



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 05:12 am BST

PDB ID : 5ZCP
Title : azide-bound cytochrome c oxidase structure determined using the crystals exposed to 20 mM azide solution for 2 days
Authors : Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on : 2018-02-19
Resolution : 1.65 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

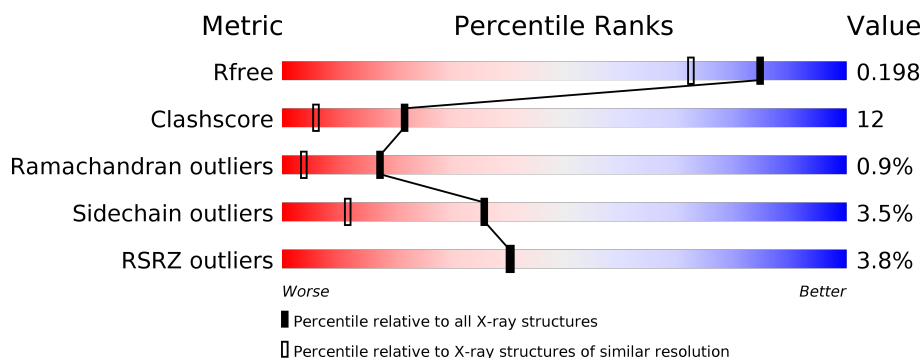
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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>80%</div> <div>17%</div> <div>.</div> </div>
1	N	514	<div> <div>79%</div> <div>18%</div> <div>.</div> </div>
2	B	227	<div> <div>3%</div> <div>68%</div> <div>27%</div> <div>..</div> </div>
2	O	227	<div> <div>3%</div> <div>78%</div> <div>18%</div> <div>.</div> </div>
3	C	261	<div> <div>%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
3	P	261	<div> <div>82%</div> <div>16%</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[A]	X	-	-	-
14	HEA	A	602[B]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
14	HEA	N	603[A]	X	-	-	-
14	HEA	N	603[B]	X	-	-	-
18	AZI	A	607[A]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
21	EDO	A	616	-	X	-	-
21	EDO	D	202	-	-	X	-
27	CDL	N	601	-	-	X	-
27	CDL	P	305	-	-	X	-
9	SAC	V	1	-	X	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33609 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	22	0
			4193	2793	649	709	42			
1	N	514	Total	C	N	O	S	0	20	0
			4179	2786	647	704	42			

- 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	9	0
			1899	1234	292	353	20			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	288	347	20			

- 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	9	0
			2185	1457	349	363	16			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

- 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	4	0
			1233	803	204	222	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	4	0
			778	481	139	152	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

- 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 686	C 440	N 130	O 114	P 1	S 1	0	1	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	0	0
			601	390	107	100	4			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	1	0
			469	302	79	85	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

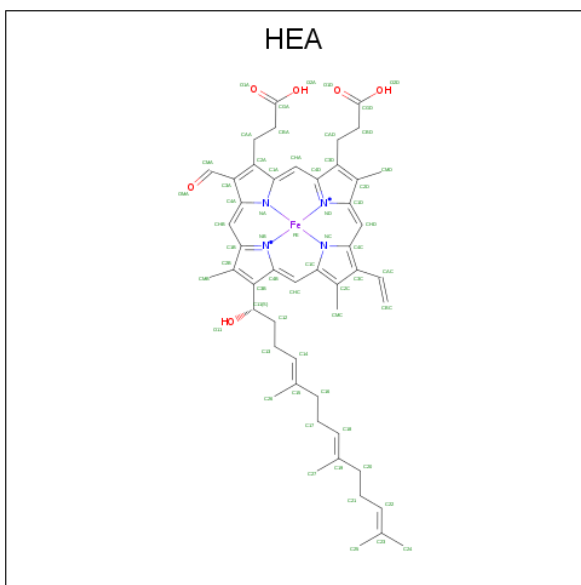
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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	1	0
			388	259	65	61	3			

- 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	C	Fe	N	O	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	1
			120	98	2	8	12		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	1
			120	98	2	8	12		

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

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

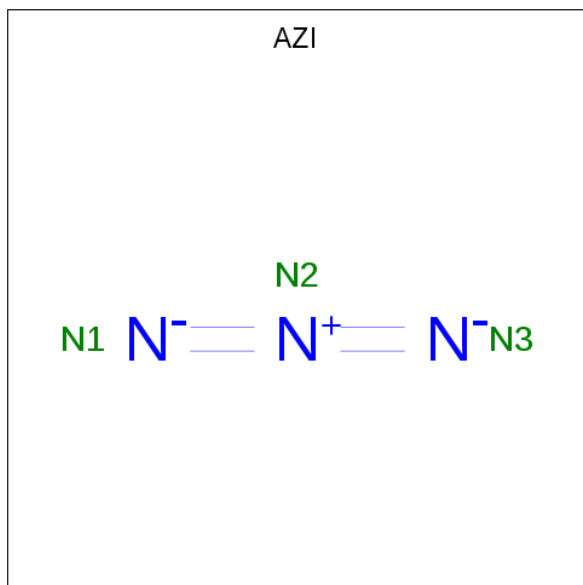
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

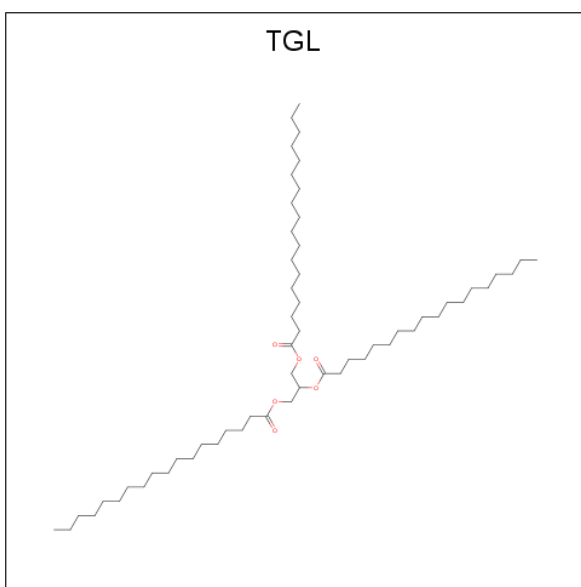
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is AZIDE ION (three-letter code: AZI) (formula: N_3).



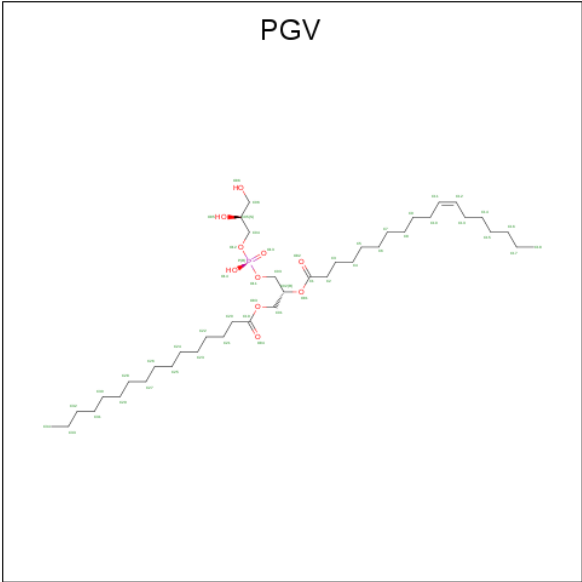
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	1
18	A	1	Total N 6 6	0	1
18	N	1	Total N 3 3	0	1
18	N	1	Total N 6 6	0	1

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



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

- Molecule 20 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
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		

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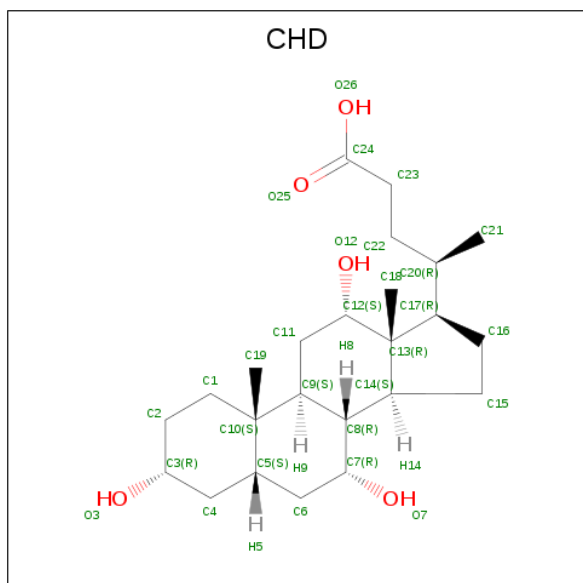
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	L	1	Total 4	C 2	O 2	0	0
21	M	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		
21	W	1	Total	C	O	0	0
			4	2	2		
21	Y	1	Total	C	O	0	0
			4	2	2		

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



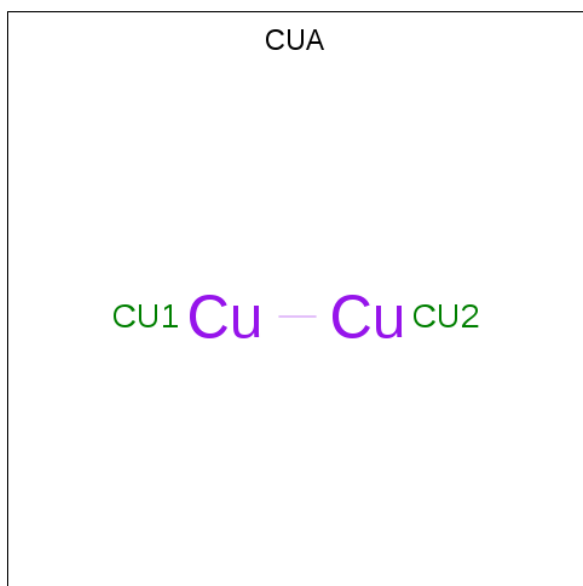
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		

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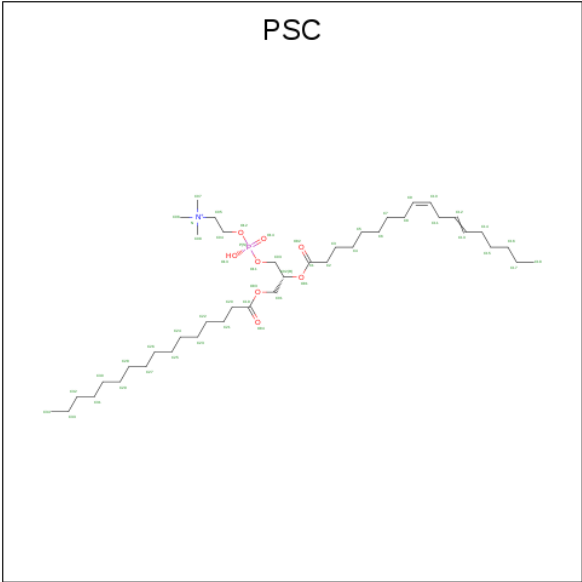
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	G	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



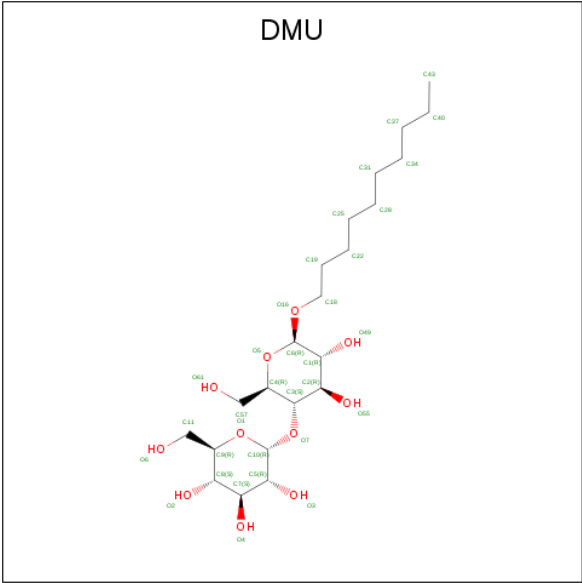
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total Cu 2 2	0	0
23	O	1	Total Cu 2 2	0	0

- Molecule 24 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: C₄₂H₈₁NO₈P).



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

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

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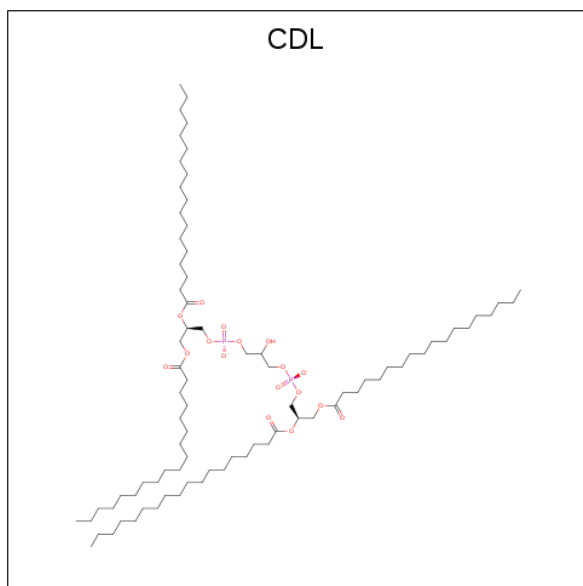
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C O 33 22 11	0	0
25	C	1	Total C O 33 22 11	0	0
25	M	1	Total C O 33 22 11	0	0
25	P	1	Total C O 33 22 11	0	0
25	P	1	Total C O 33 22 11	0	0
25	P	1	Total C O 33 22 11	0	0
25	Z	1	Total C O 33 22 11	0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

- Molecule 26 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

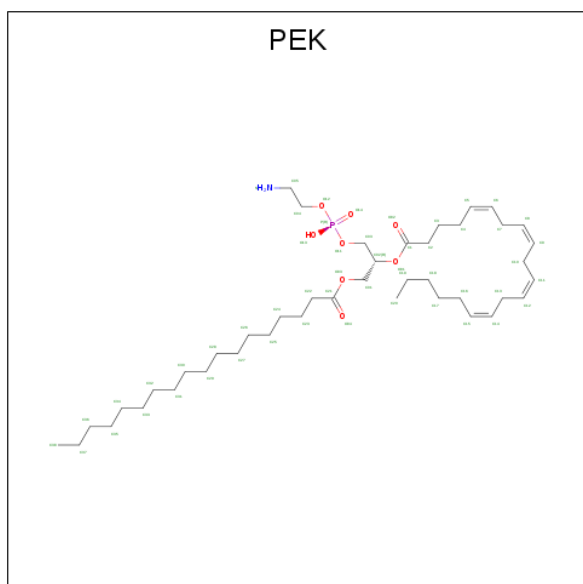
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	P	1	Total X 1 1	0	0
26	C	1	Total X 1 1	0	0

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 28 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
28	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	235	Total 235	O 235	0	0
30	B	161	Total 162	O 162	0	1
30	C	110	Total 110	O 110	0	0
30	D	118	Total 118	O 118	0	0
30	E	93	Total 93	O 93	0	0
30	F	94	Total 94	O 94	0	0
30	G	42	Total 42	O 42	0	0
30	H	42	Total 42	O 42	0	0
30	I	27	Total 27	O 27	0	0
30	J	23	Total 23	O 23	0	0
30	K	26	Total 26	O 26	0	0
30	L	38	Total 38	O 38	0	0
30	M	25	Total 25	O 25	0	0
30	N	203	Total 203	O 203	0	0
30	O	99	Total 100	O 100	0	1
30	P	95	Total 95	O 95	0	0
30	Q	29	Total 29	O 29	0	0
30	R	40	Total 40	O 40	0	0

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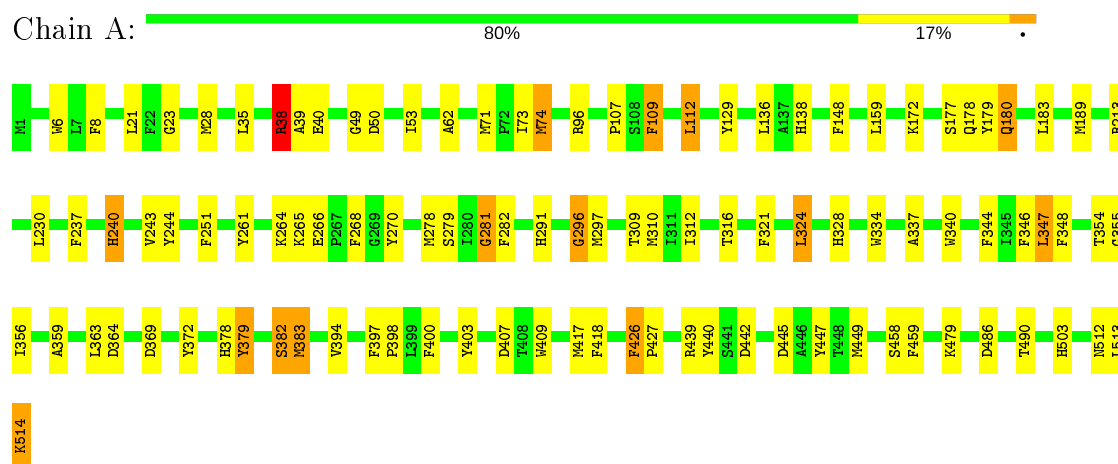
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	S	45	Total 45	O 45	0	0
30	T	35	Total 35	O 35	0	0
30	U	29	Total 29	O 29	0	0
30	V	16	Total 16	O 16	0	0
30	W	7	Total 7	O 7	0	0
30	X	11	Total 11	O 11	0	0
30	Y	12	Total 12	O 12	0	0
30	Z	12	Total 12	O 12	0	0

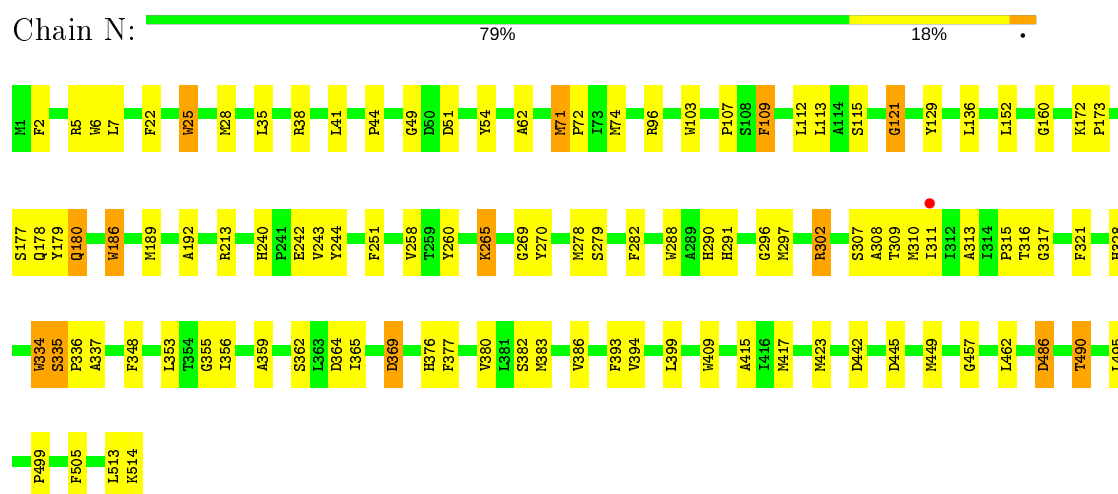
3 Residue-property plots

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

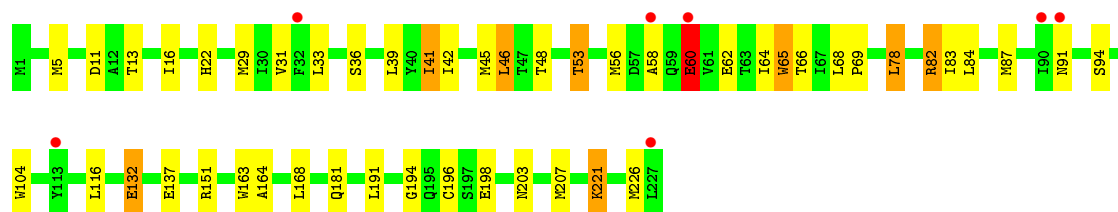
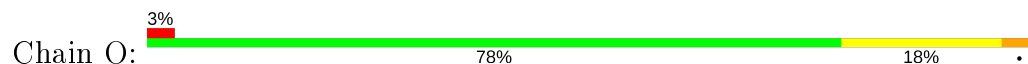


• Molecule 2: Cytochrome c oxidase subunit 2

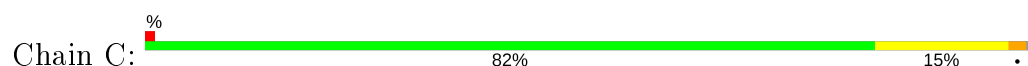




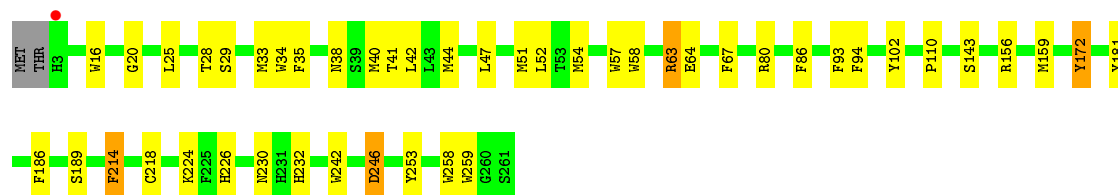
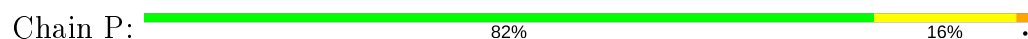
- Molecule 2: Cytochrome c oxidase subunit 2



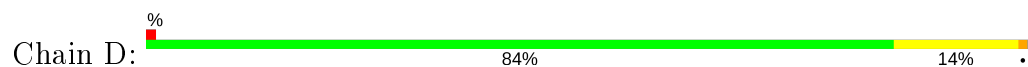
- Molecule 3: Cytochrome c oxidase subunit 3



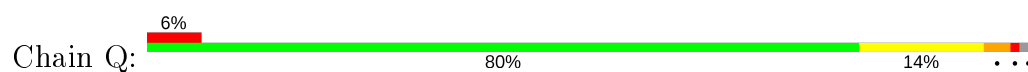
- Molecule 3: Cytochrome c oxidase subunit 3



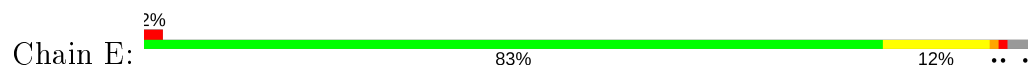
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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



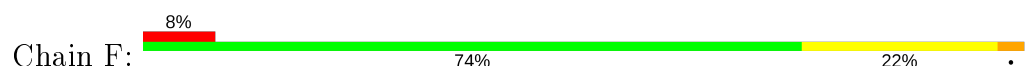
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



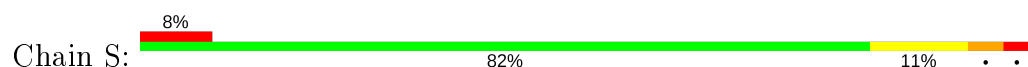
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



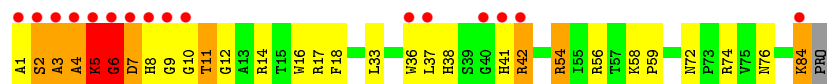
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



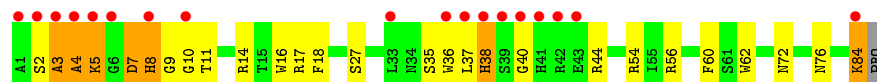
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



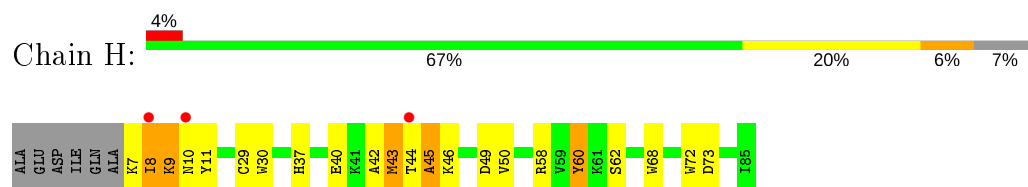
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



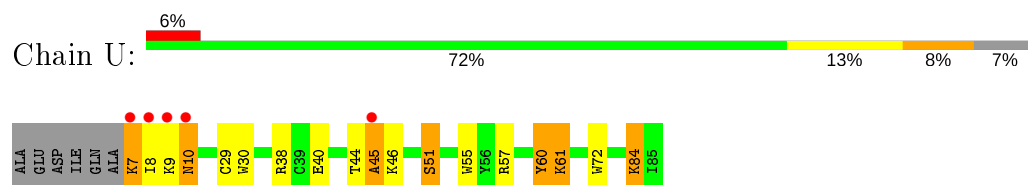
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



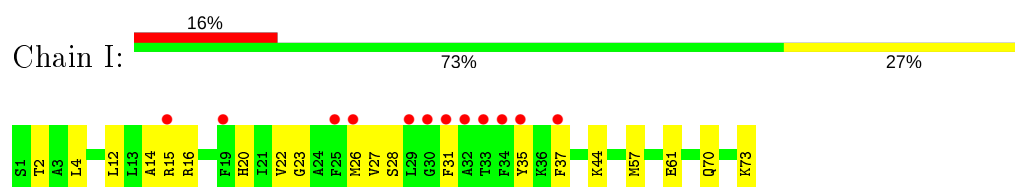
- Molecule 8: Cytochrome c oxidase subunit 6B1



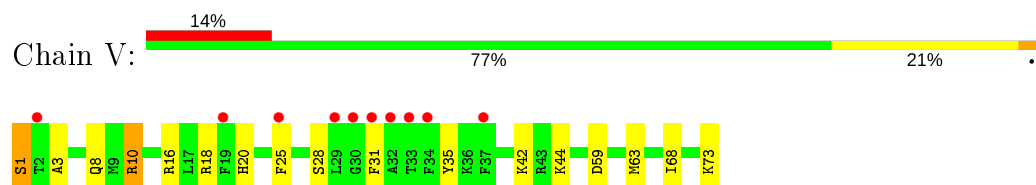
- Molecule 8: Cytochrome c oxidase subunit 6B1



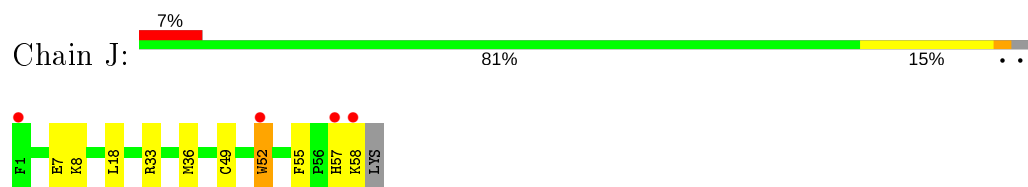
- Molecule 9: Cytochrome c oxidase subunit 6C



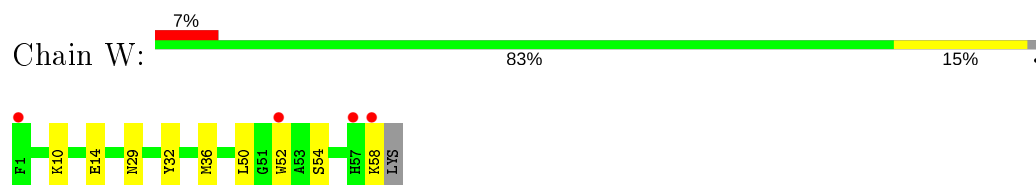
- Molecule 9: Cytochrome c oxidase subunit 6C



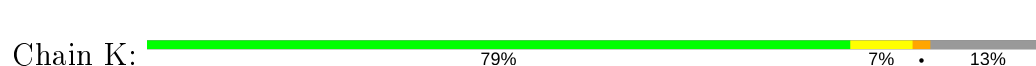
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



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

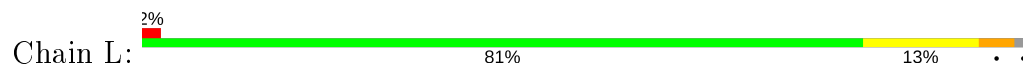




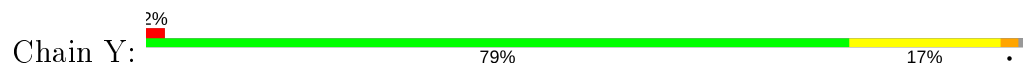
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



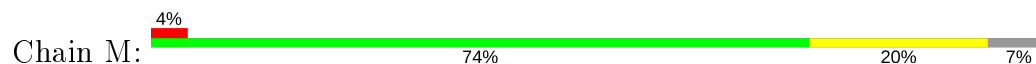
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



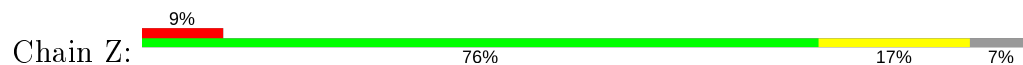
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.32Å 206.17Å 177.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.65 137.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-1.65) 99.6 (137.00-1.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.175 , 0.197 0.176 , 0.198	Depositor DCC
R_{free} test set	39973 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33609	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: AZI, ZN, CHD, HEA, SAC, TPO, PSC, PEK, MG, TGL, EDO, PGV, CDL, UNX, CUA, NA, FME, CU, DMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.62	23/4322 (0.5%)	1.43	39/5897 (0.7%)
1	N	1.58	30/4308 (0.7%)	1.39	29/5878 (0.5%)
2	B	1.52	12/1937 (0.6%)	1.37	14/2637 (0.5%)
2	O	1.30	8/1908 (0.4%)	1.16	7/2597 (0.3%)
3	C	1.53	15/2272 (0.7%)	1.28	8/3102 (0.3%)
3	P	1.57	19/2272 (0.8%)	1.32	14/3102 (0.5%)
4	D	1.51	4/1268 (0.3%)	1.29	8/1709 (0.5%)
4	Q	1.17	4/1259 (0.3%)	1.23	4/1698 (0.2%)
5	E	1.50	6/871 (0.7%)	1.62	8/1182 (0.7%)
5	R	1.33	4/882 (0.5%)	1.25	5/1196 (0.4%)
6	F	1.37	2/795 (0.3%)	1.21	1/1079 (0.1%)
6	S	1.25	0/780	1.20	2/1058 (0.2%)
7	G	1.46	3/702 (0.4%)	1.21	6/953 (0.6%)
7	T	1.51	6/702 (0.9%)	1.19	3/953 (0.3%)
8	H	1.34	4/682 (0.6%)	1.03	1/921 (0.1%)
8	U	1.12	3/682 (0.4%)	0.95	1/921 (0.1%)
9	I	1.26	2/605 (0.3%)	1.19	2/802 (0.2%)
9	V	1.09	0/605	1.11	3/802 (0.4%)
10	J	1.34	1/471 (0.2%)	1.17	1/636 (0.2%)
10	W	1.31	1/480 (0.2%)	1.20	1/648 (0.2%)
11	K	1.36	2/398 (0.5%)	1.16	1/546 (0.2%)
11	X	1.19	3/405 (0.7%)	0.93	1/556 (0.2%)
12	L	1.45	0/393	1.30	2/526 (0.4%)
12	Y	1.34	0/401	1.09	0/536
13	M	1.48	3/345 (0.9%)	1.15	0/470
13	Z	1.28	2/345 (0.6%)	0.97	0/470
All	All	1.46	157/30090 (0.5%)	1.29	161/40875 (0.4%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	N	0	2
6	F	0	1
6	S	0	2
7	G	0	1
9	V	0	1
All	All	0	11

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	SER	CB-OG	8.75	1.53	1.42
2	B	198	GLU	CD-OE2	-8.56	1.16	1.25
4	D	58	GLU	CD-OE1	8.47	1.34	1.25
1	N	409	TRP	CD2-CE2	8.41	1.51	1.41
2	B	108	TYR	CE1-CZ	8.16	1.49	1.38
11	K	29	TRP	CD2-CE2	7.97	1.50	1.41
3	C	57	TRP	CD2-CE2	7.97	1.50	1.41
1	A	403	TYR	CG-CD1	7.94	1.49	1.39
1	N	25	TRP	CD2-CE2	7.89	1.50	1.41
1	A	96	ARG	CZ-NH1	7.70	1.43	1.33
1	A	74	MET	CB-CG	7.61	1.75	1.51
3	C	35	PHE	CG-CD2	7.58	1.50	1.38
4	Q	78	TRP	CD2-CE2	7.23	1.50	1.41
5	R	69	GLU	CD-OE2	-7.22	1.17	1.25
2	B	198	GLU	CD-OE1	-7.14	1.17	1.25
7	G	16	TRP	CD2-CE2	7.06	1.49	1.41
2	O	198	GLU	CD-OE2	-6.98	1.18	1.25
5	E	15	TRP	CD2-CE2	6.91	1.49	1.41
13	M	20	SER	CA-CB	6.88	1.63	1.52
1	N	334	TRP	CD2-CE2	6.84	1.49	1.41
3	P	143	SER	CA-CB	6.83	1.63	1.52
1	N	49	GLY	C-O	6.81	1.34	1.23
3	C	57	TRP	CD1-NE1	6.79	1.49	1.38
7	T	16	TRP	CD2-CE2	6.78	1.49	1.41
5	R	27	TRP	CD2-CE2	6.77	1.49	1.41
1	A	447	TYR	CG-CD1	6.74	1.48	1.39
1	N	244	TYR	CE2-CZ	6.71	1.47	1.38
2	B	65	TRP	CD2-CE2	6.70	1.49	1.41
8	H	72	TRP	CD2-CE2	6.64	1.49	1.41
3	P	34	TRP	CD2-CE2	6.62	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	258	TRP	CD2-CE2	6.61	1.49	1.41
3	C	58	TRP	CD2-CE2	6.61	1.49	1.41
1	N	96	ARG	CZ-NH1	6.59	1.41	1.33
3	P	258	TRP	CD2-CE2	6.59	1.49	1.41
7	T	62	TRP	CD2-CE2	6.58	1.49	1.41
1	N	288	TRP	CD2-CE2	6.57	1.49	1.41
1	A	458	SER	CB-OG	6.56	1.50	1.42
13	M	32	TRP	CD2-CE2	6.54	1.49	1.41
1	N	279	SER	CA-CB	6.51	1.62	1.52
3	P	20	GLY	N-CA	6.48	1.55	1.46
7	G	36	TRP	CD2-CE2	6.46	1.49	1.41
1	N	74	MET	CB-CG	6.45	1.72	1.51
1	A	409	TRP	CD2-CE2	6.44	1.49	1.41
6	F	4	GLY	N-CA	6.41	1.55	1.46
11	X	29	TRP	CD2-CE2	6.38	1.49	1.41
1	N	6	TRP	CD2-CE2	6.37	1.49	1.41
4	D	104	TYR	CB-CG	6.34	1.61	1.51
1	A	340	TRP	CD2-CE2	6.31	1.49	1.41
2	O	65	TRP	CD2-CE2	6.27	1.48	1.41
2	O	36	SER	CB-OG	6.26	1.50	1.42
8	U	72	TRP	CD2-CE2	6.26	1.48	1.41
4	Q	138	TRP	CD2-CE2	6.26	1.48	1.41
2	O	198	GLU	CD-OE1	-6.25	1.18	1.25
7	G	56	ARG	CZ-NH1	6.24	1.41	1.33
2	B	53	THR	N-CA	6.24	1.58	1.46
1	A	74	MET	CG-SD	-6.21	1.65	1.81
4	D	138	TRP	CD2-CE2	6.19	1.48	1.41
2	B	105	TYR	CE1-CZ	6.19	1.46	1.38
1	N	335	SER	CB-OG	6.18	1.50	1.42
7	T	36	TRP	CD2-CE2	6.08	1.48	1.41
1	A	281	GLY	N-CA	6.06	1.55	1.46
1	N	317	GLY	N-CA	6.04	1.55	1.46
3	C	76	GLN	CD-OE1	6.04	1.37	1.24
2	O	163	TRP	CD2-CE2	6.04	1.48	1.41
5	R	83	PRO	N-CA	6.03	1.57	1.47
3	C	249	TRP	CD2-CE2	6.02	1.48	1.41
11	X	53	TRP	CD2-CE2	6.00	1.48	1.41
4	Q	145	TRP	CD2-CE2	5.99	1.48	1.41
3	P	35	PHE	CG-CD2	5.98	1.47	1.38
1	N	192	ALA	N-CA	5.92	1.58	1.46
1	N	242	GLU	CD-OE1	5.90	1.32	1.25
2	B	163	TRP	CD2-CE2	5.88	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	186	TRP	CD2-CE2	5.88	1.48	1.41
1	N	315	PRO	CA-CB	5.88	1.65	1.53
3	P	189	SER	CA-CB	5.87	1.61	1.52
3	C	34	TRP	CD2-CE2	5.85	1.48	1.41
3	C	102	TYR	CG-CD2	-5.84	1.31	1.39
1	N	5	ARG	CZ-NH1	5.84	1.40	1.33
7	T	60	PHE	CG-CD1	5.80	1.47	1.38
3	P	218	CYS	CB-SG	5.79	1.92	1.82
5	E	63	SER	CB-OG	5.79	1.49	1.42
3	C	46	GLY	N-CA	5.78	1.54	1.46
1	A	179	TYR	CG-CD1	5.74	1.46	1.39
9	I	4	LEU	CA-CB	5.69	1.66	1.53
1	N	270	TYR	CE1-CZ	-5.68	1.31	1.38
1	A	6	TRP	CG-CD1	5.66	1.44	1.36
3	P	172	TYR	CG-CD1	5.66	1.46	1.39
3	P	242	TRP	CD2-CE2	5.65	1.48	1.41
1	A	279	SER	CA-CB	5.63	1.61	1.52
13	Z	20	SER	CA-CB	5.63	1.61	1.52
1	N	505	PHE	CE2-CZ	5.62	1.48	1.37
13	Z	32	TRP	CD2-CE2	5.62	1.48	1.41
1	A	244	TYR	CG-CD1	5.57	1.46	1.39
3	P	232	HIS	CG-CD2	5.57	1.45	1.35
3	P	16	TRP	CG-CD2	5.57	1.53	1.43
7	T	56	ARG	CZ-NH1	5.56	1.40	1.33
2	B	220	GLU	CD-OE2	-5.54	1.19	1.25
1	A	6	TRP	CD2-CE2	5.54	1.48	1.41
1	A	237	PHE	CG-CD1	5.54	1.47	1.38
3	P	64	GLU	CD-OE2	5.53	1.31	1.25
1	N	258	VAL	C-O	5.52	1.33	1.23
3	P	226	HIS	CG-CD2	5.50	1.45	1.35
1	A	179	TYR	CE1-CZ	5.50	1.45	1.38
1	A	270	TYR	N-CA	5.50	1.57	1.46
2	B	106	TRP	CD2-CE2	5.49	1.48	1.41
3	C	105	SER	CB-OG	5.48	1.49	1.42
3	P	63	ARG	CZ-NH2	5.47	1.40	1.33
3	P	253	TYR	CE1-CZ	-5.47	1.31	1.38
8	U	30	TRP	CD2-CE2	5.46	1.48	1.41
3	P	246	ASP	CB-CG	5.46	1.63	1.51
5	E	38	GLY	N-CA	5.45	1.54	1.46
3	P	102	TYR	CG-CD2	-5.45	1.32	1.39
8	H	58	ARG	CZ-NH1	5.42	1.40	1.33
4	D	48	TRP	CD2-CE2	5.42	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	393	PHE	CG-CD2	5.39	1.46	1.38
8	U	55	TRP	CD2-CE2	5.36	1.47	1.41
11	X	40	TRP	CD2-CE2	5.36	1.47	1.41
10	J	52	TRP	CD2-CE2	5.35	1.47	1.41
5	E	84	TYR	CG-CD1	5.34	1.46	1.39
10	W	52	TRP	CD2-CE2	5.33	1.47	1.41
1	A	372	TYR	CG-CD1	5.32	1.46	1.39
1	A	383[A]	MET	CG-SD	-5.30	1.67	1.81
1	A	383[B]	MET	CG-SD	-5.30	1.67	1.81
4	Q	48	TRP	CD2-CE2	5.29	1.47	1.41
1	A	334	TRP	CD2-CE2	5.29	1.47	1.41
1	N	270	TYR	CB-CG	5.28	1.59	1.51
2	O	132	GLU	CD-OE2	5.25	1.31	1.25
5	E	78	HIS	N-CA	5.25	1.56	1.46
1	N	22	PHE	CG-CD1	5.25	1.46	1.38
8	H	30	TRP	CD2-CE2	5.23	1.47	1.41
11	K	31	TYR	CG-CD1	5.22	1.46	1.39
3	P	186	PHE	CG-CD1	5.20	1.46	1.38
2	B	202	SER	CA-CB	5.20	1.60	1.52
1	N	173	PRO	CA-CB	5.19	1.64	1.53
5	E	89	LEU	CA-CB	5.15	1.65	1.53
2	O	53	THR	N-CA	5.14	1.56	1.46
1	N	269	GLY	CA-C	5.14	1.60	1.51
7	T	27	SER	CB-OG	5.14	1.49	1.42
13	M	32	TRP	CG-CD1	5.13	1.44	1.36
1	N	160	GLY	N-CA	5.13	1.53	1.46
3	P	57	TRP	CD2-CE2	5.12	1.47	1.41
1	N	288	TRP	CE3-CZ3	5.11	1.47	1.38
2	B	197	SER	CB-OG	5.10	1.48	1.42
5	R	63	SER	CB-OG	5.06	1.48	1.42
8	H	68	TRP	CD2-CE2	5.06	1.47	1.41
9	I	28	SER	CB-OG	5.06	1.48	1.42
1	N	103	TRP	NE1-CE2	-5.05	1.30	1.37
6	F	3	GLY	N-CA	5.05	1.53	1.46
2	B	24	HIS	CG-CD2	5.05	1.44	1.35
1	N	179	TYR	CE1-CZ	5.04	1.45	1.38
1	N	121	GLY	N-CA	5.03	1.53	1.46
1	A	266	GLU	CB-CG	5.03	1.61	1.52
3	C	16	TRP	CD1-NE1	5.03	1.46	1.38
3	C	99	TRP	CD2-CE2	5.03	1.47	1.41
1	A	264	LYS	CD-CE	5.02	1.63	1.51
2	O	60	GLU	CD-OE1	5.02	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	259	TRP	CD2-CE2	5.01	1.47	1.41

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	90	ARG	NE-CZ-NH1	25.98	133.29	120.30
4	Q	20	ARG	NE-CZ-NH2	-19.33	110.63	120.30
5	E	90	ARG	NE-CZ-NH2	-19.32	110.64	120.30
1	N	71	MET	CG-SD-CE	-16.18	74.31	100.20
4	Q	20	ARG	NE-CZ-NH1	16.03	128.32	120.30
1	A	71	MET	CG-SD-CE	-15.21	75.86	100.20
11	K	47	ARG	NE-CZ-NH1	12.69	126.64	120.30
1	A	189	MET	CG-SD-CE	-11.67	81.53	100.20
2	B	29[A]	MET	CG-SD-CE	11.41	118.45	100.20
2	B	29[B]	MET	CG-SD-CE	11.41	118.45	100.20
5	R	90	ARG	NE-CZ-NH2	-10.91	114.84	120.30
4	Q	21	ASP	CB-CG-OD2	10.43	127.69	118.30
9	I	16	ARG	NE-CZ-NH2	-10.23	115.19	120.30
3	C	63	ARG	NE-CZ-NH2	-10.20	115.20	120.30
2	O	82	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	N	189	MET	CG-SD-CE	-8.64	86.38	100.20
1	A	213	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	A	213	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	346	PHE	CB-CG-CD2	-8.18	115.08	120.80
1	A	8	PHE	CB-CG-CD2	-8.14	115.10	120.80
1	A	445	ASP	CB-CG-OD1	8.08	125.57	118.30
5	E	90	ARG	CD-NE-CZ	8.02	134.83	123.60
12	L	20	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	129	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	N	302[A]	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	N	302[B]	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	344	PHE	CB-CG-CD2	-7.71	115.41	120.80
4	Q	20	ARG	CG-CD-NE	-7.62	95.79	111.80
9	V	10	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	A	112	LEU	CD1-CG-CD2	-7.54	87.89	110.50
12	L	20	ARG	CG-CD-NE	-7.49	96.08	111.80
10	J	36	MET	CG-SD-CE	-7.47	88.25	100.20
3	P	63	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	N	5	ARG	NE-CZ-NH2	-7.43	116.58	120.30
2	B	42	ILE	CG1-CB-CG2	-7.43	95.05	111.40
4	D	20	ARG	NE-CZ-NH1	-7.38	116.61	120.30
7	T	7	ASP	N-CA-C	7.33	130.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	MET	CB-CG-SD	-7.32	90.43	112.40
5	R	90	ARG	NE-CZ-NH1	7.29	123.94	120.30
3	C	127	LEU	CB-CG-CD1	7.15	123.15	111.00
1	N	51	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	310	MET	CG-SD-CE	-7.07	88.89	100.20
5	R	60	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	8	PHE	CB-CG-CD1	7.03	125.72	120.80
5	R	52	LEU	CB-CG-CD2	7.02	122.94	111.00
3	C	94	PHE	CB-CG-CD1	-6.97	115.92	120.80
1	N	129	TYR	CB-CG-CD2	-6.97	116.82	121.00
3	P	63	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	96	ARG	NE-CZ-NH2	-6.95	116.83	120.30
4	D	61	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	38	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	324	LEU	CB-CG-CD2	6.87	122.68	111.00
2	O	82	ARG	NE-CZ-NH1	6.85	123.73	120.30
3	C	214	PHE	CB-CG-CD1	6.84	125.59	120.80
3	P	35	PHE	CB-CG-CD1	6.84	125.59	120.80
2	B	173	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	439	ARG	NE-CZ-NH2	-6.76	116.92	120.30
5	E	90	ARG	CB-CG-CD	6.70	129.02	111.60
1	N	41	LEU	CB-CG-CD1	-6.64	99.72	111.00
3	C	214	PHE	CB-CG-CD2	-6.60	116.18	120.80
1	N	302[A]	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	N	302[B]	ARG	NE-CZ-NH2	-6.58	117.01	120.30
3	P	86	PHE	CB-CG-CD1	-6.55	116.21	120.80
1	N	310	MET	CG-SD-CE	-6.54	89.73	100.20
1	N	348	PHE	CB-CG-CD1	-6.54	116.22	120.80
3	P	94	PHE	CZ-CE2-CD2	-6.53	112.27	120.10
2	B	65	TRP	CB-CA-C	6.52	123.44	110.40
1	A	347	LEU	CA-CB-CG	-6.42	100.52	115.30
3	P	93	PHE	CB-CG-CD2	-6.37	116.34	120.80
4	D	21	ASP	CB-CG-OD2	6.35	124.01	118.30
9	V	10	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	N	270	TYR	CB-CG-CD1	-6.28	117.23	121.00
5	E	49	ASP	CB-CG-OD1	6.27	123.95	118.30
2	B	139	ASP	CB-CG-OD1	6.26	123.93	118.30
1	N	369	ASP	CB-CG-OD1	6.26	123.93	118.30
7	G	6	GLY	N-CA-C	6.22	128.65	113.10
3	P	35	PHE	CB-CG-CD2	-6.18	116.47	120.80
1	N	251	PHE	CB-CG-CD2	-6.18	116.47	120.80
1	A	251	PHE	CB-CG-CD2	-6.17	116.48	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	ARG	NE-CZ-NH2	-6.15	117.22	120.30
3	P	214	PHE	CB-CG-CD2	-6.14	116.50	120.80
3	P	80[A]	ARG	NE-CZ-NH1	-6.14	117.23	120.30
3	P	80[B]	ARG	NE-CZ-NH1	-6.14	117.23	120.30
6	F	18	ARG	NE-CZ-NH2	-6.13	117.24	120.30
5	E	14	ARG	NE-CZ-NH1	6.11	123.36	120.30
6	S	17	GLU	OE1-CD-OE2	6.11	130.63	123.30
3	P	214	PHE	CB-CG-CD1	6.10	125.07	120.80
4	D	16	TYR	CB-CG-CD1	-6.08	117.35	121.00
9	V	59	ASP	CB-CG-OD1	5.95	123.66	118.30
1	N	7	LEU	CB-CG-CD1	5.94	121.09	111.00
1	A	38	ARG	NE-CZ-NH2	-5.88	117.36	120.30
3	P	28	THR	CA-CB-CG2	-5.86	104.19	112.40
2	B	152	MET	CG-SD-CE	5.86	109.58	100.20
7	G	14	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	268	PHE	CB-CG-CD2	-5.82	116.73	120.80
6	S	94	HIS	N-CA-C	5.82	126.71	111.00
2	B	45	MET	CG-SD-CE	5.81	109.50	100.20
1	A	310	MET	CA-CB-CG	-5.79	103.45	113.30
1	A	379	TYR	CB-CG-CD2	-5.78	117.53	121.00
8	H	73	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	N	244	TYR	CZ-CE2-CD2	-5.76	114.62	119.80
7	G	18	PHE	CB-CG-CD2	-5.75	116.78	120.80
5	E	73	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	N	213	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	N	189	MET	CB-CG-SD	-5.68	95.35	112.40
1	N	490	THR	CA-CB-CG2	-5.68	104.45	112.40
1	A	442	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	N	445	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	74	MET	CG-SD-CE	-5.66	91.15	100.20
1	A	50	ASP	CB-CG-OD1	5.65	123.39	118.30
2	B	33	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	49	GLY	N-CA-C	-5.60	99.10	113.10
7	T	40	GLY	N-CA-C	-5.59	99.11	113.10
5	R	36	LEU	CB-CG-CD2	-5.58	101.51	111.00
11	X	11	ASP	CB-CG-OD1	5.57	123.31	118.30
2	O	46	LEU	CB-CG-CD1	-5.55	101.56	111.00
1	A	348	PHE	CG-CD1-CE1	-5.55	114.69	120.80
4	D	54	ASP	CB-CG-OD1	5.54	123.29	118.30
1	N	109	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	A	347	LEU	CB-CG-CD2	5.51	120.38	111.00
2	O	65	TRP	CB-CA-C	5.43	121.26	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	LEU	CB-CG-CD1	-5.43	101.78	111.00
2	O	198	GLU	OE1-CD-OE2	-5.42	116.80	123.30
3	C	102	TYR	CB-CG-CD1	-5.41	117.75	121.00
2	B	73	LEU	CB-CG-CD1	-5.41	101.81	111.00
7	T	14	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	N	113[A]	LEU	CB-CA-C	5.40	120.46	110.20
1	N	113[B]	LEU	CB-CA-C	5.40	120.46	110.20
1	A	426	PHE	CB-CG-CD1	-5.39	117.02	120.80
1	A	354	THR	CA-CB-CG2	-5.39	104.86	112.40
1	N	152	LEU	CB-CG-CD2	5.38	120.15	111.00
1	A	40	GLU	OE1-CD-OE2	5.37	129.75	123.30
1	N	74	MET	CB-CG-SD	-5.37	96.30	112.40
7	G	54	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	N	260	TYR	CB-CG-CD1	-5.32	117.81	121.00
2	B	110	TYR	CB-CG-CD2	-5.32	117.81	121.00
3	C	215	LEU	CB-CG-CD1	-5.30	101.98	111.00
1	A	109	PHE	CB-CG-CD2	-5.30	117.09	120.80
4	D	20	ARG	NE-CZ-NH2	5.29	122.95	120.30
2	O	41	ILE	CA-CB-CG1	-5.29	100.96	111.00
2	O	11	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	21	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	A	183	LEU	CB-CG-CD1	-5.20	102.16	111.00
3	P	181	TYR	CG-CD1-CE1	-5.20	117.14	121.30
3	P	94	PHE	CB-CG-CD1	-5.19	117.17	120.80
1	A	296	GLY	O-C-N	-5.18	114.41	122.70
2	B	158	ASP	CB-CG-OD1	5.16	122.95	118.30
5	E	40	ASP	CB-CG-OD1	5.16	122.95	118.30
1	N	442	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	N	486	ASP	CB-CG-OD1	5.15	122.94	118.30
9	I	16	ARG	NE-CZ-NH1	5.14	122.87	120.30
8	U	38	ARG	NE-CZ-NH2	-5.13	117.73	120.30
10	W	36	MET	CG-SD-CE	-5.13	92.00	100.20
4	D	58	GLU	CA-CB-CG	-5.12	102.13	113.40
1	A	400	PHE	CB-CG-CD2	-5.12	117.22	120.80
2	B	59	GLN	N-CA-CB	5.12	119.81	110.60
3	C	90	GLU	OE1-CD-OE2	5.10	129.42	123.30
4	D	118	LYS	CD-CE-NZ	-5.07	100.04	111.70
7	G	5	LYS	CB-CA-C	5.05	120.50	110.40
7	G	56	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	35	LEU	CB-CG-CD2	5.03	119.55	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	379	TYR	Mainchain
1	A	38	ARG	Sidechain
6	F	93	PRO	Peptide
7	G	11	TPO	Peptide
1	N	240	HIS	Sidechain
1	N	296	GLY	Mainchain
6	S	93	PRO	Peptide
6	S	94	HIS	Peptide
9	V	1	SAC	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4162	97	0
1	N	4179	0	4154	95	0
2	B	1899	0	1898	63	0
2	O	1870	0	1868	45	0
3	C	2185	0	2097	46	0
3	P	2185	0	2097	34	0
4	D	1233	0	1223	37	0
4	Q	1224	0	1211	20	0
5	E	852	0	845	4	0
5	R	863	0	857	6	0
6	F	778	0	754	26	0
6	S	763	0	742	22	0
7	G	686	0	652	28	0
7	T	686	0	651	23	0
8	H	662	0	623	18	0
8	U	662	0	623	9	0
9	I	601	0	613	19	0
9	V	601	0	613	14	0
10	J	460	0	459	7	0
10	W	469	0	464	4	0
11	K	384	0	366	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	X	391	0	374	3	0
12	L	380	0	380	16	0
12	Y	388	0	388	13	0
13	M	335	0	352	8	0
13	Z	335	0	352	8	0
14	A	180	0	162	25	0
14	N	180	0	162	28	0
15	A	1	0	0	1	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	9	0	0	8	0
18	N	9	0	0	3	0
19	A	126	0	220	11	0
19	D	63	0	110	13	0
19	N	63	0	110	7	0
19	Q	63	0	110	12	0
19	Y	63	0	110	20	0
20	A	102	0	152	13	0
20	C	102	0	152	4	0
20	N	102	0	152	10	0
20	P	102	0	152	3	0
21	A	36	0	52	8	0
21	B	16	0	24	2	0
21	C	4	0	6	0	0
21	D	8	0	12	9	0
21	E	12	0	18	0	0
21	F	12	0	18	0	0
21	G	8	0	12	3	0
21	L	4	0	6	0	0
21	M	4	0	6	0	0
21	N	36	0	54	1	0
21	O	4	0	6	0	0
21	P	8	0	12	0	0
21	R	4	0	6	0	0
21	S	12	0	18	0	0
21	T	4	0	6	0	0
21	W	4	0	6	0	0
21	Y	4	0	6	0	0
22	B	29	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	58	0	78	6	0
22	G	29	0	39	1	0
22	J	29	0	38	1	0
22	P	58	0	78	6	0
22	W	29	0	38	1	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	15	0
24	N	52	0	80	16	0
25	C	99	0	126	15	0
25	M	33	0	42	0	0
25	P	99	0	126	15	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0
26	P	1	0	0	1	0
27	C	100	0	156	17	0
27	N	100	0	156	29	0
27	P	100	0	156	24	0
27	T	100	0	156	16	0
28	C	106	0	154	15	0
28	G	106	0	154	8	0
28	P	53	0	77	6	0
28	T	53	0	77	3	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	235	0	0	32	0
30	B	162	0	0	25	2
30	C	110	0	0	3	0
30	D	118	0	0	13	1
30	E	93	0	0	1	0
30	F	94	0	0	5	0
30	G	42	0	0	5	0
30	H	42	0	0	1	0
30	I	27	0	0	5	1
30	J	23	0	0	2	0
30	K	26	0	0	1	0
30	L	38	0	0	4	1
30	M	25	0	0	7	1
30	N	203	0	0	14	0
30	O	100	0	0	1	0
30	P	95	0	0	3	0
30	Q	29	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	R	40	0	0	1	0
30	S	45	0	0	3	0
30	T	35	0	0	3	0
30	U	29	0	0	0	0
30	V	16	0	0	3	0
30	W	7	0	0	0	0
30	X	11	0	0	0	0
30	Y	12	0	0	0	0
30	Z	12	0	0	0	0
All	All	33609	0	32570	772	3

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 12.

