



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:55 pm BST

PDB ID : 6NMF
Title : SFX structure of reduced cytochrome c oxidase at room temperature
Authors : Rousseau, D.L.; Yeh, S.-R.; Ishigami, I.
Deposited on : 2019-01-10
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

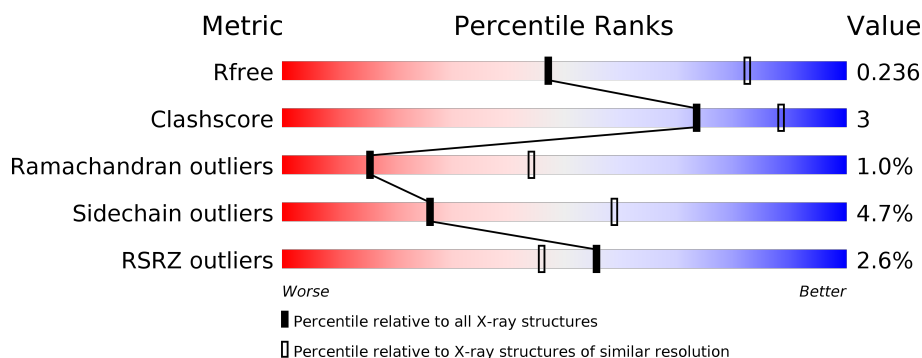
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



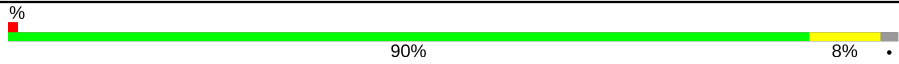

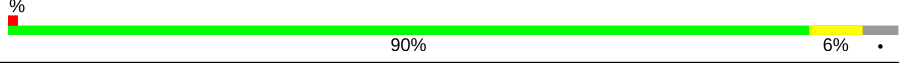
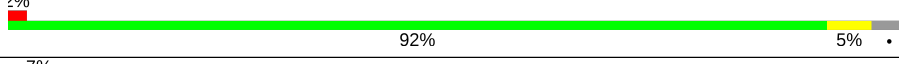


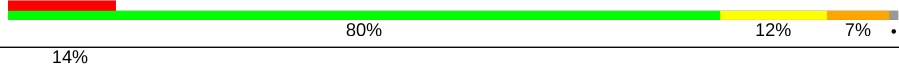

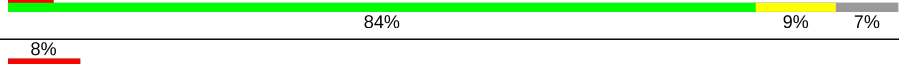

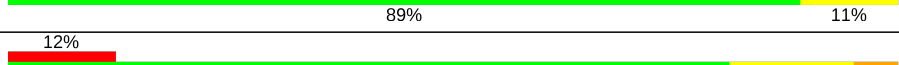
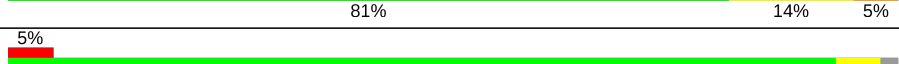
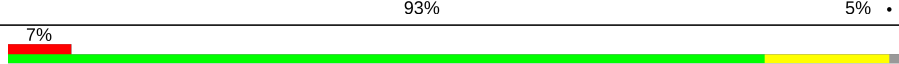
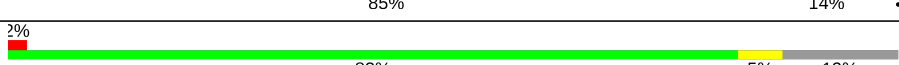

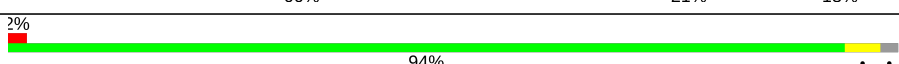
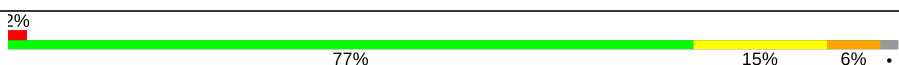
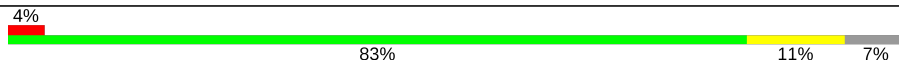
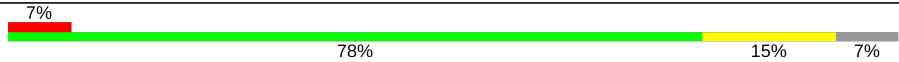

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>93%</div> <div>7%</div> </div>
1	N	514	<div> <div>89%</div> <div>11%</div> </div>
2	B	227	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	O	227	<div> <div>%</div> <div>84%</div> <div>15%</div> </div>
3	C	261	<div> <div>95%</div> <div>5%</div> <div>.</div> </div>
3	P	261	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
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
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-
14	HEA	N	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
20	CDL	P	305	-	-	X	-
22	CHD	W	101	-	-	-	X
24	DMU	C	301	-	-	-	X
24	DMU	P	303	-	-	-	X
25	PEK	G	103	-	-	-	X
25	PEK	T	101	-	-	-	X
7	TPO	G	11	-	-	-	X
7	TPO	T	11	-	-	-	X
9	SAC	I	1	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 32083 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	12	0
			4124	2753	638	693	40			
1	N	514	Total	C	N	O	S	0	13	0
			4131	2757	639	694	41			

- 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	6	0
			1874	1216	289	350	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	289	348	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	8	0
			2174	1451	345	364	14			
3	P	259	Total	C	N	O	S	0	8	0
			2173	1451	344	363	15			

- 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	6	0
			1249	814	206	224	5			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	197	219	5			

- 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	1	0
			863	550	148	163	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	5	0
			789	489	142	152	6			
6	S	98	Total	C	N	O	S	0	1	0
			755	468	135	147	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 706	C 454	N 133	O 117	P 1	S 1	0	3	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	1	0
			609	395	108	101	5			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	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	1	0
			391	255	66	68	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

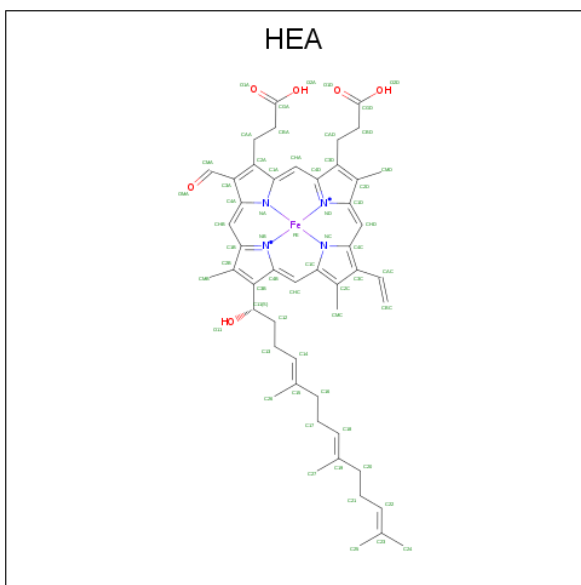
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

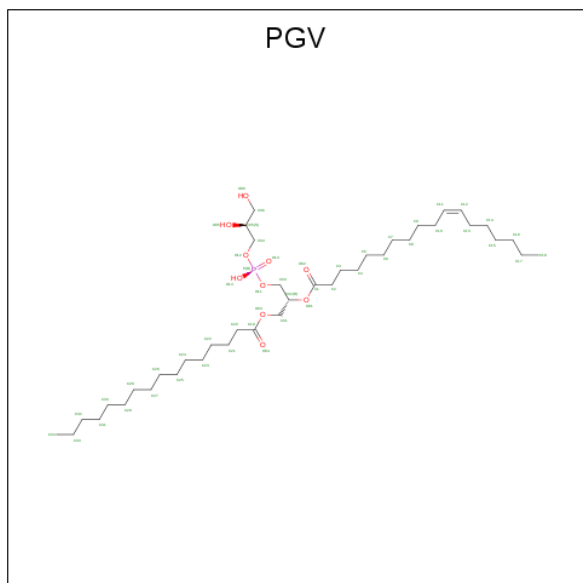
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

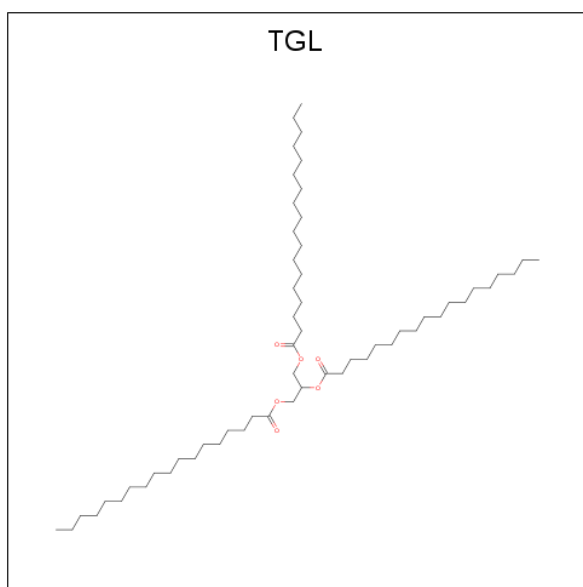
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

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



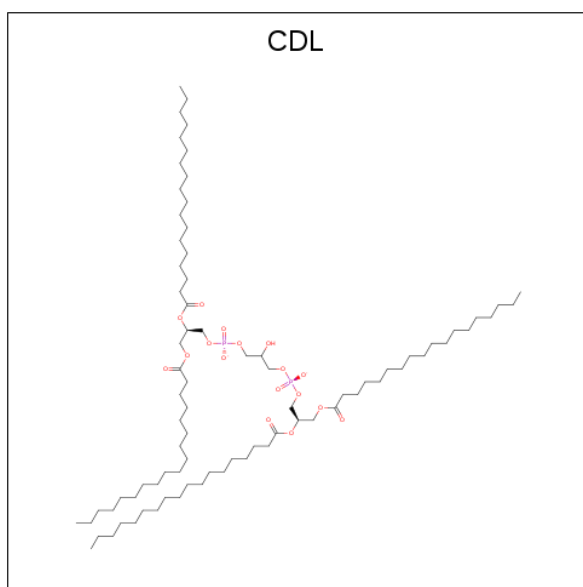
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



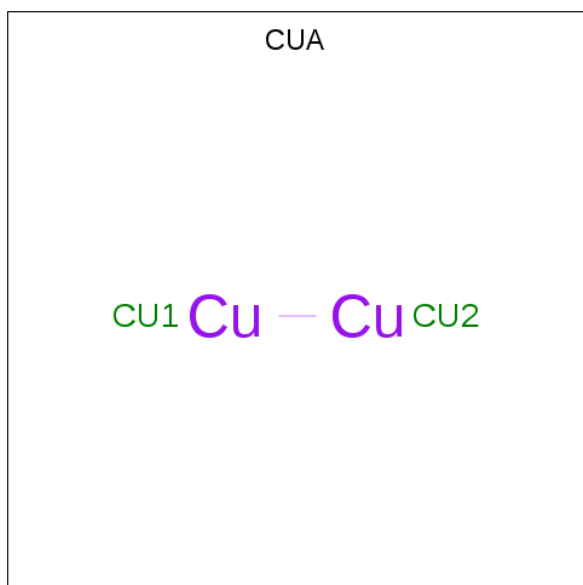
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	B	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	V	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



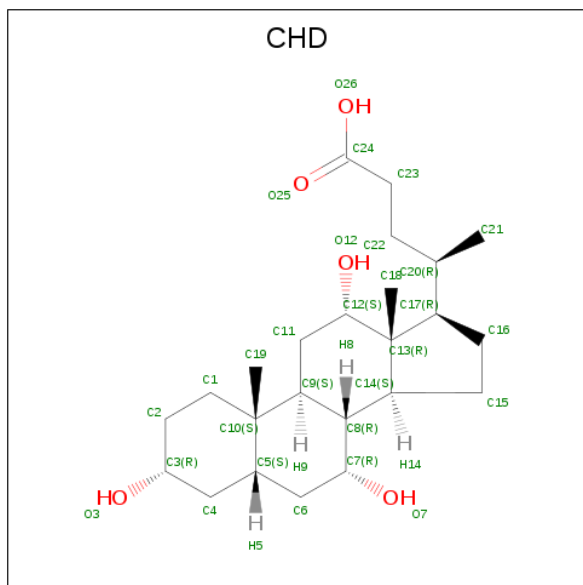
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			100	81	17	2		
20	C	1	Total	C	O	P	0	0
			100	81	17	2		
20	G	1	Total	C	O	P	0	0
			100	81	17	2		
20	P	1	Total	C	O	P	0	0
			100	81	17	2		

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



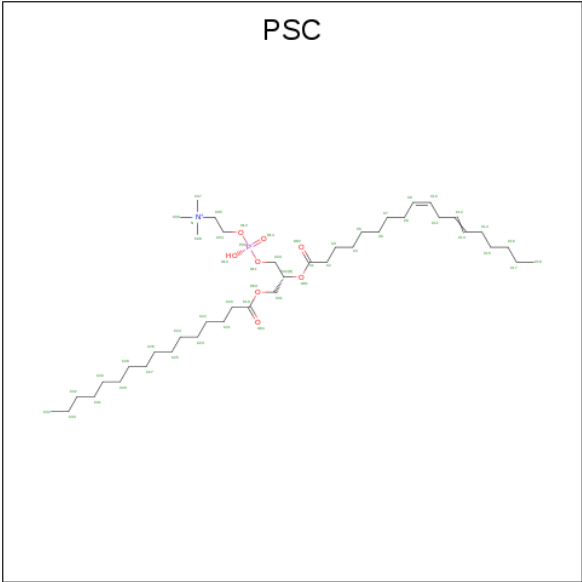
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	O	1	Total Cu 2 2	0	0

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



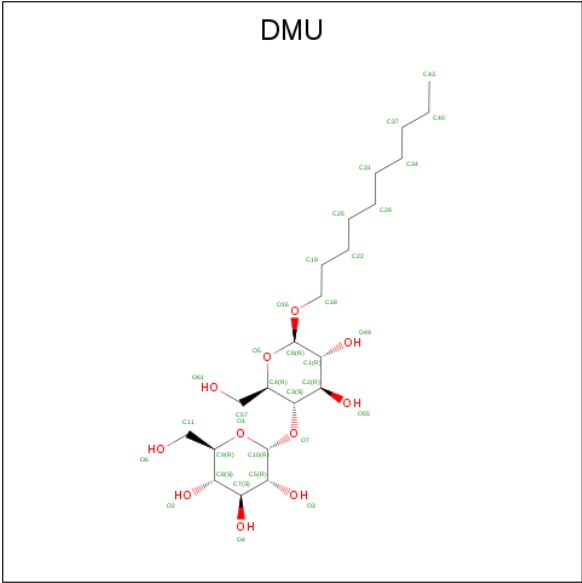
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	G	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- 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 (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



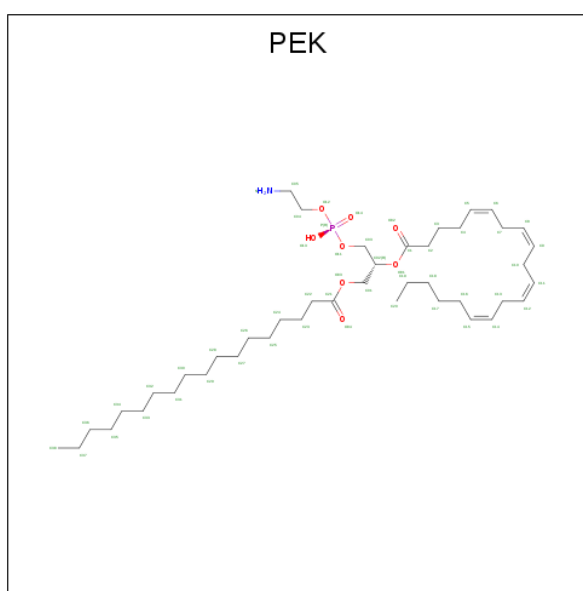
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Q	1	Total	C	O	0	0
			33	22	11		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	123	Total 123	O 123	0	0
27	B	74	Total 74	O 74	0	0
27	C	57	Total 57	O 57	0	0
27	D	32	Total 32	O 32	0	0
27	E	28	Total 28	O 28	0	0
27	F	28	Total 28	O 28	0	0
27	G	24	Total 24	O 24	0	0
27	H	21	Total 21	O 21	0	0
27	I	20	Total 20	O 20	0	0
27	J	11	Total 11	O 11	0	0
27	K	2	Total 2	O 2	0	0
27	L	24	Total 24	O 24	0	0
27	M	4	Total 4	O 4	0	0
27	N	83	Total 83	O 83	0	0
27	O	52	Total 52	O 52	0	0
27	P	39	Total 39	O 39	0	0
27	Q	22	Total 22	O 22	0	0
27	R	14	Total 14	O 14	0	0

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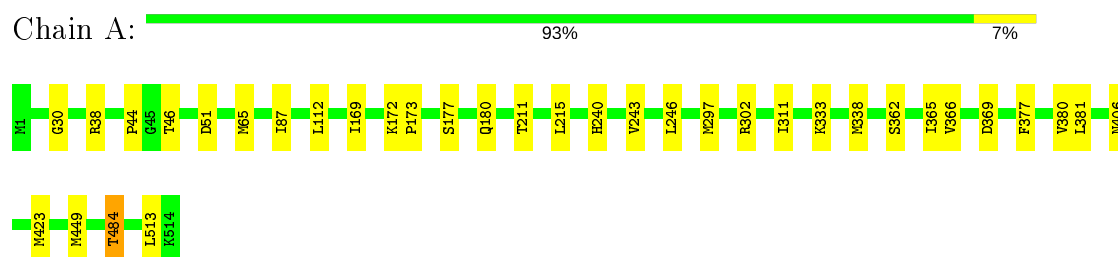
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	S	21	Total 21	O 21	0	0
27	T	20	Total 20	O 20	0	0
27	U	13	Total 13	O 13	0	0
27	V	16	Total 16	O 16	0	0
27	W	5	Total 5	O 5	0	0
27	X	5	Total 5	O 5	0	0
27	Y	2	Total 2	O 2	0	0
27	Z	4	Total 4	O 4	0	0

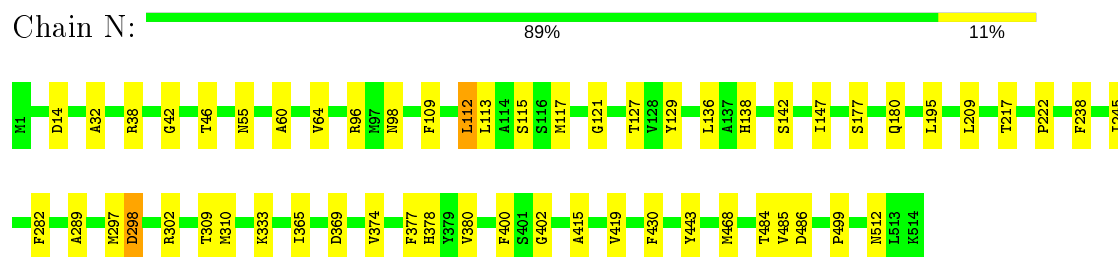
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

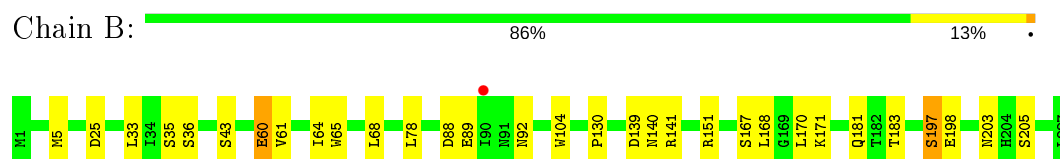
• Molecule 1: Cytochrome c oxidase subunit 1



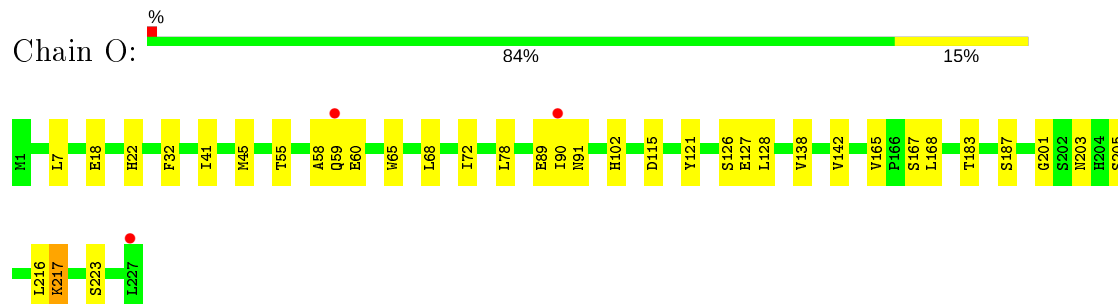
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2




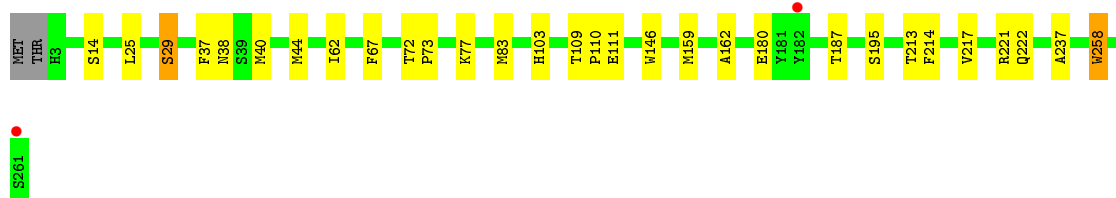
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C:  95% 5% .




- Molecule 3: Cytochrome c oxidase subunit 3

Chain P:  88% 11% ..




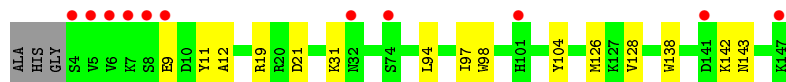
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:  90% 8% .




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

Chain Q:  88% 10% .




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

Chain E:  90% 6% .

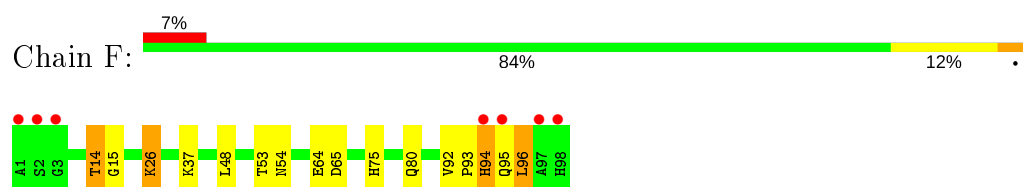


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

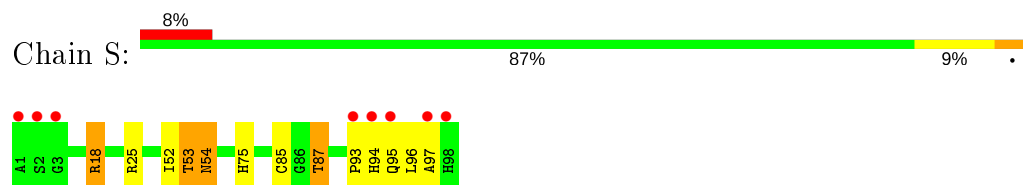
Chain R:  92% 5% .



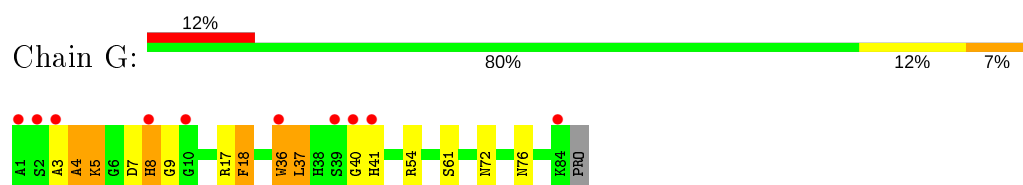
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



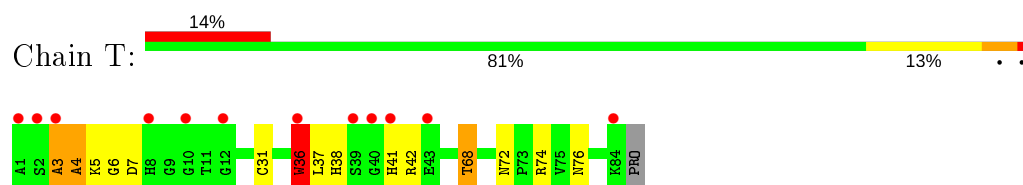
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



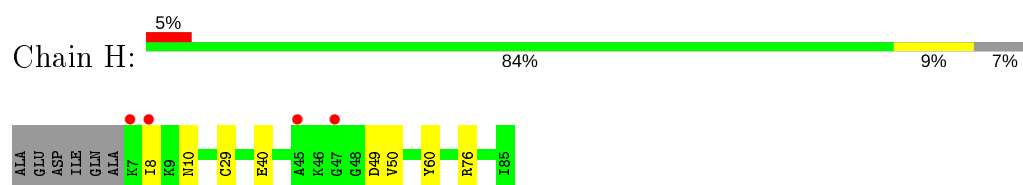
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



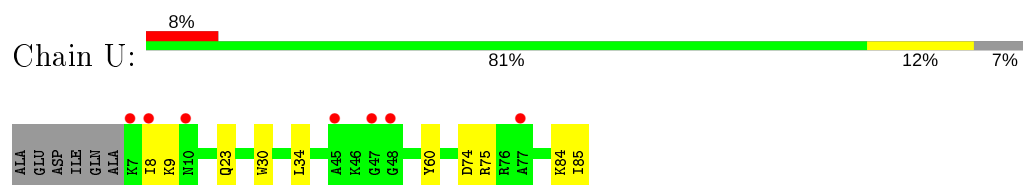
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



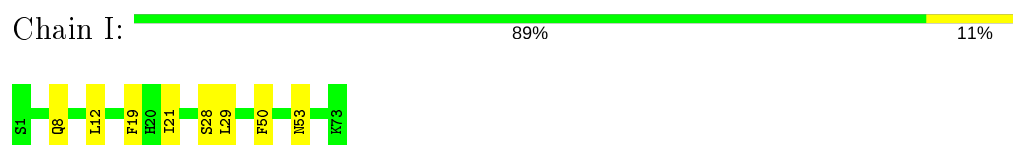
- Molecule 8: Cytochrome c oxidase subunit 6B1



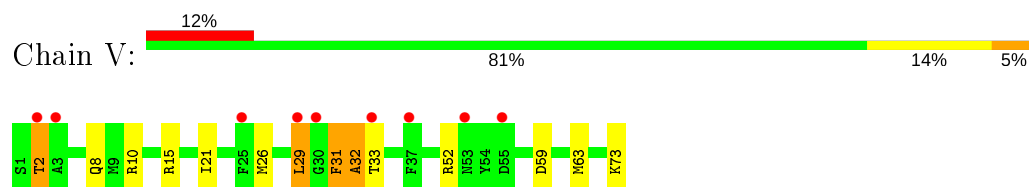
- Molecule 8: Cytochrome c oxidase subunit 6B1



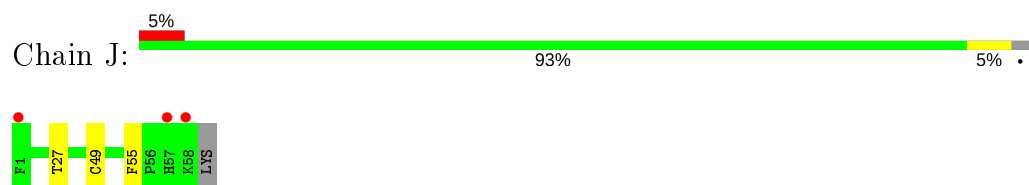
- Molecule 9: Cytochrome c oxidase subunit 6C



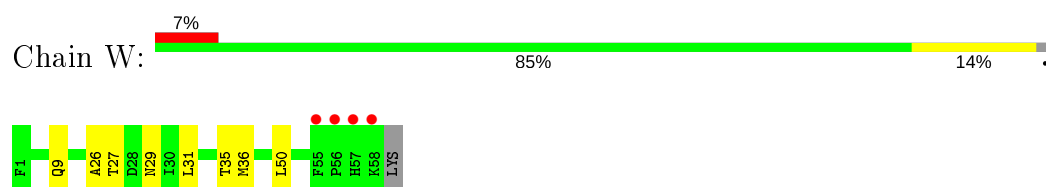
- Molecule 9: Cytochrome c oxidase subunit 6C



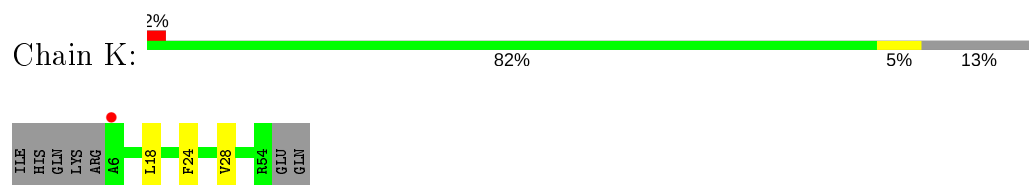
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



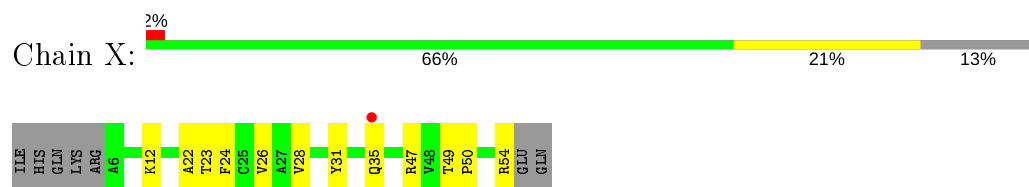
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



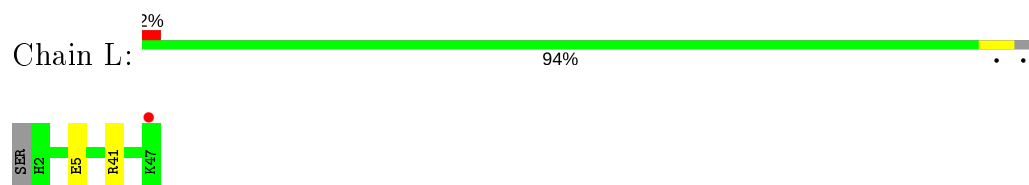
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



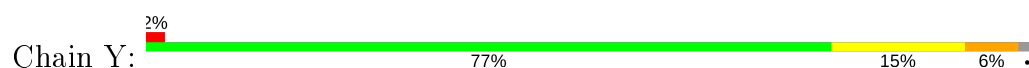
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

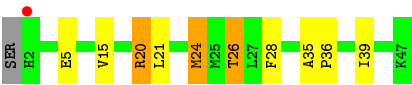


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

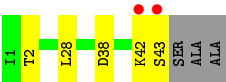
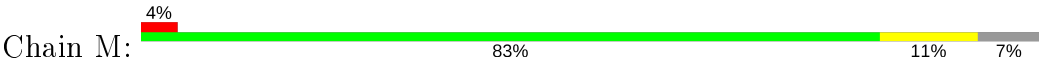


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

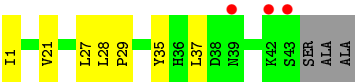
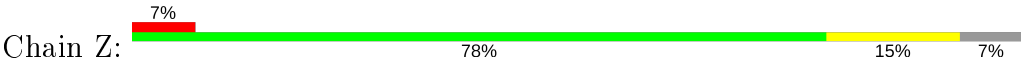




