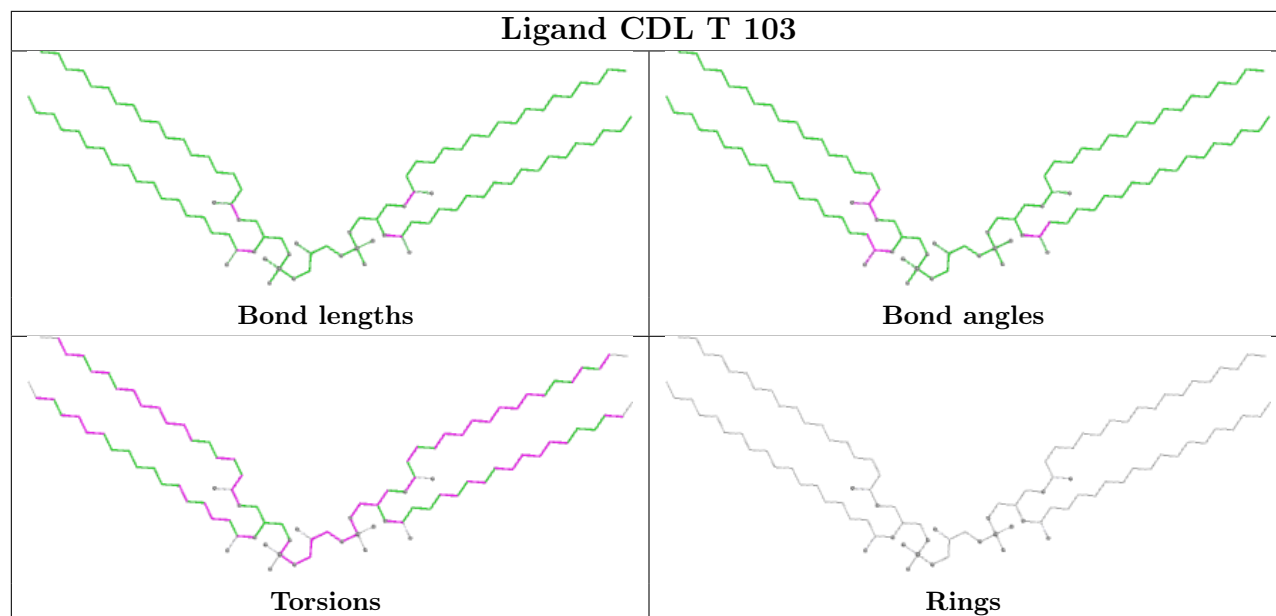
Ligand PEK P 302

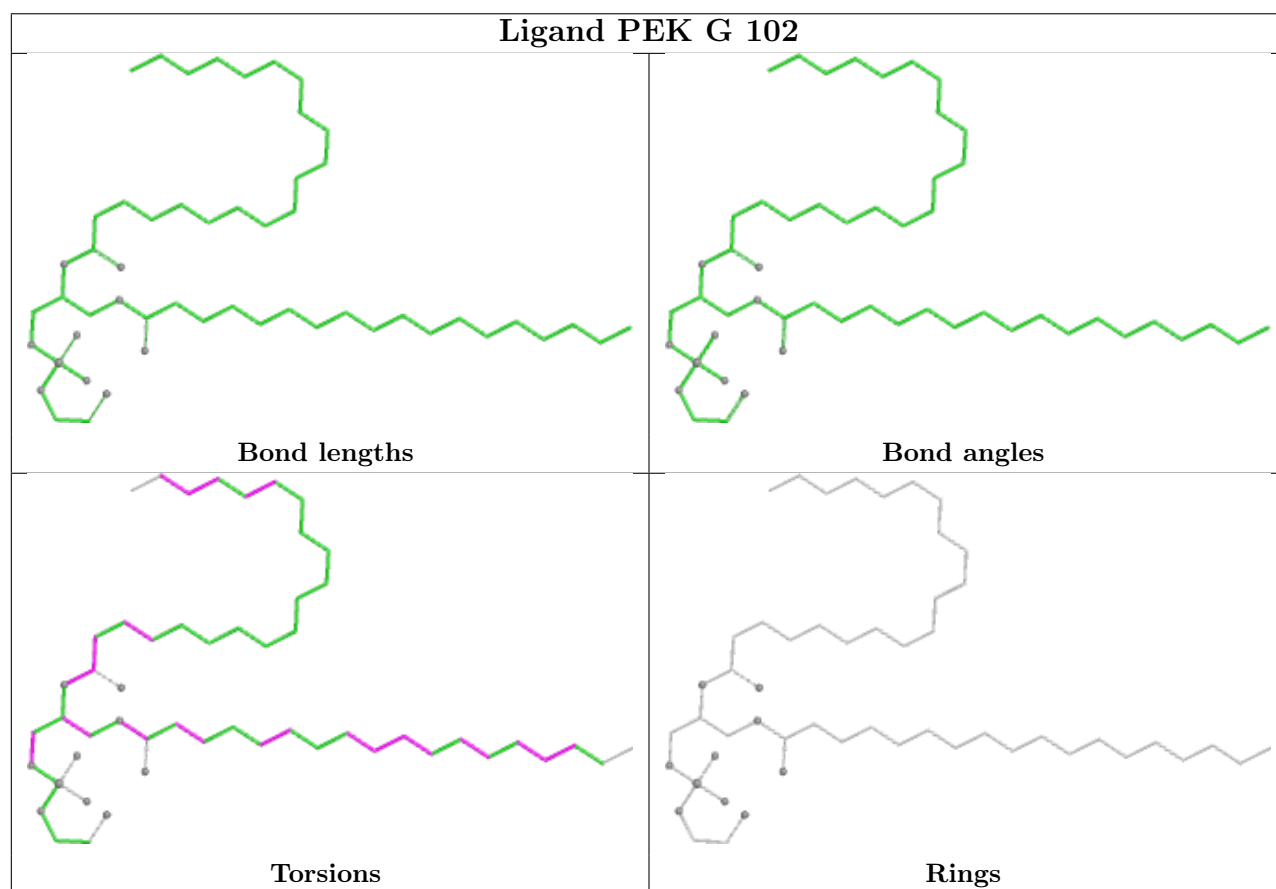
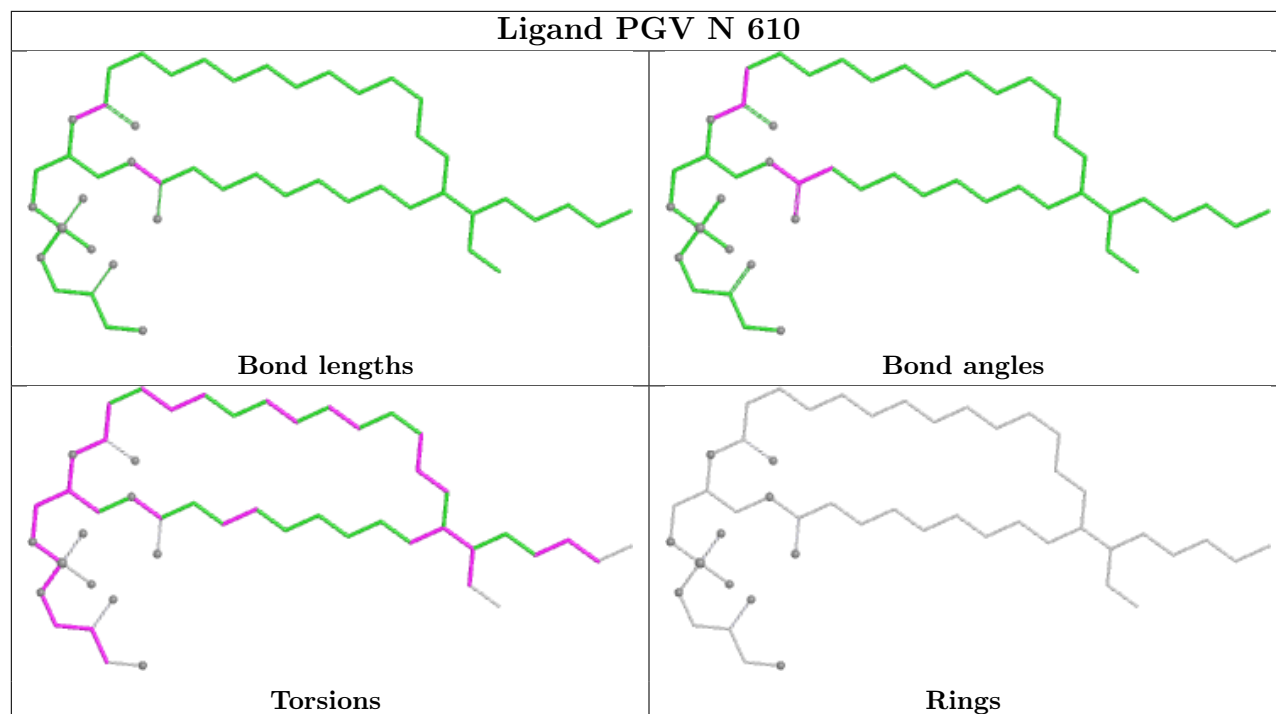