All (772) 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)
1:A:74:MET:CG	1:A:74:MET:CB	1.75	1.61
6:S:43:LYS:CD	6:S:43:LYS:H	1.08	1.49
20:N:609:PGV:C2	20:N:609:PGV:H011	1.38	1.33
24:B:303:PSC:O02	9:I:14:ALA:HB2	1.16	1.31
30:A:709:HOH:O	19:D:201:TGL:HG11	1.23	1.29
19:A:611:TGL:HC32	12:L:20:ARG:NH2	1.50	1.27
1:A:297[B]:MET:CB	30:A:794:HOH:O	1.75	1.26
1:A:39:ALA:HA	21:D:202:EDO:O1	1.33	1.26
21:B:304:EDO:H12	30:C:412:HOH:O	1.13	1.25
1:A:512:ASN:HB3	30:A:701:HOH:O	1.35	1.22
20:N:609:PGV:C01	20:N:609:PGV:H21	1.70	1.21
19:D:201:TGL:HG31	30:D:366:HOH:O	1.34	1.20
6:S:43:LYS:CD	6:S:43:LYS:N	1.90	1.17
27:P:305:CDL:H272	27:P:305:CDL:H381	1.21	1.15
26:P:303:UNX:UNK	30:P:441:HOH:O	1.28	1.14
1:N:297[B]:MET:HB2	30:N:765:HOH:O	1.44	1.14
2:B:98:LYS:HG3	30:B:522:HOH:O	1.47	1.13
19:N:611:TGL:H281	19:N:611:TGL:HB92	1.31	1.13
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD2	1.50	1.11
4:D:19[A]:ARG:HD2	4:D:21:ASP:OD1	1.51	1.11
19:N:611:TGL:HC42	30:N:903:HOH:O	1.51	1.11
6:S:43:LYS:H	6:S:43:LYS:HD3	0.98	1.10
2:B:32[A]:PHE:O	2:B:35[A]:SER:OG	1.67	1.10
3:P:33[A]:MET:HE1	3:P:42:LEU:H	1.15	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297[B]:MET:HB3	30:A:794:HOH:O	1.41	1.10
1:N:302[B]:ARG:HH12	1:N:365:ILE:HD11	1.00	1.10
1:N:297[B]:MET:CB	30:N:765:HOH:O	1.97	1.08
2:B:160:LEU:HB2	30:B:424:HOH:O	1.53	1.08
1:A:512:ASN:CB	30:A:701:HOH:O	1.88	1.08
3:P:67:PHE:HE2	27:P:305:CDL:H1	1.10	1.08
1:A:74:MET:SD	1:A:74:MET:CB	2.41	1.07
19:A:611:TGL:HC32	12:L:20:ARG:HH22	0.97	1.07
27:N:601:CDL:H371	2:O:78:LEU:HD12	1.34	1.07
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:CD	2.03	1.06
8:H:9:LYS:HG3	8:H:10:ASN:H	1.11	1.06
1:N:302[B]:ARG:NH1	1:N:365:ILE:HD11	1.71	1.05
20:N:609:PGV:H011	20:N:609:PGV:H22	1.39	1.04
3:C:67:PHE:HE2	27:C:305:CDL:H1	1.15	1.04
1:A:39:ALA:HA	21:D:202:EDO:HO1	0.92	1.04
6:S:95:GLN:HE21	6:S:95:GLN:HA	1.21	1.04
6:S:43:LYS:H	6:S:43:LYS:HD2	0.88	1.03
5:E:90:ARG:HD2	30:E:374:HOH:O	1.56	1.03
1:A:513:LEU:O	1:A:514:LYS:HB2	1.50	1.03
24:N:612:PSC:H343	24:N:612:PSC:H1	1.37	1.02
24:B:303:PSC:O02	9:I:14:ALA:CB	2.07	1.01
6:S:43:LYS:N	6:S:43:LYS:HD2	1.50	1.01
7:G:10:GLY:O	7:G:11:TPO:HB	1.56	1.00
4:D:4:SER:HB3	30:D:302:HOH:O	1.60	1.00
1:A:297[B]:MET:HB2	30:A:794:HOH:O	1.42	1.00
1:N:513:LEU:O	1:N:514:LYS:HB2	1.61	1.00
25:P:307:DMU:H35	25:P:307:DMU:H29	1.43	0.99
1:N:486:ASP:OD2	4:Q:19[B]:ARG:HD2	1.61	0.99
20:N:609:PGV:C2	20:N:609:PGV:C01	2.25	0.99
3:P:67:PHE:CE2	27:P:305:CDL:H1	1.98	0.98
4:Q:19[A]:ARG:HG2	4:Q:21:ASP:OD1	1.61	0.98
1:A:39:ALA:CA	21:D:202:EDO:O1	2.11	0.98
3:P:224:LYS:CD	27:P:305:CDL:HB31	1.94	0.97
19:N:611:TGL:HB92	19:N:611:TGL:C28	1.94	0.97
1:A:512:ASN:ND2	30:A:701:HOH:O	1.96	0.97
30:B:423:HOH:O	8:H:62:SER:HA	1.63	0.96
9:I:73:LYS:HE2	30:I:104:HOH:O	1.65	0.96
19:A:611:TGL:HC31	12:L:14:SER:H	1.28	0.96
10:J:55:PHE:HB2	30:J:208:HOH:O	1.65	0.95
6:S:43:LYS:N	6:S:43:LYS:HD3	1.61	0.95
1:A:479:LYS:HB2	30:M:201:HOH:O	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:19[A]:ARG:CG	4:Q:21:ASP:OD1	2.14	0.94
1:A:282:PHE:HA	7:T:4:ALA:CB	1.97	0.94
1:A:328:HIS:NE2	24:B:303:PSC:H31	1.83	0.94
28:G:103:PEK:H272	28:G:103:PEK:H312	1.50	0.93
1:A:136[B]:LEU:HD11	30:A:933:HOH:O	1.67	0.93
2:B:49:LYS:HE2	30:D:395:HOH:O	1.68	0.93
3:C:67:PHE:CE2	27:C:305:CDL:H1	2.03	0.93
30:A:925:HOH:O	19:D:201:TGL:HC31	1.68	0.93
19:Y:101:TGL:HA31	19:Y:101:TGL:HG11	1.48	0.93
27:N:601:CDL:H661	27:N:601:CDL:H611	1.50	0.92
11:K:6:ALA:N	30:K:101:HOH:O	2.01	0.92
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	2.10	0.91
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.52	0.91
24:B:303:PSC:H62	24:B:303:PSC:H261	1.50	0.91
27:N:601:CDL:H321	27:N:601:CDL:OA7	1.70	0.90
19:N:611:TGL:H281	19:N:611:TGL:CB9	2.01	0.90
2:B:200:CYS:HB3	30:B:402:HOH:O	1.70	0.90
19:A:611:TGL:CC3	12:L:20:ARG:HH22	1.82	0.90
1:A:503:HIS:CD2	30:A:903:HOH:O	2.24	0.89
1:A:398:PRO:HG3	30:A:738:HOH:O	1.70	0.89
20:A:610:PGV:H221	30:M:222:HOH:O	1.72	0.89
20:N:609:PGV:H011	20:N:609:PGV:H21	0.89	0.89
2:B:161:HIS:HA	30:B:402:HOH:O	1.74	0.88
1:A:503:HIS:HD2	30:A:903:HOH:O	1.56	0.88
22:C:306:CHD:H231	22:C:306:CHD:H162	1.56	0.87
1:A:230:LEU:HB3	30:A:704:HOH:O	1.74	0.87
3:C:51[B]:MET:HE2	27:C:305:CDL:H392	1.54	0.87
21:A:616:EDO:H11	30:M:220:HOH:O	1.75	0.87
3:C:33[A]:MET:HB2	25:C:302:DMU:C22	2.05	0.87
8:H:9:LYS:HG3	8:H:10:ASN:N	1.88	0.86
1:N:417[A]:MET:CE	30:N:788:HOH:O	2.21	0.86
18:N:607[B]:AZI:N1	30:N:701:HOH:O	2.08	0.86
7:G:84:LYS:HD2	7:G:84:LYS:H	1.37	0.85
1:N:302[B]:ARG:HH12	1:N:365:ILE:CD1	1.86	0.85
7:G:84:LYS:N	7:G:84:LYS:HD2	1.90	0.85
1:N:136[B]:LEU:HG	30:T:222:HOH:O	1.76	0.85
27:N:601:CDL:C66	27:N:601:CDL:H611	2.05	0.85
3:P:224:LYS:HD2	27:P:305:CDL:HB31	1.58	0.85
3:C:33[A]:MET:HB2	25:C:302:DMU:H13	1.58	0.85
12:Y:45:LEU:HD22	13:Z:42:LYS:HE3	1.57	0.84
1:A:514:LYS:NZ	30:A:702:HOH:O	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:ARG:HE	27:C:305:CDL:HA21	1.43	0.84
3:C:51[B]:MET:CE	27:C:305:CDL:H392	2.08	0.84
4:D:4:SER:HA	30:D:387:HOH:O	1.78	0.84
1:N:136[B]:LEU:HD11	30:N:902:HOH:O	1.78	0.84
28:T:101:PEK:H12	28:T:101:PEK:H242	1.60	0.83
6:S:75:HIS:H	6:S:80:GLN:HE22	1.25	0.83
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.19	0.83
24:N:612:PSC:H02	24:N:612:PSC:H212	1.61	0.83
7:T:72:ASN:H	7:T:76:ASN:HD22	1.27	0.83
1:A:112:LEU:HG	30:A:906:HOH:O	1.78	0.83
19:A:608:TGL:HA91	19:A:608:TGL:HA42	1.60	0.82
15:A:603:CU:CU	18:A:607[B]:AZI:N1	1.44	0.81
14:N:603[B]:HEA:HBD2	14:N:603[B]:HEA:HMD1	1.60	0.81
4:Q:19[A]:ARG:CD	4:Q:21:ASP:OD1	2.28	0.81
27:T:102:CDL:H361	27:T:102:CDL:H121	1.63	0.80
14:A:602[A]:HEA:HMC1	14:A:602[A]:HEA:HBC1	1.63	0.80
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD3	1.80	0.80
4:D:19[A]:ARG:CD	4:D:21:ASP:OD1	2.28	0.80
7:G:7:ASP:HB2	1:N:178[A]:GLN:HG2	1.61	0.80
19:N:611:TGL:CC4	30:N:903:HOH:O	2.16	0.80
7:G:72:ASN:H	7:G:76:ASN:HD22	1.30	0.79
1:N:178[B]:GLN:HG3	1:N:186:TRP:CZ2	2.17	0.79
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	1.64	0.79
7:T:76:ASN:HD21	28:T:101:PEK:HN2	1.28	0.79
7:T:11:TPO:HA	7:T:11:TPO:O3P	1.82	0.79
8:H:43:MET:O	8:H:45:ALA:N	2.14	0.79
4:D:4:SER:CB	30:D:302:HOH:O	2.23	0.78
4:D:34:SER:H	4:D:37:GLN:HE21	1.31	0.78
27:T:102:CDL:OB3	27:T:102:CDL:H161	1.84	0.78
3:C:63:ARG:HE	27:C:305:CDL:CA2	1.96	0.78
28:P:308:PEK:H042	6:S:1:ALA:H1	1.48	0.78
2:B:174:ALA:HB1	30:B:528:HOH:O	1.84	0.78
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.66	0.78
7:T:38:HIS:CE1	27:T:102:CDL:H141	2.19	0.77
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.67	0.77
6:F:92:VAL:HG21	30:F:290:HOH:O	1.83	0.77
27:P:305:CDL:H272	27:P:305:CDL:C38	2.11	0.77
20:A:609:PGV:H183	28:G:101:PEK:H322	1.65	0.77
3:P:33[B]:MET:SD	25:P:307:DMU:H8	2.25	0.76
24:N:612:PSC:C07	9:V:10:ARG:HH21	1.98	0.76
14:N:603[A]:HEA:HBC1	14:N:603[A]:HEA:HMC1	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:601:CDL:H761	27:N:601:CDL:H591	1.68	0.76
3:C:161[A]:GLN:HE22	28:C:307:PEK:H41	1.51	0.76
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.68	0.76
14:A:601:HEA:HBC1	14:A:601:HEA:HMC1	1.67	0.75
22:P:306:CHD:H162	22:P:306:CHD:H231	1.67	0.75
27:P:305:CDL:H351	27:P:305:CDL:H391	1.66	0.75
6:S:95:GLN:NE2	6:S:95:GLN:HA	2.00	0.75
27:N:601:CDL:C65	27:N:601:CDL:H611	2.16	0.75
3:P:33[A]:MET:HE1	3:P:42:LEU:N	1.98	0.75
24:N:612:PSC:H343	24:N:612:PSC:C13	2.16	0.75
27:T:102:CDL:OB3	27:T:102:CDL:H142	1.86	0.75
20:A:609:PGV:H343	28:G:101:PEK:H382	1.69	0.75
7:G:76:ASN:HD21	28:G:101:PEK:HN2	1.33	0.75
3:P:63:ARG:HE	27:P:305:CDL:HA21	1.51	0.74
3:C:33[A]:MET:HB2	25:C:302:DMU:C25	2.15	0.74
3:C:224:LYS:HD2	27:C:305:CDL:HB31	1.68	0.74
30:B:553:HOH:O	19:D:201:TGL:C28	2.34	0.74
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.67	0.74
6:F:75:HIS:H	6:F:80:GLN:HE22	1.33	0.74
2:B:53:THR:HG21	30:D:311:HOH:O	1.87	0.74
20:C:304:PGV:H181	27:C:305:CDL:H652	1.68	0.74
12:Y:20:ARG:HH12	19:Y:101:TGL:HC32	1.51	0.73
1:A:178[B]:GLN:H	1:A:178[B]:GLN:CD	1.90	0.73
1:N:359:ALA:HA	14:N:603[B]:HEA:OMA	1.88	0.73
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.25	0.72
4:Q:6:VAL:O	4:Q:7:LYS:HB2	1.88	0.72
6:S:43:LYS:HE3	30:S:225:HOH:O	1.89	0.72
1:A:39:ALA:CA	21:D:202:EDO:HO1	1.87	0.72
9:V:18:ARG:HG3	30:V:110:HOH:O	1.89	0.72
2:B:148:MET:HE2	30:B:547:HOH:O	1.89	0.72
9:I:73:LYS:O	30:I:102:HOH:O	2.07	0.72
3:P:63:ARG:HE	27:P:305:CDL:CA2	2.03	0.71
28:C:307:PEK:H382	27:N:601:CDL:H271	1.71	0.71
2:O:16:ILE:HD12	2:O:87[A]:MET:HG2	1.71	0.71
28:P:308:PEK:H042	6:S:1:ALA:N	2.06	0.71
7:G:38:HIS:CE1	27:N:601:CDL:H141	2.25	0.71
4:Q:78:TRP:CA	19:Q:201:TGL:HB22	2.21	0.70
1:N:307:SER:CB	27:N:601:CDL:H191	2.22	0.70
4:D:100[B]:LYS:HE3	30:D:358:HOH:O	1.91	0.70
6:F:1:ALA:HB3	6:S:65:ASP:OD2	1.92	0.70
9:V:18:ARG:HD3	30:V:114:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:ALA:CB	30:B:528:HOH:O	2.37	0.69
2:B:57:ASP:H	24:B:303:PSC:H221	1.56	0.69
8:H:9:LYS:HA	8:H:9:LYS:HZ1	1.58	0.69
6:F:1:ALA:HA	7:G:17:ARG:NH1	2.08	0.69
19:N:611:TGL:C28	19:N:611:TGL:CB9	2.66	0.69
30:B:553:HOH:O	19:D:201:TGL:H281	1.91	0.69
7:G:38:HIS:HE1	27:N:601:CDL:H141	1.58	0.69
4:D:99:GLU:OE2	21:D:202:EDO:H22	1.93	0.68
19:Y:101:TGL:OC1	19:Y:101:TGL:HC41	1.92	0.68
27:N:601:CDL:C37	2:O:78:LEU:HD12	2.19	0.68
3:C:3:HIS:N	30:C:402:HOH:O	2.26	0.68
3:C:224:LYS:CD	27:C:305:CDL:HB31	2.24	0.68
1:A:243:VAL:HB	14:A:602[B]:HEA:HAC	1.75	0.67
4:D:100[B]:LYS:CE	30:D:358:HOH:O	2.42	0.67
3:P:224:LYS:HD3	27:P:305:CDL:HB31	1.75	0.67
3:C:37:PHE:CG	25:C:302:DMU:H8	2.30	0.67
4:D:100[B]:LYS:HE3	30:D:301:HOH:O	1.94	0.67
1:N:136[B]:LEU:HD11	30:T:233:HOH:O	1.95	0.67
13:M:8:THR:OG1	30:M:201:HOH:O	2.13	0.67
1:A:324:LEU:HD22	2:B:42:ILE:HG13	1.76	0.67
3:P:33[A]:MET:HB2	25:P:307:DMU:H9	1.77	0.67
8:H:9:LYS:NZ	8:H:9:LYS:HA	2.09	0.66
14:A:602[B]:HEA:HBD2	14:A:602[B]:HEA:HMD1	1.78	0.66
3:C:47:LEU:O	3:C:51[A]:MET:HG2	1.95	0.66
19:Q:201:TGL:H352	9:V:16:ARG:HE	1.60	0.66
9:I:15:ARG:NH2	30:I:101:HOH:O	1.99	0.66
27:P:305:CDL:H411	27:P:305:CDL:H452	1.75	0.66
1:A:459:PHE:CE1	21:D:202:EDO:H11	2.30	0.66
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	1.94	0.66
24:B:303:PSC:C1	9:I:14:ALA:HB2	2.17	0.66
1:N:136[B]:LEU:CD1	30:N:902:HOH:O	2.40	0.66
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	1.93	0.65
24:N:612:PSC:H111	24:N:612:PSC:C32	2.26	0.65
30:A:877:HOH:O	4:D:17[A]:VAL:CG1	2.45	0.65
2:B:101:GLY:HA3	30:B:528:HOH:O	1.97	0.65
4:D:100[A]:LYS:NZ	30:D:301:HOH:O	1.88	0.65
3:C:180[B]:GLU:HG2	30:C:428:HOH:O	1.95	0.65
27:P:305:CDL:OB9	27:P:305:CDL:H532	1.96	0.65
1:N:309:THR:HG22	14:N:603[B]:HEA:HMB2	1.79	0.65
1:N:362[B]:SER:OG	30:N:702:HOH:O	2.15	0.65
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HD12	30:A:707:HOH:O	1.96	0.65
9:I:73:LYS:CE	30:I:104:HOH:O	2.31	0.65
1:N:297[B]:MET:HB3	30:N:765:HOH:O	1.78	0.65
19:Y:101:TGL:HG11	19:Y:101:TGL:CA3	2.23	0.65
1:A:177:SER:H	1:A:180:GLN:HE21	1.45	0.64
27:C:305:CDL:HB21	27:C:305:CDL:OB6	1.97	0.64
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.94	0.64
1:A:417[B]:MET:CE	30:A:873:HOH:O	2.45	0.64
8:H:46:LYS:NZ	8:U:51:SER:O	2.29	0.64
2:O:39:LEU:HD11	19:Q:201:TGL:H221	1.79	0.64
3:P:33[A]:MET:HB2	25:P:307:DMU:C19	2.27	0.64
20:A:610:PGV:H311	13:M:19:LEU:HD23	1.79	0.64
14:N:602:HEA:H122	14:N:602:HEA:H262	1.80	0.64
24:N:612:PSC:C34	24:N:612:PSC:H1	2.22	0.64
7:G:8:HIS:CD2	7:G:9:GLY:H	2.15	0.64
7:T:7:ASP:O	7:T:9:GLY:N	2.25	0.64
1:A:513:LEU:O	1:A:514:LYS:CB	2.32	0.64
14:N:603[B]:HEA:CBD	14:N:603[B]:HEA:HMD1	2.28	0.64
19:Q:201:TGL:HG31	30:Q:302:HOH:O	1.97	0.64
27:C:305:CDL:H211	27:C:305:CDL:H772	1.80	0.64
27:C:305:CDL:HB21	27:C:305:CDL:CB3	2.28	0.64
27:N:601:CDL:H161	27:N:601:CDL:OB3	1.97	0.63
22:C:306:CHD:C23	22:C:306:CHD:H162	2.28	0.63
12:L:47:LYS:HB3	30:L:222:HOH:O	1.98	0.63
4:D:19[A]:ARG:HH21	4:D:21:ASP:CG	2.01	0.63
27:N:601:CDL:H322	2:O:82:ARG:HA	1.80	0.63
1:N:382[B]:SER:HB2	1:N:383[B]:MET:HE2	1.80	0.63
9:I:35:TYR:C	9:I:35:TYR:CD1	2.72	0.63
7:G:8:HIS:O	1:N:178[A]:GLN:NE2	2.32	0.63
2:B:198:GLU:O	30:B:402:HOH:O	2.16	0.63
3:C:80[B]:ARG:HG2	3:C:233:PHE:CE1	2.33	0.63
20:A:610:PGV:O14	20:A:610:PGV:H062	1.99	0.63
19:Y:101:TGL:HA31	19:Y:101:TGL:CG1	2.27	0.62
1:N:177:SER:H	1:N:180:GLN:HE21	1.46	0.62
2:O:83:ILE:O	2:O:87[A]:MET:HG3	1.99	0.62
28:C:307:PEK:N	28:C:307:PEK:O14	2.32	0.62
7:G:4:ALA:CB	1:N:282:PHE:HA	2.28	0.62
1:N:28:MET:CE	14:N:602:HEA:H271	2.30	0.62
27:C:305:CDL:HB21	27:C:305:CDL:HB32	1.80	0.62
1:N:302[B]:ARG:HE	2:O:84:LEU:HD11	1.62	0.62
19:A:608:TGL:HA72	19:A:608:TGL:H101	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33[A]:MET:CB	25:C:302:DMU:H11	2.29	0.62
27:P:305:CDL:H252	27:P:305:CDL:H392	1.81	0.62
3:C:33[B]:MET:HA	25:C:302:DMU:H11	1.82	0.62
19:Q:201:TGL:H362	9:V:20:HIS:CE1	2.35	0.62
10:W:10:LYS:O	10:W:14[B]:GLU:HG3	2.00	0.62
2:B:1:FME:HE3	2:B:133:LEU:HD22	1.82	0.61
7:G:12:GLY:N	30:G:202:HOH:O	2.30	0.61
1:A:407:ASP:OD2	21:A:619:EDO:H11	2.00	0.61
2:B:16[B]:ILE:HG23	30:B:523:HOH:O	1.99	0.61
24:B:303:PSC:H211	24:B:303:PSC:H251	1.83	0.61
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG2	1.83	0.61
19:Y:101:TGL:OG3	19:Y:101:TGL:OG1	2.18	0.61
4:Q:78:TRP:HB3	19:Q:201:TGL:HB22	1.81	0.61
28:P:308:PEK:H041	7:T:17:ARG:HH22	1.66	0.61
6:F:87[A]:THR:HG21	30:F:266:HOH:O	1.99	0.61
1:N:417[A]:MET:HE1	30:N:788:HOH:O	1.92	0.61
1:A:359:ALA:HA	14:A:602[B]:HEA:OMA	2.00	0.61
1:N:178[B]:GLN:CG	1:N:186:TRP:CZ2	2.83	0.61
4:D:100[B]:LYS:HD2	4:D:100[B]:LYS:O	2.00	0.61
3:P:67:PHE:HE2	27:P:305:CDL:C1	2.01	0.61
2:B:60:GLU:CD	2:B:60:GLU:H	2.04	0.61
28:C:309:PEK:H351	7:T:5:LYS:HG3	1.83	0.61
21:A:618:EDO:O1	30:A:703:HOH:O	2.16	0.61
7:G:8:HIS:HD2	7:G:9:GLY:H	1.49	0.60
12:L:47:LYS:NZ	12:L:47:LYS:HB3	2.15	0.60
19:Y:101:TGL:CC4	19:Y:101:TGL:OC1	2.49	0.60
27:T:102:CDL:H111	27:T:102:CDL:OA5	2.01	0.60
1:A:261:TYR:OH	21:A:616:EDO:H12	2.01	0.60
2:O:13:THR:HB	2:O:168:LEU:HD23	1.84	0.60
12:Y:24[A]:MET:SD	19:Y:101:TGL:H172	2.42	0.60
1:A:172:LYS:HZ2	1:A:178[A]:GLN:HE22	1.49	0.60
28:C:307:PEK:P	28:C:307:PEK:HN1	2.24	0.60
1:N:307:SER:HB3	27:N:601:CDL:H191	1.84	0.60
2:B:87[B]:MET:HB3	30:B:494:HOH:O	2.02	0.60
7:T:38:HIS:HE1	27:T:102:CDL:H141	1.64	0.60
19:D:201:TGL:H242	19:D:201:TGL:HA91	1.83	0.59
30:L:225:HOH:O	13:M:43:SER:HB2	2.02	0.59
1:A:28:MET:CE	14:A:601:HEA:C27	2.80	0.59
30:A:706:HOH:O	6:F:96:LEU:HD13	2.02	0.59
1:N:311[A]:ILE:HD13	27:N:601:CDL:H221	1.83	0.59
1:A:281:GLY:C	7:T:4:ALA:HB1	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:MET:CE	14:A:601:HEA:H271	2.33	0.59
30:A:877:HOH:O	4:D:17[A]:VAL:HG11	2.02	0.59
22:P:306:CHD:C16	22:P:306:CHD:H231	2.32	0.59
20:N:609:PGV:H311	13:Z:19:LEU:HD23	1.85	0.59
4:Q:19[A]:ARG:HD2	4:Q:21:ASP:OD1	2.01	0.59
2:B:96:THR:HG22	30:B:522:HOH:O	2.01	0.58
1:N:364:ASP:OD1	14:N:603[B]:HEA:O1A	2.21	0.58
1:N:178[B]:GLN:HG3	1:N:186:TRP:CE2	2.37	0.58
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.38	0.58
1:N:243:VAL:HB	14:N:603[B]:HEA:HAC	1.83	0.58
1:A:514:LYS:CE	30:A:702:HOH:O	2.47	0.58
1:A:397:PHE:HD2	30:A:738:HOH:O	1.85	0.58
20:A:610:PGV:H322	20:A:610:PGV:H152	1.84	0.58
22:C:306:CHD:H231	22:C:306:CHD:C16	2.30	0.58
1:A:112:LEU:C	1:A:112:LEU:HD23	2.24	0.58
6:F:87[B]:THR:HG21	30:F:262:HOH:O	2.04	0.58
4:Q:78:TRP:CB	19:Q:201:TGL:HB22	2.33	0.58
2:B:198:GLU:HG3	30:B:424:HOH:O	2.04	0.57
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.86	0.57
3:C:33[B]:MET:HG2	3:C:39:SER:O	2.03	0.57
4:Q:78:TRP:HA	19:Q:201:TGL:HB22	1.86	0.57
1:A:28:MET:HE2	14:A:601:HEA:C27	2.35	0.57
3:C:33[A]:MET:HB2	25:C:302:DMU:H11	1.80	0.57
8:H:43:MET:HE3	8:H:49:ASP:N	2.19	0.57
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	2.87	0.57
2:B:82:ARG:HD2	2:B:86:MET:HE3	1.86	0.57
20:C:304:PGV:H12	20:C:304:PGV:H171	1.87	0.57
1:N:177:SER:H	1:N:180:GLN:NE2	2.03	0.57
13:Z:36:HIS:HD2	13:Z:39:ASN:ND2	2.02	0.57
20:A:609:PGV:H312	20:C:304:PGV:H321	1.86	0.57
30:A:706:HOH:O	6:F:96:LEU:CD1	2.53	0.57
1:N:307:SER:O	1:N:311[B]:ILE:HG23	2.04	0.57
27:P:305:CDL:H222	27:P:305:CDL:H651	1.86	0.57
13:M:8:THR:N	30:M:201:HOH:O	2.38	0.57
19:A:611:TGL:HC31	12:L:14:SER:N	2.10	0.56
22:P:306:CHD:H212	22:P:306:CHD:H12	1.86	0.56
4:D:34:SER:H	4:D:37:GLN:NE2	2.02	0.56
4:D:78:TRP:CA	19:D:201:TGL:HB21	2.35	0.56
24:B:303:PSC:H061	5:E:5:HIS:N	2.20	0.56
12:L:47:LYS:CB	30:L:222:HOH:O	2.52	0.56
2:B:140:ASN:HB3	30:B:520:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:178[B]:GLN:HG3	1:N:178[B]:GLN:O	2.04	0.56
1:A:177:SER:H	1:A:180:GLN:NE2	2.03	0.56
1:A:514:LYS:HE3	30:A:702:HOH:O	2.04	0.56
25:P:309:DMU:H12	25:P:309:DMU:H20	1.88	0.56
4:Q:109:HIS:HD2	30:Q:319:HOH:O	1.88	0.56
24:N:612:PSC:H211	2:O:56:MET:HG2	1.87	0.56
21:A:619:EDO:H12	30:A:796:HOH:O	2.05	0.56
12:L:47:LYS:HB3	12:L:47:LYS:HZ2	1.70	0.56
1:N:172:LYS:HZ2	1:N:178[A]:GLN:HE22	1.54	0.56
3:P:33[B]:MET:SD	25:P:307:DMU:C19	2.93	0.56
21:A:620:EDO:H22	6:F:32:ASN:HD21	1.71	0.56
9:I:31:PHE:CD2	9:I:31:PHE:C	2.79	0.56
27:T:102:CDL:OA7	27:T:102:CDL:H321	2.05	0.56
24:B:303:PSC:H41	24:B:303:PSC:H011	1.88	0.55
1:A:291:HIS:NE2	18:A:607[B]:AZI:N1	2.53	0.55
1:A:291:HIS:CE1	18:A:607[B]:AZI:N2	2.74	0.55
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.41	0.55
22:C:306:CHD:C23	22:C:306:CHD:C16	2.84	0.55
1:N:115[A]:SER:O	1:N:121:GLY:HA2	2.06	0.55
14:N:603[B]:HEA:HMC1	14:N:603[B]:HEA:HBC1	1.88	0.55
1:A:514:LYS:HG3	6:F:38:ALA:CB	2.37	0.55
19:Q:201:TGL:H362	9:V:20:HIS:HE1	1.70	0.55
21:A:618:EDO:C1	30:A:703:HOH:O	2.54	0.55
3:C:157:LYS:NZ	28:C:307:PEK:H051	2.22	0.55
7:G:84:LYS:H	7:G:84:LYS:CD	2.17	0.55
28:P:308:PEK:H382	27:T:102:CDL:H271	1.88	0.55
2:B:81:LEU:HD12	27:T:102:CDL:H382	1.88	0.54
2:B:85:TYR:CE2	27:T:102:CDL:H112	2.41	0.54
4:D:78:TRP:N	19:D:201:TGL:HB21	2.23	0.54
4:Q:19[B]:ARG:NH1	30:Q:301:HOH:O	2.26	0.54
14:A:601:HEA:H262	14:A:601:HEA:H122	1.89	0.54
7:G:59:PRO:O	21:G:105:EDO:H12	2.07	0.54
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.89	0.54
4:Q:9:GLU:HG3	4:Q:11:TYR:CE2	2.41	0.54
21:N:621:EDO:H11	12:Y:10:ASN:HD22	1.72	0.54
11:X:47:ARG:CZ	11:X:47:ARG:HB3	2.35	0.54
1:N:54:TYR:HB2	30:N:859:HOH:O	2.07	0.54
3:P:33[A]:MET:CB	25:P:307:DMU:H9	2.37	0.54
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.07	0.54
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.90	0.54
1:A:282:PHE:CA	7:T:4:ALA:CB	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASP:N	24:B:303:PSC:H221	2.22	0.54
28:C:309:PEK:H292	30:T:201:HOH:O	2.06	0.54
5:R:6:GLU:HA	5:R:10:GLU:OE1	2.08	0.54
1:A:178[B]:GLN:HG2	7:T:7:ASP:OD1	2.07	0.53
27:N:601:CDL:H511	27:N:601:CDL:H222	1.90	0.53
1:N:449:MET:SD	2:O:5:MET:HG2	2.48	0.53
27:T:102:CDL:H782	27:T:102:CDL:H571	1.90	0.53
24:B:303:PSC:H32	9:I:14:ALA:HA	1.90	0.53
1:A:449:MET:SD	2:B:5:MET:HG2	2.48	0.53
4:D:19[A]:ARG:HG3	4:D:21:ASP:OD1	2.08	0.53
28:P:308:PEK:C04	6:S:1:ALA:N	2.70	0.53
28:C:307:PEK:N	28:C:307:PEK:P	2.82	0.53
24:N:612:PSC:H342	2:O:41:ILE:HD13	1.91	0.53
24:N:612:PSC:H342	2:O:41:ILE:CD1	2.39	0.53
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.91	0.53
1:A:178[B]:GLN:OE1	7:T:10:GLY:HA3	2.09	0.53
1:A:356:ILE:HD13	14:A:602[B]:HEA:HMB1	1.90	0.53
3:P:52:LEU:HG	27:P:305:CDL:H382	1.90	0.52
1:A:459:PHE:CE1	21:D:202:EDO:C1	2.93	0.52
4:D:19[A]:ARG:CG	4:D:21:ASP:OD1	2.57	0.52
8:H:8:ILE:O	8:H:8:ILE:CG2	2.57	0.52
11:X:7:PRO:HB2	11:X:12:LYS:NZ	2.24	0.52
21:A:619:EDO:H22	30:M:220:HOH:O	2.08	0.52
2:B:116:LEU:HD11	2:B:226:MET:HB3	1.92	0.52
9:I:70:GLN:NE2	30:I:103:HOH:O	2.41	0.52
24:N:612:PSC:H111	24:N:612:PSC:H322	1.91	0.52
25:P:307:DMU:H29	25:P:307:DMU:C9	2.28	0.52
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.52
24:B:303:PSC:H232	24:B:303:PSC:O03	2.09	0.52
28:G:101:PEK:O04	30:G:201:HOH:O	2.19	0.52
27:N:601:CDL:C61	27:N:601:CDL:H661	2.32	0.52
3:P:40:MET:O	3:P:44[B]:MET:HG3	2.09	0.52
18:A:606[B]:AZI:N1	30:A:707:HOH:O	2.34	0.52
20:A:610:PGV:C22	30:M:222:HOH:O	2.46	0.52
1:A:324:LEU:CD2	2:B:42:ILE:HG13	2.40	0.52
3:C:95:THR:HG21	20:C:308:PGV:H312	1.91	0.52
1:N:307:SER:HB2	27:N:601:CDL:H191	1.90	0.51
3:C:33[A]:MET:CB	25:C:302:DMU:C22	2.80	0.51
2:O:221:LYS:O	2:O:221:LYS:HD2	2.10	0.51
28:G:101:PEK:H161	28:G:101:PEK:H12	1.90	0.51
3:P:38:ASN:O	25:P:310:DMU:H32	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:D:201:TGL:H363	9:I:20:HIS:HE1	1.75	0.51
1:N:514:LYS:HE2	30:S:212:HOH:O	2.11	0.51
27:N:601:CDL:H371	2:O:78:LEU:CD1	2.24	0.51
9:V:1:SAC:OAC	9:V:3:ALA:HB3	2.10	0.51
2:B:26:HIS:O	2:B:29[B]:MET:HB3	2.10	0.51
8:H:9:LYS:CG	8:H:10:ASN:N	2.69	0.51
3:P:224:LYS:HD3	27:P:305:CDL:CB3	2.41	0.51
13:Z:36:HIS:CD2	13:Z:39:ASN:ND2	2.79	0.51
1:N:112:LEU:HD23	1:N:112:LEU:C	2.32	0.51
1:N:28:MET:CE	14:N:602:HEA:C27	2.89	0.51
1:N:513:LEU:O	1:N:514:LYS:CB	2.39	0.51
5:E:86:ILE:O	5:E:90:ARG:HG2	2.11	0.51
1:A:28:MET:HE2	14:A:601:HEA:H273	1.93	0.50
14:A:601:HEA:H122	14:A:601:HEA:HHC	1.93	0.50
10:J:52:TRP:O	10:J:57:HIS:HE1	1.94	0.50
1:N:28:MET:HE1	14:N:602:HEA:C27	2.41	0.50
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.46	0.50
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.77	0.50
20:N:609:PGV:C01	20:N:609:PGV:H22	2.18	0.50
2:O:29[B]:MET:HG2	2:O:29[B]:MET:O	2.10	0.50
7:T:3:ALA:O	7:T:4:ALA:CB	2.59	0.50
4:D:100[B]:LYS:HE2	30:D:358:HOH:O	2.10	0.50
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.94	0.50
20:A:610:PGV:H312	13:M:16:ALA:HA	1.92	0.50
1:N:302[B]:ARG:HE	2:O:84:LEU:CD1	2.24	0.50
28:T:101:PEK:H71	28:T:101:PEK:H32	1.91	0.50
30:P:447:HOH:O	8:U:84:LYS:HE3	2.11	0.50
1:A:74:MET:SD	1:A:74:MET:HB2	2.45	0.50
11:K:42:PRO:O	11:K:47:ARG:NH2	2.45	0.50
27:P:305:CDL:HB21	27:P:305:CDL:OB6	2.11	0.50
1:A:309:THR:HG22	14:A:602[A]:HEA:HMB2	1.94	0.50
7:T:3:ALA:O	7:T:4:ALA:HB2	2.12	0.50
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.94	0.49
2:B:198:GLU:CG	30:B:424:HOH:O	2.58	0.49
4:D:78:TRP:HA	19:D:201:TGL:HB21	1.94	0.49
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.46	0.49
8:U:57:ARG:O	8:U:61:LYS:HB2	2.13	0.49
20:P:302:PGV:H22	20:P:302:PGV:H72	1.94	0.49
27:P:305:CDL:H411	27:P:305:CDL:C45	2.41	0.49
4:Q:17[A]:VAL:HG23	4:Q:17[A]:VAL:O	2.12	0.49
3:C:156:ARG:HE	22:C:306:CHD:C24	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.32	0.49
1:N:313:ALA:HB2	1:N:356:ILE:HD11	1.94	0.49
1:A:309:THR:HG22	14:A:602[B]:HEA:HMB2	1.93	0.49
3:C:37:PHE:CD2	25:C:302:DMU:H8	2.47	0.49
12:L:26:THR:HG23	13:M:25:SER:CB	2.43	0.49
12:Y:20:ARG:HH22	19:Y:101:TGL:HC82	1.76	0.49
3:C:76:GLN:O	3:C:80[A]:ARG:HG3	2.12	0.49
3:C:157:LYS:HZ2	28:C:307:PEK:C05	2.25	0.49
2:B:32[B]:PHE:C	2:B:32[B]:PHE:CD1	2.87	0.49
2:O:64:ILE:HG23	2:O:68:LEU:HD13	1.94	0.49
1:N:362[A]:SER:OG	2:O:87[A]:MET:HE2	2.12	0.49
25:P:307:DMU:O6	25:P:310:DMU:H40	2.13	0.49
30:A:877:HOH:O	4:D:17[A]:VAL:HG12	2.09	0.48
25:C:302:DMU:H12	10:J:49:CYS:HB3	1.94	0.48
20:A:610:PGV:H202	20:A:610:PGV:H231	1.61	0.48
3:C:253:TYR:HE2	27:N:601:CDL:H641	1.77	0.48
6:S:95:GLN:CA	6:S:95:GLN:HE21	2.09	0.48
1:A:347:LEU:HD11	1:A:418:PHE:CE2	2.48	0.48
28:G:101:PEK:H101	28:G:101:PEK:H42	1.95	0.48
8:H:40:GLU:OE1	8:H:50:VAL:HG11	2.13	0.48
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.31	0.48
3:C:161[A]:GLN:NE2	28:C:307:PEK:H41	2.23	0.48
1:A:378:HIS:O	1:A:383[B]:MET:HG2	2.13	0.48
12:Y:14:SER:H	19:Y:101:TGL:HC31	1.78	0.48
1:A:240:HIS:ND1	18:A:607[B]:AZI:N1	2.62	0.48
1:N:321:PHE:CD1	24:N:612:PSC:H332	2.49	0.48
2:B:1:FME:CE	2:B:133:LEU:HD13	2.43	0.48
2:B:60:GLU:CD	2:B:60:GLU:N	2.66	0.48
4:D:17[A]:VAL:O	4:D:17[A]:VAL:HG23	2.13	0.48
4:D:78:TRP:HB3	19:D:201:TGL:CB2	2.39	0.48
28:C:309:PEK:H361	27:T:102:CDL:H871	1.95	0.48
7:T:72:ASN:H	7:T:76:ASN:ND2	2.04	0.47
4:D:99:GLU:OE2	21:D:202:EDO:C2	2.61	0.47
9:I:22:VAL:O	9:I:26:MET:HG2	2.14	0.47
2:B:161:HIS:HB3	30:B:403:HOH:O	2.12	0.47
27:N:601:CDL:H342	27:N:601:CDL:OA7	2.15	0.47
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.49	0.47
27:P:305:CDL:C27	27:P:305:CDL:H381	2.15	0.47
4:Q:19[A]:ARG:HD2	4:Q:21:ASP:CG	2.35	0.47
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.97	0.47
2:B:56:MET:HG2	24:B:303:PSC:H231	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100[B]:LYS:O	4:D:100[B]:LYS:CD	2.63	0.47
6:F:54[A]:ASN:H	6:F:54[A]:ASN:ND2	2.13	0.47
6:F:75:HIS:H	6:F:80:GLN:NE2	2.08	0.47
3:P:63:ARG:HE	27:P:305:CDL:HA22	1.78	0.47
1:A:417[B]:MET:HE1	30:A:873:HOH:O	2.13	0.47
6:F:92:VAL:O	6:F:92:VAL:HG23	2.14	0.47
7:G:1:ALA:O	7:G:3:ALA:N	2.47	0.47
8:H:37:HIS:HD2	30:H:101:HOH:O	1.96	0.47
24:N:612:PSC:H12	2:O:64:ILE:HG21	1.97	0.47
4:Q:34:SER:O	4:Q:38:LYS:HG3	2.15	0.47
1:A:355:GLY:C	14:A:602[B]:HEA:HMB3	2.36	0.47
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.97	0.47
14:A:602[B]:HEA:CBD	14:A:602[B]:HEA:HMD1	2.44	0.47
3:C:51[A]:MET:SD	27:C:305:CDL:H612	2.54	0.47
3:C:157:LYS:NZ	28:C:307:PEK:C05	2.77	0.47
27:N:601:CDL:H241	27:N:601:CDL:H531	1.97	0.47
24:N:612:PSC:H111	24:N:612:PSC:H321	1.97	0.47
20:N:609:PGV:H291	13:Z:16:ALA:HA	1.97	0.47
14:N:603[A]:HEA:C4B	18:N:608[A]:AZI:N1	2.64	0.47
14:A:602[A]:HEA:H11	14:A:602[A]:HEA:HMB1	1.79	0.46
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.97	0.46
25:P:309:DMU:H36	25:P:309:DMU:H34	1.35	0.46
2:B:83:ILE:O	2:B:87[B]:MET:HB2	2.16	0.46
2:O:53:THR:HG21	30:Q:308:HOH:O	2.14	0.46
3:P:41:THR:HA	3:P:44[B]:MET:HE2	1.97	0.46
2:B:153:LEU:HD12	30:B:522:HOH:O	2.16	0.46
5:R:14[B]:ARG:HG2	30:R:303:HOH:O	2.15	0.46
6:S:85:CYS:SG	6:S:87[B]:THR:HG22	2.55	0.46
1:N:243:VAL:HG11	18:N:608[B]:AZI:N2	2.30	0.46
1:N:308:ALA:O	1:N:311[B]:ILE:HG12	2.15	0.46
19:N:611:TGL:HB92	19:N:611:TGL:H283	1.92	0.46
7:G:3:ALA:O	7:G:4:ALA:CB	2.64	0.46
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.97	0.46
20:N:610:PGV:H262	20:P:304:PGV:H292	1.97	0.46
6:F:64:GLU:O	6:F:65:ASP:HB2	2.15	0.46
7:G:12:GLY:N	30:G:203:HOH:O	2.35	0.46
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.98	0.46
3:C:258:TRP:CZ3	27:N:601:CDL:H642	2.49	0.46
12:Y:24[B]:MET:SD	19:Y:101:TGL:HC21	2.56	0.46
24:N:612:PSC:H22	30:N:890:HOH:O	2.15	0.46
2:O:39:LEU:CD1	19:Q:201:TGL:H221	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:47:LYS:OXT	12:Y:47:LYS:HG3	2.16	0.46
21:B:304:EDO:H22	30:B:527:HOH:O	2.16	0.46
25:C:310:DMU:H36	25:C:310:DMU:H34	0.99	0.46
22:G:102:CHD:H212	22:G:102:CHD:H12	1.98	0.46
1:N:62:ALA:HB2	14:N:602:HEA:HBD1	1.97	0.46
5:R:41:LEU:HA	30:V:109:HOH:O	2.15	0.46
12:Y:20:ARG:HH22	19:Y:101:TGL:HC62	1.80	0.46
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.97	0.46
1:A:356:ILE:HA	14:A:602[B]:HEA:HMB3	1.98	0.45
1:A:378:HIS:HA	1:A:382[B]:SER:HB2	1.98	0.45
3:C:51[B]:MET:HE3	27:C:305:CDL:H392	1.91	0.45
2:O:58:ALA:O	2:O:62:GLU:HG3	2.15	0.45
7:G:42:ARG:HB2	7:G:42:ARG:NH1	2.30	0.45
1:N:172:LYS:NZ	1:N:178[A]:GLN:NE2	2.63	0.45
1:N:386:VAL:HG21	14:N:602:HEA:H261	1.98	0.45
19:A:608:TGL:HA52	19:A:608:TGL:HA22	1.86	0.45
7:T:44:ARG:HH22	7:T:84:LYS:HZ1	1.63	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.45
25:C:310:DMU:H32	25:C:310:DMU:H29	1.98	0.45
3:C:63:ARG:HE	27:C:305:CDL:HA22	1.76	0.45
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.81	0.45
1:A:364:ASP:OD1	14:A:602[B]:HEA:O1A	2.34	0.45
19:A:611:TGL:HC32	12:L:20:ARG:HH21	1.64	0.45
3:P:33[A]:MET:CE	3:P:41:THR:HB	2.47	0.45
8:U:44:THR:C	8:U:46:LYS:H	2.18	0.45
6:F:21[B]:MET:HB2	6:F:21[B]:MET:HE2	1.54	0.45
19:Y:101:TGL:CG1	19:Y:101:TGL:CA3	2.91	0.45
1:A:148:PHE:HB3	3:C:28:THR:HB	1.98	0.45
19:A:608:TGL:HC22	30:A:919:HOH:O	2.15	0.45
12:L:26:THR:HG23	13:M:25:SER:HB3	1.99	0.45
1:N:311[A]:ILE:CD1	27:N:601:CDL:H221	2.45	0.45
24:N:612:PSC:C34	24:N:612:PSC:C13	2.87	0.45
3:P:156:ARG:HE	22:P:306:CHD:C24	2.29	0.45
22:P:306:CHD:C23	22:P:306:CHD:C16	2.94	0.45
9:V:31:PHE:CD2	9:V:31:PHE:C	2.89	0.45
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.46	0.45
20:N:609:PGV:C31	13:Z:19:LEU:HD23	2.46	0.45
1:N:309:THR:HG22	14:N:603[A]:HEA:HMB2	1.98	0.45
8:U:9:LYS:HG3	8:U:10:ASN:N	2.31	0.45
1:N:382[B]:SER:HB3	14:N:602:HEA:C2C	2.47	0.45
1:N:28:MET:HE2	14:N:602:HEA:H271	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.98	0.44
7:G:11:TPO:C	30:G:202:HOH:O	2.64	0.44
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.99	0.44
9:V:25:PHE:O	9:V:28:SER:HB2	2.18	0.44
1:N:415:ALA:HB1	19:Q:201:TGL:H132	1.99	0.44
19:Y:101:TGL:OA1	19:Y:101:TGL:H181	2.17	0.44
4:D:99:GLU:OE1	21:D:202:EDO:H11	2.17	0.44
1:N:311[B]:ILE:HD11	27:N:601:CDL:H232	1.99	0.44
2:B:160:LEU:HD22	30:B:463:HOH:O	2.17	0.44
1:A:281:GLY:O	7:T:4:ALA:HB1	2.17	0.44
2:B:82:ARG:HH11	2:B:86:MET:CE	2.30	0.44
3:C:33[B]:MET:CG	3:C:39:SER:HB3	2.48	0.44
7:G:42:ARG:HB2	7:G:42:ARG:HH11	1.82	0.44
27:N:601:CDL:H561	27:N:601:CDL:H591	1.76	0.44
2:O:29[B]:MET:HB2	9:V:35:TYR:CE1	2.52	0.44
3:P:33[B]:MET:CB	25:P:307:DMU:H9	2.46	0.44
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.00	0.44
4:D:7:LYS:NZ	30:D:303:HOH:O	2.41	0.44
3:P:29:SER:HB2	25:P:307:DMU:H21	1.98	0.44
8:U:60:TYR:CD1	8:U:60:TYR:C	2.90	0.44
1:A:74:MET:CG	1:A:74:MET:CA	2.81	0.44
6:F:87[A]:THR:HG21	30:F:209:HOH:O	2.17	0.44
2:O:48:THR:HB	9:V:16:ARG:CZ	2.47	0.44
7:G:58:LYS:HG2	21:G:105:EDO:H21	2.00	0.44
24:N:612:PSC:H011	24:N:612:PSC:O02	2.18	0.44
8:U:7:LYS:HE3	8:U:7:LYS:HA	1.98	0.44
1:A:136[B]:LEU:CD1	30:A:933:HOH:O	2.43	0.44
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.74	0.44
22:P:301:CHD:H12	22:P:301:CHD:H212	2.00	0.44
27:T:102:CDL:H602	27:T:102:CDL:H651	2.00	0.44
2:B:32[A]:PHE:HA	2:B:32[A]:PHE:HD1	1.50	0.43
10:J:7:GLU:HG3	30:J:213:HOH:O	2.18	0.43
1:N:316:THR:HG21	14:N:603[A]:HEA:H14	2.00	0.43
2:O:191:LEU:HG	9:V:68:ILE:HD12	1.99	0.43
27:P:305:CDL:C65	27:P:305:CDL:H222	2.48	0.43
8:U:44:THR:C	8:U:46:LYS:N	2.71	0.43
10:W:54:SER:O	12:Y:46:LYS:HE2	2.18	0.43
1:A:243:VAL:HG11	18:A:607[B]:AZI:N3	2.33	0.43
3:C:33[A]:MET:HE3	25:C:302:DMU:H10	2.01	0.43
30:B:423:HOH:O	8:H:62:SER:CA	2.41	0.43
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:116:LEU:HD13	2:O:226:MET:HG2	2.01	0.43
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.48	0.43
10:W:29:ASN:HD22	10:W:29:ASN:H	1.66	0.43
27:N:601:CDL:H181	27:N:601:CDL:HB32	2.00	0.43
27:T:102:CDL:H752	27:T:102:CDL:H562	1.99	0.43
2:B:28:LEU:HG	2:B:32[A]:PHE:CE2	2.53	0.43
2:B:91:ASN:OD1	2:B:183[B]:THR:HG21	2.18	0.43
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.00	0.43
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.75	0.43
20:A:609:PGV:H343	28:G:101:PEK:C38	2.44	0.43
6:F:43:LYS:HE2	6:F:43:LYS:HB2	1.59	0.43
6:F:54[A]:ASN:H	6:F:54[A]:ASN:HD22	1.65	0.43
1:N:356:ILE:HA	14:N:603[B]:HEA:HMB3	2.00	0.43
1:A:426:PHE:N	1:A:427:PRO:CD	2.81	0.43
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.00	0.43
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.43
3:P:259:TRP:CD1	25:P:309:DMU:H30	2.53	0.43
2:B:56:MET:HB3	24:B:303:PSC:H252	2.00	0.43
28:C:307:PEK:H02	28:C:307:PEK:H31	1.99	0.43
1:N:112:LEU:HG	30:N:881:HOH:O	2.17	0.43
14:N:603[B]:HEA:CBC	14:N:603[B]:HEA:HMC1	2.49	0.43
4:Q:93:ALA:O	4:Q:97:ILE:HG13	2.19	0.43
13:Z:36:HIS:HD2	13:Z:39:ASN:HD22	1.67	0.43
1:A:356:ILE:HD13	14:A:602[B]:HEA:CMB	2.49	0.43
14:A:602[A]:HEA:HAD2	14:A:602[A]:HEA:HHA	1.69	0.43
7:G:59:PRO:HB2	21:G:105:EDO:H22	2.01	0.43
7:G:6:GLY:H	1:N:278[B]:MET:HE1	1.83	0.43
2:B:91:ASN:HD22	2:B:92:ASN:N	2.17	0.43
8:H:9:LYS:HE3	8:H:11:TYR:H	1.83	0.43
3:P:54[B]:MET:HB3	3:P:58:TRP:CZ3	2.54	0.43
6:S:52:ILE:O	6:S:94:HIS:CE1	2.72	0.43
1:A:512:ASN:OD1	1:A:514:LYS:HD2	2.19	0.42
28:C:307:PEK:H382	27:N:601:CDL:C27	2.43	0.42
10:J:33:ARG:HG2	22:J:101:CHD:H151	2.00	0.42
2:O:60:GLU:H	2:O:60:GLU:CD	2.21	0.42
27:P:305:CDL:H651	27:P:305:CDL:C22	2.49	0.42
2:B:16[A]:ILE:CD1	2:B:87[A]:MET:HG2	2.48	0.42
22:C:301:CHD:H12	22:C:301:CHD:H212	2.00	0.42
9:I:23:GLY:O	9:I:27:VAL:HG23	2.19	0.42
1:N:328:HIS:HB2	2:O:45:MET:SD	2.59	0.42
19:A:608:TGL:HA92	19:A:608:TGL:H242	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:303:PSC:H042	24:B:303:PSC:H062	1.72	0.42
4:D:17[A]:VAL:O	4:D:17[A]:VAL:CG2	2.67	0.42
1:N:316:THR:HG21	14:N:603[A]:HEA:C14	2.49	0.42
3:P:54[A]:MET:HE1	20:P:304:PGV:H131	2.01	0.42
1:A:514:LYS:HG3	6:F:38:ALA:HB3	2.01	0.42
14:N:603[B]:HEA:HMB1	14:N:603[B]:HEA:H11	1.87	0.42
6:S:94:HIS:HA	30:S:223:HOH:O	2.20	0.42
2:B:148:MET:HB3	30:B:547:HOH:O	2.19	0.42
3:C:3:HIS:HD2	3:C:4:GLN:O	2.02	0.42
1:N:353:LEU:HB3	2:O:31:VAL:HG13	2.00	0.42
12:Y:20:ARG:NH1	19:Y:101:TGL:HC32	2.27	0.42
1:N:423[A]:MET:HG2	1:N:457:GLY:CA	2.50	0.42
1:N:355:GLY:C	14:N:603[B]:HEA:HMB3	2.39	0.42
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.42
3:P:172:TYR:CD2	28:P:308:PEK:H15	2.55	0.42
28:C:309:PEK:C35	7:T:5:LYS:HG3	2.49	0.42
8:H:7:LYS:HG2	8:U:45:ALA:O	2.20	0.42
12:Y:24[B]:MET:SD	19:Y:101:TGL:CC2	3.07	0.42
1:A:316:THR:HG21	14:A:602[A]:HEA:C14	2.50	0.42
4:D:100[B]:LYS:HA	4:D:100[B]:LYS:HD2	1.82	0.42
1:N:311[B]:ILE:HG22	27:N:601:CDL:H442	2.02	0.42
20:A:610:PGV:C3	20:A:610:PGV:H011	2.50	0.42
27:C:305:CDL:OB9	27:C:305:CDL:H522	2.20	0.42
7:G:41:HIS:HB3	7:G:74:ARG:CZ	2.50	0.42
10:J:18:LEU:HA	10:J:18:LEU:HD23	1.92	0.42
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	2.02	0.42
2:O:151:ARG:CD	2:O:181:GLN:HE21	2.33	0.42
3:P:224:LYS:HE3	27:P:305:CDL:OA7	2.19	0.42
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.54	0.42
12:L:2:HIS:CG	12:L:3:TYR:H	2.38	0.41
14:N:602:HEA:H122	14:N:602:HEA:HHC	2.02	0.41
27:T:102:CDL:H452	27:T:102:CDL:H421	1.73	0.41
1:A:243:VAL:HG21	18:A:607[A]:AZI:N2	2.35	0.41
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.34	0.41
1:N:335:SER:HB2	1:N:336:PRO:HD2	2.02	0.41
5:R:74:LYS:HD2	5:R:74:LYS:HA	1.85	0.41
1:N:25:TRP:CE3	19:Y:101:TGL:HB91	2.55	0.41
2:B:49:LYS:CE	30:D:395:HOH:O	2.47	0.41
10:J:8:LYS:HD3	10:J:8:LYS:HA	1.87	0.41
5:R:31:LYS:HE2	6:S:83:PRO:O	2.19	0.41
19:Y:101:TGL:HC32	19:Y:101:TGL:HC62	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:ILE:HD13	2:B:42:ILE:HG21	1.77	0.41
8:H:7:LYS:O	8:H:8:ILE:HD12	2.20	0.41
3:P:246:ASP:HB2	30:P:486:HOH:O	2.19	0.41
3:C:33[A]:MET:HE3	25:C:302:DMU:O16	2.20	0.41
9:I:57:MET:O	9:I:61:GLU:HG2	2.20	0.41
20:A:610:PGV:H241	13:M:12:PRO:HG3	2.01	0.41
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	2.02	0.41
19:Q:201:TGL:HB51	19:Q:201:TGL:HA32	2.03	0.41
1:A:321:PHE:CD2	2:B:65:TRP:HB2	2.56	0.41
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.46	0.41
7:T:44:ARG:HH22	7:T:84:LYS:NZ	2.18	0.41
1:A:378:HIS:HA	1:A:382[B]:SER:CB	2.51	0.41
1:A:243:VAL:HG11	14:A:602[B]:HEA:HMD2	2.03	0.41
4:D:17[B]:VAL:HG22	4:D:19[B]:ARG:HG3	2.02	0.41
3:C:155:ASP:OD2	6:F:2:SER:HA	2.21	0.41
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.03	0.41
2:B:82:ARG:HH11	2:B:86:MET:HE1	1.85	0.41
3:C:188:ILE:HG21	30:G:201:HOH:O	2.19	0.41
8:H:42:ALA:C	8:H:43:MET:O	2.59	0.41
14:A:602[B]:HEA:HMC1	14:A:602[B]:HEA:HBC1	2.02	0.41
3:C:34:TRP:CD1	3:C:40:MET:HG3	2.56	0.41
11:X:7:PRO:HB2	11:X:12:LYS:HZ2	1.85	0.41
1:A:243:VAL:HG11	18:A:607[A]:AZI:N3	2.36	0.41
8:H:60:TYR:C	8:H:60:TYR:CD1	2.94	0.41
1:N:382[B]:SER:CB	1:N:383[B]:MET:HE2	2.49	0.41
2:O:53:THR:CG2	30:Q:308:HOH:O	2.69	0.41
3:P:33[A]:MET:HB2	25:P:307:DMU:H8	2.00	0.41
19:Y:101:TGL:HC51	19:Y:101:TGL:OC1	2.21	0.41
12:L:46:LYS:HA	30:L:203:HOH:O	2.20	0.41
12:L:47:LYS:NZ	12:L:47:LYS:CB	2.83	0.41
1:N:2:PHE:HZ	19:Y:101:TGL:HG32	1.86	0.41
1:N:399:LEU:O	1:N:499:PRO:HA	2.21	0.41
14:N:603[B]:HEA:C24	2:O:69:PRO:HB3	2.51	0.41
2:B:174:ALA:HB3	30:B:528:HOH:O	2.14	0.40
5:E:81:ILE:HD11	9:I:12:LEU:HD11	2.03	0.40
6:F:87[B]:THR:HG21	30:F:266:HOH:O	2.21	0.40
10:W:32:TYR:OH	22:W:101:CHD:H213	2.21	0.40
1:N:423[A]:MET:HG2	1:N:457:GLY:HA3	2.03	0.40
2:O:66:THR:HG22	30:O:493:HOH:O	2.20	0.40
1:A:278[B]:MET:HE3	7:T:5:LYS:HB3	2.02	0.40
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41[B]:ILE:O	2:B:42:ILE:C	2.54	0.40
2:B:16[A]:ILE:HA	2:B:16[A]:ILE:HD13	1.93	0.40
2:B:81:LEU:HD13	27:T:102:CDL:H151	2.03	0.40
9:I:31:PHE:CZ	9:I:35:TYR:HB2	2.56	0.40
1:N:362[A]:SER:CB	2:O:87[A]:MET:HE1	2.52	0.40
5:R:77:PRO:O	5:R:79:LYS:HD2	2.22	0.40
3:C:258:TRP:CH2	25:C:310:DMU:H12	2.57	0.40
1:N:28:MET:HE1	14:N:602:HEA:H271	2.01	0.40
2:O:221:LYS:C	2:O:221:LYS:HD2	2.42	0.40
2:O:41:ILE:O	2:O:42:ILE:C	2.58	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:491:HOH:O	30:D:341:HOH:O[2_584]	1.22	0.98
30:I:126:HOH:O	30:M:216:HOH:O[2_584]	1.92	0.28
30:B:541:HOH:O	30:L:228:HOH:O[2_584]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	534/514 (104%)	516 (97%)	18 (3%)	0	100	100
1	N	532/514 (104%)	515 (97%)	17 (3%)	0	100	100
2	B	234/227 (103%)	227 (97%)	5 (2%)	2 (1%)	17	4
2	O	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	262 (98%)	4 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	146/147 (99%)	142 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	145/147 (99%)	138 (95%)	4 (3%)	3 (2%)	7	0
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	104/109 (95%)	103 (99%)	0	1 (1%)	15	3
6	F	100/98 (102%)	96 (96%)	1 (1%)	3 (3%)	4	0
6	S	98/98 (100%)	91 (93%)	3 (3%)	4 (4%)	3	0
7	G	82/85 (96%)	68 (83%)	9 (11%)	5 (6%)	1	0
7	T	82/85 (96%)	70 (85%)	8 (10%)	4 (5%)	2	0
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	0
8	U	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	2	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	6	0
13	M	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	6	0
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3597/3614 (100%)	3457 (96%)	109 (3%)	31 (1%)	17	4