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.70 Å 189.80 Å 211.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (15.00-2.80) 100.0 (15.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.176 , 0.232 0.186 , 0.236	Depositor DCC
R_{free} test set	8641 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32083	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: ZN, TPO, CHD, TGL, CDL, PSC, PEK, MG, PGV, SAC, DMU, CUA, NA, FME, CU, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.56	0/4253	0.71	1/5805 (0.0%)
1	N	0.57	0/4260	0.73	2/5814 (0.0%)
2	B	0.60	2/1912 (0.1%)	0.84	2/2603 (0.1%)
2	O	0.58	0/1908	0.78	0/2599
3	C	0.55	0/2261	0.67	0/3090
3	P	0.57	0/2260	0.70	0/3088
4	D	0.54	0/1284	0.73	1/1730 (0.1%)
4	Q	0.53	0/1237	0.69	0/1668
5	E	0.51	0/882	0.74	0/1196
5	R	0.49	0/871	0.72	1/1182 (0.1%)
6	F	0.60	0/806	0.83	0/1093
6	S	0.55	0/772	0.79	1/1048 (0.1%)
7	G	0.63	1/702 (0.1%)	0.75	0/953
7	T	0.69	2/724 (0.3%)	0.83	0/984
8	H	0.56	0/682	0.75	0/921
8	U	0.55	0/682	0.74	0/921
9	I	0.61	0/605	0.82	0/802
9	V	0.64	0/613	0.87	2/812 (0.2%)
10	J	0.51	0/471	0.69	0/636
10	W	0.54	0/471	0.69	0/636
11	K	0.61	0/405	0.67	0/556
11	X	0.61	0/405	0.69	0/556
12	L	0.59	0/393	0.75	1/526 (0.2%)
12	Y	0.58	0/393	0.72	0/526
13	M	0.56	0/345	0.72	0/470
13	Z	0.51	0/345	0.66	0/470
All	All	0.57	5/29942 (0.0%)	0.74	11/40685 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	1
6	F	0	1
6	S	0	1
7	T	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	36[A]	TRP	CB-CG	7.10	1.63	1.50
7	T	36[B]	TRP	CB-CG	7.10	1.63	1.50
2	B	198	GLU	C-O	6.27	1.35	1.23
7	G	36	TRP	CB-CG	5.88	1.60	1.50
2	B	197	SER	CB-OG	5.11	1.48	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	96	ARG	NE-CZ-NH2	-5.86	117.37	120.30
6	S	18	ARG	NE-CZ-NH1	5.69	123.14	120.30
9	V	10	ARG	NE-CZ-NH2	-5.63	117.48	120.30
4	D	20	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	B	141	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	B	25	ASP	CB-CG-OD1	5.34	123.11	118.30
12	L	41	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	38	ARG	NE-CZ-NH1	5.24	122.92	120.30
9	V	10	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	N	14	ASP	CB-CG-OD2	-5.08	113.73	118.30
5	R	14	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
2	O	91	ASN	Peptide
6	S	94	HIS	Peptide
7	T	6	GLY	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	4124	0	4102	17	0
1	N	4131	0	4107	30	0
2	B	1874	0	1869	12	0
2	O	1870	0	1867	13	0
3	C	2174	0	2082	6	0
3	P	2173	0	2083	25	0
4	D	1249	0	1242	9	0
4	Q	1203	0	1191	9	0
5	E	863	0	857	2	0
5	R	852	0	845	1	0
6	F	789	0	769	9	0
6	S	755	0	734	7	0
7	G	686	0	651	8	0
7	T	706	0	664	9	0
8	H	662	0	623	2	0
8	U	662	0	623	4	0
9	I	601	0	613	4	0
9	V	609	0	621	6	0
10	J	460	0	459	1	0
10	W	460	0	459	4	0
11	K	391	0	374	2	0
11	X	391	0	374	4	0
12	L	380	0	380	0	0
12	Y	380	0	380	6	0
13	M	335	0	352	2	0
13	Z	335	0	352	5	0
14	A	120	0	108	2	0
14	N	120	0	108	4	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	102	0	152	1	0
18	C	102	0	152	0	0
18	N	51	0	76	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	P	153	0	228	6	0
19	A	63	0	110	2	0
19	B	63	0	110	0	0
19	D	63	0	110	0	0
19	N	63	0	110	0	0
19	V	63	0	110	3	0
19	Y	63	0	110	1	0
20	A	100	0	156	5	0
20	C	100	0	156	0	0
20	G	100	0	156	4	0
20	P	100	0	156	22	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	0	0
22	G	29	0	39	1	0
22	J	29	0	39	2	0
22	P	58	0	78	1	0
22	W	29	0	38	1	0
23	B	52	0	80	0	0
23	N	52	0	80	0	0
24	C	33	0	42	2	0
24	M	33	0	42	0	0
24	P	33	0	42	1	0
24	Q	33	0	42	3	0
25	C	53	0	77	1	0
25	G	106	0	154	1	0
25	P	106	0	154	3	0
25	T	53	0	77	0	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	A	123	0	0	6	0
27	B	74	0	0	2	0
27	C	57	0	0	3	0
27	D	32	0	0	1	0
27	E	28	0	0	0	0
27	F	28	0	0	1	0
27	G	24	0	0	1	0
27	H	21	0	0	1	0
27	I	20	0	0	1	0
27	J	11	0	0	2	0
27	K	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	L	24	0	0	2	0
27	M	4	0	0	1	0
27	N	83	0	0	0	0
27	O	52	0	0	4	0
27	P	39	0	0	6	0
27	Q	22	0	0	2	0
27	R	14	0	0	0	0
27	S	21	0	0	1	0
27	T	20	0	0	0	0
27	U	13	0	0	1	0
27	V	16	0	0	6	0
27	W	5	0	0	2	0
27	X	5	0	0	0	0
27	Y	2	0	0	0	0
27	Z	4	0	0	0	0
All	All	32083	0	31882	208	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (208) 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)
20:P:305:CDL:H641	20:P:305:CDL:H531	1.21	1.14
1:A:65:MET:SD	27:A:811:HOH:O	2.24	0.95
3:P:258:TRP:CG	27:P:424:HOH:O	2.26	0.89
20:P:305:CDL:C64	20:P:305:CDL:H531	2.02	0.88
1:A:423:MET:SD	27:A:804:HOH:O	2.30	0.87
6:F:92[A]:VAL:HG23	6:F:92[A]:VAL:O	1.74	0.86
6:F:92[B]:VAL:HG12	6:F:92[B]:VAL:O	1.75	0.86
1:N:113[B]:LEU:HD12	1:N:113[B]:LEU:O	1.78	0.84
3:P:62:ILE:HD11	20:P:305:CDL:H662	1.65	0.78
20:P:305:CDL:H641	20:P:305:CDL:C53	2.09	0.77
3:P:221:ARG:HD2	20:P:305:CDL:H673	1.68	0.76
19:V:101:TGL:HG11	27:V:212:HOH:O	1.86	0.75
2:O:18[A]:GLU:OE2	2:O:22[A]:HIS:NE2	2.19	0.74
20:P:305:CDL:H622	20:P:305:CDL:H551	1.66	0.74
19:V:101:TGL:CC1	27:V:204:HOH:O	2.35	0.74
1:N:113[B]:LEU:C	1:N:113[B]:LEU:HD12	2.08	0.74
4:Q:19:ARG:NH2	27:Q:301:HOH:O	2.19	0.74
3:P:221:ARG:CD	20:P:305:CDL:H673	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131[A]:ILE:HD12	4:D:131[A]:ILE:N	2.06	0.71
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.71	0.71
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.74	0.70
6:F:75:HIS:H	6:F:80[B]:GLN:HE22	1.36	0.70
4:D:131[A]:ILE:HD12	4:D:131[A]:ILE:H	1.56	0.69
6:S:54:ASN:HD22	6:S:54:ASN:C	1.96	0.68
10:W:36:MET:HB2	27:W:202:HOH:O	1.93	0.67
18:P:304:PGV:C3	20:P:305:CDL:H651	2.26	0.65
3:P:258:TRP:CD2	27:P:424:HOH:O	2.47	0.64
14:N:601:HEA:HMC1	14:N:601:HEA:HBC1	1.80	0.64
4:Q:19:ARG:NH1	4:Q:21:ASP:OD2	2.30	0.64
3:P:213:THR:O	3:P:217:VAL:HG23	1.98	0.63
25:C:302:PEK:HN2	7:G:76:ASN:HD21	1.47	0.63
3:C:232:HIS:NE2	27:C:401:HOH:O	2.30	0.62
1:N:302[B]:ARG:NH2	8:U:23:GLN:HE21	1.98	0.62
18:P:304:PGV:H31	20:P:305:CDL:H651	1.83	0.60
7:G:72:ASN:H	7:G:76:ASN:HD22	1.49	0.59
19:V:101:TGL:CG1	27:V:212:HOH:O	2.48	0.59
22:J:101:CHD:H212	27:J:205:HOH:O	2.02	0.59
3:C:3:HIS:N	27:C:402:HOH:O	2.37	0.58
2:O:165:VAL:HG11	2:O:168:LEU:HD12	1.86	0.58
1:N:60:ALA:O	1:N:64:VAL:HG23	2.04	0.58
2:B:33:LEU:HD12	9:I:28:SER:HB3	1.86	0.58
1:N:289:ALA:HB1	1:N:297[A]:MET:HE1	1.86	0.58
20:P:305:CDL:H622	20:P:305:CDL:C55	2.34	0.57
2:B:170:LEU:HD13	27:B:469:HOH:O	2.05	0.57
10:W:26:ALA:HA	10:W:29:ASN:HD22	1.69	0.57
2:O:187:SER:HA	27:O:433:HOH:O	2.04	0.57
1:N:298[A]:ASP:OD1	1:N:298[A]:ASP:N	2.38	0.57
4:Q:19:ARG:CZ	27:Q:301:HOH:O	2.53	0.56
20:P:305:CDL:H601	20:P:305:CDL:C55	2.35	0.56
24:C:301:DMU:H10	10:J:49:CYS:HB3	1.87	0.56
2:O:72:ILE:HG22	27:O:440:HOH:O	2.05	0.56
1:N:309:THR:CG2	14:N:602:HEA:HMB2	2.36	0.56
3:P:258:TRP:CD1	27:P:424:HOH:O	2.55	0.56
14:A:601:HEA:HBC1	14:A:601:HEA:HMC1	1.88	0.56
18:P:304:PGV:H52	20:P:305:CDL:C65	2.35	0.56
5:E:78:HIS:CD2	9:I:12:LEU:HD22	2.40	0.56
1:N:400:PHE:HB3	19:Y:101:TGL:H283	1.86	0.56
18:P:304:PGV:H52	20:P:305:CDL:H651	1.87	0.56
3:P:237:ALA:HB1	27:P:426:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLY:HA3	27:A:811:HOH:O	2.06	0.55
12:Y:26:THR:HG21	13:Z:21:VAL:HG12	1.88	0.55
2:O:142:VAL:HG13	27:O:418:HOH:O	2.07	0.55
12:Y:15:VAL:HG12	12:Y:21:LEU:HD22	1.86	0.55
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.42	0.55
7:T:36[B]:TRP:O	7:T:36[B]:TRP:CG	2.60	0.55
3:P:217:VAL:HG11	20:P:305:CDL:H652	1.88	0.55
2:B:139:ASP:OD1	2:B:140:ASN:N	2.39	0.54
1:N:127:THR:HB	1:N:129:TYR:CD1	2.41	0.54
13:M:28:LEU:HG	27:M:204:HOH:O	2.07	0.54
3:P:187:THR:HB	7:T:68:THR:HG21	1.89	0.54
10:W:31:LEU:O	10:W:35:THR:OG1	2.22	0.54
25:P:308:PEK:HN2	7:T:76:ASN:HD21	1.55	0.54
3:P:221:ARG:HD3	20:P:305:CDL:H673	1.88	0.54
20:P:305:CDL:C64	20:P:305:CDL:C53	2.75	0.54
6:F:92[A]:VAL:CG2	6:F:92[A]:VAL:O	2.46	0.53
20:A:609:CDL:H532	7:T:31:CYS:SG	2.48	0.53
7:T:72:ASN:H	7:T:76:ASN:HD22	1.56	0.52
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.89	0.52
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.92	0.52
9:V:32:ALA:O	27:V:201:HOH:O	2.19	0.52
3:P:217:VAL:HG11	20:P:305:CDL:C65	2.40	0.52
20:A:609:CDL:H322	20:A:609:CDL:OA7	2.10	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HD3	2.44	0.51
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	1.92	0.51
8:U:30:TRP:CE2	8:U:34:LEU:HD11	2.45	0.51
1:A:297[A]:MET:HE3	27:A:799:HOH:O	2.11	0.50
4:D:71:MET:SD	27:D:330:HOH:O	2.59	0.50
6:S:25:ARG:NH1	27:S:202:HOH:O	2.44	0.50
25:P:308:PEK:C05	7:T:76:ASN:HD21	2.25	0.50
20:A:609:CDL:OA7	20:A:609:CDL:C32	2.60	0.50
22:J:101:CHD:C21	27:J:205:HOH:O	2.56	0.50
1:N:147:ILE:HD11	1:N:209:LEU:HD23	1.94	0.50
4:Q:94:LEU:HA	4:Q:97:ILE:HD12	1.93	0.50
6:F:94:HIS:O	6:F:96:LEU:HD12	2.11	0.49
20:G:102:CDL:C78	20:G:102:CDL:H561	2.43	0.49
2:O:58:ALA:O	2:O:60:GLU:N	2.45	0.49
9:V:59:ASP:O	9:V:63[B]:MET:HG3	2.12	0.49
3:C:161[B]:GLN:NE2	27:C:403:HOH:O	2.45	0.49
9:V:32:ALA:O	9:V:33:THR:C	2.51	0.49
2:B:151:ARG:HE	2:B:181:GLN:NE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.95	0.49
6:S:53:THR:OG1	6:S:54:ASN:N	2.39	0.49
1:N:55:ASN:ND2	2:O:201:GLY:O	2.45	0.48
19:A:608:TGL:HC21	27:L:109:HOH:O	2.12	0.48
3:P:62:ILE:HD11	20:P:305:CDL:C66	2.40	0.48
9:V:8:GLN:HG2	9:V:15:ARG:NH2	2.28	0.48
6:F:92[B]:VAL:O	6:F:92[B]:VAL:CG1	2.47	0.48
1:A:366:VAL:HB	27:A:714:HOH:O	2.13	0.48
1:A:377:PHE:HA	1:A:380:VAL:HG12	1.96	0.48
1:N:430:PHE:CE1	2:O:7:LEU:HD22	2.49	0.48
2:O:126:SER:O	2:O:128:LEU:N	2.47	0.47
8:H:10:ASN:N	27:H:101:HOH:O	2.39	0.47
1:N:402:GLY:CA	1:N:499:PRO:HD3	2.44	0.47
20:P:305:CDL:C62	20:P:305:CDL:H551	2.39	0.47
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.97	0.47
19:A:608:TGL:CC2	27:L:109:HOH:O	2.63	0.47
2:O:41:ILE:O	2:O:45:MET:HG2	2.14	0.47
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.50	0.47
22:G:104:CHD:H212	22:G:104:CHD:H12	1.96	0.47
9:V:31:PHE:CD2	27:V:205:HOH:O	2.67	0.47
3:P:40[B]:MET:O	3:P:44[B]:MET:HG3	2.15	0.47
4:D:131[A]:ILE:N	4:D:131[A]:ILE:CD1	2.77	0.46
1:A:240:HIS:O	1:A:243:VAL:HG22	2.16	0.46
4:D:131[B]:ILE:HD13	9:I:50:PHE:CG	2.51	0.46
4:Q:12:ALA:O	6:S:75:HIS:NE2	2.35	0.46
3:C:33:MET:SD	24:C:301:DMU:H8	2.55	0.46
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.50	0.46
2:O:32[B]:PHE:HD1	2:O:32[B]:PHE:O	1.99	0.46
6:S:95:GLN:O	6:S:97:ALA:N	2.49	0.46
1:N:222:PRO:O	3:P:111:GLU:OE2	2.33	0.46
1:N:302[A]:ARG:NH2	1:N:365:ILE:HD11	2.31	0.45
11:X:22:ALA:O	11:X:26:VAL:HG23	2.16	0.45
20:G:102:CDL:H782	20:G:102:CDL:H561	1.98	0.45
3:P:222:GLN:CD	27:P:419:HOH:O	2.55	0.45
1:A:169:ILE:O	1:A:172:LYS:NZ	2.49	0.45
1:N:127:THR:HB	1:N:129:TYR:CE1	2.51	0.45
1:A:211:THR:HG22	1:A:215:LEU:HD12	1.99	0.45
1:A:377:PHE:O	1:A:381:LEU:HB3	2.17	0.45
24:Q:201:DMU:H14	13:Z:27:LEU:HD22	1.98	0.45
1:A:406:ASN:HD21	18:A:607:PGV:H22	1.82	0.45
1:N:113[B]:LEU:HD13	12:Y:39:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131[A]:ILE:H	4:D:131[A]:ILE:CD1	2.26	0.45
4:D:33:LEU:HA	4:D:37:GLN:HE21	1.82	0.45
1:A:87:ILE:O	1:A:173:PRO:HD3	2.17	0.45
2:O:217:LYS:HB2	27:O:452:HOH:O	2.16	0.45
3:P:37:PHE:CD1	24:P:303:DMU:H10	2.52	0.44
6:S:85:CYS:SG	6:S:87[B]:THR:HG22	2.57	0.44
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.52	0.44
1:A:484:THR:HB	13:M:2:THR:OG1	2.16	0.44
18:P:304:PGV:C4	20:P:305:CDL:H651	2.47	0.44
2:B:92:ASN:N	2:B:92:ASN:HD22	2.16	0.44
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.99	0.44
1:N:177:SER:H	1:N:180:GLN:NE2	2.16	0.44
11:K:24:PHE:O	11:K:28[A]:VAL:HG12	2.18	0.44
13:Z:1:ILE:O	13:Z:1:ILE:HG23	2.18	0.44
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.57	0.43
2:B:168:LEU:HG	27:B:438:HOH:O	2.18	0.43
2:B:35[B]:SER:O	2:B:36[B]:SER:C	2.56	0.43
3:P:83:MET:SD	27:P:426:HOH:O	2.62	0.43
2:B:151:ARG:HE	2:B:181:GLN:HE21	1.66	0.43
12:Y:20:ARG:NH2	12:Y:24:MET:SD	2.91	0.43
7:G:18[A]:PHE:O	7:G:18[A]:PHE:HD1	2.02	0.43
20:P:305:CDL:H601	20:P:305:CDL:H552	2.00	0.43
11:X:24:PHE:CE1	11:X:28[B]:VAL:HG21	2.54	0.43
18:P:304:PGV:C5	20:P:305:CDL:H651	2.48	0.43
20:A:609:CDL:C53	7:T:31:CYS:SG	3.07	0.42
20:G:102:CDL:H591	20:G:102:CDL:H632	2.00	0.42
7:G:8:HIS:N	27:G:202:HOH:O	2.52	0.42
6:F:54[B]:ASN:ND2	27:F:201:HOH:O	2.53	0.42
7:G:37:LEU:HD23	20:G:102:CDL:H372	2.01	0.42
9:I:29:LEU:CB	27:I:120:HOH:O	2.67	0.42
3:C:151:LEU:HD21	3:C:232:HIS:CG	2.54	0.42
6:F:14:THR:OG1	6:F:15:GLY:N	2.51	0.42
8:U:85:ILE:HG23	27:U:112:HOH:O	2.19	0.42
3:P:25:LEU:O	3:P:29:SER:OG	2.35	0.42
1:A:302[B]:ARG:NH2	1:A:365:ILE:HD11	2.35	0.42
4:D:83:GLY:HA3	11:K:18:LEU:HA	2.02	0.42
1:N:415:ALA:O	1:N:419:VAL:HG23	2.20	0.42
1:N:115[A]:SER:O	1:N:121:GLY:HA2	2.20	0.41
1:N:180:GLN:HB2	1:N:180:GLN:HE21	1.60	0.41
20:A:609:CDL:HA61	27:A:820:HOH:O	2.20	0.41
3:P:103:HIS:ND1	22:P:307:CHD:O26	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:67:ILE:O	5:R:70:VAL:HG12	2.21	0.41
11:X:31:TYR:CD1	11:X:35:GLN:HG3	2.55	0.41
4:Q:98:TRP:CE2	24:Q:201:DMU:H11	2.56	0.41
1:N:113[B]:LEU:HD11	1:N:117[B]:MET:SD	2.61	0.41
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.56	0.41
1:A:44:PRO:HG2	4:D:111:PHE:CZ	2.55	0.41
8:H:40:GLU:HG3	8:H:50:VAL:HG13	2.03	0.41
1:N:112:LEU:O	1:N:115[B]:SER:HB3	2.21	0.41
1:N:378:HIS:CE1	14:N:601:HEA:NA	2.88	0.41
6:F:64:GLU:O	6:F:65:ASP:HB2	2.20	0.41
1:N:195:LEU:HD23	1:N:245:ILE:HD13	2.03	0.41
3:P:72:THR:HB	3:P:73:PRO:CD	2.51	0.41
1:A:246:LEU:HD13	1:A:381:LEU:HD11	2.02	0.41
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.56	0.41
3:P:67:PHE:HA	10:W:9:GLN:HG2	2.03	0.40
7:T:3:ALA:O	7:T:4:ALA:CB	2.68	0.40
9:V:32:ALA:HA	27:V:208:HOH:O	2.20	0.40
7:G:5:LYS:HD2	25:G:103:PEK:H381	2.03	0.40
1:N:217:THR:HB	3:P:195:SER:HB3	2.03	0.40
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.21	0.40
6:S:54:ASN:ND2	6:S:54:ASN:C	2.68	0.40
2:B:61:VAL:HA	2:B:64:ILE:HD12	2.04	0.40
24:Q:201:DMU:H36	13:Z:35:TYR:CD2	2.57	0.40
2:O:121:TYR:O	2:O:138:VAL:HA	2.22	0.40
25:P:308:PEK:O14	7:T:68:THR:HB	2.21	0.40
22:W:101:CHD:C21	27:W:204: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	524/514 (102%)	504 (96%)	20 (4%)	0	100	100
1	N	525/514 (102%)	499 (95%)	26 (5%)	0	100	100
2	B	231/227 (102%)	215 (93%)	13 (6%)	3 (1%)	12	36
2	O	230/227 (101%)	209 (91%)	17 (7%)	4 (2%)	9	29
3	C	265/261 (102%)	258 (97%)	5 (2%)	2 (1%)	19	49
3	P	265/261 (102%)	256 (97%)	8 (3%)	1 (0%)	34	66
4	D	148/147 (101%)	143 (97%)	5 (3%)	0	100	100
4	Q	143/147 (97%)	134 (94%)	8 (6%)	1 (1%)	22	53
5	E	104/109 (95%)	99 (95%)	5 (5%)	0	100	100
5	R	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
6	F	101/98 (103%)	87 (86%)	11 (11%)	3 (3%)	4	15
6	S	97/98 (99%)	91 (94%)	4 (4%)	2 (2%)	7	23
7	G	82/85 (96%)	68 (83%)	7 (8%)	7 (8%)	1	1
7	T	84/85 (99%)	70 (83%)	10 (12%)	4 (5%)	2	7
8	H	77/85 (91%)	72 (94%)	4 (5%)	1 (1%)	12	36
8	U	77/85 (91%)	72 (94%)	4 (5%)	1 (1%)	12	36
9	I	71/73 (97%)	64 (90%)	7 (10%)	0	100	100
9	V	72/73 (99%)	59 (82%)	10 (14%)	3 (4%)	3	9
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
11	K	48/56 (86%)	43 (90%)	5 (10%)	0	100	100
11	X	48/56 (86%)	43 (90%)	4 (8%)	1 (2%)	7	23
12	L	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	1 (2%)	1 (2%)	6	21
13	M	41/46 (89%)	40 (98%)	0	1 (2%)	6	20
13	Z	41/46 (89%)	37 (90%)	4 (10%)	0	100	100
All	All	3577/3614 (99%)	3351 (94%)	191 (5%)	35 (1%)	15	44

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	G	8	HIS

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Mol	Chain	Res	Type
2	O	59	GLN
2	O	89	GLU
6	S	96	LEU
7	T	3	ALA
7	T	4	ALA
7	T	7	ASP
7	T	41	HIS
9	V	32	ALA
7	G	41	HIS
2	O	127	GLU
4	Q	11	TYR
2	B	88	ASP
7	G	7	ASP
3	P	38	ASN
9	V	2	THR
2	B	60	GLU
2	B	89	GLU
6	F	26	LYS
7	G	3	ALA
9	V	29	LEU
11	X	12	LYS
3	C	128	GLU
6	F	96	LEU
8	H	8	ILE
13	M	42	LYS
2	O	90	ILE
6	S	93	PRO
12	Y	28	PHE
3	C	154	GLY
7	G	40	GLY
7	G	9	GLY
8	U	8	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/426 (103%)	425 (97%)	13 (3%)	41	75
1	N	439/426 (103%)	417 (95%)	22 (5%)	24	56
2	B	216/210 (103%)	205 (95%)	11 (5%)	24	55
2	O	215/210 (102%)	201 (94%)	14 (6%)	17	44
3	C	232/226 (103%)	228 (98%)	4 (2%)	60	87
3	P	232/226 (103%)	223 (96%)	9 (4%)	32	66
4	D	134/129 (104%)	129 (96%)	5 (4%)	34	68
4	Q	129/129 (100%)	125 (97%)	4 (3%)	40	74
5	E	93/95 (98%)	88 (95%)	5 (5%)	22	53
5	R	92/95 (97%)	90 (98%)	2 (2%)	52	83
6	F	86/81 (106%)	79 (92%)	7 (8%)	11	33
6	S	82/81 (101%)	76 (93%)	6 (7%)	14	38
7	G	68/68 (100%)	61 (90%)	7 (10%)	7	21
7	T	70/68 (103%)	62 (89%)	8 (11%)	5	18
8	H	71/75 (95%)	67 (94%)	4 (6%)	21	51
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	40
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	40
9	V	58/57 (102%)	51 (88%)	7 (12%)	5	15
10	J	49/50 (98%)	47 (96%)	2 (4%)	30	64
10	W	49/50 (98%)	47 (96%)	2 (4%)	30	64
11	K	40/46 (87%)	40 (100%)	0	100	100
11	X	40/46 (87%)	36 (90%)	4 (10%)	7	22
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	79
12	Y	39/40 (98%)	35 (90%)	4 (10%)	7	21
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	53
13	Z	37/38 (97%)	36 (97%)	1 (3%)	44	78
All	All	3113/3082 (101%)	2960 (95%)	153 (5%)	26	57

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	51	ASP
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	177	SER
1	A	180	GLN
1	A	311[A]	ILE
1	A	311[B]	ILE
1	A	333	LYS
1	A	338	MET
1	A	362	SER
1	A	369	ASP
1	A	484	THR
1	A	513	LEU
2	B	43	SER
2	B	60	GLU
2	B	65	TRP
2	B	68	LEU
2	B	78	LEU
2	B	130	PRO
2	B	167	SER
2	B	171	LYS
2	B	183	THR
2	B	197	SER
2	B	205	SER
3	C	38	ASN
3	C	127	LEU
3	C	159	MET
3	C	258	TRP
4	D	4	SER
4	D	36	SER
4	D	107	ILE
4	D	143	ASN
4	D	147	LYS
5	E	5	HIS
5	E	14[A]	ARG
5	E	14[B]	ARG
5	E	70	VAL
5	E	87	GLN
6	F	14	THR
6	F	26	LYS
6	F	37[A]	LYS
6	F	37[B]	LYS
6	F	48	LEU
6	F	53	THR
6	F	95	GLN

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Mol	Chain	Res	Type
7	G	5	LYS
7	G	18[A]	PHE
7	G	18[B]	PHE
7	G	36	TRP
7	G	37	LEU
7	G	54	ARG
7	G	61	SER
8	H	29	CYS
8	H	49	ASP
8	H	60	TYR
8	H	76	ARG
9	I	8	GLN
9	I	19	PHE
9	I	21	ILE
9	I	53	ASN
10	J	27	THR
10	J	55	PHE
12	L	5	GLU
13	M	38	ASP
13	M	43	SER
1	N	38	ARG
1	N	46	THR
1	N	98	ASN
1	N	109	PHE
1	N	112	LEU
1	N	136[A]	LEU
1	N	136[B]	LEU
1	N	138	HIS
1	N	142	SER
1	N	238	PHE
1	N	298[A]	ASP
1	N	298[B]	ASP
1	N	310	MET
1	N	333	LYS
1	N	369	ASP
1	N	380	VAL
1	N	443	TYR
1	N	468	MET
1	N	484	THR
1	N	485	VAL
1	N	486	ASP
1	N	512	ASN

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Mol	Chain	Res	Type
2	O	55	THR
2	O	65	TRP
2	O	68	LEU
2	O	78	LEU
2	O	102	HIS
2	O	115	ASP
2	O	167	SER
2	O	183	THR
2	O	203[A]	ASN
2	O	203[B]	ASN
2	O	205	SER
2	O	216	LEU
2	O	217	LYS
2	O	223	SER
3	P	14	SER
3	P	29	SER
3	P	77	LYS
3	P	109	THR
3	P	159	MET
3	P	180[A]	GLU
3	P	180[B]	GLU
3	P	214	PHE
3	P	258	TRP
4	Q	9	GLU
4	Q	31	LYS
4	Q	142	LYS
4	Q	143	ASN
5	R	5	HIS
5	R	7	THR
6	S	18	ARG
6	S	52	ILE
6	S	53	THR
6	S	54	ASN
6	S	87[A]	THR
6	S	87[B]	THR
7	T	5	LYS
7	T	36[A]	TRP
7	T	36[B]	TRP
7	T	37	LEU
7	T	38	HIS
7	T	42	ARG
7	T	68	THR

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Mol	Chain	Res	Type
7	T	74	ARG
8	U	9	LYS
8	U	60	TYR
8	U	74	ASP
8	U	75	ARG
8	U	84	LYS
9	V	2	THR
9	V	21	ILE
9	V	26	MET
9	V	29	LEU
9	V	31	PHE
9	V	52	ARG
9	V	73	LYS
10	W	27	THR
10	W	50	LEU
11	X	23	THR
11	X	47	ARG
11	X	49	THR
11	X	54	ARG
12	Y	5	GLU
12	Y	20	ARG
12	Y	24	MET
12	Y	26	THR
13	Z	37	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	512	ASN
2	B	10	GLN
2	B	92	ASN
2	B	181	GLN
3	C	68	GLN
4	D	32	ASN
4	D	37	GLN
5	E	78	HIS
5	E	94	ASN
7	G	34	ASN
7	G	76	ASN
8	H	32	ASN

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Mol	Chain	Res	Type
9	I	8	GLN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	52	HIS
2	O	59	GLN
2	O	92	ASN
2	O	181	GLN
2	O	195	GLN
3	P	12	ASN
3	P	68	GLN
3	P	148	HIS
3	P	161	GLN
4	Q	32	ASN
4	Q	37	GLN
5	R	94	ASN
6	S	54	ASN
7	T	34	ASN
7	T	66	ASN
7	T	76	ASN
8	U	23	GLN
8	U	31	GLN
8	U	32	ASN
8	U	37	HIS
10	W	29	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	SAC	I	1	9	7,8,9	2.04	1 (14%)	8,9,11	2.17	3 (37%)
1	FME	A	1	1	8,9,10	0.53	0	7,9,11	1.83	3 (42%)
7	TPO	T	11	7	8,10,11	1.26	1 (12%)	10,14,16	1.32	2 (20%)
2	FME	B	1	2	8,9,10	0.73	0	7,9,11	2.69	3 (42%)
1	FME	N	1	1	8,9,10	0.65	0	7,9,11	2.03	3 (42%)
2	FME	O	1	2	8,9,10	0.65	0	7,9,11	1.02	0
7	TPO	G	11	7	8,10,11	1.34	1 (12%)	10,14,16	1.55	2 (20%)
9	SAC	V	1	9	7,8,9	1.86	1 (14%)	8,9,11	1.62	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SAC	I	1	9	-	2/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	3/9/11/13	-
9	SAC	V	1	9	-	4/7/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-N	4.76	1.53	1.46
9	V	1	SAC	CA-N	4.38	1.52	1.46
7	T	11	TPO	P-OG1	2.71	1.64	1.59
7	G	11	TPO	P-OG1	2.32	1.63	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-5.64	114.15	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CA-N-CN	4.11	129.15	122.82
9	I	1	SAC	OAC-C1A-C2A	-3.53	115.51	122.06
9	I	1	SAC	C-CA-N	3.50	116.05	109.73
7	G	11	TPO	CG2-CB-CA	3.27	119.61	113.16
9	I	1	SAC	C2A-C1A-N	3.13	121.39	116.10
2	B	1	FME	C-CA-N	3.10	115.33	109.73
7	G	11	TPO	P-OG1-CB	-3.01	114.12	123.21
1	A	1	FME	CA-N-CN	2.75	127.05	122.82
1	N	1	FME	C-CA-N	2.55	114.34	109.73
7	T	11	TPO	CG2-CB-CA	2.53	118.15	113.16
1	A	1	FME	CE-SD-CG	2.46	108.86	100.40
9	V	1	SAC	OAC-C1A-C2A	-2.44	117.53	122.06
2	B	1	FME	O1-CN-N	-2.34	119.11	125.27
7	T	11	TPO	P-OG1-CB	-2.33	116.17	123.21
1	A	1	FME	O-C-CA	-2.32	118.70	124.78
1	N	1	FME	O-C-CA	-2.22	118.95	124.78
9	V	1	SAC	O-C-CA	-2.13	119.19	124.78

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
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	V	1	SAC	O-C-CA-CB
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
1	A	1	FME	CB-CG-SD-CE
9	V	1	SAC	C-CA-CB-OG
1	N	1	FME	CB-CG-SD-CE
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
7	T	11	TPO	O-C-CA-CB
1	N	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	TGL	N	607	-	62,62,62	1.18	3 (4%)	65,65,65	1.14	8 (12%)
18	PGV	P	301	-	50,50,50	0.91	2 (4%)	53,56,56	1.05	3 (5%)
18	PGV	A	607	-	50,50,50	1.08	2 (4%)	53,56,56	1.08	4 (7%)
21	CUA	B	302	2	0,1,1	0.00	-	-		
20	CDL	P	305	-	99,99,99	1.09	4 (4%)	105,111,111	1.21	10 (9%)
25	PEK	T	101	-	52,52,52	1.13	2 (3%)	55,57,57	1.10	5 (9%)
22	CHD	G	104	-	29,32,32	0.78	0	48,51,51	1.55	10 (20%)
18	PGV	C	307	-	50,50,50	1.12	2 (4%)	53,56,56	0.91	3 (5%)
18	PGV	C	303	-	50,50,50	0.90	2 (4%)	53,56,56	0.90	3 (5%)
23	PSC	B	304	-	51,51,51	0.99	2 (3%)	57,59,59	1.74	8 (14%)
18	PGV	N	606	-	50,50,50	0.99	2 (4%)	53,56,56	0.97	4 (7%)
25	PEK	C	302	-	52,52,52	0.85	2 (3%)	55,57,57	1.06	3 (5%)
22	CHD	P	307	-	29,32,32	0.62	0	48,51,51	1.34	6 (12%)
25	PEK	G	103	-	52,52,52	1.10	2 (3%)	55,57,57	1.50	6 (10%)
25	PEK	P	308	-	52,52,52	0.87	2 (3%)	55,57,57	1.01	2 (3%)
19	TGL	Y	101	-	62,62,62	1.13	3 (4%)	65,65,65	1.02	5 (7%)
19	TGL	V	101	-	62,62,62	1.13	3 (4%)	65,65,65	1.25	8 (12%)
24	DMU	P	303	-	34,34,34	1.69	1 (2%)	45,45,45	1.46	5 (11%)
24	DMU	C	301	-	34,34,34	1.89	6 (17%)	45,45,45	2.26	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DMU	Q	201	-	34,34,34	0.83	1 (2%)	45,45,45	1.02	2 (4%)
22	CHD	J	101	-	29,32,32	0.71	0	48,51,51	1.63	5 (10%)
18	PGV	P	304	-	50,50,50	0.97	2 (4%)	53,56,56	0.93	2 (3%)
19	TGL	D	201	-	62,62,62	1.21	3 (4%)	65,65,65	1.17	6 (9%)
25	PEK	G	101	-	52,52,52	1.04	2 (3%)	55,57,57	1.19	4 (7%)
23	PSC	N	608	-	51,51,51	1.09	2 (3%)	57,59,59	1.79	9 (15%)
18	PGV	A	606	-	50,50,50	0.93	2 (4%)	53,56,56	0.90	3 (5%)
25	PEK	P	309	-	52,52,52	1.13	2 (3%)	55,57,57	1.40	6 (10%)
22	CHD	W	101	-	29,32,32	0.73	1 (3%)	48,51,51	2.16	15 (31%)
21	CUA	O	301	2	0,1,1	0.00	-	-	-	-
22	CHD	C	306	-	29,32,32	0.82	0	48,51,51	1.24	7 (14%)
18	PGV	P	302	-	50,50,50	1.10	2 (4%)	53,56,56	1.16	5 (9%)
22	CHD	B	303	-	29,32,32	0.64	1 (3%)	48,51,51	1.46	6 (12%)
20	CDL	G	102	-	99,99,99	1.09	4 (4%)	105,111,111	1.08	8 (7%)
14	HEA	N	602	1	44,67,67	1.65	9 (20%)	37,103,103	2.25	7 (18%)
19	TGL	B	301	-	62,62,62	1.17	3 (4%)	65,65,65	1.19	6 (9%)
19	TGL	A	608	-	62,62,62	1.20	3 (4%)	65,65,65	1.14	5 (7%)
14	HEA	N	601	1	44,67,67	1.84	11 (25%)	37,103,103	2.09	9 (24%)
14	HEA	A	602	1	44,67,67	1.64	9 (20%)	37,103,103	2.40	8 (21%)
22	CHD	P	306	-	29,32,32	0.45	0	48,51,51	1.74	15 (31%)
20	CDL	C	304	-	99,99,99	1.10	4 (4%)	105,111,111	1.02	5 (4%)
14	HEA	A	601	1	44,67,67	1.86	9 (20%)	37,103,103	2.16	7 (18%)
22	CHD	C	305	-	29,32,32	0.57	0	48,51,51	1.59	9 (18%)
24	DMU	M	101	-	34,34,34	1.08	1 (2%)	45,45,45	1.17	3 (6%)
20	CDL	A	609	-	99,99,99	1.11	4 (4%)	105,111,111	1.15	8 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	N	607	-	-	36/65/65/65	-
18	PGV	P	301	-	-	13/55/55/55	-
18	PGV	A	607	-	-	30/55/55/55	-
20	CDL	P	305	-	-	52/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	T	101	-	-	21/56/56/56	-
22	CHD	G	104	-	-	0/7/74/74	0/4/4/4
18	PGV	C	307	-	-	30/55/55/55	-
18	PGV	C	303	-	-	15/55/55/55	-
23	PSC	B	304	-	-	26/55/55/55	-
18	PGV	N	606	-	-	27/55/55/55	-
25	PEK	C	302	-	-	18/56/56/56	-
22	CHD	P	307	-	-	0/7/74/74	0/4/4/4
25	PEK	G	103	-	-	30/56/56/56	-
25	PEK	P	308	-	-	16/56/56/56	-
19	TGL	Y	101	-	-	35/65/65/65	-
19	TGL	V	101	-	-	32/65/65/65	-
24	DMU	C	301	-	-	12/19/59/59	0/2/2/2
24	DMU	Q	201	-	-	7/19/59/59	0/2/2/2
22	CHD	J	101	-	-	4/7/74/74	0/4/4/4
18	PGV	P	304	-	-	15/55/55/55	-
19	TGL	D	201	-	-	36/65/65/65	-
25	PEK	G	101	-	-	23/56/56/56	-
23	PSC	N	608	-	-	29/55/55/55	-
18	PGV	A	606	-	-	9/55/55/55	-
25	PEK	P	309	-	-	22/56/56/56	-
22	CHD	W	101	-	-	5/7/74/74	0/4/4/4
24	DMU	P	303	-	-	6/19/59/59	0/2/2/2
22	CHD	C	306	-	-	0/7/74/74	0/4/4/4
18	PGV	P	302	-	-	32/55/55/55	-
22	CHD	B	303	-	-	2/7/74/74	0/4/4/4
20	CDL	G	102	-	-	56/110/110/110	-
14	HEA	N	602	1	3/3/7/16	0/24/76/76	-
19	TGL	B	301	-	-	35/65/65/65	-
19	TGL	A	608	-	-	33/65/65/65	-
14	HEA	N	601	1	3/3/7/16	0/24/76/76	-
14	HEA	A	602	1	3/3/7/16	2/24/76/76	-
22	CHD	P	306	-	-	3/7/74/74	0/4/4/4
20	CDL	C	304	-	-	65/110/110/110	-
14	HEA	A	601	1	3/3/7/16	0/24/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	C	305	-	-	6/7/74/74	0/4/4/4
24	DMU	M	101	-	-	9/19/59/59	0/2/2/2
20	CDL	A	609	-	-	59/110/110/110	-

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	301	DMU	O16-C6	8.30	1.54	1.40
24	P	303	DMU	O16-C6	8.13	1.54	1.40
14	A	601	HEA	C3B-C11	-6.45	1.47	1.52
25	P	309	PEK	O01-C1	5.49	1.49	1.34
14	N	601	HEA	C3C-C2C	5.36	1.47	1.40
20	P	305	CDL	OA6-CA5	5.35	1.49	1.34
19	A	608	TGL	OG2-CB1	5.30	1.49	1.34
19	B	301	TGL	OG2-CB1	5.24	1.49	1.34
14	N	601	HEA	C3B-C11	-5.21	1.48	1.52
20	C	304	CDL	OA6-CA5	5.18	1.48	1.34
18	A	607	PGV	O03-C19	5.16	1.48	1.33
25	T	101	PEK	O01-C1	5.15	1.48	1.34
19	D	201	TGL	OG2-CB1	5.12	1.48	1.34
14	A	602	HEA	C3B-C11	-5.09	1.48	1.52
14	N	601	HEA	C3A-C2A	5.08	1.47	1.40
20	G	102	CDL	OA6-CA5	5.07	1.48	1.34
20	A	609	CDL	OB6-CB5	5.06	1.48	1.34
14	A	601	HEA	C3C-C2C	5.02	1.47	1.40
19	N	607	TGL	OG3-CC1	5.01	1.48	1.33
19	Y	101	TGL	OG2-CB1	5.00	1.48	1.34
20	G	102	CDL	OB6-CB5	4.96	1.48	1.34
19	D	201	TGL	OG3-CC1	4.96	1.47	1.33
20	G	102	CDL	OA8-CA7	4.94	1.47	1.33
25	G	101	PEK	O01-C1	4.92	1.48	1.34
19	D	201	TGL	OG1-CA1	4.91	1.47	1.33
19	N	607	TGL	OG2-CB1	4.91	1.48	1.34
19	A	608	TGL	OG1-CA1	4.90	1.47	1.33
20	P	305	CDL	OA8-CA7	4.87	1.47	1.33
18	P	302	PGV	O01-C1	4.87	1.48	1.34
20	A	609	CDL	OB8-CB7	4.87	1.47	1.33
20	C	304	CDL	OB8-CB7	4.86	1.47	1.33
18	N	606	PGV	O03-C19	4.86	1.47	1.33
25	G	103	PEK	O03-C21	4.84	1.47	1.33
25	T	101	PEK	O03-C21	4.82	1.47	1.33
18	P	304	PGV	O01-C1	4.82	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C3A-C2A	4.80	1.47	1.40
20	A	609	CDL	OA8-CA7	4.78	1.47	1.33
25	G	103	PEK	O01-C1	4.78	1.47	1.34
19	V	101	TGL	OG2-CB1	4.78	1.47	1.34
18	C	307	PGV	O01-C1	4.77	1.47	1.34
19	Y	101	TGL	OG3-CC1	4.77	1.47	1.33
23	N	608	PSC	O03-C19	4.76	1.47	1.33
19	A	608	TGL	OG3-CC1	4.75	1.47	1.33
20	C	304	CDL	OA8-CA7	4.75	1.47	1.33
18	C	307	PGV	O03-C19	4.71	1.47	1.33
23	N	608	PSC	O01-C1	4.71	1.47	1.34
24	M	101	DMU	O16-C6	4.62	1.48	1.40
19	B	301	TGL	OG1-CA1	4.57	1.46	1.33
20	P	305	CDL	OB8-CB7	4.55	1.46	1.33
19	V	101	TGL	OG3-CC1	4.55	1.46	1.33
25	P	309	PEK	O03-C21	4.54	1.46	1.33
19	Y	101	TGL	OG1-CA1	4.48	1.46	1.33
18	A	607	PGV	O01-C1	4.48	1.46	1.34
18	P	302	PGV	O03-C19	4.48	1.46	1.33
23	B	304	PSC	O01-C1	4.47	1.46	1.34
14	A	602	HEA	C3C-C2C	4.46	1.46	1.40
19	N	607	TGL	OG1-CA1	4.43	1.46	1.33
20	G	102	CDL	OB8-CB7	4.41	1.46	1.33
20	A	609	CDL	OA6-CA5	4.39	1.46	1.34
14	N	602	HEA	C3B-C11	-4.39	1.49	1.52
20	C	304	CDL	OB6-CB5	4.37	1.46	1.34
20	P	305	CDL	OB6-CB5	4.36	1.46	1.34
14	N	602	HEA	C3A-C2A	4.36	1.46	1.40
19	V	101	TGL	OG1-CA1	4.28	1.45	1.33
25	G	101	PEK	O03-C21	4.28	1.45	1.33
25	C	302	PEK	O01-C1	4.28	1.46	1.34
18	C	303	PGV	O01-C1	4.23	1.46	1.34
18	A	606	PGV	O03-C19	4.21	1.45	1.33
23	B	304	PSC	O03-C19	4.19	1.45	1.33
18	P	301	PGV	O03-C19	4.16	1.45	1.33
25	P	308	PEK	O03-C21	4.09	1.45	1.33
18	A	606	PGV	O01-C1	4.03	1.45	1.34
19	B	301	TGL	OG3-CC1	3.97	1.44	1.33
14	N	602	HEA	C3C-C2C	3.96	1.45	1.40
18	P	301	PGV	O01-C1	3.92	1.45	1.34
18	C	303	PGV	O03-C19	3.78	1.44	1.33
18	N	606	PGV	O01-C1	3.77	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	308	PEK	O01-C1	3.75	1.44	1.34
18	P	304	PGV	O03-C19	3.70	1.44	1.33
25	C	302	PEK	O03-C21	3.39	1.43	1.33
24	C	301	DMU	C8-C9	3.37	1.60	1.53
14	A	601	HEA	C3D-C2D	3.30	1.47	1.37
14	N	601	HEA	C1A-C2A	3.24	1.49	1.42
14	N	602	HEA	C1A-C2A	3.15	1.49	1.42
14	A	602	HEA	C3A-C2A	3.08	1.44	1.40
14	N	601	HEA	C3D-C2D	3.01	1.46	1.37
14	N	602	HEA	C1B-CHB	2.90	1.49	1.41
14	A	602	HEA	C3D-C2D	2.87	1.46	1.37
14	N	602	HEA	C3D-C2D	2.87	1.46	1.37
24	Q	201	DMU	O16-C6	2.80	1.45	1.40
14	A	601	HEA	C4B-C3B	2.80	1.48	1.42
24	C	301	DMU	C2-C1	2.79	1.59	1.52
14	A	602	HEA	C1A-C2A	2.61	1.48	1.42
24	C	301	DMU	C6-C1	2.59	1.59	1.52
14	A	602	HEA	C1C-CHC	2.55	1.48	1.41
14	A	602	HEA	C1D-C2D	2.54	1.48	1.42
14	A	602	HEA	C4D-CHA	2.49	1.47	1.41
22	W	101	CHD	C20-C17	2.47	1.58	1.54
14	N	601	HEA	C1D-C2D	2.47	1.48	1.42
14	N	601	HEA	C4B-C3B	2.40	1.48	1.42
14	A	601	HEA	C1D-C2D	2.40	1.48	1.42
14	A	601	HEA	C1A-C2A	2.39	1.48	1.42
22	B	303	CHD	C13-C14	-2.38	1.51	1.55
14	N	601	HEA	C1B-CHB	2.36	1.47	1.41
14	N	602	HEA	C4B-C3B	2.34	1.47	1.42
14	N	601	HEA	C1C-CHC	2.33	1.47	1.41
14	N	601	HEA	C4C-CHD	2.32	1.47	1.41
14	A	602	HEA	C4B-C3B	2.32	1.47	1.42
14	N	601	HEA	C4D-CHA	2.26	1.47	1.41
14	A	601	HEA	C1C-CHC	2.26	1.47	1.41
24	C	301	DMU	O5-C6	2.21	1.47	1.41
14	N	602	HEA	C1D-C2D	2.13	1.47	1.42
14	N	602	HEA	CAD-C3D	-2.13	1.48	1.52
24	C	301	DMU	O1-C9	2.12	1.49	1.44
14	A	601	HEA	C4C-CHD	2.06	1.46	1.41