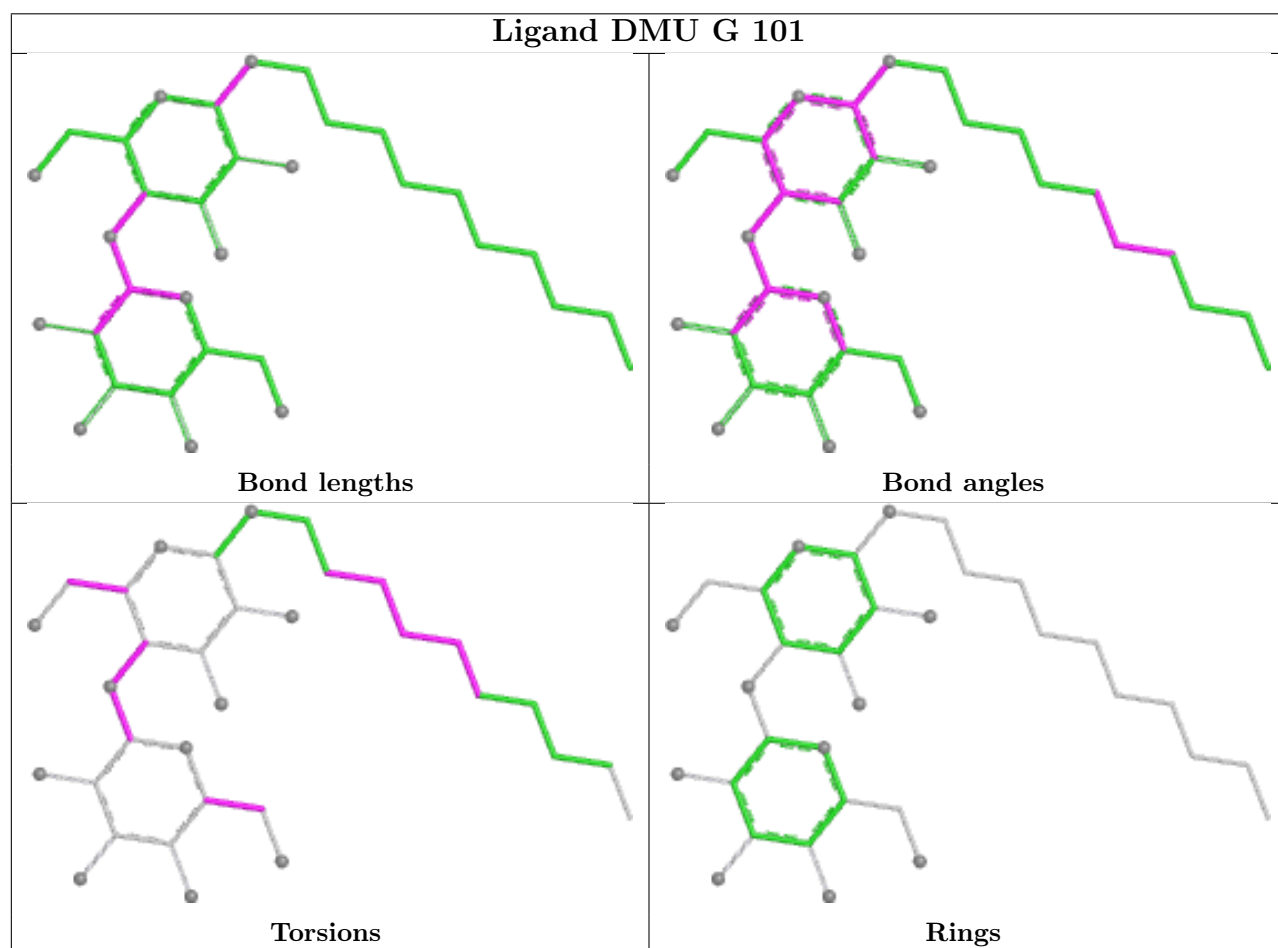
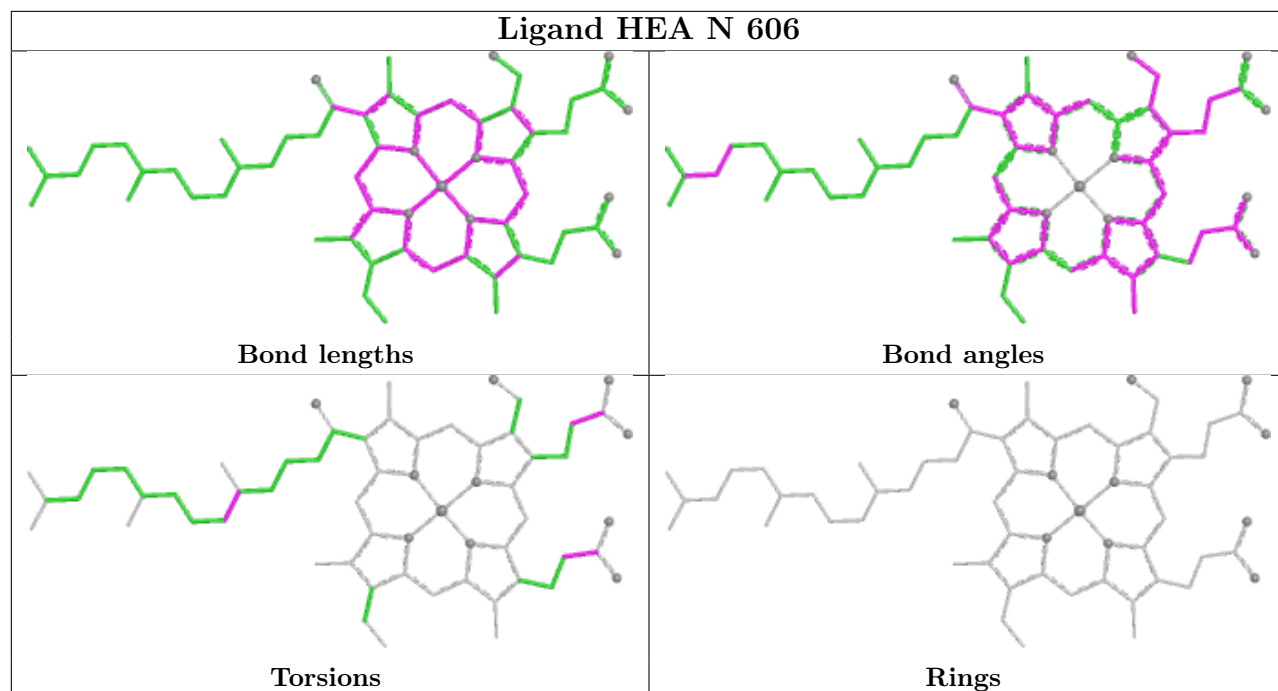