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	2	SER
7	G	3	ALA
7	G	4	ALA
7	G	5	LYS
8	H	43	MET
8	H	44	THR
13	M	42	LYS
4	Q	7	LYS
6	S	94	HIS
6	S	95	GLN

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Mol	Chain	Res	Type
7	T	3	ALA
7	T	5	LYS
7	T	8	HIS
8	U	10	ASN
12	Y	46	LYS
5	R	6	GLU
6	S	96	LEU
7	T	4	ALA
8	U	8	ILE
6	F	95	GLN
8	H	45	ALA
6	F	96	LEU
4	Q	8	SER
8	U	45	ALA
8	U	51	SER
2	B	87[A]	MET
2	B	87[B]	MET
7	G	6	GLY
4	Q	6	VAL
6	S	93	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/426 (105%)	438 (98%)	9 (2%)	55	32
1	N	445/426 (104%)	439 (99%)	6 (1%)	69	50
2	B	219/210 (104%)	209 (95%)	10 (5%)	27	6
2	O	215/210 (102%)	208 (97%)	7 (3%)	38	12
3	C	233/226 (103%)	229 (98%)	4 (2%)	60	39
3	P	233/226 (103%)	229 (98%)	4 (2%)	60	39
4	D	132/129 (102%)	130 (98%)	2 (2%)	65	44
4	Q	131/129 (102%)	125 (95%)	6 (5%)	27	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	12
5	R	93/95 (98%)	88 (95%)	5 (5%)	22	4
6	F	85/81 (105%)	81 (95%)	4 (5%)	26	6
6	S	83/81 (102%)	73 (88%)	10 (12%)	5	0
7	G	68/68 (100%)	61 (90%)	7 (10%)	7	1
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	1
8	H	71/75 (95%)	67 (94%)	4 (6%)	21	4
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	1
9	I	57/57 (100%)	55 (96%)	2 (4%)	36	11
9	V	57/57 (100%)	54 (95%)	3 (5%)	22	4
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	32
10	W	50/50 (100%)	48 (96%)	2 (4%)	31	9
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	37 (92%)	3 (8%)	13	2
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	21
12	Y	40/40 (100%)	39 (98%)	1 (2%)	47	22
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	37 (100%)	0	100	100
All	All	3131/3082 (102%)	3023 (97%)	108 (3%)	36	12

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	363	LEU
1	A	369	ASP
1	A	382[A]	SER
1	A	382[B]	SER
1	A	514	LYS
2	B	42	ILE
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP

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Mol	Chain	Res	Type
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	17	PRO
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
4	D	31	LYS
4	D	147	LYS
5	E	5	HIS
5	E	90	ARG
5	E	109	VAL
6	F	37	LYS
6	F	43	LYS
6	F	78	GLU
6	F	80	GLN
7	G	2	SER
7	G	7	ASP
7	G	33	LEU
7	G	37	LEU
7	G	42	ARG
7	G	54	ARG
7	G	84	LYS
8	H	8	ILE
8	H	9	LYS
8	H	29	CYS
8	H	60	TYR
9	I	2	THR
9	I	37	PHE
10	J	58	LYS
12	L	47	LYS
1	N	38	ARG
1	N	109	PHE
1	N	180	GLN
1	N	265	LYS
1	N	369	ASP
1	N	495	LEU
2	O	33	LEU
2	O	60	GLU

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Mol	Chain	Res	Type
2	O	65	TRP
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	221	LYS
3	P	110	PRO
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	7	LYS
4	Q	20	ARG
4	Q	51	LEU
4	Q	142	LYS
4	Q	143	ASN
4	Q	147	LYS
5	R	6	GLU
5	R	45	PRO
5	R	79	LYS
5	R	90	ARG
5	R	108	LYS
6	S	37	LYS
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
6	S	87[A]	THR
6	S	87[B]	THR
6	S	93	PRO
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	2	SER
7	T	8	HIS
7	T	18	PHE
7	T	35	SER
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	7	LYS
8	U	29	CYS
8	U	40	GLU
8	U	60	TYR

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Mol	Chain	Res	Type
8	U	61	LYS
8	U	84	LYS
9	V	8	GLN
9	V	42	LYS
9	V	73	LYS
10	W	50	LEU
10	W	58	LYS
11	X	51	LYS
11	X	52	GLU
11	X	54	ARG
12	Y	16	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	10	GLN
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
5	E	94	ASN
6	F	80	GLN
7	G	8	HIS
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
9	I	20	HIS
10	J	29	ASN
10	J	57	HIS
1	N	180	GLN
2	O	10	GLN
2	O	52	HIS
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN

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Mol	Chain	Res	Type
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	88	HIS
6	S	94	HIS
6	S	95	GLN
6	S	98	HIS
7	T	8	HIS
7	T	76	ASN
8	U	22	ASN
8	U	37	HIS
10	W	29	ASN
13	Z	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SAC	V	1	9	7,8,9	1.66	1 (14%)	8,9,11	1.35	2 (25%)
2	FME	B	1	2	8,9,10	2.06	4 (50%)	7,9,11	1.90	2 (28%)
1	FME	N	1	1	8,9,10	1.26	1 (12%)	7,9,11	1.30	1 (14%)
7	TPO	T	11	7	8,10,11	1.74	2 (25%)	10,14,16	1.28	1 (10%)
7	TPO	G	11	7	8,10,11	2.03	3 (37%)	10,14,16	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	A	1	1	8,9,10	0.96	1 (12%)	7,9,11	1.84	3 (42%)
9	SAC	I	1	9	7,8,9	1.50	1 (14%)	8,9,11	1.89	2 (25%)
2	FME	O	1	2	8,9,10	1.26	1 (12%)	7,9,11	2.00	2 (28%)

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	V	1	9	-	7/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	2/7/9/11	-
9	SAC	I	1	9	-	4/7/8/10	-
2	FME	O	1	2	-	0/7/9/11	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.24	1.52	1.46
2	B	1	FME	CB-CA	3.59	1.59	1.53
9	I	1	SAC	CA-N	3.50	1.51	1.46
7	G	11	TPO	P-O1P	3.29	1.61	1.50
7	T	11	TPO	P-O1P	3.09	1.60	1.50
7	G	11	TPO	P-OG1	2.78	1.64	1.59
2	B	1	FME	CB-CG	2.65	1.61	1.51
1	N	1	FME	CA-N	2.40	1.49	1.46
2	B	1	FME	O-C	2.37	1.29	1.19
7	T	11	TPO	P-OG1	2.18	1.63	1.59
7	G	11	TPO	CB-CA	2.16	1.58	1.53
1	A	1	FME	O-C	2.13	1.28	1.19
2	O	1	FME	CB-CG	2.08	1.59	1.51
2	B	1	FME	CG-SD	-2.01	1.70	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	SAC	OG-CB-CA	-3.53	101.96	110.97
9	I	1	SAC	C-CA-N	3.46	115.97	109.73
2	O	1	FME	CA-N-CN	3.36	127.98	122.82
1	A	1	FME	CE-SD-CG	3.23	111.50	100.40
2	B	1	FME	C-CA-N	-3.20	103.96	109.73
2	B	1	FME	CG-CB-CA	-3.02	104.55	112.95
9	V	1	SAC	CA-N-C1A	2.62	127.99	123.15
2	O	1	FME	CG-CB-CA	-2.59	105.74	112.95
1	A	1	FME	O-C-CA	-2.42	118.44	124.78
1	A	1	FME	C-CA-N	2.26	113.81	109.73
1	N	1	FME	O-C-CA	-2.11	119.26	124.78
7	T	11	TPO	CG2-CB-CA	2.08	117.27	113.16
9	V	1	SAC	O-C-CA	-2.00	119.54	124.78

There are no chirality outliers.

All (26) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
9	V	1	SAC	C-CA-N-C1A

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1	SAC	1	0
2	B	1	FME	2	0
7	T	11	TPO	1	0
7	G	11	TPO	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 101 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	DMU	C	310	-	34,34,34	0.91	1 (2%)	45,45,45	2.51	13 (28%)
21	EDO	Y	102	-	3,3,3	0.53	0	2,2,2	0.61	0
21	EDO	E	202	-	3,3,3	0.93	0	2,2,2	0.66	0
14	HEA	A	601	1	44,67,67	1.37	6 (13%)	37,103,103	2.65	15 (40%)
20	PGV	A	610	-	50,50,50	1.41	5 (10%)	53,56,56	1.88	7 (13%)
22	CHD	J	101	-	29,32,32	0.84	0	48,51,51	2.31	19 (39%)
27	CDL	N	601	-	99,99,99	1.53	15 (15%)	105,111,111	1.51	16 (15%)
21	EDO	D	202	-	3,3,3	1.05	0	2,2,2	0.36	0
22	CHD	C	306	-	29,32,32	1.15	3 (10%)	48,51,51	4.08	17 (35%)
21	EDO	G	104	-	3,3,3	0.99	0	2,2,2	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	A	617	-	3,3,3	1.38	0	2,2,2	0.41	0
21	EDO	W	102	-	3,3,3	0.49	0	2,2,2	0.65	0
19	TGL	Q	201	-	62,62,62	1.51	4 (6%)	65,65,65	1.47	7 (10%)
21	EDO	O	302	-	3,3,3	0.65	0	2,2,2	0.58	0
21	EDO	N	614	-	3,3,3	0.47	0	2,2,2	1.07	0
27	CDL	T	102	-	99,99,99	1.45	13 (13%)	105,111,111	1.36	17 (16%)
24	PSC	N	612	-	51,51,51	1.29	3 (5%)	57,59,59	1.19	4 (7%)
22	CHD	C	301	-	29,32,32	1.74	5 (17%)	48,51,51	2.52	19 (39%)
21	EDO	N	617	-	3,3,3	0.65	0	2,2,2	0.84	0
21	EDO	P	311	-	3,3,3	0.87	0	2,2,2	0.50	0
24	PSC	B	303	-	51,51,51	1.28	4 (7%)	57,59,59	1.38	4 (7%)
21	EDO	M	102	-	3,3,3	0.24	0	2,2,2	1.04	0
21	EDO	C	312	-	3,3,3	0.64	0	2,2,2	0.60	0
21	EDO	B	304	-	3,3,3	0.16	0	2,2,2	1.40	0
19	TGL	N	611	-	62,62,62	1.12	4 (6%)	65,65,65	1.69	10 (15%)
22	CHD	W	101	-	29,32,32	1.25	4 (13%)	48,51,51	2.71	27 (56%)
25	DMU	M	101	-	34,34,34	0.90	1 (2%)	45,45,45	1.44	6 (13%)
21	EDO	A	614	-	3,3,3	1.58	1 (33%)	2,2,2	0.78	0
21	EDO	S	104	-	3,3,3	0.63	0	2,2,2	1.66	1 (50%)
21	EDO	F	103	-	3,3,3	1.11	0	2,2,2	0.11	0
18	AZI	N	607[B]	14	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	S	102	-	3,3,3	1.07	0	2,2,2	0.43	0
25	DMU	C	311	-	34,34,34	1.04	1 (2%)	45,45,45	2.33	13 (28%)
18	AZI	A	606[B]	14	0,2,2	0.00	-	0,1,1	0.00	-
20	PGV	C	304	-	50,50,50	0.98	3 (6%)	53,56,56	1.12	4 (7%)
21	EDO	T	103	-	3,3,3	1.00	0	2,2,2	0.82	0
28	PEK	C	309	-	52,52,52	1.19	2 (3%)	55,57,57	1.37	5 (9%)
21	EDO	F	102	-	3,3,3	0.94	0	2,2,2	0.20	0
19	TGL	A	611	-	62,62,62	1.28	3 (4%)	65,65,65	1.83	13 (20%)
21	EDO	N	615	-	3,3,3	0.69	0	2,2,2	1.27	0
18	AZI	N	608[B]	15	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	A	618	-	3,3,3	0.41	0	2,2,2	1.03	0
28	PEK	G	103	-	52,52,52	1.11	2 (3%)	55,57,57	1.19	4 (7%)
21	EDO	F	104	-	3,3,3	0.68	0	2,2,2	0.34	0
21	EDO	A	615	-	3,3,3	0.62	0	2,2,2	1.83	1 (50%)
14	HEA	N	603[A]	1,18	44,67,67	1.22	4 (9%)	37,103,103	2.26	14 (37%)
27	CDL	P	305	-	99,99,99	1.53	18 (18%)	105,111,111	1.63	18 (17%)
18	AZI	A	607[A]	15,14	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DMU	C	302	-	34,34,34	0.75	1 (2%)	45,45,45	1.47	7 (15%)
18	AZI	A	607[B]	15	0,2,2	0.00	-	0,1,1	0.00	-
19	TGL	A	608	-	62,62,62	1.31	6 (9%)	65,65,65	2.24	10 (15%)
21	EDO	E	203	-	3,3,3	0.77	0	2,2,2	0.53	0
14	HEA	N	602	1	44,67,67	1.49	11 (25%)	37,103,103	2.44	15 (40%)
22	CHD	B	301	-	29,32,32	1.83	10 (34%)	48,51,51	2.33	21 (43%)
21	EDO	B	306	-	3,3,3	0.58	0	2,2,2	0.30	0
22	CHD	P	306	-	29,32,32	1.41	4 (13%)	48,51,51	4.24	20 (41%)
20	PGV	P	304	-	50,50,50	1.07	4 (8%)	53,56,56	1.35	6 (11%)
21	EDO	L	101	-	3,3,3	0.74	0	2,2,2	0.84	0
21	EDO	P	312	-	3,3,3	0.77	0	2,2,2	1.65	1 (50%)
23	CUA	O	301	2	0,1,1	0.00	-	-	-	-
20	PGV	N	609	-	50,50,50	1.20	2 (4%)	53,56,56	1.23	6 (11%)
22	CHD	G	102	-	29,32,32	2.04	9 (31%)	48,51,51	2.08	14 (29%)
21	EDO	D	203	-	3,3,3	0.56	0	2,2,2	0.35	0
21	EDO	A	619	-	3,3,3	0.26	0	2,2,2	0.78	0
19	TGL	Y	101	-	62,62,62	1.49	5 (8%)	65,65,65	1.81	10 (15%)
28	PEK	T	101	-	52,52,52	1.37	6 (11%)	55,57,57	2.47	8 (14%)
21	EDO	R	201	-	3,3,3	0.87	0	2,2,2	0.63	0
20	PGV	A	609	-	50,50,50	1.19	5 (10%)	53,56,56	1.30	6 (11%)
23	CUA	B	302	2,30	0,1,1	0.00	-	-	-	-
25	DMU	P	309	-	34,34,34	0.81	1 (2%)	45,45,45	2.15	12 (26%)
28	PEK	G	101	-	52,52,52	1.08	6 (11%)	55,57,57	1.45	8 (14%)
25	DMU	P	307	-	34,34,34	0.94	1 (2%)	45,45,45	1.46	8 (17%)
21	EDO	E	201	-	3,3,3	0.70	0	2,2,2	0.77	0
22	CHD	P	301	-	29,32,32	1.51	7 (24%)	48,51,51	2.20	16 (33%)
21	EDO	B	305	-	3,3,3	1.59	0	2,2,2	0.24	0
14	HEA	A	602[A]	1,18	44,67,67	1.12	3 (6%)	37,103,103	2.27	12 (32%)
21	EDO	N	613	-	3,3,3	1.61	1 (33%)	2,2,2	0.51	0
14	HEA	A	602[B]	1,18	44,67,67	1.19	5 (11%)	37,103,103	2.44	12 (32%)
21	EDO	S	103	-	3,3,3	1.30	0	2,2,2	0.49	0
21	EDO	A	613	-	3,3,3	0.58	0	2,2,2	1.32	0
25	DMU	Z	101	-	34,34,34	0.80	1 (2%)	45,45,45	1.21	3 (6%)
21	EDO	N	620	-	3,3,3	0.57	0	2,2,2	0.05	0
21	EDO	N	621	-	3,3,3	0.79	0	2,2,2	1.29	0
25	DMU	P	310	-	34,34,34	1.11	2 (5%)	45,45,45	1.79	10 (22%)
27	CDL	C	305	-	99,99,99	1.50	17 (17%)	105,111,111	1.53	15 (14%)
20	PGV	C	308	-	50,50,50	1.26	2 (4%)	53,56,56	1.44	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	AZI	N	608[A]	15,14	0,2,2	0.00	-	0,1,1	0.00	-
19	TGL	D	201	-	62,62,62	2.00	5 (8%)	65,65,65	2.58	11 (16%)
21	EDO	G	105	-	3,3,3	0.59	0	2,2,2	0.30	0
21	EDO	A	616	-	3,3,3	3.00	1 (33%)	2,2,2	5.57	1 (50%)
14	HEA	N	603[B]	1,18	44,67,67	1.22	1 (2%)	37,103,103	2.27	11 (29%)
21	EDO	N	619	-	3,3,3	1.21	0	2,2,2	0.19	0
28	PEK	P	308	-	52,52,52	1.24	2 (3%)	55,57,57	1.37	5 (9%)
21	EDO	B	307	-	3,3,3	0.67	0	2,2,2	0.04	0
20	PGV	N	610	-	50,50,50	1.15	6 (12%)	53,56,56	1.48	9 (16%)
21	EDO	N	616	-	3,3,3	1.04	0	2,2,2	0.19	0
21	EDO	N	618	-	3,3,3	0.64	0	2,2,2	0.66	0
28	PEK	C	307	-	52,52,52	1.50	4 (7%)	55,57,57	1.50	9 (16%)
20	PGV	P	302	-	50,50,50	1.16	2 (4%)	53,56,56	1.32	4 (7%)
21	EDO	A	620	-	3,3,3	0.45	0	2,2,2	0.84	0
21	EDO	A	612	-	3,3,3	0.40	0	2,2,2	1.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DMU	C	310	-	-	7/19/59/59	0/2/2/2
21	EDO	Y	102	-	-	1/1/1/1	-
21	EDO	E	202	-	-	1/1/1/1	-
14	HEA	A	601	1	3/3/7/16	2/24/76/76	-
20	PGV	A	610	-	-	28/55/55/55	-
22	CHD	J	101	-	-	3/7/74/74	0/4/4/4
27	CDL	N	601	-	-	59/110/110/110	-
21	EDO	D	202	-	-	1/1/1/1	-
22	CHD	C	306	-	-	3/7/74/74	0/4/4/4
21	EDO	G	104	-	-	0/1/1/1	-
21	EDO	A	617	-	-	0/1/1/1	-
21	EDO	W	102	-	-	0/1/1/1	-
19	TGL	Q	201	-	-	30/65/65/65	-
21	EDO	O	302	-	-	0/1/1/1	-
21	EDO	N	614	-	-	0/1/1/1	-
27	CDL	T	102	-	-	51/110/110/110	-
24	PSC	N	612	-	-	28/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	C	301	-	-	0/7/74/74	0/4/4/4
21	EDO	N	617	-	-	0/1/1/1	-
21	EDO	P	311	-	-	0/1/1/1	-
24	PSC	B	303	-	-	33/55/55/55	-
21	EDO	M	102	-	-	0/1/1/1	-
21	EDO	C	312	-	-	0/1/1/1	-
21	EDO	B	304	-	-	1/1/1/1	-
19	TGL	N	611	-	-	39/65/65/65	-
22	CHD	W	101	-	-	6/7/74/74	0/4/4/4
25	DMU	M	101	-	-	4/19/59/59	0/2/2/2
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
25	DMU	C	311	-	-	8/19/59/59	0/2/2/2
20	PGV	C	304	-	-	17/55/55/55	-
21	EDO	T	103	-	-	0/1/1/1	-
21	EDO	G	105	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
19	TGL	A	611	-	-	39/65/65/65	-
21	EDO	N	615	-	-	0/1/1/1	-
21	EDO	A	618	-	-	1/1/1/1	-
28	PEK	G	103	-	-	31/56/56/56	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	A	615	-	-	1/1/1/1	-
14	HEA	N	603[A]	1,18	3/3/7/16	0/24/76/76	-
27	CDL	P	305	-	-	54/110/110/110	-
25	DMU	C	302	-	-	9/19/59/59	0/2/2/2
19	TGL	A	608	-	-	34/65/65/65	-
21	EDO	E	203	-	-	0/1/1/1	-
14	HEA	N	602	1	3/3/7/16	3/24/76/76	-
22	CHD	B	301	-	-	0/7/74/74	0/4/4/4
21	EDO	B	306	-	-	0/1/1/1	-
22	CHD	P	306	-	-	3/7/74/74	0/4/4/4
20	PGV	P	304	-	-	13/55/55/55	-
21	EDO	L	101	-	-	1/1/1/1	-
21	EDO	P	312	-	-	0/1/1/1	-
20	PGV	N	609	-	-	35/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	G	102	-	-	0/7/74/74	0/4/4/4
21	EDO	D	203	-	-	0/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
19	TGL	Y	101	-	-	34/65/65/65	-
28	PEK	T	101	-	-	23/56/56/56	-
21	EDO	R	201	-	-	0/1/1/1	-
20	PGV	A	609	-	-	8/55/55/55	-
25	DMU	P	309	-	-	7/19/59/59	0/2/2/2
28	PEK	G	101	-	-	19/56/56/56	-
25	DMU	P	307	-	-	5/19/59/59	0/2/2/2
21	EDO	E	201	-	-	0/1/1/1	-
22	CHD	P	301	-	-	1/7/74/74	0/4/4/4
21	EDO	B	305	-	-	1/1/1/1	-
14	HEA	A	602[A]	1,18	2/2/7/16	1/24/76/76	-
21	EDO	N	613	-	-	0/1/1/1	-
14	HEA	A	602[B]	1,18	3/3/7/16	2/24/76/76	-
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	A	613	-	-	1/1/1/1	-
25	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
21	EDO	N	620	-	-	0/1/1/1	-
21	EDO	N	621	-	-	1/1/1/1	-
25	DMU	P	310	-	-	10/19/59/59	0/2/2/2
27	CDL	C	305	-	-	53/110/110/110	-
20	PGV	C	308	-	-	23/55/55/55	-
19	TGL	D	201	-	-	36/65/65/65	-
28	PEK	C	309	-	-	26/56/56/56	-
21	EDO	A	616	-	-	1/1/1/1	-
14	HEA	N	603[B]	1,18	2/2/7/16	3/24/76/76	-
21	EDO	N	619	-	-	0/1/1/1	-
28	PEK	P	308	-	-	25/56/56/56	-
21	EDO	B	307	-	-	0/1/1/1	-
20	PGV	N	610	-	-	11/55/55/55	-
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	N	618	-	-	1/1/1/1	-
28	PEK	C	307	-	-	31/56/56/56	-
20	PGV	P	302	-	-	24/55/55/55	-
21	EDO	A	620	-	-	0/1/1/1	-
21	EDO	A	612	-	-	1/1/1/1	-

All (232) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	10.00	1.52	1.22
19	D	201	TGL	OG2-CB1	7.60	1.55	1.34
19	Y	101	TGL	OG2-CB1	6.73	1.53	1.34
19	Q	201	TGL	OG2-CB1	6.52	1.52	1.34
28	C	307	PEK	O01-C1	6.35	1.52	1.34
19	D	201	TGL	OG1-CA1	6.26	1.51	1.33
19	A	611	TGL	OG2-CB1	6.21	1.51	1.34
19	Y	101	TGL	OG3-CC1	6.00	1.50	1.33
20	N	609	PGV	O03-C19	5.93	1.50	1.33
20	A	610	PGV	O01-C1	5.92	1.51	1.34
28	C	307	PEK	O03-C21	5.87	1.50	1.33
27	N	601	CDL	OB8-CB7	5.79	1.50	1.33
27	N	601	CDL	OB6-CB5	5.76	1.50	1.34
19	Q	201	TGL	OB1-CB1	5.76	1.39	1.22
28	T	101	PEK	C2-C1	5.63	1.67	1.50
27	P	305	CDL	OA8-CA7	5.63	1.49	1.33
27	P	305	CDL	OB8-CB7	5.62	1.49	1.33
24	N	612	PSC	O01-C1	5.52	1.49	1.34
28	P	308	PEK	O01-C1	5.49	1.49	1.34
14	N	603[B]	HEA	C3B-C11	-5.48	1.48	1.52
27	T	102	CDL	OB8-CB7	5.47	1.49	1.33
27	T	102	CDL	OB6-CB5	5.35	1.49	1.34
20	C	308	PGV	O01-C1	5.35	1.49	1.34
20	C	308	PGV	O03-C19	5.18	1.48	1.33
27	C	305	CDL	OA8-CA7	5.17	1.48	1.33
27	T	102	CDL	OA6-CA5	5.12	1.48	1.34
28	C	309	PEK	O01-C1	5.12	1.48	1.34
19	A	608	TGL	OG1-CA1	5.12	1.48	1.33
28	C	309	PEK	O03-C21	5.06	1.48	1.33
21	A	616	EDO	C2-C1	5.02	1.83	1.48
27	N	601	CDL	OA6-CA5	5.00	1.48	1.34
22	G	102	CHD	C8-C7	4.83	1.61	1.53
24	N	612	PSC	O03-C19	4.80	1.47	1.33
27	T	102	CDL	OA8-CA7	4.79	1.47	1.33
27	N	601	CDL	OA8-CA7	4.78	1.47	1.33
28	G	103	PEK	O01-C1	4.78	1.47	1.34
19	N	611	TGL	OG1-CA1	4.75	1.47	1.33
19	Q	201	TGL	OG1-CA1	4.73	1.47	1.33
22	C	301	CHD	C11-C12	4.72	1.61	1.53
20	P	302	PGV	O01-C1	4.71	1.47	1.34
28	P	308	PEK	O03-C21	4.70	1.47	1.33
24	B	303	PSC	O01-C1	4.69	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	302	PGV	O03-C19	4.68	1.47	1.33
19	A	611	TGL	OG3-CC1	4.66	1.47	1.33
20	A	610	PGV	O03-C19	4.65	1.46	1.33
19	Q	201	TGL	OG3-CC1	4.64	1.46	1.33
27	C	305	CDL	PB2-OB3	4.60	1.67	1.50
27	P	305	CDL	OA6-CA5	4.58	1.47	1.34
19	A	608	TGL	OG2-CB1	4.53	1.47	1.34
28	G	103	PEK	O03-C21	4.53	1.46	1.33
24	B	303	PSC	O03-C19	4.49	1.46	1.33
19	A	611	TGL	OG1-CA1	4.45	1.46	1.33
19	Y	101	TGL	OG1-CA1	4.39	1.46	1.33
19	N	611	TGL	OG2-CB1	4.35	1.46	1.34
27	C	305	CDL	OA6-CA5	4.25	1.46	1.34
25	C	311	DMU	O16-C6	4.21	1.47	1.40
20	N	609	PGV	O01-C1	4.15	1.46	1.34
27	C	305	CDL	OB8-CB7	3.97	1.45	1.33
24	B	303	PSC	C13-C12	3.96	1.54	1.31
27	C	305	CDL	OB6-CB5	3.94	1.45	1.34
24	N	612	PSC	C13-C12	3.83	1.54	1.31
19	A	608	TGL	OG3-CC1	3.75	1.44	1.33
22	G	102	CHD	C4-C5	3.75	1.59	1.53
27	P	305	CDL	PB2-OB3	3.74	1.64	1.50
14	N	603[A]	HEA	O11-C11	3.70	1.51	1.42
19	N	611	TGL	OG3-CC1	3.68	1.44	1.33
22	G	102	CHD	C11-C9	3.65	1.59	1.53
19	D	201	TGL	OG3-CC1	3.62	1.43	1.33
25	P	307	DMU	O16-C6	3.57	1.46	1.40
25	P	310	DMU	O16-C6	3.52	1.46	1.40
22	B	301	CHD	O7-C7	3.47	1.50	1.43
27	P	305	CDL	OB6-CB5	3.41	1.43	1.34
22	G	102	CHD	O7-C7	3.33	1.50	1.43
22	P	306	CHD	C11-C9	3.30	1.59	1.53
22	G	102	CHD	C1-C2	3.29	1.60	1.53
28	T	101	PEK	P-O14	3.29	1.62	1.50
19	A	608	TGL	OG2-CG2	3.23	1.54	1.46
28	G	101	PEK	O01-C02	3.19	1.54	1.46
22	G	102	CHD	C19-C10	3.18	1.59	1.54
22	P	301	CHD	C11-C12	3.17	1.58	1.53
27	N	601	CDL	C59-C58	-3.17	1.33	1.51
27	N	601	CDL	C22-C21	-3.16	1.33	1.51
27	C	305	CDL	C79-C78	-3.16	1.33	1.51
20	N	610	PGV	C01-C02	3.13	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	301	CHD	C8-C7	3.12	1.58	1.53
27	T	102	CDL	C59-C58	-3.11	1.34	1.51
25	C	310	DMU	O16-C6	3.09	1.45	1.40
20	P	304	PGV	O05-C05	3.08	1.52	1.43
27	C	305	CDL	C59-C58	-3.07	1.34	1.51
14	N	602	HEA	CMB-C2B	3.07	1.58	1.51
27	C	305	CDL	O1-C1	3.04	1.52	1.43
22	P	301	CHD	C11-C9	3.04	1.58	1.53
20	A	609	PGV	C01-C02	3.04	1.60	1.50
27	P	305	CDL	C19-C18	-3.02	1.34	1.51
22	C	301	CHD	C11-C9	3.01	1.58	1.53
20	N	610	PGV	O01-C1	3.01	1.42	1.34
22	B	301	CHD	C19-C10	2.99	1.59	1.54
22	B	301	CHD	C10-C9	-2.99	1.50	1.56
27	C	305	CDL	C82-C81	-2.98	1.34	1.51
27	T	102	CDL	C79-C78	-2.98	1.34	1.51
20	A	610	PGV	O02-C1	2.97	1.31	1.22
25	M	101	DMU	O16-C6	2.97	1.45	1.40
27	C	305	CDL	C62-C61	-2.97	1.34	1.51
14	A	601	HEA	C3B-C2B	-2.97	1.31	1.41
27	N	601	CDL	C82-C81	-2.96	1.35	1.51
22	P	306	CHD	C16-C17	2.94	1.60	1.54
27	P	305	CDL	C62-C61	-2.94	1.35	1.51
20	N	610	PGV	O03-C01	2.93	1.51	1.45
14	A	601	HEA	C12-C13	2.92	1.63	1.53
27	P	305	CDL	C42-C41	-2.91	1.35	1.51
27	P	305	CDL	C22-C21	-2.91	1.35	1.51
27	T	102	CDL	C22-C21	-2.89	1.35	1.51
27	N	601	CDL	C79-C78	-2.89	1.35	1.51
27	N	601	CDL	C19-C18	-2.89	1.35	1.51
19	A	608	TGL	OC1-CC1	-2.88	1.14	1.22
28	T	101	PEK	C3-C2	2.87	1.62	1.52
28	G	101	PEK	P-O14	2.86	1.61	1.50
27	N	601	CDL	C62-C61	-2.86	1.35	1.51
28	T	101	PEK	O11-C03	2.85	1.55	1.44
14	A	601	HEA	CAD-C3D	2.85	1.56	1.52
27	C	305	CDL	C22-C21	-2.83	1.35	1.51
20	P	304	PGV	C01-C02	2.83	1.59	1.50
22	C	301	CHD	C8-C7	2.83	1.58	1.53
27	P	305	CDL	C59-C58	-2.82	1.35	1.51
27	N	601	CDL	C42-C41	-2.79	1.35	1.51
20	A	609	PGV	O01-C1	2.78	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	305	CDL	C19-C18	-2.77	1.36	1.51
22	C	301	CHD	C2-C3	2.77	1.58	1.51
25	P	310	DMU	C10-C5	2.77	1.60	1.52
27	T	102	CDL	C62-C61	-2.76	1.36	1.51
25	Z	101	DMU	O16-C6	2.75	1.44	1.40
22	C	301	CHD	C4-C3	2.75	1.57	1.51
27	T	102	CDL	C39-C38	-2.73	1.36	1.51
22	C	306	CHD	C16-C17	2.73	1.60	1.54
27	N	601	CDL	C39-C38	-2.73	1.36	1.51
27	P	305	CDL	C39-C38	-2.72	1.36	1.51
22	P	301	CHD	C6-C7	2.69	1.57	1.52
20	P	304	PGV	O01-C02	-2.68	1.39	1.46
22	P	301	CHD	C16-C17	2.67	1.59	1.54
27	P	305	CDL	C79-C78	-2.65	1.36	1.51
14	N	602	HEA	C3A-CMA	2.64	1.52	1.46
20	C	304	PGV	O01-C02	-2.63	1.40	1.46
28	G	101	PEK	O01-C1	2.63	1.41	1.34
27	C	305	CDL	C42-C41	-2.63	1.36	1.51
27	T	102	CDL	C42-C41	-2.61	1.36	1.51
19	Y	101	TGL	CG3-CG2	2.57	1.58	1.50
19	Y	101	TGL	CB2-CB1	2.57	1.58	1.50
20	C	304	PGV	O05-C05	2.56	1.51	1.43
14	A	602[B]	HEA	C3A-C2A	-2.55	1.36	1.40
27	T	102	CDL	C19-C18	-2.55	1.37	1.51
28	C	307	PEK	O02-C1	2.53	1.30	1.22
14	A	602[B]	HEA	C18-C19	2.53	1.39	1.33
27	P	305	CDL	C82-C81	-2.52	1.37	1.51
20	P	304	PGV	O03-C19	2.52	1.40	1.33
27	C	305	CDL	C39-C38	-2.51	1.37	1.51
20	A	609	PGV	C3-C2	2.50	1.61	1.52
14	A	601	HEA	C3C-CAC	2.50	1.53	1.47
27	C	305	CDL	CB2-C1	2.49	1.60	1.51
22	B	301	CHD	C18-C13	2.49	1.58	1.54
21	N	613	EDO	O2-C2	2.49	1.54	1.42
22	B	301	CHD	C20-C17	2.47	1.58	1.54
28	T	101	PEK	C3-C4	2.47	1.62	1.52
28	T	101	PEK	O03-C21	2.43	1.40	1.33
27	T	102	CDL	C82-C81	-2.42	1.38	1.51
14	N	602	HEA	C12-C13	2.40	1.61	1.53
27	P	305	CDL	PA1-OA5	2.40	1.69	1.59
21	A	614	EDO	O2-C2	2.40	1.54	1.42
22	C	306	CHD	C20-C17	2.40	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	608	TGL	CG3-CG2	2.39	1.58	1.50
27	C	305	CDL	PB2-OB2	2.39	1.69	1.59
14	N	602	HEA	C3B-C11	-2.39	1.51	1.52
22	C	306	CHD	C4-C3	2.33	1.56	1.51
20	A	610	PGV	P-O11	2.33	1.68	1.59
14	A	601	HEA	C3A-C2A	-2.32	1.37	1.40
22	W	101	CHD	C8-C14	2.32	1.58	1.53
22	P	301	CHD	C8-C7	2.30	1.57	1.53
24	B	303	PSC	C3-C2	2.30	1.60	1.52
14	N	602	HEA	O11-C11	2.30	1.48	1.42
22	W	101	CHD	C13-C17	2.29	1.59	1.55
20	A	610	PGV	C2-C1	-2.29	1.44	1.50
27	P	305	CDL	CB2-C1	2.29	1.59	1.51
20	N	610	PGV	C3-C2	2.28	1.60	1.52
27	P	305	CDL	O1-C1	2.27	1.50	1.43
14	N	602	HEA	CAA-C2A	-2.27	1.48	1.52
27	N	601	CDL	CB3-CB4	2.27	1.57	1.50
14	N	602	HEA	C22-C23	2.26	1.38	1.32
22	P	306	CHD	C4-C5	2.26	1.57	1.53
22	B	301	CHD	C13-C17	-2.25	1.51	1.55
20	N	610	PGV	C06-C05	2.25	1.61	1.51
19	D	201	TGL	OC1-CC1	2.25	1.29	1.22
28	G	101	PEK	O11-C03	2.23	1.53	1.44
22	W	101	CHD	C20-C17	2.22	1.58	1.54
20	A	609	PGV	O03-C19	2.22	1.39	1.33
28	C	307	PEK	C2-C1	2.21	1.57	1.50
14	N	603[A]	HEA	C3C-C2C	-2.21	1.37	1.40
27	P	305	CDL	PB2-OB2	2.21	1.68	1.59
27	C	305	CDL	PA1-OA5	2.20	1.68	1.59
14	A	602[A]	HEA	C3A-C2A	-2.19	1.37	1.40
27	N	601	CDL	CB6-CB4	2.18	1.57	1.50
27	P	305	CDL	OB8-CB6	2.17	1.50	1.45
22	B	301	CHD	C21-C20	2.16	1.58	1.53
22	P	301	CHD	C1-C10	-2.14	1.50	1.54
28	G	101	PEK	C05-C04	2.13	1.58	1.50
14	N	602	HEA	C27-C19	2.13	1.56	1.50
19	N	611	TGL	OC1-CC1	-2.12	1.16	1.22
14	A	602[A]	HEA	C18-C19	2.12	1.38	1.33
27	T	102	CDL	CB6-CB4	2.11	1.57	1.50
22	W	101	CHD	C8-C7	2.11	1.57	1.53
20	C	304	PGV	O03-C19	2.10	1.39	1.33
14	A	602[B]	HEA	C4B-C3B	-2.10	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	102	CHD	C20-C17	2.08	1.58	1.54
14	A	601	HEA	C16-C17	-2.08	1.46	1.53
14	A	602[B]	HEA	CMC-C2C	2.07	1.55	1.51
14	N	602	HEA	CMD-C2D	2.07	1.56	1.51
22	G	102	CHD	O3-C3	2.06	1.49	1.43
22	B	301	CHD	C16-C15	2.06	1.59	1.54
14	A	602[A]	HEA	C1C-CHC	2.06	1.46	1.41
20	N	610	PGV	O03-C19	2.05	1.39	1.33
25	C	302	DMU	O16-C6	2.04	1.43	1.40
14	N	603[A]	HEA	CAA-C2A	2.04	1.55	1.52
22	B	301	CHD	C16-C17	2.04	1.58	1.54
14	N	602	HEA	C3B-C2B	-2.03	1.34	1.41
22	G	102	CHD	C16-C17	2.02	1.58	1.54
14	N	603[A]	HEA	C4C-NC	-2.02	1.32	1.36
25	P	309	DMU	O16-C6	2.02	1.43	1.40
20	A	609	PGV	O03-C01	2.02	1.49	1.45
22	P	306	CHD	O12-C12	2.02	1.47	1.43
14	N	602	HEA	C16-C17	-2.01	1.46	1.53
27	N	601	CDL	C71-CB7	2.01	1.56	1.50
28	G	101	PEK	P-O13	-2.01	1.45	1.55
22	P	301	CHD	C16-C15	2.00	1.59	1.54
14	A	602[B]	HEA	C14-C15	2.00	1.37	1.33