All (261) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	301	DMU	C18-O16-C6	10.11	130.61	113.84
14	N	601	HEA	C4B-C3B-C2B	-8.42	100.98	106.87
14	A	601	HEA	C4B-C3B-C2B	-7.94	101.32	106.87
14	N	602	HEA	C4B-C3B-C2B	-7.28	101.78	106.87
25	G	103	PEK	O01-C1-C2	7.17	126.96	111.50
20	P	305	CDL	OA6-CA5-C11	6.61	125.75	111.50
23	N	608	PSC	C08-N-C06	-6.61	91.98	108.97
14	N	602	HEA	CAD-CBD-CGD	-6.46	101.84	112.67
14	A	602	HEA	C1B-C2B-C3B	-6.41	102.54	107.00
14	A	602	HEA	C4B-C3B-C2B	-6.34	102.44	106.87
23	N	608	PSC	C08-N-C07	-6.32	92.73	108.97
24	C	301	DMU	O16-C6-C1	6.24	118.05	108.30
22	W	101	CHD	C22-C20-C17	6.18	123.06	110.28
14	A	602	HEA	CAD-CBD-CGD	-6.14	102.37	112.67
23	B	304	PSC	C08-N-C06	-6.09	93.31	108.97
23	B	304	PSC	C08-N-C07	-6.07	93.38	108.97
19	V	101	TGL	OG2-CB1-CB2	5.94	124.31	111.50
25	P	309	PEK	O01-C1-C2	5.87	124.15	111.50
22	C	305	CHD	C16-C17-C20	5.80	121.12	112.15
20	A	609	CDL	OA6-CA5-C11	5.45	123.26	111.50
25	G	101	PEK	O01-C1-C2	5.43	123.20	111.50
20	C	304	CDL	OA6-CA5-C11	5.32	122.97	111.50
25	C	302	PEK	O01-C1-C2	5.19	122.69	111.50
20	A	609	CDL	OB6-CB5-C51	5.02	122.32	111.50
14	A	601	HEA	C1B-C2B-C3B	-4.98	103.53	107.00
20	G	102	CDL	OA6-CA5-C11	4.96	122.20	111.50
24	P	303	DMU	O16-C6-C1	4.95	116.03	108.30
22	J	101	CHD	C22-C20-C17	4.95	120.51	110.28
25	T	101	PEK	O01-C1-C2	4.93	122.12	111.50
22	W	101	CHD	C5-C6-C7	-4.76	109.21	114.46
23	B	304	PSC	O01-C1-C2	4.70	121.62	111.50
18	P	302	PGV	O01-C1-C2	4.65	121.53	111.50
14	N	602	HEA	C1B-C2B-C3B	-4.64	103.77	107.00
23	N	608	PSC	C07-N-C06	4.63	120.89	108.97
19	Y	101	TGL	OG2-CB1-CB2	4.58	121.38	111.50
18	A	607	PGV	O01-C1-C2	4.47	121.13	111.50
19	N	607	TGL	OG2-CB1-CB2	4.41	121.00	111.50
25	G	103	PEK	O01-C1-O02	-4.36	113.16	123.70
22	B	303	CHD	C6-C5-C4	-4.36	106.17	111.19
23	N	608	PSC	O01-C1-C2	4.35	120.88	111.50
14	N	601	HEA	C1B-C2B-C3B	-4.33	103.98	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	C3C-C4C-NC	4.30	114.77	109.21
14	A	602	HEA	CBD-CAD-C3D	4.28	120.37	112.49
25	P	309	PEK	O03-C21-C22	4.26	125.29	111.91
20	P	305	CDL	OB6-CB5-C51	4.26	120.67	111.50
18	P	302	PGV	O03-C19-C20	4.25	125.24	111.91
25	P	308	PEK	O01-C1-C2	4.22	120.60	111.50
19	D	201	TGL	OG3-CC1-CC2	4.21	125.13	111.91
18	P	301	PGV	O01-C1-C2	4.21	120.58	111.50
24	C	301	DMU	O1-C9-C8	4.11	117.17	109.69
22	W	101	CHD	C13-C17-C20	4.10	124.39	119.50
22	W	101	CHD	C10-C9-C8	4.09	116.21	111.82
14	A	602	HEA	C13-C12-C11	-4.09	108.21	114.35
23	B	304	PSC	C08-N-C05	-4.02	93.48	109.92
14	A	602	HEA	C3C-C4C-NC	3.96	114.33	109.21
19	V	101	TGL	CG2-OG2-CB1	3.94	127.49	117.79
14	N	601	HEA	C3C-C4C-NC	3.91	114.27	109.21
14	A	601	HEA	CMC-C2C-C3C	3.90	131.98	124.68
23	B	304	PSC	C07-N-C06	3.90	119.00	108.97
25	G	101	PEK	O03-C21-C22	3.89	124.13	111.91
19	B	301	TGL	OG2-CB1-CB2	3.88	119.87	111.50
19	B	301	TGL	OG1-CA1-CA2	3.88	124.09	111.91
22	J	101	CHD	C16-C17-C20	3.86	118.12	112.15
18	N	606	PGV	O03-C19-C20	3.83	123.93	111.91
19	A	608	TGL	OG2-CB1-CB2	3.78	119.66	111.50
25	G	103	PEK	C02-O01-C1	3.78	127.10	117.79
20	G	102	CDL	OB6-CB5-C51	3.76	119.61	111.50
24	P	303	DMU	C18-O16-C6	3.75	120.06	113.84
19	A	608	TGL	OG1-CA1-CA2	3.72	123.58	111.91
20	G	102	CDL	OA8-CA7-C31	3.69	123.50	111.91
22	P	306	CHD	C9-C8-C7	3.68	116.27	111.88
22	W	101	CHD	C16-C17-C20	3.66	117.81	112.15
25	P	309	PEK	O03-C21-O04	-3.65	114.37	123.59
19	D	201	TGL	OG2-CB1-CB2	3.61	119.28	111.50
22	G	104	CHD	C6-C5-C4	-3.61	107.03	111.19
22	W	101	CHD	C4-C5-C10	3.59	116.47	112.66
22	B	303	CHD	C19-C10-C1	-3.57	102.50	108.26
18	C	307	PGV	O01-C1-C2	3.57	119.20	111.50
22	W	101	CHD	C1-C10-C5	3.55	113.01	107.77
20	C	304	CDL	OB6-CB5-C51	3.54	119.13	111.50
23	N	608	PSC	C08-N-C05	-3.53	95.49	109.92
14	A	601	HEA	CAA-CBA-CGA	-3.51	106.79	112.67
25	P	308	PEK	O03-C21-C22	3.50	122.89	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	309	PEK	C03-C02-C01	-3.49	103.53	111.79
25	G	103	PEK	O03-C21-C22	3.42	122.64	111.91
22	C	305	CHD	C6-C5-C4	-3.41	107.26	111.19
22	P	306	CHD	C11-C9-C8	-3.41	105.89	110.88
19	N	607	TGL	OG1-CA1-CA2	3.40	122.57	111.91
22	P	307	CHD	C11-C12-C13	3.39	114.73	111.24
22	B	303	CHD	C22-C20-C17	3.37	117.25	110.28
25	G	101	PEK	O03-C21-O04	-3.36	115.12	123.59
22	G	104	CHD	C19-C10-C1	-3.33	102.89	108.26
19	B	301	TGL	OG3-CC1-OC1	-3.33	115.20	123.59
20	C	304	CDL	OB8-CB7-C71	3.24	122.08	111.91
18	A	606	PGV	O03-C19-C20	3.21	121.99	111.91
18	A	607	PGV	O03-C19-C20	3.20	121.95	111.91
24	C	301	DMU	C6-C1-C2	3.19	116.65	110.00
22	G	104	CHD	C4-C3-C2	3.19	114.36	110.55
19	B	301	TGL	CG2-OG2-CB1	3.19	125.64	117.79
19	D	201	TGL	OG1-CG1-CG2	3.17	117.66	108.43
18	P	302	PGV	O03-C19-O04	-3.14	115.66	123.59
14	N	602	HEA	CBD-CAD-C3D	3.13	118.25	112.49
22	J	101	CHD	C6-C5-C4	-3.12	107.60	111.19
18	C	307	PGV	O03-C19-C20	3.10	121.64	111.91
19	B	301	TGL	OG1-CA1-OA1	-3.10	115.77	123.59
14	A	601	HEA	C3C-C4C-NC	3.09	113.21	109.21
22	P	306	CHD	C17-C13-C12	3.09	120.48	117.67
22	W	101	CHD	O7-C7-C8	3.09	116.32	109.43
22	C	306	CHD	C5-C6-C7	3.09	117.87	114.46
18	P	301	PGV	O03-C19-C20	3.05	121.48	111.91
24	C	301	DMU	C1-C2-C3	3.04	116.63	109.68
22	C	305	CHD	C23-C22-C20	-3.04	110.63	114.72
19	N	607	TGL	OG3-CC1-CC2	2.99	121.30	111.91
22	B	303	CHD	C1-C2-C3	2.99	114.31	110.47
22	J	101	CHD	C21-C20-C17	-2.98	108.36	112.92
20	P	305	CDL	OB8-CB7-C71	2.96	121.19	111.91
19	D	201	TGL	OG1-CA1-CA2	2.95	121.17	111.91
24	C	301	DMU	C10-O1-C9	2.94	119.45	113.69
19	D	201	TGL	CG3-OG3-CC1	2.93	127.96	117.12
22	P	306	CHD	C1-C2-C3	2.91	114.21	110.47
22	P	306	CHD	C11-C12-C13	2.88	114.20	111.24
19	V	101	TGL	OG2-CB1-OB1	-2.87	116.76	123.70
19	N	607	TGL	OG1-CA1-OA1	-2.87	116.36	123.59
22	P	307	CHD	C23-C22-C20	-2.85	110.88	114.72
19	A	608	TGL	OG3-CC1-CC2	2.84	120.83	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	301	TGL	OG3-CC1-CC2	2.84	120.83	111.91
22	P	307	CHD	C18-C13-C12	2.82	111.94	109.07
20	G	102	CDL	OA8-CA7-OA9	-2.81	116.51	123.59
24	C	301	DMU	C7-C8-C9	2.79	115.21	110.24
22	C	306	CHD	C19-C10-C1	-2.77	103.80	108.26
14	A	601	HEA	CBD-CAD-C3D	-2.76	107.39	112.49
24	M	101	DMU	C22-C19-C18	-2.76	101.26	113.49
19	V	101	TGL	OG1-CA1-CA2	2.76	120.55	111.91
14	N	601	HEA	CAA-CBA-CGA	-2.72	108.10	112.67
18	C	303	PGV	O01-C1-C2	2.71	117.34	111.50
22	G	104	CHD	C14-C13-C12	-2.70	104.88	107.40
25	T	101	PEK	O03-C21-C22	2.69	120.35	111.91
14	A	602	HEA	CMC-C2C-C3C	2.67	129.67	124.68
20	G	102	CDL	CA6-OA8-CA7	2.66	126.97	117.12
22	W	101	CHD	C14-C13-C12	2.66	109.87	107.40
20	A	609	CDL	OA8-CA7-C31	2.65	120.22	111.91
19	Y	101	TGL	OG3-CC1-CC2	2.65	120.21	111.91
18	P	304	PGV	O01-C1-C2	2.64	117.18	111.50
19	D	201	TGL	OG3-CC1-OC1	-2.63	116.95	123.59
18	P	304	PGV	C4-C3-C2	2.63	122.63	113.19
19	V	101	TGL	CG3-OG3-CC1	2.61	126.80	117.12
20	P	305	CDL	OA8-CA7-C31	2.61	120.09	111.91
20	A	609	CDL	OA6-CA5-OA7	-2.60	117.41	123.70
20	A	609	CDL	OB8-CB6-CB4	2.59	115.98	108.43
14	N	601	HEA	OMA-CMA-C3A	-2.59	119.27	124.91
24	C	301	DMU	C28-C25-C22	-2.59	101.29	114.42
18	P	302	PGV	O03-C01-C02	2.59	115.97	108.43
20	P	305	CDL	CA4-OA6-CA5	2.59	124.16	117.79
22	W	101	CHD	O7-C7-C6	-2.56	103.58	109.94
14	N	602	HEA	OMA-CMA-C3A	-2.56	119.34	124.91
22	G	104	CHD	C6-C7-C8	2.55	114.20	111.48
22	C	306	CHD	C19-C10-C9	2.55	114.69	111.18
19	Y	101	TGL	OG1-CA1-CA2	2.54	119.89	111.91
19	V	101	TGL	OG3-CC1-CC2	2.54	119.87	111.91
25	P	309	PEK	O03-C01-C02	2.53	115.79	108.43
19	N	607	TGL	CG3-OG3-CC1	2.53	126.48	117.12
23	B	304	PSC	C06-N-C05	2.52	120.23	109.92
22	G	104	CHD	C1-C10-C9	2.51	115.30	111.35
14	N	602	HEA	C20-C19-C18	-2.51	116.03	121.12
14	N	601	HEA	CMC-C2C-C3C	2.51	129.37	124.68
22	W	101	CHD	C14-C8-C7	2.51	115.13	111.81
14	N	601	HEA	CAD-CBD-CGD	-2.48	108.51	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	606	PGV	O03-C01-C02	2.47	115.64	108.43
22	P	307	CHD	C21-C20-C22	-2.46	106.50	110.36
22	J	101	CHD	O7-C7-C8	2.45	114.89	109.43
22	C	306	CHD	C14-C13-C12	-2.44	105.13	107.40
25	T	101	PEK	O01-C1-O02	-2.44	117.81	123.70
22	P	306	CHD	C9-C10-C5	2.43	112.00	108.58
22	W	101	CHD	C1-C10-C9	-2.43	107.53	111.35
22	C	305	CHD	C4-C5-C10	2.43	115.24	112.66
22	P	306	CHD	C6-C5-C4	-2.42	108.40	111.19
18	N	606	PGV	O01-C1-C2	2.42	116.72	111.50
22	P	306	CHD	C11-C9-C10	2.41	116.21	113.73
19	A	608	TGL	OG3-CG3-CG2	2.41	115.45	108.43
20	A	609	CDL	OB8-CB7-OB9	-2.41	117.51	123.59
22	C	305	CHD	C10-C9-C8	2.40	114.40	111.82
23	B	304	PSC	C07-N-C05	2.40	119.73	109.92
19	N	607	TGL	OG3-CC1-OC1	-2.39	117.55	123.59
22	P	306	CHD	C13-C17-C20	2.38	122.33	119.50
18	C	303	PGV	O12-P-O13	-2.37	99.79	109.07
18	P	302	PGV	O01-C1-O02	-2.36	117.99	123.70
22	P	306	CHD	C16-C17-C20	-2.36	108.49	112.15
22	G	104	CHD	C21-C20-C17	-2.36	109.31	112.92
25	G	103	PEK	O01-C02-C01	2.35	116.89	108.40
19	N	607	TGL	OG1-CG1-CG2	2.33	115.22	108.43
22	P	306	CHD	C1-C10-C9	2.32	115.01	111.35
25	G	103	PEK	O03-C01-C02	2.32	115.18	108.43
22	C	305	CHD	C22-C23-C24	-2.31	108.62	113.59
18	P	301	PGV	O01-C1-O02	-2.31	118.13	123.70
24	P	303	DMU	C1-C2-C3	2.30	114.94	109.68
22	P	306	CHD	C4-C3-C2	-2.29	107.81	110.55
20	A	609	CDL	OA8-CA6-CA4	2.29	115.10	108.43
24	P	303	DMU	C34-C31-C28	-2.29	102.82	114.42
22	G	104	CHD	C9-C8-C7	-2.28	109.15	111.88
20	C	304	CDL	OA8-CA7-C31	2.28	119.05	111.91
20	G	102	CDL	OB8-CB7-C71	2.27	119.04	111.91
24	Q	201	DMU	O7-C10-O1	2.27	117.01	110.67
19	A	608	TGL	OG1-CG1-CG2	2.27	115.03	108.43
25	C	302	PEK	O03-C21-C22	2.26	119.00	111.91
22	P	306	CHD	C10-C9-C8	2.26	114.24	111.82
22	G	104	CHD	C18-C13-C14	2.25	114.73	111.21
19	N	607	TGL	OG2-CB1-OB1	-2.25	118.27	123.70
23	N	608	PSC	C06-N-C05	2.25	119.11	109.92
25	G	101	PEK	C03-C02-C01	-2.25	106.47	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	304	CDL	CA6-OA8-CA7	2.24	125.43	117.12
22	C	306	CHD	C6-C5-C4	-2.24	108.61	111.19
14	A	602	HEA	OMA-CMA-C3A	-2.24	120.04	124.91
24	M	101	DMU	C10-O1-C9	2.22	118.05	113.69
22	P	306	CHD	C2-C1-C10	2.22	116.59	112.78
18	A	607	PGV	O03-C01-C02	2.22	114.89	108.43
22	B	303	CHD	C4-C5-C10	2.21	115.00	112.66
23	N	608	PSC	C07-N-C05	2.21	118.96	109.92
18	C	307	PGV	O03-C19-O04	-2.20	118.04	123.59
24	M	101	DMU	C6-O5-C4	2.20	118.00	113.69
22	C	305	CHD	C19-C10-C1	-2.18	104.74	108.26
20	P	305	CDL	OB6-CB5-OB7	-2.18	118.44	123.70
20	P	305	CDL	C62-C61-C60	2.17	125.42	114.42
22	P	307	CHD	C6-C7-C8	2.15	113.77	111.48
18	A	606	PGV	O01-C1-C2	2.14	116.12	111.50
22	P	307	CHD	C14-C13-C12	-2.14	105.41	107.40
22	C	306	CHD	C4-C5-C10	2.13	114.92	112.66
19	V	101	TGL	OG1-CA1-OA1	-2.13	118.22	123.59
20	P	305	CDL	OA7-CA5-C11	-2.13	115.43	123.73
25	T	101	PEK	O03-C01-C02	2.11	114.59	108.43
22	B	303	CHD	C11-C12-C13	2.11	113.41	111.24
22	P	306	CHD	C14-C8-C9	-2.10	106.83	109.71
22	W	101	CHD	C19-C10-C5	-2.10	106.80	110.36
18	C	303	PGV	O14-P-O13	2.10	122.60	112.24
23	N	608	PSC	C01-O03-C19	2.09	124.87	117.12
24	Q	201	DMU	O5-C4-C57	2.09	111.62	106.44
22	C	305	CHD	C13-C17-C20	-2.08	117.01	119.50
22	C	306	CHD	C22-C20-C17	-2.07	106.00	110.28
22	G	104	CHD	C22-C20-C17	2.07	114.56	110.28
22	W	101	CHD	C15-C14-C8	2.07	121.22	118.33
14	A	601	HEA	CAD-CBD-CGD	-2.07	109.20	112.67
19	Y	101	TGL	CG3-OG3-CC1	2.06	124.77	117.12
22	C	305	CHD	C1-C10-C9	2.06	114.60	111.35
25	T	101	PEK	O03-C21-O04	-2.06	118.39	123.59
20	P	305	CDL	OA6-CA5-OA7	-2.06	118.73	123.70
19	Y	101	TGL	OG3-CC1-OC1	-2.05	118.42	123.59
22	W	101	CHD	C4-C3-C2	-2.05	108.11	110.55
25	C	302	PEK	O13-P-O14	2.05	122.36	112.24
24	P	303	DMU	C11-C9-C8	-2.04	108.22	113.00
23	N	608	PSC	O03-C19-C20	2.03	118.29	111.91
20	P	305	CDL	OA8-CA7-OA9	-2.03	118.46	123.59
18	A	606	PGV	O03-C01-C02	2.03	114.34	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	101	TGL	OG2-CG2-CG1	2.03	115.74	108.40
20	G	102	CDL	OB8-CB6-CB4	2.03	114.33	108.43
18	N	606	PGV	O04-C19-C20	-2.02	115.84	123.73
20	G	102	CDL	OB8-CB7-OB9	-2.02	118.50	123.59
20	A	609	CDL	OB8-CB7-C71	2.02	118.24	111.91
14	N	601	HEA	CMD-C2D-C3D	2.02	128.74	124.94
25	P	309	PEK	O02-C1-C2	-2.01	115.87	123.73
18	A	607	PGV	O01-C1-O02	-2.01	118.84	123.70
23	B	304	PSC	O01-C1-O02	-2.01	118.84	123.70
14	N	601	HEA	C13-C12-C11	-2.00	111.34	114.35

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	602	HEA	ND
14	N	602	HEA	NA
14	N	602	HEA	NB
14	N	601	HEA	ND
14	N	601	HEA	NA
14	N	601	HEA	NB
14	A	602	HEA	ND
14	A	602	HEA	NA
14	A	602	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	601	HEA	NB

All (851) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	N	607	TGL	CB2-CB1-OG2-CG2
19	N	607	TGL	CG1-CG2-OG2-CB1
19	N	607	TGL	CC2-CC1-OG3-CG3
19	N	607	TGL	OC1-CC1-OG3-CG3
18	A	607	PGV	C03-O11-P-O14
18	A	607	PGV	C02-C03-O11-P
18	A	607	PGV	C04-C05-C06-O06
18	A	607	PGV	O05-C05-C06-O06
18	A	607	PGV	O02-C1-O01-C02
18	A	607	PGV	C20-C19-O03-C01
20	P	305	CDL	O1-C1-CA2-OA2
20	P	305	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
20	P	305	CDL	CA2-OA2-PA1-OA3
20	P	305	CDL	C11-CA5-OA6-CA4
20	P	305	CDL	CB3-OB5-PB2-OB3
25	T	101	PEK	C04-O12-P-O14
25	T	101	PEK	O03-C01-C02-O01
25	T	101	PEK	C9-C10-C11-C12
18	C	307	PGV	C03-O11-P-O14
18	C	307	PGV	C04-O12-P-O13
18	C	307	PGV	O03-C01-C02-O01
18	C	307	PGV	C02-C03-O11-P
18	C	307	PGV	O12-C04-C05-O05
18	C	307	PGV	C04-C05-C06-O06
18	C	307	PGV	O05-C05-C06-O06
18	C	303	PGV	C04-C05-C06-O06
18	C	303	PGV	O05-C05-C06-O06
24	M	101	DMU	O5-C6-O16-C18
23	B	304	PSC	C03-O11-P-O14
23	B	304	PSC	O12-C04-C05-N
18	N	606	PGV	C03-O11-P-O12
18	N	606	PGV	C02-C03-O11-P
18	N	606	PGV	O02-C1-O01-C02
18	N	606	PGV	C2-C1-O01-C02
25	G	103	PEK	C03-O11-P-O14
25	G	103	PEK	C04-O12-P-O13
25	G	103	PEK	O02-C1-O01-C02
25	G	103	PEK	C2-C1-O01-C02
25	G	103	PEK	C5-C6-C7-C8
19	V	101	TGL	CB2-CB1-OG2-CG2
24	C	301	DMU	C1-C6-O16-C18
24	C	301	DMU	C19-C18-O16-C6
22	J	101	CHD	C13-C17-C20-C22
22	J	101	CHD	C16-C17-C20-C22
19	D	201	TGL	OG1-CG1-CG2-OG2
19	D	201	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	OC1-CC1-OG3-CG3
25	G	101	PEK	C04-O12-P-O11
25	G	101	PEK	C04-O12-P-O14
25	G	101	PEK	O12-C04-C05-N
23	N	608	PSC	C03-O11-P-O12
23	N	608	PSC	C05-C04-O12-P
25	P	309	PEK	C03-O11-P-O14
25	P	309	PEK	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
25	P	309	PEK	C2-C1-O01-C02
22	W	101	CHD	C13-C17-C20-C22
22	W	101	CHD	C16-C17-C20-C21
18	P	302	PGV	C04-O12-P-O11
18	P	302	PGV	C02-C03-O11-P
18	P	302	PGV	C04-C05-C06-O06
20	G	102	CDL	OA9-CA7-OA8-CA6
20	G	102	CDL	C31-CA7-OA8-CA6
20	G	102	CDL	C1-CB2-OB2-PB2
20	G	102	CDL	CB2-OB2-PB2-OB3
20	G	102	CDL	CB2-OB2-PB2-OB4
20	G	102	CDL	CB2-OB2-PB2-OB5
20	G	102	CDL	CB3-OB5-PB2-OB3
14	A	602	HEA	C3B-C11-C12-C13
20	C	304	CDL	CA2-C1-CB2-OB2
20	C	304	CDL	CA2-OA2-PA1-OA4
20	C	304	CDL	C11-CA5-OA6-CA4
20	C	304	CDL	OB5-CB3-CB4-OB6
22	C	305	CHD	C13-C17-C20-C21
22	C	305	CHD	C16-C17-C20-C22
20	A	609	CDL	C11-CA5-OA6-CA4
20	A	609	CDL	CB3-OB5-PB2-OB2
20	A	609	CDL	CB3-OB5-PB2-OB3
20	A	609	CDL	CB3-OB5-PB2-OB4
20	A	609	CDL	CB4-CB3-OB5-PB2
18	A	607	PGV	O04-C19-O03-C01
23	N	608	PSC	C20-C19-O03-C01
18	N	606	PGV	O04-C19-O03-C01
23	N	608	PSC	O04-C19-O03-C01
19	B	301	TGL	OC1-CC1-OG3-CG3
20	A	609	CDL	OB9-CB7-OB8-CB6
22	C	305	CHD	C16-C17-C20-C21
22	W	101	CHD	C16-C17-C20-C22
19	N	607	TGL	OB1-CB1-OG2-CG2
20	P	305	CDL	OA7-CA5-OA6-CA4
19	V	101	TGL	OB1-CB1-OG2-CG2
19	A	608	TGL	OB1-CB1-OG2-CG2
20	C	304	CDL	OA7-CA5-OA6-CA4
20	A	609	CDL	OA7-CA5-OA6-CA4
18	N	606	PGV	C20-C19-O03-C01
20	A	609	CDL	C71-CB7-OB8-CB6
18	A	607	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	CB2-CB1-OG2-CG2
22	C	305	CHD	C13-C17-C20-C22
19	Y	101	TGL	CA2-CA1-OG1-CG1
19	B	301	TGL	CC2-CC1-OG3-CG3
19	N	607	TGL	OA1-CA1-OG1-CG1
19	Y	101	TGL	OA1-CA1-OG1-CG1
19	A	608	TGL	OA1-CA1-OG1-CG1
18	P	302	PGV	O12-C04-C05-O05
20	C	304	CDL	O1-C1-CB2-OB2
19	N	607	TGL	CA2-CA1-OG1-CG1
25	T	101	PEK	C22-C21-O03-C01
25	T	101	PEK	C29-C30-C31-C32
24	P	303	DMU	O16-C18-C19-C22
20	P	305	CDL	C51-CB5-OB6-CB4
20	C	304	CDL	C51-CB5-OB6-CB4
22	C	305	CHD	C21-C20-C22-C23
24	Q	201	DMU	C3-C4-C57-O61
22	J	101	CHD	C16-C17-C20-C21
19	A	608	TGL	CA2-CA1-OG1-CG1
24	Q	201	DMU	O5-C4-C57-O61
20	P	305	CDL	OB7-CB5-OB6-CB4
25	T	101	PEK	O04-C21-O03-C01
20	P	305	CDL	C31-CA7-OA8-CA6
23	B	304	PSC	C20-C19-O03-C01
22	C	305	CHD	C17-C20-C22-C23
19	D	201	TGL	C20-C21-C22-C23
18	P	302	PGV	O12-C04-C05-C06
20	C	304	CDL	CB2-C1-CA2-OA2
20	C	304	CDL	OB7-CB5-OB6-CB4
20	G	102	CDL	C71-CB7-OB8-CB6
24	P	303	DMU	O5-C4-C57-O61
18	N	606	PGV	O12-C04-C05-O05
20	G	102	CDL	O1-C1-CB2-OB2
20	A	609	CDL	O1-C1-CB2-OB2
20	G	102	CDL	CB7-C71-C72-C73
20	G	102	CDL	OB6-CB4-CB6-OB8
23	B	304	PSC	O04-C19-O03-C01
19	A	608	TGL	CC2-CC3-CC4-CC5
23	B	304	PSC	C1-C2-C3-C4
20	G	102	CDL	OB9-CB7-OB8-CB6
24	C	301	DMU	O6-C11-C9-O1
19	B	301	TGL	CA2-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
18	A	607	PGV	C1-C2-C3-C4
19	B	301	TGL	CC1-CC2-CC3-CC4
23	B	304	PSC	C19-C20-C21-C22
19	D	201	TGL	CC1-CC2-CC3-CC4
22	P	306	CHD	C17-C20-C22-C23
20	G	102	CDL	C31-C32-C33-C34
18	A	606	PGV	C19-C20-C21-C22
19	A	608	TGL	CB1-CB2-CB3-CB4
22	J	101	CHD	C13-C17-C20-C21
20	A	609	CDL	C79-C80-C81-C82
22	P	306	CHD	C21-C20-C22-C23
18	A	607	PGV	O12-C04-C05-O05
20	C	304	CDL	O1-C1-CA2-OA2
22	W	101	CHD	C13-C17-C20-C21
20	P	305	CDL	OA9-CA7-OA8-CA6
18	P	304	PGV	C12-C13-C14-C15
24	M	101	DMU	O16-C18-C19-C22
19	A	608	TGL	C20-C21-C22-C23
24	C	301	DMU	O1-C10-O7-C3
19	B	301	TGL	OA1-CA1-OG1-CG1
18	C	307	PGV	C2-C1-O01-C02
23	B	304	PSC	C2-C1-O01-C02
25	G	101	PEK	C2-C1-O01-C02
18	A	607	PGV	C03-O11-P-O12
18	A	607	PGV	C04-O12-P-O11
18	C	307	PGV	C03-O11-P-O12
23	B	304	PSC	C03-O11-P-O12
25	P	309	PEK	C03-O11-P-O12
25	P	309	PEK	C04-O12-P-O11
18	P	302	PGV	C03-O11-P-O12
20	G	102	CDL	CA3-OA5-PA1-OA2
20	C	304	CDL	CA2-OA2-PA1-OA5
20	C	304	CDL	CA3-OA5-PA1-OA2
20	C	304	CDL	CB3-OB5-PB2-OB2
20	A	609	CDL	CA3-OA5-PA1-OA2
20	P	305	CDL	CB2-C1-CA2-OA2
18	C	307	PGV	O02-C1-O01-C02
25	G	101	PEK	O02-C1-O01-C02
23	N	608	PSC	C04-C05-N-C06
23	N	608	PSC	C04-C05-N-C08
20	A	609	CDL	C31-CA7-OA8-CA6
25	G	103	PEK	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
22	P	306	CHD	C20-C22-C23-C24
18	C	303	PGV	C12-C13-C14-C15
20	C	304	CDL	C12-C13-C14-C15
19	Y	101	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	CA6-CA7-CA8-CA9
19	D	201	TGL	CB6-CB7-CB8-CB9
18	P	302	PGV	C29-C30-C31-C32
19	B	301	TGL	CA4-CA5-CA6-CA7
20	A	609	CDL	C17-C18-C19-C20
19	N	607	TGL	CC6-CC7-CC8-CC9
19	N	607	TGL	C23-C24-C25-C26
18	C	307	PGV	C26-C27-C28-C29
18	N	606	PGV	C25-C26-C27-C28
19	V	101	TGL	CB6-CB7-CB8-CB9
19	V	101	TGL	CC5-CC6-CC7-CC8
25	G	101	PEK	C34-C35-C36-C37
18	P	302	PGV	C4-C5-C6-C7
19	A	608	TGL	C11-C10-CB9-CB8
20	C	304	CDL	C53-C54-C55-C56
20	A	609	CDL	C77-C78-C79-C80
25	G	103	PEK	C01-C02-O01-C1
19	V	101	TGL	CG1-CG2-OG2-CB1
23	B	304	PSC	O02-C1-O01-C02
19	Y	101	TGL	OB1-CB1-OG2-CG2
19	A	608	TGL	CC1-CC2-CC3-CC4
25	T	101	PEK	C25-C26-C27-C28
18	C	303	PGV	C22-C23-C24-C25
18	N	606	PGV	C14-C15-C16-C17
25	C	302	PEK	C24-C25-C26-C27
25	G	101	PEK	C30-C31-C32-C33
19	B	301	TGL	C11-C12-C13-C14
20	C	304	CDL	C34-C35-C36-C37
25	P	308	PEK	C23-C24-C25-C26
25	G	101	PEK	C29-C30-C31-C32
18	P	302	PGV	C24-C25-C26-C27
20	G	102	CDL	C15-C16-C17-C18
19	A	608	TGL	C21-C20-CA9-CA8
20	P	305	CDL	C54-C55-C56-C57
18	A	606	PGV	C21-C22-C23-C24
19	B	301	TGL	CC4-CC5-CC6-CC7
20	C	304	CDL	C59-C60-C61-C62
19	N	607	TGL	CC7-CC8-CC9-C15

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Mol	Chain	Res	Type	Atoms
20	P	305	CDL	C59-C60-C61-C62
20	G	102	CDL	C75-C76-C77-C78
20	C	304	CDL	C75-C76-C77-C78
18	A	607	PGV	C22-C23-C24-C25
18	A	607	PGV	C26-C27-C28-C29
18	N	606	PGV	C2-C3-C4-C5
25	C	302	PEK	C27-C28-C29-C30
19	Y	101	TGL	C12-C13-C14-C29
18	P	304	PGV	C7-C8-C9-C10
19	D	201	TGL	CB5-CB6-CB7-CB8
20	G	102	CDL	C18-C19-C20-C21
20	G	102	CDL	C39-C40-C41-C42
19	A	608	TGL	CA6-CA7-CA8-CA9
19	A	608	TGL	CC9-C15-C16-C17
20	C	304	CDL	C58-C59-C60-C61
23	N	608	PSC	C19-C20-C21-C22
19	N	607	TGL	C15-C16-C17-C18
20	P	305	CDL	C75-C76-C77-C78
19	D	201	TGL	CB2-CB3-CB4-CB5
25	P	309	PEK	C34-C35-C36-C37
19	B	301	TGL	CA9-C20-C21-C22
19	D	201	TGL	C15-C16-C17-C18
19	B	301	TGL	C20-C21-C22-C23
18	N	606	PGV	C04-C05-C06-O06
19	N	607	TGL	C21-C22-C23-C24
18	C	303	PGV	C25-C26-C27-C28
24	M	101	DMU	C31-C34-C37-C40
19	V	101	TGL	CC3-CC4-CC5-CC6
19	D	201	TGL	CC2-CC3-CC4-CC5
25	G	101	PEK	C27-C28-C29-C30
20	G	102	CDL	C14-C15-C16-C17
20	C	304	CDL	C78-C79-C80-C81
24	M	101	DMU	C3-C4-C57-O61
18	N	606	PGV	C11-C10-C9-C8
18	A	606	PGV	C11-C10-C9-C8
25	P	309	PEK	C2-C3-C4-C5
18	P	301	PGV	C19-C20-C21-C22
19	N	607	TGL	C24-C25-C26-C27
20	P	305	CDL	C37-C38-C39-C40
23	B	304	PSC	C3-C4-C5-C6
25	C	302	PEK	C25-C26-C27-C28
20	G	102	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
20	G	102	CDL	C43-C44-C45-C46
19	B	301	TGL	CB4-CB5-CB6-CB7
19	A	608	TGL	CB5-CB6-CB7-CB8
24	C	301	DMU	O5-C6-O16-C18
25	G	103	PEK	C34-C35-C36-C37
19	Y	101	TGL	C24-C25-C26-C27
19	V	101	TGL	CC7-CC8-CC9-C15
20	G	102	CDL	C54-C55-C56-C57
19	A	608	TGL	CC6-CC7-CC8-CC9
20	P	305	CDL	C43-C44-C45-C46
19	Y	101	TGL	C13-C14-C29-C30
19	B	301	TGL	CA7-CA8-CA9-C20
20	P	305	CDL	CB7-C71-C72-C73
20	A	609	CDL	CB7-C71-C72-C73
23	B	304	PSC	C2-C3-C4-C5
23	B	304	PSC	C29-C30-C31-C32
20	C	304	CDL	C71-CB7-OB8-CB6
20	P	305	CDL	C38-C39-C40-C41
18	C	307	PGV	C3-C4-C5-C6
25	G	103	PEK	C27-C28-C29-C30
19	D	201	TGL	CA9-C20-C21-C22
19	A	608	TGL	CA2-CA3-CA4-CA5
20	C	304	CDL	C36-C37-C38-C39
18	C	307	PGV	C24-C25-C26-C27
18	P	302	PGV	C23-C24-C25-C26
19	N	607	TGL	CC3-CC4-CC5-CC6
20	P	305	CDL	C17-C18-C19-C20
25	T	101	PEK	C28-C29-C30-C31
19	Y	101	TGL	CC4-CC5-CC6-CC7
20	A	609	CDL	C37-C38-C39-C40
20	G	102	CDL	C80-C81-C82-C83
19	Y	101	TGL	C10-C11-C12-C13
20	A	609	CDL	C36-C37-C38-C39
20	A	609	CDL	OA9-CA7-OA8-CA6
18	N	606	PGV	C7-C8-C9-C10
19	D	201	TGL	CA3-CA4-CA5-CA6
19	Y	101	TGL	CA3-CA4-CA5-CA6
20	G	102	CDL	C20-C21-C22-C23
20	A	609	CDL	C15-C16-C17-C18
18	C	303	PGV	C11-C10-C9-C8
18	P	304	PGV	C11-C10-C9-C8
19	B	301	TGL	CA1-CA2-CA3-CA4

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Mol	Chain	Res	Type	Atoms
25	T	101	PEK	C34-C35-C36-C37
20	A	609	CDL	CB5-C51-C52-C53
18	N	606	PGV	C22-C23-C24-C25
18	P	304	PGV	C2-C3-C4-C5
18	C	307	PGV	C14-C15-C16-C17
24	M	101	DMU	C19-C22-C25-C28
25	G	103	PEK	C29-C30-C31-C32
19	V	101	TGL	CA5-CA6-CA7-CA8
24	P	303	DMU	C19-C22-C25-C28
18	A	606	PGV	C13-C14-C15-C16
19	A	608	TGL	CC3-CC4-CC5-CC6
20	A	609	CDL	C16-C17-C18-C19
20	C	304	CDL	CA5-C11-C12-C13
19	Y	101	TGL	C16-C15-CC9-CC8
20	A	609	CDL	C51-CB5-OB6-CB4
20	G	102	CDL	C11-C12-C13-C14
19	A	608	TGL	CB3-CB4-CB5-CB6
20	C	304	CDL	OB9-CB7-OB8-CB6
19	N	607	TGL	CB1-CB2-CB3-CB4
18	C	307	PGV	C1-C2-C3-C4
18	C	303	PGV	C1-C2-C3-C4
18	P	304	PGV	C3-C4-C5-C6
23	N	608	PSC	C29-C30-C31-C32
18	P	302	PGV	C14-C15-C16-C17
19	V	101	TGL	C18-C19-C33-C34
20	C	304	CDL	C13-C14-C15-C16
20	C	304	CDL	C37-C38-C39-C40
18	A	607	PGV	C11-C10-C9-C8
23	N	608	PSC	O02-C1-O01-C02
19	Y	101	TGL	CA1-CA2-CA3-CA4
18	C	307	PGV	C20-C19-O03-C01
20	A	609	CDL	C53-C54-C55-C56
19	N	607	TGL	C17-C18-C19-C33
20	P	305	CDL	C19-C20-C21-C22
25	T	101	PEK	C26-C27-C28-C29
19	N	607	TGL	CC2-CC3-CC4-CC5
20	P	305	CDL	C14-C15-C16-C17
20	A	609	CDL	C52-C53-C54-C55
25	P	309	PEK	C28-C29-C30-C31
18	P	302	PGV	C26-C27-C28-C29
20	G	102	CDL	C55-C56-C57-C58
19	A	608	TGL	C18-C19-C33-C34

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Mol	Chain	Res	Type	Atoms
19	N	607	TGL	C12-C13-C14-C29
19	N	607	TGL	C20-C21-C22-C23
19	B	301	TGL	CC9-C15-C16-C17
20	A	609	CDL	C58-C59-C60-C61
23	N	608	PSC	C2-C1-O01-C02
19	B	301	TGL	CB2-CB1-OG2-CG2
25	G	101	PEK	C16-C17-C18-C19
19	B	301	TGL	CA5-CA6-CA7-CA8
20	P	305	CDL	C53-C54-C55-C56
25	G	101	PEK	C32-C33-C34-C35
25	P	309	PEK	C33-C34-C35-C36
19	B	301	TGL	C16-C15-CC9-CC8
18	P	302	PGV	O03-C01-C02-O01
19	Y	101	TGL	CC2-CC3-CC4-CC5
19	V	101	TGL	CA7-CA8-CA9-C20
18	C	307	PGV	C11-C10-C9-C8
18	C	307	PGV	C12-C13-C14-C15
25	P	308	PEK	C2-C3-C4-C5
18	A	606	PGV	C12-C13-C14-C15
24	C	301	DMU	C5-C10-O7-C3
20	C	304	CDL	C55-C56-C57-C58
18	A	606	PGV	C02-C01-O03-C19
18	P	302	PGV	C20-C21-C22-C23
19	B	301	TGL	CC2-CC3-CC4-CC5
24	P	303	DMU	C3-C4-C57-O61
24	M	101	DMU	O5-C4-C57-O61
19	B	301	TGL	OB1-CB1-OG2-CG2
20	A	609	CDL	OB7-CB5-OB6-CB4
20	P	305	CDL	C11-C12-C13-C14
20	P	305	CDL	C40-C41-C42-C43
24	C	301	DMU	C25-C28-C31-C34
19	A	608	TGL	C12-C13-C14-C29
20	P	305	CDL	CA2-OA2-PA1-OA5
20	P	305	CDL	CB3-OB5-PB2-OB2
25	T	101	PEK	C04-O12-P-O11
25	G	103	PEK	C03-O11-P-O12
25	G	103	PEK	C04-O12-P-O11
19	Y	101	TGL	CB9-C10-C11-C12
20	A	609	CDL	C22-C23-C24-C25
20	G	102	CDL	CB4-CB3-OB5-PB2
18	A	607	PGV	C5-C6-C7-C8
19	Y	101	TGL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	A	607	PGV	C01-C02-C03-O11
25	G	103	PEK	C01-C02-C03-O11
25	G	101	PEK	C01-C02-C03-O11
18	P	302	PGV	C01-C02-C03-O11
20	C	304	CDL	OB5-CB3-CB4-CB6
20	A	609	CDL	OB5-CB3-CB4-CB6
19	V	101	TGL	CA3-CA4-CA5-CA6
19	V	101	TGL	CB1-CB2-CB3-CB4
18	N	606	PGV	C23-C24-C25-C26
25	G	103	PEK	C16-C17-C18-C19
25	P	309	PEK	C24-C25-C26-C27
18	P	302	PGV	C12-C13-C14-C15
20	G	102	CDL	CA2-C1-CB2-OB2
18	P	301	PGV	C14-C15-C16-C17
18	C	303	PGV	C24-C25-C26-C27
19	V	101	TGL	CB9-C10-C11-C12
20	C	304	CDL	C21-C22-C23-C24
20	C	304	CDL	C72-C73-C74-C75
18	C	307	PGV	O04-C19-O03-C01
19	D	201	TGL	CA2-CA3-CA4-CA5
20	G	102	CDL	C13-C14-C15-C16
20	A	609	CDL	C82-C83-C84-C85
25	T	101	PEK	O03-C01-C02-C03
18	C	307	PGV	O03-C01-C02-C03
19	V	101	TGL	OG1-CG1-CG2-CG3
19	D	201	TGL	OG1-CG1-CG2-CG3
25	P	309	PEK	O03-C01-C02-C03
20	G	102	CDL	CB3-CB4-CB6-OB8
23	N	608	PSC	C23-C24-C25-C26
24	C	301	DMU	C34-C37-C40-C43
19	D	201	TGL	C21-C22-C23-C24
20	G	102	CDL	C64-C65-C66-C67
23	N	608	PSC	C31-C32-C33-C34
19	V	101	TGL	C16-C17-C18-C19
18	P	304	PGV	C15-C16-C17-C18
19	V	101	TGL	CB3-CB4-CB5-CB6
19	N	607	TGL	CA9-C20-C21-C22
20	A	609	CDL	C60-C61-C62-C63
18	A	607	PGV	C12-C13-C14-C15
25	G	103	PEK	C2-C3-C4-C5
18	C	307	PGV	C28-C29-C30-C31
19	Y	101	TGL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	N	607	TGL	C33-C34-C35-C36
25	C	302	PEK	C22-C21-O03-C01
18	A	607	PGV	C20-C21-C22-C23
20	A	609	CDL	C61-C62-C63-C64
23	B	304	PSC	C31-C32-C33-C34
18	C	307	PGV	C23-C24-C25-C26
20	C	304	CDL	CA4-CA3-OA5-PA1
23	N	608	PSC	C4-C5-C6-C7
20	G	102	CDL	C35-C36-C37-C38
20	G	102	CDL	C62-C63-C64-C65
20	A	609	CDL	C42-C43-C44-C45
25	C	302	PEK	C26-C27-C28-C29
19	Y	101	TGL	C33-C34-C35-C36
20	A	609	CDL	C20-C21-C22-C23
19	N	607	TGL	C10-C11-C12-C13
19	B	301	TGL	C25-C26-C27-C28
25	P	309	PEK	C35-C36-C37-C38
24	P	303	DMU	C1-C6-O16-C18
25	P	309	PEK	O03-C01-C02-O01
20	C	304	CDL	OB6-CB4-CB6-OB8
20	G	102	CDL	C61-C62-C63-C64
18	A	607	PGV	C7-C8-C9-C10
18	P	302	PGV	C6-C7-C8-C9
20	C	304	CDL	C16-C17-C18-C19
18	C	307	PGV	C13-C14-C15-C16
24	C	301	DMU	C31-C34-C37-C40
20	C	304	CDL	C24-C25-C26-C27
18	A	607	PGV	O12-C04-C05-C06
18	C	307	PGV	O12-C04-C05-C06
25	P	308	PEK	C22-C21-O03-C01
20	G	102	CDL	C40-C41-C42-C43
20	P	305	CDL	OA5-CA3-CA4-CA6
18	N	606	PGV	C19-C20-C21-C22
20	G	102	CDL	C56-C57-C58-C59
20	C	304	CDL	C79-C80-C81-C82
19	D	201	TGL	CA2-CA1-OG1-CG1
20	P	305	CDL	C36-C37-C38-C39
25	G	101	PEK	C1-C2-C3-C4
20	C	304	CDL	CA7-C31-C32-C33
20	P	305	CDL	C79-C80-C81-C82
25	G	103	PEK	C22-C21-O03-C01
20	P	305	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
18	N	606	PGV	C3-C4-C5-C6
25	P	309	PEK	C23-C24-C25-C26
18	P	302	PGV	C21-C22-C23-C24
18	P	304	PGV	C02-C03-O11-P
20	A	609	CDL	C1-CB2-OB2-PB2
20	G	102	CDL	C73-C74-C75-C76
20	G	102	CDL	C57-C58-C59-C60
19	B	301	TGL	CB2-CB3-CB4-CB5
20	C	304	CDL	C56-C57-C58-C59
19	A	608	TGL	CA9-C20-C21-C22
19	N	607	TGL	CG1-CG2-CG3-OG3
19	D	201	TGL	CG1-CG2-CG3-OG3
18	P	302	PGV	O03-C01-C02-C03
20	G	102	CDL	CA3-CA4-CA6-OA8
18	C	303	PGV	C20-C21-C22-C23
20	A	609	CDL	C39-C40-C41-C42
20	A	609	CDL	C51-C52-C53-C54
19	Y	101	TGL	CB4-CB5-CB6-CB7
19	B	301	TGL	C13-C14-C29-C30
18	P	301	PGV	C29-C30-C31-C32
25	P	309	PEK	C16-C17-C18-C19
20	G	102	CDL	C59-C60-C61-C62
25	T	101	PEK	C12-C13-C14-C15
23	B	304	PSC	C9-C10-C11-C12
23	B	304	PSC	C10-C11-C12-C13
25	C	302	PEK	C6-C7-C8-C9
25	C	302	PEK	C11-C12-C13-C14
25	G	103	PEK	C11-C10-C9-C8
25	G	103	PEK	C11-C12-C13-C14
25	P	308	PEK	C6-C7-C8-C9
25	G	101	PEK	C11-C10-C9-C8
23	N	608	PSC	C9-C10-C11-C12
23	N	608	PSC	C10-C11-C12-C13
25	P	309	PEK	C11-C12-C13-C14
24	Q	201	DMU	C22-C25-C28-C31
20	G	102	CDL	C63-C64-C65-C66
20	A	609	CDL	C62-C63-C64-C65
18	P	302	PGV	O05-C05-C06-O06
25	C	302	PEK	C32-C33-C34-C35
20	C	304	CDL	OA5-CA3-CA4-OA6
20	A	609	CDL	OB5-CB3-CB4-OB6
20	A	609	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
20	P	305	CDL	CA5-C11-C12-C13
18	P	302	PGV	C5-C6-C7-C8
20	G	102	CDL	C38-C39-C40-C41
19	A	608	TGL	C22-C23-C24-C25
19	V	101	TGL	C21-C20-CA9-CA8
25	C	302	PEK	O04-C21-O03-C01
20	P	305	CDL	C24-C25-C26-C27
18	P	302	PGV	C22-C23-C24-C25
18	A	607	PGV	O03-C01-C02-O01
20	P	305	CDL	OB6-CB4-CB6-OB8
19	D	201	TGL	OG2-CG2-CG3-OG3
20	G	102	CDL	OA6-CA4-CA6-OA8
18	A	607	PGV	C2-C3-C4-C5
20	C	304	CDL	C23-C24-C25-C26
20	G	102	CDL	C72-C73-C74-C75
25	G	103	PEK	C17-C18-C19-C20
19	B	301	TGL	CC7-CC8-CC9-C15
19	D	201	TGL	CB4-CB5-CB6-CB7
25	C	302	PEK	C16-C17-C18-C19
19	Y	101	TGL	C11-C10-CB9-CB8
20	P	305	CDL	CA4-CA3-OA5-PA1
20	A	609	CDL	C1-CA2-OA2-PA1
23	B	304	PSC	C26-C27-C28-C29
19	Y	101	TGL	C23-C24-C25-C26
25	P	309	PEK	C25-C26-C27-C28
20	A	609	CDL	C23-C24-C25-C26
19	D	201	TGL	CC6-CC7-CC8-CC9
19	Y	101	TGL	CC1-CC2-CC3-CC4
18	P	301	PGV	C30-C31-C32-C33
18	C	303	PGV	C7-C8-C9-C10
18	C	303	PGV	C27-C28-C29-C30
24	M	101	DMU	C22-C25-C28-C31
18	N	606	PGV	C28-C29-C30-C31
19	B	301	TGL	C21-C20-CA9-CA8
20	P	305	CDL	C58-C59-C60-C61
18	N	606	PGV	C01-C02-C03-O11
20	G	102	CDL	OB5-CB3-CB4-CB6
20	C	304	CDL	OA5-CA3-CA4-CA6
25	G	103	PEK	C3-C4-C5-C6
25	G	103	PEK	O04-C21-O03-C01
25	C	302	PEK	C23-C24-C25-C26
20	P	305	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
20	P	305	CDL	C41-C42-C43-C44
25	T	101	PEK	C32-C33-C34-C35
24	C	301	DMU	O16-C18-C19-C22
25	C	302	PEK	C22-C23-C24-C25
20	P	305	CDL	CA3-CA4-OA6-CA5
18	N	606	PGV	C21-C22-C23-C24
18	P	302	PGV	C7-C8-C9-C10
23	N	608	PSC	C14-C15-C16-C17
19	A	608	TGL	CC7-CC8-CC9-C15
20	C	304	CDL	C77-C78-C79-C80
18	N	606	PGV	C13-C14-C15-C16
19	Y	101	TGL	CA7-CA8-CA9-C20
19	V	101	TGL	C17-C18-C19-C33
25	T	101	PEK	C2-C3-C4-C5
18	A	607	PGV	C28-C29-C30-C31
20	P	305	CDL	CB3-CB4-CB6-OB8
25	P	308	PEK	O04-C21-O03-C01
18	N	606	PGV	C20-C21-C22-C23
20	G	102	CDL	C83-C84-C85-C86
25	T	101	PEK	O01-C02-C03-O11
18	N	606	PGV	O12-C04-C05-C06
20	P	305	CDL	C56-C57-C58-C59
23	B	304	PSC	C5-C6-C7-C8
20	A	609	CDL	C64-C65-C66-C67
25	P	308	PEK	C17-C18-C19-C20
19	A	608	TGL	CA3-CA4-CA5-CA6
25	G	103	PEK	O03-C01-C02-O01
25	P	309	PEK	C32-C33-C34-C35
19	V	101	TGL	CB2-CB3-CB4-CB5
18	P	301	PGV	C11-C10-C9-C8
25	C	302	PEK	C15-C16-C17-C18
20	P	305	CDL	C81-C82-C83-C84
23	N	608	PSC	C5-C6-C7-C8
18	A	606	PGV	C29-C30-C31-C32
20	G	102	CDL	C81-C82-C83-C84
19	D	201	TGL	OA1-CA1-OG1-CG1
18	P	302	PGV	C31-C32-C33-C34
20	G	102	CDL	C36-C37-C38-C39
18	P	304	PGV	C1-C2-C3-C4
19	D	201	TGL	CB1-CB2-CB3-CB4
19	A	608	TGL	CA7-CA8-CA9-C20
25	P	308	PEK	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
24	C	301	DMU	C22-C25-C28-C31
25	P	309	PEK	C29-C30-C31-C32
20	A	609	CDL	C56-C57-C58-C59
25	T	101	PEK	C03-O11-P-O12
18	C	307	PGV	C04-O12-P-O11
19	N	607	TGL	C14-C29-C30-C31
20	C	304	CDL	C1-CA2-OA2-PA1
19	B	301	TGL	CC3-CC4-CC5-CC6
18	A	607	PGV	C04-O12-P-O13
23	B	304	PSC	C03-O11-P-O13
18	N	606	PGV	C03-O11-P-O14
25	G	103	PEK	C03-O11-P-O13
25	G	103	PEK	C04-O12-P-O14
23	N	608	PSC	C03-O11-P-O13
25	P	309	PEK	C04-O12-P-O14
18	P	302	PGV	C03-O11-P-O13
18	P	302	PGV	C04-O12-P-O14
20	G	102	CDL	CA3-OA5-PA1-OA3
20	G	102	CDL	CB3-OB5-PB2-OB4
20	C	304	CDL	CA3-OA5-PA1-OA3
20	C	304	CDL	CB3-OB5-PB2-OB3
20	A	609	CDL	CA3-OA5-PA1-OA3
19	N	607	TGL	C18-C19-C33-C34
25	T	101	PEK	C01-C02-C03-O11
23	N	608	PSC	C01-C02-C03-O11
20	C	304	CDL	C84-C85-C86-C87
25	P	308	PEK	C21-C22-C23-C24
19	D	201	TGL	C24-C25-C26-C27
23	N	608	PSC	C21-C22-C23-C24
25	P	308	PEK	C1-C2-C3-C4
19	B	301	TGL	CB7-CB8-CB9-C10
18	A	607	PGV	O01-C02-C03-O11
18	N	606	PGV	O01-C02-C03-O11
25	G	103	PEK	O01-C02-C03-O11
25	G	101	PEK	O01-C02-C03-O11
23	N	608	PSC	O01-C02-C03-O11
18	P	302	PGV	O01-C02-C03-O11
18	P	302	PGV	C1-C2-C3-C4
20	G	102	CDL	OB5-CB3-CB4-OB6
19	Y	101	TGL	CC3-CC4-CC5-CC6
19	V	101	TGL	C14-C29-C30-C31
19	B	301	TGL	C17-C18-C19-C33