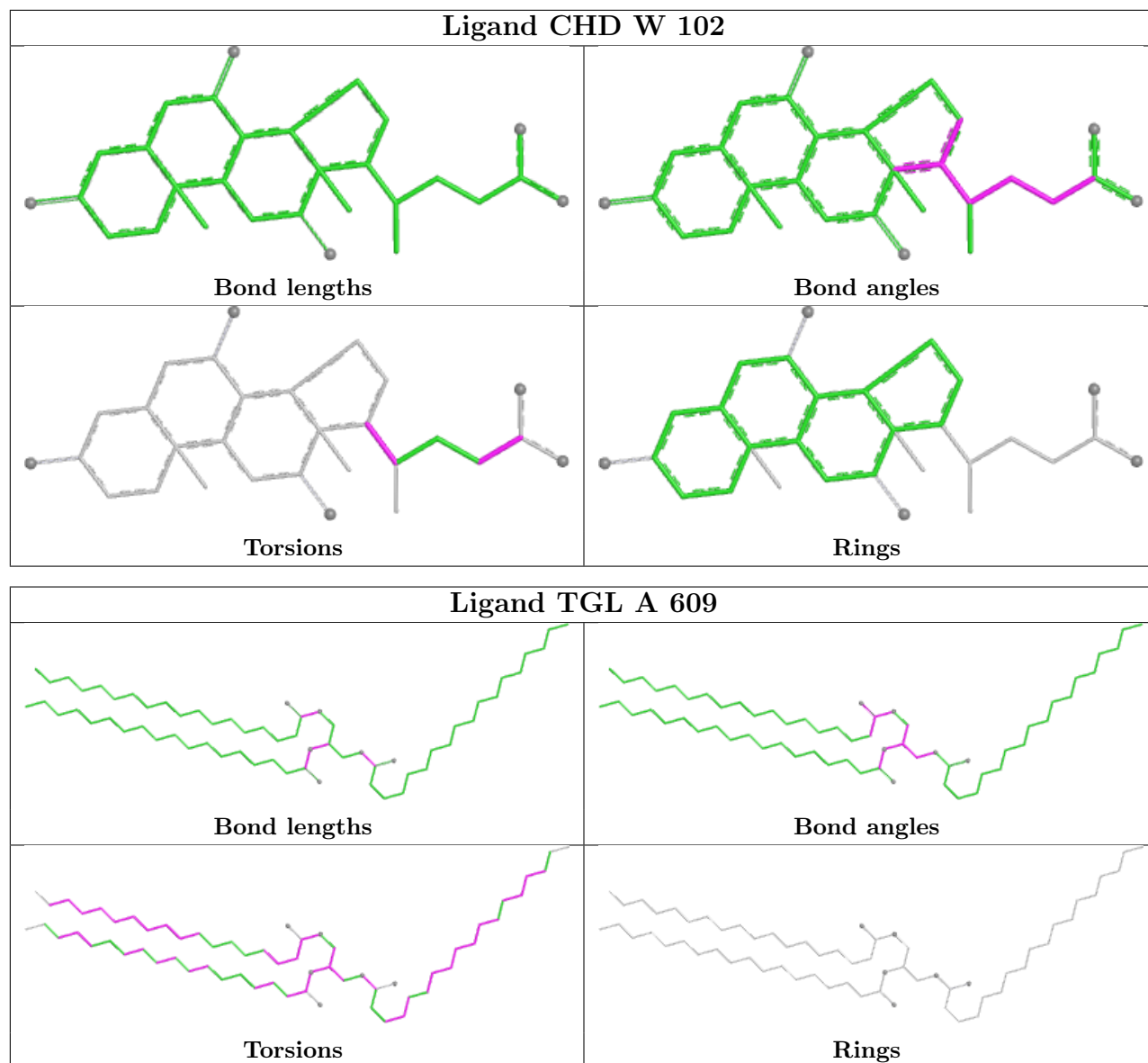


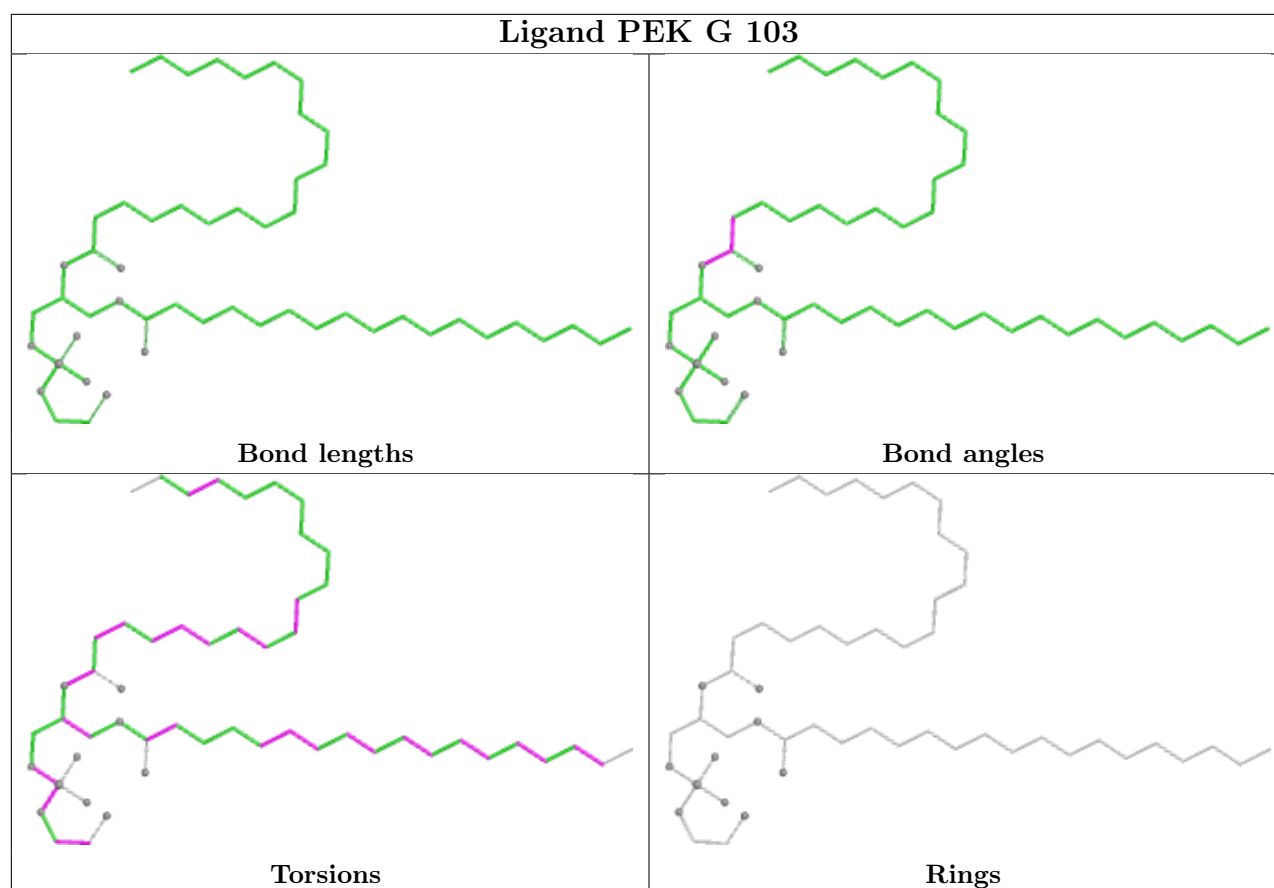












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-1.06	0 100 100	35, 43, 55, 103	0
1	N	513/514 (99%)	-0.82	0 100 100	41, 57, 75, 129	0
2	B	226/227 (99%)	-0.91	1 (0%) 88 86	36, 50, 84, 158	0
2	O	226/227 (99%)	-0.56	2 (0%) 81 78	48, 70, 109, 160	0
3	C	259/261 (99%)	-0.97	0 100 100	39, 48, 66, 114	0
3	P	259/261 (99%)	-0.82	0 100 100	45, 59, 86, 127	0
4	D	144/147 (97%)	-0.91	0 100 100	43, 54, 81, 124	0
4	Q	139/147 (94%)	-0.45	0 100 100	62, 86, 118, 135	0
5	E	105/109 (96%)	-0.94	0 100 100	41, 54, 92, 147	0
5	R	105/109 (96%)	-0.72	0 100 100	53, 73, 97, 152	0
6	F	96/98 (97%)	-0.70	2 (2%) 63 59	42, 55, 103, 145	0
6	S	94/98 (95%)	-0.67	1 (1%) 78 75	50, 70, 112, 153	0
7	G	83/85 (97%)	-0.43	2 (2%) 59 55	44, 59, 156, 192	0
7	T	83/85 (97%)	-0.28	3 (3%) 46 41	49, 74, 152, 192	0
8	H	78/85 (91%)	-0.67	1 (1%) 75 71	44, 59, 126, 160	0
8	U	79/85 (92%)	-0.44	1 (1%) 75 71	51, 78, 144, 179	0
9	I	72/73 (98%)	-0.63	1 (1%) 73 70	50, 62, 95, 118	0
9	V	72/73 (98%)	-0.33	2 (2%) 55 50	50, 82, 115, 137	0
10	J	58/59 (98%)	-0.71	0 100 100	50, 62, 112, 160	0
10	W	58/59 (98%)	-0.26	0 100 100	64, 81, 124, 158	0
11	K	49/56 (87%)	-0.70	0 100 100	41, 58, 78, 110	0
11	X	49/56 (87%)	-0.31	0 100 100	73, 86, 109, 144	0
12	L	46/47 (97%)	-0.87	0 100 100	41, 49, 78, 137	0
12	Y	46/47 (97%)	-0.40	0 100 100	56, 80, 108, 144	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%)	-0.82	0 100 100	44, 51, 89, 143	0
13	Z	43/46 (93%)	-0.26	0 100 100	67, 81, 126, 158	0
All	All	3538/3614 (97%)	-0.76	16 (0%) 87 85	35, 58, 105, 192	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	94	HIS	4.5
9	I	37	PHE	3.6
7	T	8	HIS	3.5
7	T	36	TRP	3.4
7	G	8	HIS	3.1
6	F	96	LEU	2.8
8	U	8	ILE	2.7
7	G	3	ALA	2.7
6	S	93	PRO	2.6
7	T	3	ALA	2.6
9	V	25	PHE	2.4
2	B	59	GLN	2.4
9	V	37	PHE	2.3
8	H	8	ILE	2.2
2	O	59	GLN	2.1
2	O	58	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.40	0.17	140,158,175,179	0
7	TPO	G	11	11/12	0.66	0.21	116,142,176,188	0
9	SAC	I	1	9/10	0.69	0.16	128,141,151,154	0
7	TPO	T	11	11/12	0.74	0.20	139,157,180,188	0
1	FME	N	1	10/11	0.78	0.12	89,103,132,152	0
1	FME	A	1	10/11	0.88	0.10	69,80,105,120	0
2	FME	O	1	10/11	0.95	0.07	59,73,86,88	0
2	FME	B	1	10/11	0.96	0.06	48,54,56,64	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	PEK	G	103	53/53	0.75	0.13	78,133,201,215	0
28	DMU	T	101	33/33	0.76	0.11	117,166,199,205	0
19	TGL	N	609	63/63	0.79	0.11	91,125,149,159	0
19	TGL	A	609	63/63	0.81	0.11	75,106,129,133	0
26	CDL	T	103	100/100	0.82	0.11	86,134,181,206	0
18	PGV	N	610	51/51	0.82	0.12	67,113,153,166	0
25	PEK	P	303	53/53	0.83	0.12	78,129,162,178	0
26	CDL	N	601	100/100	0.83	0.10	90,125,171,189	0
24	CHD	J	102	29/29	0.84	0.10	97,115,137,144	0
26	CDL	P	305	100/100	0.84	0.11	54,129,159,162	0
24	CHD	W	102	29/29	0.84	0.11	98,143,157,162	0
25	PEK	T	102	53/53	0.84	0.11	72,147,234,241	0
25	PEK	C	302	53/53	0.85	0.11	80,123,194,208	0
19	TGL	Y	101	63/63	0.86	0.11	74,117,173,182	0
23	PSC	B	302	52/52	0.86	0.13	78,132,259,284	0
18	PGV	U	101	51/51	0.86	0.11	75,119,151,156	0
18	PGV	A	608	51/51	0.87	0.10	76,120,154,156	0
19	TGL	B	303	63/63	0.87	0.12	47,99,151,158	0
19	TGL	L	101	63/63	0.87	0.12	58,95,149,160	0
26	CDL	C	304	100/100	0.87	0.11	59,124,167,174	0
24	CHD	J	101	29/29	0.88	0.10	89,107,119,123	0
19	TGL	N	607	63/63	0.88	0.10	53,109,152,162	0
18	PGV	A	606	51/51	0.88	0.11	53,107,152,185	0
23	PSC	O	302	52/52	0.88	0.11	73,139,232,252	0
28	DMU	G	101	33/33	0.89	0.10	101,139,187,198	0
24	CHD	W	101	29/29	0.90	0.08	102,115,125,128	0
28	DMU	Q	201	33/33	0.92	0.07	96,111,126,131	0
24	CHD	P	301	29/29	0.94	0.06	51,58,61,64	0
16	NA	N	604	1/1	0.94	0.12	62,62,62,62	0
25	PEK	G	102	53/53	0.95	0.07	40,83,126,143	0
28	DMU	M	101	33/33	0.95	0.06	56,65,83,87	0
24	CHD	C	301	29/29	0.95	0.06	41,48,54,61	0

Continued on next page...

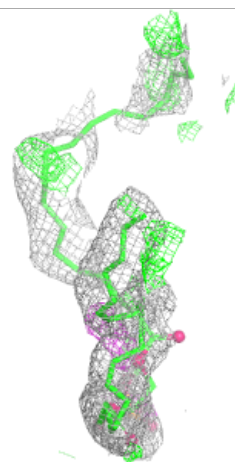
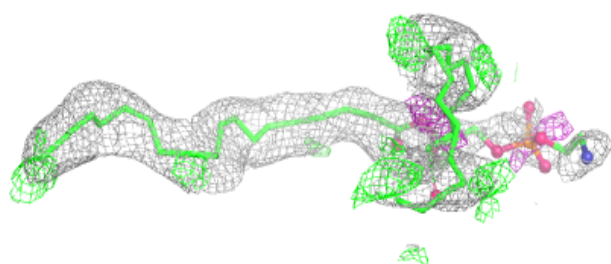
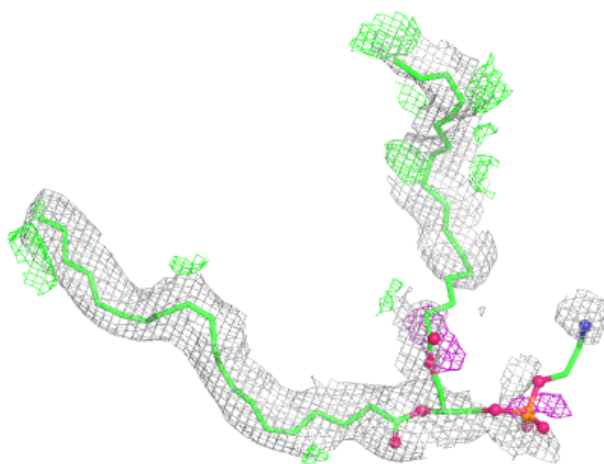
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	PEK	P	302	53/53	0.95	0.08	54,94,153,177	0
18	PGV	P	304	51/51	0.96	0.06	45,59,172,183	0
18	PGV	N	608	51/51	0.96	0.06	43,73,91,94	0
18	PGV	C	303	51/51	0.97	0.06	38,54,123,140	0
24	CHD	G	104	29/29	0.97	0.04	45,52,60,66	0
24	CHD	B	304	29/29	0.97	0.04	46,50,60,66	0
17	HEA	A	604	60/60	0.98	0.04	32,39,75,81	0
17	HEA	N	605	60/60	0.98	0.05	45,56,74,86	0
16	NA	A	603	1/1	0.98	0.03	45,45,45,45	0
18	PGV	A	607	51/51	0.98	0.05	32,68,86,90	0
15	MG	N	603	1/1	0.99	0.02	55,55,55,55	0
17	HEA	N	606	60/60	0.99	0.04	42,46,56,60	0
15	MG	A	602	1/1	0.99	0.02	38,38,38,38	0
17	HEA	A	605	60/60	0.99	0.04	32,39,51,55	0
20	O	N	611	1/1	0.99	0.05	50,50,50,50	0
21	OH	A	611	1/1	0.99	0.04	44,44,44,44	0
22	CUA	B	301	2/2	0.99	0.03	42,42,42,45	0
22	CUA	O	301	2/2	0.99	0.03	59,59,59,61	0
27	ZN	F	101	1/1	1.00	0.02	58,58,58,58	0
27	ZN	S	101	1/1	1.00	0.02	64,64,64,64	0
14	CU	N	602	1/1	1.00	0.03	58,58,58,58	0
21	OH	N	612	1/1	1.00	0.06	64,64,64,64	0
20	O	A	610	1/1	1.00	0.04	35,35,35,35	0
14	CU	A	601	1/1	1.00	0.02	46,46,46,46	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.

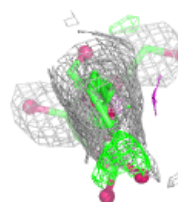
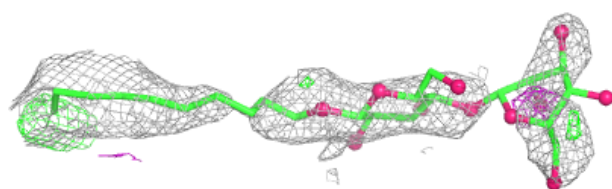
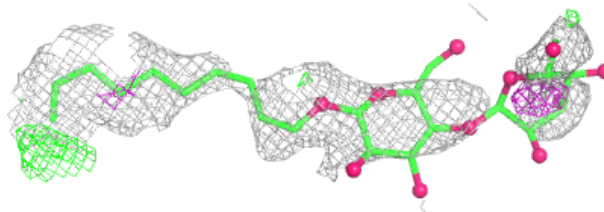
Electron density around PEK G 103:

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

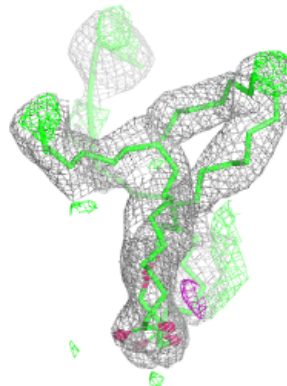
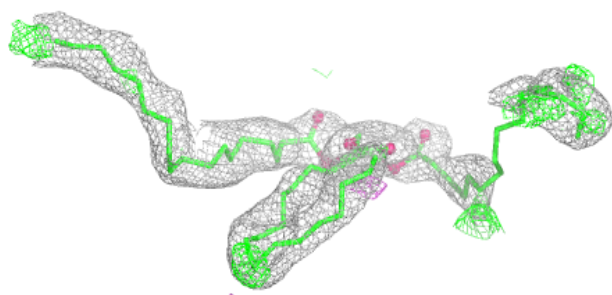
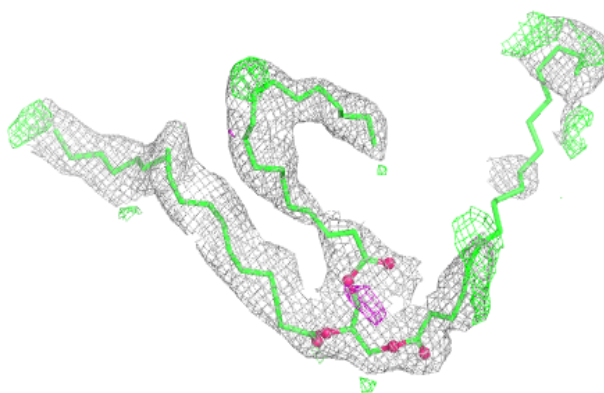


Electron density around DMU T 101:

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

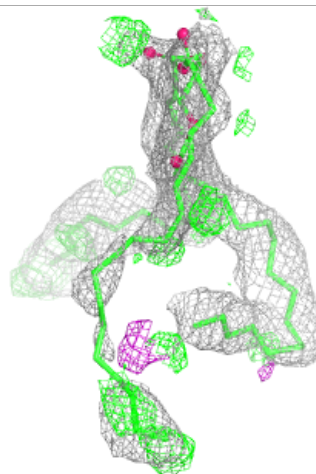
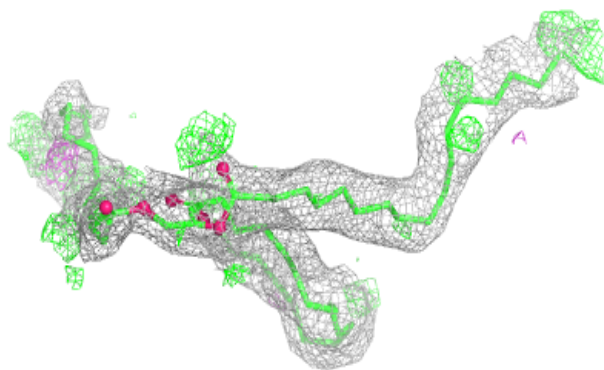
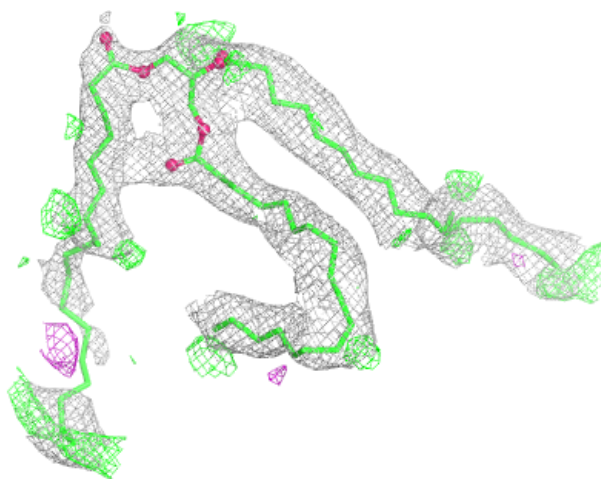
**Electron density around TGL N 609:**

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



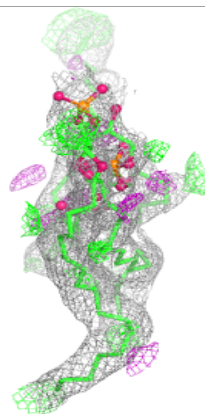
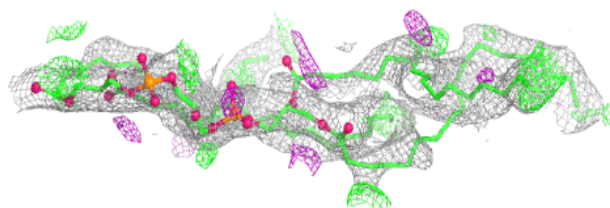
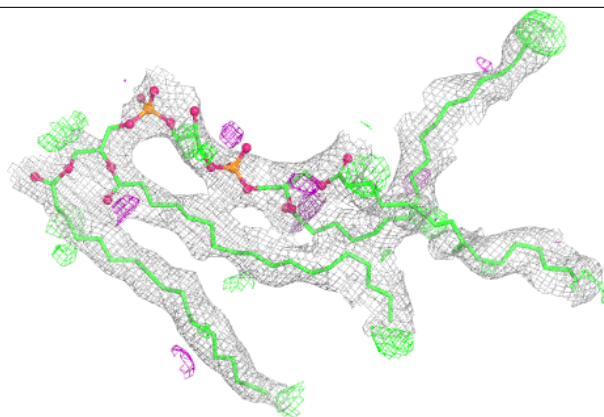
Electron density around TGL A 609:

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

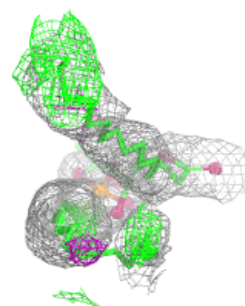
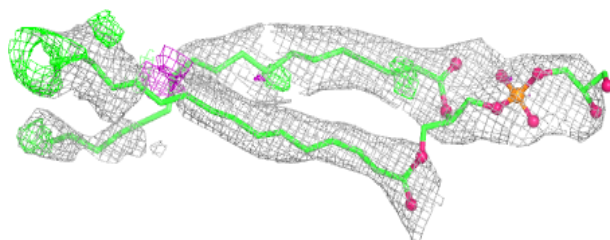
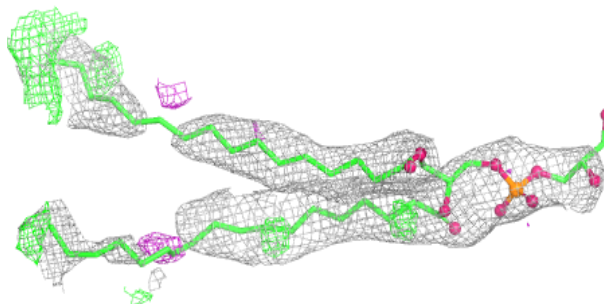


Electron density around CDL T 103:

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

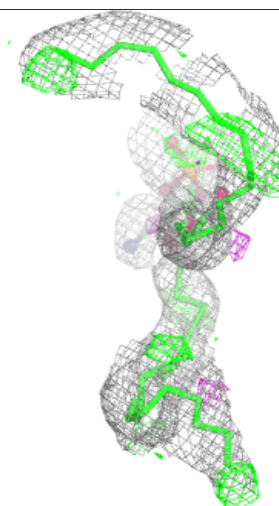
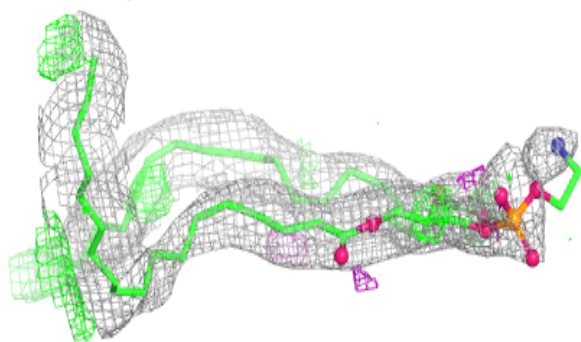
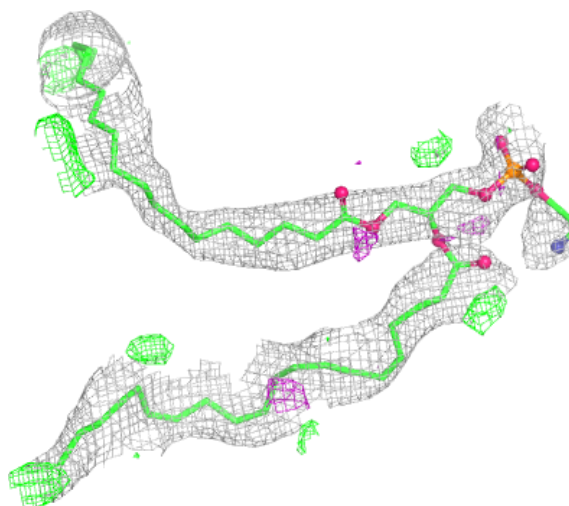
**Electron density around PGV N 610:**

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



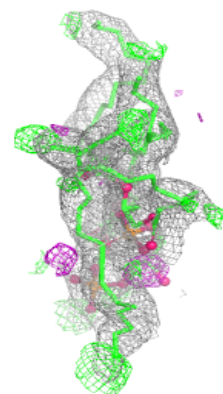
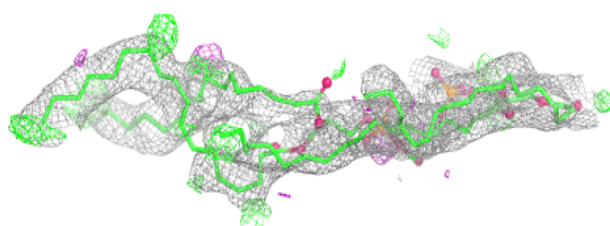
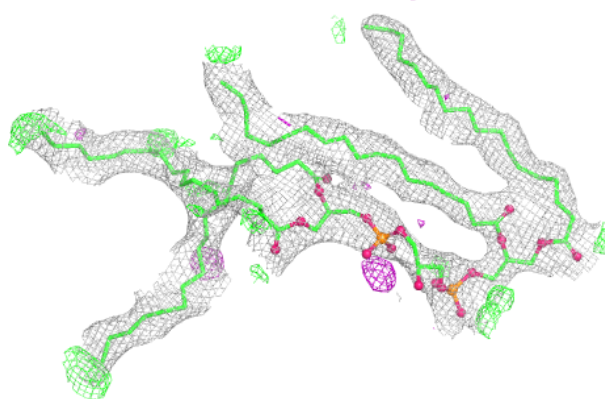
Electron density around PEK P 303:

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

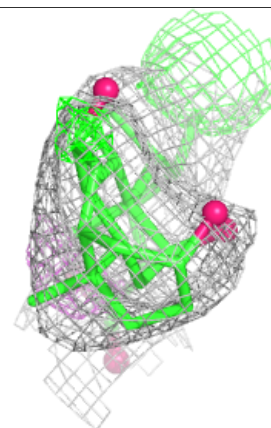
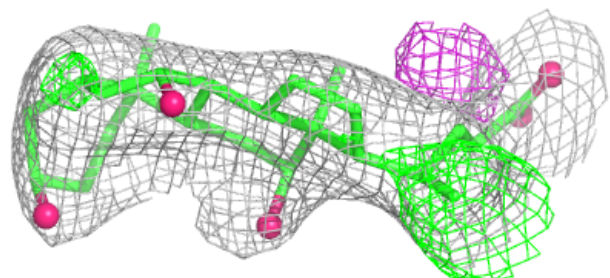
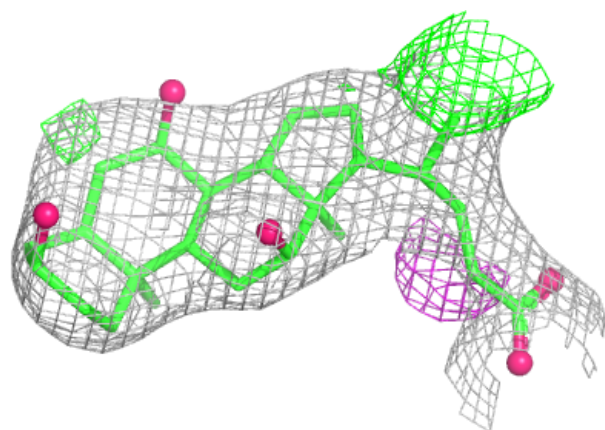


Electron density around CDL N 601:

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

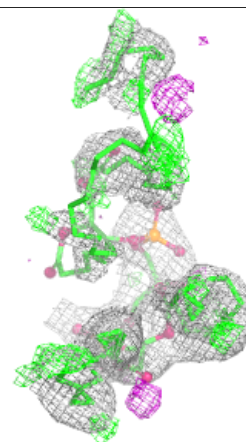
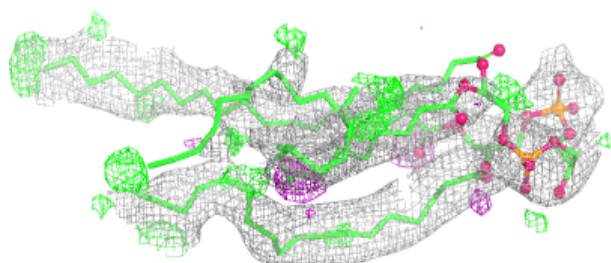
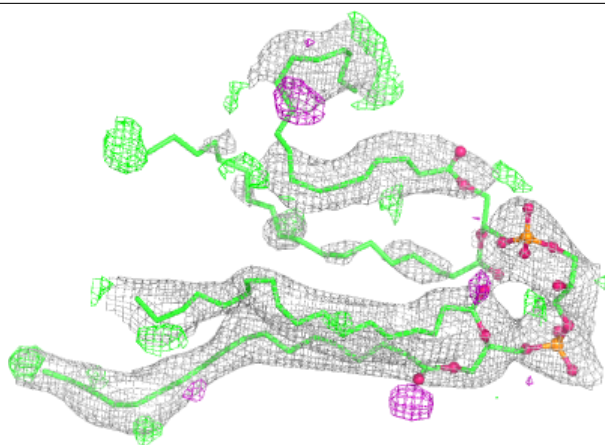
**Electron density around CHD J 102:**