All (531) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	306	CHD	C23-C22-C20	-24.48	81.74	114.72
22	P	306	CHD	C23-C22-C20	-24.31	81.97	114.72
28	T	101	PEK	C2-C3-C4	15.35	140.59	113.23
19	D	201	TGL	OG2-CB1-CB2	-12.32	84.94	111.50
25	C	311	DMU	O16-C6-C1	11.07	125.59	108.30
19	D	201	TGL	OG2-CB1-OB1	10.53	149.14	123.70
20	A	610	PGV	C02-O01-C1	9.46	141.09	117.79
19	A	608	TGL	OG2-CB1-CB2	8.87	130.61	111.50
19	A	608	TGL	OG3-CC1-OC1	-8.38	102.44	123.59
25	C	310	DMU	C10-O1-C9	-8.02	97.95	113.69
22	W	101	CHD	C13-C17-C20	7.93	128.96	119.50
21	A	616	EDO	O1-C1-C2	-7.88	55.25	111.91
19	Y	101	TGL	OG2-CB1-CB2	7.70	128.10	111.50
22	C	301	CHD	C23-C22-C20	-6.98	105.32	114.72
24	B	303	PSC	O01-C1-C2	6.79	126.14	111.50
19	D	201	TGL	CB3-CB2-CB1	6.72	138.04	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	309	PEK	O01-C1-C2	6.71	125.96	111.50
25	C	310	DMU	C10-C5-C7	-6.70	96.03	110.00
28	P	308	PEK	O01-C1-C2	6.67	125.88	111.50
25	C	310	DMU	O7-C10-C5	6.52	125.00	108.10
14	A	602[A]	HEA	OMA-CMA-C3A	-6.45	110.85	124.91
19	Q	201	TGL	OG2-CB1-CB2	-6.36	97.79	111.50
22	P	301	CHD	C23-C22-C20	-6.35	106.17	114.72
14	N	603[A]	HEA	CAD-CBD-CGD	-6.29	102.11	112.67
27	C	305	CDL	OA2-PA1-OA3	6.28	133.60	109.07
19	N	611	TGL	OG2-CB1-CB2	6.28	125.03	111.50
22	C	306	CHD	C21-C20-C17	6.25	122.49	112.92
19	A	608	TGL	OG2-CG2-CG3	6.15	130.68	108.40
14	N	603[B]	HEA	C27-C19-C20	6.08	125.50	115.27
14	N	603[B]	HEA	C13-C12-C11	-6.07	105.24	114.35
20	P	302	PGV	O03-C19-C20	5.96	130.61	111.91
14	A	602[B]	HEA	C13-C12-C11	-5.93	105.45	114.35
28	G	103	PEK	O01-C1-C2	5.89	124.20	111.50
22	P	301	CHD	C6-C7-C8	-5.88	105.20	111.48
19	A	611	TGL	CC4-CC3-CC2	-5.87	92.07	113.19
14	N	603[A]	HEA	C26-C15-C16	5.85	125.11	115.27
14	A	601	HEA	C3C-C4C-NC	5.81	116.72	109.21
14	N	602	HEA	OMA-CMA-C3A	-5.75	112.38	124.91
25	P	309	DMU	O16-C6-C1	5.72	117.24	108.30
14	A	602[B]	HEA	CAA-CBA-CGA	-5.68	103.15	112.67
25	P	309	DMU	O7-C10-C5	5.65	122.75	108.10
14	A	601	HEA	C13-C12-C11	-5.58	105.97	114.35
25	C	310	DMU	O16-C6-C1	5.58	117.01	108.30
22	J	101	CHD	C17-C13-C14	-5.55	94.50	100.09
27	N	601	CDL	OB6-CB5-C51	5.54	123.45	111.50
19	A	611	TGL	OG2-CB1-CB2	5.52	123.40	111.50
22	W	101	CHD	C1-C10-C5	5.50	115.91	107.77
27	P	305	CDL	OA6-CA5-C11	5.50	123.36	111.50
22	C	301	CHD	C6-C7-C8	-5.42	105.69	111.48
20	A	610	PGV	O01-C1-O02	5.41	136.78	123.70
22	J	101	CHD	C13-C17-C20	5.40	125.94	119.50
14	A	601	HEA	CAD-CBD-CGD	-5.37	103.66	112.67
28	C	307	PEK	O01-C1-C2	5.34	123.00	111.50
14	A	602[B]	HEA	C27-C19-C20	5.33	124.23	115.27
19	N	611	TGL	CG3-CG2-CG1	-5.32	99.21	111.79
22	G	102	CHD	C19-C10-C1	-5.30	99.71	108.26
22	P	301	CHD	C22-C20-C17	-5.20	99.54	110.28
25	P	310	DMU	O7-C10-C5	5.19	121.56	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	309	DMU	C10-O1-C9	-5.11	103.65	113.69
24	N	612	PSC	O01-C1-C2	5.11	122.51	111.50
22	B	301	CHD	C11-C9-C10	-5.08	108.49	113.73
19	Q	201	TGL	OG2-CB1-OB1	5.06	135.94	123.70
14	N	603[B]	HEA	C3C-C4C-NC	5.04	115.72	109.21
19	N	611	TGL	OG3-CC1-OC1	-5.03	110.89	123.59
22	P	306	CHD	C15-C14-C13	5.03	108.49	103.55
27	C	305	CDL	OA6-CA5-C11	5.01	122.30	111.50
27	N	601	CDL	CB2-C1-CA2	-5.00	98.08	112.79
22	P	301	CHD	C21-C20-C22	-4.91	102.67	110.36
22	W	101	CHD	C13-C14-C8	4.91	121.00	114.74
14	N	602	HEA	CMB-C2B-C1B	-4.90	120.93	128.46
22	C	301	CHD	C22-C23-C24	-4.86	103.14	113.59
14	N	602	HEA	C3C-C4C-NC	4.84	115.47	109.21
19	A	611	TGL	OG3-CC1-CC2	4.84	127.10	111.91
22	P	306	CHD	C13-C17-C20	-4.84	113.72	119.50
19	A	608	TGL	CG3-CG2-CG1	-4.79	100.47	111.79
20	N	610	PGV	O01-C1-O02	-4.78	112.15	123.70
22	B	301	CHD	C13-C17-C20	-4.74	113.83	119.50
19	Y	101	TGL	OG2-CB1-OB1	-4.73	112.26	123.70
19	A	608	TGL	OG3-CC1-CC2	4.73	126.75	111.91
22	B	301	CHD	C19-C10-C1	-4.69	100.70	108.26
22	G	102	CHD	C23-C22-C20	-4.65	108.46	114.72
22	B	301	CHD	C23-C22-C20	-4.64	108.47	114.72
14	A	601	HEA	C13-C14-C15	-4.57	116.66	127.66
25	P	310	DMU	O3-C5-C10	4.56	121.12	110.05
22	P	306	CHD	C5-C4-C3	-4.54	106.09	112.76
19	N	611	TGL	OG1-CA1-CA2	4.53	126.12	111.91
25	P	309	DMU	O49-C1-C2	-4.52	99.90	110.35
19	Y	101	TGL	CG2-OG2-CB1	4.51	128.90	117.79
27	N	601	CDL	CB4-OB6-CB5	4.49	128.85	117.79
14	N	602	HEA	CMB-C2B-C3B	4.47	133.44	124.69
28	G	101	PEK	C24-C23-C22	-4.45	97.20	113.19
14	N	602	HEA	C20-C21-C22	-4.44	97.28	111.88
22	J	101	CHD	C1-C10-C5	4.44	114.34	107.77
20	C	308	PGV	O01-C1-C2	4.44	121.06	111.50
22	C	301	CHD	C5-C6-C7	4.41	119.32	114.46
28	C	307	PEK	O03-C21-C22	4.40	125.71	111.91
22	C	306	CHD	C1-C10-C5	4.38	114.24	107.77
19	A	608	TGL	CG3-OG3-CC1	4.37	133.32	117.12
19	D	201	TGL	OG1-CA1-CA2	4.37	125.63	111.91
22	W	101	CHD	C18-C13-C14	-4.37	104.37	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	306	CHD	C19-C10-C9	-4.36	105.18	111.18
27	P	305	CDL	OB8-CB7-C71	4.35	125.57	111.91
14	N	602	HEA	C13-C14-C15	-4.34	117.21	127.66
22	C	301	CHD	C11-C9-C10	-4.33	109.26	113.73
19	N	611	TGL	OG3-CC1-CC2	4.28	125.35	111.91
22	G	102	CHD	C6-C5-C10	4.28	117.20	112.66
22	G	102	CHD	C6-C5-C4	-4.28	106.27	111.19
27	N	601	CDL	CB6-OB8-CB7	4.27	132.95	117.12
22	P	306	CHD	C16-C17-C20	4.26	118.74	112.15
19	D	201	TGL	CG1-OG1-CA1	4.24	132.82	117.12
22	W	101	CHD	C11-C12-C13	4.22	115.58	111.24
14	A	602[A]	HEA	C1B-C2B-C3B	-4.21	104.07	107.00
14	A	602[A]	HEA	C26-C15-C16	4.21	122.35	115.27
22	J	101	CHD	C18-C13-C17	4.20	117.79	111.21
27	T	102	CDL	OA6-CA5-C11	4.20	120.56	111.50
19	Q	201	TGL	OG3-CC1-CC2	4.19	125.07	111.91
22	P	306	CHD	C21-C20-C17	4.17	119.30	112.92
14	A	602[B]	HEA	CAD-CBD-CGD	-4.17	105.68	112.67
14	A	601	HEA	CMB-C2B-C1B	-4.14	122.10	128.46
22	C	301	CHD	C1-C2-C3	-4.13	105.17	110.47
22	P	306	CHD	C16-C17-C13	4.11	107.58	103.55
25	P	309	DMU	C18-O16-C6	-4.08	107.07	113.84
14	A	602[A]	HEA	CAD-CBD-CGD	-4.08	105.83	112.67
24	B	303	PSC	O01-C1-O02	-4.07	113.86	123.70
25	C	311	DMU	C18-O16-C6	4.06	120.58	113.84
20	C	308	PGV	O03-C19-C20	4.05	124.62	111.91
14	A	601	HEA	CMB-C2B-C3B	4.05	132.62	124.69
14	A	601	HEA	C27-C19-C20	-4.03	108.48	115.27
28	T	101	PEK	O03-C21-C22	4.03	124.56	111.91
19	D	201	TGL	CG3-OG3-CC1	4.03	132.04	117.12
22	C	306	CHD	C6-C7-C8	4.01	115.76	111.48
22	C	301	CHD	C9-C11-C12	-4.00	109.01	114.30
14	N	603[A]	HEA	CMC-C2C-C3C	3.99	132.15	124.68
27	N	601	CDL	OA6-CA5-C11	3.99	120.10	111.50
14	N	603[B]	HEA	CAA-CBA-CGA	-3.97	106.01	112.67
27	T	102	CDL	OB6-CB5-C51	3.96	120.03	111.50
14	N	603[B]	HEA	C20-C19-C18	-3.95	113.12	121.12
14	A	602[B]	HEA	C20-C19-C18	-3.95	113.12	121.12
27	C	305	CDL	OA5-PA1-OA3	-3.95	93.65	109.07
22	W	101	CHD	C6-C7-C8	3.93	115.67	111.48
25	C	302	DMU	C18-O16-C6	-3.92	107.34	113.84
19	A	608	TGL	OG2-CB1-OB1	-3.89	114.29	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	301	CHD	C9-C8-C7	-3.89	107.23	111.88
19	Y	101	TGL	OG3-CG3-CG2	3.88	119.74	108.43
19	Y	101	TGL	OG3-CC1-CC2	3.88	124.08	111.91
20	N	610	PGV	O03-C19-O04	-3.88	113.81	123.59
22	P	306	CHD	C14-C13-C12	3.87	111.00	107.40
25	P	310	DMU	C1-C2-C3	3.86	118.50	109.68
22	W	101	CHD	C6-C5-C10	3.80	116.70	112.66
20	P	304	PGV	O01-C1-O02	-3.80	114.51	123.70
19	A	611	TGL	OG3-CC1-OC1	-3.77	114.07	123.59
22	B	301	CHD	O12-C12-C13	-3.77	104.66	111.03
22	J	101	CHD	C6-C5-C10	3.76	116.65	112.66
14	A	602[A]	HEA	C20-C19-C18	-3.74	113.54	121.12
28	T	101	PEK	O01-C1-O02	-3.73	114.68	123.70
14	A	601	HEA	C20-C19-C18	3.71	128.62	121.12
14	A	602[A]	HEA	C27-C19-C20	3.70	121.49	115.27
22	B	301	CHD	C18-C13-C12	-3.69	105.31	109.07
28	G	103	PEK	O01-C1-O02	-3.68	114.81	123.70
22	J	101	CHD	C16-C17-C13	3.68	107.16	103.55
22	C	306	CHD	C16-C17-C20	3.66	117.81	112.15
25	P	310	DMU	O16-C6-C1	3.63	113.97	108.30
22	J	101	CHD	C6-C5-C4	-3.63	107.02	111.19
22	C	301	CHD	C18-C13-C12	3.62	112.76	109.07
19	Q	201	TGL	OG1-CA1-CA2	3.61	123.25	111.91
14	A	602[A]	HEA	C13-C14-C15	-3.61	118.97	127.66
22	W	101	CHD	C17-C13-C12	3.59	120.94	117.67
14	A	602[B]	HEA	CMD-C2D-C3D	3.58	131.69	124.94
20	P	304	PGV	C03-C02-C01	-3.58	103.32	111.79
22	G	102	CHD	C2-C1-C10	-3.57	106.66	112.78
25	M	101	DMU	O49-C1-C6	-3.56	101.39	110.05
22	B	301	CHD	C19-C10-C9	3.56	116.09	111.18
25	C	310	DMU	C7-C8-C9	3.55	116.57	110.24
25	M	101	DMU	C18-O16-C6	-3.54	107.97	113.84
22	J	101	CHD	C1-C10-C9	-3.53	105.80	111.35
27	P	305	CDL	CB6-CB4-CB3	-3.53	103.44	111.79
14	A	601	HEA	CBD-CAD-C3D	-3.53	105.98	112.49
22	G	102	CHD	C9-C8-C7	-3.51	107.67	111.88
25	M	101	DMU	C22-C19-C18	-3.50	97.96	113.49
25	C	302	DMU	C25-C22-C19	-3.49	96.69	114.42
22	P	306	CHD	O3-C3-C4	-3.49	102.89	109.85
20	P	302	PGV	O01-C1-C2	3.48	119.00	111.50
14	A	602[B]	HEA	C12-C13-C14	-3.47	103.08	112.23
20	A	610	PGV	C4-C3-C2	-3.47	100.73	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	306	CHD	C4-C5-C10	3.46	116.33	112.66
22	C	301	CHD	C17-C13-C14	-3.46	96.61	100.09
27	P	305	CDL	OB8-CB7-OB9	-3.45	114.88	123.59
14	A	602[B]	HEA	C4B-C3B-C2B	-3.44	104.47	106.87
14	N	603[A]	HEA	CAA-CBA-CGA	-3.41	106.95	112.67
22	W	101	CHD	C10-C9-C8	3.41	115.48	111.82
22	P	301	CHD	C18-C13-C12	3.40	112.52	109.07
28	G	101	PEK	C02-O01-C1	-3.39	109.43	117.79
20	N	609	PGV	C3-C2-C1	-3.39	101.28	113.62
22	C	306	CHD	C5-C4-C3	-3.39	107.79	112.76
20	C	304	PGV	C30-C29-C28	-3.38	97.25	114.42
19	D	201	TGL	OG3-CC1-OC1	-3.37	115.09	123.59
22	C	301	CHD	C22-C20-C17	-3.36	103.34	110.28
25	C	302	DMU	C10-O7-C3	-3.35	109.67	117.96
27	P	305	CDL	OA8-CA7-C31	3.34	122.39	111.91
28	T	101	PEK	O02-C1-C2	3.34	136.75	123.73
27	P	305	CDL	C56-C55-C54	3.33	131.34	114.42
19	A	611	TGL	CG2-OG2-CB1	3.33	125.98	117.79
25	P	309	DMU	C10-C5-C7	-3.32	103.08	110.00
22	G	102	CHD	C1-C2-C3	-3.32	106.21	110.47
20	N	610	PGV	O02-C1-C2	3.31	136.66	123.73
22	W	101	CHD	C4-C5-C10	3.31	116.17	112.66
19	Q	201	TGL	OG3-CC1-OC1	-3.31	115.24	123.59
20	P	302	PGV	O04-C19-C20	-3.31	110.83	123.73
19	A	611	TGL	OG1-CA1-CA2	3.30	122.28	111.91
14	A	602[B]	HEA	CBA-CAA-C2A	-3.29	106.41	112.48
27	P	305	CDL	OA6-CA5-OA7	-3.29	115.74	123.70
20	A	610	PGV	O02-C1-C2	-3.29	110.90	123.73
28	G	101	PEK	O01-C1-O02	3.28	131.63	123.70
20	C	308	PGV	O03-C01-C02	3.28	117.98	108.43
25	P	309	DMU	C8-C7-C5	-3.27	105.11	110.82
22	J	101	CHD	C16-C17-C20	3.26	117.20	112.15
20	N	609	PGV	O03-C19-C20	3.25	122.11	111.91
22	B	301	CHD	C17-C13-C12	3.25	120.63	117.67
22	P	306	CHD	C1-C10-C9	3.25	116.46	111.35
20	C	308	PGV	O03-C19-O04	-3.25	115.40	123.59
27	P	305	CDL	C83-C82-C81	3.24	130.88	114.42
28	C	309	PEK	C2-C3-C4	3.24	119.00	113.23
14	N	603[A]	HEA	C4B-C3B-C2B	-3.24	104.60	106.87
22	C	301	CHD	C15-C14-C8	-3.23	113.81	118.33
22	C	306	CHD	C15-C14-C13	3.23	106.72	103.55
22	B	301	CHD	C2-C1-C10	-3.22	107.26	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	611	TGL	C26-C25-C24	-3.22	98.10	114.42
20	N	609	PGV	O01-C02-C01	3.22	120.04	108.40
25	C	311	DMU	O1-C9-C11	3.21	114.42	106.44
25	P	307	DMU	O16-C18-C19	3.21	120.81	109.56
28	P	308	PEK	O03-C21-O04	-3.20	115.52	123.59
22	J	101	CHD	C4-C5-C10	3.20	116.05	112.66
20	A	609	PGV	O03-C19-O04	-3.20	115.52	123.59
25	C	311	DMU	O16-C18-C19	3.20	120.76	109.56
22	B	301	CHD	C16-C17-C20	-3.18	107.22	112.15
27	T	102	CDL	CB6-OB8-CB7	3.17	128.86	117.12
14	A	601	HEA	CAA-CBA-CGA	-3.17	107.35	112.67
22	G	102	CHD	C11-C12-C13	3.16	114.49	111.24
25	C	311	DMU	O5-C4-C57	3.15	114.27	106.44
27	C	305	CDL	OB2-PB2-OB3	3.15	121.36	109.07
28	C	307	PEK	O03-C21-O04	-3.14	115.68	123.59
20	C	304	PGV	C22-C21-C20	-3.13	101.93	113.19
14	N	602	HEA	C25-C23-C24	-3.13	107.70	114.60
22	P	306	CHD	C6-C7-C8	3.12	114.81	111.48
25	C	311	DMU	C6-C1-C2	3.11	116.48	110.00
25	C	311	DMU	O5-C4-C3	-3.11	103.19	109.75
20	N	610	PGV	O03-C19-C20	3.11	121.67	111.91
22	C	306	CHD	C4-C5-C10	3.10	115.95	112.66
22	W	101	CHD	C23-C22-C20	3.09	118.89	114.72
27	C	305	CDL	CB6-CB4-CB3	-3.09	104.48	111.79
19	A	608	TGL	OG1-CA1-CA2	3.08	121.58	111.91
20	A	610	PGV	O03-C19-C20	3.08	121.57	111.91
14	N	603[A]	HEA	CMC-C2C-C1C	-3.08	123.74	128.46
22	C	301	CHD	C5-C4-C3	-3.07	108.25	112.76
22	W	101	CHD	C19-C10-C5	-3.07	105.15	110.36
19	A	611	TGL	CA4-CA3-CA2	-3.07	102.17	113.19
20	C	308	PGV	C03-C02-C01	-3.06	104.54	111.79
19	Q	201	TGL	OG1-CA1-OA1	-3.06	115.86	123.59
19	N	611	TGL	OG1-CA1-OA1	-3.06	115.86	123.59
25	P	307	DMU	O55-C2-C3	3.06	118.05	109.94
14	N	603[B]	HEA	CBA-CAA-C2A	-3.05	106.86	112.48
19	A	608	TGL	CC3-CC2-CC1	3.05	124.72	113.62
22	J	101	CHD	C21-C20-C17	-3.05	108.25	112.92
22	C	301	CHD	C16-C15-C14	-3.05	99.09	105.13
28	G	101	PEK	O03-C21-O04	-3.05	115.91	123.59
22	C	306	CHD	C19-C10-C5	-3.05	105.20	110.36
20	A	609	PGV	O01-C1-O02	-3.04	116.34	123.70
25	P	310	DMU	O1-C9-C11	3.03	113.97	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	101	CHD	C6-C5-C4	-3.03	107.70	111.19
25	C	310	DMU	O7-C10-O1	3.02	119.11	110.67
22	P	306	CHD	C18-C13-C12	-3.01	106.00	109.07
27	P	305	CDL	OA2-PA1-OA3	2.99	120.74	109.07
28	T	101	PEK	O11-P-O14	-2.99	97.40	109.07
20	P	302	PGV	C21-C20-C19	-2.99	102.76	113.62
22	W	101	CHD	C14-C8-C7	2.98	115.75	111.81
24	B	303	PSC	O01-C02-C03	2.97	119.17	108.40
28	G	101	PEK	O11-P-O14	-2.96	97.49	109.07
27	P	305	CDL	C53-C52-C51	2.96	123.83	113.19
22	P	301	CHD	C17-C13-C12	-2.96	114.97	117.67
19	Y	101	TGL	CG3-OG3-CC1	2.94	128.02	117.12
27	C	305	CDL	OA6-CA5-OA7	-2.94	116.61	123.70
28	C	307	PEK	C02-O01-C1	2.93	125.01	117.79
22	P	301	CHD	C5-C4-C3	-2.92	108.46	112.76
14	A	601	HEA	C1B-C2B-C3B	-2.92	104.96	107.00
27	C	305	CDL	C39-C38-C37	2.92	129.26	114.42
25	C	310	DMU	O2-C8-C7	2.92	117.10	110.35
19	Y	101	TGL	CB4-CB3-CB2	2.91	123.67	113.19
19	A	611	TGL	C25-C24-C23	-2.90	99.71	114.42
27	T	102	CDL	OB8-CB6-CB4	2.89	116.84	108.43
27	N	601	CDL	OA8-CA7-C31	2.89	120.97	111.91
22	W	101	CHD	C9-C11-C12	2.88	118.11	114.30
25	P	307	DMU	C2-C3-C4	-2.88	104.32	110.93
14	N	602	HEA	C27-C19-C18	-2.86	116.33	123.68
27	P	305	CDL	PA1-OA2-CA2	2.86	138.46	121.68
20	P	304	PGV	C27-C26-C25	-2.86	99.90	114.42
25	P	309	DMU	O7-C3-C4	-2.85	101.64	109.45
14	A	601	HEA	C16-C17-C18	-2.85	102.52	111.88
28	P	308	PEK	O01-C1-O02	-2.85	116.82	123.70
22	G	102	CHD	C1-C10-C9	2.85	115.83	111.35
22	J	101	CHD	C22-C20-C17	2.84	116.15	110.28
20	C	308	PGV	O01-C02-C01	2.83	118.66	108.40
22	J	101	CHD	C10-C9-C8	2.81	114.84	111.82
14	N	603[B]	HEA	OMA-CMA-C3A	-2.81	118.79	124.91
25	P	309	DMU	O4-C7-C8	2.81	116.83	110.35
27	T	102	CDL	C83-C82-C81	2.80	128.66	114.42
27	C	305	CDL	PA1-OA2-CA2	2.80	138.10	121.68
14	N	602	HEA	CMD-C2D-C3D	2.80	130.22	124.94
22	G	102	CHD	C4-C5-C10	-2.79	109.69	112.66
14	N	603[A]	HEA	C12-C11-C3B	2.78	119.85	112.56
28	C	307	PEK	C36-C35-C34	-2.78	100.33	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	310	DMU	O55-C2-C1	2.77	116.75	110.35
20	N	609	PGV	C01-O03-C19	2.76	127.35	117.12
14	A	601	HEA	C21-C20-C19	2.76	122.06	112.98
22	C	306	CHD	C16-C17-C13	2.76	106.26	103.55
20	A	609	PGV	O03-C19-C20	2.76	120.56	111.91
27	T	102	CDL	OB8-CB7-C71	2.75	120.54	111.91
25	P	309	DMU	O5-C6-O16	-2.74	103.48	109.97
14	A	602[B]	HEA	OMA-CMA-C3A	-2.73	118.97	124.91
25	Z	101	DMU	C10-O7-C3	-2.72	111.22	117.96
27	C	305	CDL	O1-C1-CB2	2.72	119.10	109.56
24	B	303	PSC	O03-C19-C20	2.72	120.44	111.91
28	C	309	PEK	O03-C21-C22	2.71	120.41	111.91
14	N	603[B]	HEA	C1B-C2B-C3B	-2.70	105.12	107.00
22	P	301	CHD	C22-C23-C24	-2.68	107.83	113.59
20	A	610	PGV	C3-C2-C1	2.67	123.35	113.62
22	B	301	CHD	C16-C17-C13	2.67	106.17	103.55
14	A	601	HEA	CMD-C2D-C3D	2.67	129.97	124.94
25	C	302	DMU	C6-C1-C2	-2.66	104.46	110.00
25	C	311	DMU	O49-C1-C2	-2.66	104.20	110.35
25	M	101	DMU	C31-C28-C25	-2.65	100.95	114.42
22	P	306	CHD	C11-C12-C13	-2.65	108.52	111.24
14	N	602	HEA	C20-C19-C18	2.65	126.47	121.12
20	C	304	PGV	O14-P-O13	2.64	125.30	112.24
22	C	306	CHD	C2-C1-C10	-2.63	108.26	112.78
19	D	201	TGL	OC1-CC1-CC2	2.62	133.97	123.73
28	C	307	PEK	O01-C1-O02	-2.62	117.37	123.70
25	C	302	DMU	O55-C2-C3	2.61	116.87	109.94
20	N	610	PGV	C4-C3-C2	-2.61	103.81	113.19
25	P	310	DMU	O5-C6-C1	-2.61	104.83	110.35
19	A	611	TGL	C20-CA9-CA8	-2.61	101.19	114.42
25	C	311	DMU	O49-C1-C6	-2.60	103.73	110.05
22	G	102	CHD	C13-C17-C20	-2.60	116.39	119.50
25	P	307	DMU	C8-C7-C5	2.60	115.36	110.82
22	W	101	CHD	C2-C1-C10	2.59	117.23	112.78
27	P	305	CDL	OA8-CA6-CA4	2.59	115.98	108.43
22	C	306	CHD	C14-C13-C12	2.59	109.81	107.40
22	B	301	CHD	O3-C3-C4	-2.59	104.70	109.85
20	A	609	PGV	C30-C29-C28	2.58	127.53	114.42
27	N	601	CDL	C23-C22-C21	2.57	127.48	114.42
28	G	101	PEK	O03-C01-C02	-2.57	100.95	108.43
27	C	305	CDL	C42-C41-C40	2.56	127.43	114.42
22	P	301	CHD	C10-C9-C8	-2.56	109.07	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	301	CHD	C22-C23-C24	-2.55	108.10	113.59
22	C	301	CHD	C11-C9-C8	2.55	114.60	110.88
22	C	306	CHD	C5-C6-C7	2.54	117.27	114.46
25	C	311	DMU	C10-O7-C3	-2.54	111.69	117.96
25	C	311	DMU	C6-O5-C4	-2.53	108.72	113.69
24	N	612	PSC	C02-O01-C1	2.53	124.02	117.79
22	C	306	CHD	C13-C17-C20	-2.52	116.48	119.50
20	N	610	PGV	C03-C02-C01	-2.52	105.82	111.79
22	W	101	CHD	C19-C10-C1	-2.52	104.20	108.26
22	P	301	CHD	C11-C12-C13	-2.52	108.66	111.24
22	P	306	CHD	C11-C9-C10	2.52	116.32	113.73
14	A	602[B]	HEA	C3C-C4C-NC	2.51	112.46	109.21
28	C	307	PEK	C24-C23-C22	2.51	122.20	113.19
14	A	602[B]	HEA	C1B-C2B-C3B	-2.50	105.26	107.00
14	N	602	HEA	C12-C13-C14	2.50	118.83	112.23
25	Z	101	DMU	C34-C31-C28	-2.50	101.75	114.42
24	N	612	PSC	O03-C19-C20	2.49	119.72	111.91
22	B	301	CHD	C1-C10-C9	2.48	115.26	111.35
27	N	601	CDL	C44-C43-C42	-2.48	101.82	114.42
28	G	103	PEK	O03-C21-C22	2.48	119.69	111.91
14	N	603[A]	HEA	OMA-CMA-C3A	-2.48	119.51	124.91
25	P	307	DMU	O16-C6-C1	2.46	112.15	108.30
27	C	305	CDL	OB6-CB5-OB7	-2.46	117.75	123.70
22	G	102	CHD	C11-C9-C10	-2.46	111.19	113.73
25	C	311	DMU	C1-C2-C3	2.46	115.30	109.68
22	J	101	CHD	C11-C9-C8	2.45	114.46	110.88
14	A	602[A]	HEA	CMB-C2B-C1B	2.45	132.23	128.46
25	Z	101	DMU	O3-C5-C7	2.44	116.00	110.35
14	A	602[A]	HEA	CAD-C3D-C2D	2.43	134.23	127.25
22	C	301	CHD	C6-C5-C10	-2.43	110.08	112.66
27	T	102	CDL	C63-C62-C61	2.43	126.76	114.42
19	Y	101	TGL	OG3-CC1-OC1	-2.43	117.47	123.59
22	B	301	CHD	O7-C7-C6	2.43	115.96	109.94
14	N	603[A]	HEA	C1B-C2B-C3B	-2.42	105.31	107.00
19	N	611	TGL	OG1-CG1-CG2	2.42	115.48	108.43
27	T	102	CDL	OA8-CA7-C31	2.42	119.49	111.91
27	P	305	CDL	OB2-PB2-OB3	2.42	118.51	109.07
22	J	101	CHD	C15-C14-C13	2.41	105.92	103.55
27	P	305	CDL	C39-C38-C37	2.41	126.67	114.42
22	W	101	CHD	C14-C8-C9	2.41	113.02	109.71
27	N	601	CDL	C80-C79-C78	2.40	126.63	114.42
22	G	102	CHD	C22-C23-C24	-2.40	108.43	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	301	CHD	C4-C3-C2	-2.40	107.69	110.55
28	C	309	PEK	O01-C1-O02	-2.40	117.90	123.70
19	Y	101	TGL	OG2-CG2-CG3	2.40	117.08	108.40
20	P	304	PGV	O03-C01-C02	-2.39	101.47	108.43
20	P	304	PGV	C22-C21-C20	-2.39	104.59	113.19
28	T	101	PEK	O03-C21-O04	-2.39	117.56	123.59
14	N	603[A]	HEA	C27-C19-C20	2.39	119.29	115.27
20	N	610	PGV	C5-C4-C3	-2.38	102.34	114.42
20	N	610	PGV	O01-C02-C03	2.38	117.02	108.40
22	W	101	CHD	C17-C13-C14	-2.38	97.69	100.09
22	W	101	CHD	C9-C10-C5	2.38	111.92	108.58
20	N	609	PGV	C03-C02-C01	-2.38	106.17	111.79
25	C	310	DMU	C8-C7-C5	-2.38	106.67	110.82
25	C	302	DMU	C7-C8-C9	2.37	114.47	110.24
22	P	306	CHD	C15-C14-C8	2.37	121.64	118.33
22	B	301	CHD	C22-C20-C17	2.37	115.17	110.28
14	N	602	HEA	CAA-CBA-CGA	-2.36	108.71	112.67
20	A	609	PGV	C34-C33-C32	-2.36	95.52	113.42
14	N	603[A]	HEA	C16-C17-C18	2.35	119.60	111.88
27	C	305	CDL	OA8-CA7-C31	2.35	119.27	111.91
28	C	307	PEK	C01-O03-C21	2.34	125.80	117.12
22	W	101	CHD	C15-C14-C13	-2.34	101.26	103.55
25	C	310	DMU	O5-C4-C57	2.34	112.25	106.44
25	P	310	DMU	C10-O1-C9	-2.34	109.10	113.69
27	T	102	CDL	C12-C11-CA5	2.33	122.10	113.62
21	P	312	EDO	O1-C1-C2	-2.33	95.15	111.91
22	P	301	CHD	C14-C8-C7	-2.33	108.72	111.81
27	N	601	CDL	OB7-CB5-C51	-2.33	114.65	123.73
25	M	101	DMU	O3-C5-C10	-2.32	104.40	110.05
20	N	610	PGV	C3-C2-C1	-2.32	105.20	113.62
28	C	307	PEK	C3-C2-C1	2.31	122.03	113.62
22	C	306	CHD	O12-C12-C13	-2.31	107.13	111.03
28	C	309	PEK	C01-O03-C21	2.31	125.66	117.12
22	W	101	CHD	C1-C10-C9	-2.29	107.75	111.35
27	C	305	CDL	C43-C42-C41	2.29	126.06	114.42
22	C	301	CHD	O3-C3-C2	-2.28	104.36	110.16
19	D	201	TGL	CB5-CB4-CB3	2.28	125.98	114.42
22	W	101	CHD	C5-C6-C7	2.27	116.97	114.46
22	B	301	CHD	C15-C14-C13	2.27	105.78	103.55
14	N	602	HEA	C16-C17-C18	-2.27	104.42	111.88
25	P	310	DMU	C10-C5-C7	2.27	114.72	110.00
27	P	305	CDL	CB4-OB6-CB5	2.27	123.37	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	310	DMU	O5-C4-C3	-2.27	104.97	109.75
19	D	201	TGL	OG1-CA1-OA1	-2.27	117.87	123.59
27	T	102	CDL	C80-C79-C78	2.27	125.93	114.42
14	N	603[B]	HEA	C12-C13-C14	-2.27	106.25	112.23
14	N	602	HEA	CAD-CBD-CGD	-2.26	108.87	112.67
19	A	608	TGL	OB1-CB1-CB2	-2.26	114.90	123.73
25	M	101	DMU	O3-C5-C7	2.26	115.58	110.35
14	N	603[A]	HEA	C12-C13-C14	-2.26	106.28	112.23
25	P	307	DMU	O1-C9-C11	2.25	112.04	106.44
27	P	305	CDL	OA5-PA1-OA3	-2.25	100.27	109.07
22	G	102	CHD	C16-C17-C20	-2.25	108.67	112.15
22	P	306	CHD	C21-C20-C22	2.24	113.87	110.36
27	N	601	CDL	OA6-CA5-OA7	-2.24	118.30	123.70
14	A	602[A]	HEA	C12-C11-C3B	2.24	118.43	112.56
25	P	309	DMU	C7-C8-C9	2.24	114.23	110.24
19	Q	201	TGL	OG2-CG2-CG3	2.23	116.48	108.40
19	N	611	TGL	OG2-CB1-OB1	-2.23	118.32	123.70
27	T	102	CDL	C39-C38-C37	2.22	125.71	114.42
19	A	611	TGL	OG1-CA1-OA1	-2.22	117.99	123.59
14	N	602	HEA	CBD-CAD-C3D	-2.21	108.40	112.49
27	T	102	CDL	C19-C18-C17	2.21	125.65	114.42
20	A	609	PGV	C25-C24-C23	2.21	125.65	114.42
22	B	301	CHD	C5-C4-C3	-2.21	109.52	112.76
19	N	611	TGL	CB3-CB2-CB1	-2.21	105.60	113.62
22	C	301	CHD	C19-C10-C9	-2.21	108.14	111.18
14	N	603[A]	HEA	C26-C15-C14	-2.20	118.02	123.68
27	P	305	CDL	OB6-CB4-CB3	-2.19	100.46	108.40
27	T	102	CDL	CB4-OB6-CB5	2.19	123.18	117.79
19	D	201	TGL	CG3-CG2-CG1	2.19	116.96	111.79
20	N	609	PGV	C26-C25-C24	-2.19	103.33	114.42
21	S	104	EDO	O1-C1-C2	-2.18	96.21	111.91
14	A	601	HEA	OMA-CMA-C3A	-2.18	120.16	124.91
19	Y	101	TGL	CC3-CC2-CC1	2.18	121.54	113.62
22	P	301	CHD	C1-C2-C3	-2.18	107.67	110.47
20	C	308	PGV	C26-C25-C24	2.17	125.46	114.42
22	C	306	CHD	C21-C20-C22	2.17	113.77	110.36
27	N	601	CDL	OB8-CB6-CB4	2.17	114.75	108.43
14	A	602[A]	HEA	C4B-C3B-C2B	2.16	108.38	106.87
22	B	301	CHD	C11-C12-C13	2.16	113.46	111.24
25	C	310	DMU	C6-C1-C2	-2.16	105.50	110.00
25	P	307	DMU	C31-C28-C25	-2.15	103.50	114.42
14	N	603[A]	HEA	C16-C15-C14	-2.15	116.77	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602[A]	HEA	CMC-C2C-C3C	2.15	128.70	124.68
28	T	101	PEK	O01-C02-C03	-2.14	100.66	108.40
25	P	310	DMU	C6-C1-C2	2.13	114.44	110.00
22	W	101	CHD	C18-C13-C17	2.13	114.55	111.21
27	C	305	CDL	OB4-PB2-OB5	-2.13	97.86	107.75
20	C	304	PGV	C4-C3-C2	-2.12	105.55	113.19
28	G	101	PEK	C3-C2-C1	-2.12	105.92	113.62
27	N	601	CDL	CA6-OA8-CA7	2.11	124.94	117.12
25	P	310	DMU	C6-O5-C4	2.11	117.83	113.69
28	G	101	PEK	O02-C1-C2	-2.11	115.52	123.73
22	J	101	CHD	C19-C10-C1	-2.10	104.87	108.26
20	P	304	PGV	C3-C2-C1	-2.10	105.98	113.62
22	C	301	CHD	C2-C1-C10	2.10	116.39	112.78
22	J	101	CHD	C1-C2-C3	-2.10	107.78	110.47
27	T	102	CDL	OA6-CA5-OA7	-2.09	118.65	123.70
22	P	306	CHD	C11-C9-C8	2.09	113.93	110.88
22	P	306	CHD	C18-C13-C14	2.09	114.48	111.21
22	B	301	CHD	C19-C10-C5	-2.09	106.82	110.36
28	G	103	PEK	C01-O03-C21	2.08	124.84	117.12
22	J	101	CHD	O7-C7-C8	2.08	114.08	109.43
25	P	307	DMU	C22-C19-C18	-2.08	104.28	113.49
27	T	102	CDL	CB2-C1-CA2	-2.07	106.69	112.79
22	W	101	CHD	O12-C12-C13	2.07	114.53	111.03
27	P	305	CDL	OB4-PB2-OB5	-2.07	98.12	107.75
24	N	612	PSC	C26-C25-C24	-2.07	103.91	114.42
21	A	615	EDO	O1-C1-C2	-2.07	97.02	111.91
22	P	301	CHD	C5-C6-C7	2.07	116.74	114.46
28	T	101	PEK	C24-C23-C22	-2.07	105.76	113.19
25	P	309	DMU	O5-C4-C57	2.06	111.56	106.44
27	T	102	CDL	C62-C61-C60	2.06	124.88	114.42
22	J	101	CHD	C14-C8-C7	2.06	114.53	111.81
27	N	601	CDL	C63-C62-C61	2.05	124.84	114.42
28	P	308	PEK	C35-C34-C33	2.05	124.81	114.42
19	A	611	TGL	CG3-OG3-CC1	2.04	124.68	117.12
28	P	308	PEK	O03-C21-C22	2.04	118.31	111.91
22	W	101	CHD	C21-C20-C17	2.04	116.04	112.92
25	C	311	DMU	O7-C3-C2	2.03	112.67	107.28
14	N	603[B]	HEA	CMC-C2C-C3C	2.03	128.47	124.68
22	W	101	CHD	C5-C4-C3	2.02	115.73	112.76
20	A	610	PGV	O03-C19-O04	-2.02	118.49	123.59
27	T	102	CDL	C59-C58-C57	2.02	124.68	114.42
22	P	301	CHD	C17-C13-C14	2.02	102.13	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	310	DMU	O5-C6-C1	-2.02	106.08	110.35
22	P	301	CHD	C1-C10-C5	2.02	110.75	107.77
27	C	305	CDL	C22-C21-C20	2.01	124.65	114.42
27	N	601	CDL	C43-C42-C41	2.01	124.65	114.42
14	N	603[B]	HEA	C17-C18-C19	2.01	132.50	127.66
19	N	611	TGL	OG2-CG2-CG1	2.01	115.68	108.40
19	A	611	TGL	OG2-CB1-OB1	-2.01	118.84	123.70
25	C	302	DMU	C57-C4-C3	2.01	119.17	113.33
27	N	601	CDL	C20-C19-C18	2.01	124.63	114.42
22	C	301	CHD	C4-C3-C2	-2.01	108.16	110.55
22	C	306	CHD	C18-C13-C17	-2.00	108.08	111.21

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	601	HEA	NB
14	N	603[A]	HEA	ND
14	N	603[A]	HEA	NA
14	N	603[A]	HEA	NB
14	N	602	HEA	ND
14	N	602	HEA	NA
14	N	602	HEA	NB
14	A	602[A]	HEA	ND
14	A	602[A]	HEA	NB
14	A	602[B]	HEA	ND
14	A	602[B]	HEA	NA
14	A	602[B]	HEA	NB
14	N	603[B]	HEA	ND
14	N	603[B]	HEA	NB

All (902) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	610	PGV	C04-O12-P-O11
20	A	610	PGV	C02-C03-O11-P
20	A	610	PGV	C2-C1-O01-C02
27	N	601	CDL	CB2-C1-CA2-OA2
27	N	601	CDL	CA2-OA2-PA1-OA4
27	N	601	CDL	CA3-OA5-PA1-OA3
27	N	601	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
27	N	601	CDL	C11-CA5-OA6-CA4
27	N	601	CDL	CB3-OB5-PB2-OB2
27	N	601	CDL	CB3-OB5-PB2-OB3
27	N	601	CDL	CB3-OB5-PB2-OB4
27	N	601	CDL	OB6-CB4-CB6-OB8
24	B	303	PSC	C03-O11-P-O12
24	B	303	PSC	C03-O11-P-O14
24	B	303	PSC	O12-C04-C05-N
27	T	102	CDL	CA3-OA5-PA1-OA2
27	T	102	CDL	CA3-OA5-PA1-OA3
27	T	102	CDL	OA6-CA4-CA6-OA8
27	T	102	CDL	OA7-CA5-OA6-CA4
27	T	102	CDL	CB3-OB5-PB2-OB3
24	N	612	PSC	C04-O12-P-O14
24	N	612	PSC	O12-C04-C05-N
25	C	311	DMU	C1-C6-O16-C18
25	C	311	DMU	O5-C6-O16-C18
25	C	311	DMU	C19-C18-O16-C6
28	C	309	PEK	C03-O11-P-O12
28	C	309	PEK	C03-O11-P-O13
28	C	309	PEK	C03-O11-P-O14
28	C	309	PEK	C04-O12-P-O14
28	C	309	PEK	O12-C04-C05-N
19	A	611	TGL	CB2-CB1-OG2-CG2
19	A	611	TGL	OB1-CB1-OG2-CG2
28	G	103	PEK	C04-O12-P-O11
28	G	103	PEK	C04-O12-P-O13
28	G	103	PEK	C04-O12-P-O14
28	G	103	PEK	O02-C1-O01-C02
28	G	103	PEK	C2-C1-O01-C02
27	P	305	CDL	CA2-OA2-PA1-OA5
27	P	305	CDL	CA3-OA5-PA1-OA3
27	P	305	CDL	C11-CA5-OA6-CA4
27	P	305	CDL	CB2-OB2-PB2-OB3
27	P	305	CDL	CB2-OB2-PB2-OB4
27	P	305	CDL	CB2-OB2-PB2-OB5
27	P	305	CDL	C51-CB5-OB6-CB4
20	N	609	PGV	C04-O12-P-O13
20	N	609	PGV	C04-O12-P-O14
20	N	609	PGV	C02-C03-O11-P
20	N	609	PGV	O02-C1-O01-C02
20	N	609	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
19	Y	101	TGL	CA2-CA1-OG1-CG1
19	Y	101	TGL	OA1-CA1-OG1-CG1
19	Y	101	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	OB1-CB1-OG2-CG2
28	T	101	PEK	C11-C12-C13-C14
28	T	101	PEK	C12-C13-C14-C15
28	G	101	PEK	C7-C8-C9-C10
28	G	101	PEK	C10-C11-C12-C13
28	G	101	PEK	C12-C13-C14-C15
25	P	307	DMU	O5-C6-O16-C18
14	A	602[B]	HEA	C2D-C3D-CAD-CBD
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
25	C	302	DMU	C19-C18-O16-C6
21	N	621	EDO	O1-C1-C2-O2
25	P	310	DMU	C1-C6-O16-C18
25	P	310	DMU	O5-C6-O16-C18
27	C	305	CDL	CA2-OA2-PA1-OA4
27	C	305	CDL	CA3-OA5-PA1-OA2
27	C	305	CDL	C11-CA5-OA6-CA4
27	C	305	CDL	CB2-OB2-PB2-OB3
27	C	305	CDL	CB2-OB2-PB2-OB4
27	C	305	CDL	C51-CB5-OB6-CB4
20	C	308	PGV	C03-O11-P-O13
20	C	308	PGV	C03-O11-P-O14
20	C	308	PGV	O03-C01-C02-O01
20	C	308	PGV	C02-C03-O11-P
19	D	201	TGL	CG2-CG1-OG1-CA1
14	N	603[B]	HEA	C2D-C3D-CAD-CBD
14	N	603[B]	HEA	C4D-C3D-CAD-CBD
28	P	308	PEK	C03-O11-P-O14
28	P	308	PEK	C04-O12-P-O11
28	P	308	PEK	C04-O12-P-O13
28	P	308	PEK	C04-O12-P-O14
28	P	308	PEK	O02-C1-O01-C02
28	P	308	PEK	C2-C1-O01-C02
28	C	307	PEK	C04-O12-P-O11
28	C	307	PEK	O12-C04-C05-N
28	C	307	PEK	O02-C1-O01-C02
28	C	307	PEK	C2-C1-O01-C02
20	P	302	PGV	C02-C03-O11-P
20	A	610	PGV	O04-C19-O03-C01
24	N	612	PSC	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
20	N	609	PGV	O04-C19-O03-C01
19	D	201	TGL	OC1-CC1-OG3-CG3
25	P	309	DMU	C5-C10-O7-C3
25	C	310	DMU	C5-C10-O7-C3
20	A	610	PGV	C20-C19-O03-C01
24	N	612	PSC	C20-C19-O03-C01
20	N	609	PGV	C20-C19-O03-C01
24	B	303	PSC	O04-C19-O03-C01
19	N	611	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	OA1-CA1-OG1-CG1
20	A	610	PGV	O02-C1-O01-C02
27	N	601	CDL	OA7-CA5-OA6-CA4
27	P	305	CDL	OA7-CA5-OA6-CA4
27	P	305	CDL	OB7-CB5-OB6-CB4
27	C	305	CDL	OA7-CA5-OA6-CA4
27	C	305	CDL	OB7-CB5-OB6-CB4
19	A	608	TGL	OC1-CC1-OG3-CG3
24	B	303	PSC	C20-C19-O03-C01
19	N	611	TGL	CC2-CC1-OG3-CG3
27	T	102	CDL	C11-CA5-OA6-CA4
19	Q	201	TGL	CC2-CC1-OG3-CG3
19	A	608	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	CA2-CA1-OG1-CG1
19	D	201	TGL	CC2-CC1-OG3-CG3
25	P	309	DMU	O6-C11-C9-O1
28	G	103	PEK	C7-C8-C9-C10
28	T	101	PEK	C4-C5-C6-C7
28	T	101	PEK	C7-C8-C9-C10
28	P	308	PEK	C13-C14-C15-C16
28	C	307	PEK	C4-C5-C6-C7
28	C	307	PEK	C7-C8-C9-C10
19	N	611	TGL	C20-C21-C22-C23
19	A	611	TGL	CA9-C20-C21-C22
25	C	302	DMU	C25-C28-C31-C34
19	D	201	TGL	C16-C17-C18-C19
27	T	102	CDL	C79-C80-C81-C82
19	A	611	TGL	CA2-CA1-OG1-CG1
19	Y	101	TGL	CC3-CC4-CC5-CC6
27	C	305	CDL	C76-C77-C78-C79
27	T	102	CDL	C51-CB5-OB6-CB4
19	Y	101	TGL	CC1-CC2-CC3-CC4
27	T	102	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
20	C	308	PGV	C24-C25-C26-C27
19	Q	201	TGL	OC1-CC1-OG3-CG3
20	A	610	PGV	C20-C21-C22-C23
27	N	601	CDL	C58-C59-C60-C61
25	M	101	DMU	C28-C31-C34-C37
27	P	305	CDL	C75-C76-C77-C78
19	D	201	TGL	C21-C22-C23-C24
25	P	309	DMU	O6-C11-C9-C8
24	B	303	PSC	C19-C20-C21-C22
19	Q	201	TGL	CC1-CC2-CC3-CC4
19	A	611	TGL	CC1-CC2-CC3-CC4
27	N	601	CDL	C81-C82-C83-C84
25	Z	101	DMU	O6-C11-C9-O1
14	A	601	HEA	C15-C16-C17-C18
24	B	303	PSC	C30-C31-C32-C33
22	J	101	CHD	C13-C17-C20-C22
22	C	306	CHD	C17-C20-C22-C23
22	P	306	CHD	C17-C20-C22-C23
19	A	611	TGL	OA1-CA1-OG1-CG1
25	C	302	DMU	O6-C11-C9-C8
19	A	608	TGL	CA2-CA3-CA4-CA5
24	N	612	PSC	C20-C21-C22-C23
20	A	610	PGV	O12-C04-C05-C06
27	P	305	CDL	CB2-C1-CA2-OA2
27	P	305	CDL	CA2-C1-CB2-OB2
27	C	305	CDL	CB2-C1-CA2-OA2
27	C	305	CDL	CA2-C1-CB2-OB2
27	T	102	CDL	OB7-CB5-OB6-CB4
27	T	102	CDL	C42-C43-C44-C45
27	N	601	CDL	C31-CA7-OA8-CA6
19	A	608	TGL	CA2-CA1-OG1-CG1
25	Z	101	DMU	O6-C11-C9-C8
27	N	601	CDL	C61-C62-C63-C64
22	C	306	CHD	C20-C22-C23-C24
19	D	201	TGL	CC2-CC3-CC4-CC5
22	W	101	CHD	C13-C17-C20-C21
24	B	303	PSC	C21-C22-C23-C24
20	A	610	PGV	O12-C04-C05-O05
27	N	601	CDL	O1-C1-CA2-OA2
27	P	305	CDL	O1-C1-CB2-OB2
27	C	305	CDL	O1-C1-CB2-OB2
19	N	611	TGL	CA1-CA2-CA3-CA4