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Mol	Chain	Res	Type	Atoms
19	N	607	TGL	C16-C15-CC9-CC8
20	A	609	CDL	C21-C22-C23-C24
18	A	607	PGV	O03-C01-C02-C03
19	V	101	TGL	C10-C11-C12-C13
18	A	606	PGV	C26-C27-C28-C29
19	N	607	TGL	OG2-CG2-CG3-OG3
19	V	101	TGL	OG1-CG1-CG2-OG2
19	B	301	TGL	CB5-CB6-CB7-CB8
20	A	609	CDL	C41-C42-C43-C44
18	P	304	PGV	C11-C12-C13-C14
18	C	303	PGV	C02-C03-O11-P
23	B	304	PSC	C02-C03-O11-P
25	T	101	PEK	C31-C32-C33-C34
25	P	309	PEK	C22-C23-C24-C25
19	N	607	TGL	CB4-CB5-CB6-CB7
19	Y	101	TGL	CC5-CC6-CC7-CC8
19	D	201	TGL	CC7-CC8-CC9-C15
20	G	102	CDL	C33-C34-C35-C36
20	P	305	CDL	C55-C56-C57-C58
20	P	305	CDL	C13-C14-C15-C16
25	G	103	PEK	C35-C36-C37-C38
19	N	607	TGL	CA2-CA3-CA4-CA5
20	P	305	CDL	C51-C52-C53-C54
19	Y	101	TGL	CB6-CB7-CB8-CB9
25	T	101	PEK	C17-C18-C19-C20
20	C	304	CDL	C11-C12-C13-C14
18	A	607	PGV	C03-C02-O01-C1
19	B	301	TGL	CG1-CG2-OG2-CB1
19	A	608	TGL	OC1-CC1-OG3-CG3
19	V	101	TGL	CA2-CA1-OG1-CG1
20	G	102	CDL	C52-C53-C54-C55
20	A	609	CDL	C12-C13-C14-C15
19	N	607	TGL	OG1-CA1-CA2-CA3
18	P	301	PGV	C31-C32-C33-C34
20	A	609	CDL	C40-C41-C42-C43
18	C	307	PGV	C7-C8-C9-C10
18	P	304	PGV	C20-C21-C22-C23
25	G	101	PEK	C26-C27-C28-C29
18	P	302	PGV	C20-C19-O03-C01
19	V	101	TGL	OA1-CA1-OG1-CG1
18	P	302	PGV	O04-C19-O03-C01
19	N	607	TGL	CA4-CA5-CA6-CA7

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Mol	Chain	Res	Type	Atoms
20	A	609	CDL	C59-C60-C61-C62
18	N	606	PGV	O03-C19-C20-C21
20	A	609	CDL	C44-C45-C46-C47
19	V	101	TGL	C20-C21-C22-C23
19	D	201	TGL	CC4-CC5-CC6-CC7
23	N	608	PSC	C04-O12-P-O11
20	A	609	CDL	CB2-OB2-PB2-OB5
20	G	102	CDL	C41-C42-C43-C44
19	D	201	TGL	C16-C17-C18-C19
18	P	301	PGV	O03-C19-C20-C21
25	P	308	PEK	C32-C33-C34-C35
20	C	304	CDL	C18-C19-C20-C21
24	M	101	DMU	O6-C11-C9-O1
25	G	101	PEK	C17-C18-C19-C20
20	C	304	CDL	C40-C41-C42-C43
19	N	607	TGL	CB9-C10-C11-C12
18	C	307	PGV	C22-C23-C24-C25
20	C	304	CDL	C35-C36-C37-C38
20	G	102	CDL	O1-C1-CA2-OA2
25	C	302	PEK	C30-C31-C32-C33
24	P	303	DMU	C22-C25-C28-C31
23	N	608	PSC	C27-C28-C29-C30
19	Y	101	TGL	C21-C20-CA9-CA8
19	B	301	TGL	C12-C13-C14-C29
19	A	608	TGL	C10-C11-C12-C13
24	C	301	DMU	C18-C19-C22-C25
20	P	305	CDL	C15-C16-C17-C18
23	B	304	PSC	C6-C7-C8-C9
19	N	607	TGL	CA5-CA6-CA7-CA8
19	Y	101	TGL	CB1-CB2-CB3-CB4
19	A	608	TGL	CC2-CC1-OG3-CG3
19	B	301	TGL	C18-C19-C33-C34
25	P	308	PEK	O02-C1-O01-C02
25	P	309	PEK	C3-C4-C5-C6
20	P	305	CDL	C82-C83-C84-C85
20	C	304	CDL	C64-C65-C66-C67
18	C	307	PGV	C21-C22-C23-C24
18	P	304	PGV	C4-C5-C6-C7
19	D	201	TGL	CG3-CG2-OG2-CB1
23	B	304	PSC	C04-C05-N-C07
25	G	103	PEK	C9-C10-C11-C12
25	G	101	PEK	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	C	304	CDL	C81-C82-C83-C84
24	Q	201	DMU	C19-C22-C25-C28
20	C	304	CDL	C74-C75-C76-C77
19	D	201	TGL	C12-C13-C14-C29
19	Y	101	TGL	C17-C18-C19-C33
20	A	609	CDL	C13-C14-C15-C16
25	G	101	PEK	C22-C21-O03-C01
25	G	101	PEK	O04-C21-O03-C01
25	G	103	PEK	C28-C29-C30-C31
24	Q	201	DMU	C31-C34-C37-C40
20	C	304	CDL	C20-C21-C22-C23
25	P	308	PEK	O03-C01-C02-O01
19	N	607	TGL	C11-C10-CB9-CB8
20	C	304	CDL	C42-C43-C44-C45
20	C	304	CDL	C51-C52-C53-C54
20	A	609	CDL	CA2-C1-CB2-OB2
25	P	308	PEK	C33-C34-C35-C36
19	B	301	TGL	C29-C30-C31-C32
22	B	303	CHD	C13-C17-C20-C22
19	Y	101	TGL	C11-C12-C13-C14
22	W	101	CHD	C17-C20-C22-C23
20	C	304	CDL	C57-C58-C59-C60
19	N	607	TGL	C21-C20-CA9-CA8
20	P	305	CDL	C72-C73-C74-C75
20	C	304	CDL	CB3-CB4-CB6-OB8
19	A	608	TGL	OG1-CA1-CA2-CA3
19	N	607	TGL	CB5-CB6-CB7-CB8
25	T	101	PEK	C3-C4-C5-C6
25	G	101	PEK	C3-C4-C5-C6
18	P	301	PGV	C13-C14-C15-C16
19	D	201	TGL	CB9-C10-C11-C12
18	P	302	PGV	C27-C28-C29-C30
18	N	606	PGV	O05-C05-C06-O06
24	M	101	DMU	C1-C6-O16-C18
23	B	304	PSC	C21-C22-C23-C24
25	C	302	PEK	C34-C35-C36-C37
19	D	201	TGL	C22-C23-C24-C25
24	Q	201	DMU	O6-C11-C9-C8
20	A	609	CDL	C32-C31-CA7-OA8
20	C	304	CDL	C12-C11-CA5-OA6
20	C	304	CDL	C83-C84-C85-C86
20	G	102	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	C14-C29-C30-C31
19	V	101	TGL	C21-C22-C23-C24
20	C	304	CDL	OA9-CA7-OA8-CA6
25	P	308	PEK	O03-C21-C22-C23
18	P	302	PGV	C9-C10-C11-C12
19	V	101	TGL	CC4-CC5-CC6-CC7
20	A	609	CDL	C75-C76-C77-C78
23	B	304	PSC	O01-C1-C2-C3
19	V	101	TGL	OG1-CA1-CA2-CA3
18	P	304	PGV	O03-C19-C20-C21
19	A	608	TGL	OG3-CC1-CC2-CC3
19	V	101	TGL	CA9-C20-C21-C22
19	Y	101	TGL	OG2-CB1-CB2-CB3
23	N	608	PSC	C12-C13-C14-C15
18	C	303	PGV	C30-C31-C32-C33
25	C	302	PEK	O03-C21-C22-C23
23	N	608	PSC	C04-C05-N-C07
19	B	301	TGL	CC5-CC6-CC7-CC8
25	P	308	PEK	C14-C15-C16-C17
19	D	201	TGL	C16-C15-CC9-CC8
18	P	304	PGV	C28-C29-C30-C31
19	V	101	TGL	CA2-CA3-CA4-CA5
25	G	101	PEK	C24-C25-C26-C27
23	N	608	PSC	O03-C01-C02-O01
20	C	304	CDL	C52-C51-CB5-OB6
20	C	304	CDL	C14-C15-C16-C17
18	P	304	PGV	C13-C14-C15-C16
19	B	301	TGL	CB9-C10-C11-C12
20	A	609	CDL	C52-C51-CB5-OB6
24	Q	201	DMU	C25-C28-C31-C34
19	D	201	TGL	C10-C11-C12-C13
20	A	609	CDL	C19-C20-C21-C22
18	A	606	PGV	C11-C12-C13-C14
20	P	305	CDL	C20-C21-C22-C23
23	N	608	PSC	O03-C19-C20-C21
19	A	608	TGL	OC1-CC1-CC2-CC3
18	A	607	PGV	C24-C25-C26-C27
18	A	607	PGV	C19-C20-C21-C22
23	B	304	PSC	O02-C1-C2-C3
20	C	304	CDL	C12-C11-CA5-OA7
20	C	304	CDL	C52-C51-CB5-OB7
20	C	304	CDL	C60-C61-C62-C63

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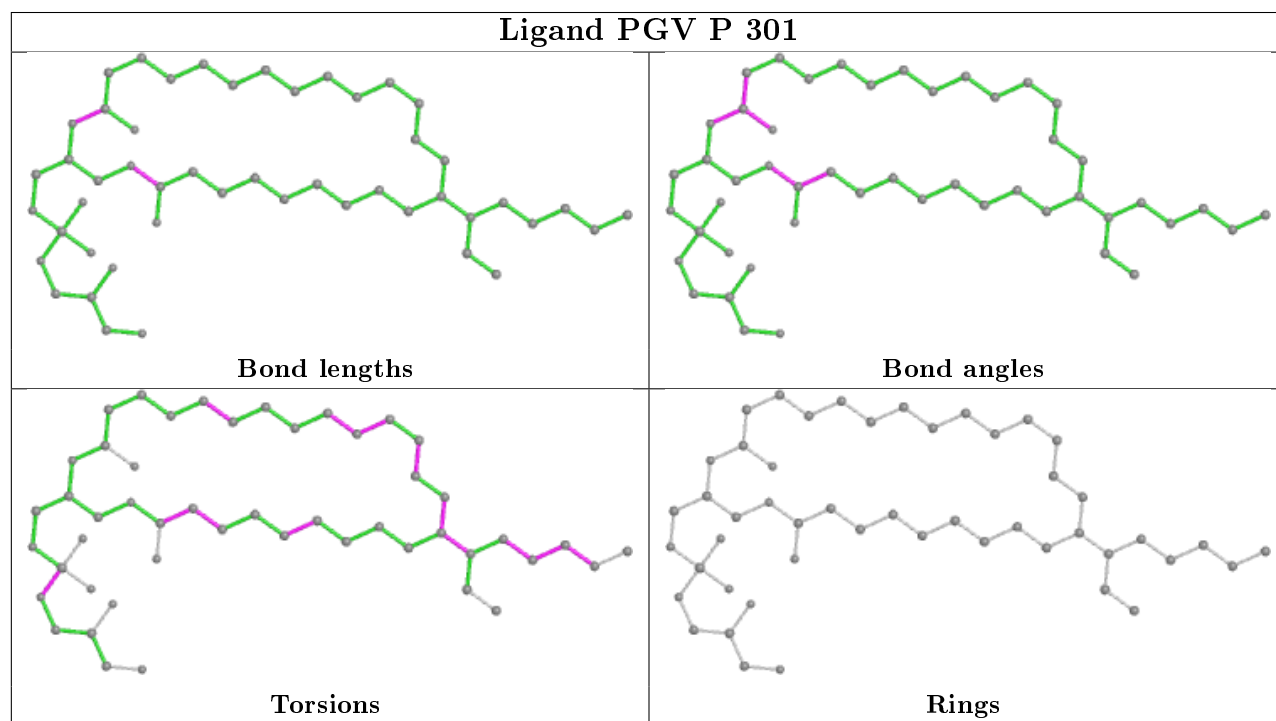
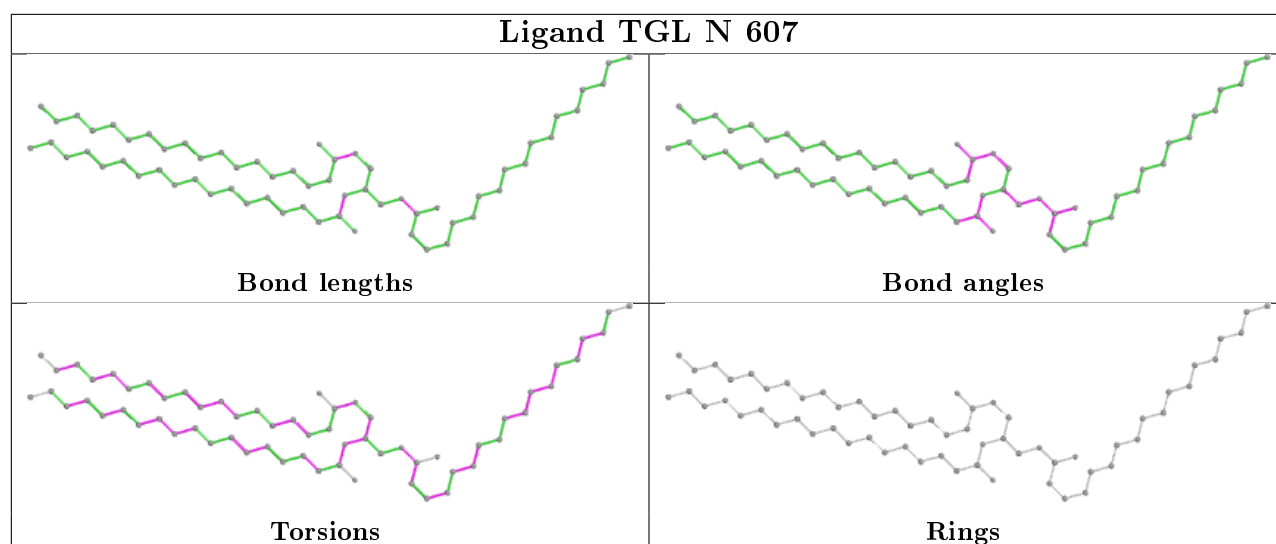
Mol	Chain	Res	Type	Atoms
20	P	305	CDL	C35-C36-C37-C38
19	B	301	TGL	CG2-CG1-OG1-CA1
25	C	302	PEK	O04-C21-C22-C23
19	Y	101	TGL	OB1-CB1-CB2-CB3
18	C	307	PGV	C20-C21-C22-C23
18	P	301	PGV	C04-O12-P-O13
20	P	305	CDL	CB3-OB5-PB2-OB4
19	Y	101	TGL	OG1-CG1-CG2-OG2
18	P	301	PGV	C22-C23-C24-C25
18	C	307	PGV	C29-C30-C31-C32
18	C	303	PGV	C31-C32-C33-C34
25	G	103	PEK	O12-C04-C05-N
19	V	101	TGL	OA1-CA1-CA2-CA3
20	A	609	CDL	C43-C44-C45-C46
19	D	201	TGL	OG3-CC1-CC2-CC3
19	A	608	TGL	CB9-C10-C11-C12
23	N	608	PSC	C3-C4-C5-C6
18	P	304	PGV	O04-C19-C20-C21
25	P	308	PEK	C34-C35-C36-C37
23	N	608	PSC	O04-C19-C20-C21
14	A	602	HEA	C26-C15-C16-C17
23	B	304	PSC	C05-C04-O12-P
19	A	608	TGL	C19-C33-C34-C35
18	P	301	PGV	C4-C5-C6-C7
20	P	305	CDL	C32-C33-C34-C35
19	Y	101	TGL	OG1-CA1-CA2-CA3
25	C	302	PEK	C31-C32-C33-C34
19	V	101	TGL	CA4-CA5-CA6-CA7
19	Y	101	TGL	OC1-CC1-CC2-CC3
19	D	201	TGL	CA4-CA5-CA6-CA7
18	C	303	PGV	O03-C19-C20-C21
19	Y	101	TGL	OG3-CC1-CC2-CC3
25	G	101	PEK	O01-C1-C2-C3
18	P	301	PGV	C9-C10-C11-C12
18	P	301	PGV	C11-C12-C13-C14
19	D	201	TGL	OC1-CC1-CC2-CC3
22	B	303	CHD	C16-C17-C20-C22
20	A	609	CDL	C52-C51-CB5-OB7
20	P	305	CDL	C12-C11-CA5-OA6
25	G	103	PEK	C31-C32-C33-C34
23	B	304	PSC	C12-C13-C14-C15

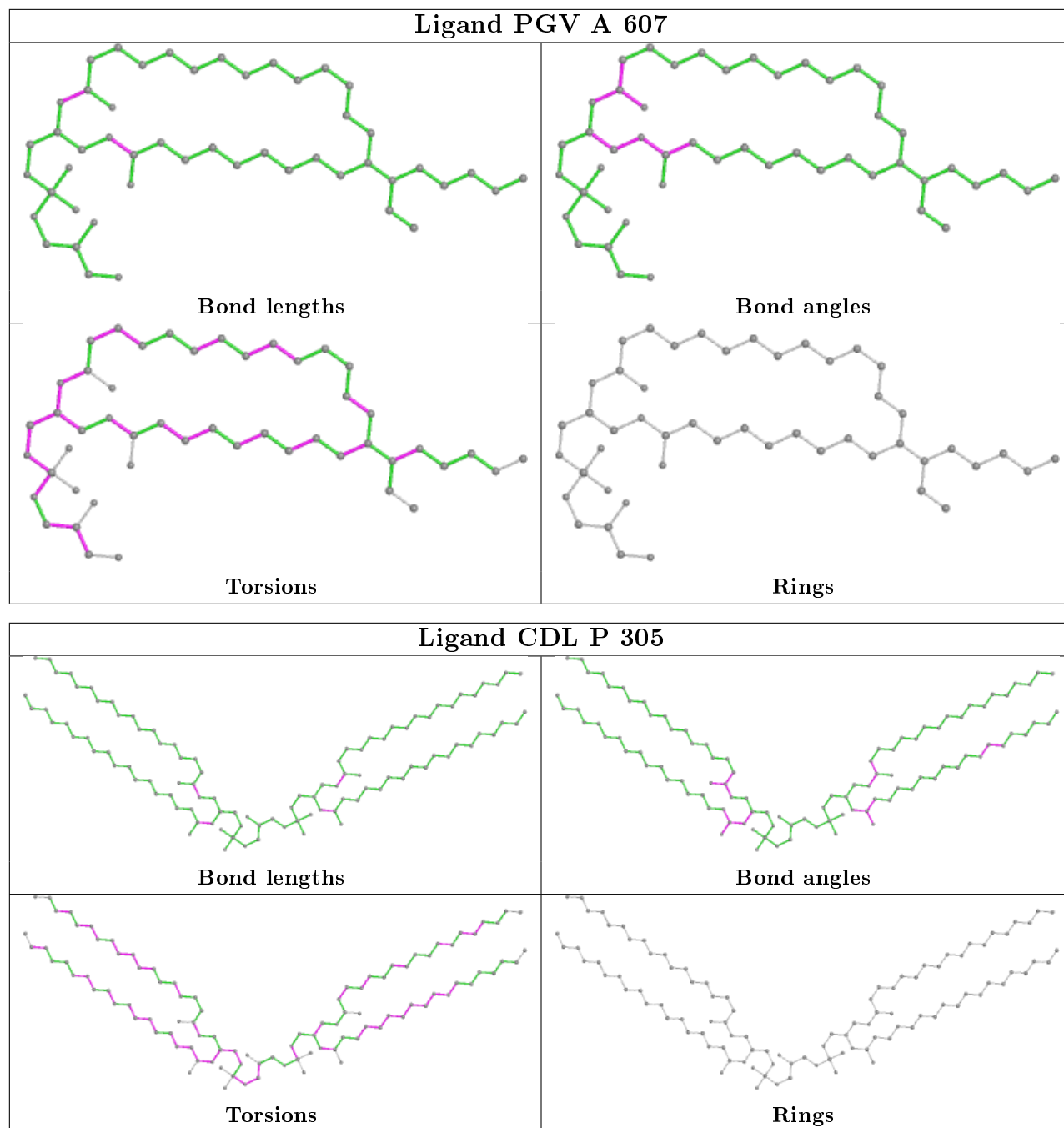
There are no ring outliers.

22 monomers are involved in 60 short contacts:

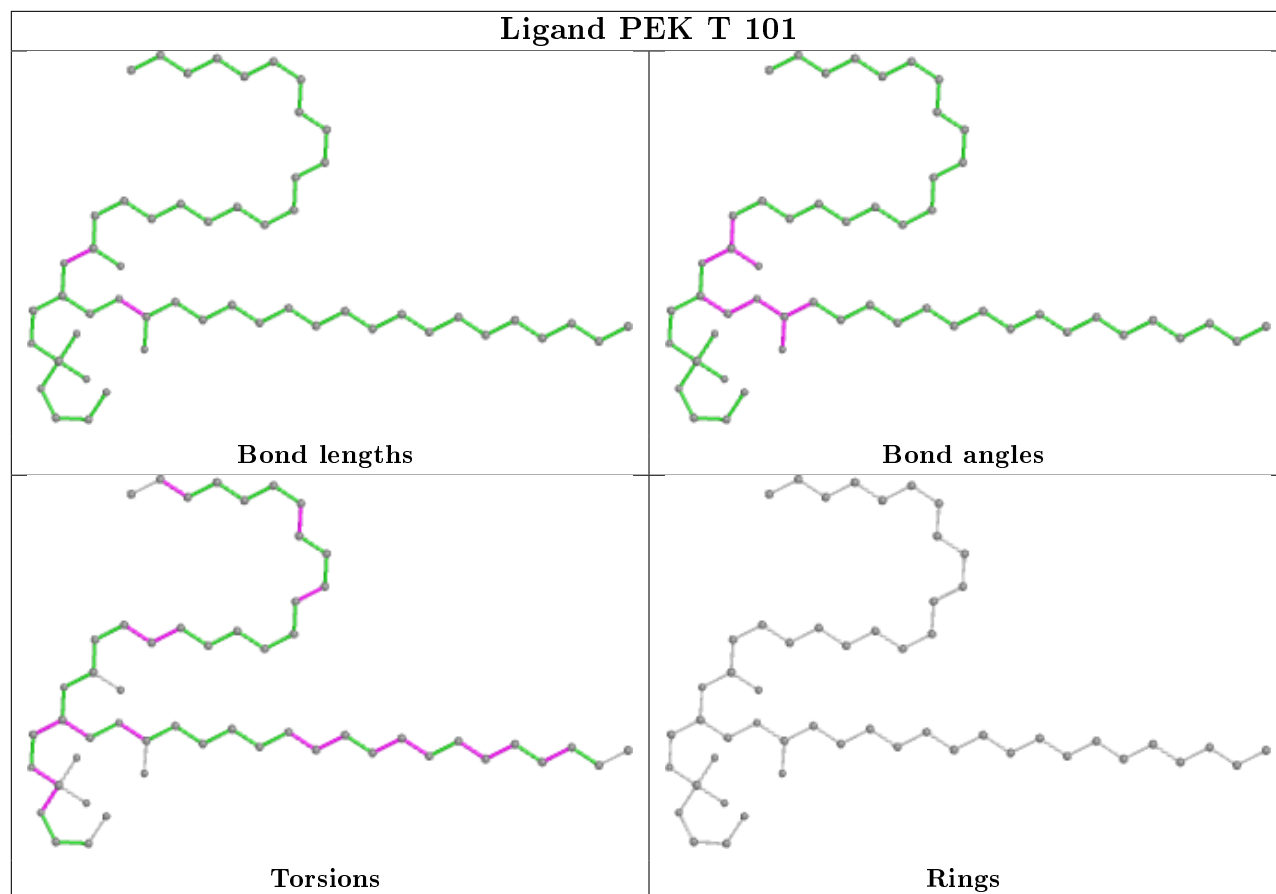
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	607	PGV	1	0
20	P	305	CDL	22	0
22	G	104	CHD	1	0
25	C	302	PEK	1	0
22	P	307	CHD	1	0
25	G	103	PEK	1	0
25	P	308	PEK	3	0
19	Y	101	TGL	1	0
19	V	101	TGL	3	0
24	P	303	DMU	1	0
24	C	301	DMU	2	0
24	Q	201	DMU	3	0
22	J	101	CHD	2	0
18	P	304	PGV	6	0
22	W	101	CHD	1	0
20	G	102	CDL	4	0
14	N	602	HEA	2	0
19	A	608	TGL	2	0
14	N	601	HEA	2	0
14	A	602	HEA	1	0
14	A	601	HEA	1	0
20	A	609	CDL	5	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.

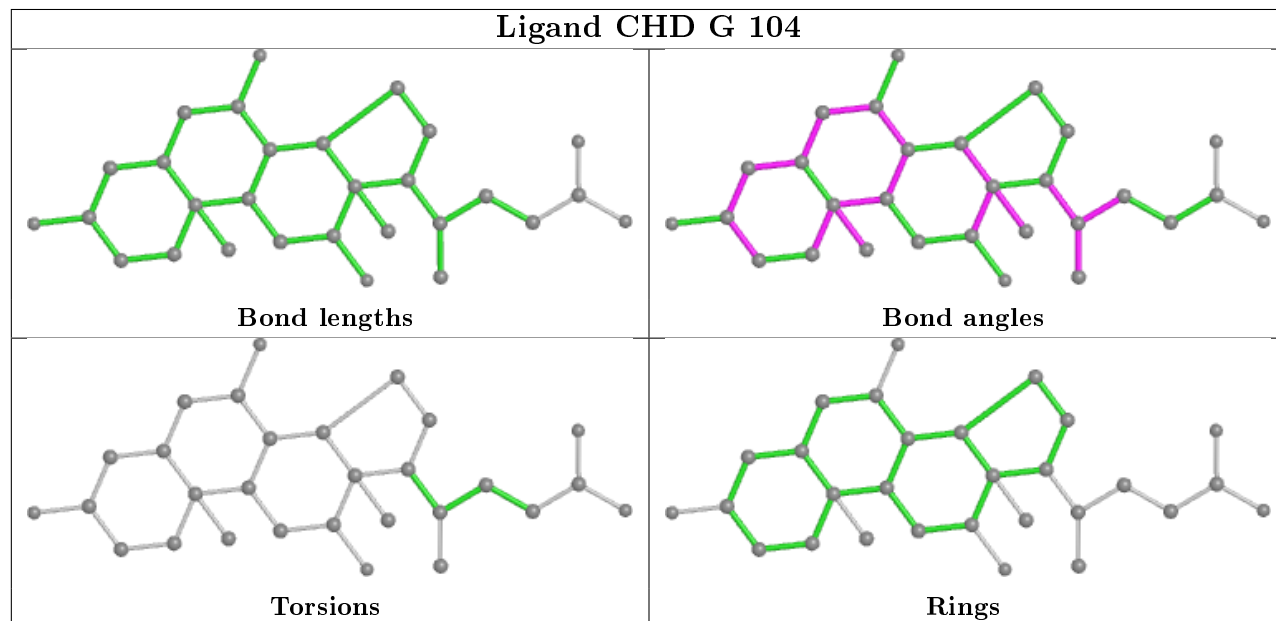


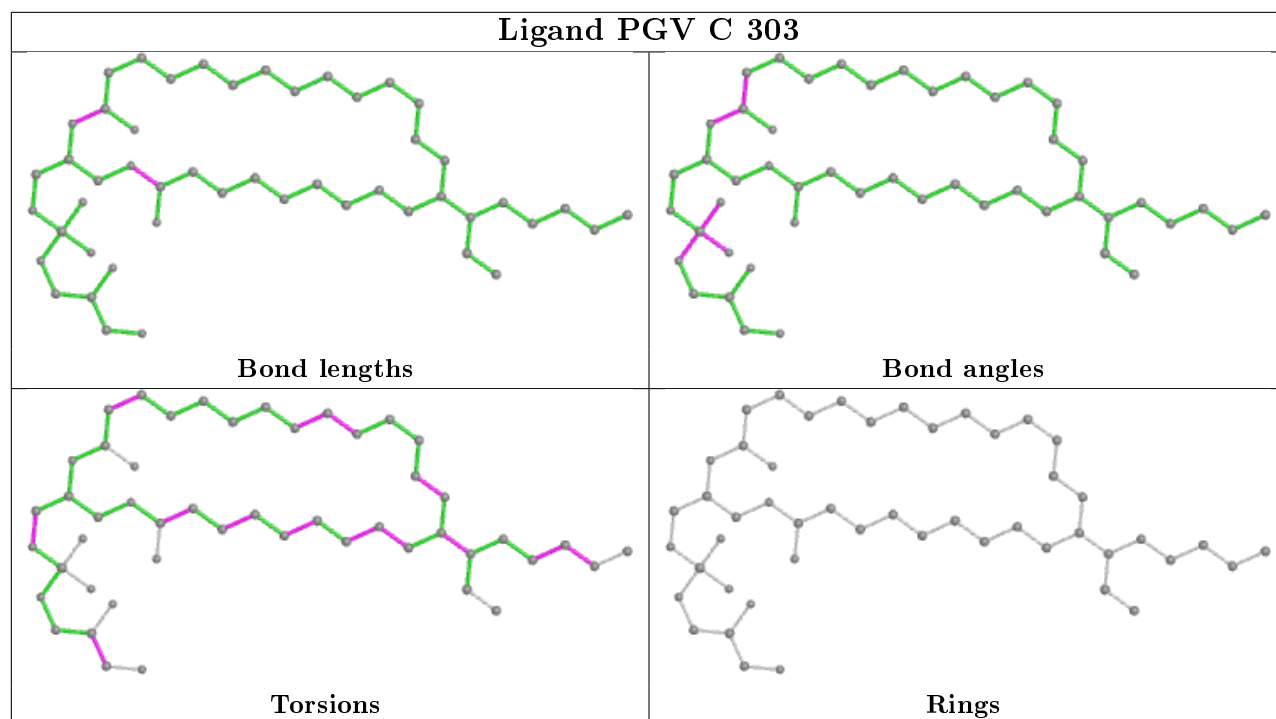
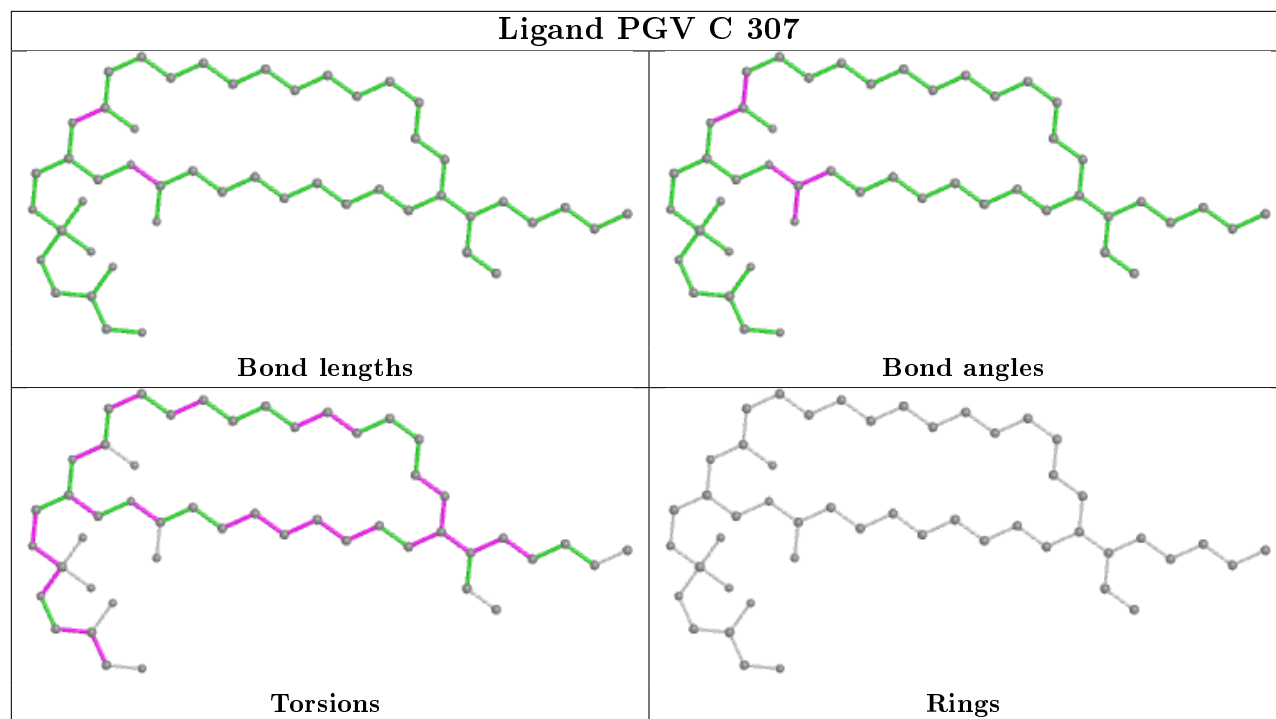


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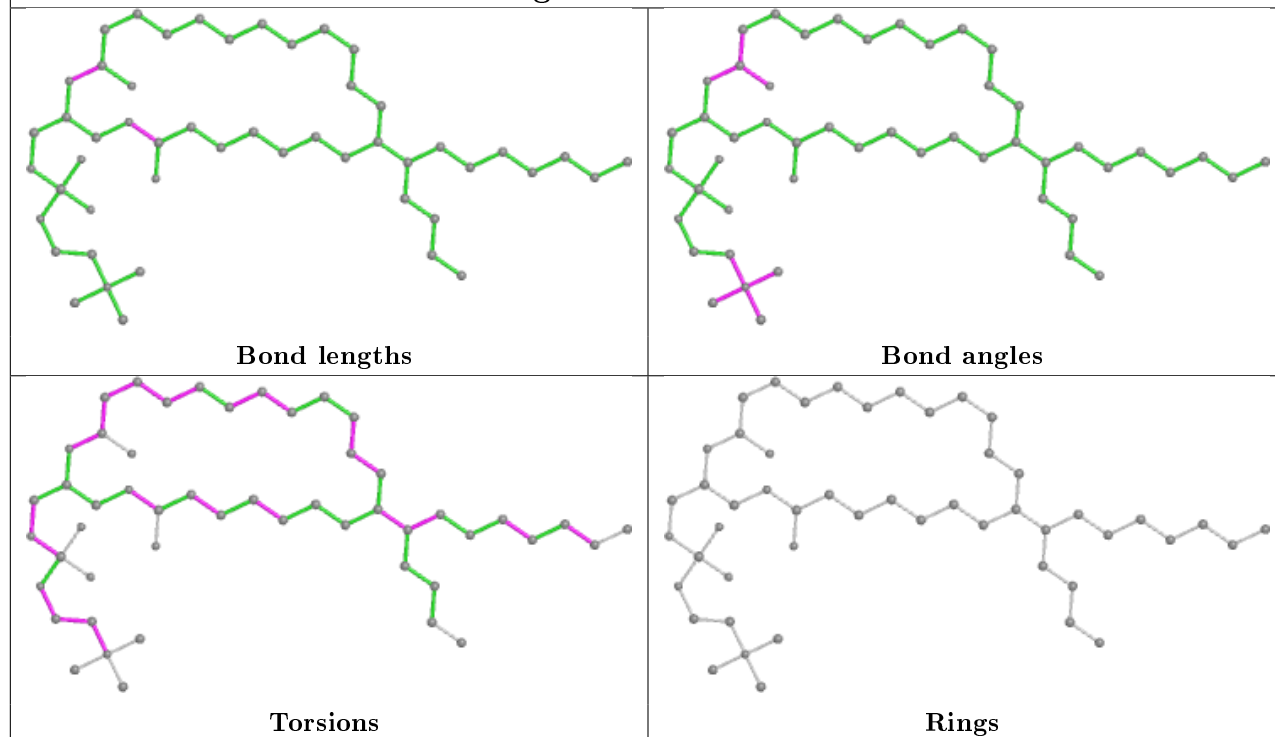