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

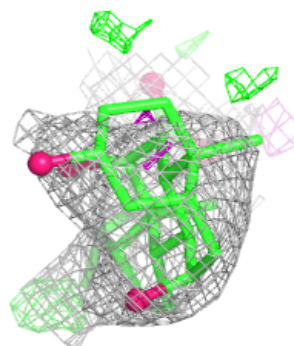
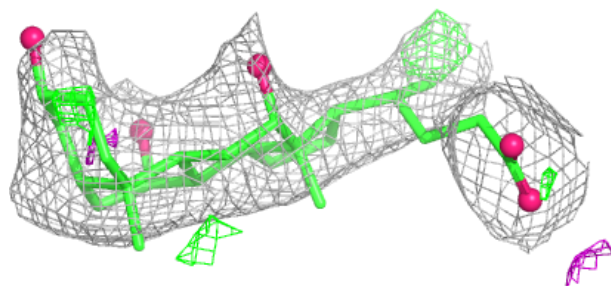
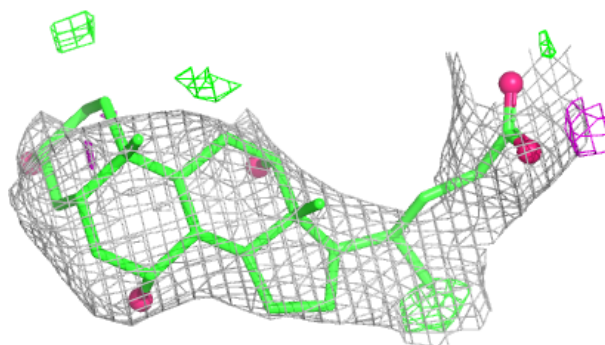


Electron density around CDL P 305:

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

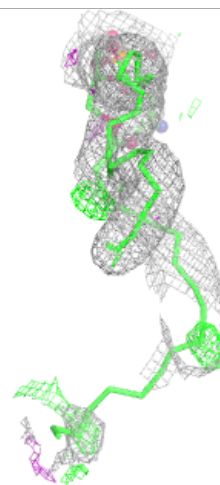
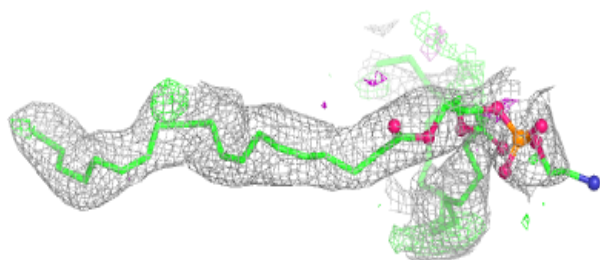
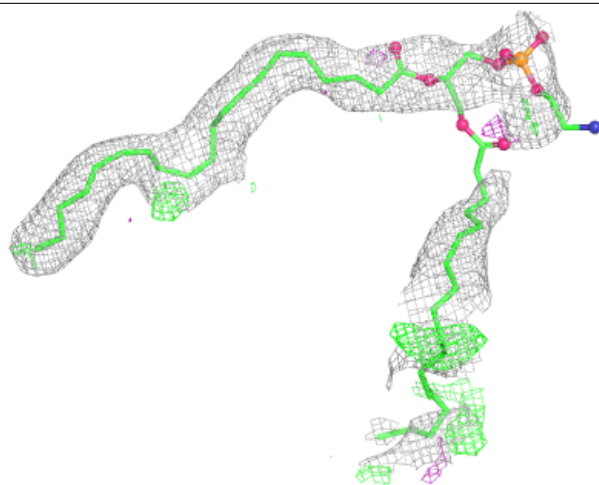
**Electron density around CHD W 102:**

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



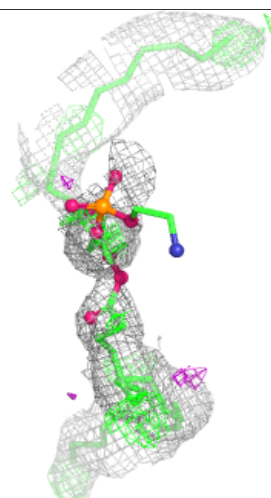
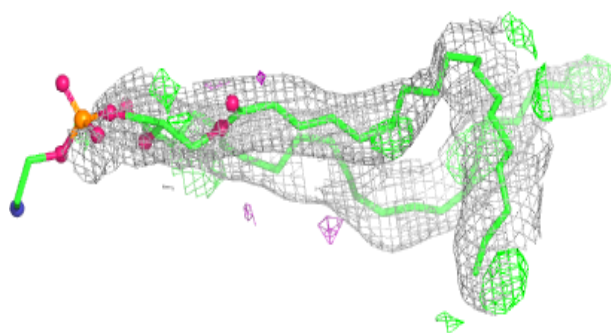
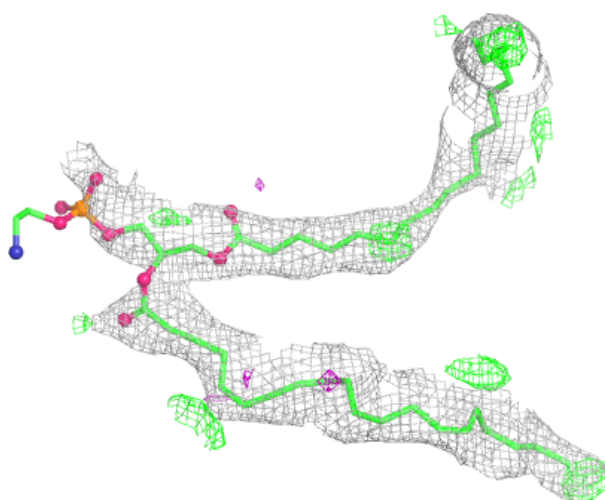
Electron density around PEK T 102:

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



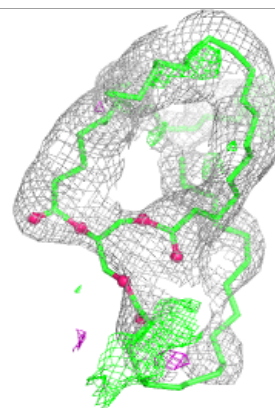
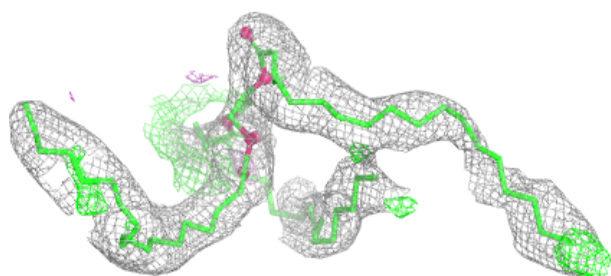
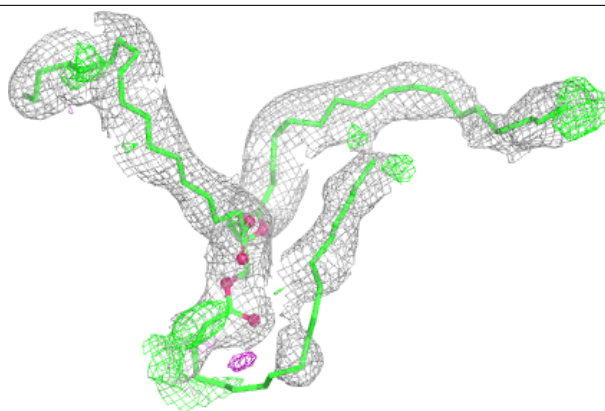
Electron density around PEK C 302:

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

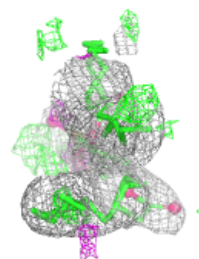
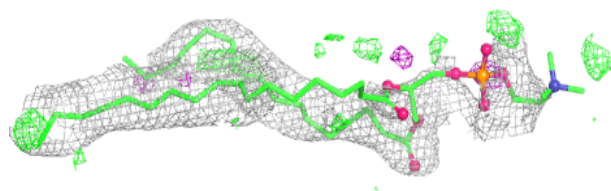
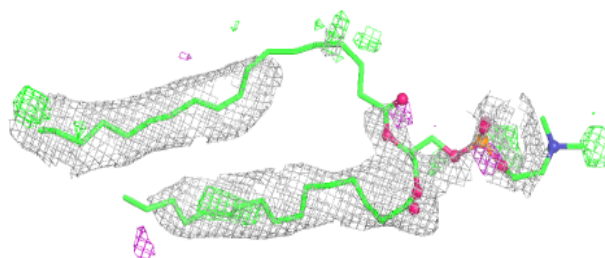


Electron density around TGL Y 101:

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

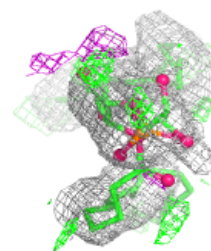
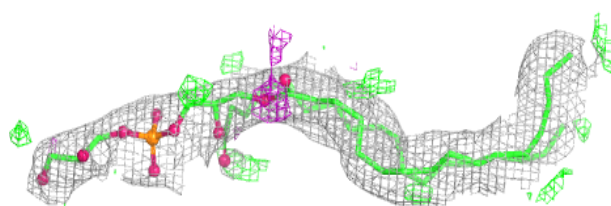
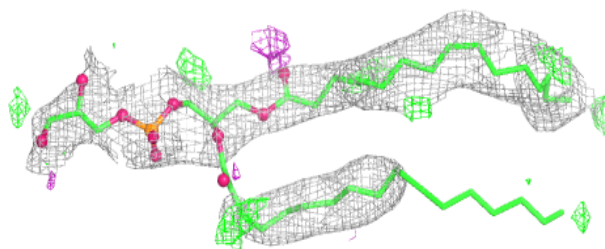
**Electron density around PSC B 302:**

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

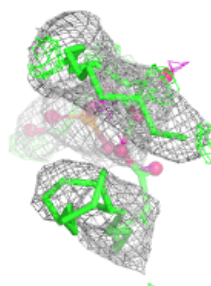
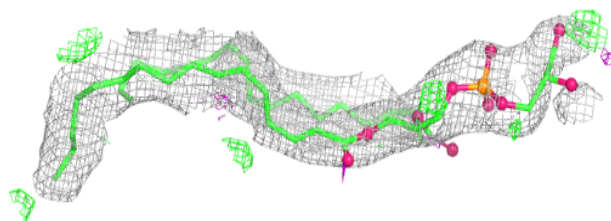
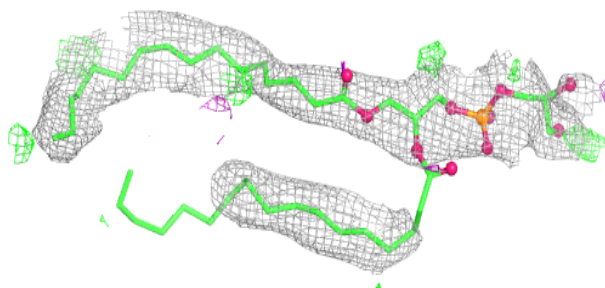


Electron density around PGV U 101:

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

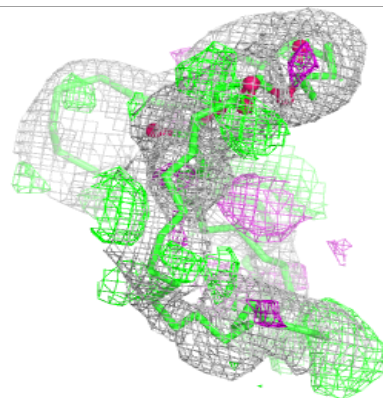
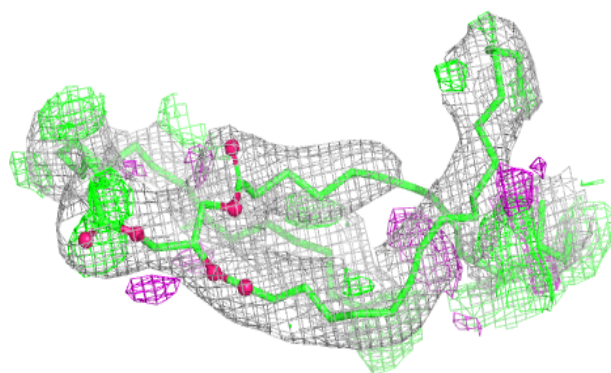
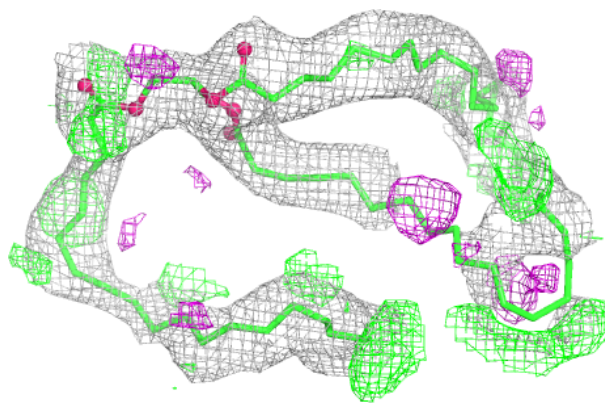
**Electron density around PGV A 608:**

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



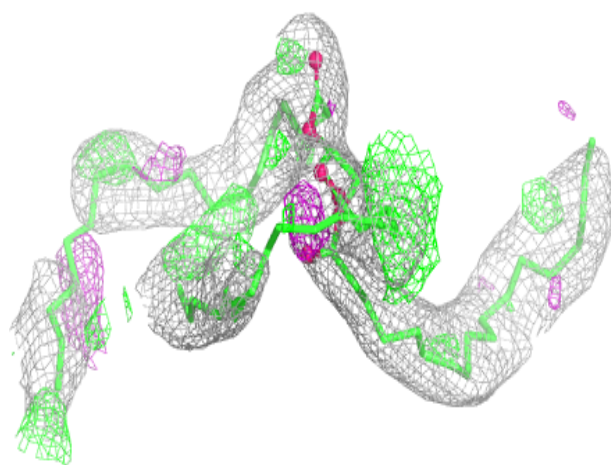
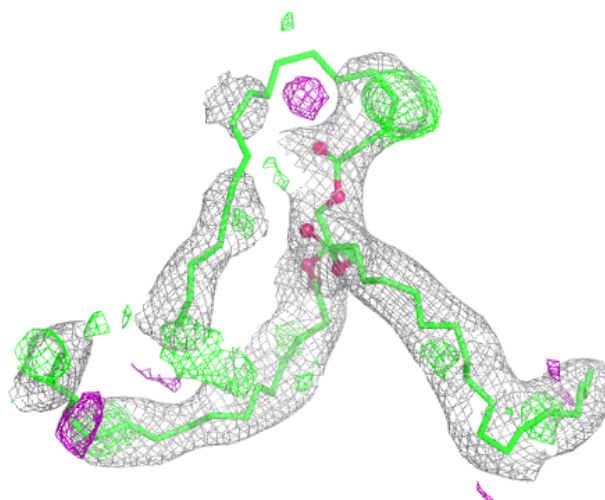
Electron density around TGL B 303:

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



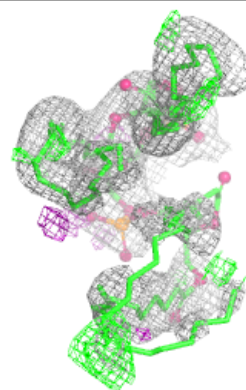
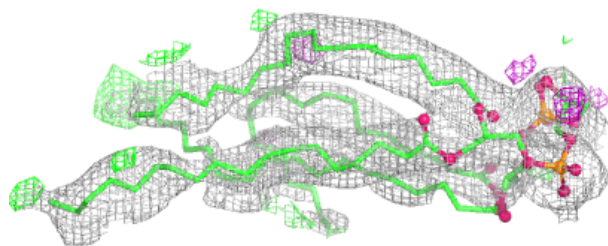
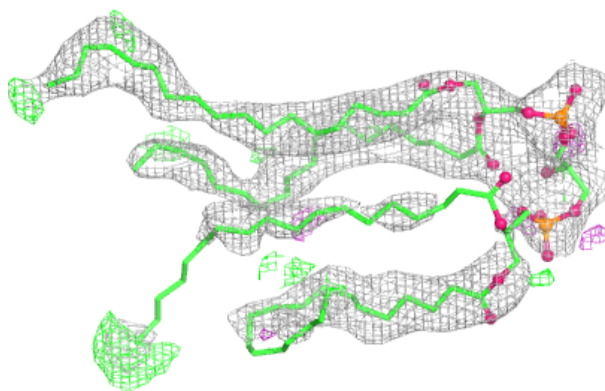
Electron density around TGL L 101:

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

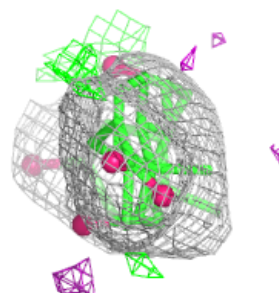
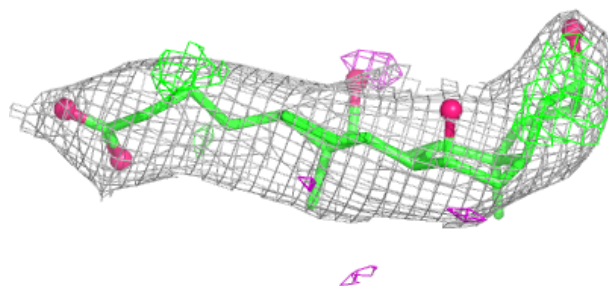
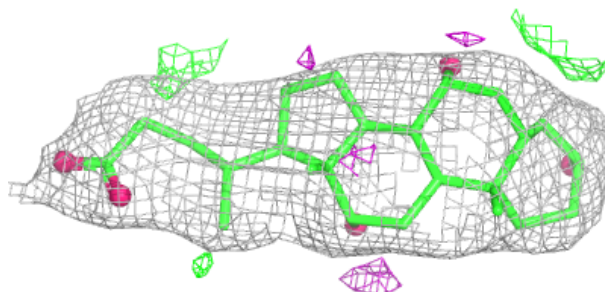


Electron density around CDL C 304:

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

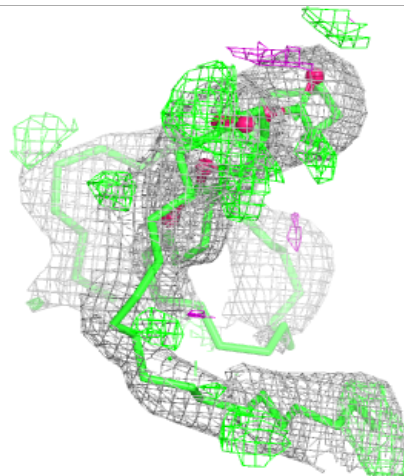
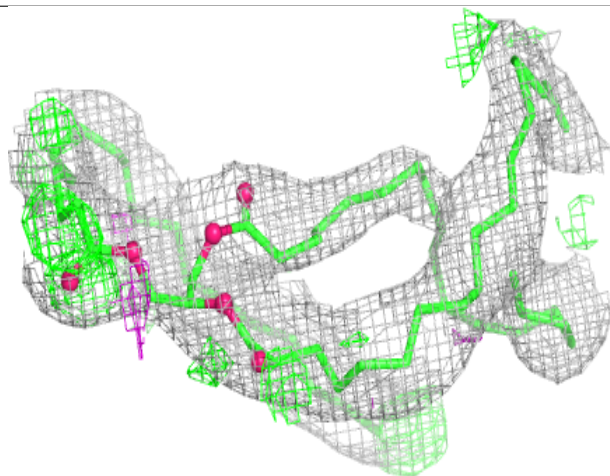
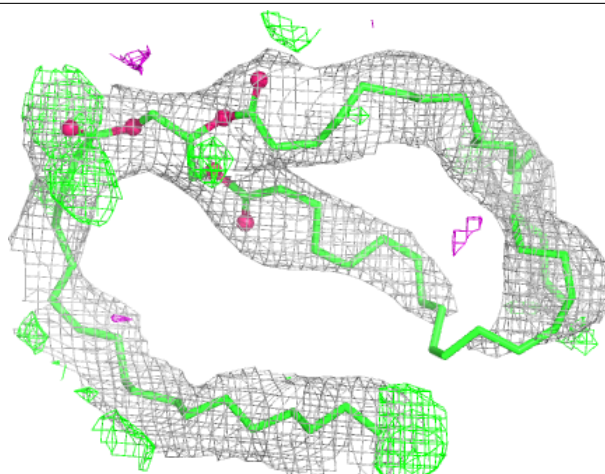
**Electron density around CHD J 101:**

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



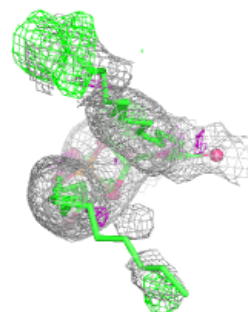
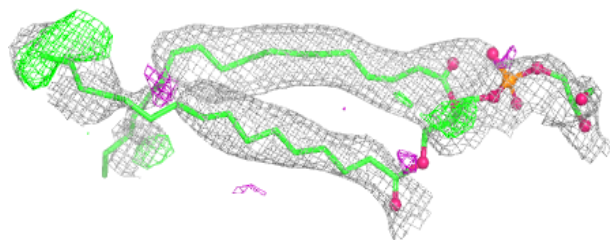
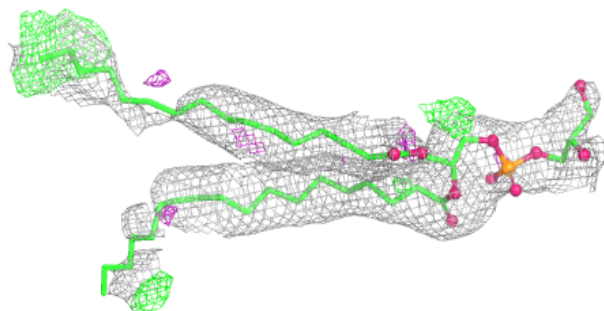
Electron density around TGL N 607:

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

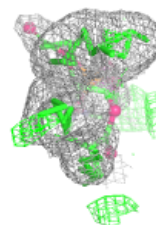
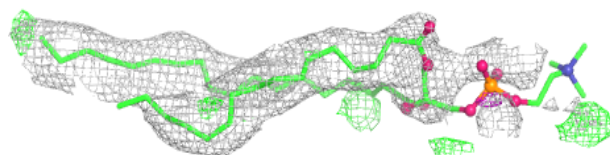
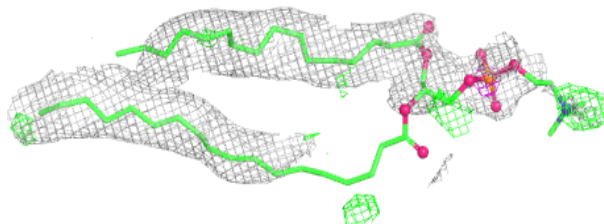


Electron density around PGV A 606:

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

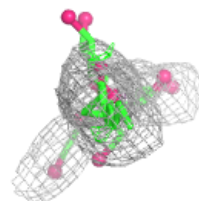
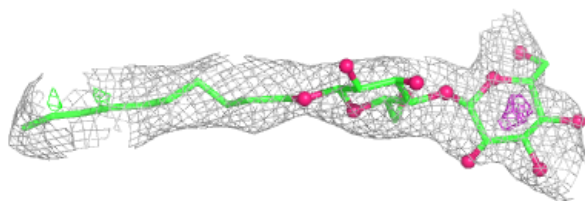
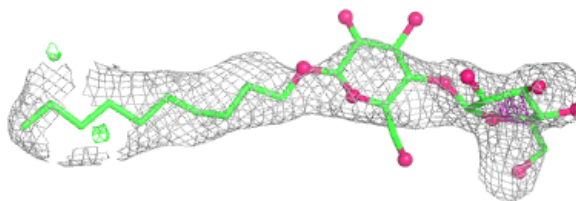
**Electron density around PSC O 302:**

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

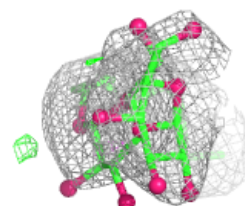
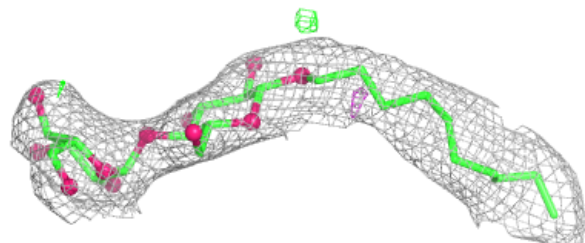
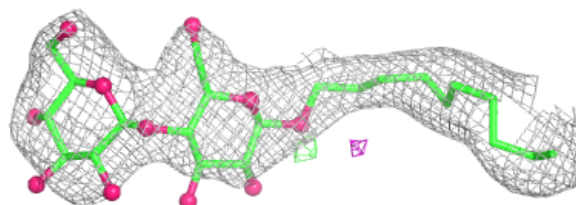


Electron density around DMU G 101:

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

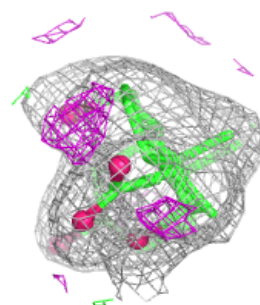
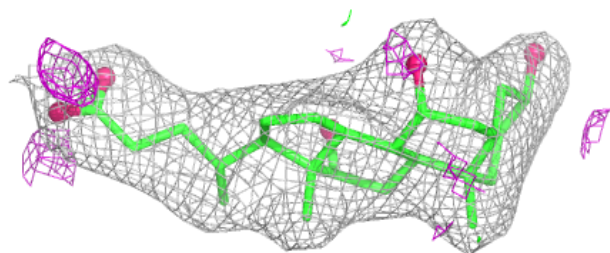
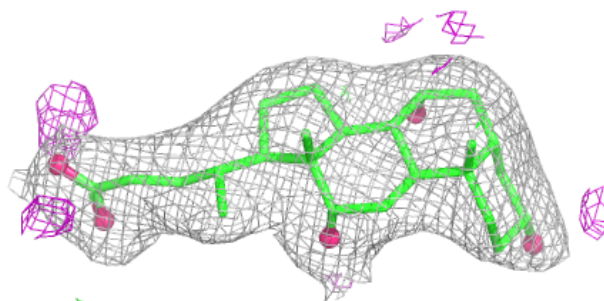
**Electron density around DMU Q 201:**

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

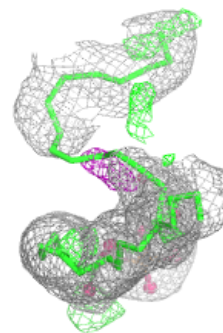
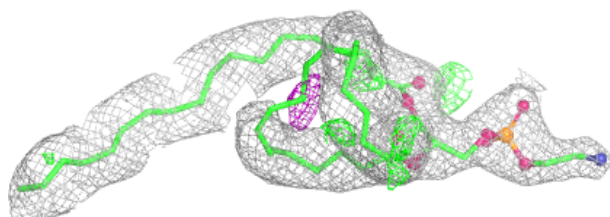
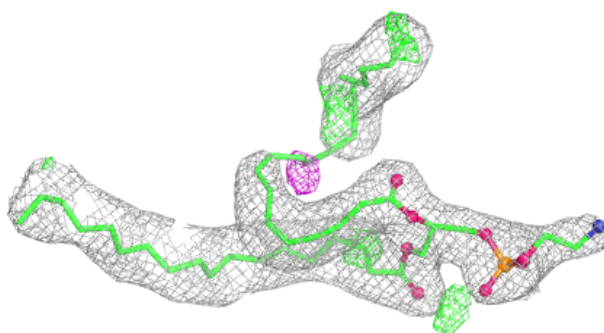


Electron density around CHD P 301:

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

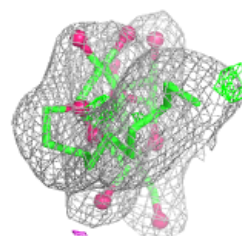
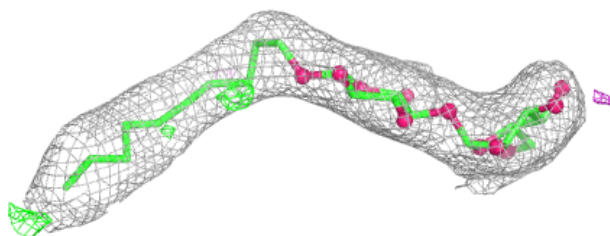
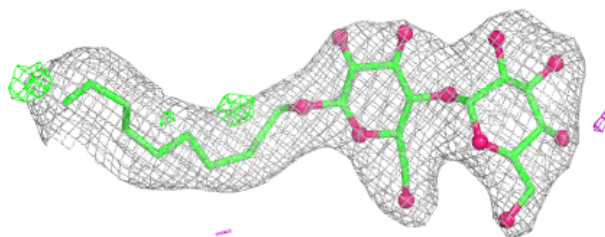
**Electron density around PEK G 102:**

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

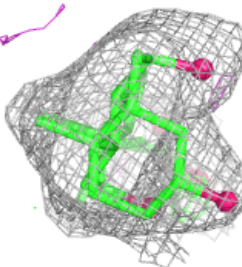
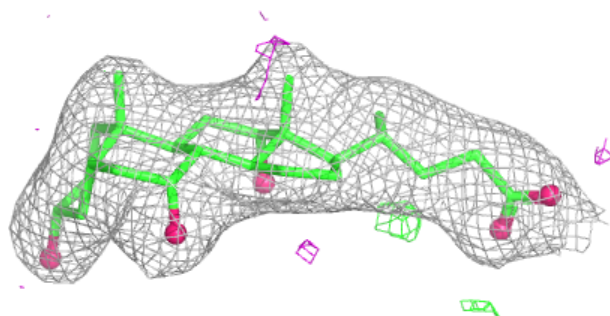
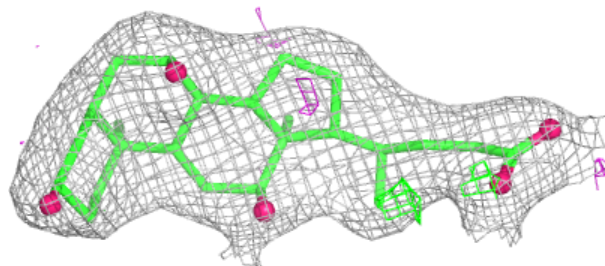


Electron density around DMU M 101:

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

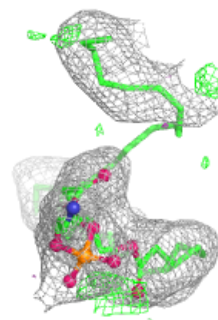
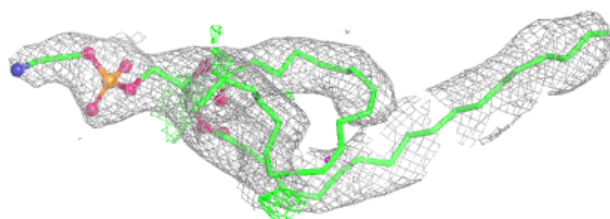
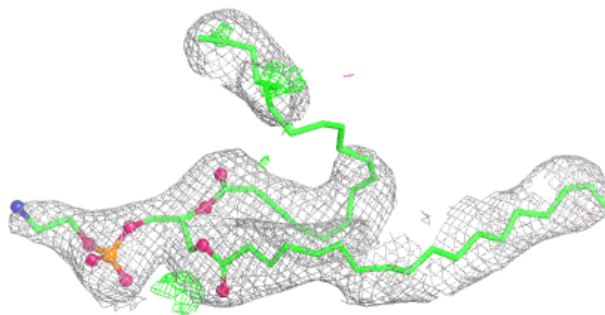
**Electron density around CHD C 301:**

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

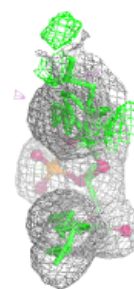
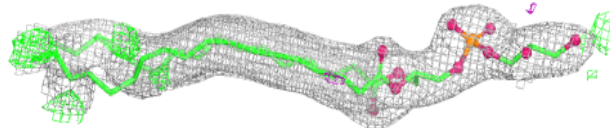
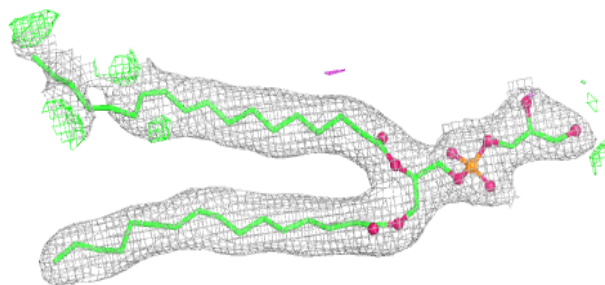


Electron density around PEK P 302:

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

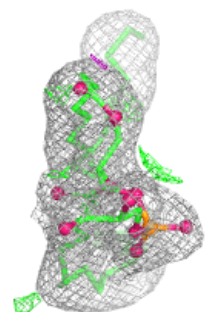
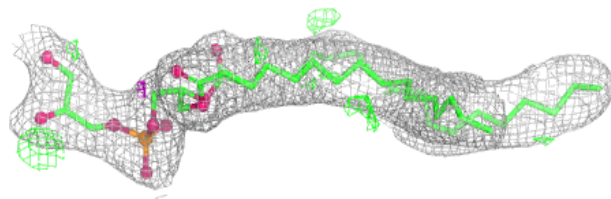
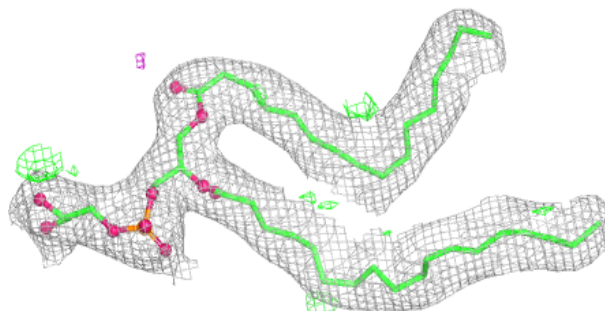
**Electron density around PGV P 304:**

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

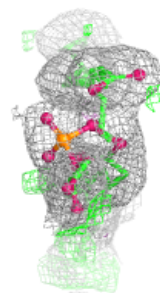
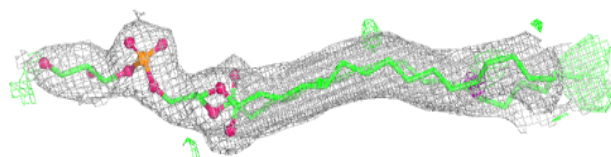
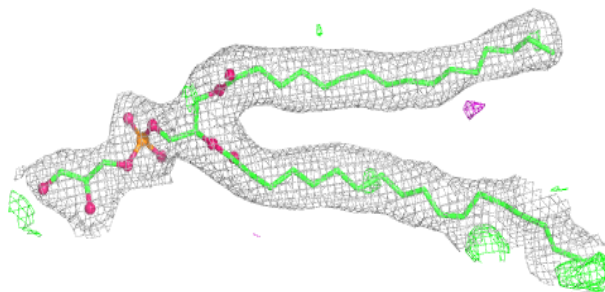