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Mol	Chain	Res	Type	Atoms
28	T	101	PEK	C1-C2-C3-C4
27	P	305	CDL	C81-C82-C83-C84
27	N	601	CDL	OA9-CA7-OA8-CA6
19	A	608	TGL	OB1-CB1-OG2-CG2
22	W	101	CHD	C13-C17-C20-C22
22	W	101	CHD	C17-C20-C22-C23
27	T	102	CDL	C31-CA7-OA8-CA6
27	N	601	CDL	CA5-C11-C12-C13
28	P	308	PEK	C21-C22-C23-C24
25	P	310	DMU	C4-C3-O7-C10
19	A	608	TGL	CA1-CA2-CA3-CA4
19	A	608	TGL	CB1-CB2-CB3-CB4
20	N	609	PGV	C19-C20-C21-C22
19	D	201	TGL	CA1-CA2-CA3-CA4
27	C	305	CDL	CA7-C31-C32-C33
27	C	305	CDL	CB7-C71-C72-C73
21	L	101	EDO	O1-C1-C2-O2
19	Y	101	TGL	CA2-CA3-CA4-CA5
25	P	310	DMU	O16-C18-C19-C22
22	C	306	CHD	C21-C20-C22-C23
22	P	306	CHD	C21-C20-C22-C23
19	A	608	TGL	OA1-CA1-OG1-CG1
28	G	103	PEK	C21-C22-C23-C24
27	P	305	CDL	O1-C1-CA2-OA2
20	N	609	PGV	O12-C04-C05-O05
27	C	305	CDL	O1-C1-CA2-OA2
22	J	101	CHD	C13-C17-C20-C21
27	T	102	CDL	OA9-CA7-OA8-CA6
25	P	310	DMU	C2-C3-O7-C10
24	B	303	PSC	C11-C10-C9-C8
20	N	609	PGV	C10-C11-C12-C13
19	A	608	TGL	CB2-CB1-OG2-CG2
20	A	609	PGV	C23-C24-C25-C26
20	A	610	PGV	C03-O11-P-O12
27	N	601	CDL	CA2-OA2-PA1-OA5
27	N	601	CDL	CB2-OB2-PB2-OB5
24	N	612	PSC	C03-O11-P-O12
28	C	309	PEK	C04-O12-P-O11
27	P	305	CDL	CA3-OA5-PA1-OA2
20	N	609	PGV	C04-O12-P-O11
27	C	305	CDL	CA2-OA2-PA1-OA5
27	C	305	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
20	C	308	PGV	C03-O11-P-O12
20	C	308	PGV	C04-O12-P-O11
20	P	302	PGV	C03-O11-P-O12
27	C	305	CDL	C71-CB7-OB8-CB6
22	W	101	CHD	C16-C17-C20-C21
20	C	308	PGV	C1-C2-C3-C4
20	N	609	PGV	O12-C04-C05-C06
22	J	101	CHD	C16-C17-C20-C21
20	P	302	PGV	C1-C2-C3-C4
19	Q	201	TGL	CC6-CC7-CC8-CC9
19	N	611	TGL	C11-C10-CB9-CB8
27	P	305	CDL	C80-C81-C82-C83
27	N	601	CDL	C14-C15-C16-C17
27	N	601	CDL	C56-C57-C58-C59
25	P	309	DMU	C19-C22-C25-C28
27	T	102	CDL	C14-C15-C16-C17
19	N	611	TGL	C21-C22-C23-C24
27	P	305	CDL	C57-C58-C59-C60
19	Y	101	TGL	CC4-CC5-CC6-CC7
19	Y	101	TGL	C14-C29-C30-C31
24	N	612	PSC	C29-C30-C31-C32
19	N	611	TGL	CB7-CB8-CB9-C10
19	A	611	TGL	CA3-CA4-CA5-CA6
19	Y	101	TGL	C21-C20-CA9-CA8
20	A	609	PGV	C26-C27-C28-C29
28	C	307	PEK	C25-C26-C27-C28
24	N	612	PSC	C01-C02-O01-C1
20	N	609	PGV	C01-C02-O01-C1
27	T	102	CDL	CA7-C31-C32-C33
19	Q	201	TGL	CB4-CB5-CB6-CB7
19	Q	201	TGL	C11-C10-CB9-CB8
20	C	304	PGV	C7-C8-C9-C10
19	A	611	TGL	CB5-CB6-CB7-CB8
19	A	608	TGL	C21-C22-C23-C24
19	Y	101	TGL	CB3-CB4-CB5-CB6
27	C	305	CDL	C56-C57-C58-C59
27	C	305	CDL	C63-C64-C65-C66
20	A	610	PGV	C05-C04-O12-P
20	P	304	PGV	C10-C11-C12-C13
28	T	101	PEK	C10-C11-C12-C13
19	N	611	TGL	C19-C33-C34-C35
28	G	103	PEK	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
27	P	305	CDL	C14-C15-C16-C17
28	G	101	PEK	C34-C35-C36-C37
27	N	601	CDL	C79-C80-C81-C82
27	P	305	CDL	C20-C21-C22-C23
19	A	608	TGL	C20-C21-C22-C23
19	Y	101	TGL	CB5-CB6-CB7-CB8
19	Y	101	TGL	CC6-CC7-CC8-CC9
25	C	302	DMU	C1-C6-O16-C18
19	Q	201	TGL	CA6-CA7-CA8-CA9
28	G	101	PEK	C16-C17-C18-C19
20	P	302	PGV	C26-C27-C28-C29
27	N	601	CDL	C22-C23-C24-C25
27	N	601	CDL	C32-C33-C34-C35
19	A	611	TGL	CC7-CC8-CC9-C15
27	P	305	CDL	C40-C41-C42-C43
27	P	305	CDL	C52-C53-C54-C55
27	N	601	CDL	C77-C78-C79-C80
19	Q	201	TGL	CC9-C15-C16-C17
20	C	304	PGV	C13-C14-C15-C16
19	A	611	TGL	C11-C10-CB9-CB8
27	P	305	CDL	C61-C62-C63-C64
20	N	609	PGV	C29-C30-C31-C32
19	Y	101	TGL	CB6-CB7-CB8-CB9
28	T	101	PEK	C26-C27-C28-C29
27	C	305	CDL	C20-C21-C22-C23
25	C	302	DMU	O6-C11-C9-O1
27	N	601	CDL	C13-C14-C15-C16
24	B	303	PSC	C5-C6-C7-C8
27	T	102	CDL	C13-C14-C15-C16
27	P	305	CDL	C82-C83-C84-C85
27	C	305	CDL	C83-C84-C85-C86
28	C	307	PEK	C32-C33-C34-C35
20	A	610	PGV	C04-C05-C06-O06
20	N	609	PGV	C04-C05-C06-O06
20	P	302	PGV	C04-C05-C06-O06
19	N	611	TGL	OB1-CB1-OG2-CG2
19	Q	201	TGL	C10-C11-C12-C13
27	T	102	CDL	C59-C60-C61-C62
19	A	608	TGL	C12-C13-C14-C29
19	Y	101	TGL	C12-C13-C14-C29
20	P	302	PGV	C2-C3-C4-C5
20	P	302	PGV	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
27	N	601	CDL	C63-C64-C65-C66
27	T	102	CDL	C36-C37-C38-C39
24	N	612	PSC	C5-C6-C7-C8
25	C	311	DMU	O16-C18-C19-C22
28	G	103	PEK	C31-C32-C33-C34
27	P	305	CDL	C17-C18-C19-C20
19	A	608	TGL	C21-C20-CA9-CA8
20	P	304	PGV	C24-C25-C26-C27
28	G	101	PEK	C23-C24-C25-C26
25	P	310	DMU	C22-C25-C28-C31
27	C	305	CDL	C71-C72-C73-C74
19	D	201	TGL	C15-C16-C17-C18
25	C	311	DMU	C18-C19-C22-C25
27	N	601	CDL	C18-C19-C20-C21
27	N	601	CDL	C55-C56-C57-C58
19	Q	201	TGL	C20-C21-C22-C23
19	Q	201	TGL	C19-C33-C34-C35
19	N	611	TGL	CA7-CA8-CA9-C20
19	A	611	TGL	C12-C13-C14-C29
19	A	608	TGL	CA5-CA6-CA7-CA8
19	D	201	TGL	CA7-CA8-CA9-C20
19	D	201	TGL	C19-C33-C34-C35
28	C	307	PEK	C28-C29-C30-C31
25	C	302	DMU	C18-C19-C22-C25
27	N	601	CDL	C17-C18-C19-C20
27	N	601	CDL	C60-C61-C62-C63
27	T	102	CDL	C41-C42-C43-C44
27	T	102	CDL	C71-C72-C73-C74
19	N	611	TGL	CA6-CA7-CA8-CA9
19	A	611	TGL	C11-C12-C13-C14
27	P	305	CDL	C15-C16-C17-C18
27	P	305	CDL	C16-C17-C18-C19
20	N	609	PGV	C25-C26-C27-C28
19	Y	101	TGL	CA3-CA4-CA5-CA6
27	C	305	CDL	C77-C78-C79-C80
19	D	201	TGL	CC7-CC8-CC9-C15
20	A	610	PGV	C19-C20-C21-C22
27	C	305	CDL	OB9-CB7-OB8-CB6
28	T	101	PEK	C30-C31-C32-C33
27	C	305	CDL	C18-C19-C20-C21
19	N	611	TGL	C16-C15-CC9-CC8
20	A	610	PGV	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	C10-C11-C12-C13
19	A	608	TGL	C16-C15-CC9-CC8
19	Y	101	TGL	C10-C11-C12-C13
27	C	305	CDL	C11-C12-C13-C14
20	P	302	PGV	C24-C25-C26-C27
27	T	102	CDL	CB3-CB4-CB6-OB8
20	A	610	PGV	C10-C11-C12-C13
28	C	309	PEK	C10-C11-C12-C13
27	T	102	CDL	C75-C76-C77-C78
19	N	611	TGL	CB9-C10-C11-C12
19	N	611	TGL	CC4-CC5-CC6-CC7
27	P	305	CDL	C78-C79-C80-C81
19	A	608	TGL	C16-C17-C18-C19
19	Y	101	TGL	C22-C23-C24-C25
19	N	611	TGL	CB1-CB2-CB3-CB4
19	Y	101	TGL	C18-C19-C33-C34
24	B	303	PSC	C2-C1-O01-C02
19	N	611	TGL	CB2-CB1-OG2-CG2
19	Q	201	TGL	CA5-CA6-CA7-CA8
27	T	102	CDL	C32-C33-C34-C35
20	N	609	PGV	O05-C05-C06-O06
19	A	608	TGL	C15-C16-C17-C18
25	Z	101	DMU	O16-C18-C19-C22
25	C	311	DMU	O5-C4-C57-O61
25	P	310	DMU	C19-C22-C25-C28
25	C	311	DMU	C3-C4-C57-O61
27	N	601	CDL	C34-C35-C36-C37
27	T	102	CDL	C52-C53-C54-C55
20	P	304	PGV	C7-C8-C9-C10
19	Y	101	TGL	C16-C17-C18-C19
25	Z	101	DMU	C28-C31-C34-C37
27	N	601	CDL	C59-C60-C61-C62
19	N	611	TGL	CC5-CC6-CC7-CC8
19	A	611	TGL	CC6-CC7-CC8-CC9
19	A	611	TGL	C21-C22-C23-C24
19	A	611	TGL	C19-C33-C34-C35
19	A	611	TGL	C15-C16-C17-C18
27	P	305	CDL	C18-C19-C20-C21
27	P	305	CDL	C51-C52-C53-C54
20	N	609	PGV	C3-C4-C5-C6
21	A	618	EDO	O1-C1-C2-O2
28	C	309	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
28	G	103	PEK	C24-C25-C26-C27
19	A	608	TGL	CC4-CC5-CC6-CC7
24	N	612	PSC	C4-C5-C6-C7
27	P	305	CDL	C60-C61-C62-C63
19	A	611	TGL	CB2-CB3-CB4-CB5
20	A	609	PGV	C28-C29-C30-C31
20	P	302	PGV	C30-C31-C32-C33
28	T	101	PEK	C13-C14-C15-C16
20	C	308	PGV	C10-C11-C12-C13
28	P	308	PEK	C10-C11-C12-C13
19	Q	201	TGL	C13-C14-C29-C30
27	T	102	CDL	C76-C77-C78-C79
25	C	311	DMU	C31-C34-C37-C40
19	Y	101	TGL	C11-C12-C13-C14
28	T	101	PEK	C22-C23-C24-C25
28	C	307	PEK	C24-C25-C26-C27
22	W	101	CHD	C16-C17-C20-C22
28	T	101	PEK	C2-C3-C4-C5
24	B	303	PSC	O02-C1-O01-C02
28	G	103	PEK	C29-C30-C31-C32
19	A	608	TGL	C14-C29-C30-C31
27	N	601	CDL	C35-C36-C37-C38
27	P	305	CDL	C19-C20-C21-C22
27	P	305	CDL	C39-C40-C41-C42
20	P	302	PGV	C22-C23-C24-C25
28	G	103	PEK	C25-C26-C27-C28
27	P	305	CDL	C31-C32-C33-C34
19	D	201	TGL	CB1-CB2-CB3-CB4
19	Q	201	TGL	CB9-C10-C11-C12
19	Y	101	TGL	CC9-C15-C16-C17
20	A	610	PGV	C22-C23-C24-C25
19	Q	201	TGL	C22-C23-C24-C25
20	N	609	PGV	C27-C28-C29-C30
19	N	611	TGL	CA5-CA6-CA7-CA8
19	A	611	TGL	CC2-CC3-CC4-CC5
28	P	308	PEK	C33-C34-C35-C36
24	N	612	PSC	C2-C1-O01-C02
27	P	305	CDL	C43-C44-C45-C46
27	N	601	CDL	C42-C43-C44-C45
25	M	101	DMU	O16-C18-C19-C22
19	A	611	TGL	C21-C20-CA9-CA8
19	Y	101	TGL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
24	N	612	PSC	O02-C1-O01-C02
27	T	102	CDL	CB5-C51-C52-C53
24	N	612	PSC	C2-C3-C4-C5
20	P	304	PGV	C22-C23-C24-C25
27	T	102	CDL	OB6-CB4-CB6-OB8
28	C	309	PEK	O03-C01-C02-O01
19	Q	201	TGL	CB5-CB6-CB7-CB8
28	C	309	PEK	C24-C25-C26-C27
28	C	309	PEK	C25-C26-C27-C28
19	A	608	TGL	CB4-CB5-CB6-CB7
20	P	304	PGV	C11-C10-C9-C8
28	C	307	PEK	C15-C16-C17-C18
25	P	307	DMU	O6-C11-C9-C8
27	N	601	CDL	C72-C73-C74-C75
19	Q	201	TGL	C17-C18-C19-C33
19	N	611	TGL	CB6-CB7-CB8-CB9
19	A	611	TGL	CC5-CC6-CC7-CC8
28	G	101	PEK	C25-C26-C27-C28
27	C	305	CDL	C19-C20-C21-C22
27	N	601	CDL	C16-C17-C18-C19
27	N	601	CDL	CA3-OA5-PA1-OA2
28	P	308	PEK	C03-O11-P-O12
27	N	601	CDL	C11-C12-C13-C14
27	C	305	CDL	C36-C37-C38-C39
20	C	304	PGV	C27-C28-C29-C30
28	G	103	PEK	C32-C33-C34-C35
20	A	609	PGV	C30-C31-C32-C33
24	B	303	PSC	C01-C02-C03-O11
27	T	102	CDL	OB5-CB3-CB4-CB6
28	C	309	PEK	C01-C02-C03-O11
19	Q	201	TGL	CC7-CC8-CC9-C15
19	A	611	TGL	C22-C23-C24-C25
28	P	308	PEK	C30-C31-C32-C33
24	B	303	PSC	C2-C3-C4-C5
28	C	309	PEK	C27-C28-C29-C30
20	C	304	PGV	C12-C13-C14-C15
28	C	307	PEK	C2-C3-C4-C5
25	C	310	DMU	O16-C18-C19-C22
19	N	611	TGL	C14-C29-C30-C31
19	D	201	TGL	C21-C20-CA9-CA8
27	P	305	CDL	C83-C84-C85-C86
19	A	611	TGL	C14-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
25	Z	101	DMU	C25-C28-C31-C34
28	C	307	PEK	C29-C30-C31-C32
20	P	302	PGV	C6-C7-C8-C9
27	C	305	CDL	C40-C41-C42-C43
28	C	307	PEK	C35-C36-C37-C38
24	B	303	PSC	O03-C01-C02-C03
27	T	102	CDL	CA3-CA4-CA6-OA8
24	N	612	PSC	O03-C01-C02-C03
19	N	611	TGL	OG1-CG1-CG2-CG3
28	C	309	PEK	O03-C01-C02-C03
27	P	305	CDL	CB3-CB4-CB6-OB8
27	P	305	CDL	C79-C80-C81-C82
19	A	608	TGL	CA6-CA7-CA8-CA9
19	A	608	TGL	C11-C12-C13-C14
20	N	609	PGV	O03-C01-C02-C03
27	C	305	CDL	CB3-CB4-CB6-OB8
27	C	305	CDL	C52-C53-C54-C55
20	C	308	PGV	O03-C01-C02-C03
19	D	201	TGL	OG1-CG1-CG2-CG3
25	C	310	DMU	C34-C37-C40-C43
27	N	601	CDL	C44-C45-C46-C47
27	T	102	CDL	C81-C82-C83-C84
20	C	304	PGV	C15-C16-C17-C18
20	A	610	PGV	C29-C30-C31-C32
19	Q	201	TGL	CB2-CB3-CB4-CB5
24	N	612	PSC	C31-C32-C33-C34
20	A	609	PGV	C31-C32-C33-C34
20	P	302	PGV	C13-C14-C15-C16
24	B	303	PSC	C25-C26-C27-C28
25	M	101	DMU	C19-C22-C25-C28
19	Y	101	TGL	C15-C16-C17-C18
28	C	307	PEK	C33-C34-C35-C36
20	P	304	PGV	C11-C12-C13-C14
28	T	101	PEK	C3-C4-C5-C6
20	P	302	PGV	O05-C05-C06-O06
19	A	611	TGL	C16-C17-C18-C19
19	A	608	TGL	C25-C26-C27-C28
28	C	307	PEK	C26-C27-C28-C29
20	A	610	PGV	C11-C10-C9-C8
28	P	308	PEK	C2-C3-C4-C5
20	N	610	PGV	C11-C10-C9-C8
20	N	610	PGV	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
20	P	304	PGV	C1-C2-C3-C4
20	C	308	PGV	C29-C30-C31-C32
19	Y	101	TGL	C25-C26-C27-C28
20	A	610	PGV	C21-C22-C23-C24
20	P	302	PGV	C29-C30-C31-C32
27	T	102	CDL	C72-C73-C74-C75
24	N	612	PSC	C15-C16-C17-C18
28	C	307	PEK	C17-C18-C19-C20
25	P	310	DMU	O6-C11-C9-C8
27	T	102	CDL	C38-C39-C40-C41
19	A	611	TGL	C23-C24-C25-C26
27	C	305	CDL	C12-C13-C14-C15
19	Y	101	TGL	C29-C30-C31-C32
28	G	103	PEK	O01-C02-C03-O11
28	P	308	PEK	O01-C02-C03-O11
28	G	101	PEK	C13-C14-C15-C16
20	C	308	PGV	C31-C32-C33-C34
21	A	612	EDO	O1-C1-C2-O2
19	Q	201	TGL	C21-C20-CA9-CA8
28	G	101	PEK	C28-C29-C30-C31
22	W	101	CHD	C21-C20-C22-C23
25	P	307	DMU	C1-C6-O16-C18
19	Q	201	TGL	C12-C13-C14-C29
20	C	304	PGV	C24-C25-C26-C27
19	N	611	TGL	OG1-CG1-CG2-OG2
19	A	611	TGL	OG1-CG1-CG2-OG2
20	P	302	PGV	O03-C01-C02-O01
27	C	305	CDL	C59-C60-C61-C62
27	N	601	CDL	C31-C32-C33-C34
19	D	201	TGL	C10-C11-C12-C13
27	C	305	CDL	C41-C42-C43-C44
19	A	611	TGL	CB1-CB2-CB3-CB4
19	N	611	TGL	CA2-CA3-CA4-CA5
28	G	103	PEK	C23-C24-C25-C26
19	N	611	TGL	CA4-CA5-CA6-CA7
27	P	305	CDL	C36-C37-C38-C39
19	D	201	TGL	C11-C10-CB9-CB8
27	T	102	CDL	C34-C35-C36-C37
19	A	611	TGL	CA2-CA3-CA4-CA5
19	A	611	TGL	CC4-CC5-CC6-CC7
19	A	608	TGL	C23-C24-C25-C26
20	C	308	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	C	304	PGV	C10-C11-C12-C13
27	T	102	CDL	C37-C38-C39-C40
27	C	305	CDL	OA5-CA3-CA4-CA6
20	C	308	PGV	C01-C02-C03-O11
28	G	101	PEK	C26-C27-C28-C29
19	N	611	TGL	C33-C34-C35-C36
19	Y	101	TGL	C13-C14-C29-C30
27	C	305	CDL	C37-C38-C39-C40
20	P	304	PGV	C02-C03-O11-P
27	N	601	CDL	CA3-CA4-CA6-OA8
27	N	601	CDL	CB3-CB4-CB6-OB8
27	P	305	CDL	CA3-CA4-CA6-OA8
19	A	608	TGL	OG1-CG1-CG2-CG3
20	P	302	PGV	O03-C01-C02-C03
27	C	305	CDL	C31-C32-C33-C34
28	C	309	PEK	C13-C14-C15-C16
20	C	308	PGV	C6-C7-C8-C9
19	A	608	TGL	C17-C18-C19-C33
19	Y	101	TGL	C11-C10-CB9-CB8
24	B	303	PSC	C9-C10-C11-C12
24	B	303	PSC	C10-C11-C12-C13
24	N	612	PSC	C10-C11-C12-C13
28	C	309	PEK	C11-C10-C9-C8
28	C	309	PEK	C9-C10-C11-C12
28	C	309	PEK	C12-C13-C14-C15
28	G	103	PEK	C6-C7-C8-C9
28	G	103	PEK	C11-C12-C13-C14
28	G	103	PEK	C12-C13-C14-C15
28	T	101	PEK	C11-C10-C9-C8
28	G	101	PEK	C9-C10-C11-C12
28	P	308	PEK	C9-C10-C11-C12
28	P	308	PEK	C12-C13-C14-C15
28	C	307	PEK	C5-C6-C7-C8
28	C	307	PEK	C6-C7-C8-C9
28	C	307	PEK	C11-C10-C9-C8
27	T	102	CDL	C21-C22-C23-C24
20	N	609	PGV	O01-C02-C03-O11
28	C	307	PEK	O01-C02-C03-O11
28	P	308	PEK	C29-C30-C31-C32
27	P	305	CDL	CB5-C51-C52-C53
27	N	601	CDL	O1-C1-CB2-OB2
19	A	611	TGL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	A	610	PGV	C15-C16-C17-C18
27	T	102	CDL	C62-C63-C64-C65
27	P	305	CDL	OA6-CA4-CA6-OA8
20	N	609	PGV	O03-C01-C02-O01
27	C	305	CDL	OB6-CB4-CB6-OB8
19	D	201	TGL	OG1-CG1-CG2-OG2
20	N	609	PGV	C20-C21-C22-C23
28	P	308	PEK	C35-C36-C37-C38
20	N	610	PGV	C30-C31-C32-C33
27	N	601	CDL	CA2-C1-CB2-OB2
20	C	308	PGV	O12-C04-C05-C06
19	Q	201	TGL	C15-C16-C17-C18
20	C	304	PGV	C22-C23-C24-C25
19	N	611	TGL	C13-C14-C29-C30
24	N	612	PSC	C02-C03-O11-P
20	C	304	PGV	C02-C03-O11-P
27	C	305	CDL	C1-CA2-OA2-PA1
24	N	612	PSC	C6-C7-C8-C9
25	Z	101	DMU	C31-C34-C37-C40
27	C	305	CDL	C53-C54-C55-C56
25	P	307	DMU	C22-C25-C28-C31
21	D	202	EDO	O1-C1-C2-O2
21	B	304	EDO	O1-C1-C2-O2
21	A	616	EDO	O1-C1-C2-O2
20	N	610	PGV	C13-C14-C15-C16
19	A	611	TGL	C33-C34-C35-C36
28	G	101	PEK	C35-C36-C37-C38
27	C	305	CDL	C24-C25-C26-C27
20	N	610	PGV	C27-C28-C29-C30
22	P	306	CHD	C20-C22-C23-C24
19	Y	101	TGL	C20-C21-C22-C23
20	N	609	PGV	C01-C02-C03-O11
20	P	302	PGV	C23-C24-C25-C26
28	C	309	PEK	C7-C8-C9-C10
19	A	611	TGL	CA6-CA7-CA8-CA9
25	P	310	DMU	C34-C37-C40-C43
20	C	308	PGV	C14-C15-C16-C17
27	T	102	CDL	C64-C65-C66-C67
19	N	611	TGL	C11-C12-C13-C14
28	G	103	PEK	C28-C29-C30-C31
27	N	601	CDL	C53-C54-C55-C56
20	N	609	PGV	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
19	Q	201	TGL	CA3-CA4-CA5-CA6
19	A	611	TGL	CB4-CB5-CB6-CB7
20	P	304	PGV	C28-C29-C30-C31
19	A	611	TGL	OG1-CG1-CG2-CG3
20	N	609	PGV	C05-C04-O12-P
19	D	201	TGL	CG1-CG2-CG3-OG3
27	N	601	CDL	C21-C22-C23-C24
27	T	102	CDL	OB5-CB3-CB4-OB6
27	C	305	CDL	OA5-CA3-CA4-OA6
20	C	308	PGV	O01-C02-C03-O11
19	N	611	TGL	CA9-C20-C21-C22
27	C	305	CDL	C84-C85-C86-C87
27	N	601	CDL	OB7-CB5-OB6-CB4
25	C	302	DMU	O16-C18-C19-C22
19	A	611	TGL	C20-C21-C22-C23
24	B	303	PSC	O03-C01-C02-O01
24	N	612	PSC	O03-C01-C02-O01
27	P	305	CDL	OB6-CB4-CB6-OB8
20	A	610	PGV	O05-C05-C06-O06
28	C	309	PEK	C22-C23-C24-C25
19	A	611	TGL	C29-C30-C31-C32
20	N	609	PGV	C11-C10-C9-C8
20	N	609	PGV	C12-C13-C14-C15
19	D	201	TGL	CA3-CA4-CA5-CA6
20	C	304	PGV	C1-C2-C3-C4
19	D	201	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	CB2-CB3-CB4-CB5
24	N	612	PSC	C11-C12-C13-C14
25	P	307	DMU	O16-C18-C19-C22
28	P	308	PEK	C26-C27-C28-C29
27	P	305	CDL	C22-C23-C24-C25
19	Y	101	TGL	CA9-C20-C21-C22
20	C	308	PGV	C3-C4-C5-C6
24	B	303	PSC	C4-C5-C6-C7
24	B	303	PSC	C6-C7-C8-C9
20	A	609	PGV	C11-C10-C9-C8
27	T	102	CDL	CB3-OB5-PB2-OB2
24	N	612	PSC	C04-O12-P-O11
27	P	305	CDL	CA5-C11-C12-C13
27	C	305	CDL	CA4-CA3-OA5-PA1
27	T	102	CDL	OB9-CB7-OB8-CB6
20	A	610	PGV	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
20	A	610	PGV	C04-O12-P-O14
27	N	601	CDL	CA2-OA2-PA1-OA3
27	N	601	CDL	CB2-OB2-PB2-OB3
24	N	612	PSC	C03-O11-P-O13
28	C	309	PEK	C04-O12-P-O13
27	P	305	CDL	CA2-OA2-PA1-OA4
27	C	305	CDL	CA3-OA5-PA1-OA3
20	C	308	PGV	C04-O12-P-O13
28	P	308	PEK	C03-O11-P-O13
28	C	307	PEK	C04-O12-P-O13
20	P	302	PGV	C03-O11-P-O13
19	Q	201	TGL	C29-C30-C31-C32
27	T	102	CDL	C55-C56-C57-C58
28	G	103	PEK	C35-C36-C37-C38
25	C	302	DMU	O5-C6-O16-C18
27	T	102	CDL	C71-CB7-OB8-CB6
28	G	103	PEK	C01-C02-C03-O11
27	P	305	CDL	OA5-CA3-CA4-CA6
28	P	308	PEK	C01-C02-C03-O11
27	N	601	CDL	C20-C21-C22-C23
21	A	619	EDO	O1-C1-C2-O2
21	N	618	EDO	O1-C1-C2-O2
27	T	102	CDL	C73-C74-C75-C76
25	M	101	DMU	C22-C25-C28-C31
28	C	307	PEK	C05-C04-O12-P
20	A	610	PGV	C12-C13-C14-C15
25	C	310	DMU	O6-C11-C9-C8
27	C	305	CDL	C55-C56-C57-C58
24	B	303	PSC	O01-C02-C03-O11
28	C	309	PEK	O01-C02-C03-O11
27	P	305	CDL	OA5-CA3-CA4-OA6
27	C	305	CDL	C17-C18-C19-C20
27	N	601	CDL	C51-CB5-OB6-CB4
20	N	609	PGV	C28-C29-C30-C31
14	A	602[A]	HEA	C2D-C3D-CAD-CBD
28	C	307	PEK	C34-C35-C36-C37
28	P	308	PEK	C4-C5-C6-C7
24	N	612	PSC	C30-C31-C32-C33
20	P	302	PGV	C9-C10-C11-C12
28	G	101	PEK	C24-C25-C26-C27
20	P	302	PGV	C31-C32-C33-C34
28	G	103	PEK	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	C33-C34-C35-C36
28	G	101	PEK	C33-C34-C35-C36
20	C	304	PGV	C20-C21-C22-C23
25	C	310	DMU	C19-C22-C25-C28
20	P	304	PGV	C12-C13-C14-C15
19	D	201	TGL	C16-C15-CC9-CC8
28	G	103	PEK	C4-C5-C6-C7
20	A	609	PGV	C10-C11-C12-C13
28	G	101	PEK	C4-C5-C6-C7
20	N	610	PGV	C10-C11-C12-C13
19	D	201	TGL	CB2-CB1-OG2-CG2
28	T	101	PEK	O03-C21-C22-C23
19	Y	101	TGL	CC5-CC6-CC7-CC8
27	N	601	CDL	C75-C76-C77-C78
19	D	201	TGL	CG3-CG2-OG2-CB1
28	T	101	PEK	O02-C1-O01-C02
19	N	611	TGL	CA2-CA1-OG1-CG1
25	Z	101	DMU	C19-C22-C25-C28
24	B	303	PSC	C02-C03-O11-P
24	B	303	PSC	C22-C23-C24-C25
21	Y	102	EDO	O1-C1-C2-O2
24	N	612	PSC	C7-C8-C9-C10
24	B	303	PSC	C04-O12-P-O11
27	T	102	CDL	CA2-OA2-PA1-OA5
27	T	102	CDL	CB2-OB2-PB2-OB5
28	G	103	PEK	C03-O11-P-O12
20	N	609	PGV	C03-O11-P-O12
28	C	307	PEK	C03-O11-P-O12
20	P	302	PGV	C04-O12-P-O11
27	C	305	CDL	CA3-CA4-CA6-OA8
19	N	611	TGL	C21-C20-CA9-CA8
20	P	302	PGV	C19-C20-C21-C22
19	D	201	TGL	OG2-CB1-CB2-CB3
20	N	610	PGV	C28-C29-C30-C31
20	P	304	PGV	C05-C04-O12-P
20	N	609	PGV	C13-C14-C15-C16
19	N	611	TGL	CB2-CB3-CB4-CB5
14	N	602	HEA	C12-C13-C14-C15
27	T	102	CDL	C80-C81-C82-C83
19	A	608	TGL	CA7-CA8-CA9-C20
19	N	611	TGL	OA1-CA1-OG1-CG1
20	P	304	PGV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	CA4-CA5-CA6-CA7
19	Q	201	TGL	OG1-CA1-CA2-CA3
19	D	201	TGL	CB5-CB6-CB7-CB8
24	B	303	PSC	C3-C4-C5-C6
25	C	302	DMU	C19-C22-C25-C28
19	A	608	TGL	C22-C23-C24-C25
27	N	601	CDL	C64-C65-C66-C67
27	T	102	CDL	C74-C75-C76-C77
25	C	310	DMU	C25-C28-C31-C34
25	P	309	DMU	C34-C37-C40-C43
27	C	305	CDL	C51-C52-C53-C54
20	C	308	PGV	C27-C28-C29-C30
22	P	301	CHD	C16-C17-C20-C22
25	P	309	DMU	O16-C18-C19-C22
20	N	610	PGV	C31-C32-C33-C34
19	N	611	TGL	C15-C16-C17-C18
20	C	304	PGV	C30-C31-C32-C33
19	D	201	TGL	CG1-CG2-OG2-CB1
20	N	610	PGV	C11-C12-C13-C14
28	T	101	PEK	C5-C6-C7-C8
28	C	307	PEK	C9-C10-C11-C12
28	C	307	PEK	C11-C12-C13-C14
20	C	304	PGV	C05-C04-O12-P
19	Q	201	TGL	OG2-CB1-CB2-CB3
19	A	611	TGL	OG1-CA1-CA2-CA3
20	P	304	PGV	C21-C22-C23-C24
28	C	307	PEK	C01-C02-C03-O11
20	N	609	PGV	C24-C25-C26-C27
27	P	305	CDL	C12-C13-C14-C15
27	P	305	CDL	C56-C57-C58-C59
19	D	201	TGL	C12-C13-C14-C29
27	P	305	CDL	C41-C42-C43-C44
28	C	309	PEK	C15-C16-C17-C18
28	G	103	PEK	C13-C14-C15-C16
27	C	305	CDL	C62-C63-C64-C65
24	B	303	PSC	C26-C27-C28-C29
19	N	611	TGL	OG1-CA1-CA2-CA3
27	N	601	CDL	C83-C84-C85-C86
20	A	609	PGV	O03-C19-C20-C21
27	T	102	CDL	C20-C21-C22-C23
24	N	612	PSC	C14-C15-C16-C17
19	D	201	TGL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C26-C15-C16-C17
28	C	307	PEK	O01-C1-C2-C3
19	Y	101	TGL	CC2-CC3-CC4-CC5
28	P	308	PEK	C32-C33-C34-C35
19	Q	201	TGL	C16-C17-C18-C19
24	N	612	PSC	C22-C23-C24-C25
28	G	101	PEK	C22-C23-C24-C25
20	C	304	PGV	C9-C10-C11-C12
28	G	103	PEK	C3-C4-C5-C6
24	B	303	PSC	C04-C05-N-C06
14	N	602	HEA	C26-C15-C16-C17
19	N	611	TGL	CC7-CC8-CC9-C15
28	G	101	PEK	O12-C04-C05-N
25	C	310	DMU	C31-C34-C37-C40
28	G	103	PEK	O03-C21-C22-C23
19	A	611	TGL	OC1-CC1-OG3-CG3
27	N	601	CDL	C78-C79-C80-C81
28	G	101	PEK	C27-C28-C29-C30
20	C	304	PGV	C25-C26-C27-C28
20	N	609	PGV	O03-C19-C20-C21
19	A	608	TGL	CC9-C15-C16-C17
28	T	101	PEK	C15-C16-C17-C18
27	C	305	CDL	C22-C23-C24-C25
28	G	101	PEK	C17-C18-C19-C20
25	P	310	DMU	C31-C34-C37-C40
24	B	303	PSC	C7-C8-C9-C10
20	C	304	PGV	C11-C12-C13-C14
19	Q	201	TGL	OB1-CB1-OG2-CG2
24	N	612	PSC	C28-C29-C30-C31
14	N	602	HEA	C11-C12-C13-C14
19	D	201	TGL	OG1-CA1-CA2-CA3
27	N	601	CDL	C41-C42-C43-C44
20	C	308	PGV	C13-C14-C15-C16
28	T	101	PEK	O01-C1-C2-C3
20	N	610	PGV	O03-C19-C20-C21
20	A	610	PGV	C24-C25-C26-C27
28	P	308	PEK	C3-C4-C5-C6
20	A	610	PGV	O03-C01-C02-C03
27	N	601	CDL	C73-C74-C75-C76
20	C	304	PGV	C28-C29-C30-C31
19	A	608	TGL	OG3-CC1-CC2-CC3
20	C	308	PGV	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
21	E	202	EDO	O1-C1-C2-O2
21	A	613	EDO	O1-C1-C2-O2
24	B	303	PSC	C12-C13-C14-C15
28	C	307	PEK	C3-C4-C5-C6
19	N	611	TGL	C22-C23-C24-C25
20	P	302	PGV	C5-C6-C7-C8
20	P	302	PGV	C11-C10-C9-C8
27	N	601	CDL	C19-C20-C21-C22
19	Q	201	TGL	CB2-CB1-OG2-CG2
19	Q	201	TGL	CC2-CC3-CC4-CC5
20	A	610	PGV	O03-C01-C02-O01
19	A	608	TGL	CB5-CB6-CB7-CB8
24	B	303	PSC	C04-C05-N-C08
27	P	305	CDL	C58-C59-C60-C61
28	T	101	PEK	C2-C1-O01-C02
28	P	308	PEK	C17-C18-C19-C20
19	D	201	TGL	CB4-CB5-CB6-CB7
27	T	102	CDL	C12-C13-C14-C15
20	N	610	PGV	C14-C15-C16-C17
24	B	303	PSC	C20-C21-C22-C23
27	P	305	CDL	C84-C85-C86-C87
28	G	103	PEK	O04-C21-C22-C23
19	D	201	TGL	OA1-CA1-CA2-CA3
28	C	309	PEK	C26-C27-C28-C29
19	A	608	TGL	OC1-CC1-CC2-CC3
19	Y	101	TGL	CG1-CG2-CG3-OG3
20	A	610	PGV	C31-C32-C33-C34
14	N	603[B]	HEA	C26-C15-C16-C17
20	N	609	PGV	O04-C19-C20-C21
24	B	303	PSC	C04-C05-N-C07
27	T	102	CDL	CA2-OA2-PA1-OA3
27	T	102	CDL	CB2-OB2-PB2-OB3
20	N	609	PGV	C03-O11-P-O13
28	C	307	PEK	C03-O11-P-O14
28	G	103	PEK	C27-C28-C29-C30
21	A	615	EDO	O1-C1-C2-O2
21	B	305	EDO	O1-C1-C2-O2
28	T	101	PEK	O04-C21-C22-C23
19	N	611	TGL	C10-C11-C12-C13
28	G	103	PEK	C05-C04-O12-P
28	T	101	PEK	C05-C04-O12-P
28	T	101	PEK	O02-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
28	T	101	PEK	C33-C34-C35-C36
27	C	305	CDL	C12-C11-CA5-OA6
19	N	611	TGL	C16-C17-C18-C19
19	N	611	TGL	OG3-CC1-CC2-CC3
28	C	309	PEK	C33-C34-C35-C36
19	A	611	TGL	C18-C19-C33-C34
28	C	309	PEK	O03-C21-C22-C23
28	G	103	PEK	C22-C23-C24-C25
27	P	305	CDL	C44-C45-C46-C47
19	D	201	TGL	OC1-CC1-CC2-CC3
19	A	611	TGL	CC2-CC1-OG3-CG3
19	Y	101	TGL	C19-C33-C34-C35
25	P	309	DMU	C25-C28-C31-C34

There are no ring outliers.

58 monomers are involved in 363 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	310	DMU	3	0
14	A	601	HEA	8	0
20	A	610	PGV	9	0
22	J	101	CHD	1	0
27	N	601	CDL	29	0
21	D	202	EDO	9	0
22	C	306	CHD	5	0
19	Q	201	TGL	12	0
27	T	102	CDL	16	0
24	N	612	PSC	16	0
22	C	301	CHD	1	0
24	B	303	PSC	15	0
21	B	304	EDO	2	0
19	N	611	TGL	7	0
22	W	101	CHD	1	0
18	N	607[B]	AZI	1	0
18	A	606[B]	AZI	1	0
20	C	304	PGV	3	0
28	C	309	PEK	4	0
19	A	611	TGL	6	0
18	N	608[B]	AZI	1	0
21	A	618	EDO	2	0
28	G	103	PEK	1	0
14	N	603[A]	HEA	5	0

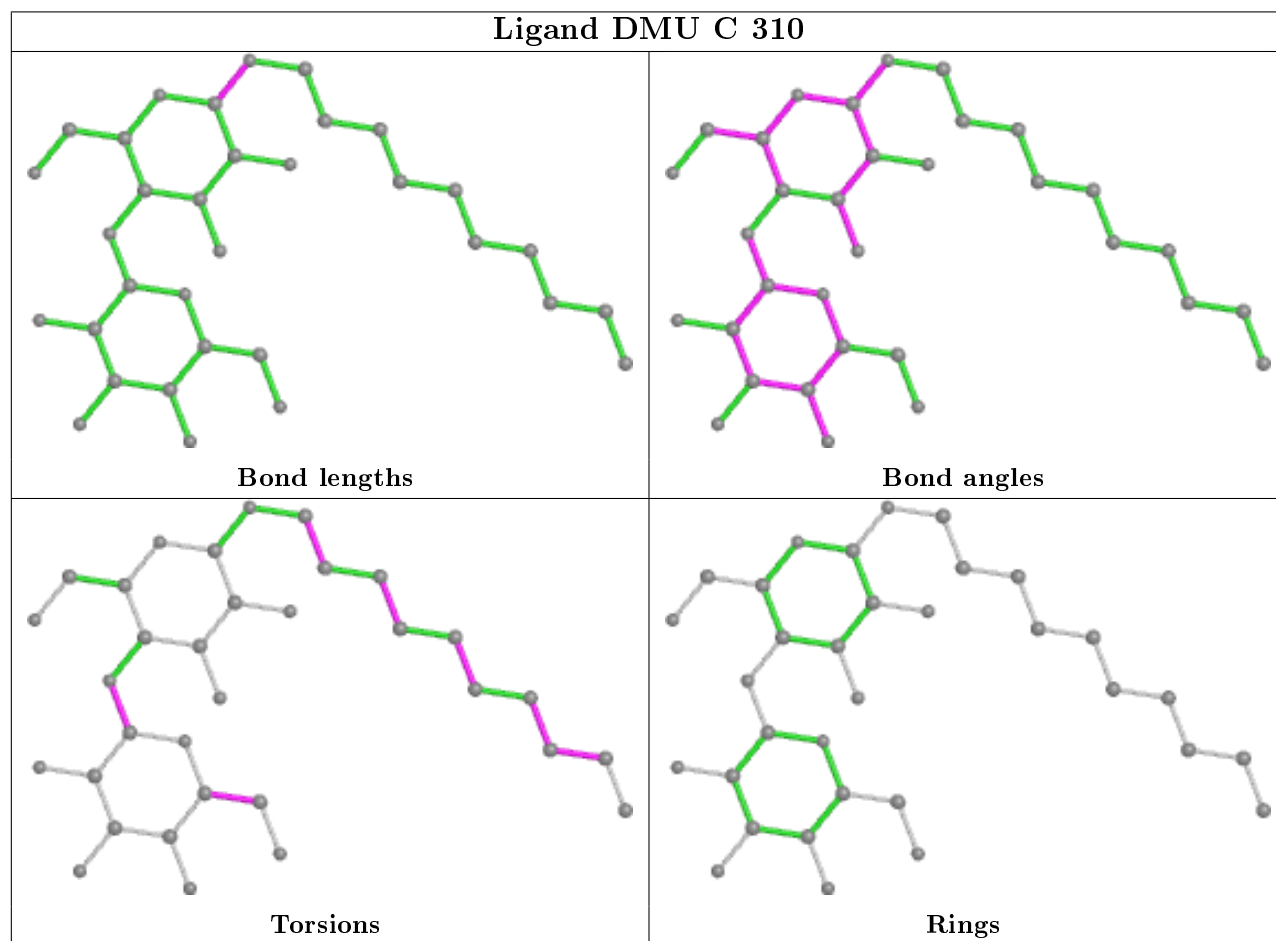
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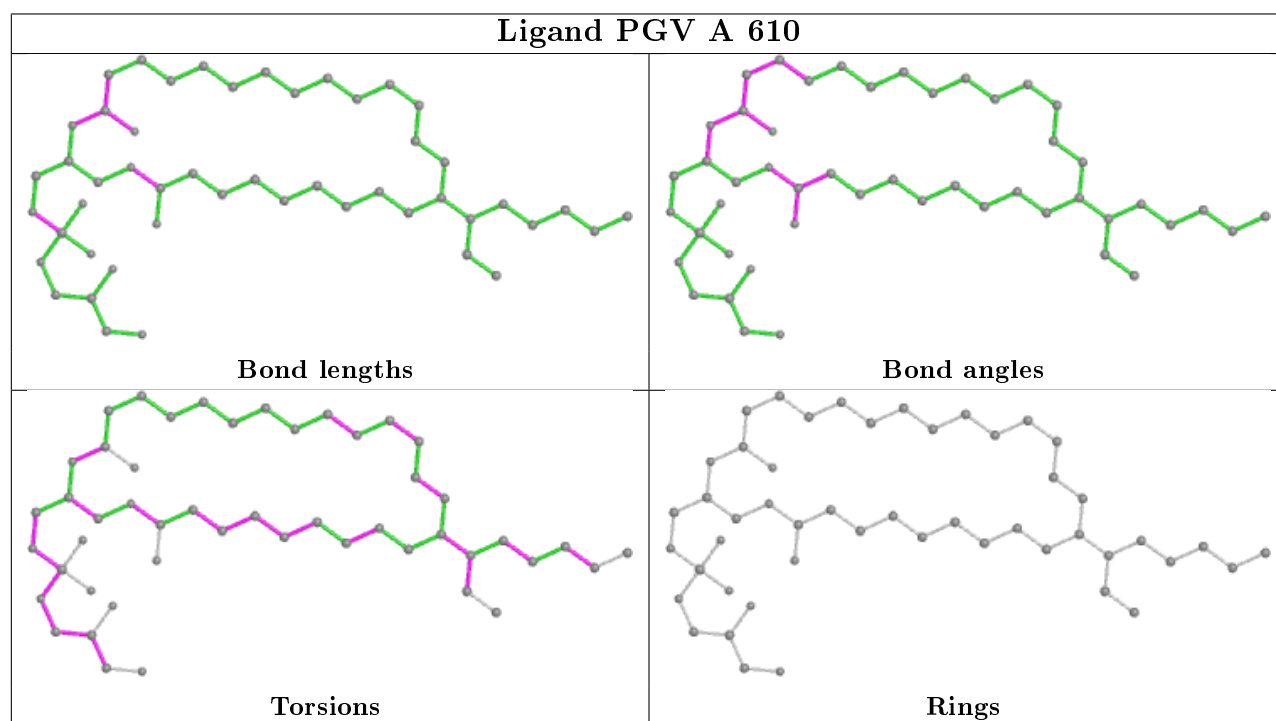
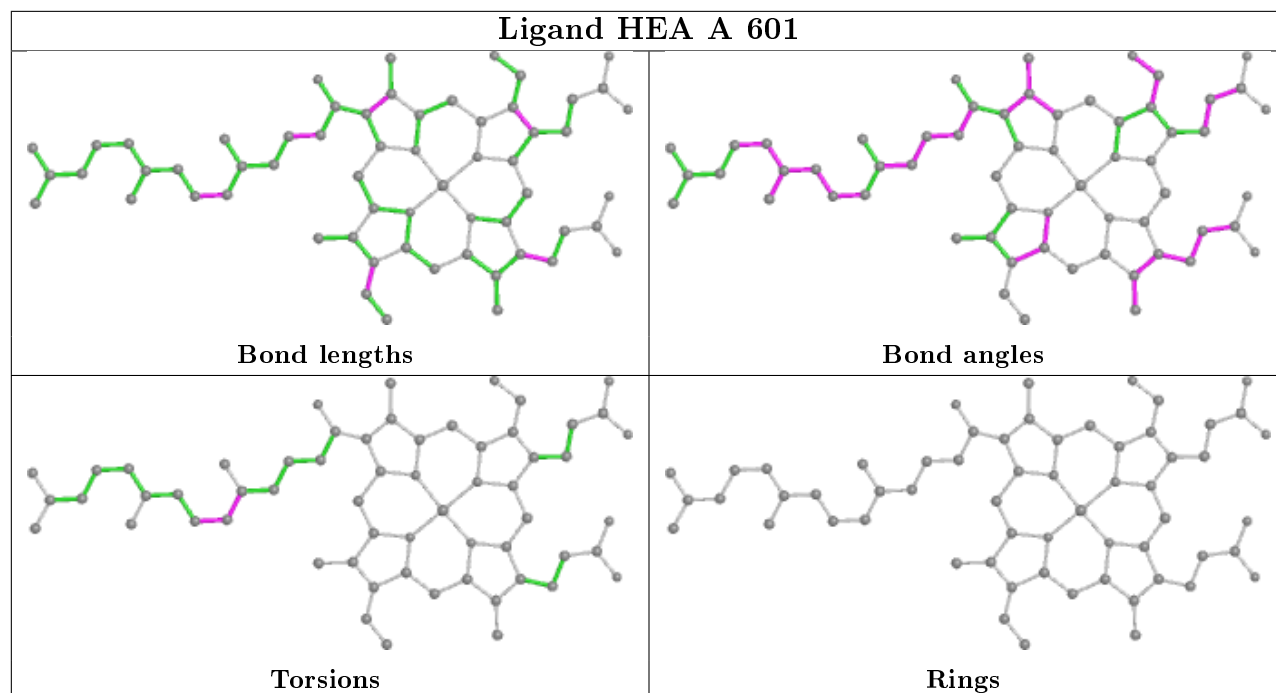
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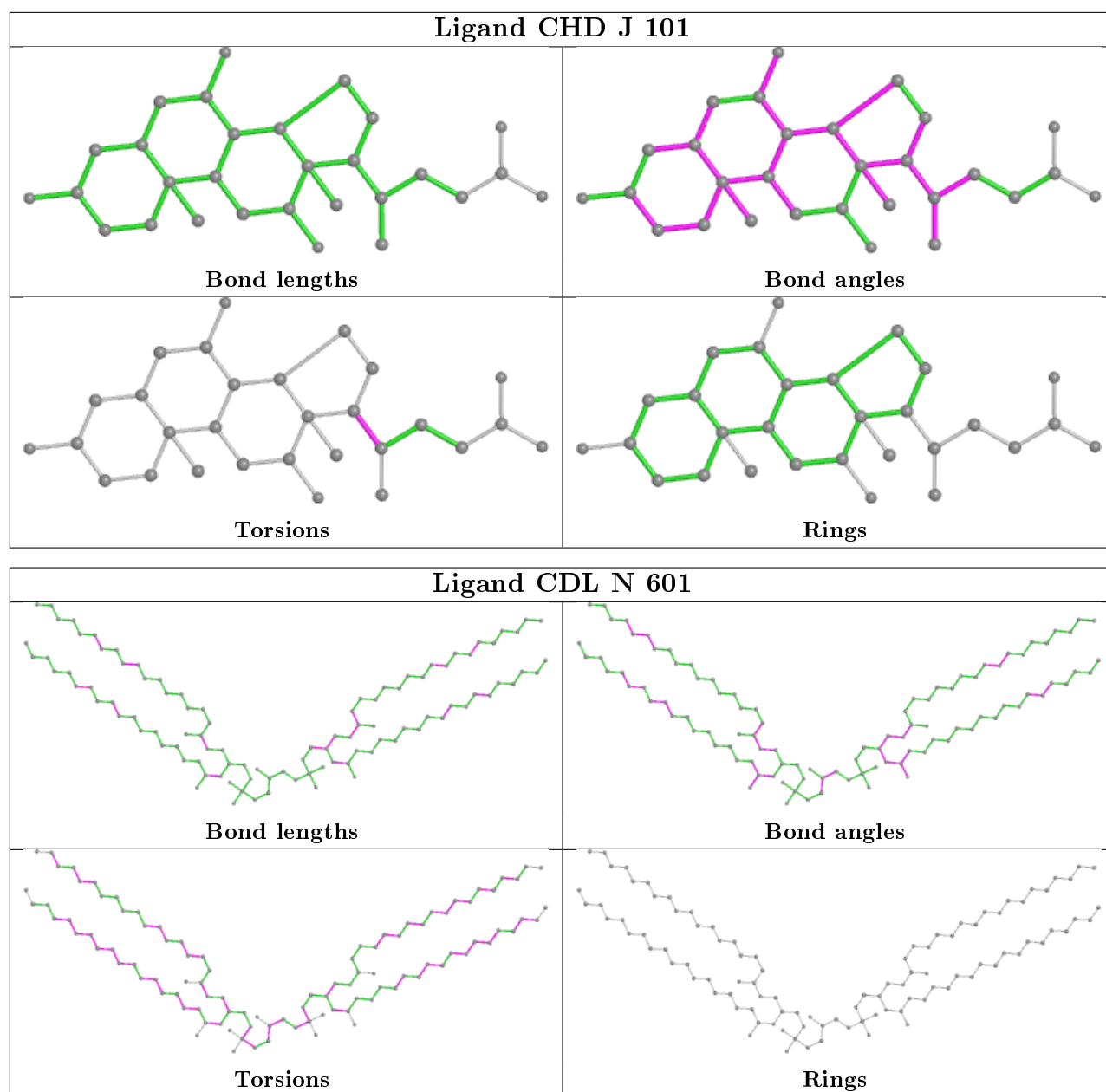
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	P	305	CDL	24	0
18	A	607[A]	AZI	2	0
25	C	302	DMU	12	0
18	A	607[B]	AZI	5	0
19	A	608	TGL	5	0
14	N	602	HEA	11	0
22	P	306	CHD	5	0
20	P	304	PGV	2	0
20	N	609	PGV	9	0
22	G	102	CHD	1	0
21	A	619	EDO	3	0
19	Y	101	TGL	20	0
28	T	101	PEK	3	0
20	A	609	PGV	4	0
25	P	309	DMU	3	0
28	G	101	PEK	7	0
25	P	307	DMU	11	0
22	P	301	CHD	1	0
14	A	602[A]	HEA	5	0
14	A	602[B]	HEA	12	0
21	N	621	EDO	1	0
25	P	310	DMU	2	0
27	C	305	CDL	17	0
20	C	308	PGV	1	0
18	N	608[A]	AZI	1	0
19	D	201	TGL	13	0
21	G	105	EDO	3	0
21	A	616	EDO	2	0
14	N	603[B]	HEA	12	0
28	P	308	PEK	6	0
20	N	610	PGV	1	0
28	C	307	PEK	11	0
20	P	302	PGV	1	0
21	A	620	EDO	1	0

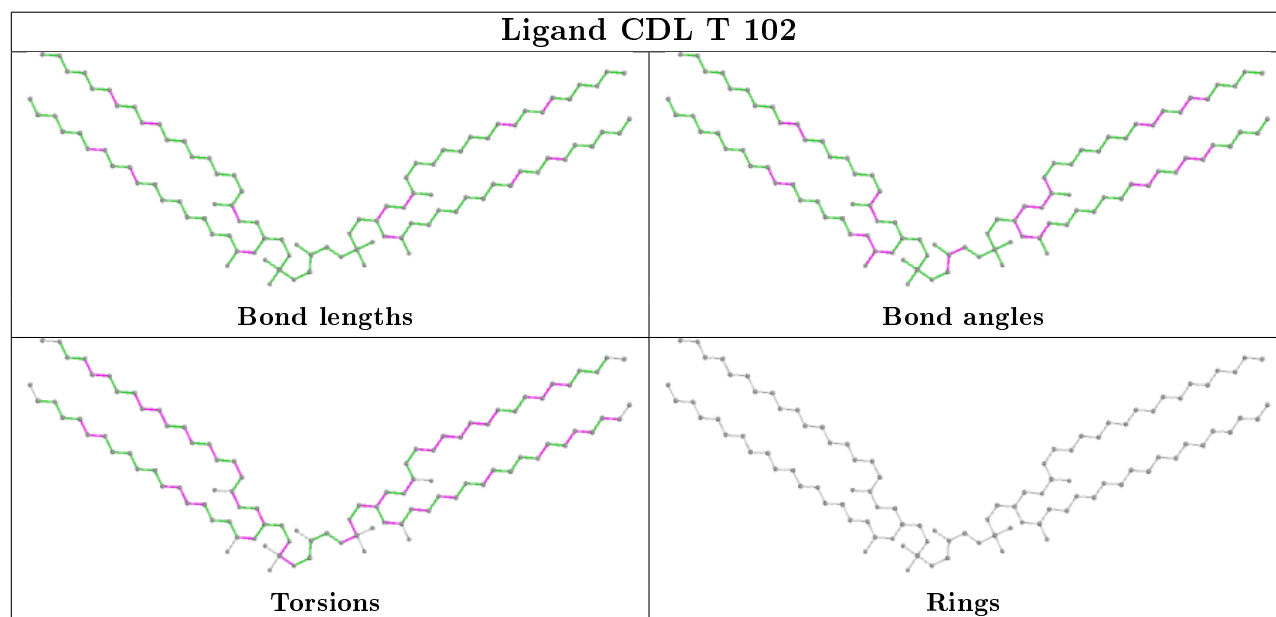
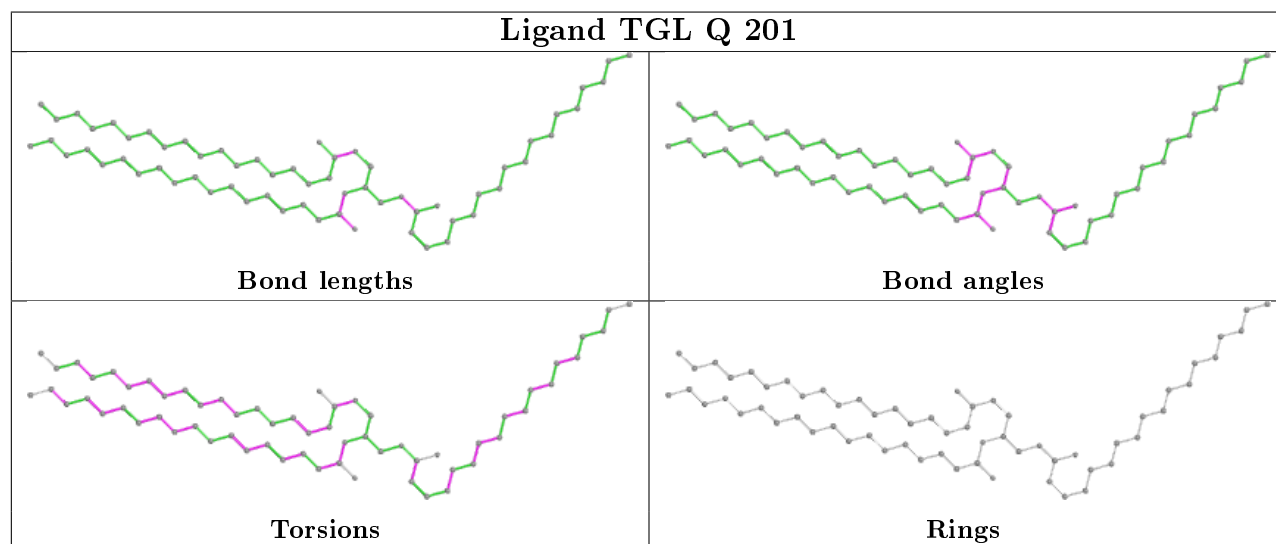
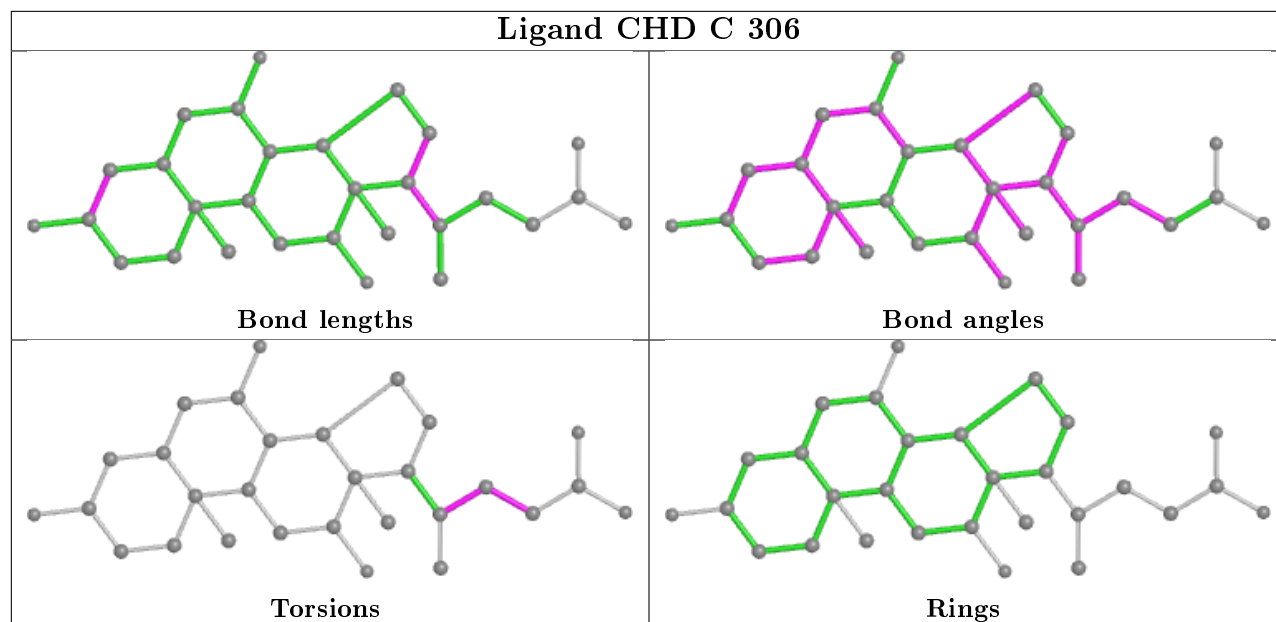
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

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

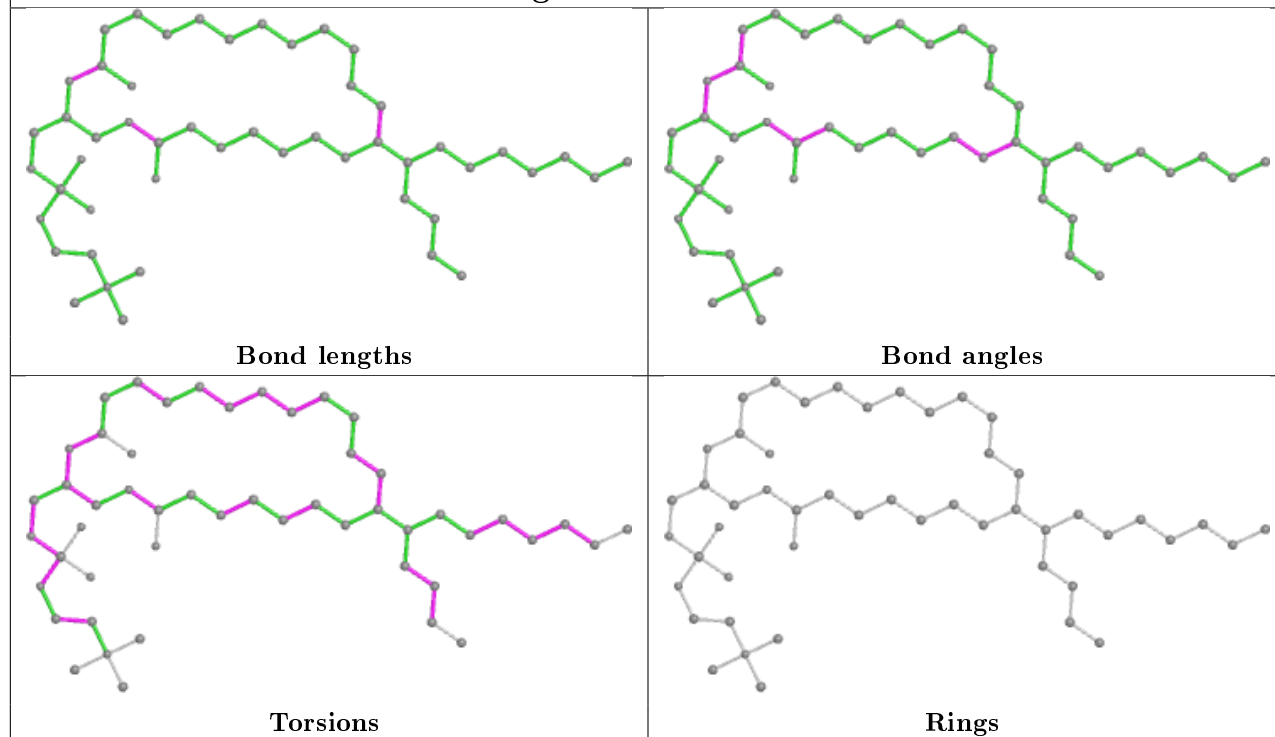




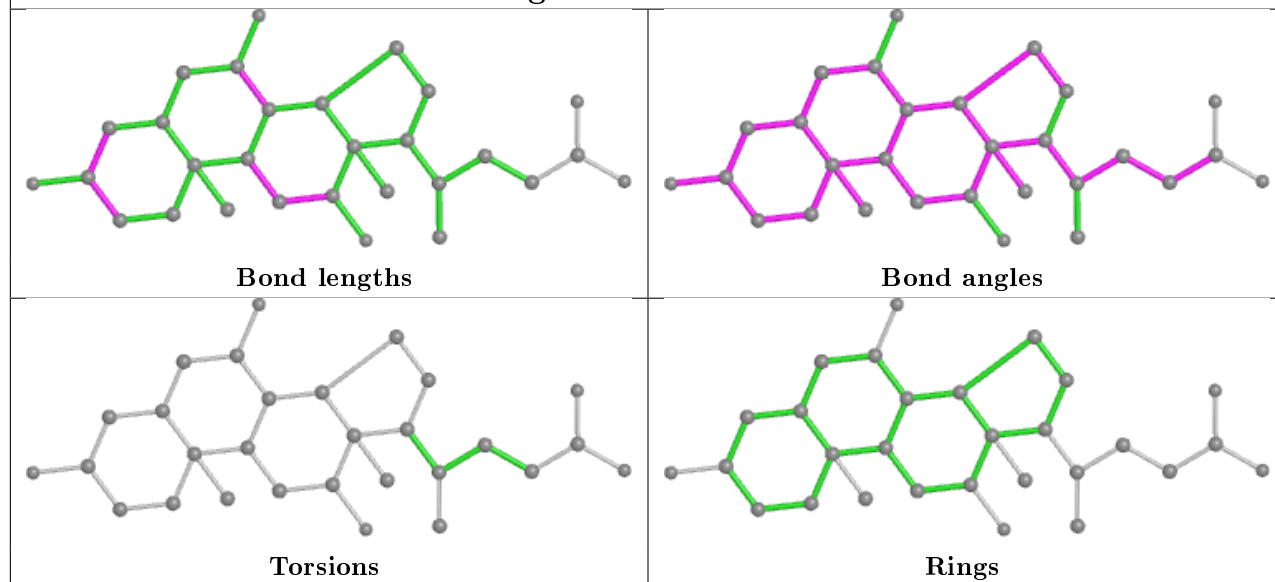


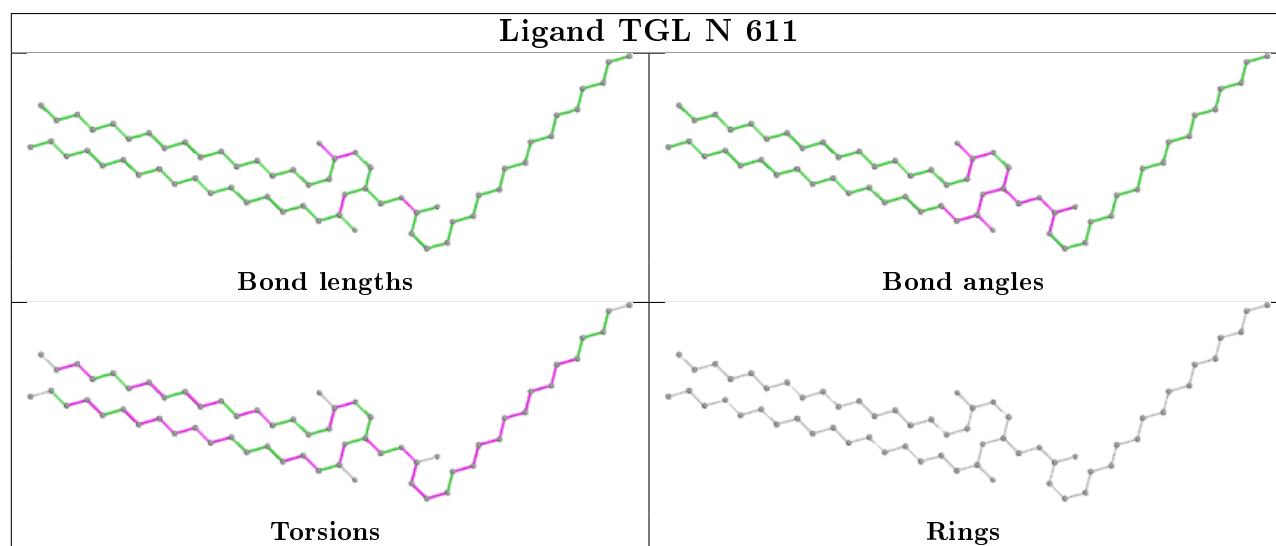
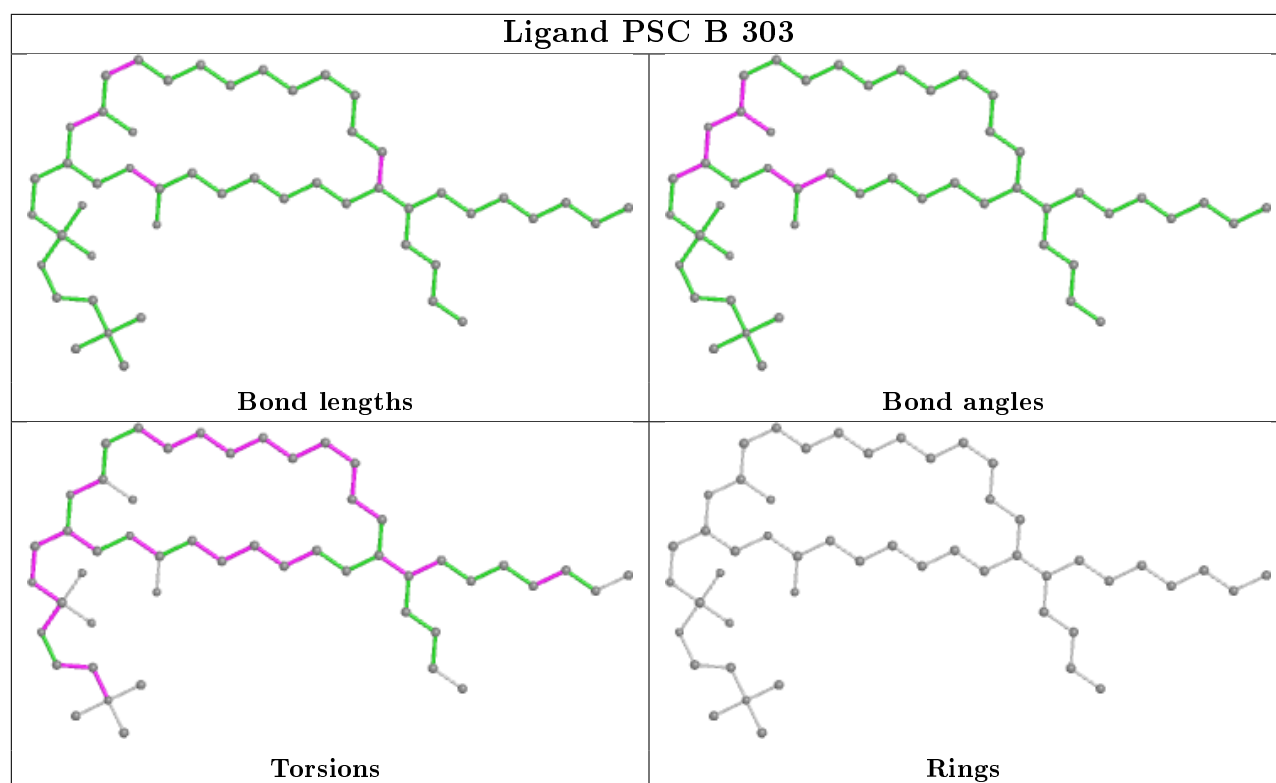