Ligand CHD G 104

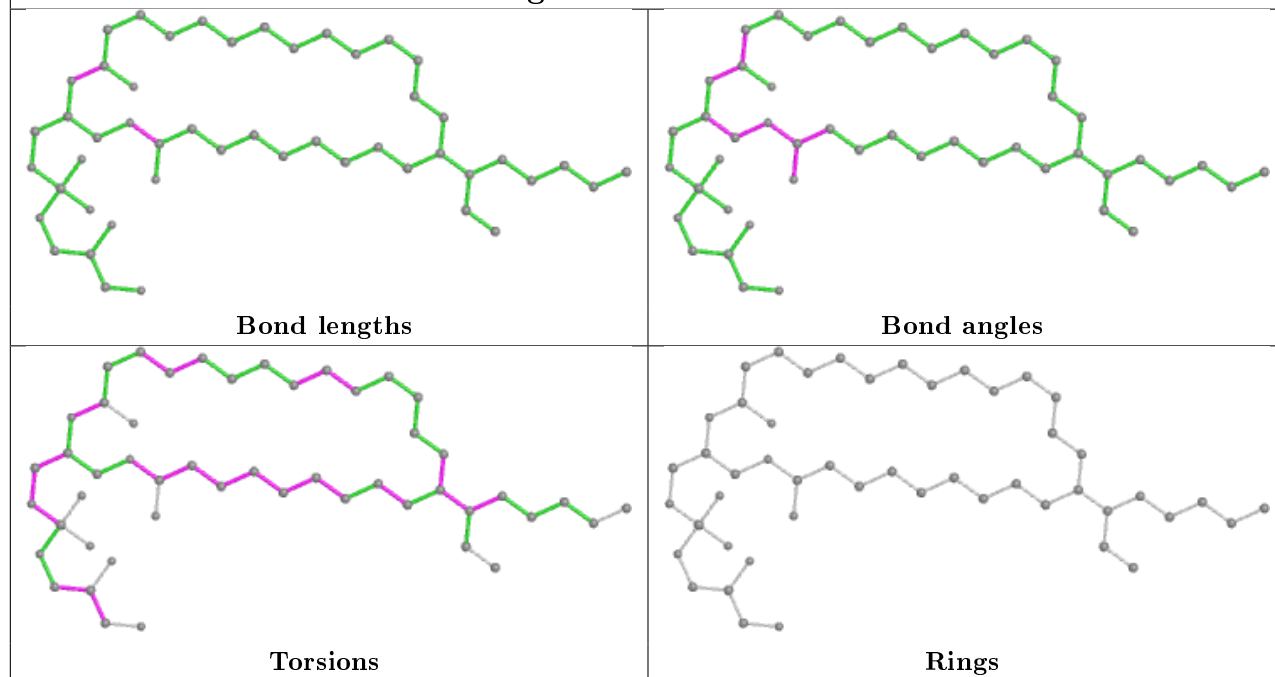




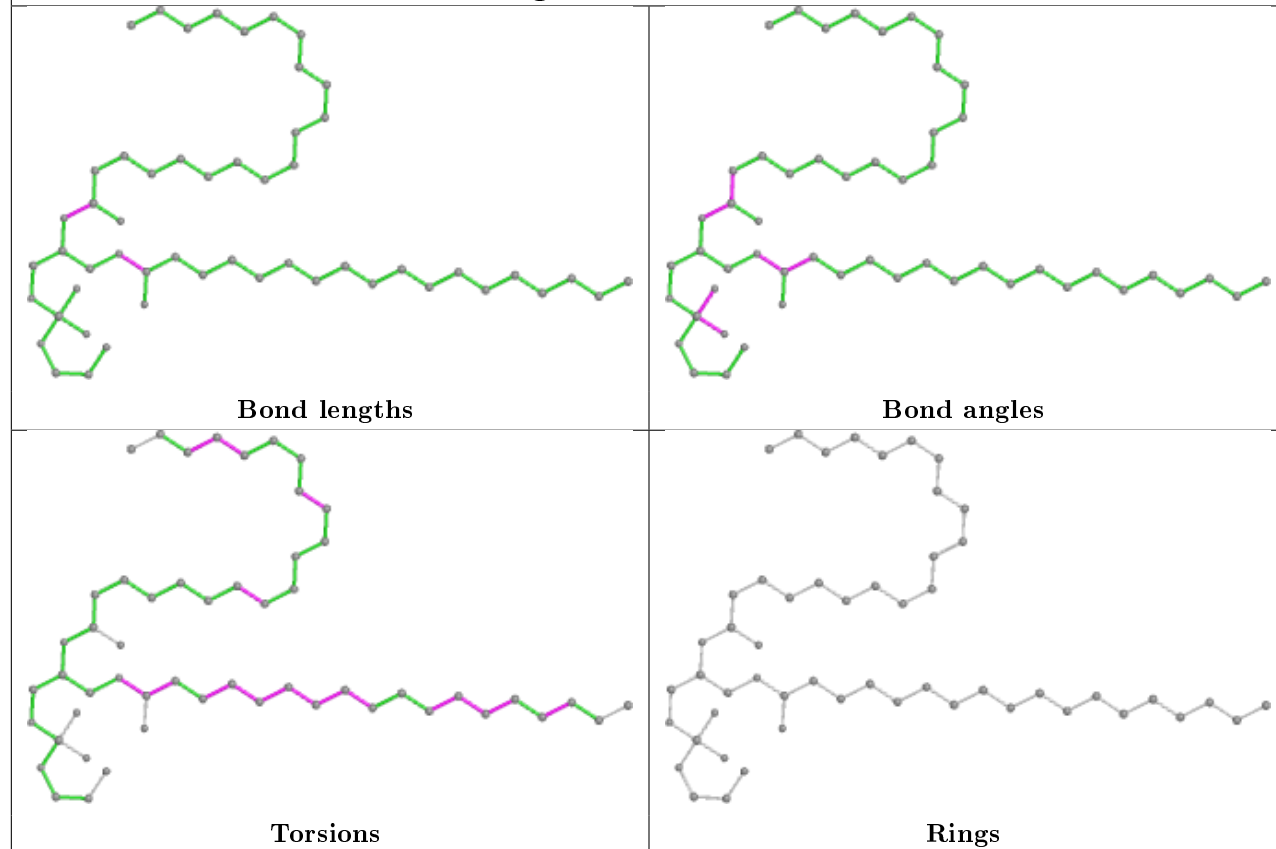
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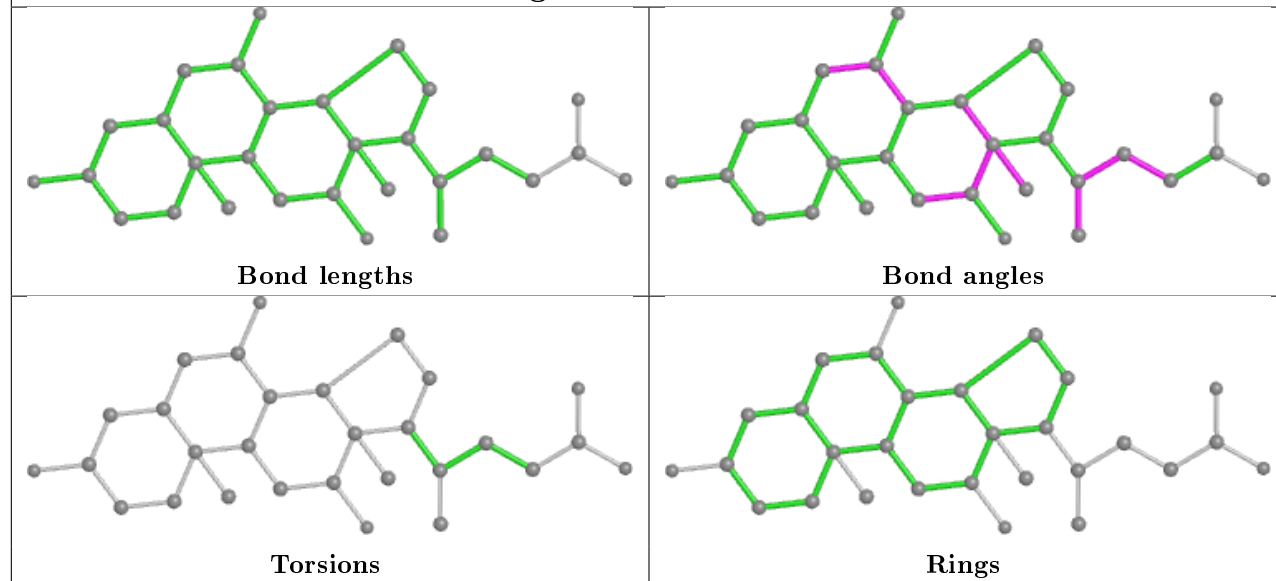
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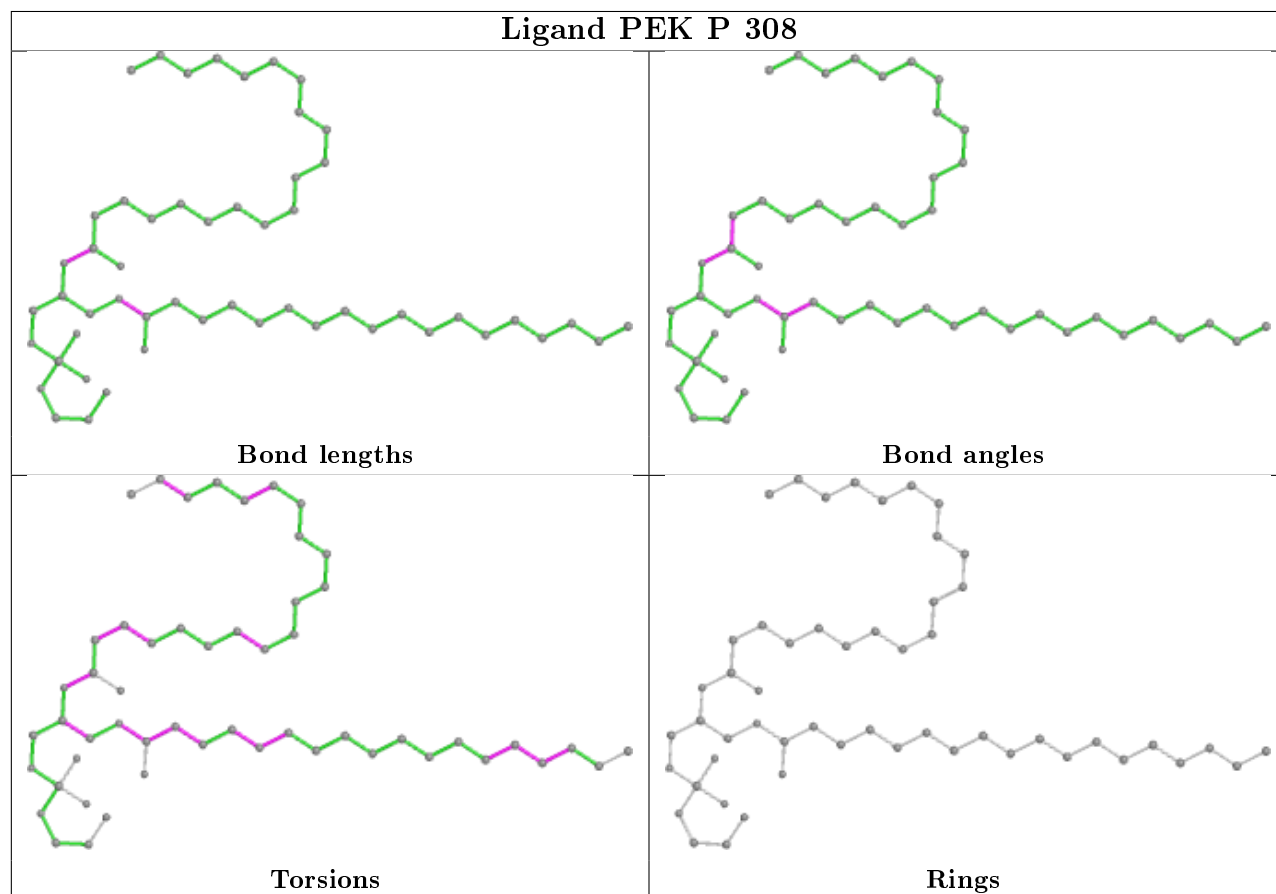
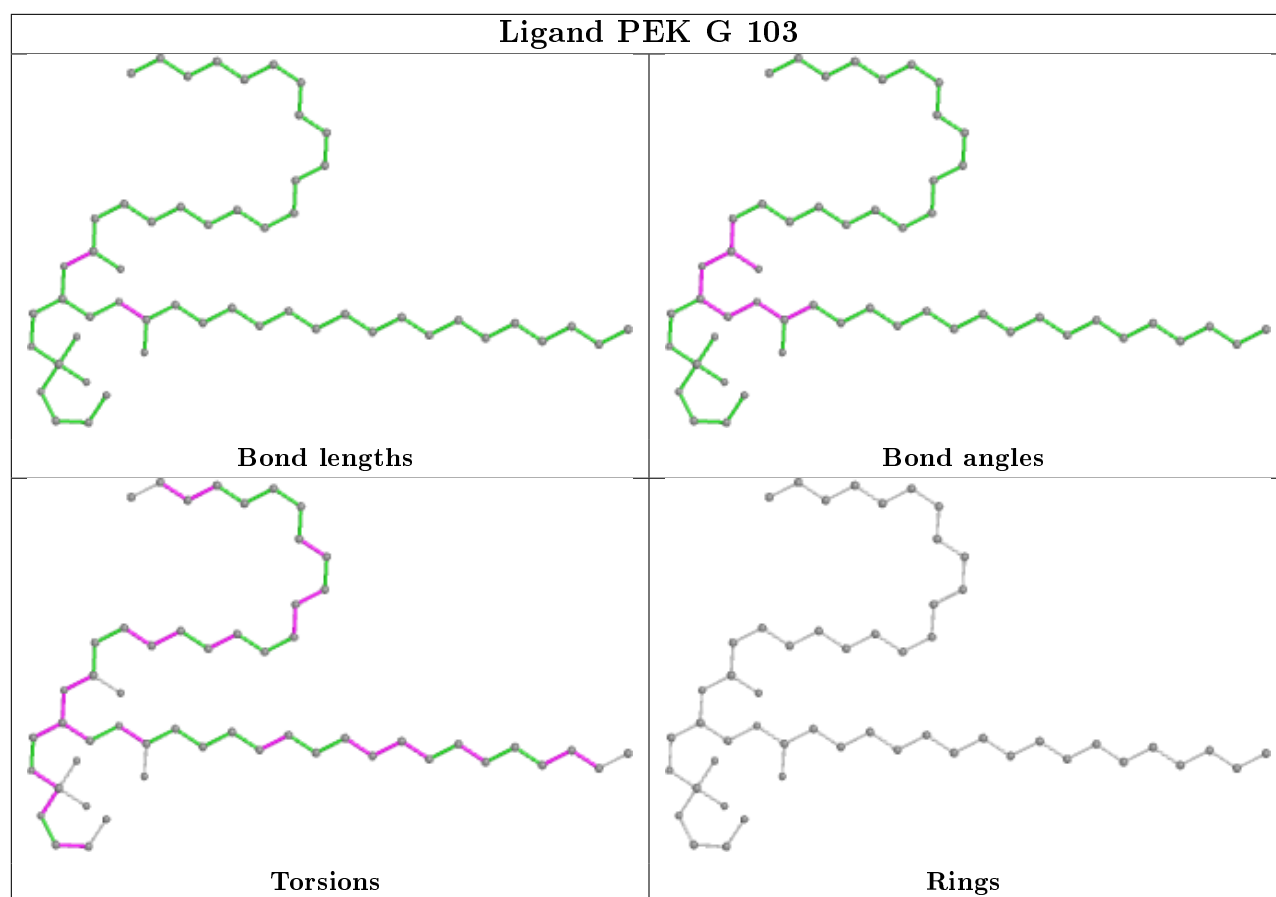


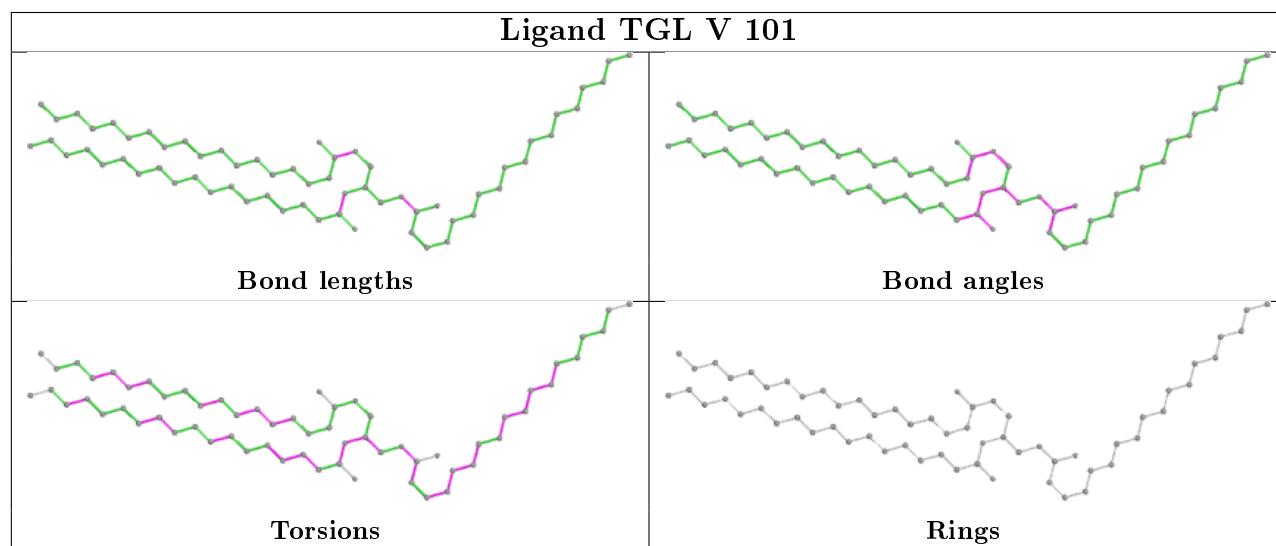
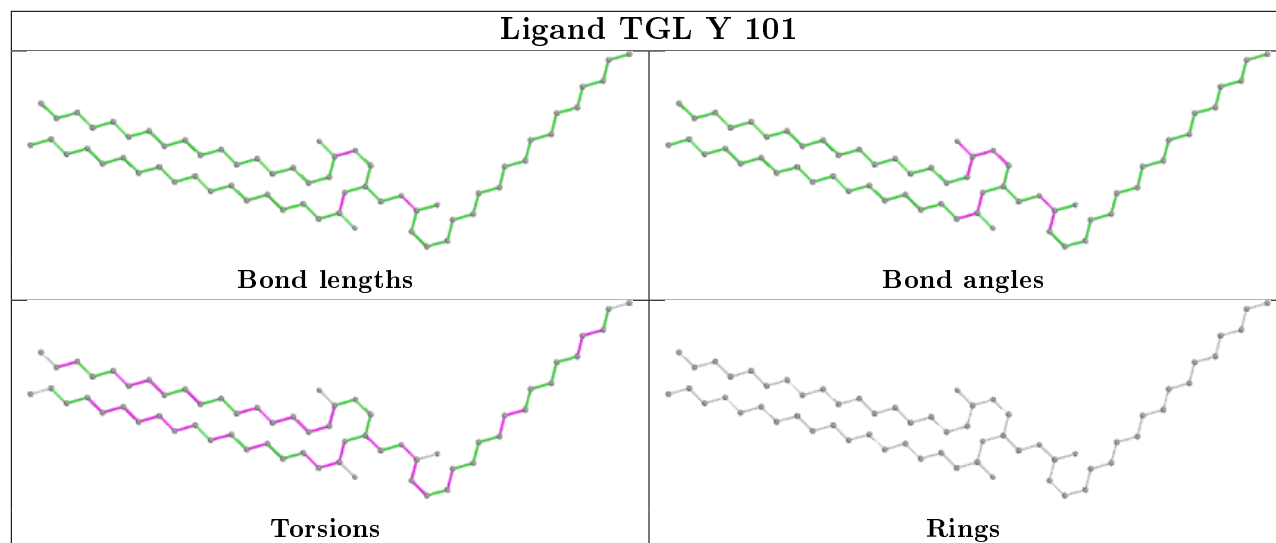
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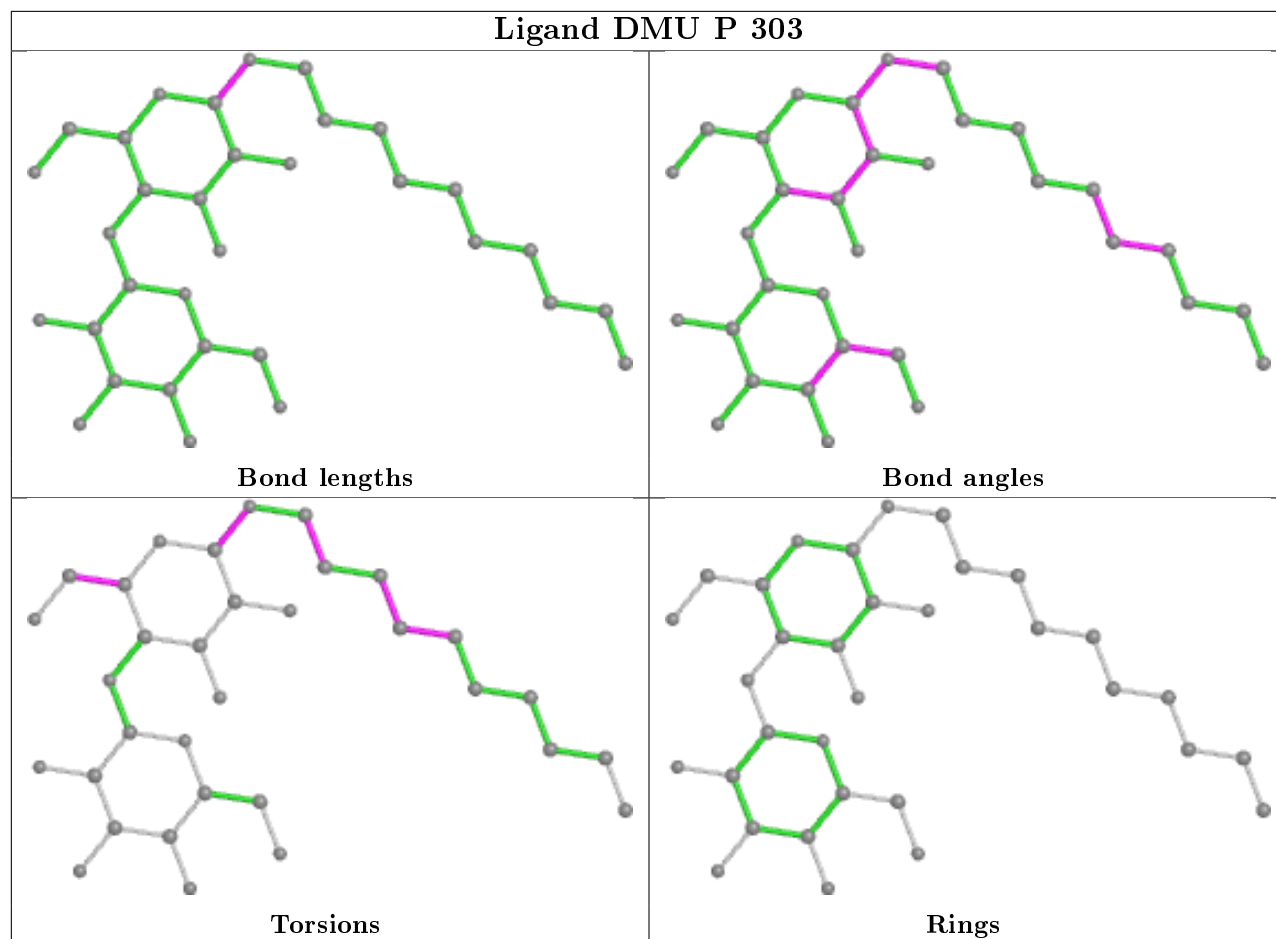


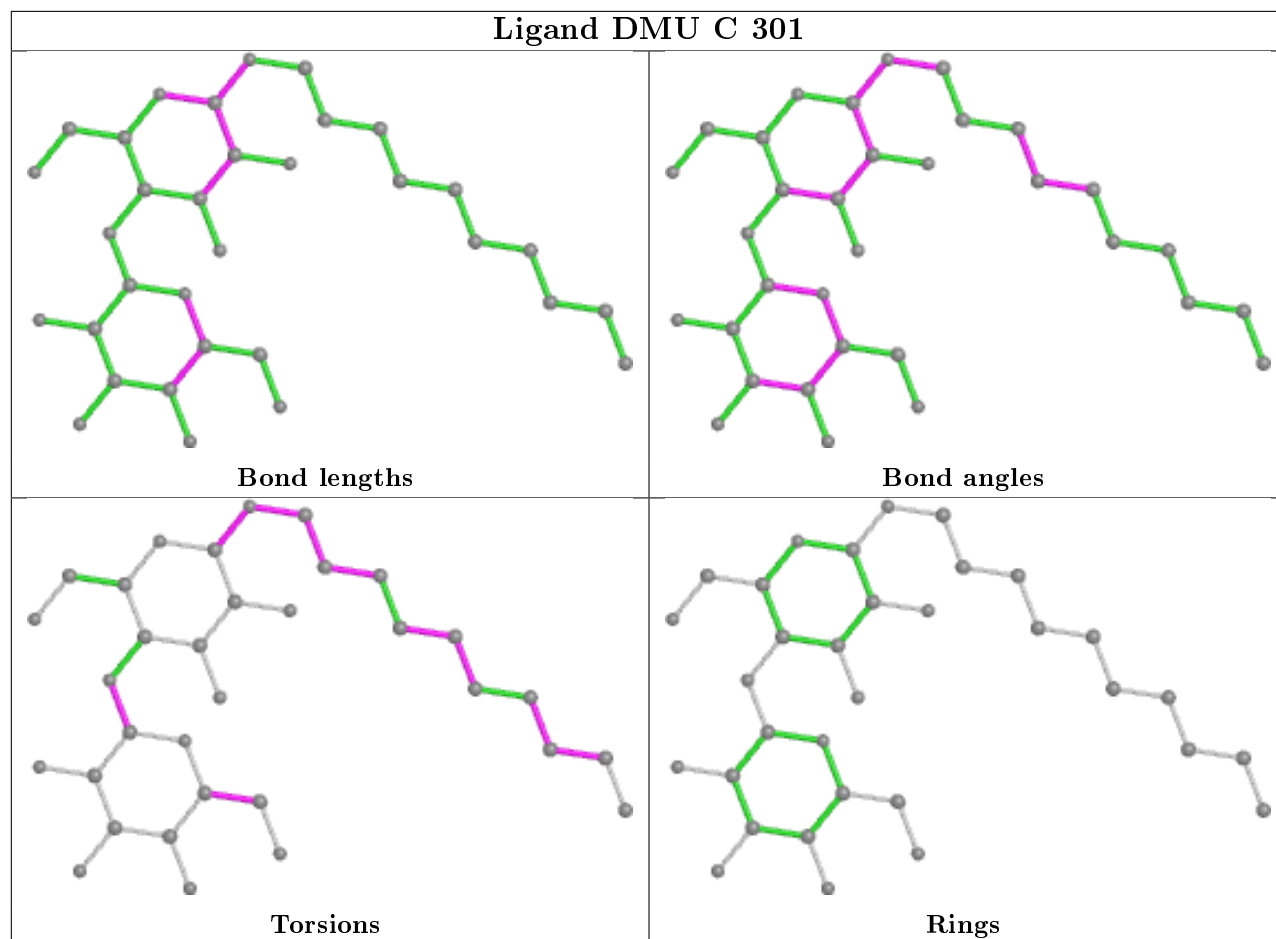
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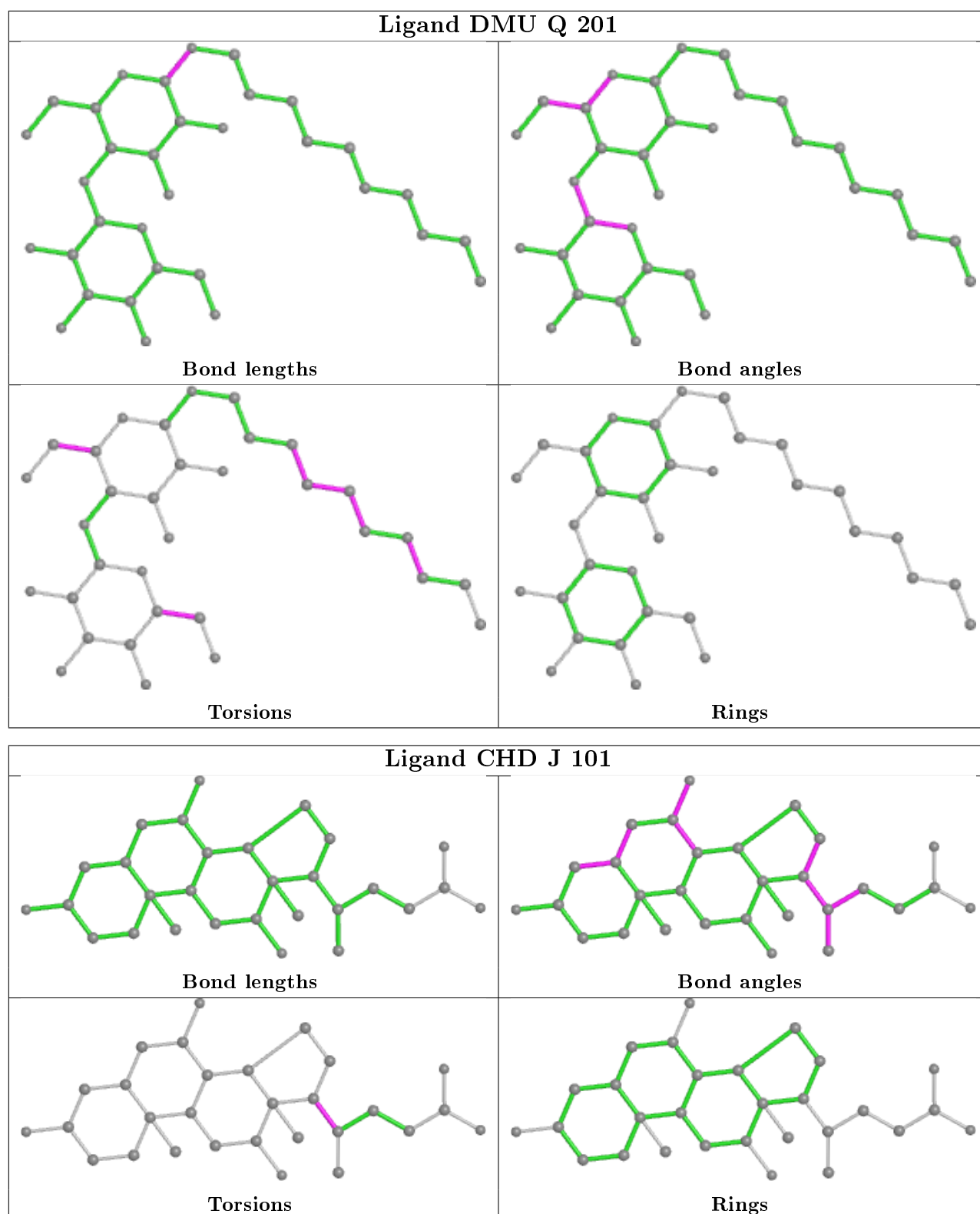


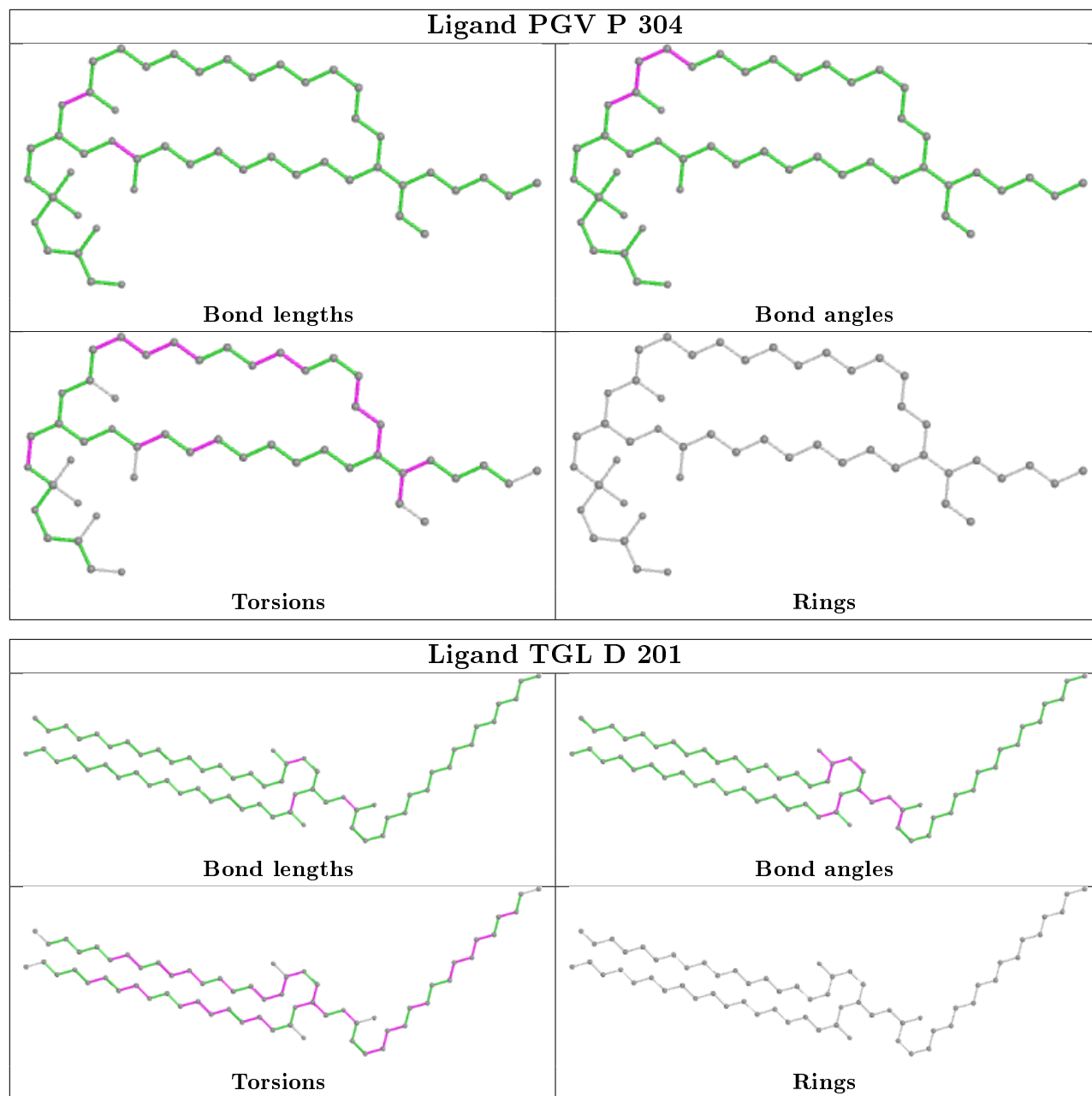


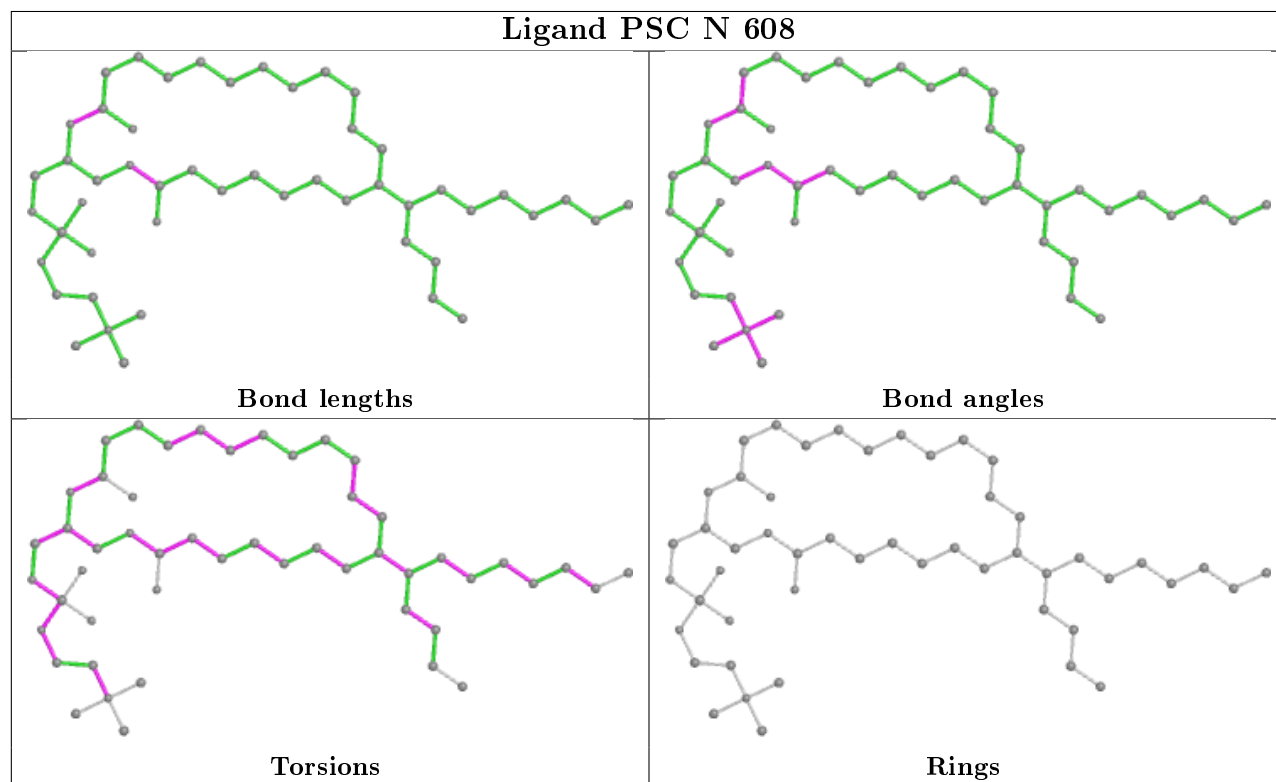
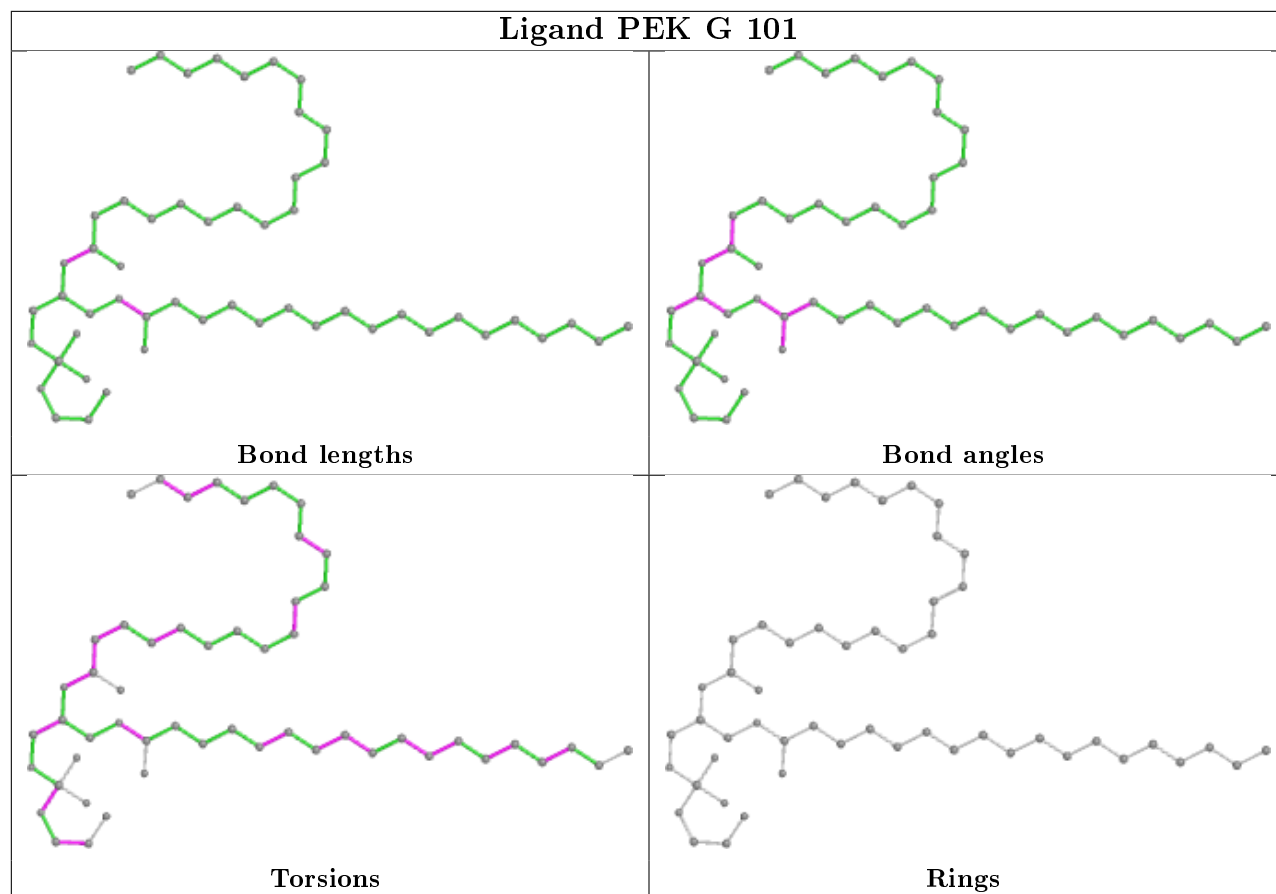