Electron density around PGV N 608:

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

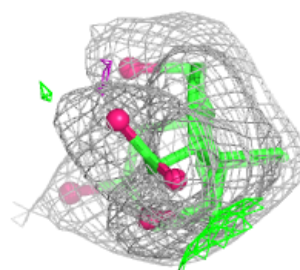
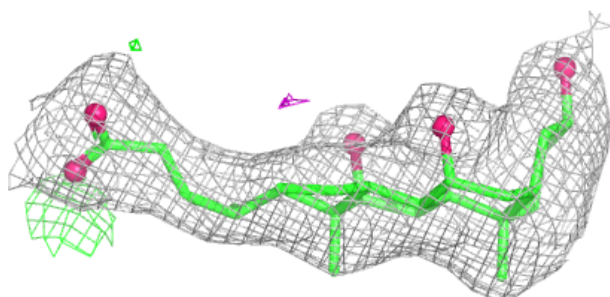
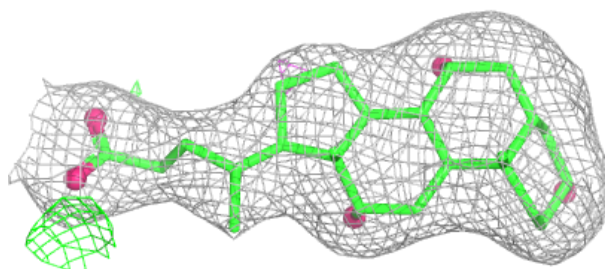
**Electron density around PGV C 303:**

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

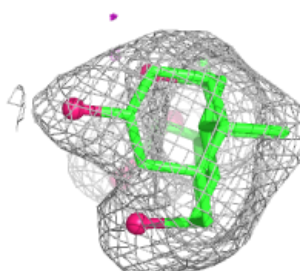
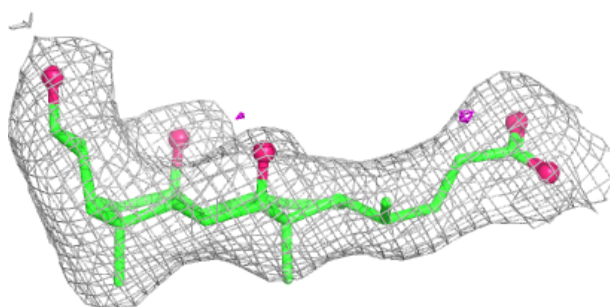
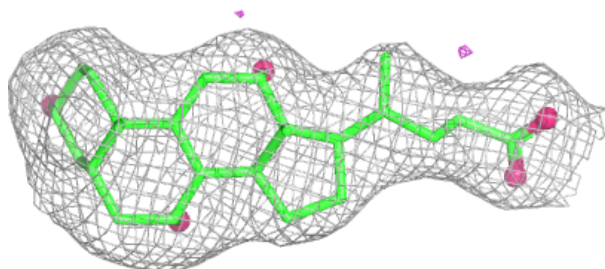


Electron density around CHD G 104:

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

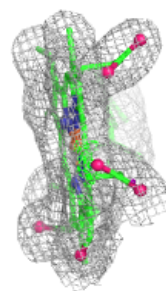
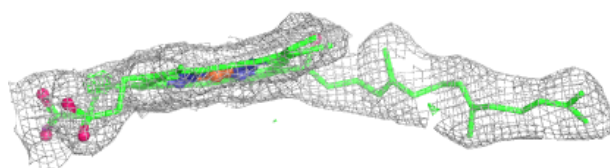
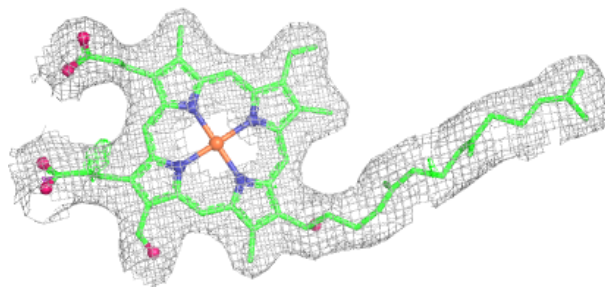
**Electron density around CHD B 304:**

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

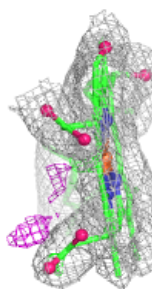
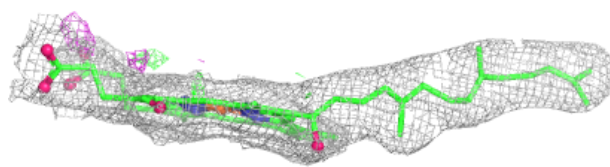
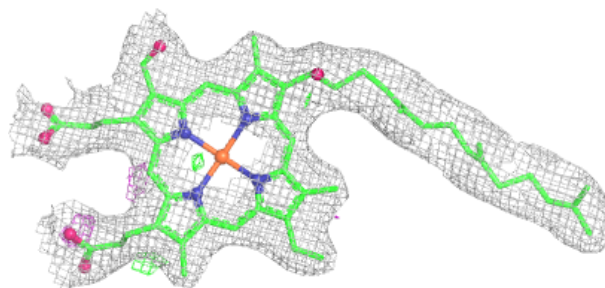


Electron density around HEA A 604:

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

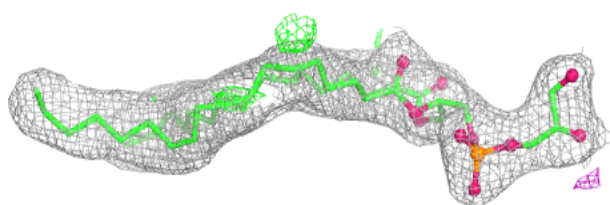
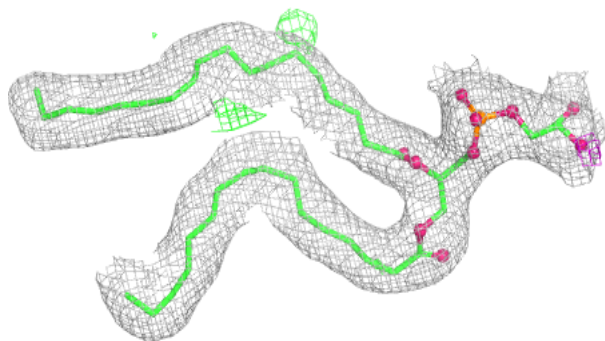
**Electron density around HEA N 605:**

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

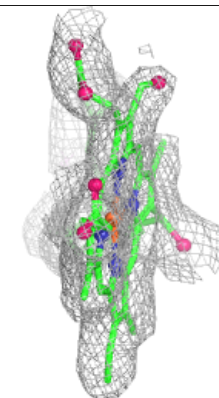
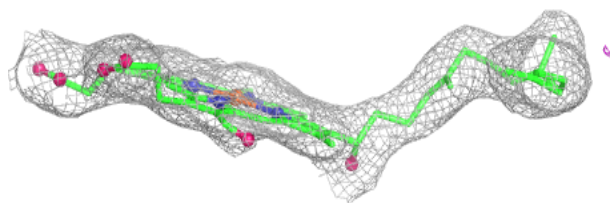
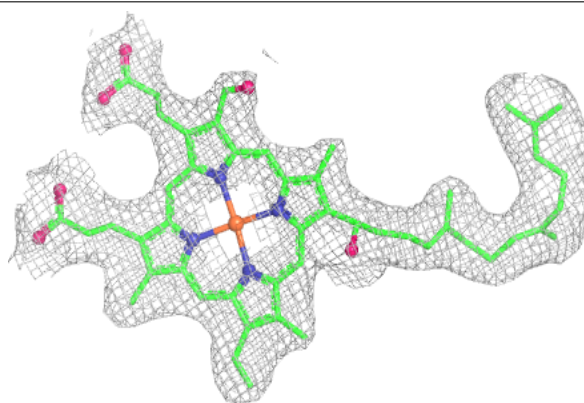


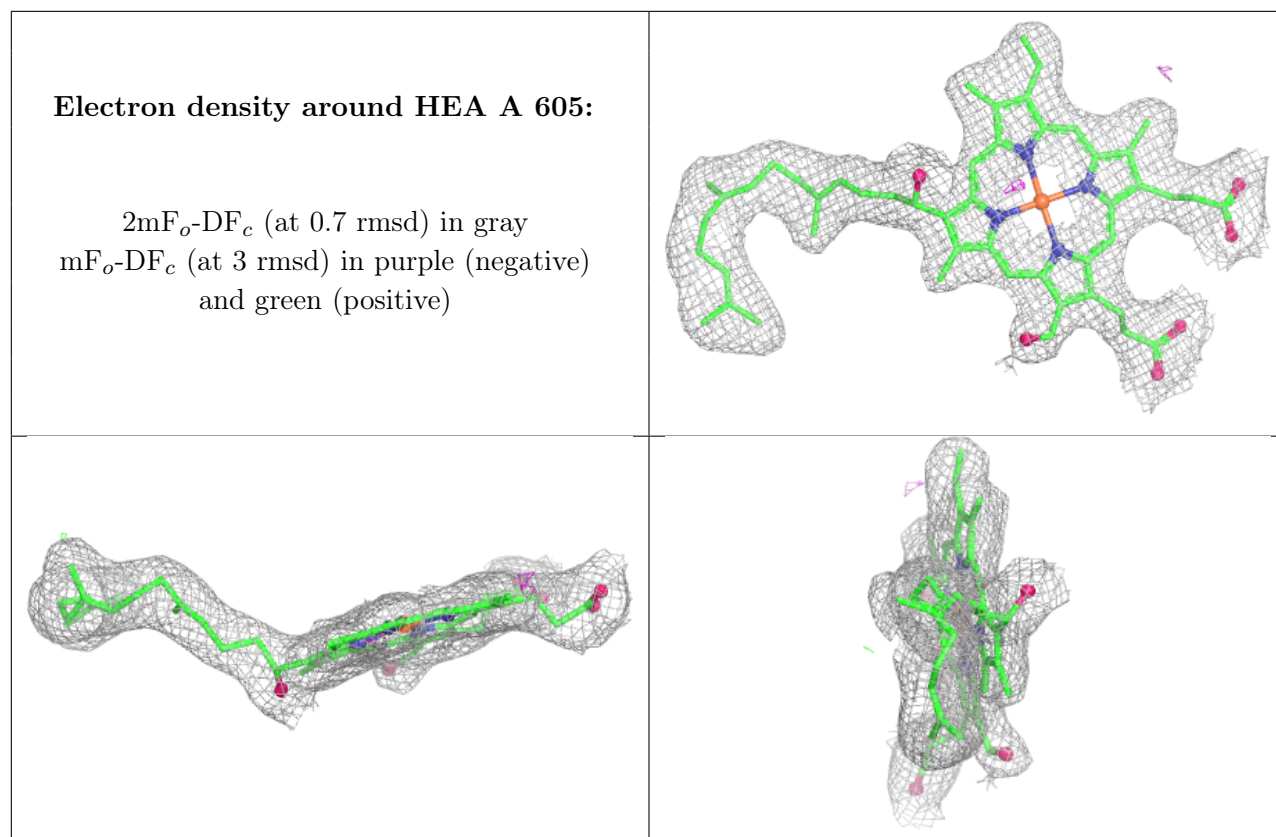
Electron density around PGV A 607:

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

**Electron density around HEA N 606:**

$2mF_o-DF_c$ (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.