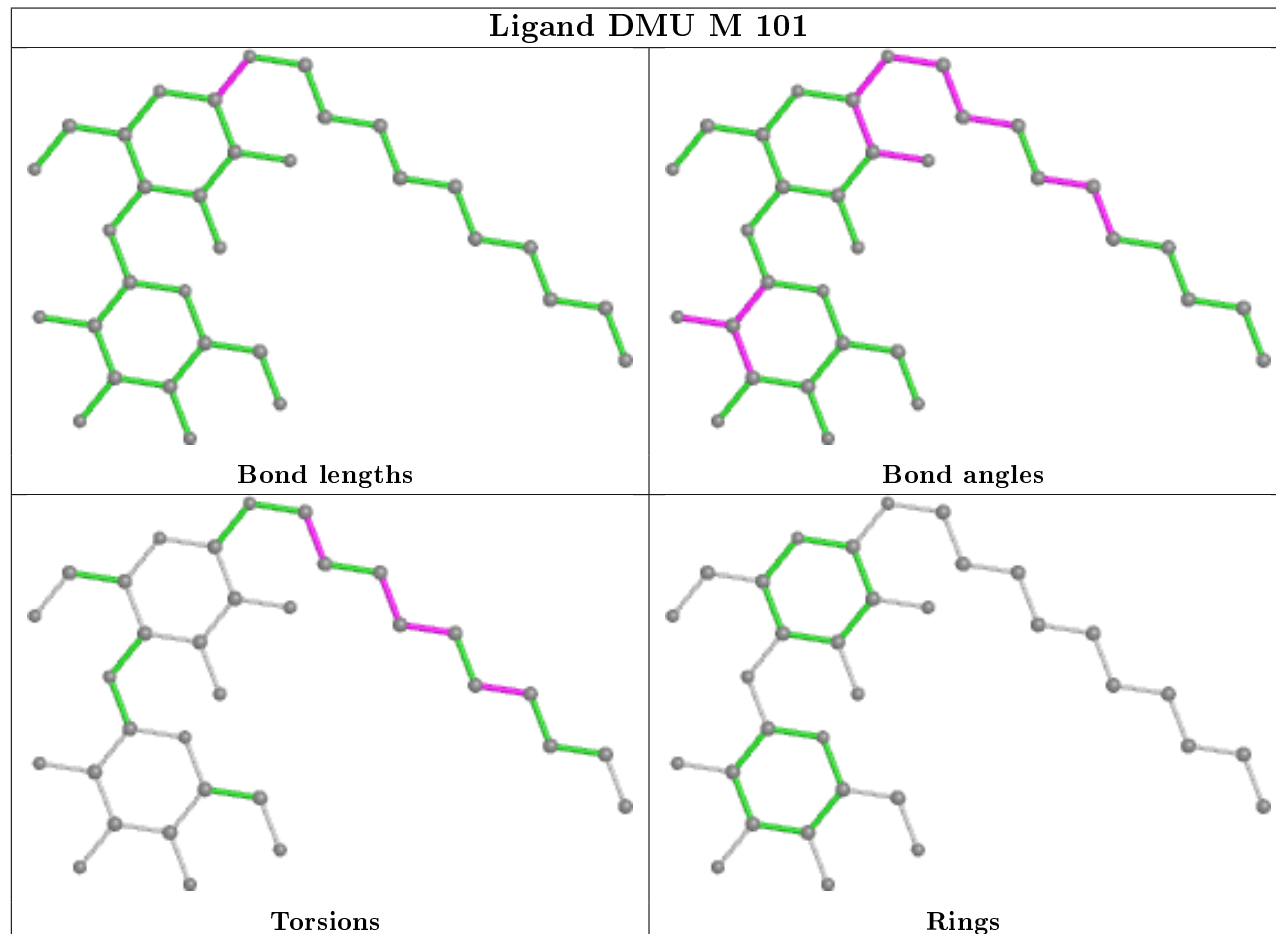
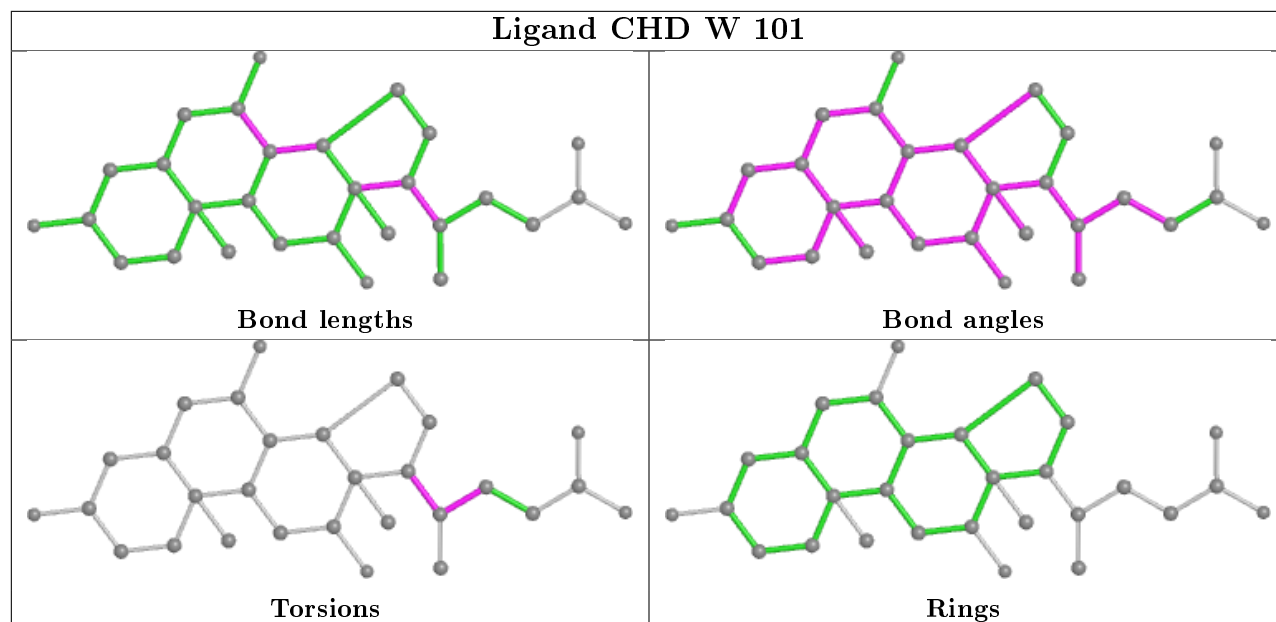
Ligand PSC N 612



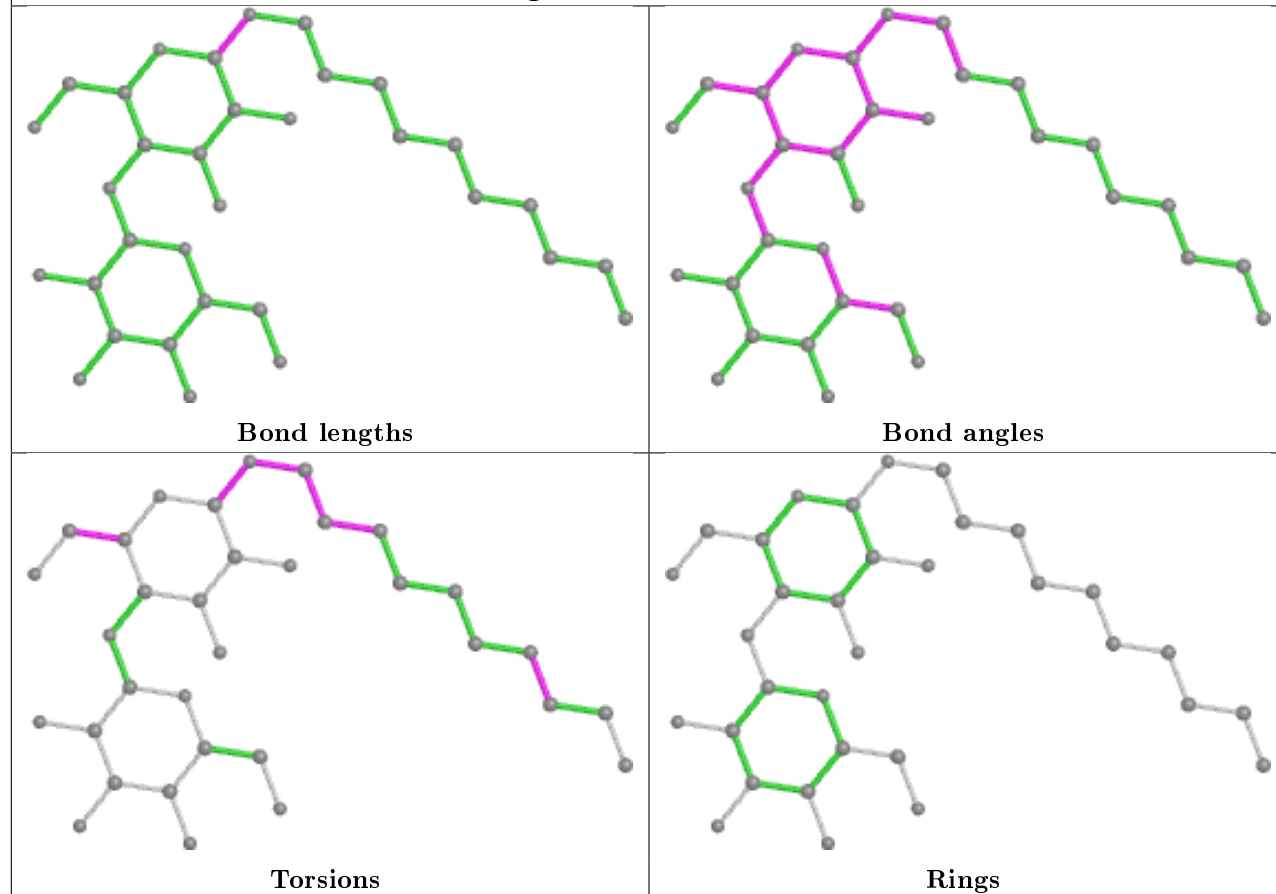
Ligand CHD C 301



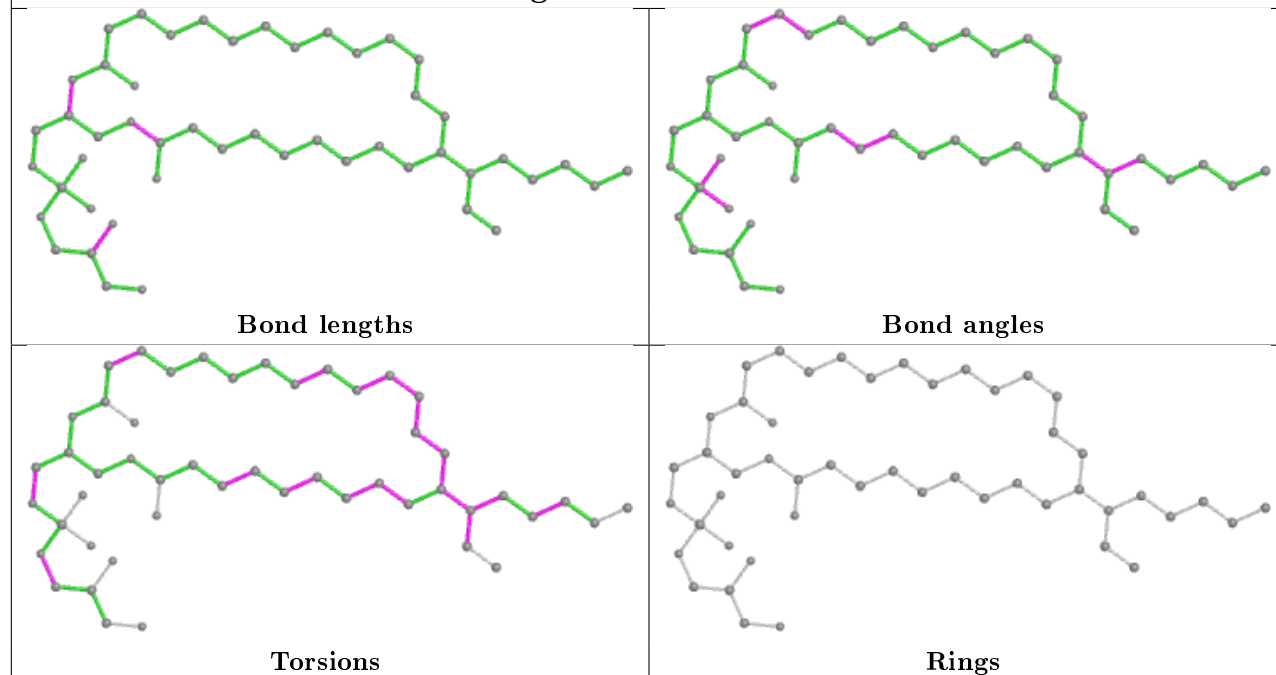




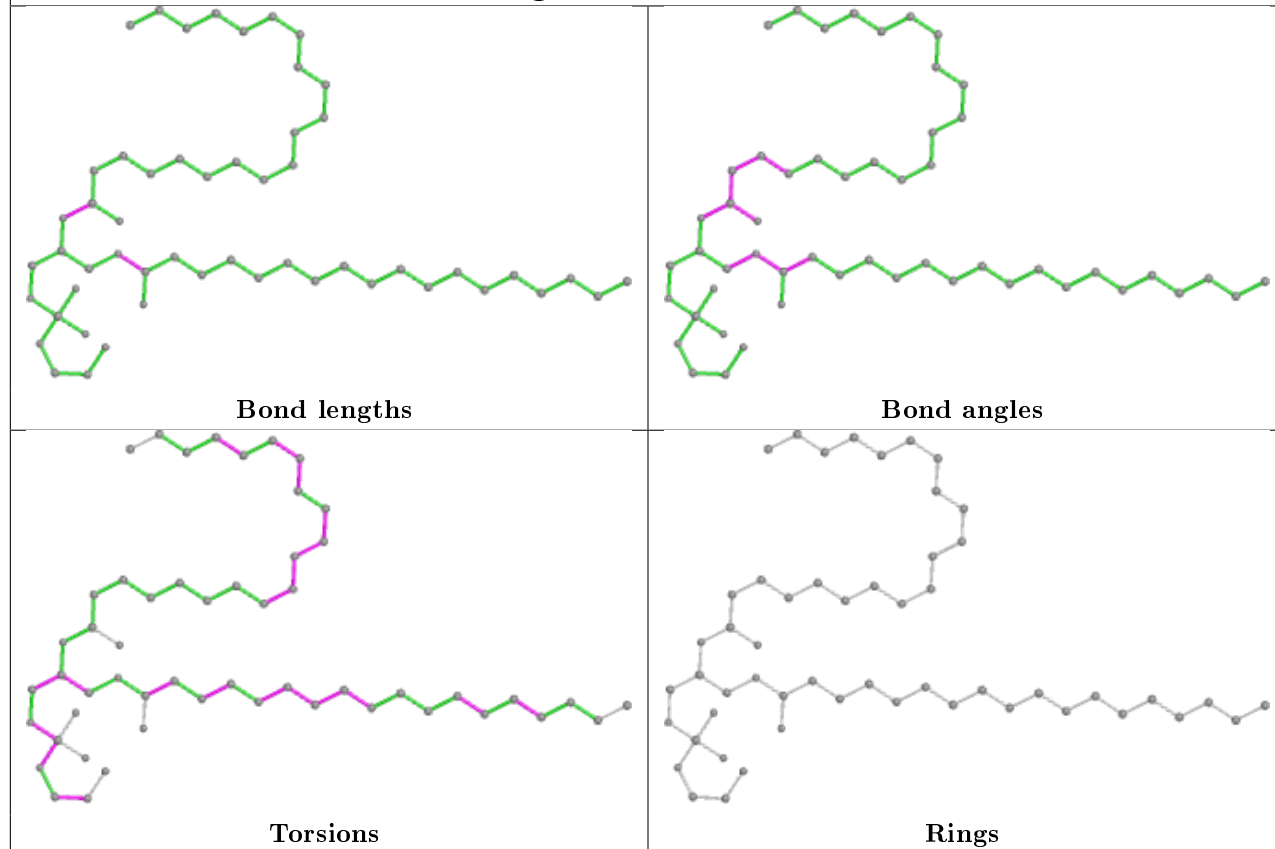
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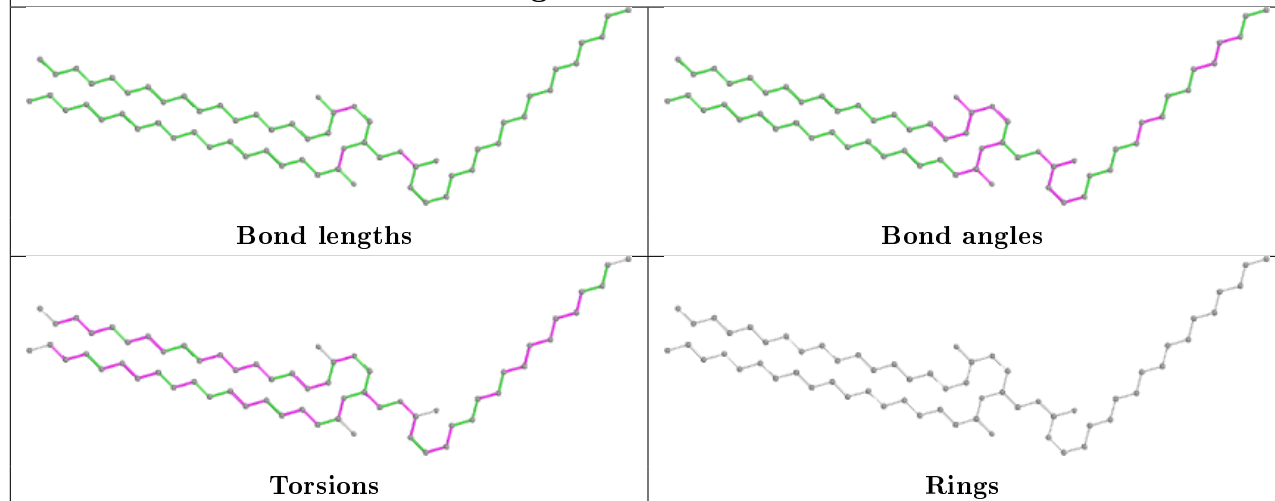
Ligand PGV C 304

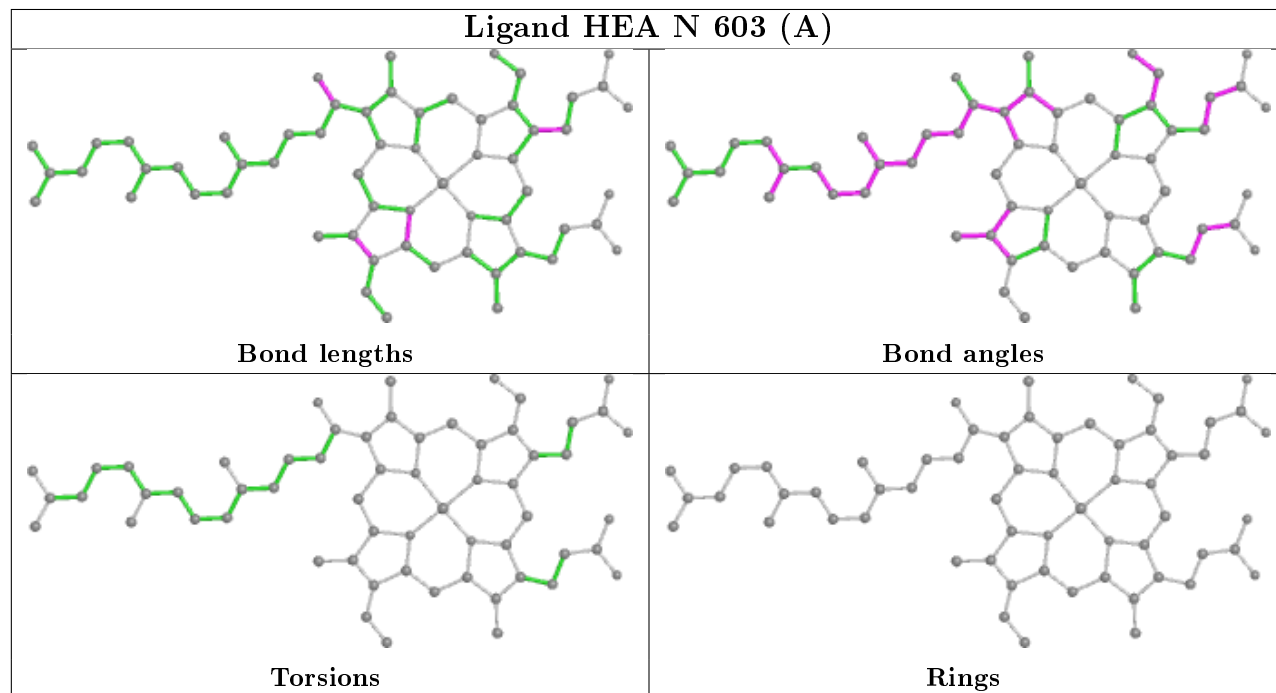
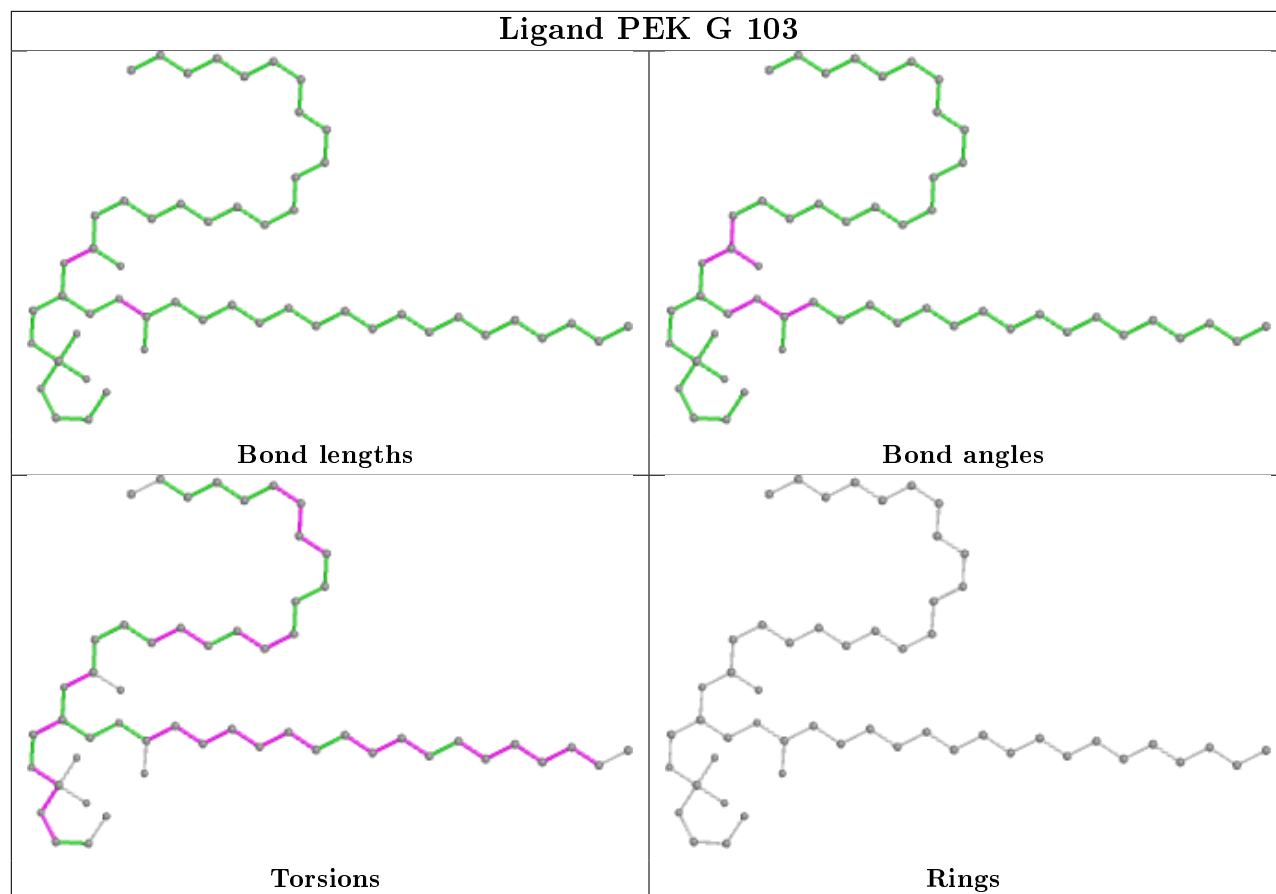


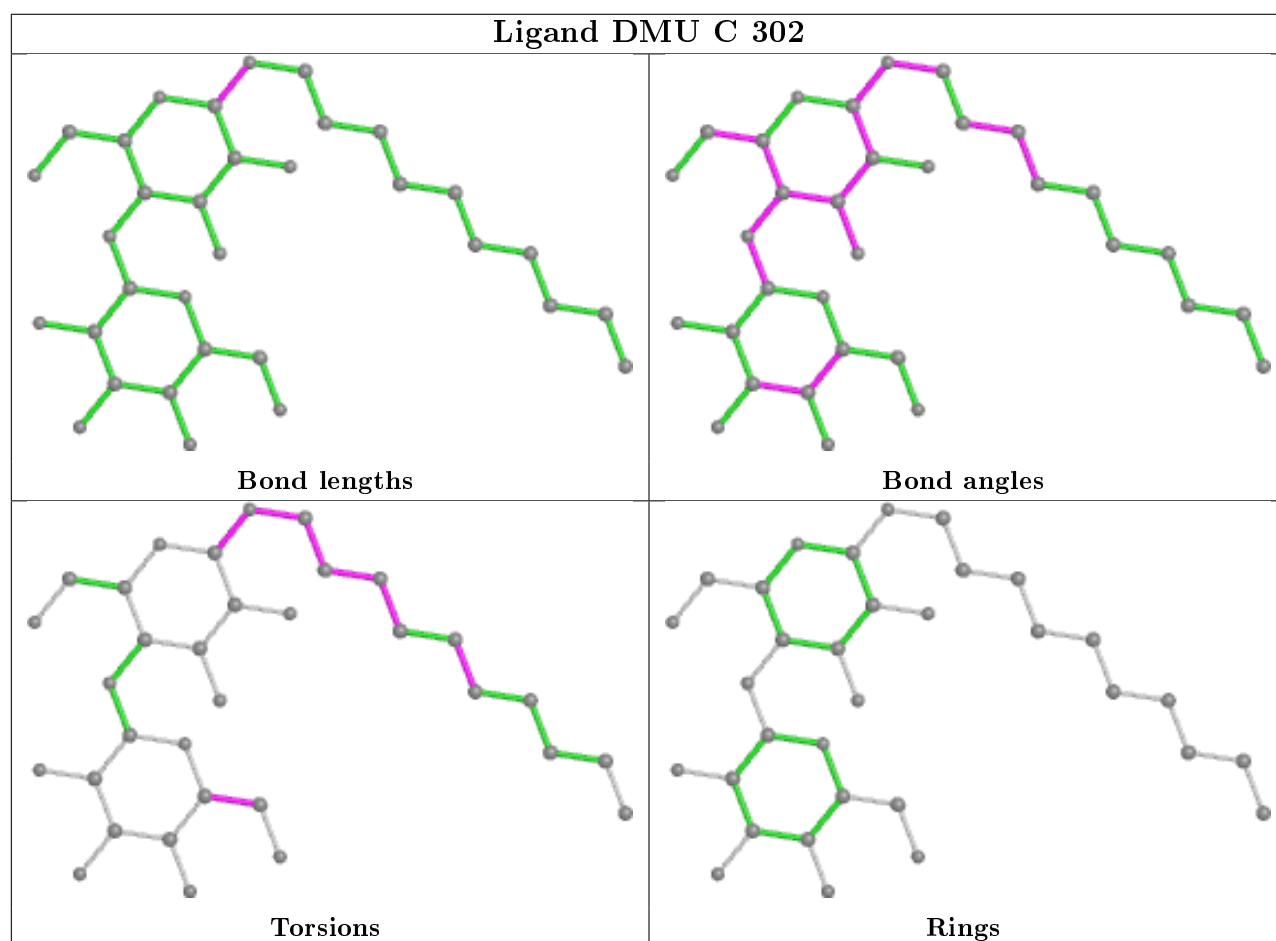
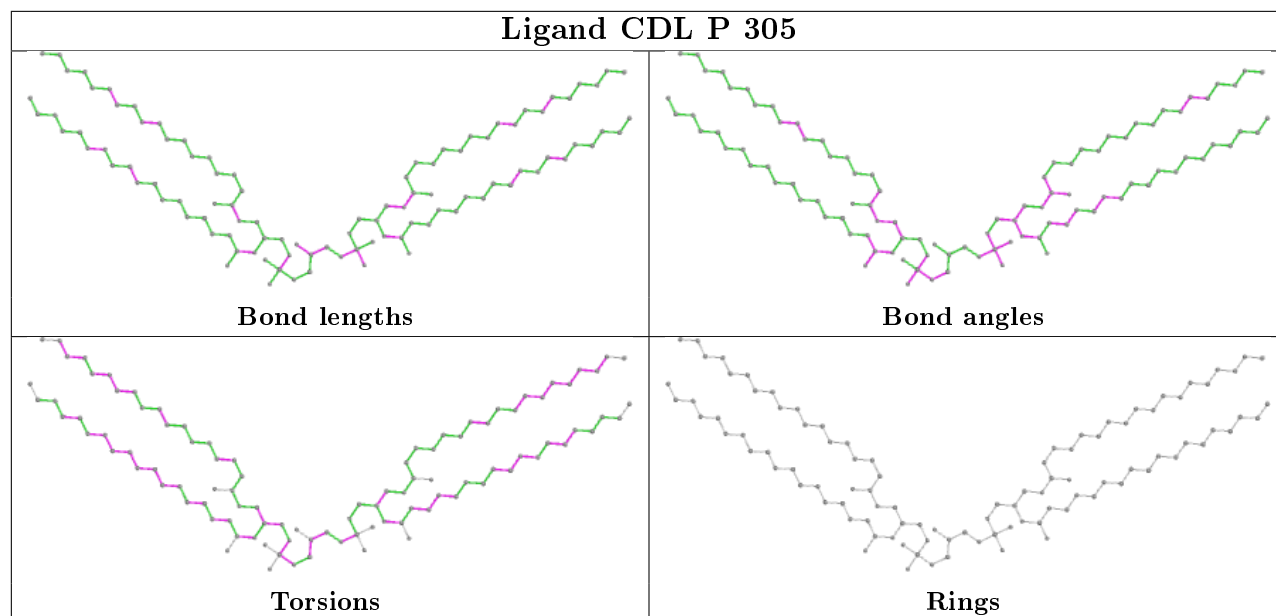
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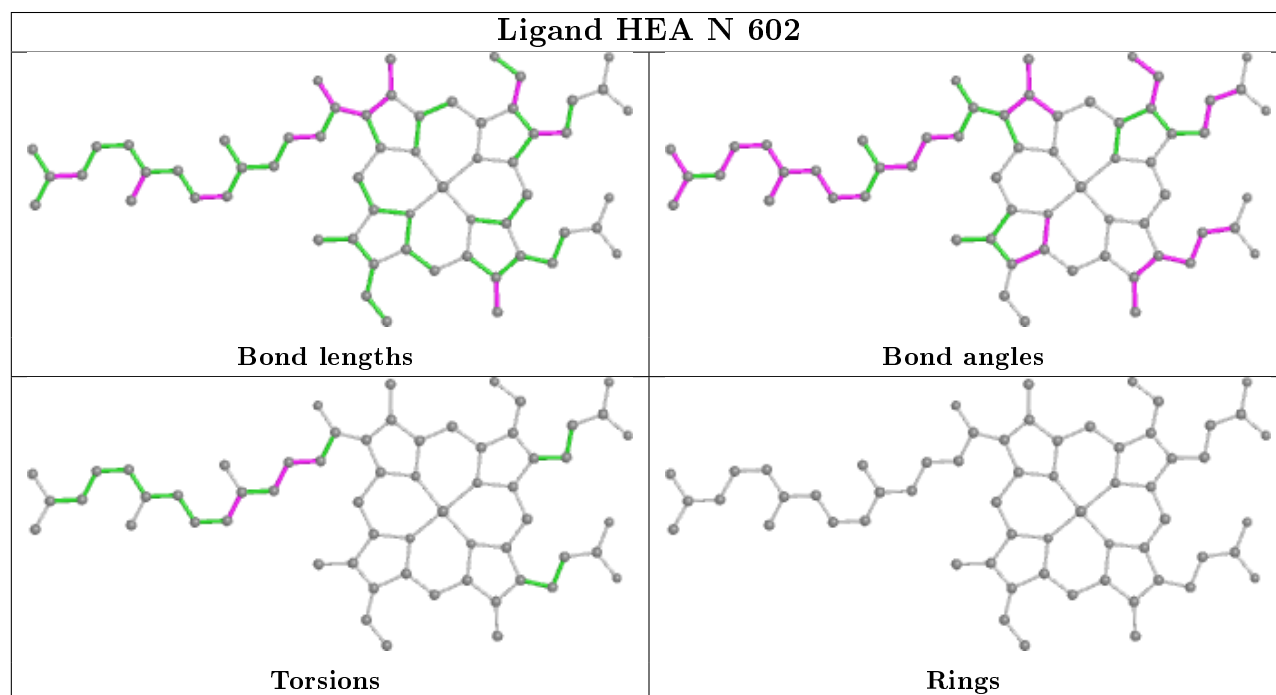
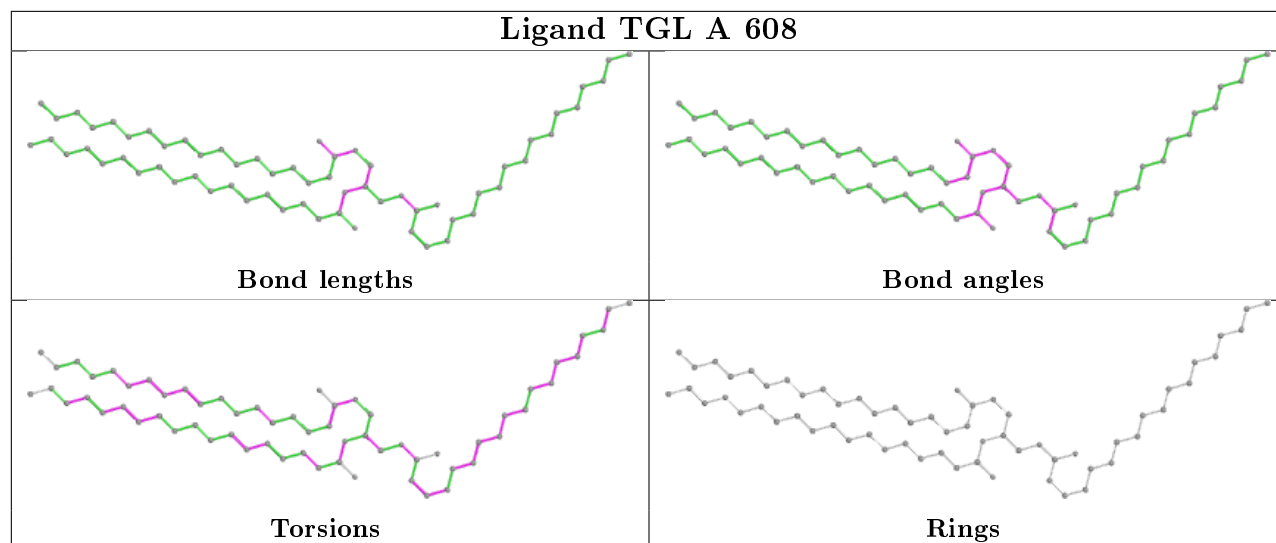


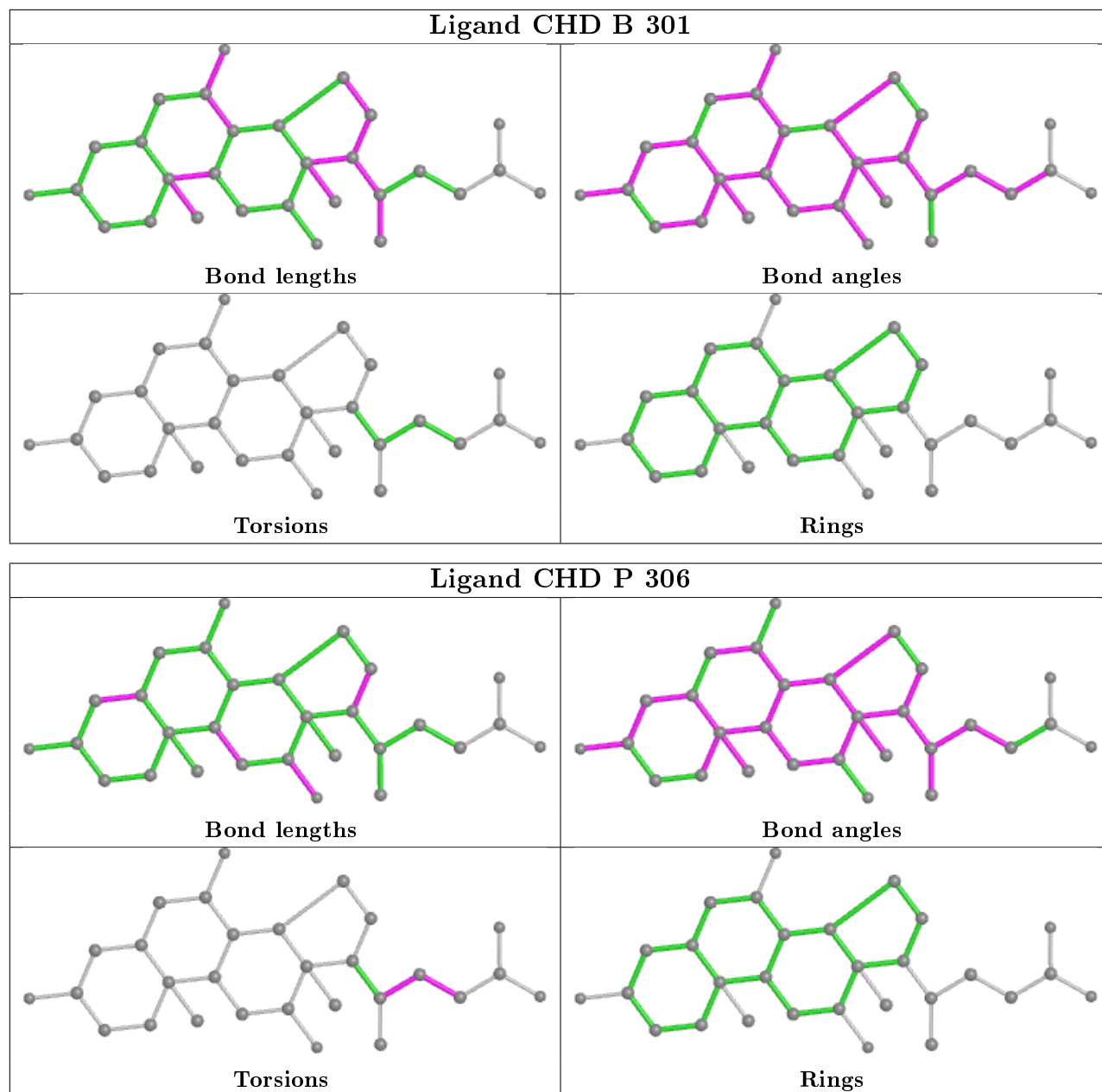
Ligand TGL A 611

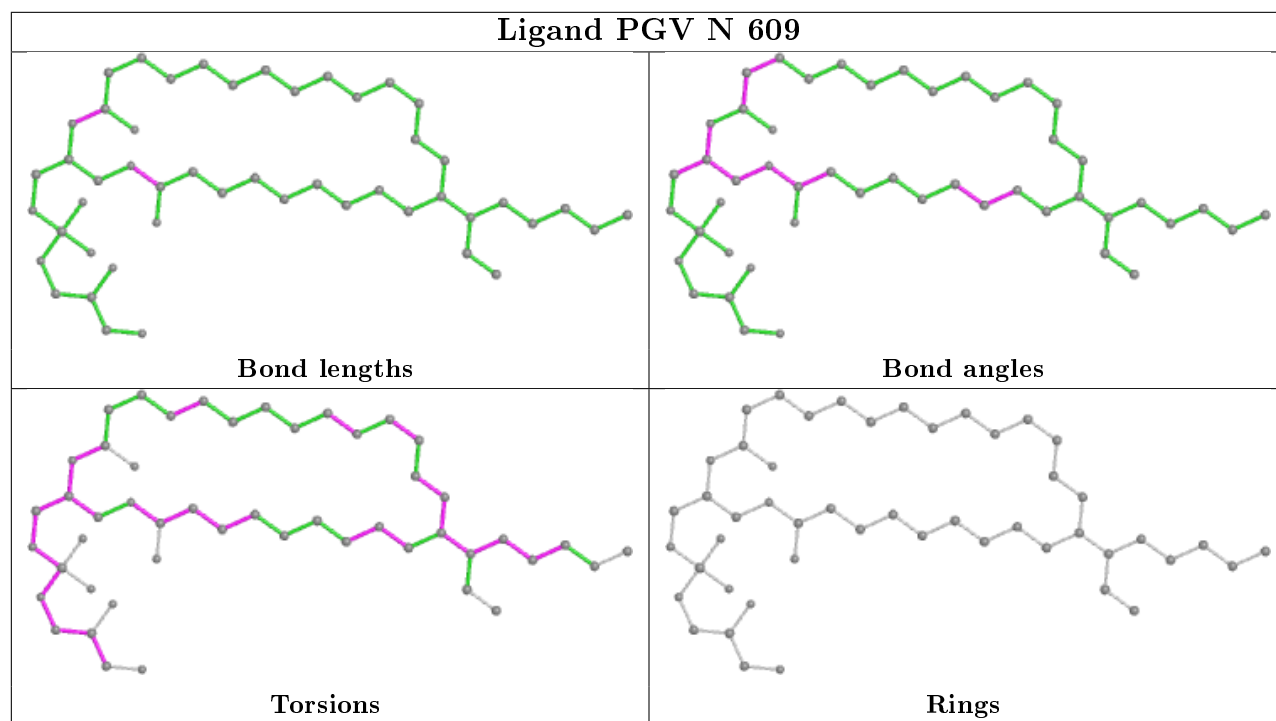
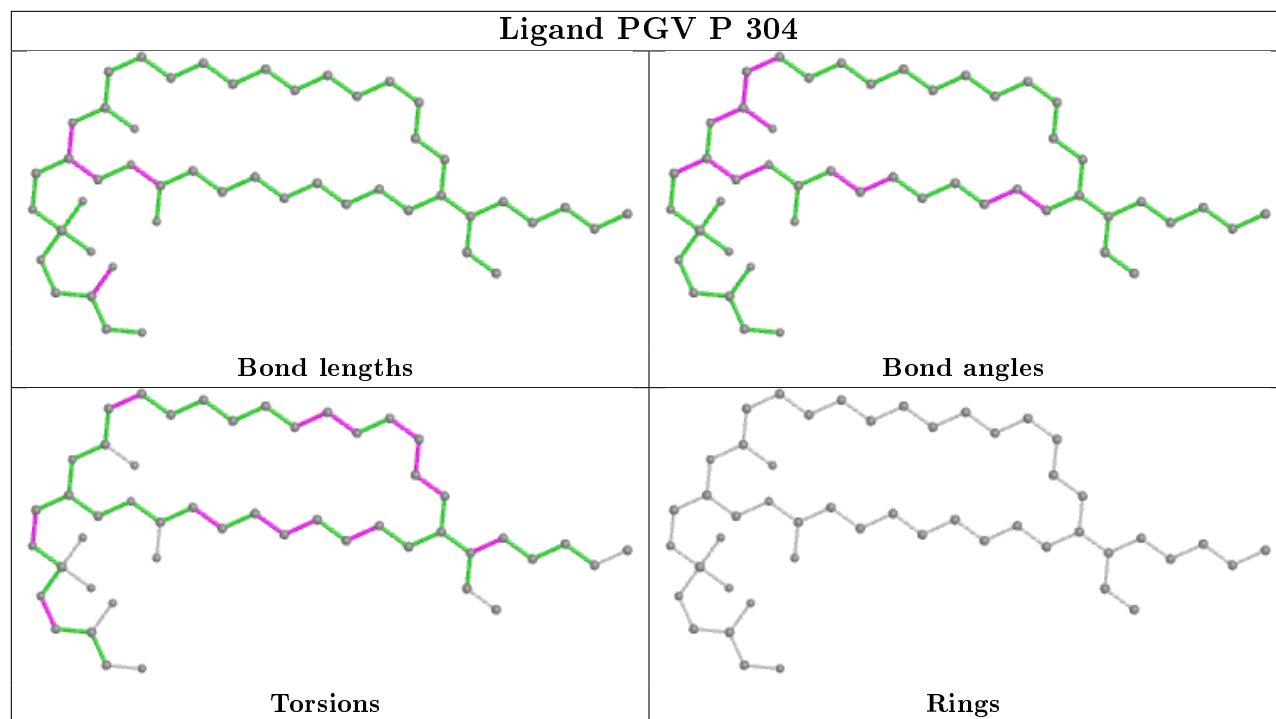


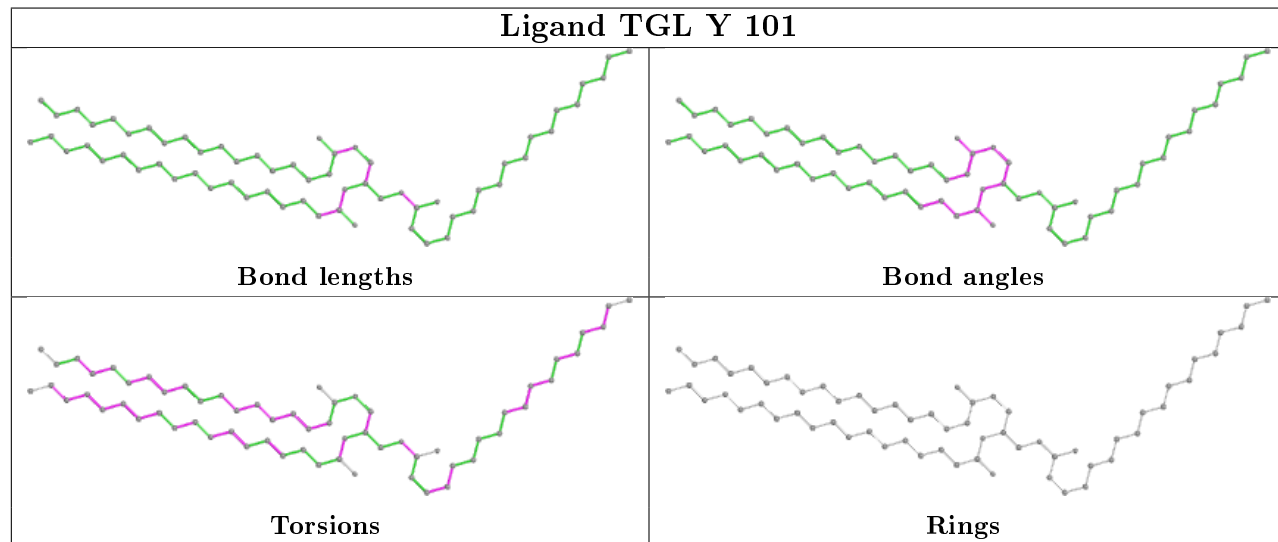
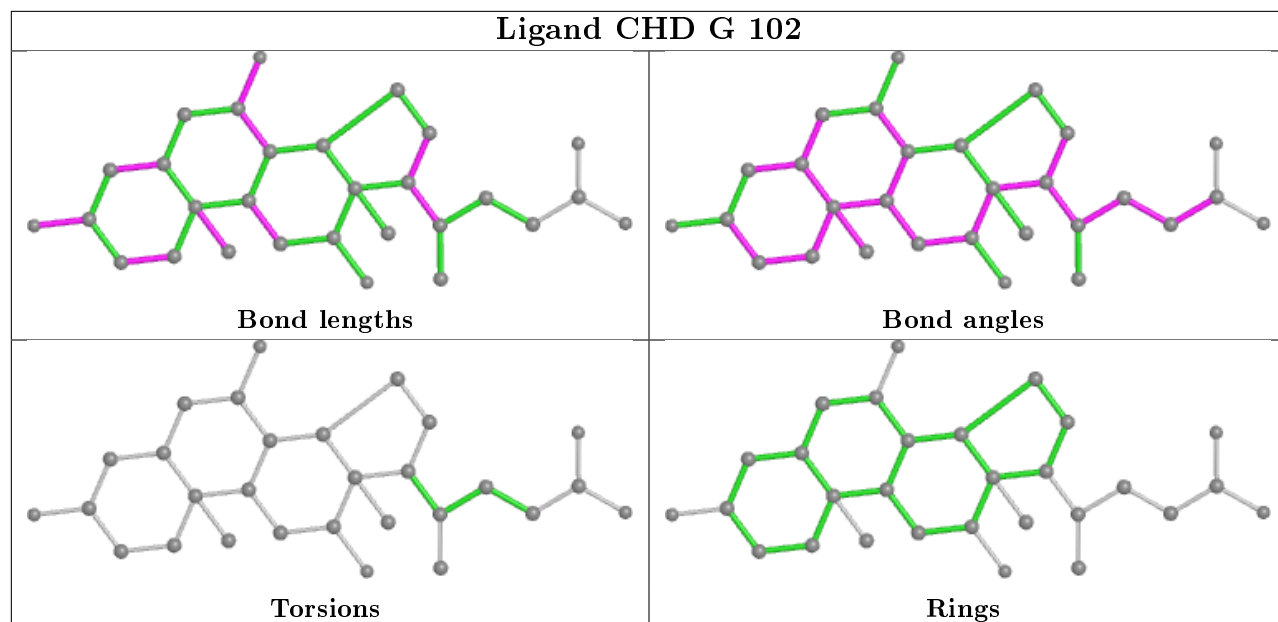