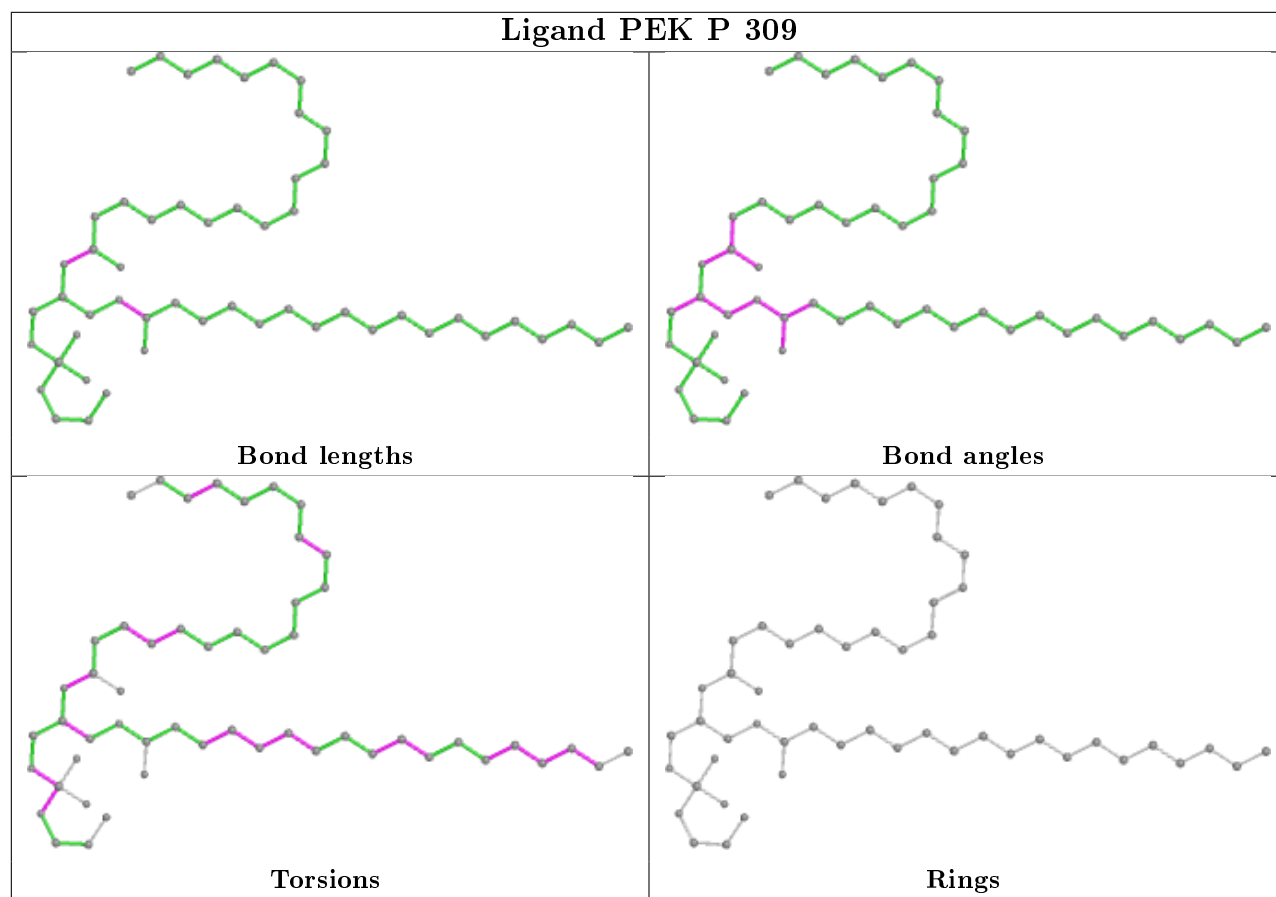
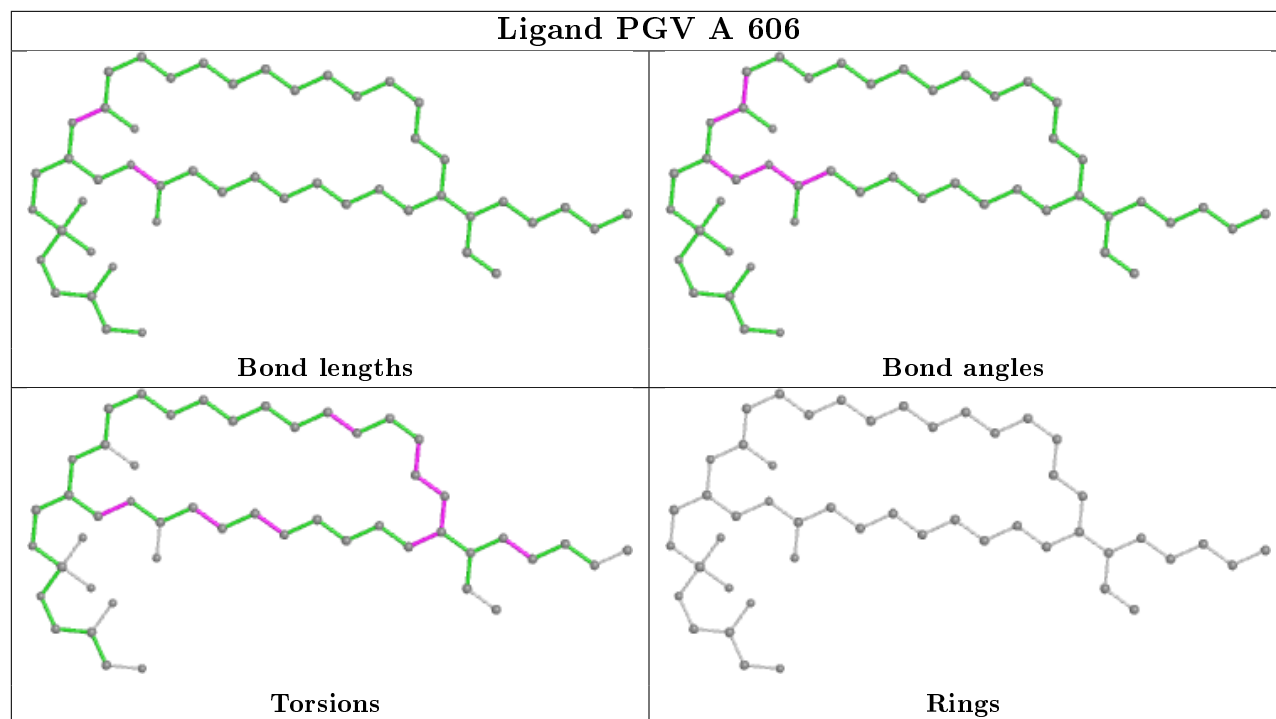




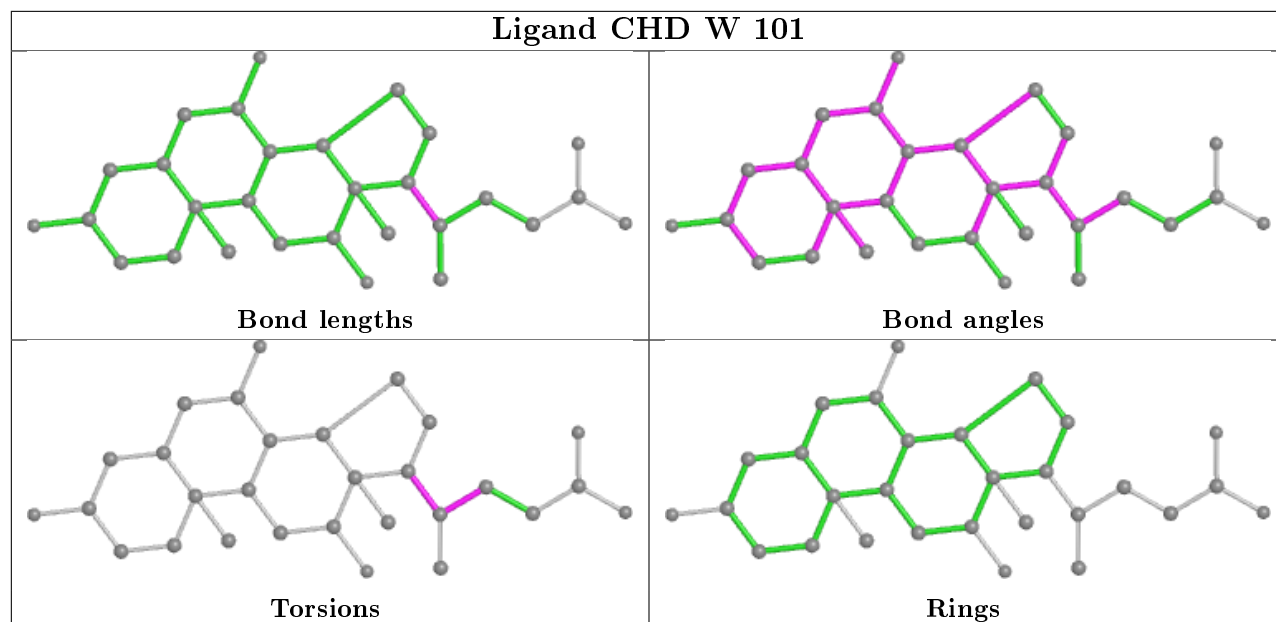




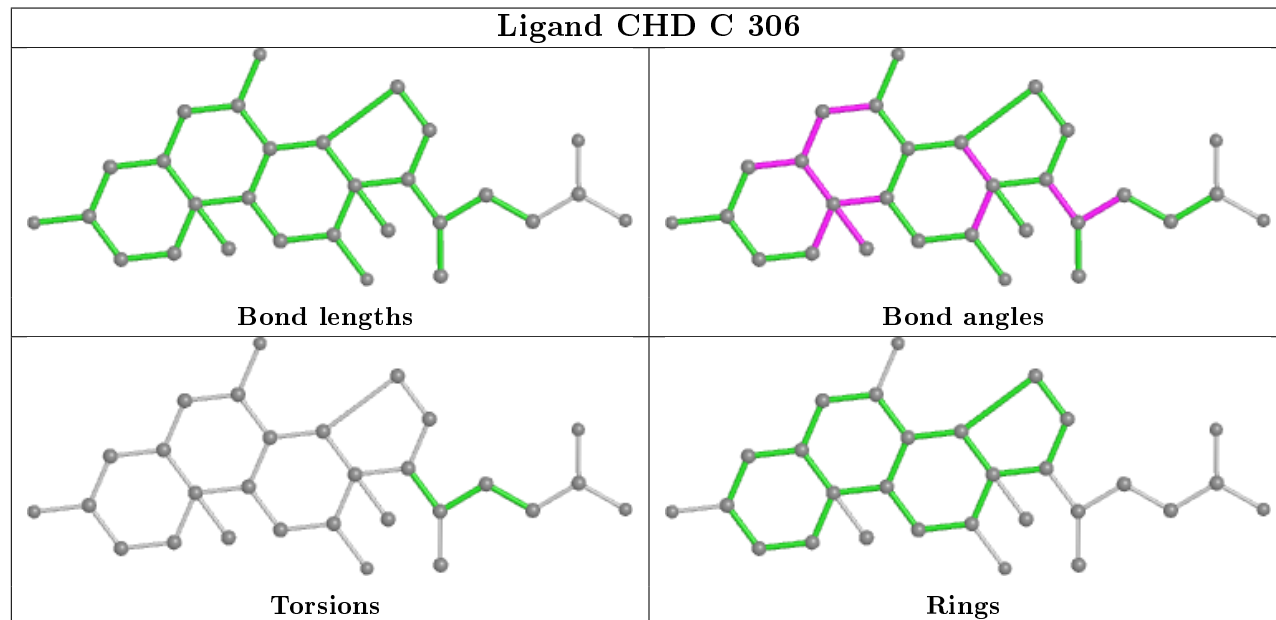




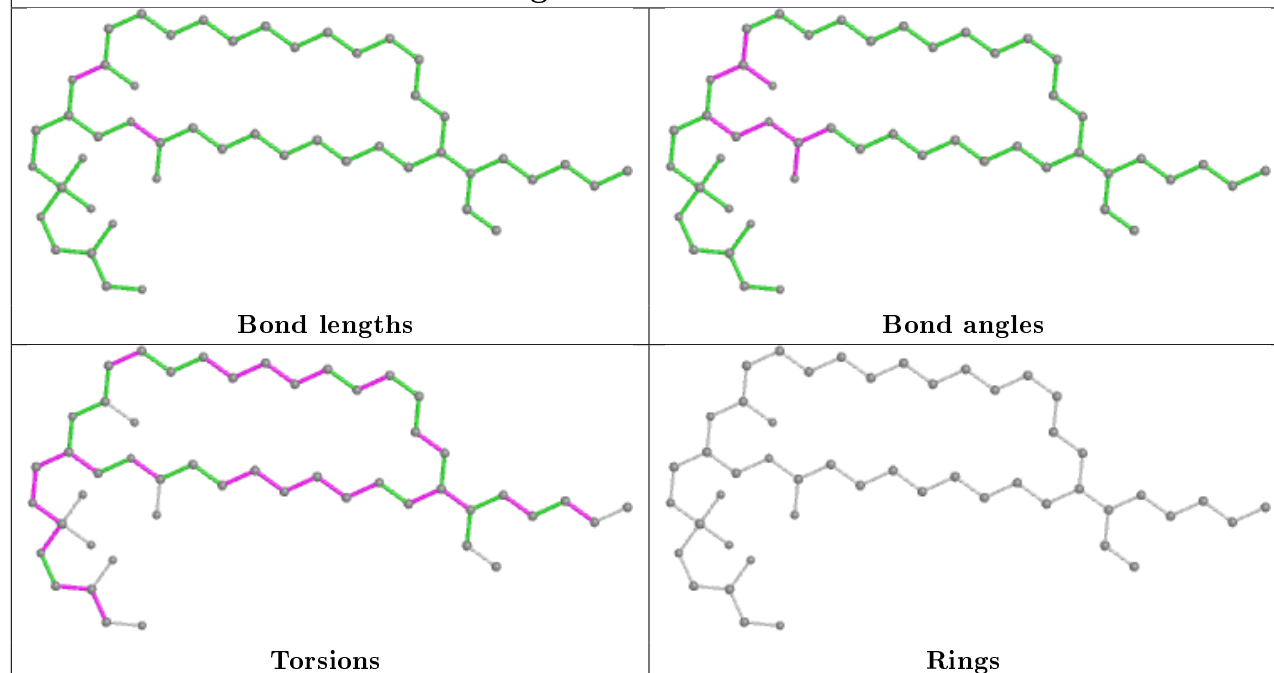
Ligand CHD W 101



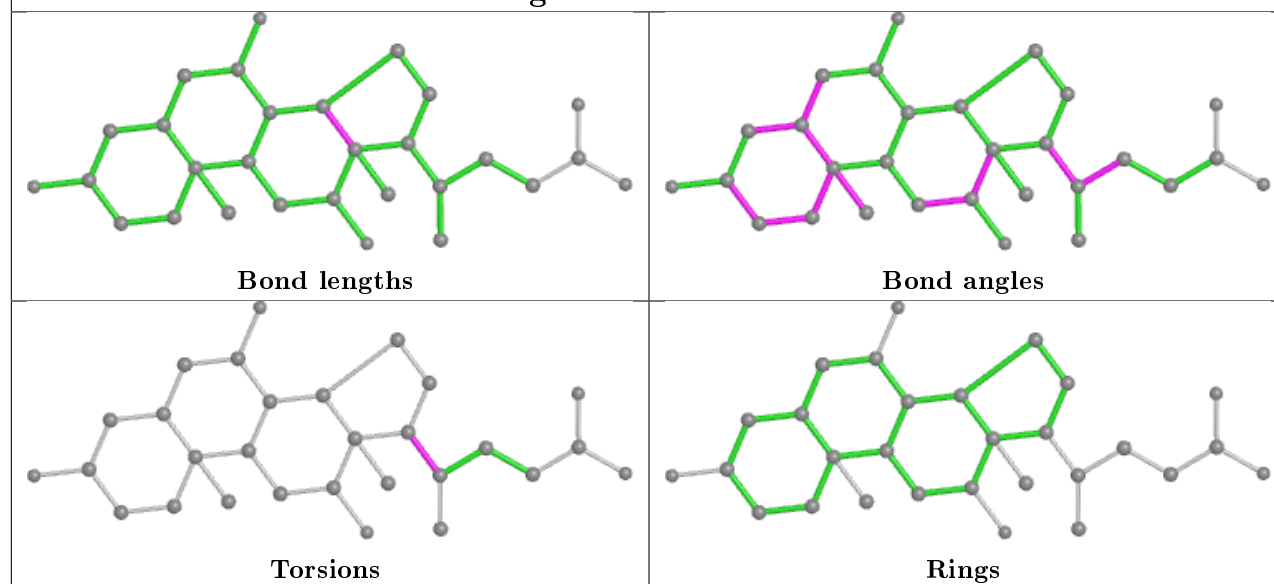
Ligand CHD C 306

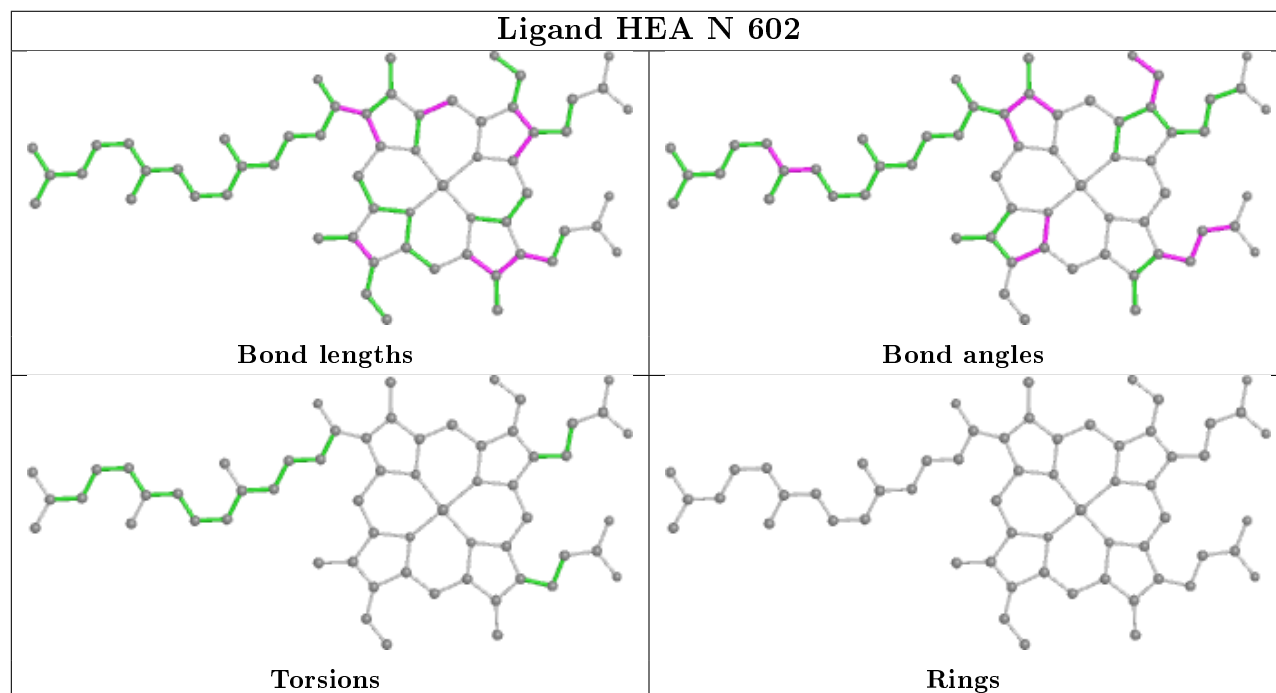
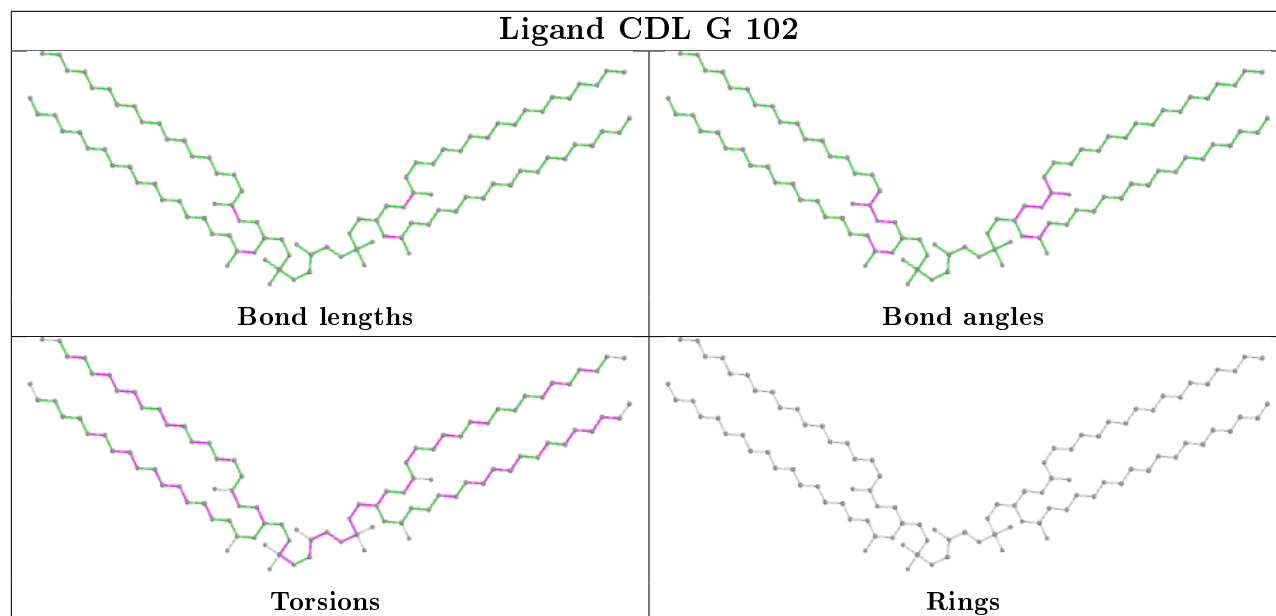


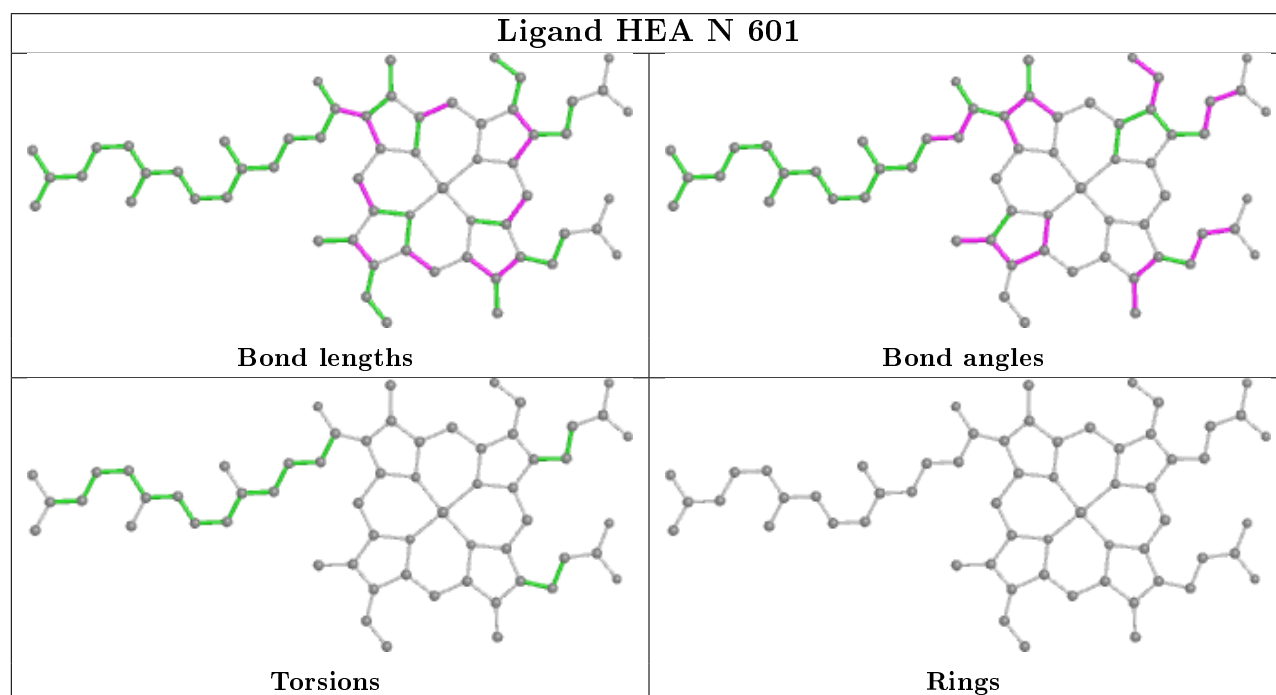
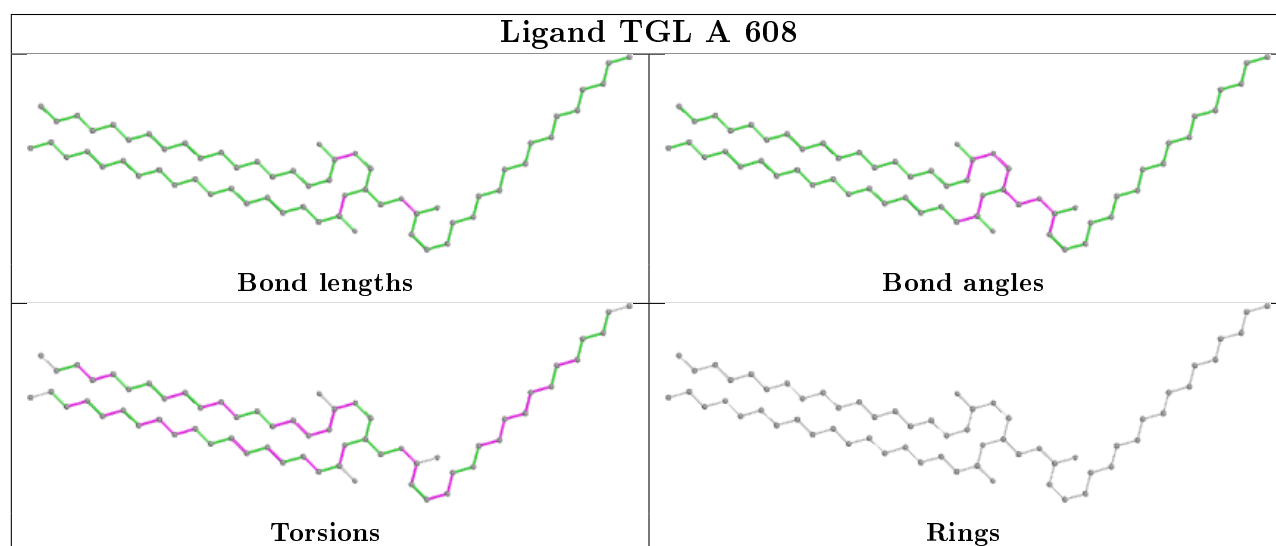
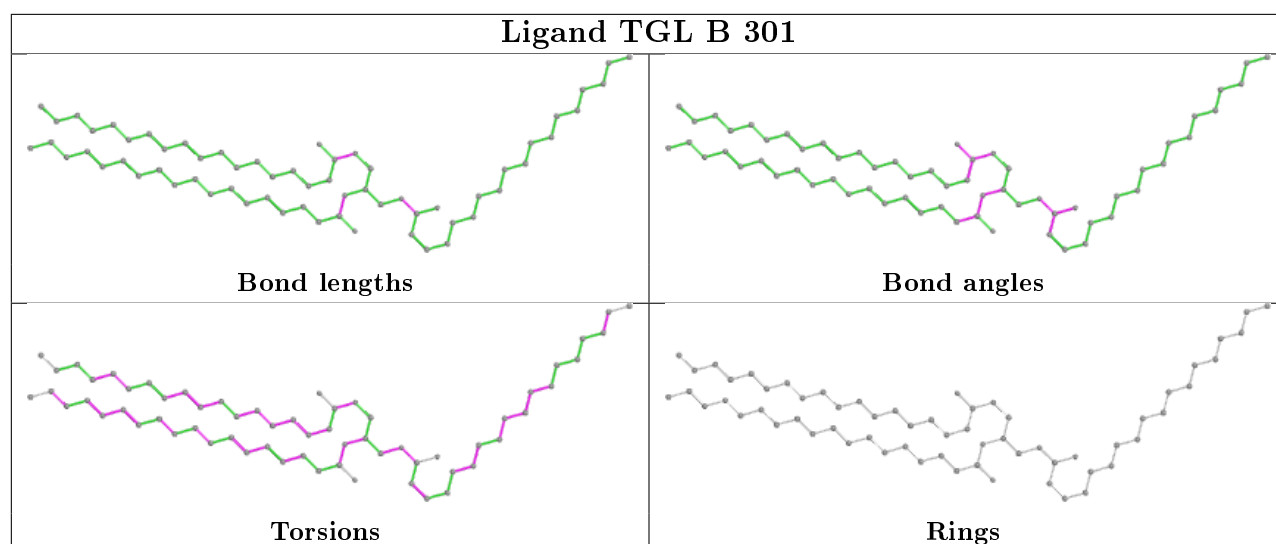
Ligand PGV P 302

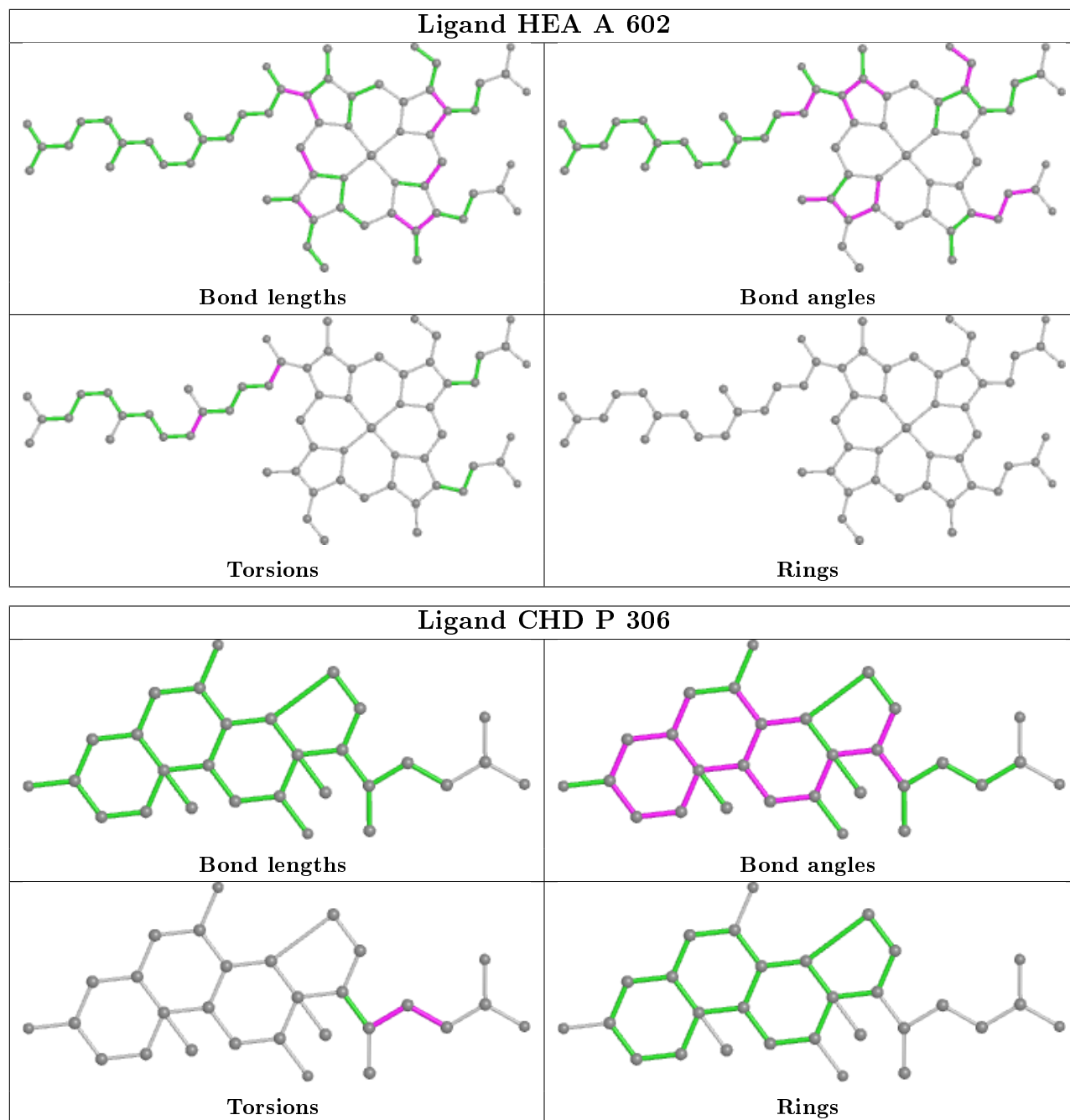


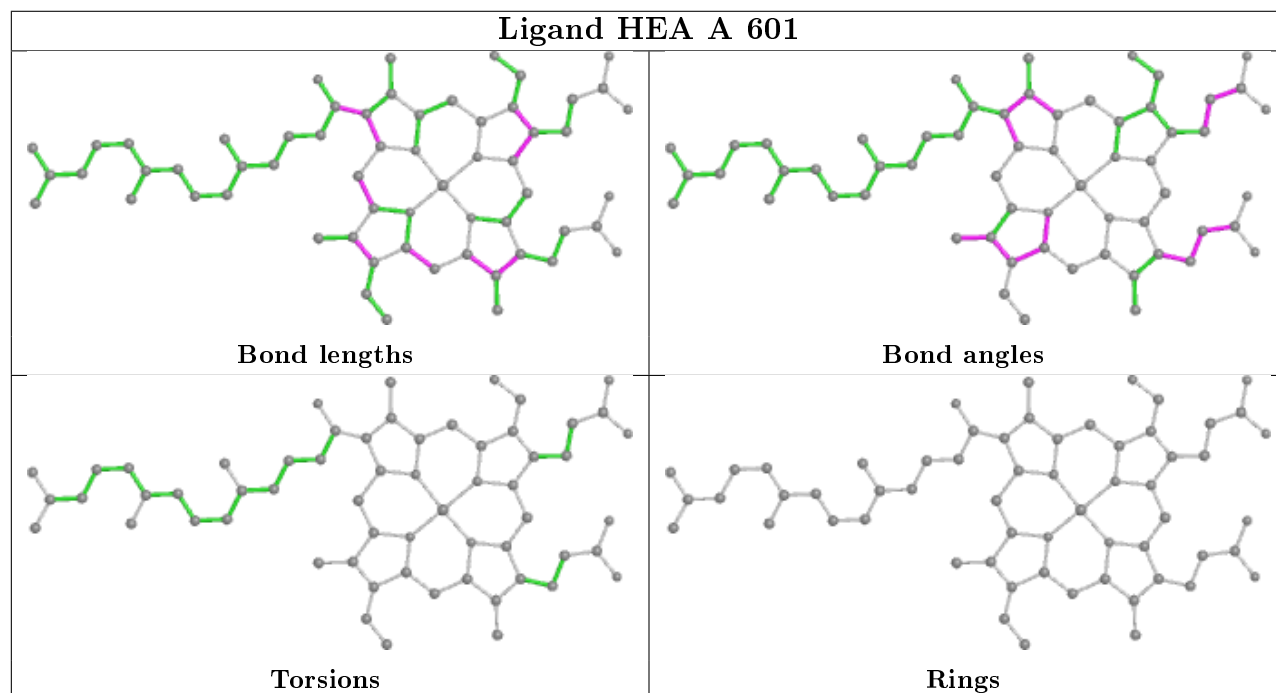
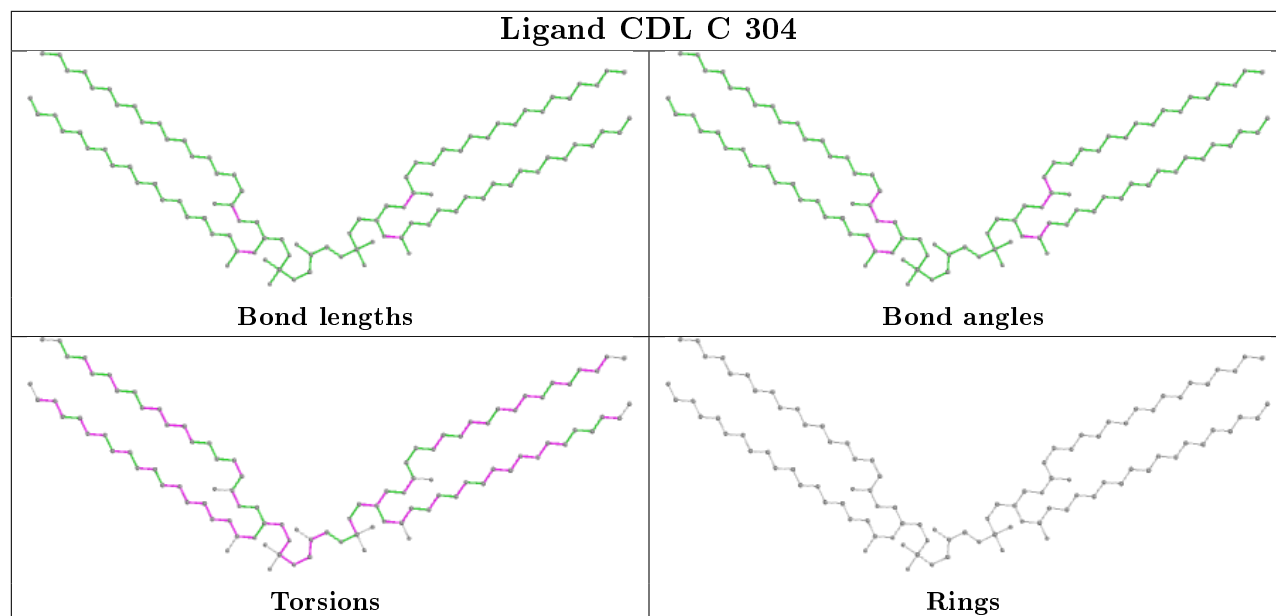
Ligand CHD B 303

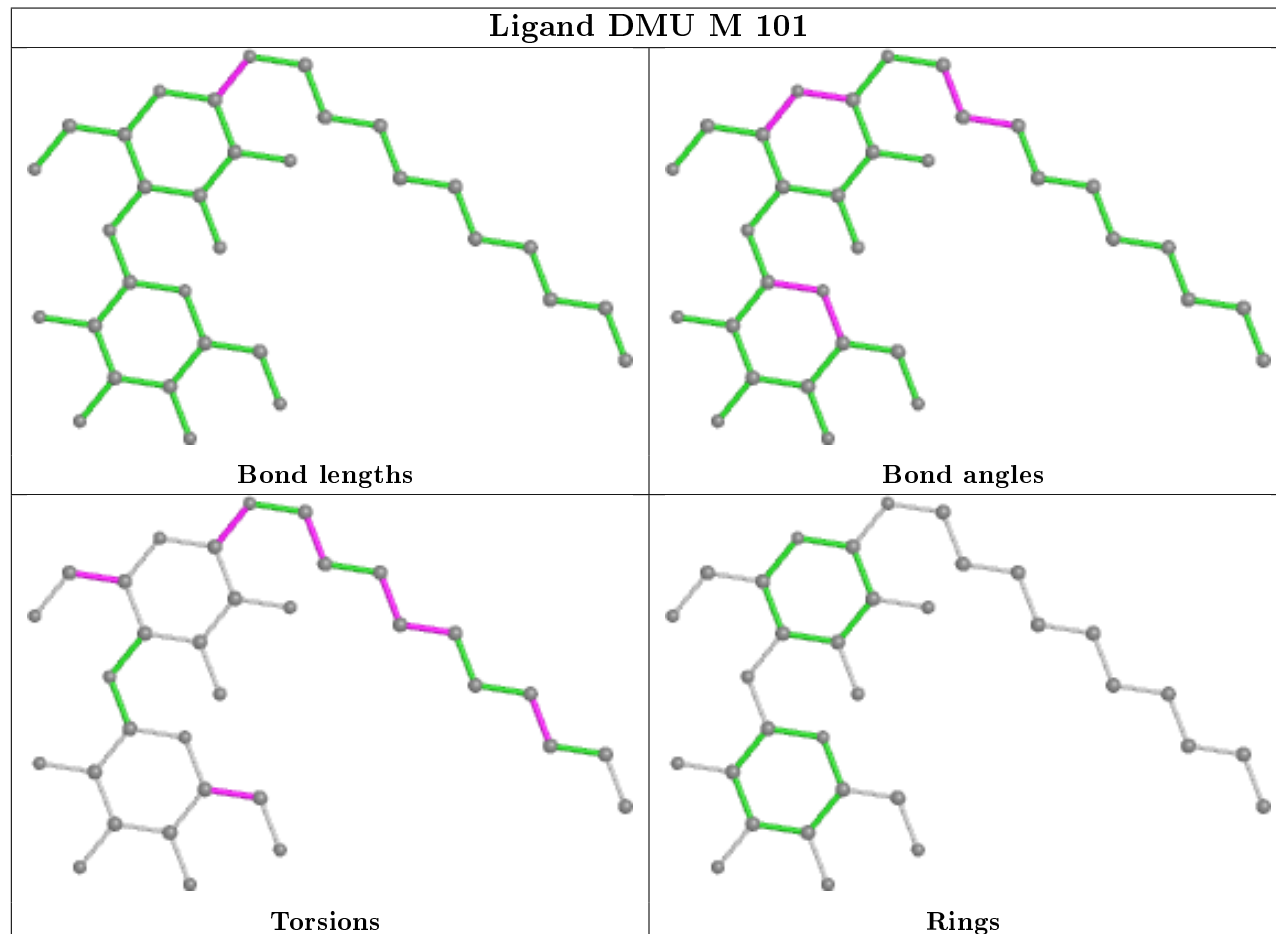
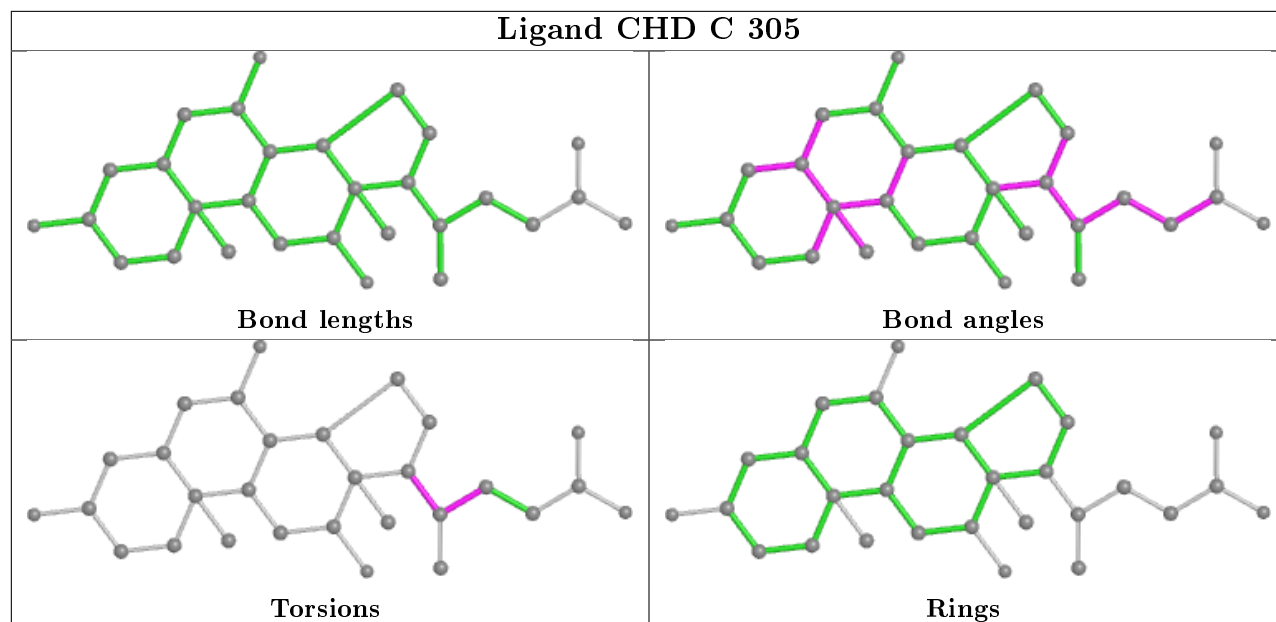