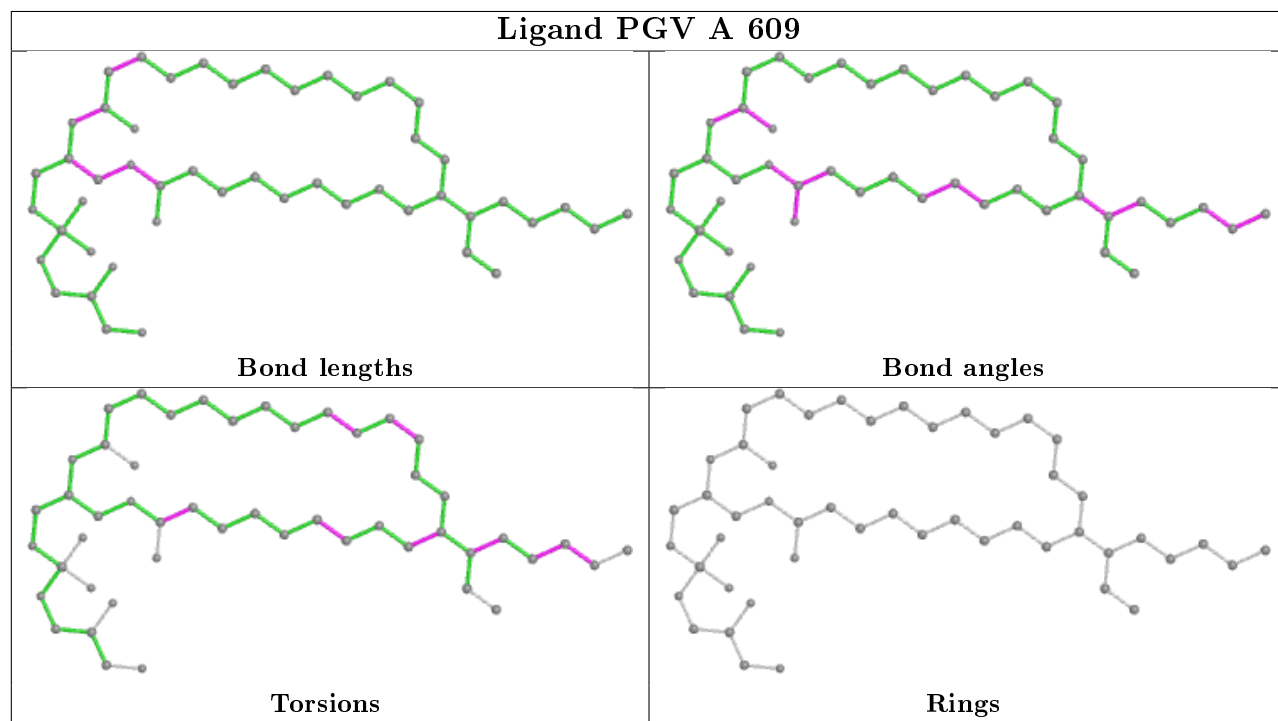
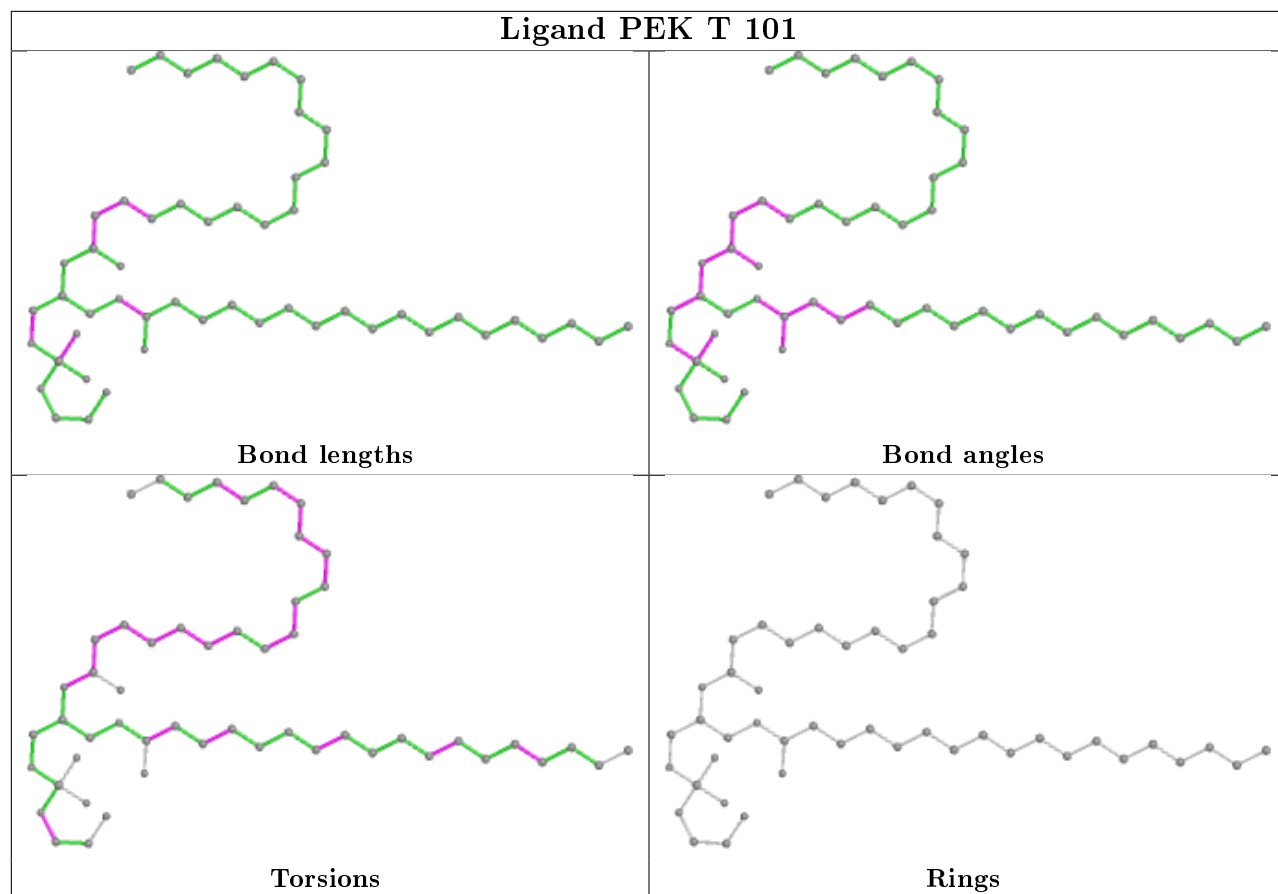


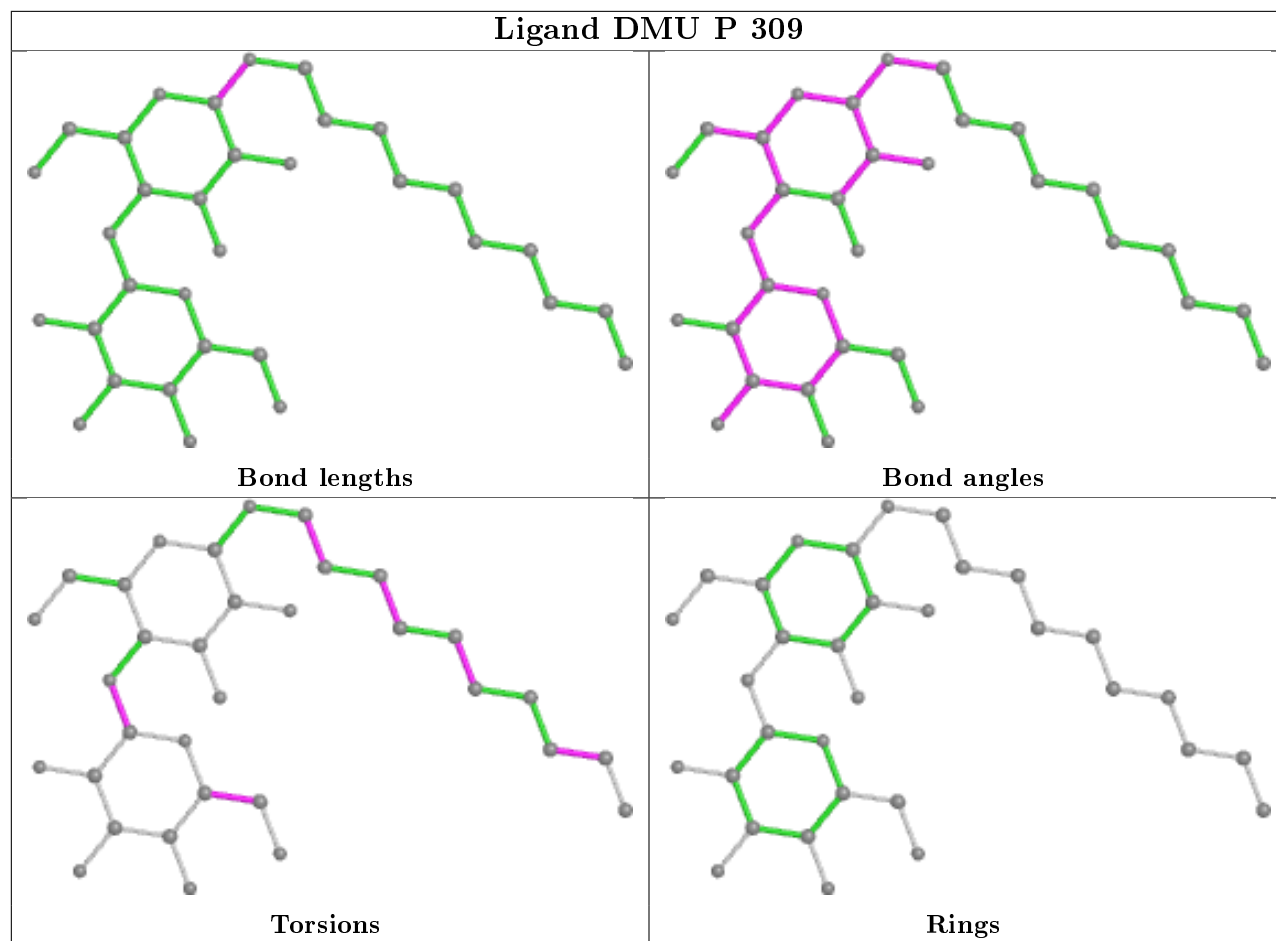


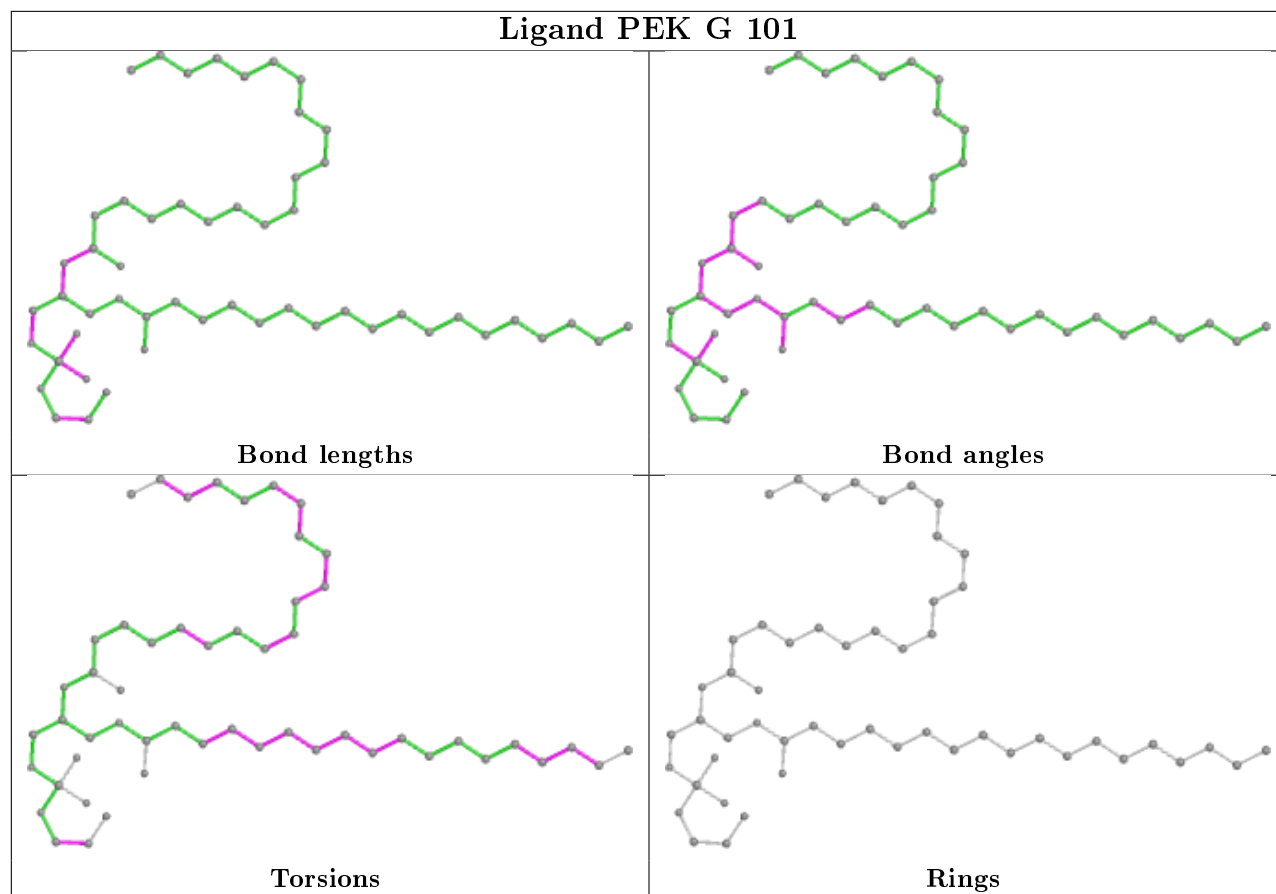




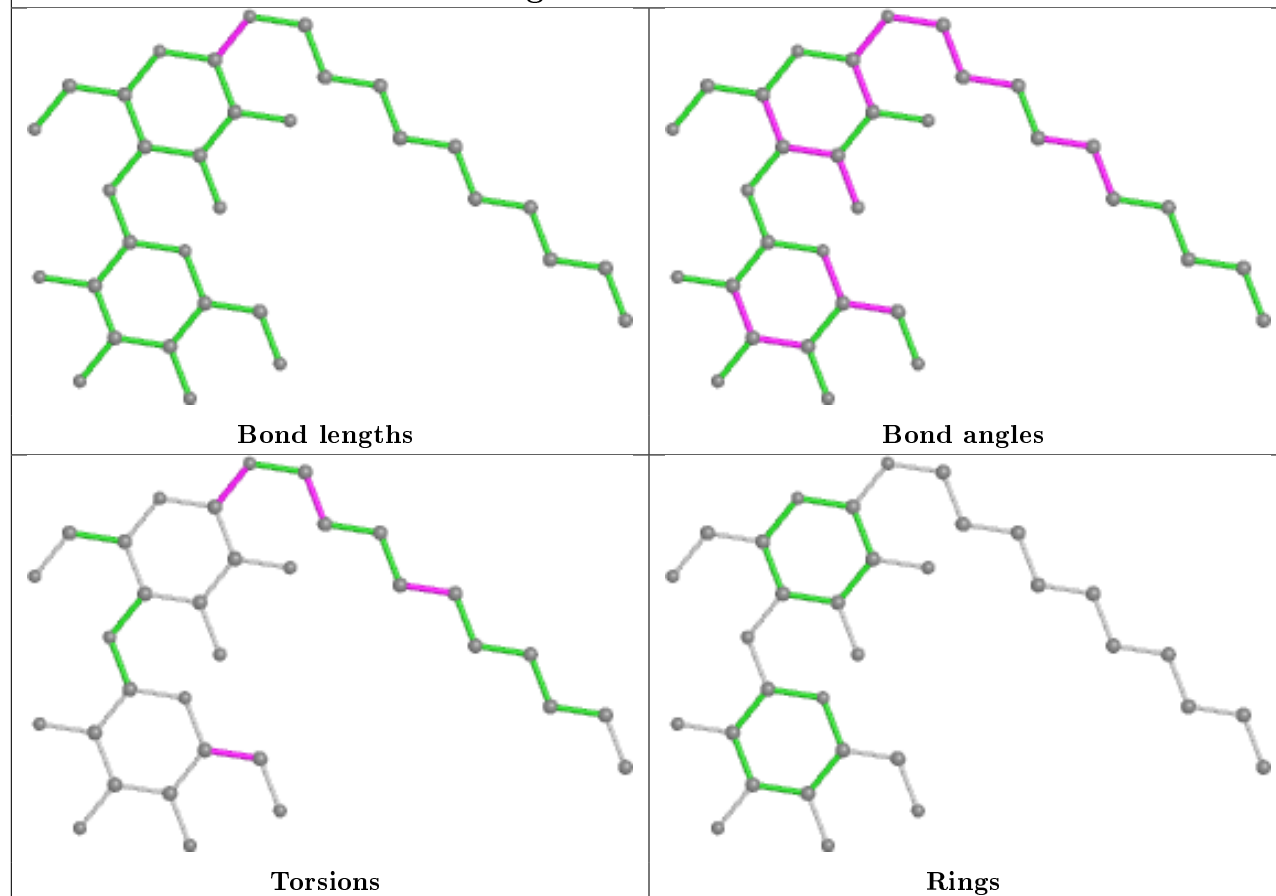




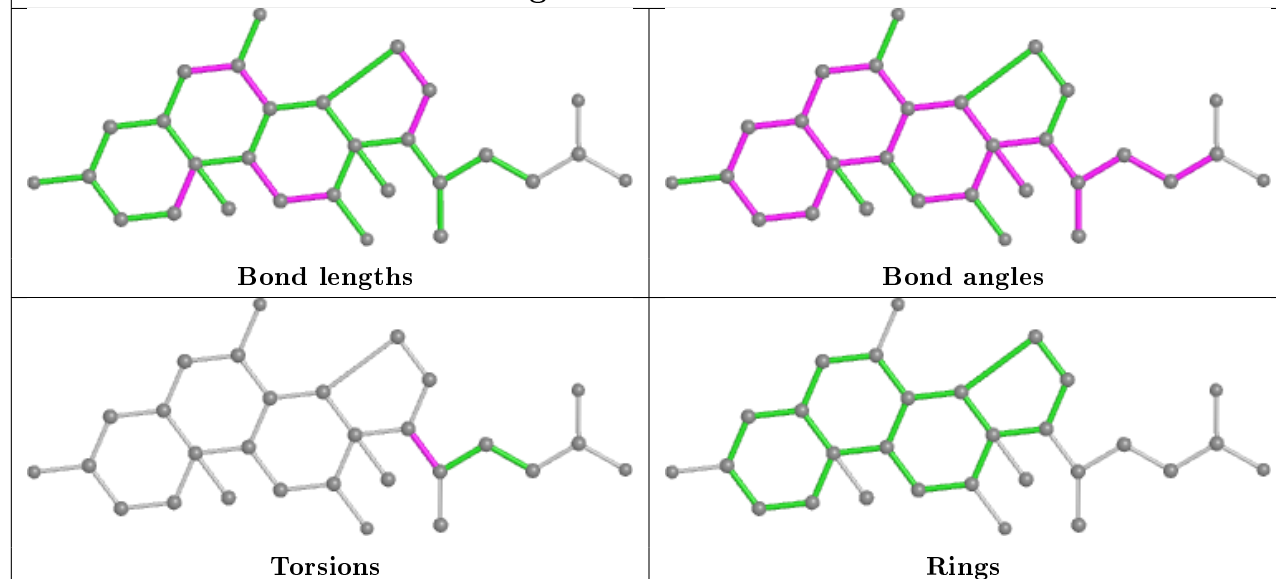


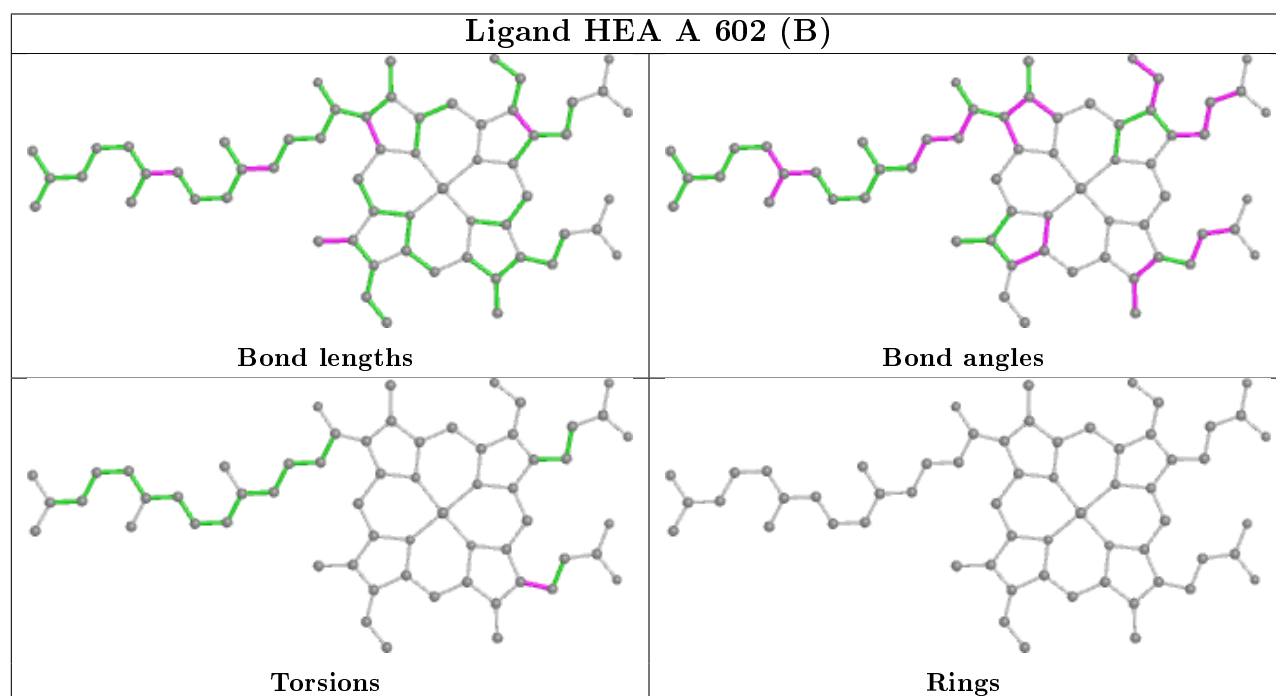
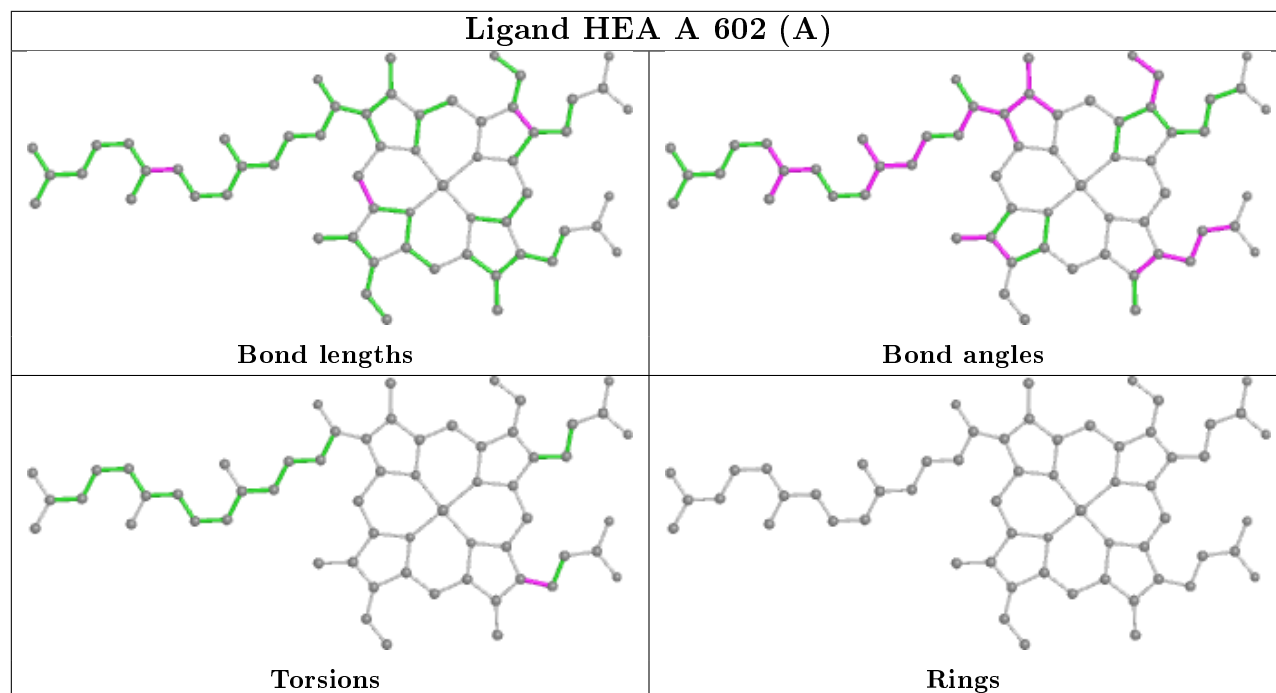


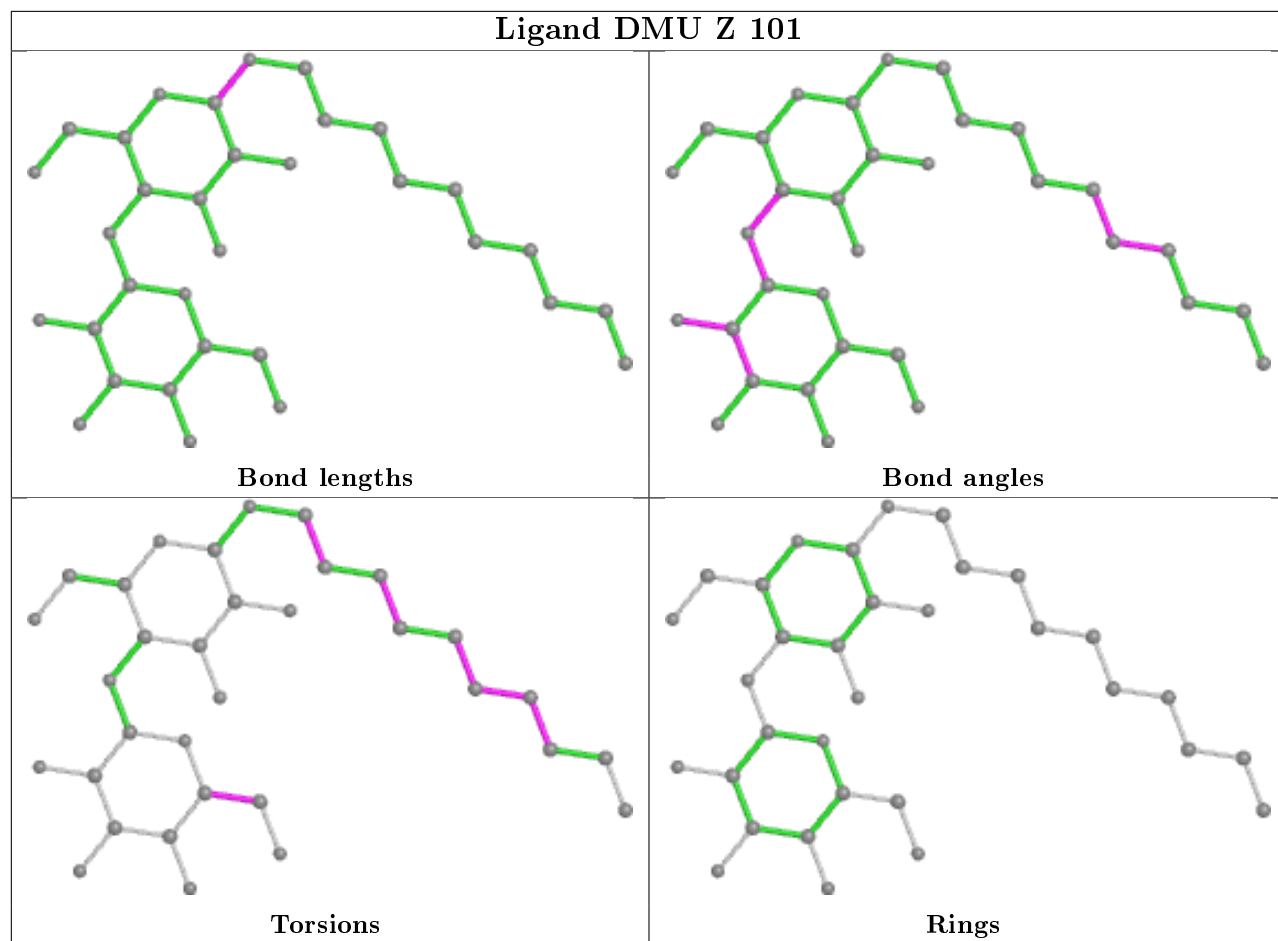
Ligand DMU P 307

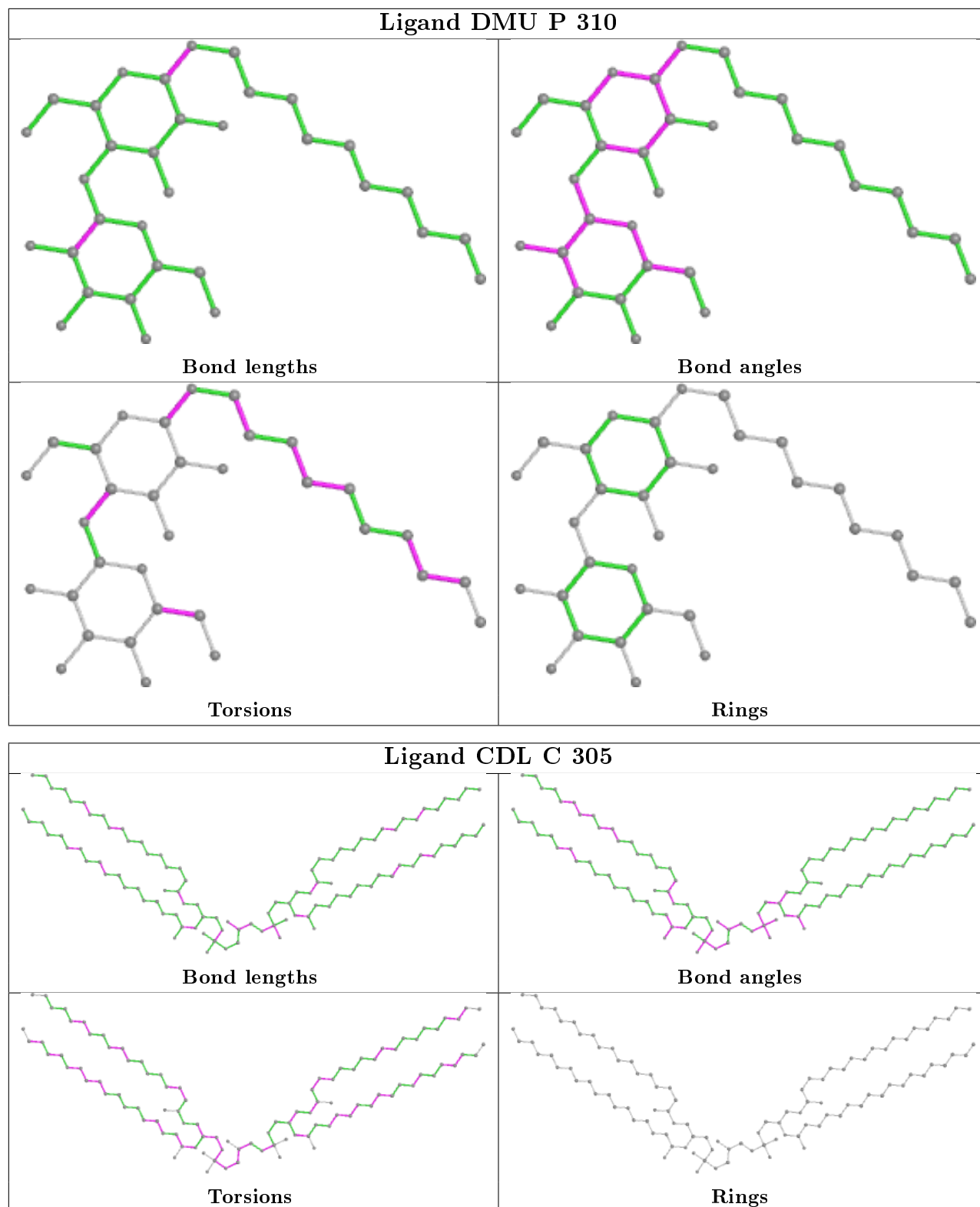


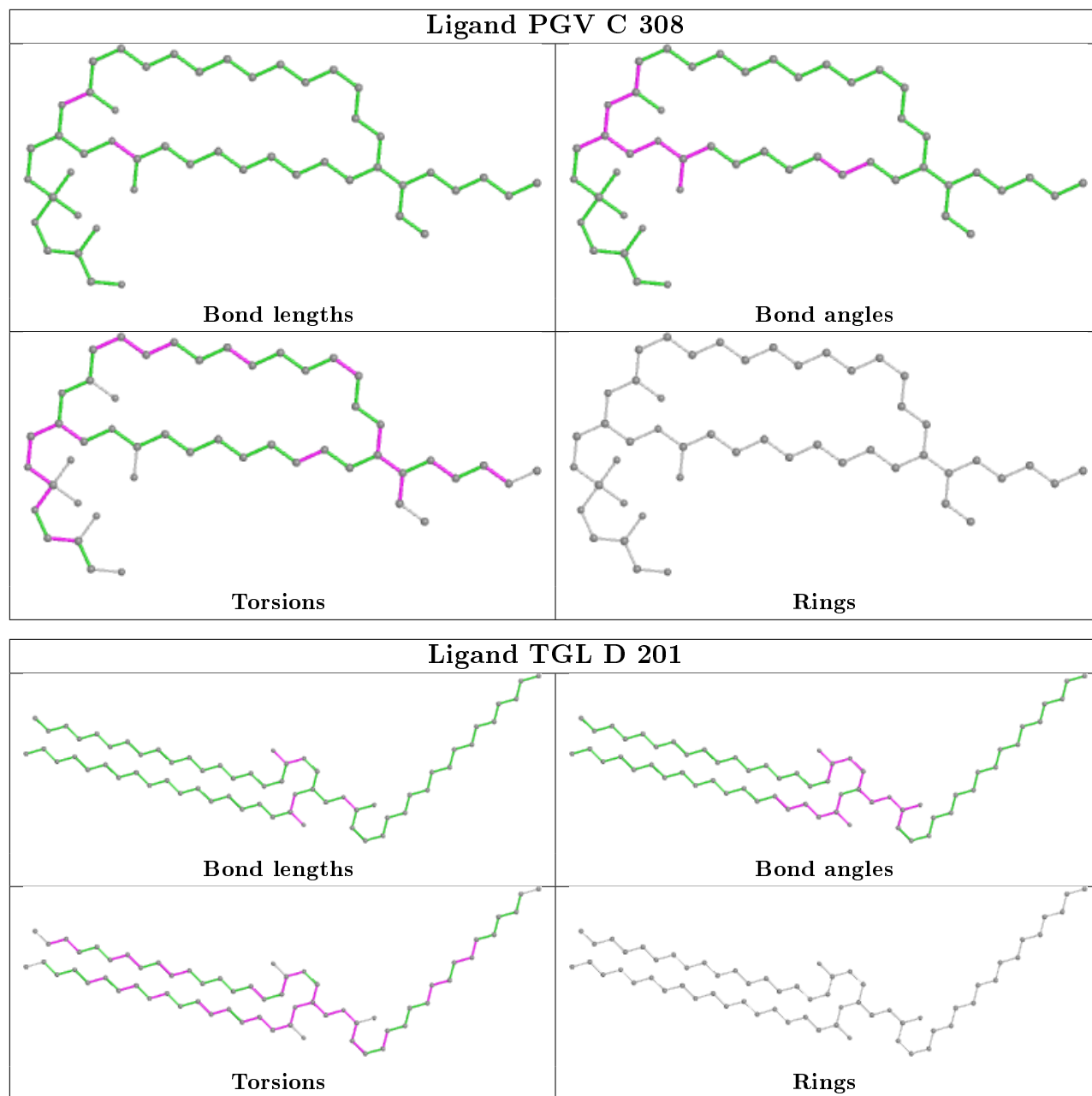
Ligand CHD P 301

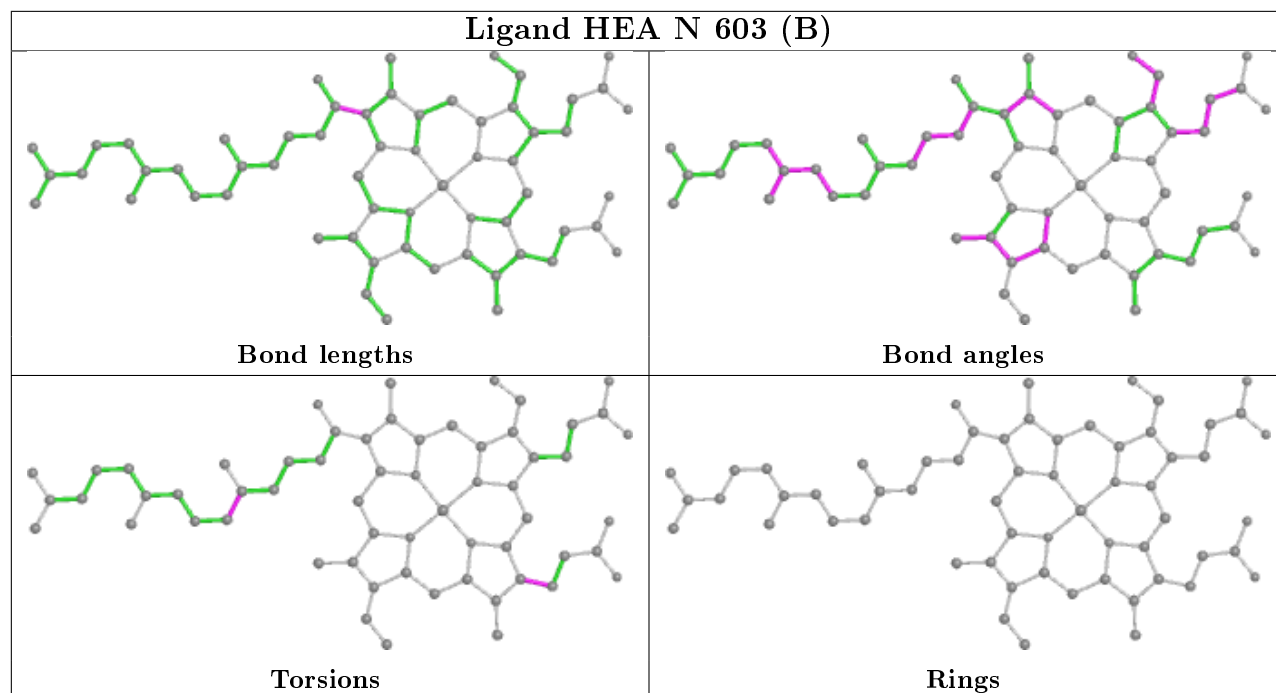
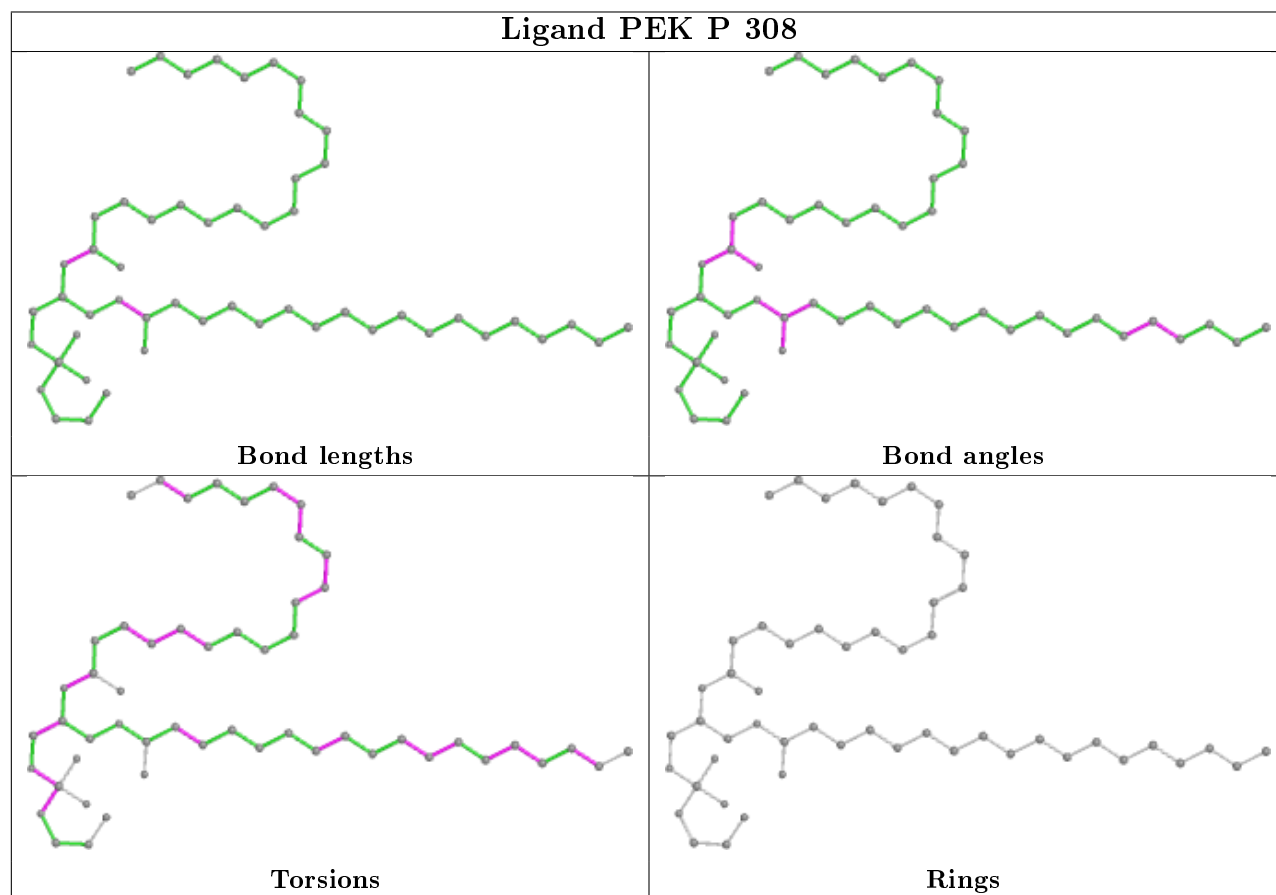


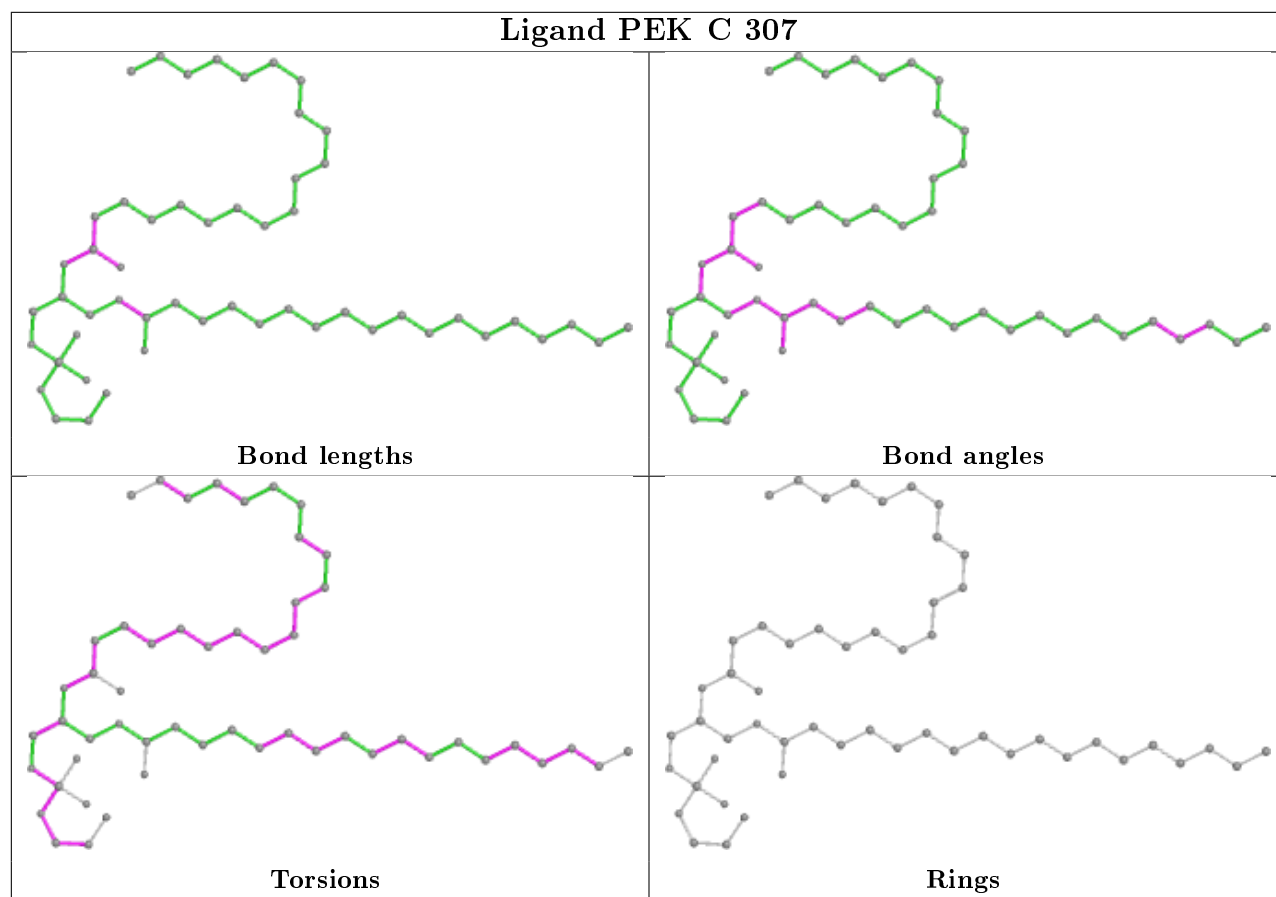
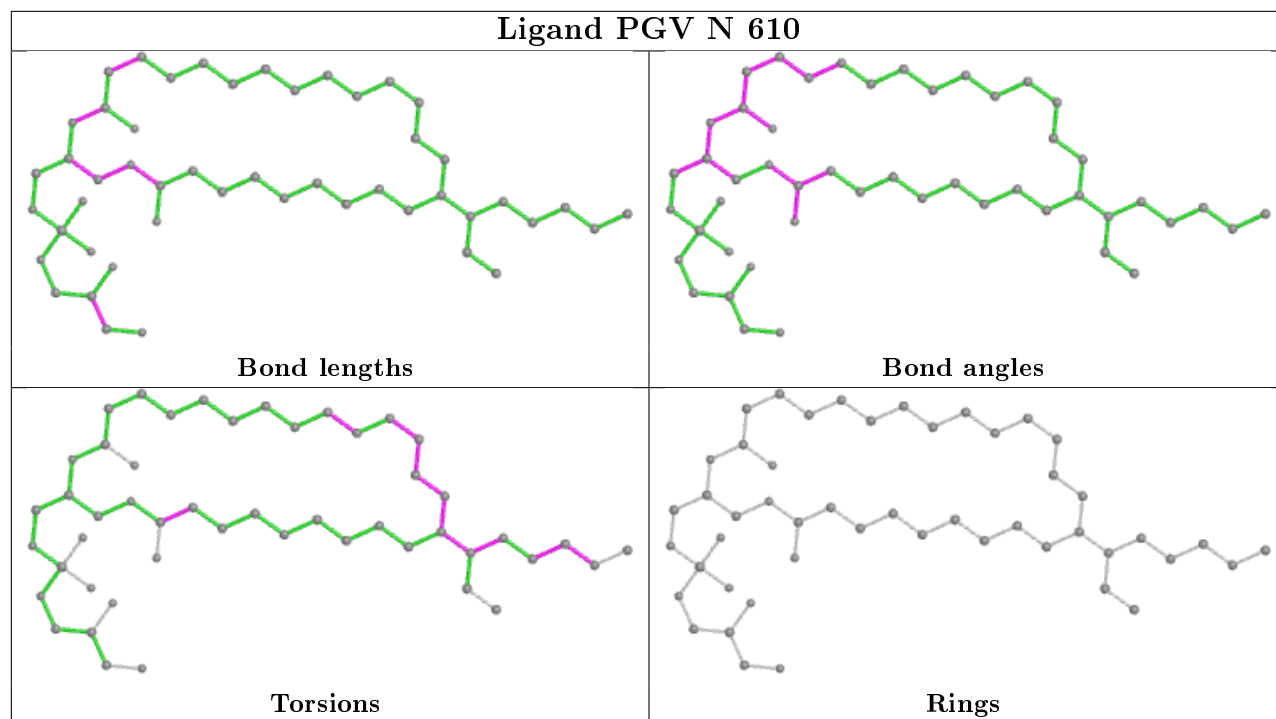


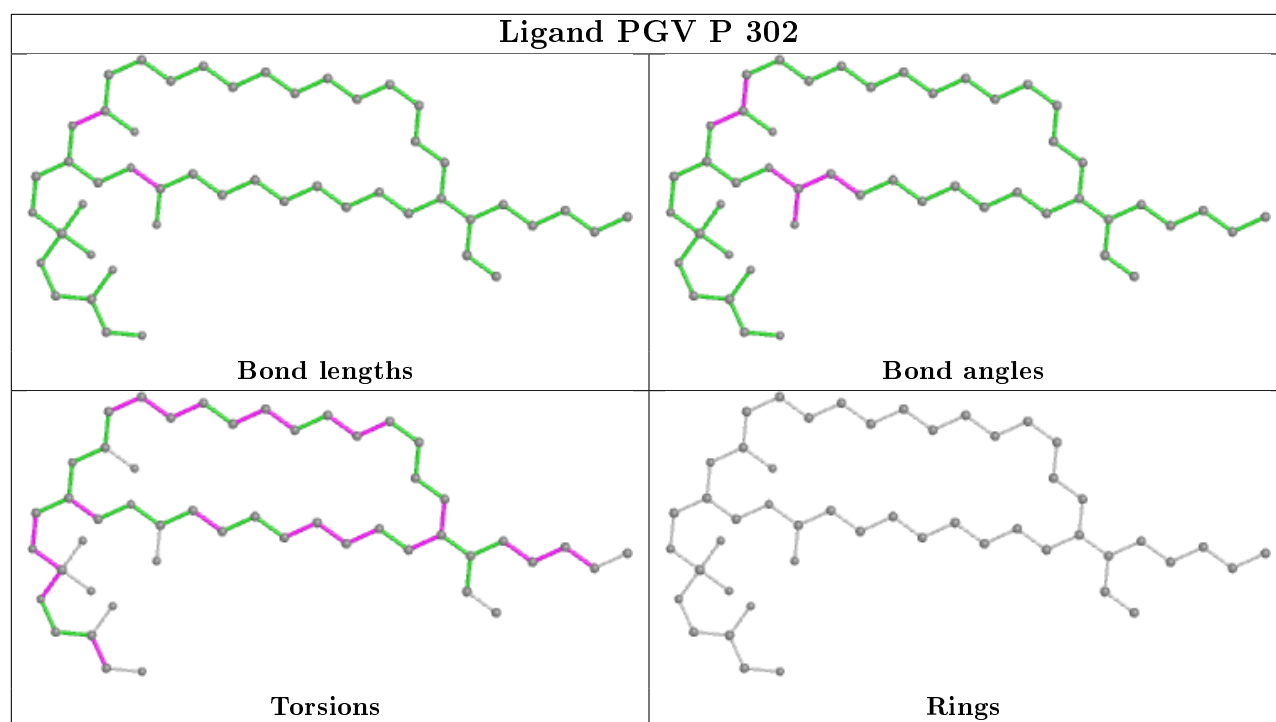






Ligand HEA N 603 (B)**Ligand PEK P 308**





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.05	0 100 100	22, 27, 35, 71	0
1	N	513/514 (99%)	-0.16	1 (0%) 95 95	24, 31, 40, 74	0
2	B	226/227 (99%)	-0.01	7 (3%) 49 49	25, 35, 54, 68	0
2	O	226/227 (99%)	0.01	7 (3%) 49 49	30, 41, 65, 88	0
3	C	259/261 (99%)	-0.11	2 (0%) 86 88	24, 30, 40, 75	0
3	P	259/261 (99%)	-0.16	1 (0%) 92 93	25, 31, 42, 80	0
4	D	144/147 (97%)	-0.23	2 (1%) 75 79	28, 35, 57, 79	0
4	Q	144/147 (97%)	0.51	9 (6%) 20 19	35, 48, 74, 136	0
5	E	105/109 (96%)	-0.25	2 (1%) 66 69	27, 34, 57, 118	0
5	R	105/109 (96%)	-0.24	2 (1%) 66 69	33, 40, 58, 121	0
6	F	98/98 (100%)	0.52	8 (8%) 11 11	27, 37, 90, 148	0
6	S	98/98 (100%)	0.61	8 (8%) 11 11	27, 37, 99, 143	0
7	G	83/85 (97%)	1.01	16 (19%) 1 1	29, 39, 108, 141	0
7	T	83/85 (97%)	0.84	18 (21%) 0 0	28, 39, 101, 131	0
8	H	79/85 (92%)	0.14	3 (3%) 40 40	33, 44, 91, 101	0
8	U	79/85 (92%)	0.14	5 (6%) 20 19	37, 47, 103, 123	0
9	I	72/73 (98%)	0.62	12 (16%) 1 1	33, 44, 83, 90	0
9	V	72/73 (98%)	0.68	10 (13%) 2 2	32, 54, 80, 104	0
10	J	58/59 (98%)	0.41	4 (6%) 16 15	30, 39, 63, 121	0
10	W	58/59 (98%)	0.25	4 (6%) 16 15	33, 43, 69, 127	0
11	K	49/56 (87%)	-0.19	0 100 100	34, 41, 54, 61	0
11	X	49/56 (87%)	0.50	5 (10%) 6 5	43, 50, 70, 81	0
12	L	46/47 (97%)	0.06	1 (2%) 62 63	28, 33, 52, 91	0
12	Y	46/47 (97%)	0.06	1 (2%) 62 63	34, 40, 65, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.17	2 (4%) 31 30	30, 33, 68, 118	0
13	Z	43/46 (93%)	0.22	4 (9%) 8 7	39, 44, 78, 108	0
All	All	3550/3614 (98%)	0.08	134 (3%) 40 40	22, 35, 66, 148	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	23.5
6	F	97	ALA	17.7
4	Q	5	VAL	17.0
6	F	2	SER	16.2
10	J	58	LYS	15.3
4	Q	6	VAL	15.2
6	S	2	SER	12.3
7	G	10	GLY	12.2
10	W	58	LYS	11.1
6	S	98	HIS	10.5
4	Q	7	LYS	10.2
7	T	3	ALA	9.8
6	F	96	LEU	9.4
7	G	3	ALA	9.2
6	S	96	LEU	8.0
4	Q	4	SER	8.0
6	F	98	HIS	7.9
6	F	1	ALA	7.7
6	S	1	ALA	7.6
7	G	42	ARG	7.5
4	Q	8	SER	6.8
6	S	94	HIS	6.5
13	Z	43	SER	6.4
12	Y	47	LYS	6.3
13	M	42	LYS	6.1
8	U	45	ALA	6.0
5	R	5	HIS	6.0
7	G	40	GLY	5.9
9	V	37	PHE	5.9
9	I	30	GLY	5.8
7	G	6	GLY	5.8
5	E	109	VAL	5.6
5	E	5	HIS	5.5
3	P	3	HIS	5.5