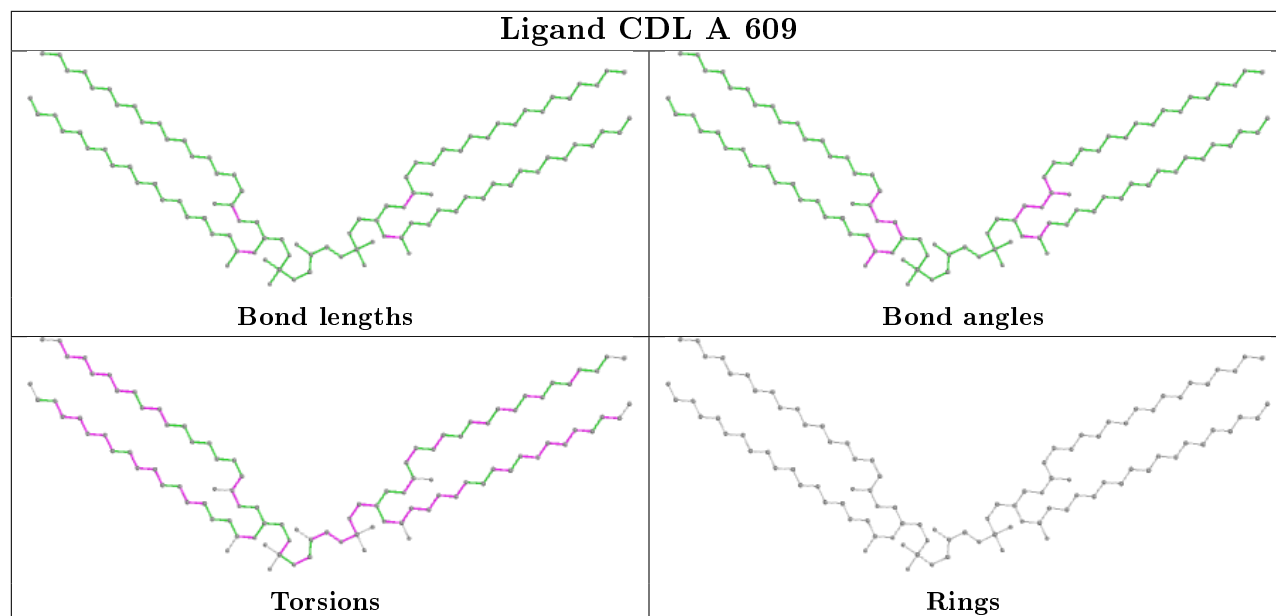












5.7 Other polymers [i](#)

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%)	-1.08	0 100 100	37, 49, 63, 102	0
1	N	513/514 (99%)	-0.97	0 100 100	48, 64, 86, 108	0
2	B	226/227 (99%)	-0.82	1 (0%) 92 91	42, 57, 86, 152	0
2	O	226/227 (99%)	-0.56	3 (1%) 77 72	57, 76, 115, 162	0
3	C	259/261 (99%)	-0.88	0 100 100	43, 54, 75, 111	0
3	P	259/261 (99%)	-0.82	2 (0%) 86 81	48, 66, 89, 144	0
4	D	144/147 (97%)	-0.61	1 (0%) 87 84	47, 62, 91, 127	0
4	Q	144/147 (97%)	-0.01	11 (7%) 13 7	67, 91, 136, 199	0
5	E	105/109 (96%)	-0.70	1 (0%) 82 77	47, 61, 98, 151	0
5	R	105/109 (96%)	-0.57	2 (1%) 66 59	57, 80, 102, 148	0
6	F	98/98 (100%)	-0.15	7 (7%) 16 9	47, 64, 144, 210	0
6	S	98/98 (100%)	-0.00	8 (8%) 11 6	54, 77, 156, 217	0
7	G	83/85 (97%)	0.02	10 (12%) 4 2	46, 65, 155, 191	0
7	T	83/85 (97%)	0.08	12 (14%) 2 1	52, 81, 152, 230	0
8	H	79/85 (92%)	-0.30	4 (5%) 28 19	49, 70, 142, 155	0
8	U	79/85 (92%)	-0.01	7 (8%) 9 5	66, 87, 145, 161	0
9	I	72/73 (98%)	-0.47	0 100 100	52, 70, 99, 126	0
9	V	72/73 (98%)	0.09	9 (12%) 3 2	63, 93, 136, 155	0
10	J	58/59 (98%)	-0.33	3 (5%) 27 18	55, 68, 132, 159	0
10	W	58/59 (98%)	-0.01	4 (6%) 16 10	75, 90, 131, 176	0
11	K	49/56 (87%)	-0.30	1 (2%) 65 56	54, 66, 90, 132	0
11	X	49/56 (87%)	0.03	1 (2%) 65 56	76, 92, 116, 129	0
12	L	46/47 (97%)	-0.75	1 (2%) 62 52	44, 57, 83, 137	0
12	Y	46/47 (97%)	-0.39	1 (2%) 62 52	68, 86, 109, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.48	2 (4%) 31 22	49, 57, 102, 141	0
13	Z	43/46 (93%)	0.01	3 (6%) 16 9	71, 86, 133, 165	0
All	All	3550/3614 (98%)	-0.62	94 (2%) 56 46	37, 65, 113, 230	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	8	SER	8.2
6	S	98	HIS	8.2
7	G	39	SER	8.1
13	Z	43	SER	7.8
6	S	2	SER	7.2
4	Q	7	LYS	7.0
6	S	97	ALA	6.7
7	G	40	GLY	6.5
6	S	95	GLN	6.3
7	T	40	GLY	5.8
7	G	3	ALA	5.6
6	F	98	HIS	5.5
6	F	1	ALA	5.5
7	T	39	SER	5.3
6	F	97	ALA	5.3
13	M	43	SER	5.1
6	S	1	ALA	5.0
6	F	94	HIS	4.9
10	W	58	LYS	4.9
13	Z	42	LYS	4.8
6	F	2	SER	4.7
10	W	57	HIS	4.6
7	T	41	HIS	4.5
8	U	7	LYS	4.5
7	G	41	HIS	4.5
5	R	5	HIS	4.4
2	O	90	ILE	4.4
9	V	33	THR	4.4
4	Q	5	VAL	4.4
7	G	10	GLY	4.4
8	U	10	ASN	4.3
4	Q	4	SER	4.3
9	V	2	THR	4.3
9	V	30	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
7	G	2	SER	4.2
7	T	84	LYS	4.2
10	J	58	LYS	4.0
4	Q	6	VAL	4.0
4	Q	147	LYS	3.7
10	J	57	HIS	3.7
11	K	6	ALA	3.7
7	T	1	ALA	3.7
2	O	59	GLN	3.6
2	B	90	ILE	3.5
7	T	3	ALA	3.5
5	E	5	HIS	3.4
7	G	36	TRP	3.4
9	V	37	PHE	3.4
8	H	8	ILE	3.3
7	T	10	GLY	3.2
13	M	42	LYS	3.2
12	Y	2	HIS	3.1
2	O	227	LEU	3.0
9	V	53	ASN	3.0
8	H	47	GLY	3.0
4	Q	9	GLU	3.0
8	U	8	ILE	2.9
11	X	35	GLN	2.8
9	V	3	ALA	2.8
8	U	48	GLY	2.8
7	T	12	GLY	2.8
8	U	45	ALA	2.7
7	T	36[A]	TRP	2.7
7	G	84	LYS	2.7
6	F	95	GLN	2.7
4	Q	32	ASN	2.6
8	H	45	ALA	2.6
6	S	3	GLY	2.6
7	T	43	GLU	2.5
9	V	29	LEU	2.4
6	S	94	HIS	2.4
7	G	8	HIS	2.4
10	J	1	PHE	2.4
3	P	261	SER	2.4
9	V	25	PHE	2.3
7	T	8	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
3	P	182	TYR	2.3
5	R	108	LYS	2.3
8	H	7	LYS	2.3
9	V	55	ASP	2.3
8	U	77	ALA	2.3
4	Q	74	SER	2.2
7	T	2	SER	2.2
10	W	56	PRO	2.2
10	W	55	PHE	2.2
4	Q	101	HIS	2.2
7	G	1	ALA	2.1
12	L	47	LYS	2.1
6	S	93	PRO	2.1
6	F	3	GLY	2.1
13	Z	39	ASN	2.1
8	U	47	GLY	2.1
4	Q	141	ASP	2.0
4	D	141	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	I	1	9/10	0.57	0.60	121,144,159,160	0
7	TPO	G	11	11/12	0.63	0.52	121,154,184,184	0
7	TPO	T	11	11/12	0.74	0.47	115,155,185,188	0
9	SAC	V	1	9/10	0.74	0.56	135,147,156,162	0
1	FME	N	1	10/11	0.91	0.43	101,115,136,144	0
1	FME	A	1	10/11	0.94	0.35	78,86,113,125	0
2	FME	O	1	10/11	0.96	0.13	67,85,98,100	0
2	FME	B	1	10/11	0.98	0.10	49,56,61,63	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.

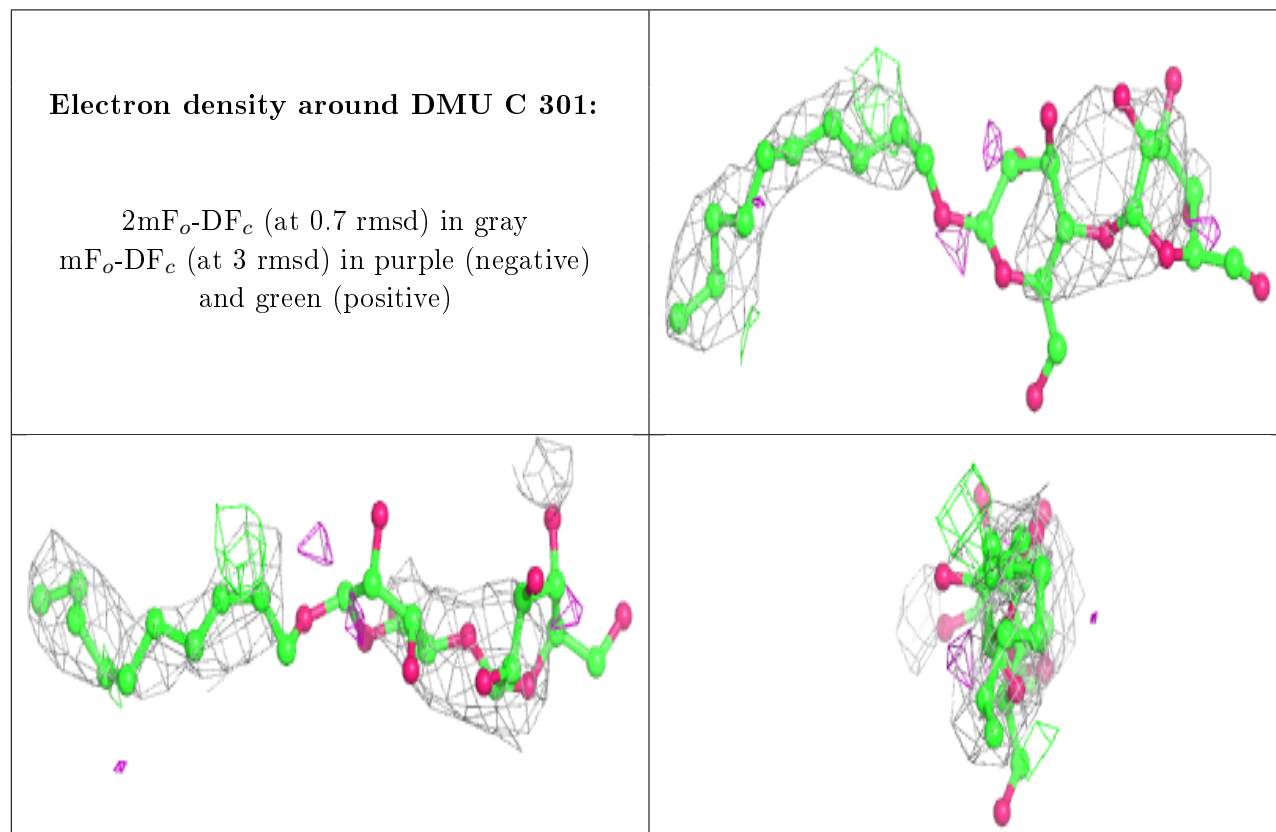
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	DMU	C	301	33/33	0.48	0.60	86,191,206,210	0
25	PEK	G	103	53/53	0.52	0.42	74,142,205,215	0
18	PGV	N	606	51/51	0.54	0.36	79,110,191,215	0
25	PEK	T	101	53/53	0.60	0.41	87,156,204,213	0
25	PEK	P	309	53/53	0.61	0.31	78,122,173,183	0
24	DMU	P	303	33/33	0.65	0.51	96,163,206,222	0
19	TGL	Y	101	63/63	0.67	0.34	83,122,160,163	0
20	CDL	A	609	100/100	0.68	0.34	96,129,187,213	0
18	PGV	A	607	51/51	0.69	0.30	72,120,163,176	0
25	PEK	G	101	53/53	0.69	0.27	74,117,202,210	0
20	CDL	C	304	100/100	0.70	0.32	68,127,168,183	0
23	PSC	N	608	52/52	0.70	0.34	83,137,241,271	0
19	TGL	N	607	63/63	0.72	0.28	84,123,138,143	0
23	PSC	B	304	52/52	0.74	0.30	81,130,210,219	0
20	CDL	G	102	100/100	0.74	0.30	105,135,187,207	0
19	TGL	V	101	63/63	0.76	0.25	53,114,164,179	0
19	TGL	B	301	63/63	0.77	0.23	47,103,141,146	0
22	CHD	W	101	29/29	0.77	0.41	110,149,184,190	0
20	CDL	P	305	100/100	0.77	0.30	84,133,190,254	0
19	TGL	D	201	63/63	0.78	0.24	72,109,128,135	0
18	PGV	C	307	51/51	0.79	0.28	81,118,146,150	0
24	DMU	Q	201	33/33	0.80	0.29	86,110,126,137	0
18	PGV	P	302	51/51	0.81	0.28	74,117,160,166	0
19	TGL	A	608	63/63	0.81	0.27	56,105,138,148	0
17	NA	N	605	1/1	0.84	0.21	81,81,81,81	0
22	CHD	J	101	29/29	0.85	0.32	87,116,136,140	0
24	DMU	M	101	33/33	0.87	0.20	62,69,85,91	0
22	CHD	C	305	29/29	0.89	0.25	99,115,136,140	0
25	PEK	P	308	53/53	0.92	0.19	65,94,152,173	0
22	CHD	P	306	29/29	0.92	0.23	102,113,124,126	0
25	PEK	C	302	53/53	0.95	0.17	49,72,125,132	0
18	PGV	P	304	51/51	0.95	0.17	55,67,117,123	0
22	CHD	G	104	29/29	0.96	0.12	49,54,62,73	0
26	ZN	S	101	1/1	0.96	0.03	72,72,72,72	0
18	PGV	P	301	51/51	0.96	0.15	47,71,94,108	0
18	PGV	C	303	51/51	0.96	0.14	45,60,107,114	0
18	PGV	A	606	51/51	0.97	0.16	40,69,89,93	0

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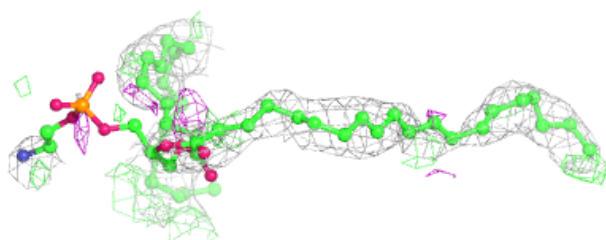
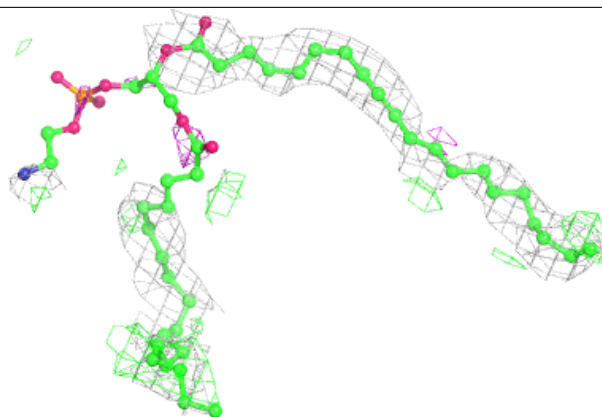
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	HEA	A	601	60/60	0.97	0.13	40,47,65,75	0
22	CHD	P	307	29/29	0.97	0.09	55,60,67,69	0
14	HEA	A	602	60/60	0.98	0.13	34,43,60,70	0
17	NA	A	605	1/1	0.98	0.06	55,55,55,55	0
22	CHD	B	303	29/29	0.98	0.10	52,55,64,72	0
22	CHD	C	306	29/29	0.98	0.10	41,52,60,68	0
14	HEA	N	602	60/60	0.98	0.11	43,52,61,64	0
21	CUA	B	302	2/2	0.98	0.04	53,53,53,57	0
21	CUA	O	301	2/2	0.98	0.04	76,76,76,76	0
14	HEA	N	601	60/60	0.98	0.12	42,62,77,82	0
16	MG	N	604	1/1	0.99	0.13	60,60,60,60	0
16	MG	A	604	1/1	0.99	0.06	43,43,43,43	0
26	ZN	F	101	1/1	0.99	0.02	65,65,65,65	0
15	CU	A	603	1/1	1.00	0.09	53,53,53,53	0
15	CU	N	603	1/1	1.00	0.09	64,64,64,64	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.

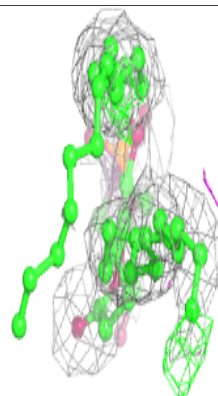
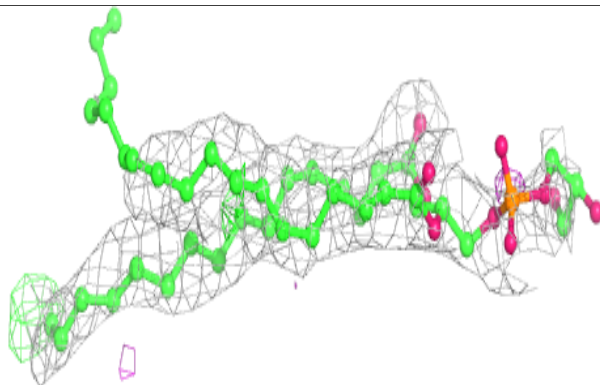
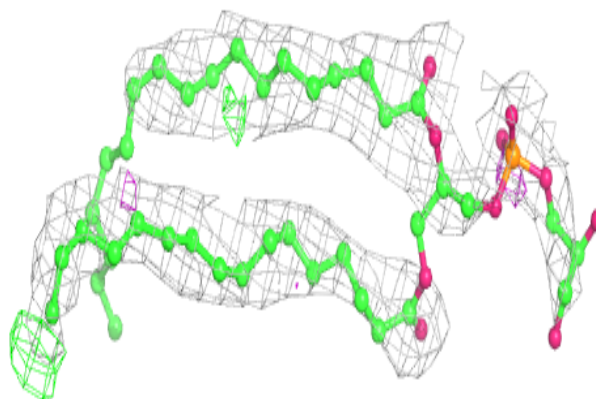


Electron density around PEK G 103:

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

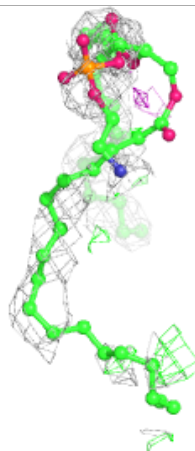
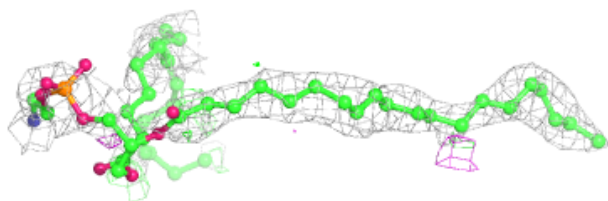
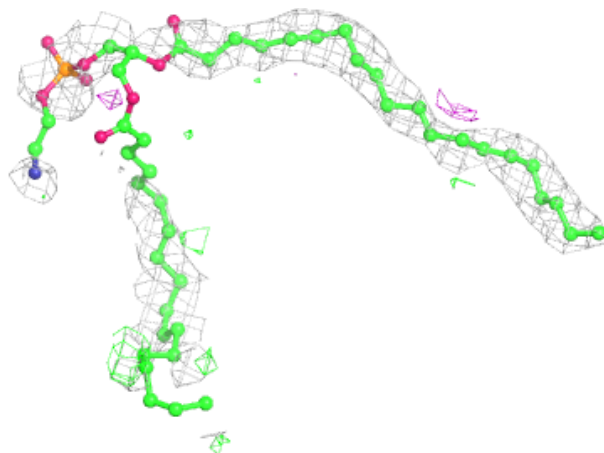
**Electron density around PGV N 606:**

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



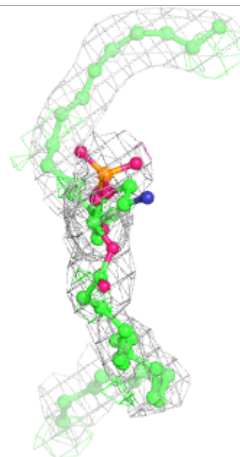
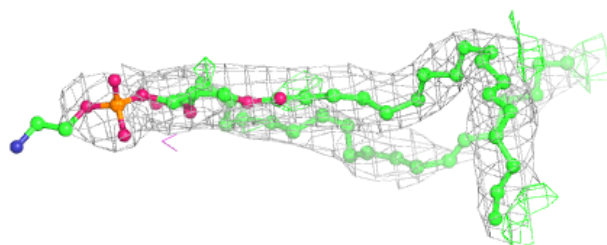
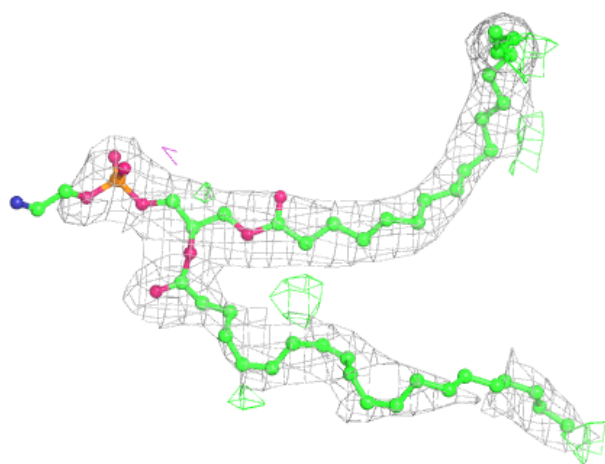
Electron density around PEK T 101:

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



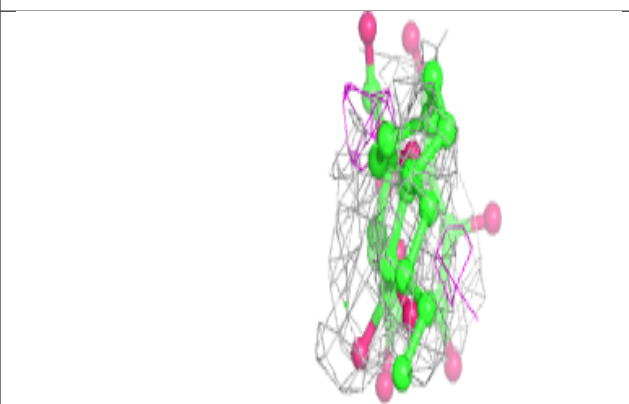
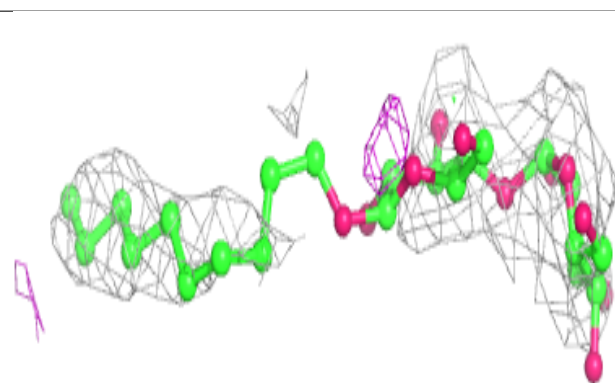
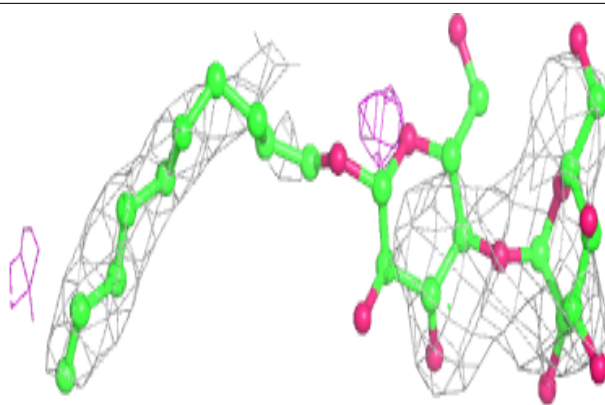
Electron density around PEK P 309:

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

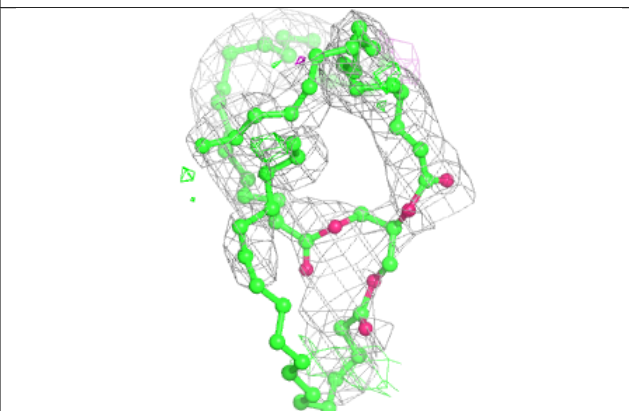
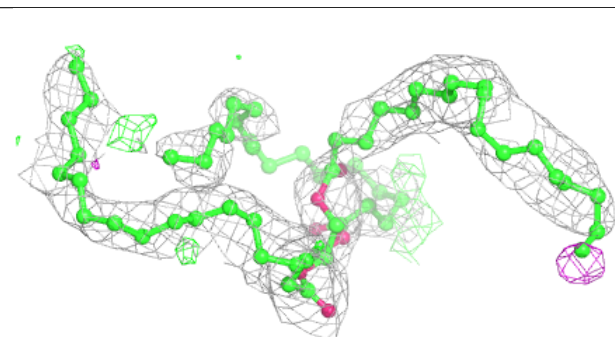
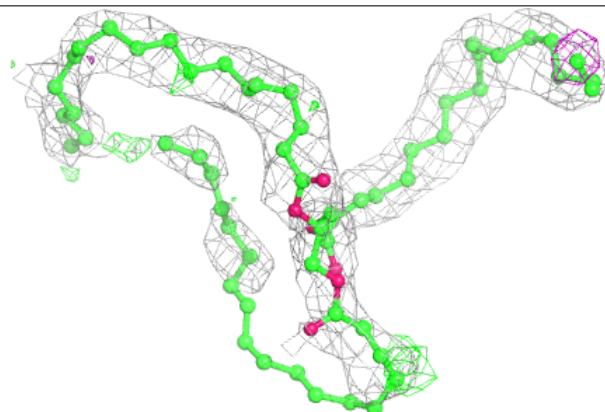


Electron density around DMU P 303:

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

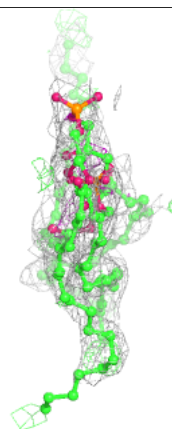
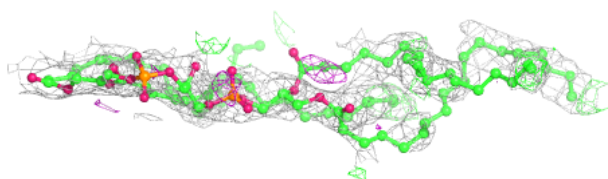
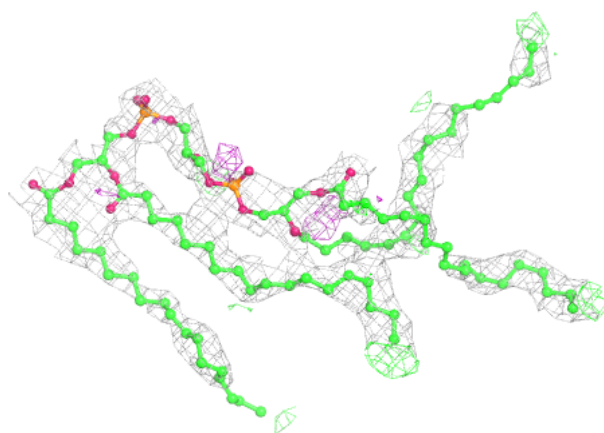
**Electron density around TGL Y 101:**

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

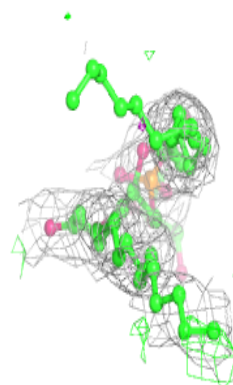
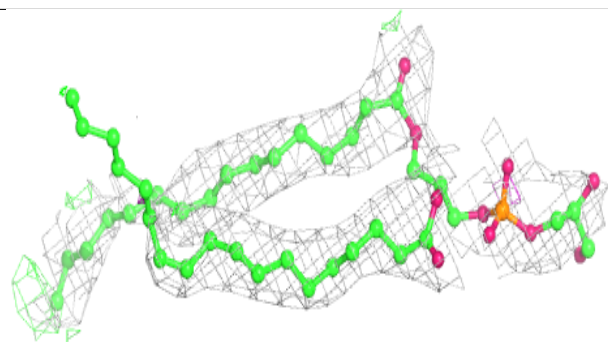
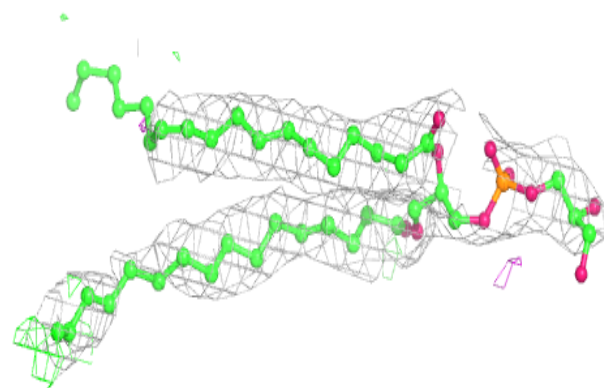


Electron density around CDL A 609:

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

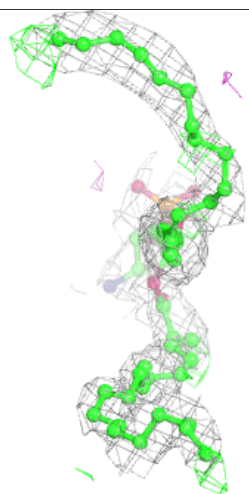
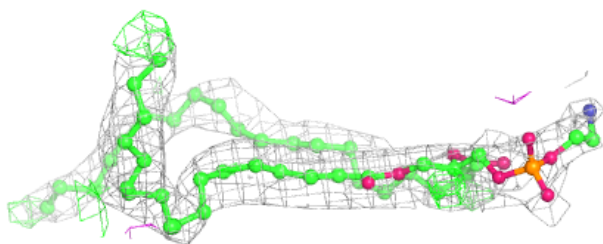
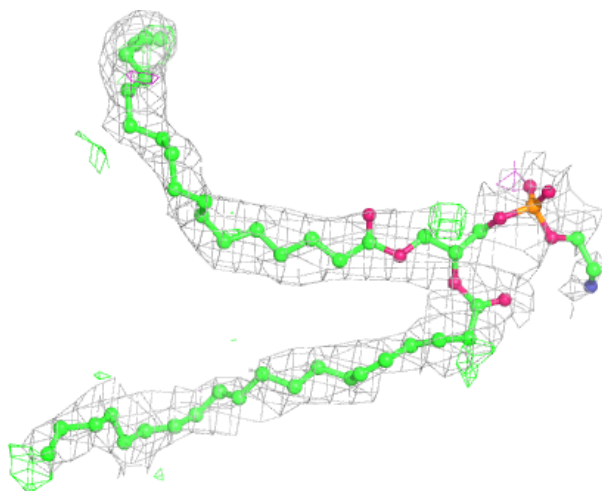
**Electron density around PGV A 607:**

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



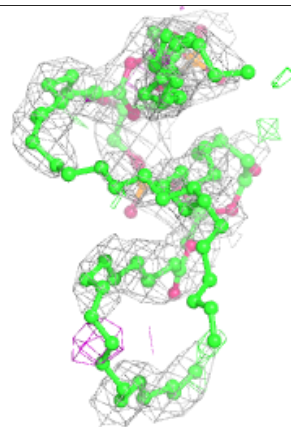
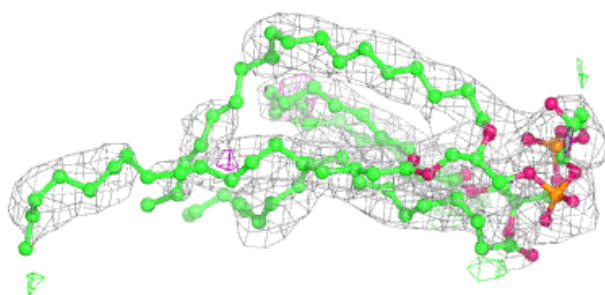
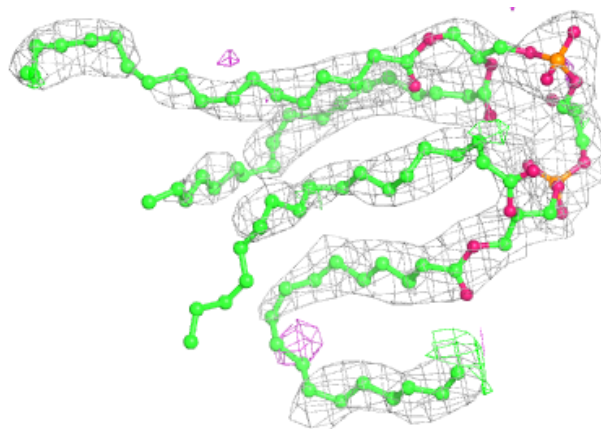
Electron density around PEK G 101:

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

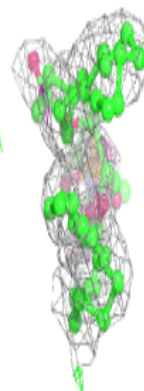
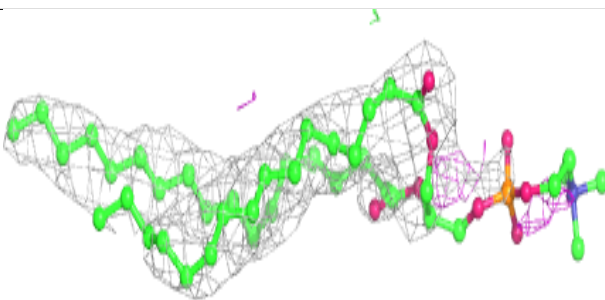
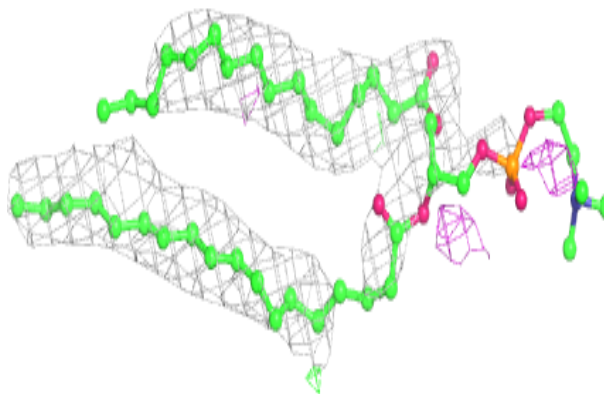


Electron density around CDL C 304:

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

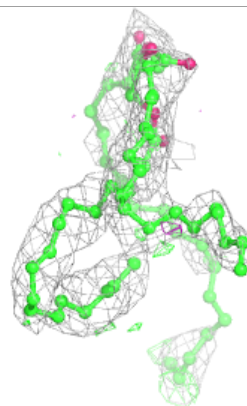
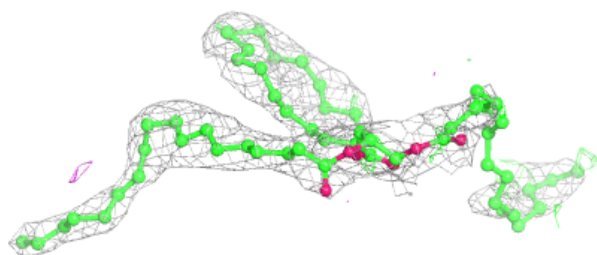
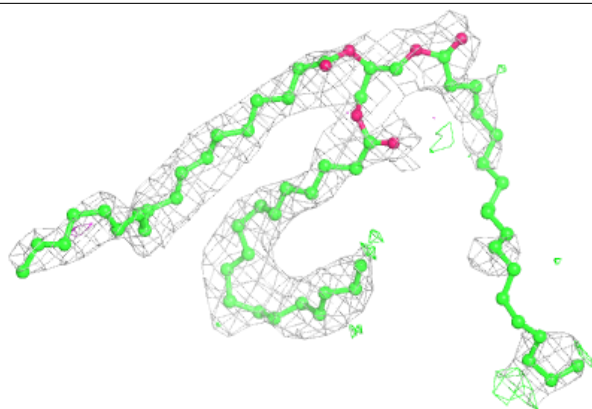
**Electron density around PSC N 608:**

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

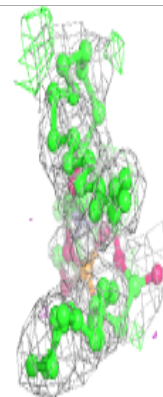
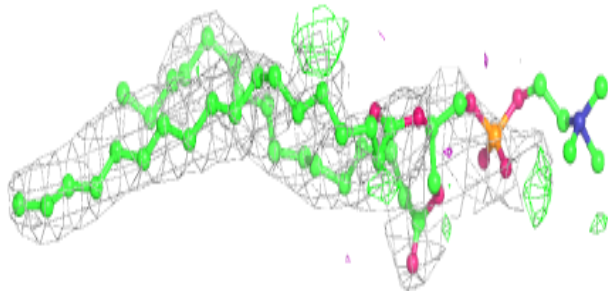
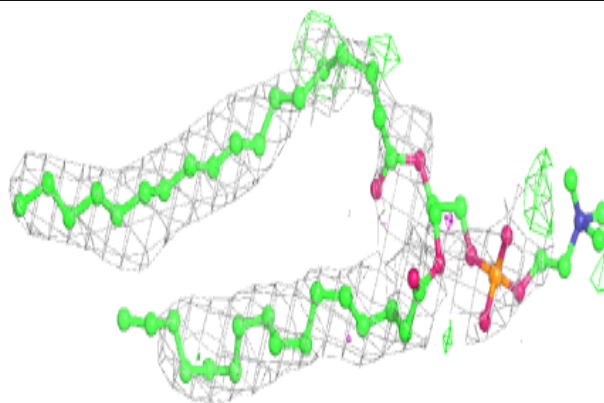


Electron density around TGL N 607:

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

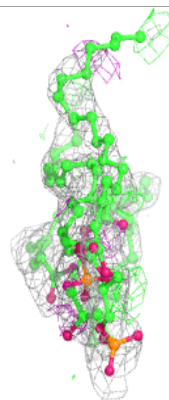
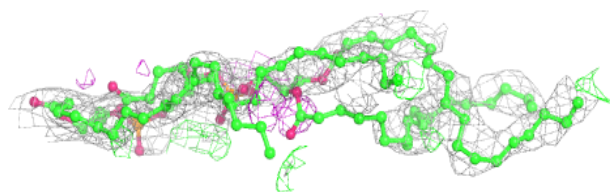
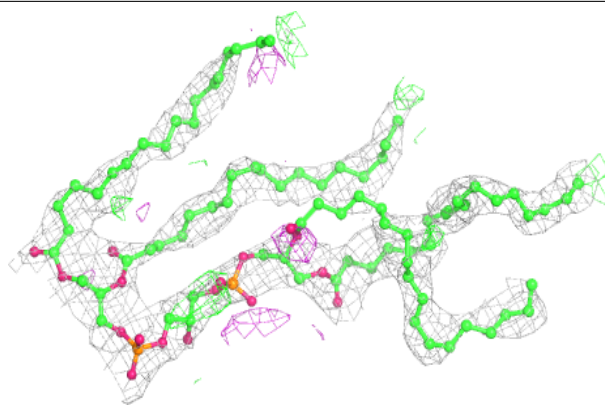
**Electron density around PSC B 304:**

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

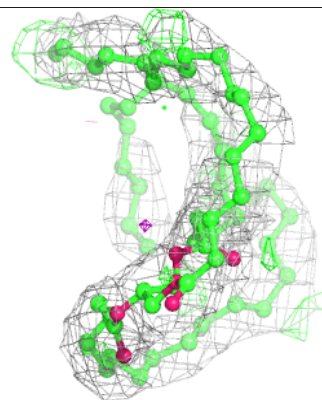
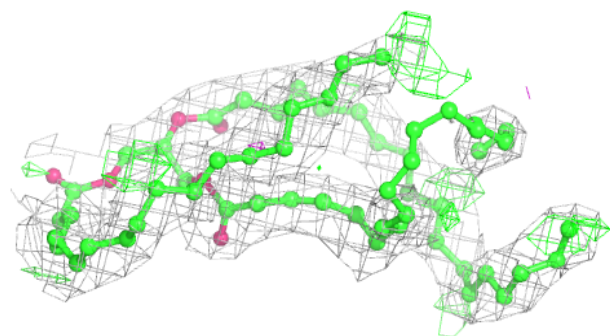
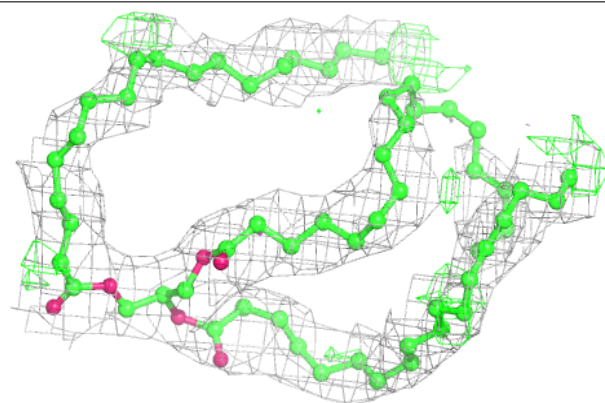


Electron density around CDL G 102:

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

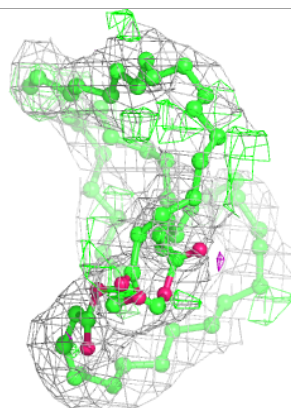
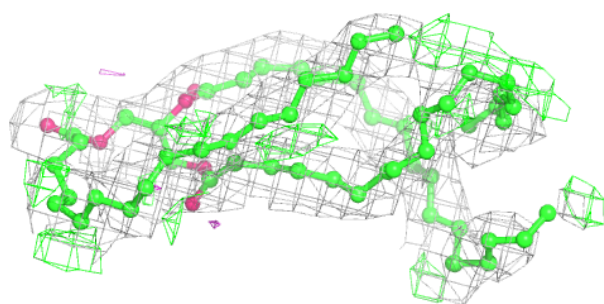
**Electron density around TGL V 101:**

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

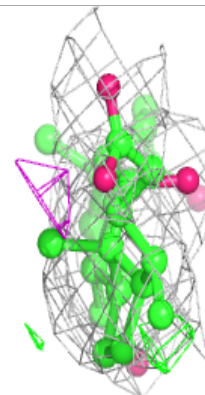
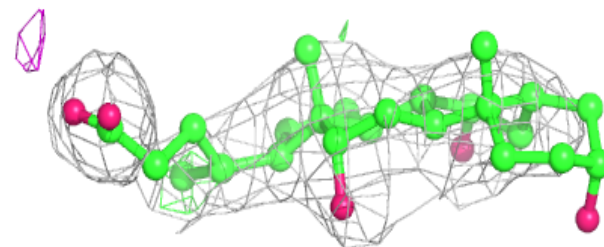
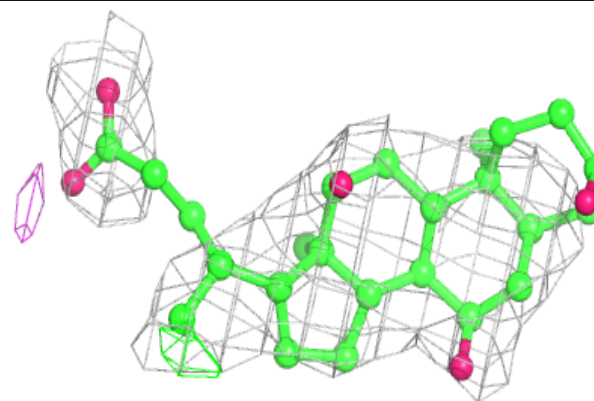


Electron density around TGL B 301:

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

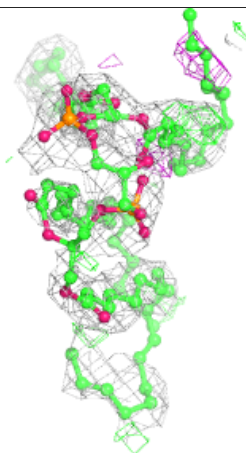
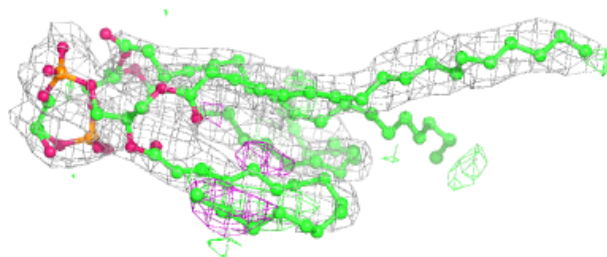
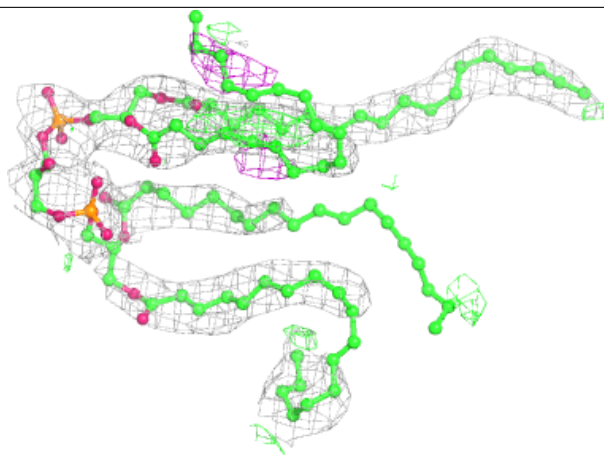
**Electron density around CHD W 101:**

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

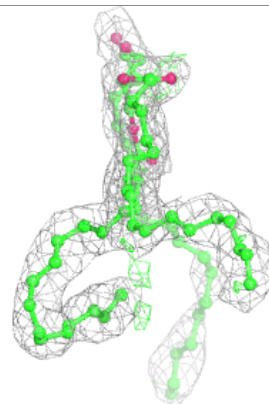
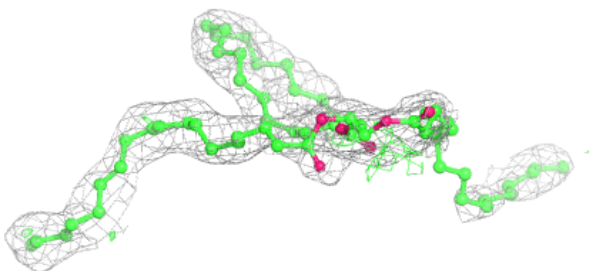


Electron density around CDL P 305:

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

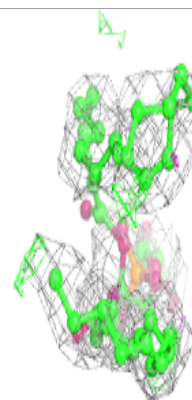
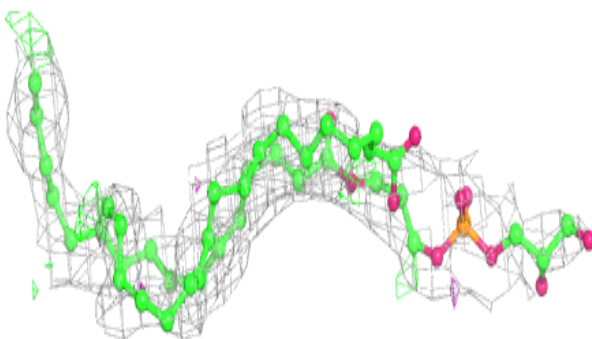
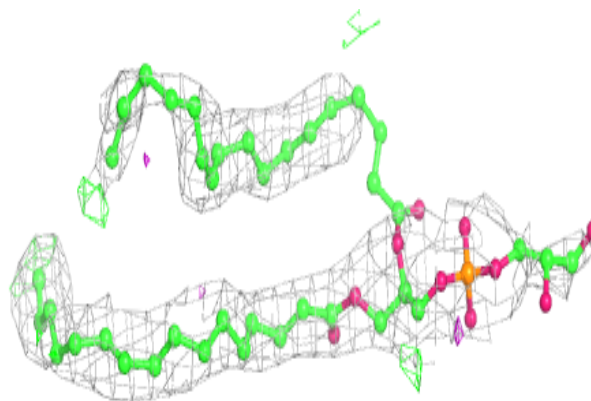
**Electron density around TGL D 201:**

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

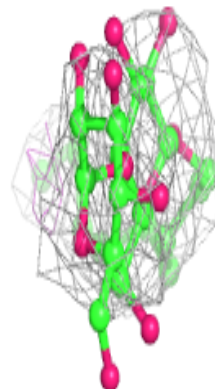
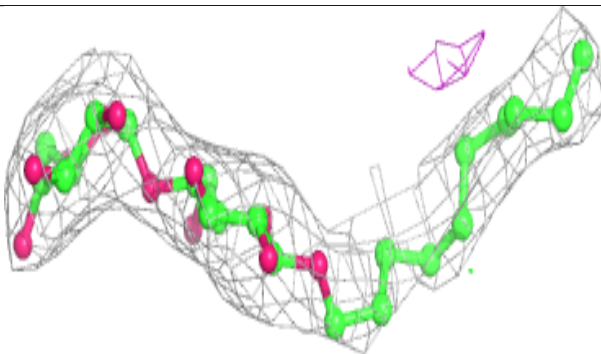
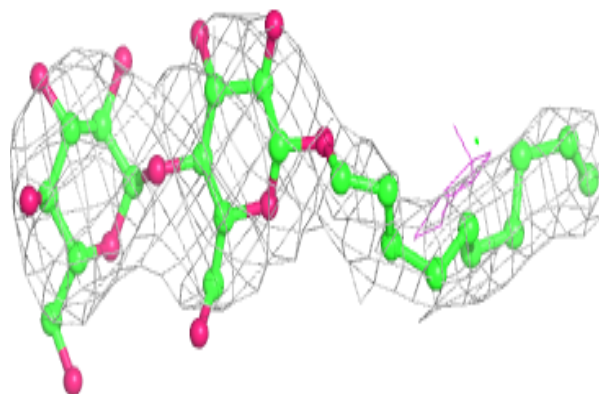


Electron density around PGV C 307:

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

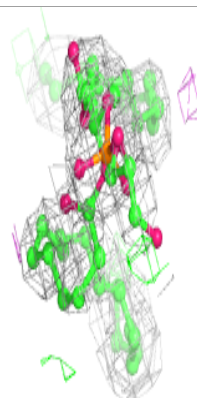
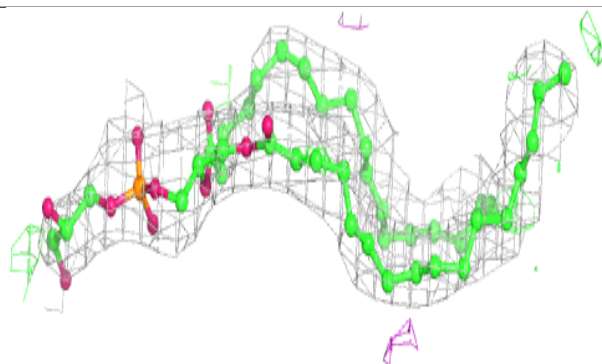
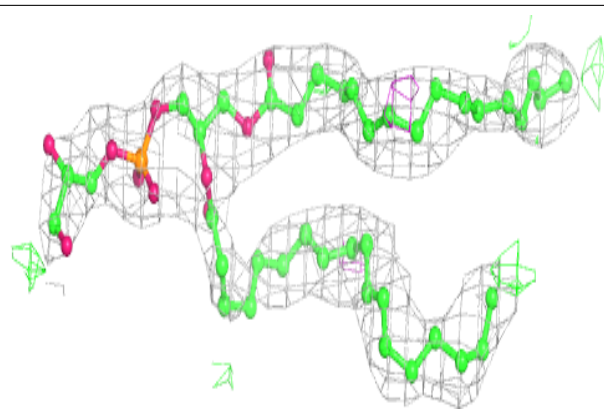
**Electron density around DMU Q 201:**

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



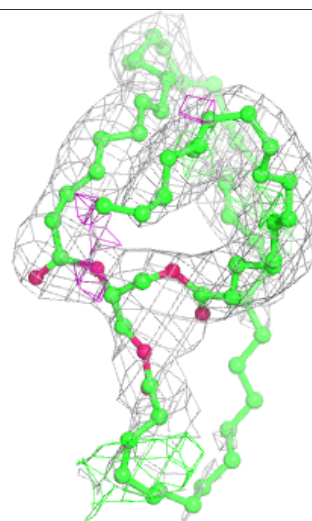
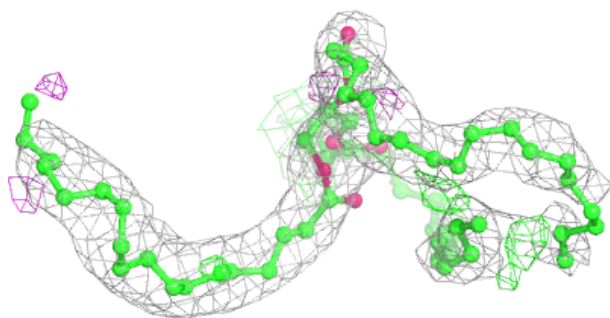
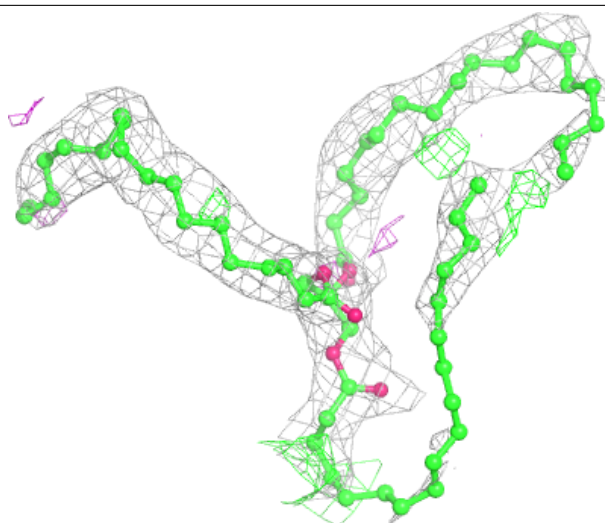
Electron density around PGV P 302:

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



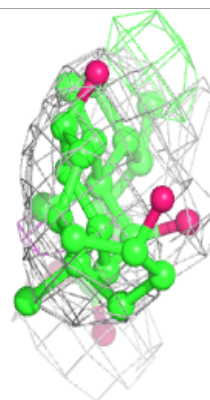
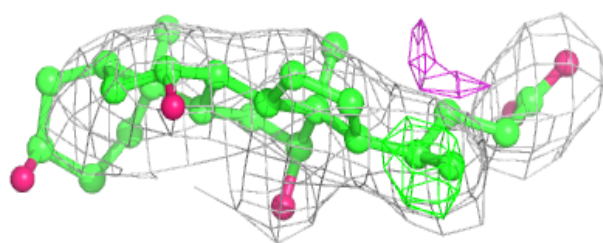
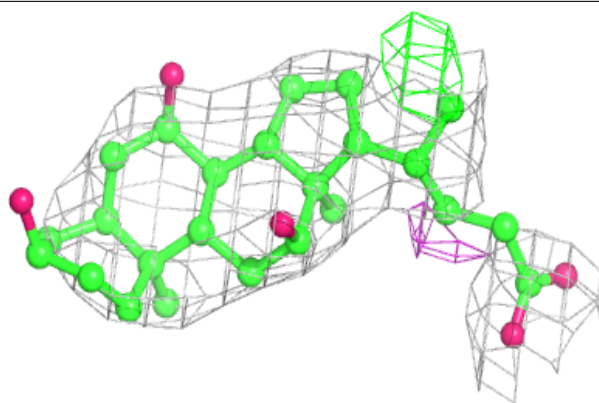
Electron density around TGL A 608:

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

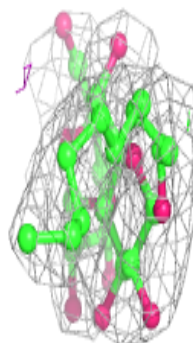
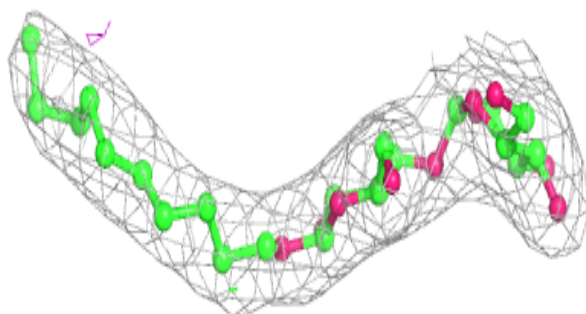
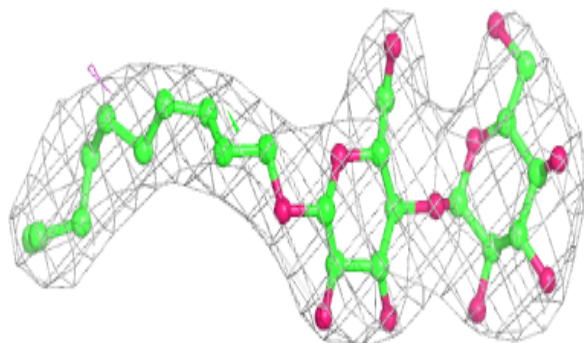


Electron density around CHD J 101:

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

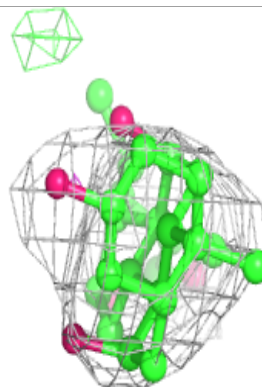
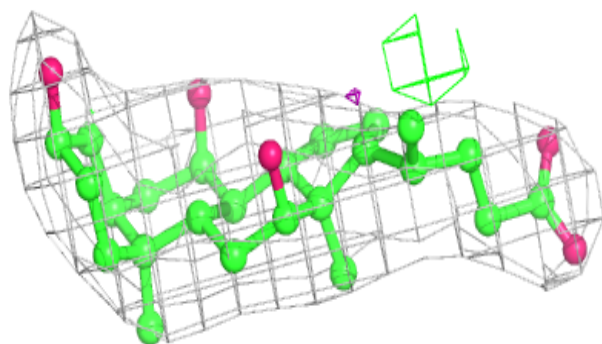
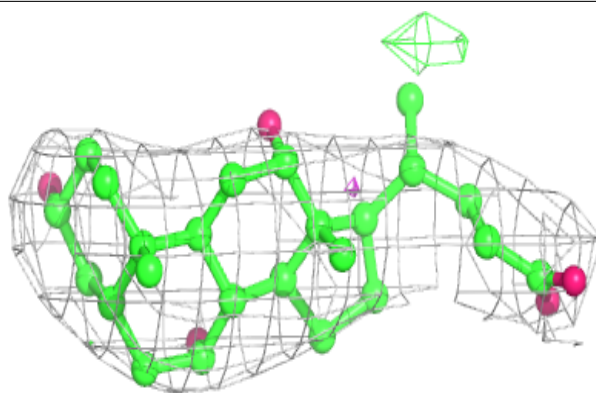
**Electron density around DMU M 101:**

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

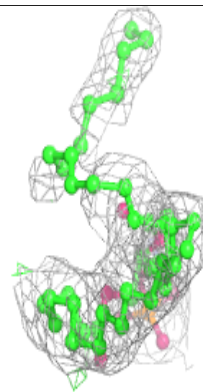
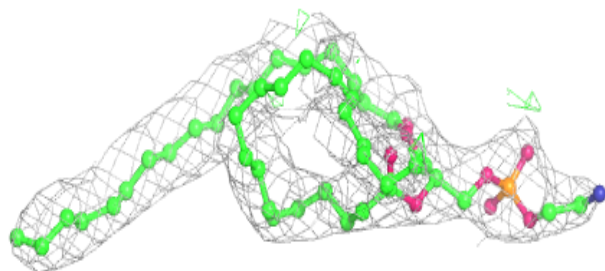
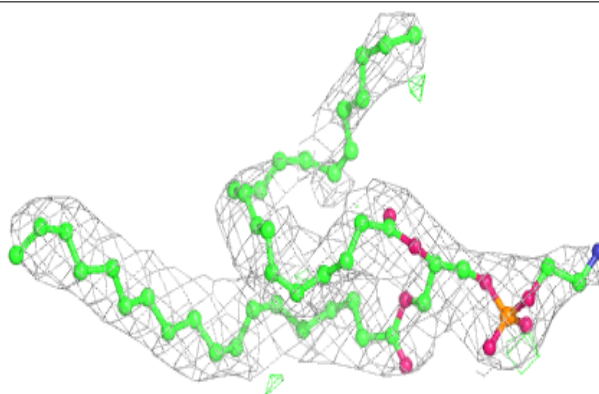


Electron density around CHD C 305:

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

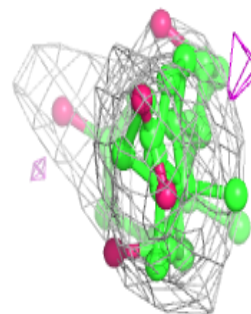
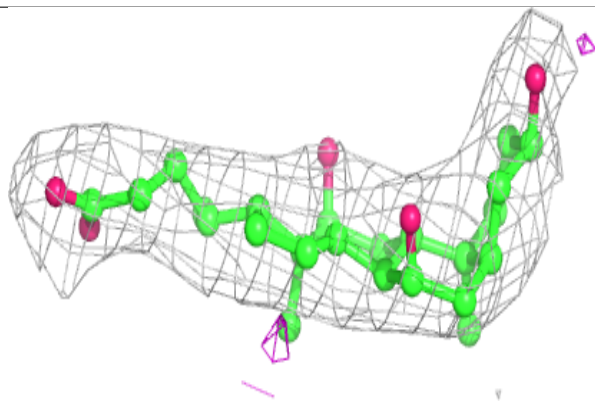
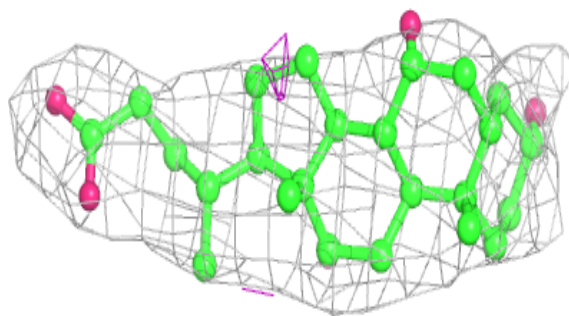
**Electron density around PEK P 308:**

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

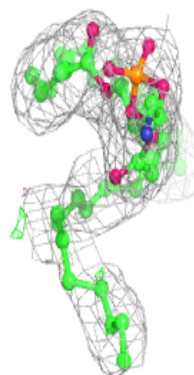
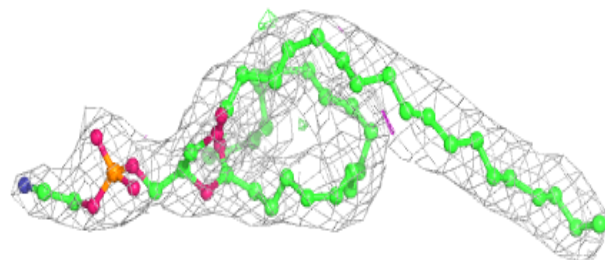
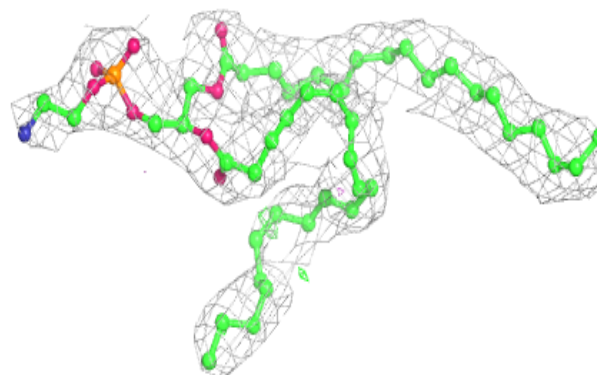


Electron density around CHD P 306:

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

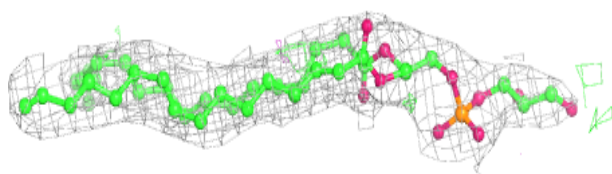
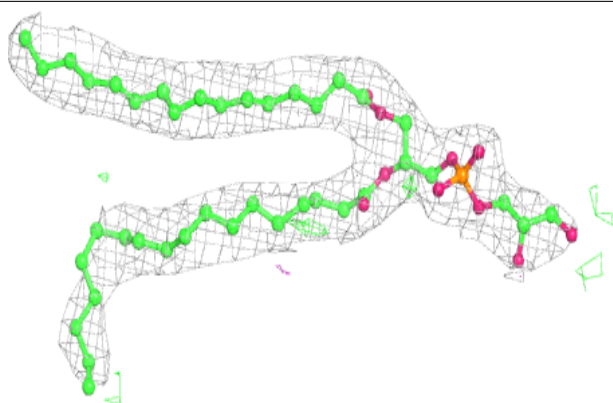
**Electron density around PEK C 302:**

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

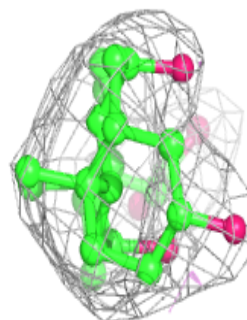
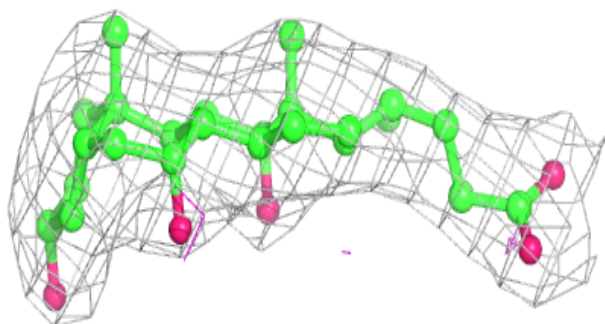
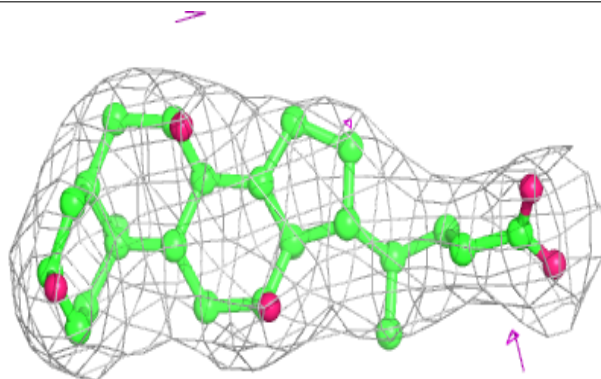


Electron density around PGV P 304:

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

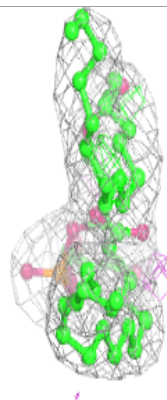
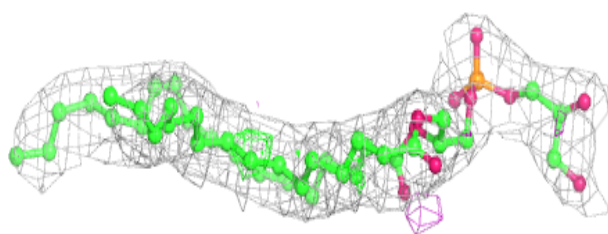
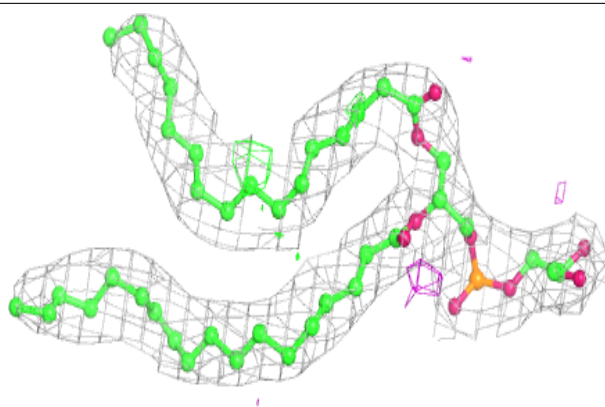
**Electron density around CHD G 104:**

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

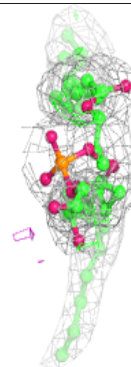
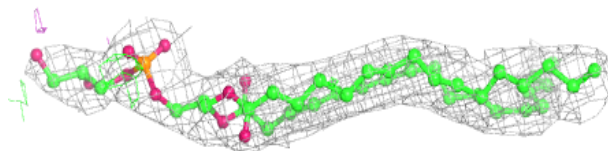
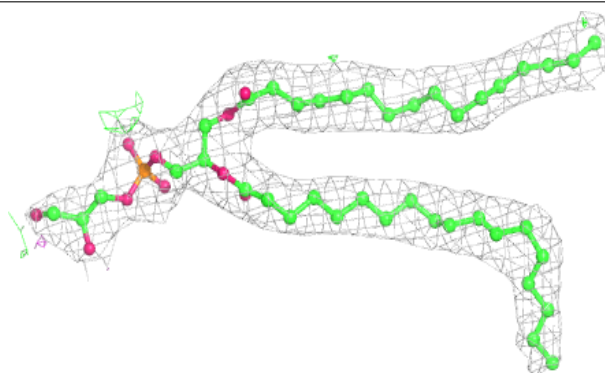


Electron density around PGV P 301:

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

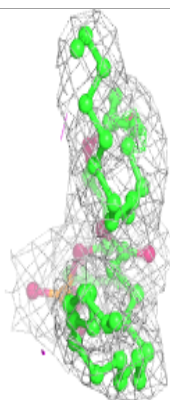
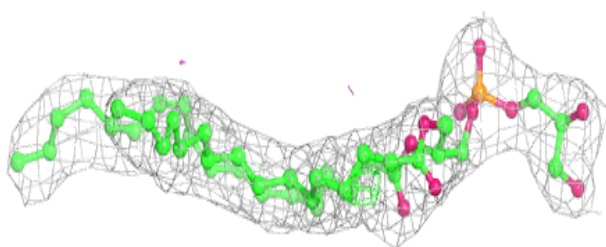
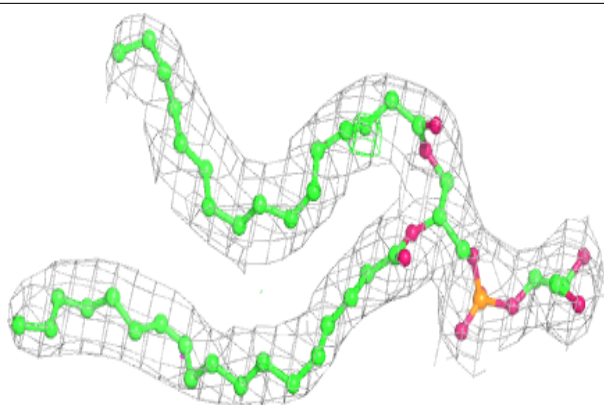
**Electron density around PGV C 303:**

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

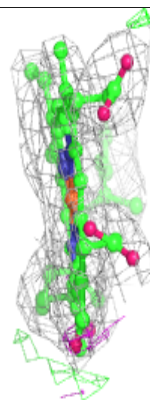
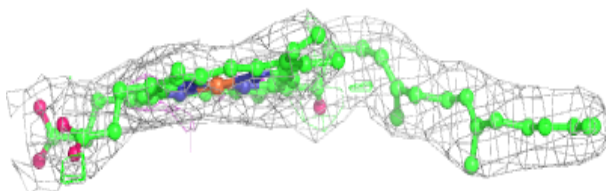
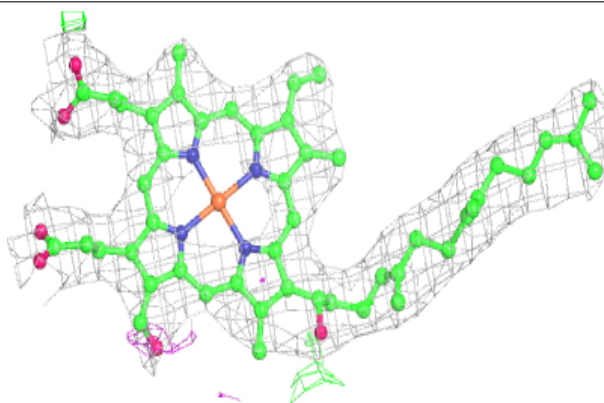


Electron density around PGV A 606:

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

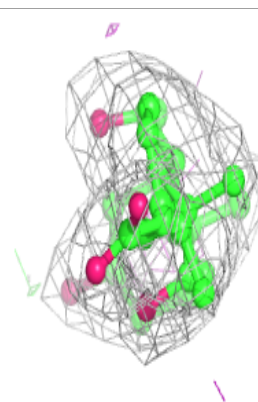
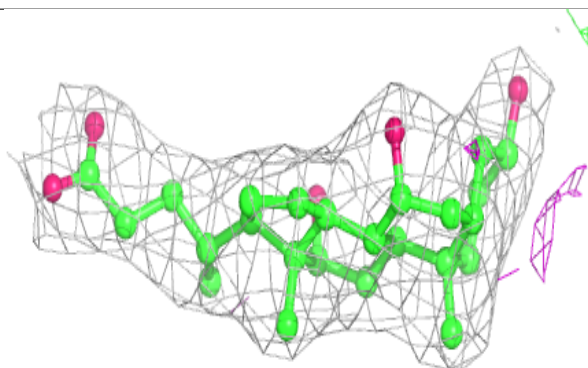
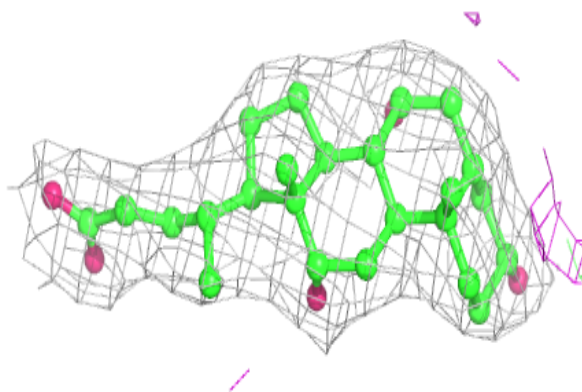
**Electron density around HEA A 601:**

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

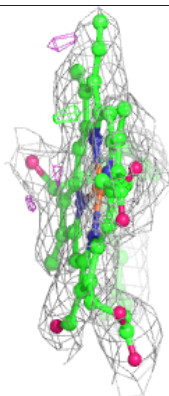
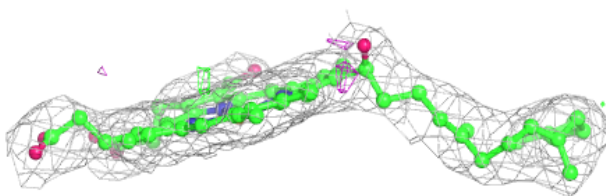
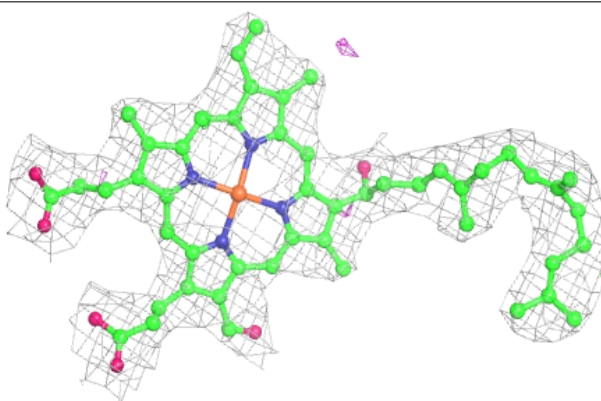


Electron density around CHD P 307:

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

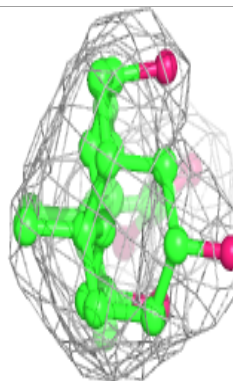
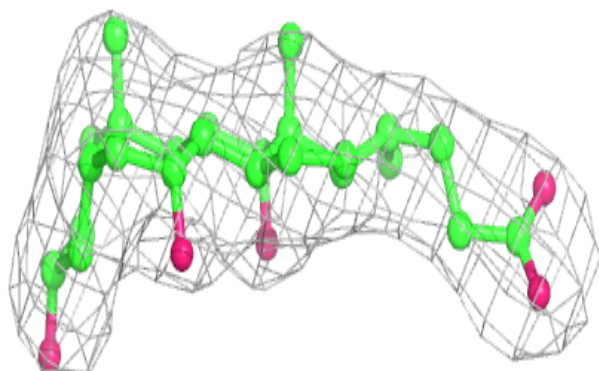
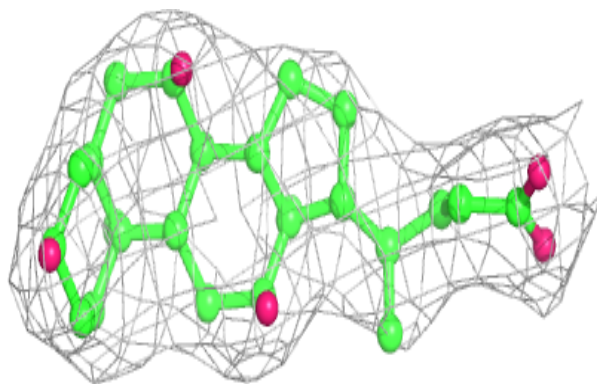
**Electron density around HEA A 602:**

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

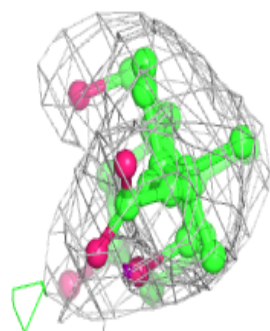
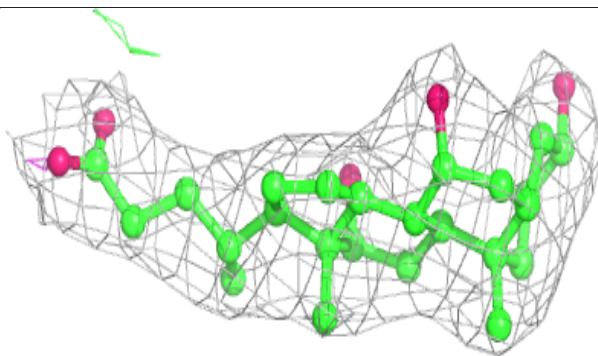
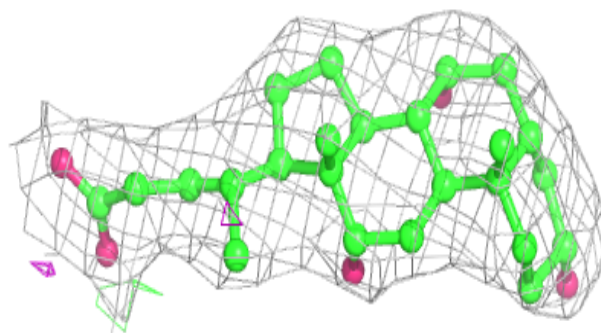


Electron density around CHD B 303:

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

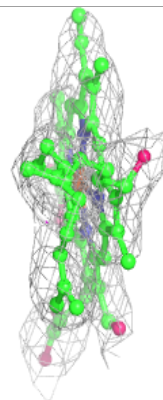
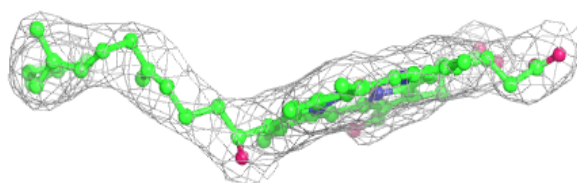
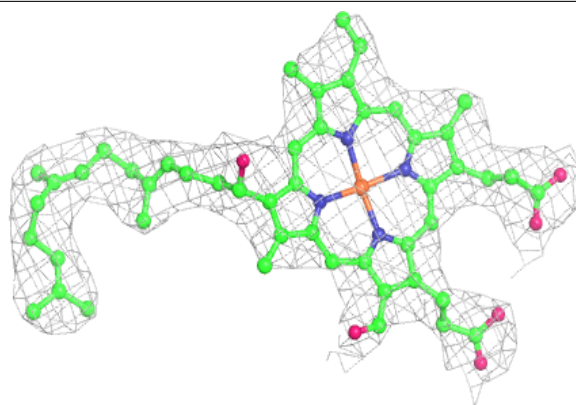
**Electron density around CHD C 306:**

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

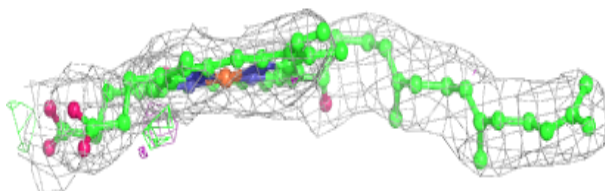
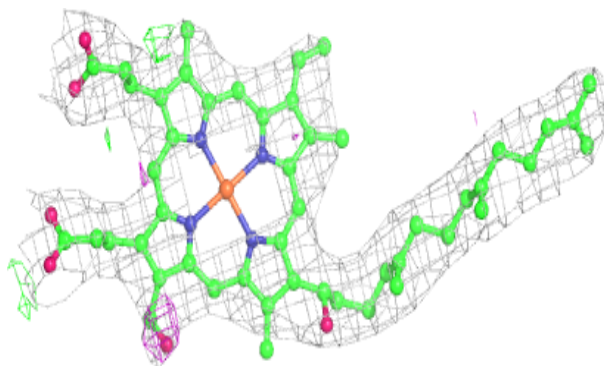


Electron density around HEA N 602:

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

**Electron density around HEA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.