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Mol	Chain	Res	Type	RSRZ
7	G	2	SER	5.4
9	V	30	GLY	5.2
6	F	95	GLN	5.2
7	T	8	HIS	5.1
7	T	42	ARG	5.0
9	I	33	THR	4.9
7	G	9	GLY	4.9
7	T	36	TRP	4.8
8	U	8	ILE	4.7
5	R	109	VAL	4.7
6	S	95	GLN	4.7
7	G	1	ALA	4.6
9	V	29	LEU	4.5
13	M	43	SER	4.5
9	I	37	PHE	4.4
6	S	93	PRO	4.3
9	I	29	LEU	4.3
13	Z	42	LYS	4.3
7	T	10	GLY	4.3
7	T	40	GLY	4.3
11	X	6	ALA	4.2
2	O	113	TYR	4.2
7	G	36	TRP	4.2
7	G	5	LYS	4.1
12	L	2	HIS	4.1
8	H	10	ASN	3.9
7	T	39	SER	3.9
8	U	7	LYS	3.9
7	T	2	SER	3.9
8	H	8	ILE	3.8
6	F	94	HIS	3.8
7	G	8	HIS	3.8
9	V	33	THR	3.8
4	D	4	SER	3.8
7	T	41	HIS	3.7
2	O	32[A]	PHE	3.7
7	T	1	ALA	3.7
7	T	6	GLY	3.7
9	V	34	PHE	3.6
8	U	10	ASN	3.6
4	Q	147	LYS	3.6
9	I	25	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
10	J	1	PHE	3.5
11	X	7	PRO	3.5
9	I	26	MET	3.5
7	T	4	ALA	3.5
7	G	7	ASP	3.4
7	G	37	LEU	3.4
2	O	91	ASN	3.4
9	V	25	PHE	3.4
9	I	32	ALA	3.3
2	B	60	GLU	3.2
9	V	32	ALA	3.1
7	T	38	HIS	3.1
7	T	5	LYS	3.0
2	O	227	LEU	3.0
9	I	31	PHE	3.0
6	F	3	GLY	3.0
4	Q	87[A]	PHE	2.9
10	J	52	TRP	2.9
2	O	90	ILE	2.8
13	Z	40	TYR	2.8
7	T	43	GLU	2.8
1	N	311[A]	ILE	2.8
10	W	57	HIS	2.7
7	G	41	HIS	2.7
13	Z	39	ASN	2.6
4	D	5	VAL	2.6
9	I	35	TYR	2.6
2	B	87[A]	MET	2.6
4	Q	10	ASP	2.5
8	H	44	THR	2.5
2	B	59	GLN	2.5
11	X	52	GLU	2.5
7	T	37	LEU	2.5
3	C	38	ASN	2.4
9	V	31	PHE	2.4
10	W	1	PHE	2.4
9	V	2	THR	2.4
9	I	19	PHE	2.4
11	X	13	TYR	2.4
2	B	16[A]	ILE	2.3
9	V	19	PHE	2.3
2	B	32[A]	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
7	G	84	LYS	2.3
3	C	33[A]	MET	2.3
9	I	15	ARG	2.3
7	T	84	LYS	2.3
8	U	9	LYS	2.3
4	Q	33	LEU	2.2
7	G	4	ALA	2.2
2	B	55	THR	2.1
10	W	52	TRP	2.1
2	O	58	ALA	2.1
7	T	33	LEU	2.1
9	I	34	PHE	2.0
10	J	57	HIS	2.0
11	X	54	ARG	2.0
2	B	113	TYR	2.0
2	O	60	GLU	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
7	TPO	G	11	11/12	0.39	0.37	90,110,131,132	0
7	TPO	T	11	11/12	0.64	0.36	94,107,122,130	0
9	SAC	V	1	9/10	0.68	0.41	102,119,126,133	0
9	SAC	I	1	9/10	0.89	0.26	60,74,81,81	0
1	FME	A	1	10/11	0.95	0.10	38,45,74,86	0
1	FME	N	1	10/11	0.96	0.13	42,51,69,79	0
2	FME	B	1	10/11	0.97	0.12	29,32,42,66	0
2	FME	O	1	10/11	0.97	0.10	38,39,48,53	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
22	CHD	W	101	29/29	0.64	0.35	61,91,115,121	0
25	DMU	C	302	33/33	0.67	0.34	30,73,105,109	0
28	PEK	C	307	53/53	0.67	0.21	38,77,135,141	0
27	CDL	T	102	100/100	0.69	0.26	49,89,137,155	0
21	EDO	D	203	4/4	0.69	0.20	63,67,71,74	0
27	CDL	N	601	100/100	0.70	0.29	54,90,129,155	0
24	PSC	B	303	52/52	0.72	0.29	36,84,154,154	0
19	TGL	Q	201	63/63	0.72	0.18	52,75,93,100	0
28	PEK	G	103	53/53	0.72	0.23	48,86,146,153	0
28	PEK	P	308	53/53	0.73	0.25	41,72,131,139	0
28	PEK	C	309	53/53	0.73	0.33	48,90,151,153	0
25	DMU	P	310	33/33	0.74	0.23	62,79,108,112	0
24	PSC	N	612	52/52	0.74	0.26	42,83,154,156	0
27	CDL	P	305	100/100	0.74	0.27	36,82,118,137	0
25	DMU	P	307	33/33	0.76	0.31	38,67,118,121	0
20	PGV	C	308	51/51	0.76	0.22	44,74,136,146	0
19	TGL	Y	101	63/63	0.79	0.23	45,74,111,138	0
22	CHD	J	101	29/29	0.79	0.24	51,75,90,93	0
27	CDL	C	305	100/100	0.79	0.23	35,75,109,115	0
20	PGV	P	302	51/51	0.80	0.26	51,81,132,151	0
21	EDO	A	613	4/4	0.81	0.20	49,53,56,57	0
20	PGV	N	609	51/51	0.82	0.24	43,77,115,131	0
25	DMU	C	310	33/33	0.82	0.25	52,73,102,105	0
19	TGL	A	611	63/63	0.83	0.18	34,60,92,110	0
25	DMU	P	309	33/33	0.83	0.19	45,72,92,97	0
21	EDO	G	105	4/4	0.83	0.26	53,56,64,79	0
21	EDO	N	621	4/4	0.84	0.26	41,51,53,61	0
21	EDO	L	101	4/4	0.84	0.24	55,62,78,81	0
21	EDO	A	618	4/4	0.85	0.32	51,51,53,63	0
20	PGV	A	610	51/51	0.85	0.21	34,75,106,125	0
25	DMU	C	311	33/33	0.85	0.18	46,77,99,109	0
19	TGL	D	201	63/63	0.85	0.18	32,62,89,92	0
21	EDO	A	615	4/4	0.86	0.13	53,63,65,70	0
21	EDO	N	616	4/4	0.86	0.16	52,54,55,56	0
19	TGL	N	611	63/63	0.87	0.17	51,77,97,104	0
25	DMU	Z	101	33/33	0.88	0.13	45,54,70,76	0
22	CHD	C	306	29/29	0.88	0.17	43,49,54,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	EDO	A	617	4/4	0.88	0.15	40,42,43,44	0
22	CHD	P	306	29/29	0.88	0.18	43,49,52,68	0
21	EDO	D	202	4/4	0.89	0.42	33,38,47,66	0
21	EDO	W	102	4/4	0.89	0.33	50,55,66,73	0
21	EDO	M	102	4/4	0.89	0.14	60,63,63,69	0
26	UNX	C	303	1/1	0.90	0.14	35,35,35,35	0
21	EDO	N	620	4/4	0.90	0.16	47,49,54,58	0
19	TGL	A	608	63/63	0.90	0.15	40,75,93,101	0
21	EDO	B	305	4/4	0.90	0.19	35,45,48,51	0
21	EDO	Y	102	4/4	0.90	0.26	61,65,66,67	0
21	EDO	A	619	4/4	0.90	0.32	44,60,74,82	0
21	EDO	N	617	4/4	0.91	0.17	52,55,58,61	0
21	EDO	A	614	4/4	0.92	0.10	30,31,32,37	0
25	DMU	M	101	33/33	0.92	0.08	38,44,58,67	0
21	EDO	B	306	4/4	0.93	0.19	50,51,55,57	0
21	EDO	F	104	4/4	0.94	0.11	36,36,38,42	0
21	EDO	B	304	4/4	0.94	0.25	46,59,60,85	0
21	EDO	E	203	4/4	0.94	0.08	42,42,50,55	0
21	EDO	P	312	4/4	0.94	0.12	33,36,43,49	0
21	EDO	A	620	4/4	0.94	0.15	52,56,57,64	0
21	EDO	N	613	4/4	0.95	0.10	33,34,37,41	0
21	EDO	S	104	4/4	0.95	0.17	40,52,60,65	0
21	EDO	F	103	4/4	0.95	0.09	37,41,42,52	0
21	EDO	A	616	4/4	0.95	0.12	22,27,28,42	0
21	EDO	N	619	4/4	0.95	0.13	40,43,46,49	0
28	PEK	T	101	53/53	0.95	0.13	29,49,85,92	0
21	EDO	B	307	4/4	0.95	0.11	29,30,35,37	0
21	EDO	R	201	4/4	0.95	0.08	44,45,45,45	0
21	EDO	E	202	4/4	0.95	0.08	38,40,44,47	0
22	CHD	P	301	29/29	0.95	0.07	28,32,36,39	0
21	EDO	S	103	4/4	0.95	0.07	39,42,45,47	0
21	EDO	N	614	4/4	0.96	0.12	29,33,36,36	0
18	AZI	N	607[B]	3/3	0.96	0.10	23,23,27,28	3
21	EDO	N	618	4/4	0.96	0.13	37,40,43,45	0
22	CHD	C	301	29/29	0.96	0.08	27,30,34,36	0
21	EDO	T	103	4/4	0.96	0.09	36,37,42,44	0
21	EDO	O	302	4/4	0.96	0.10	38,39,40,42	0
21	EDO	C	312	4/4	0.97	0.40	41,43,72,85	0
18	AZI	A	606[B]	3/3	0.97	0.11	22,22,23,24	3
20	PGV	N	610	51/51	0.97	0.11	27,35,68,72	0
20	PGV	C	304	51/51	0.97	0.12	27,34,86,96	0
22	CHD	B	301	29/29	0.97	0.09	25,30,33,41	0

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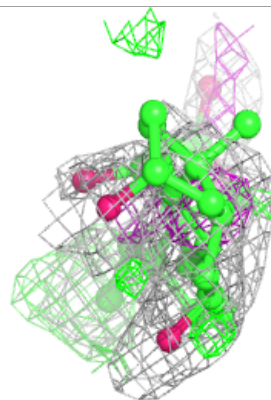
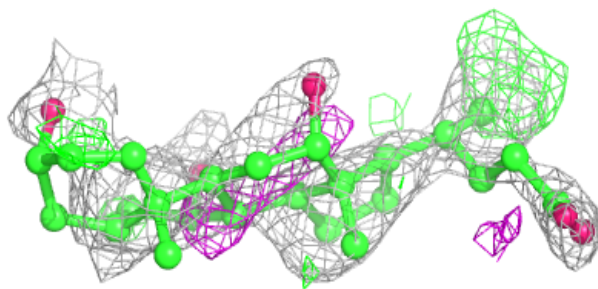
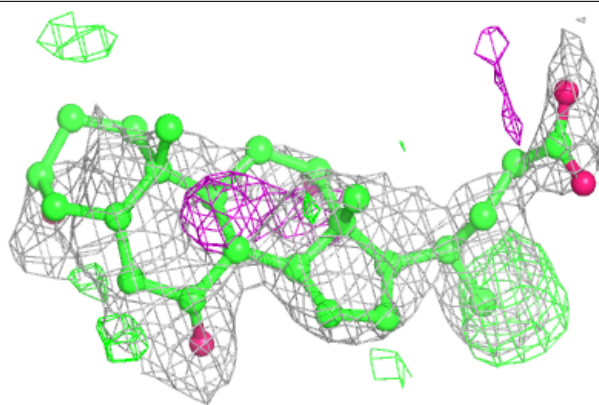
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	PEK	G	101	53/53	0.97	0.12	29,46,79,95	0
22	CHD	G	102	29/29	0.97	0.09	28,30,36,39	0
21	EDO	N	615	4/4	0.97	0.10	41,53,57,60	0
21	EDO	A	612	4/4	0.97	0.12	37,41,41,53	0
21	EDO	P	311	4/4	0.98	0.10	39,42,43,46	0
26	UNX	P	303	1/1	0.98	0.06	32,32,32,32	0
18	AZI	N	608[A]	3/3	0.98	0.16	29,29,38,40	3
21	EDO	E	201	4/4	0.98	0.10	40,41,43,44	0
21	EDO	G	104	4/4	0.98	0.10	34,37,38,41	0
14	HEA	N	602	60/60	0.98	0.10	26,30,49,52	0
14	HEA	N	603[B]	60/60	0.98	0.11	24,29,42,46	60
14	HEA	A	602[A]	60/60	0.98	0.11	18,22,26,28	60
14	HEA	A	601	60/60	0.98	0.10	21,24,48,50	0
14	HEA	A	602[B]	60/60	0.98	0.11	21,25,34,37	60
17	NA	A	605	1/1	0.98	0.06	30,30,30,30	0
14	HEA	N	603[A]	60/60	0.98	0.11	21,25,28,30	60
16	MG	N	605	1/1	0.98	0.06	31,31,31,31	0
20	PGV	P	304	51/51	0.98	0.11	26,36,79,89	0
18	AZI	N	608[B]	3/3	0.98	0.16	24,24,26,26	3
20	PGV	A	609	51/51	0.98	0.11	25,33,67,71	0
17	NA	N	606	1/1	0.98	0.05	35,35,35,35	0
21	EDO	S	102	4/4	0.99	0.07	29,29,30,30	0
18	AZI	A	607[B]	3/3	0.99	0.12	23,23,24,29	3
16	MG	A	604	1/1	0.99	0.09	26,26,26,26	0
21	EDO	F	102	4/4	0.99	0.11	27,27,28,30	0
18	AZI	A	607[A]	3/3	0.99	0.12	20,20,24,27	3
29	ZN	F	101	1/1	0.99	0.12	31,31,31,31	0
29	ZN	S	101	1/1	0.99	0.13	33,33,33,33	0
15	CU	N	604	1/1	1.00	0.16	30,30,30,30	0
23	CUA	B	302	2/2	1.00	0.15	27,27,27,28	0
15	CU	A	603	1/1	1.00	0.15	26,26,26,26	0
23	CUA	O	301	2/2	1.00	0.12	32,32,32,32	0

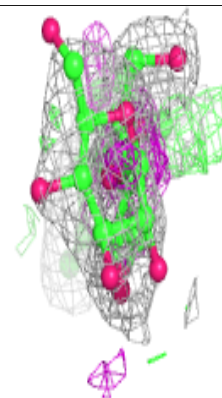
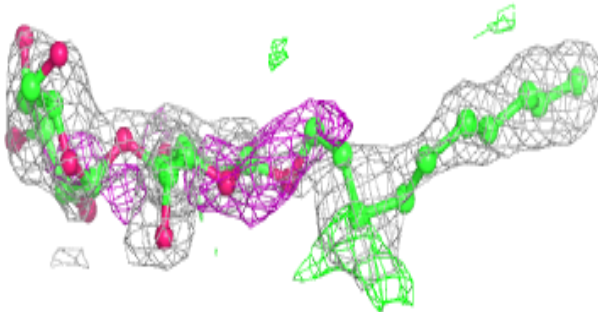
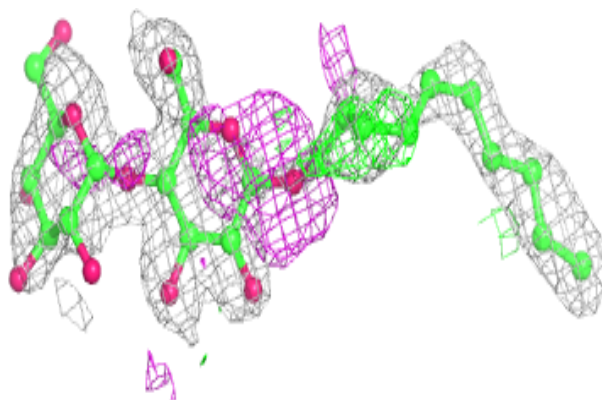
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 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)

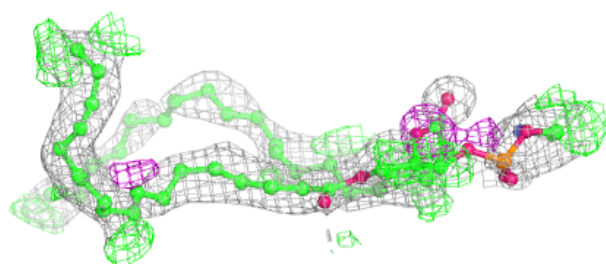
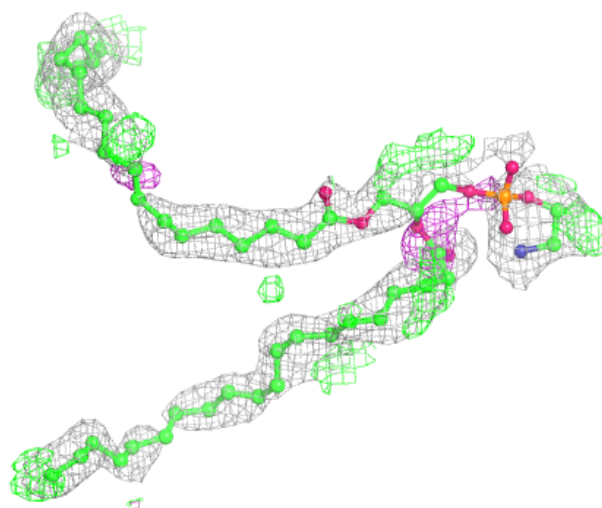
**Electron density around DMU C 302:**

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



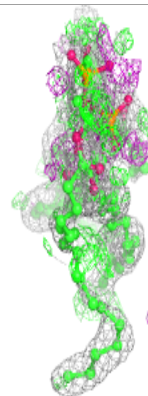
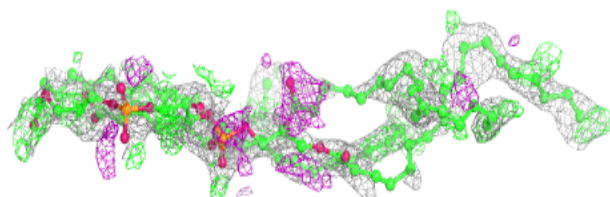
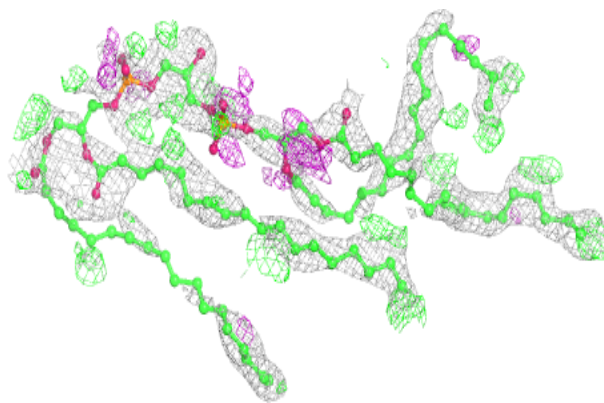
Electron density around PEK C 307:

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

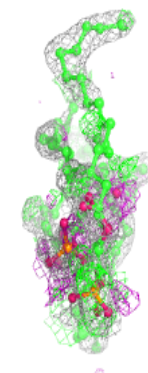
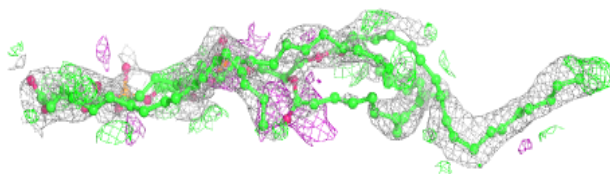
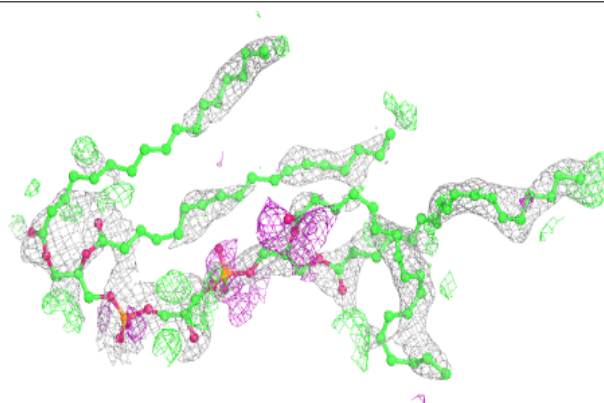


Electron density around CDL T 102:

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

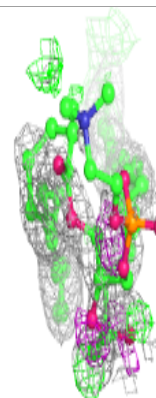
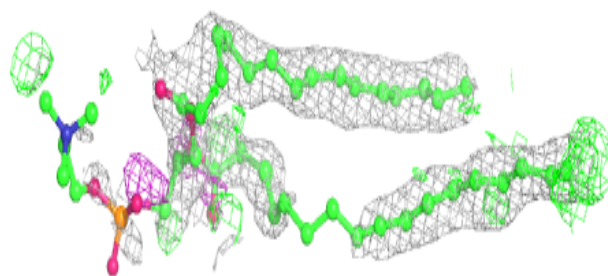
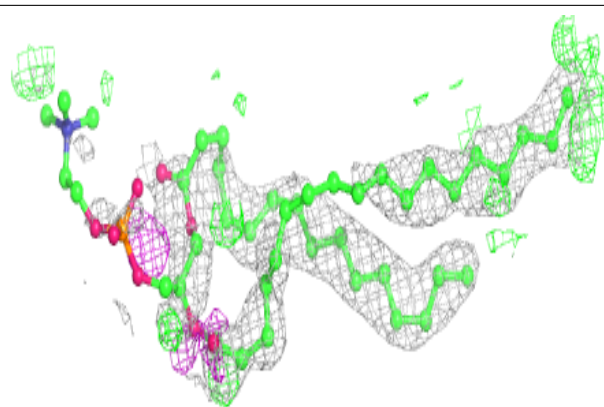
**Electron density around CDL N 601:**

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

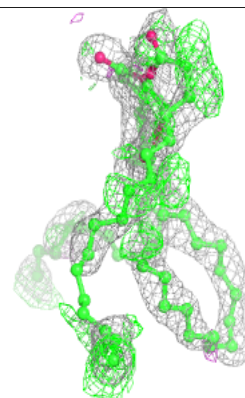
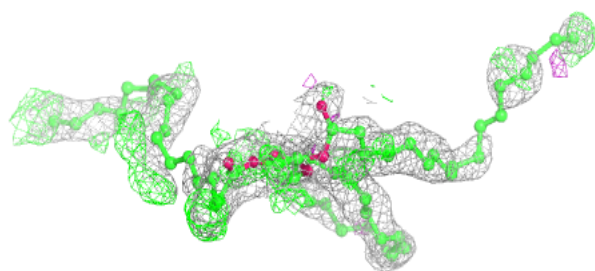
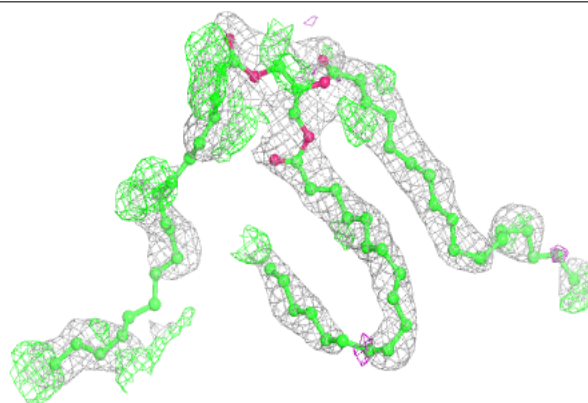


Electron density around PSC B 303:

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

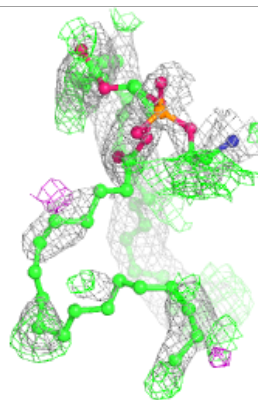
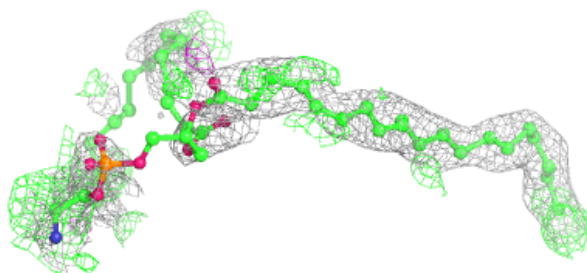
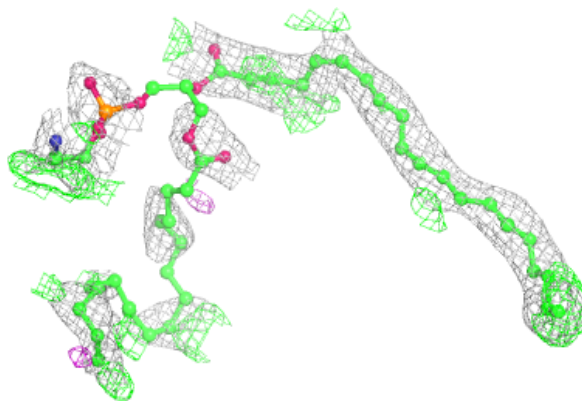
**Electron density around TGL Q 201:**

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

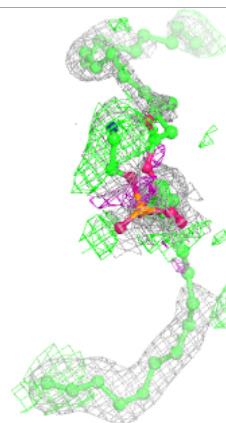
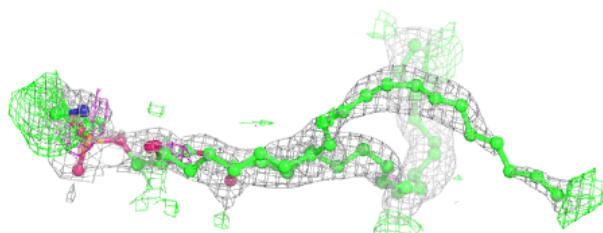
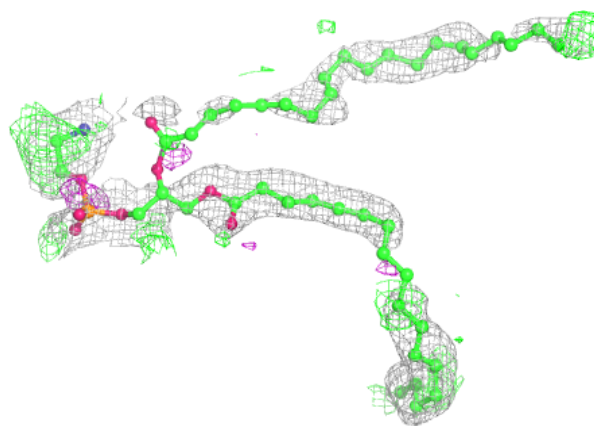


Electron density around PEK G 103:

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

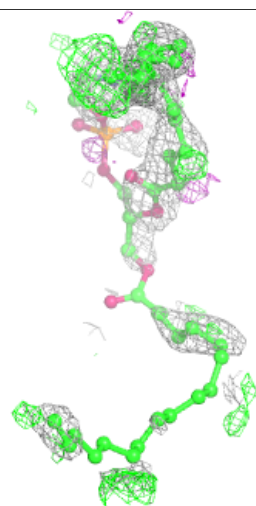
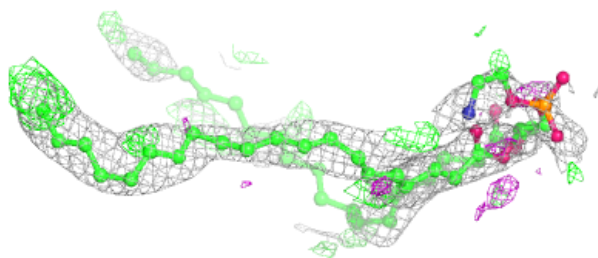
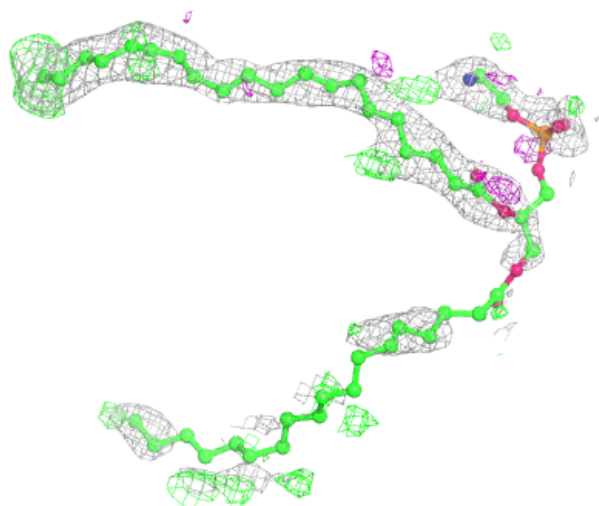
**Electron density around PEK P 308:**

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



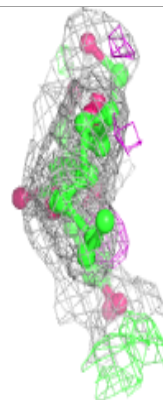
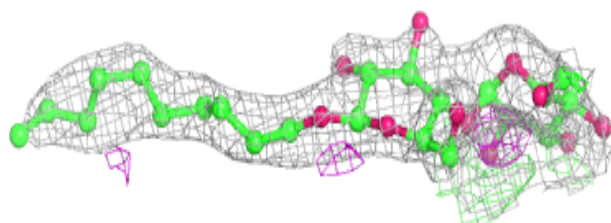
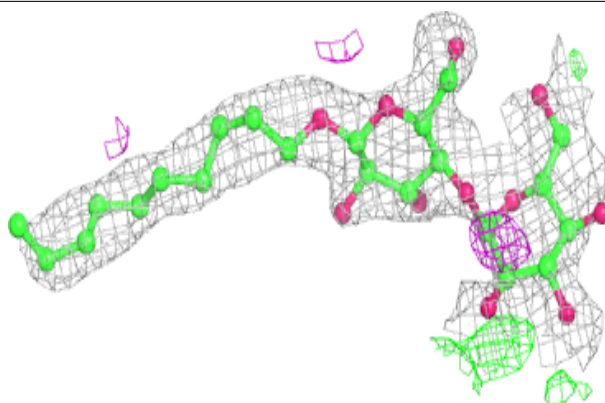
Electron density around PEK C 309:

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

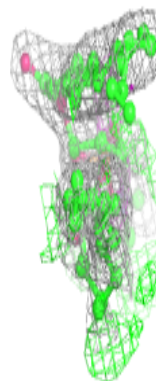
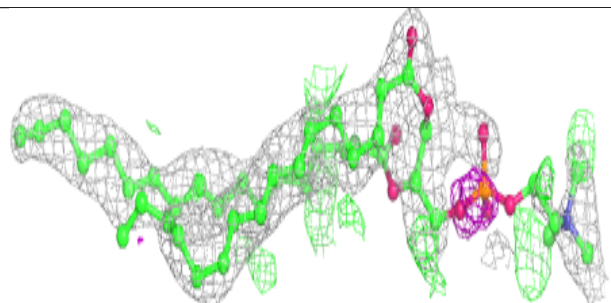
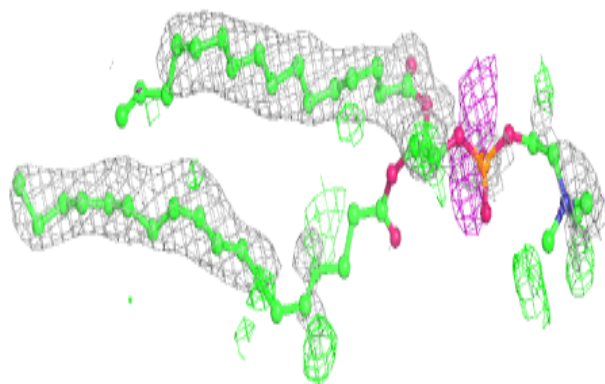


Electron density around DMU P 310:

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

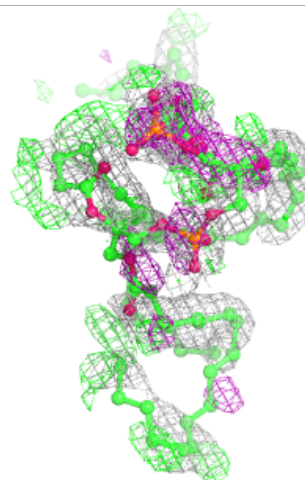
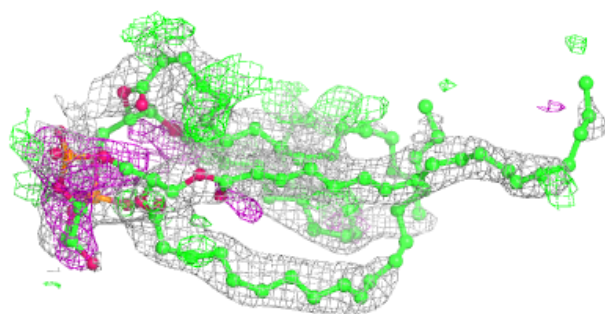
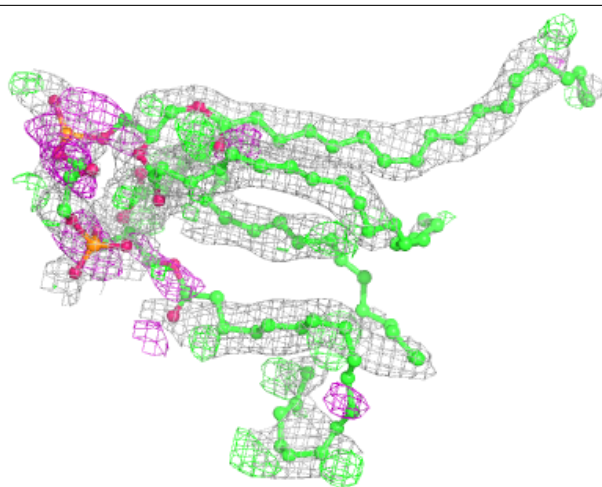
**Electron density around PSC N 612:**

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



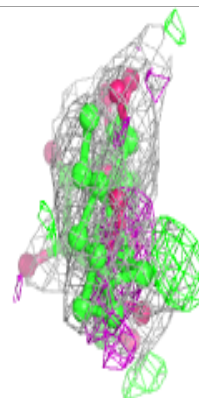
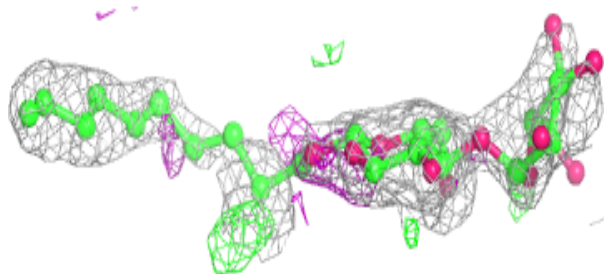
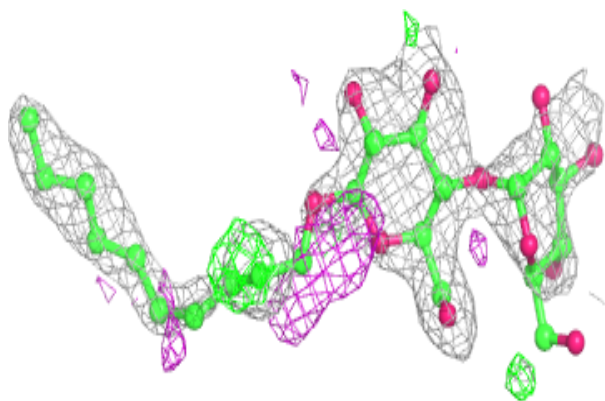
Electron density around CDL P 305:

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

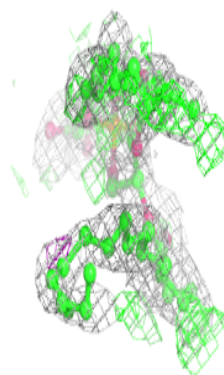
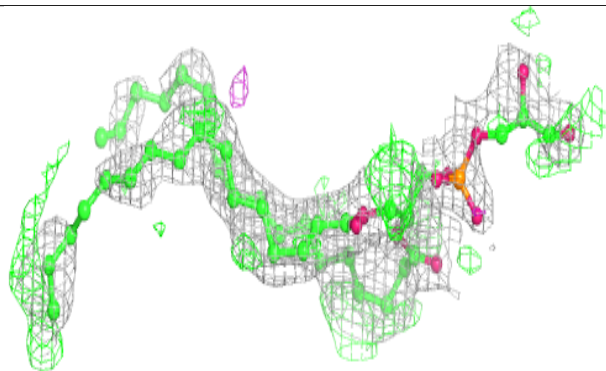
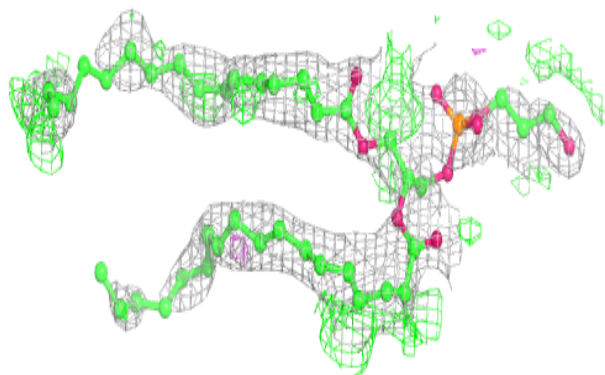


Electron density around DMU P 307:

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

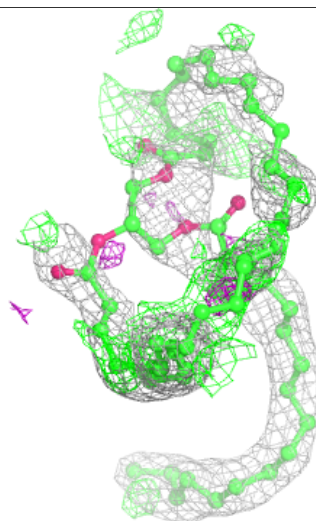
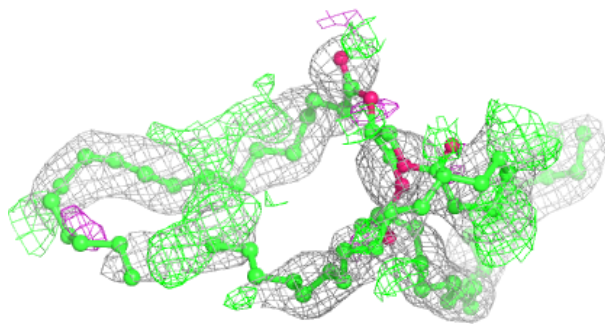
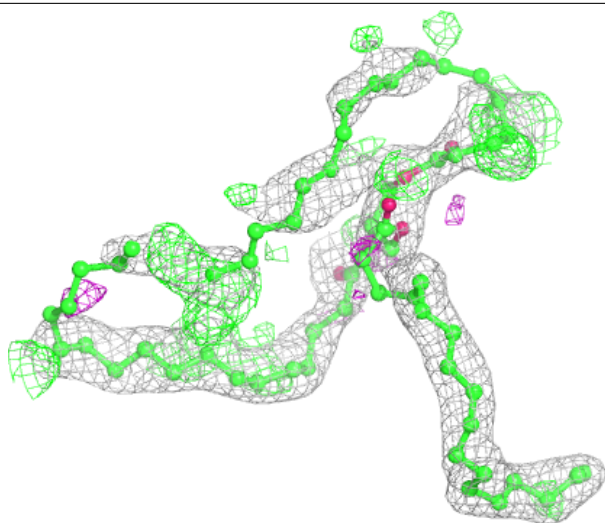
**Electron density around PGV C 308:**

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



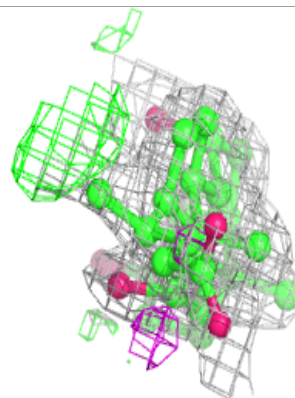
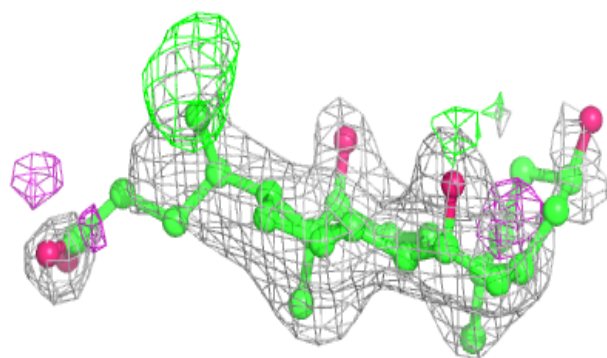
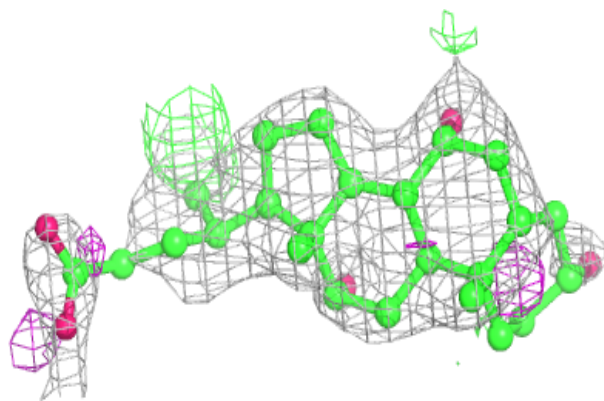
Electron density around TGL Y 101:

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



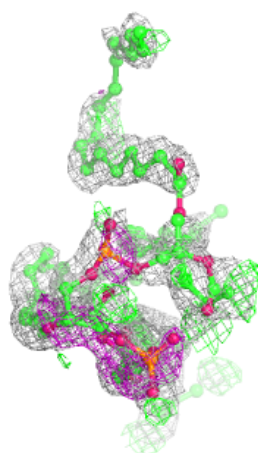
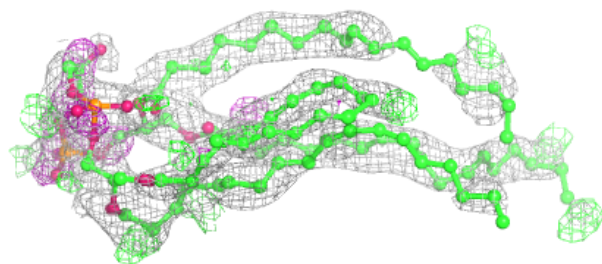
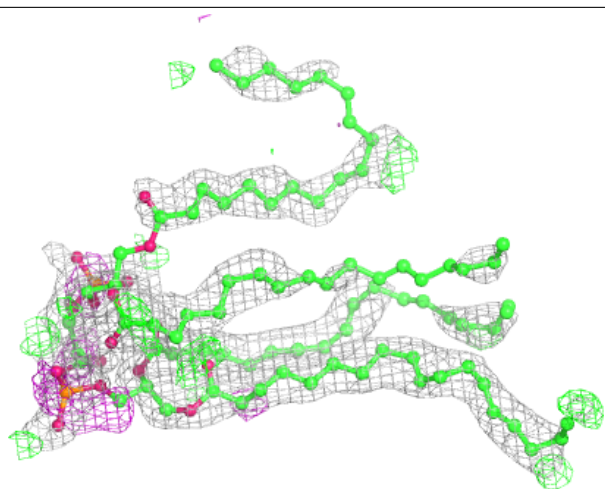
Electron density around CHD J 101:

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



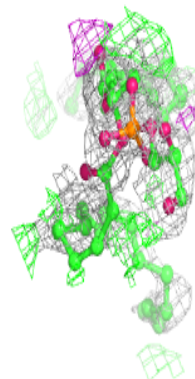
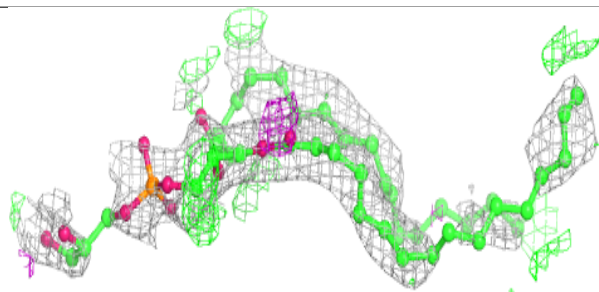
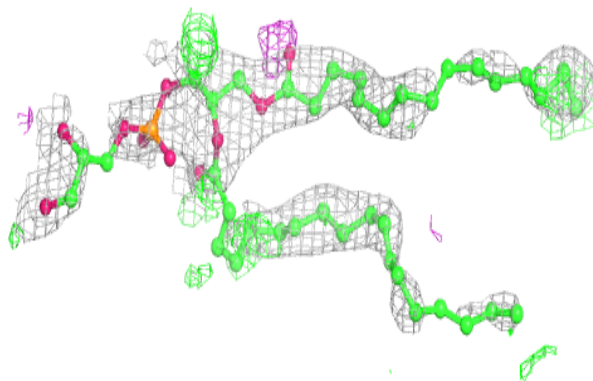
Electron density around CDL C 305:

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

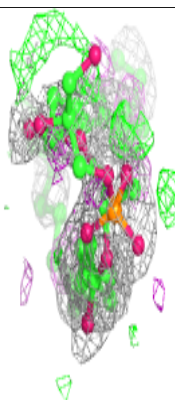
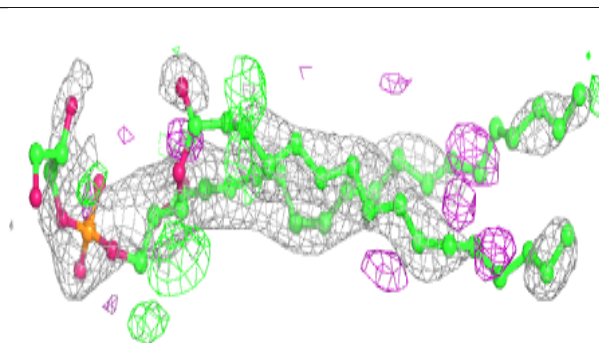
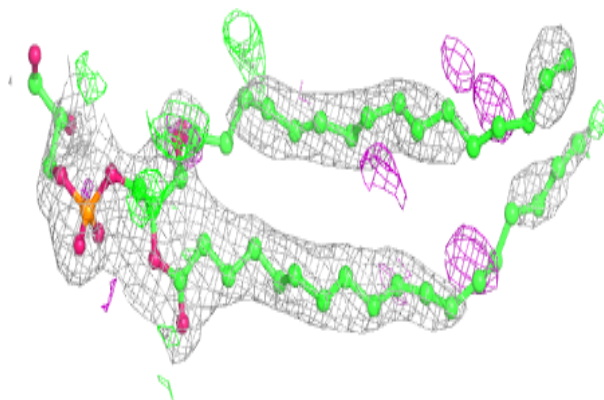


Electron density around PGV P 302:

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

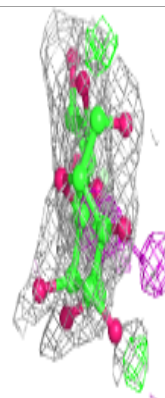
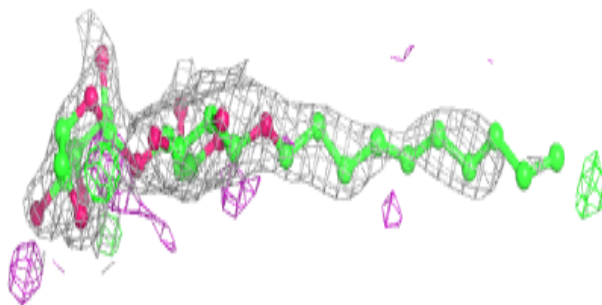
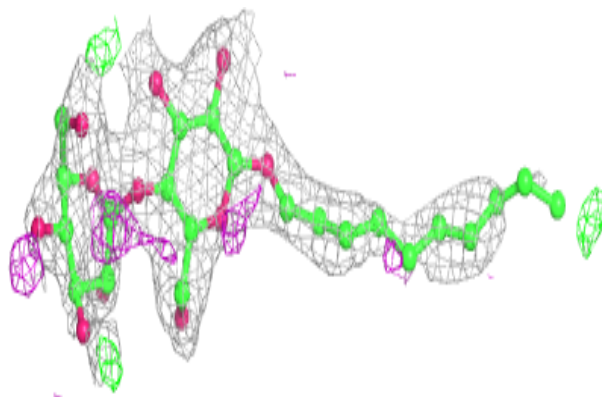
**Electron density around PGV N 609:**

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



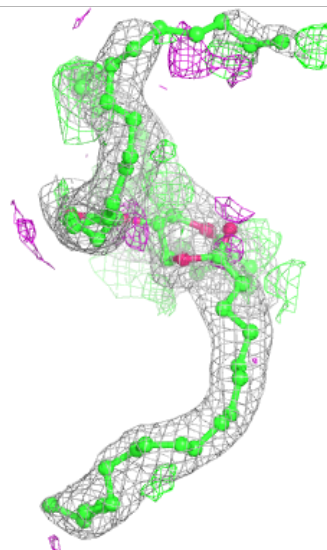
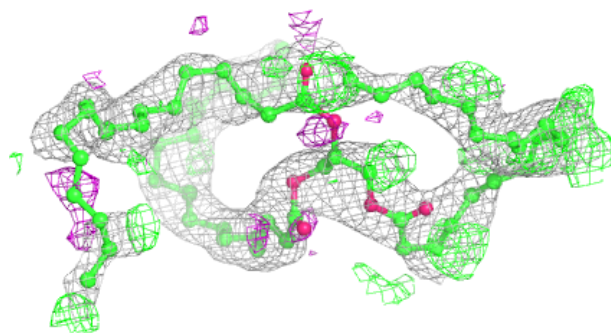
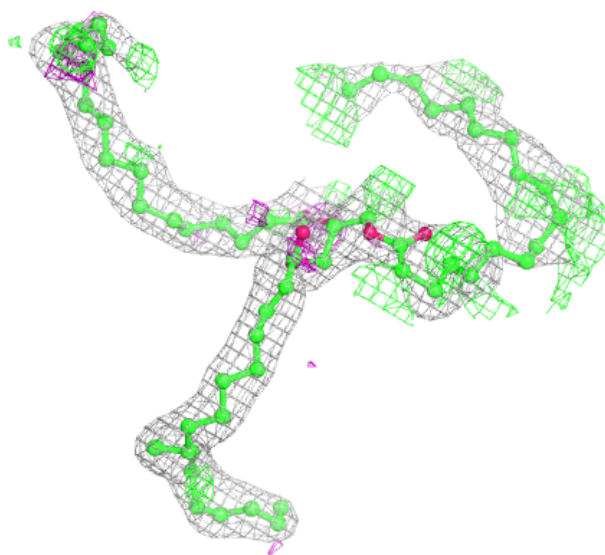
Electron density around DMU C 310:

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



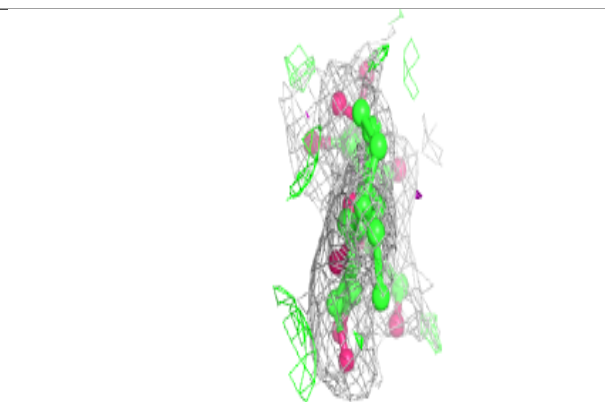
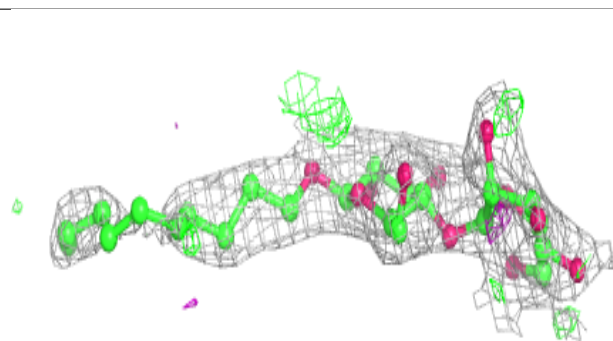
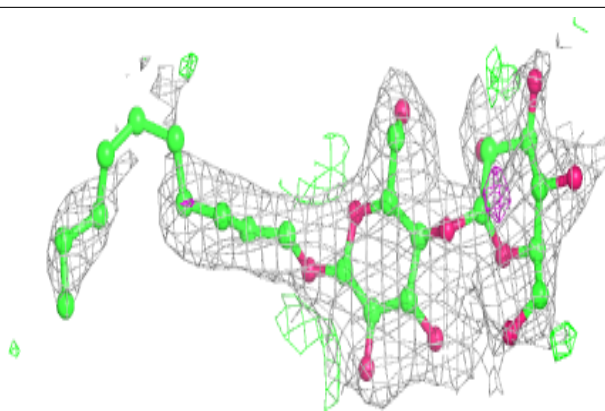
Electron density around TGL A 611:

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

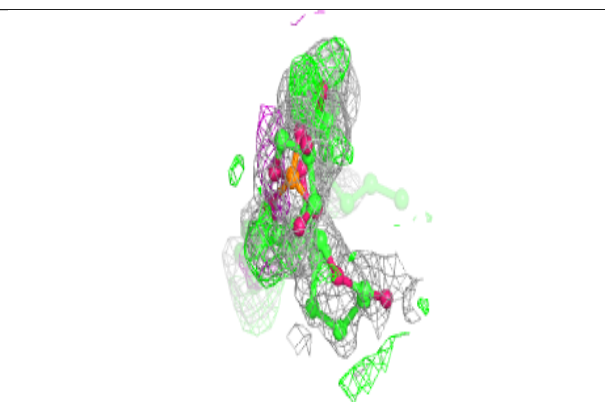
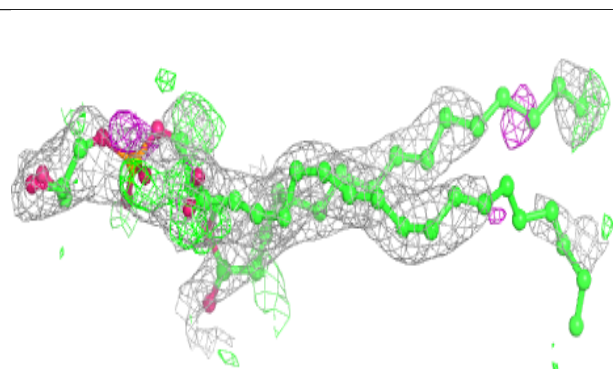
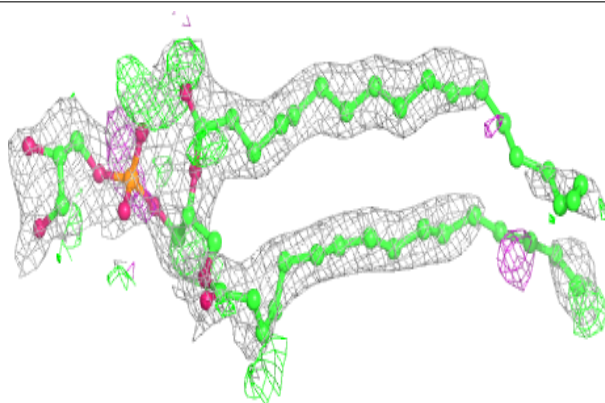


Electron density around DMU P 309:

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

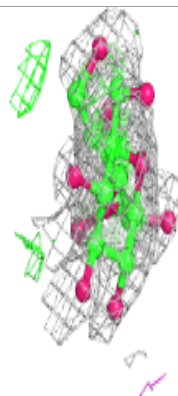
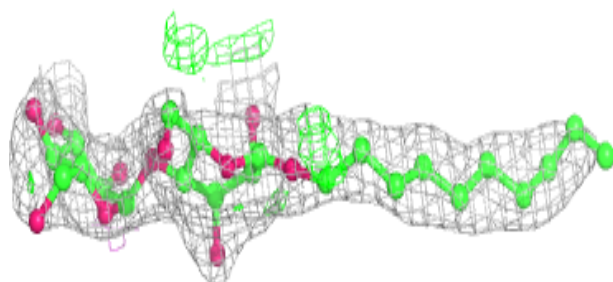
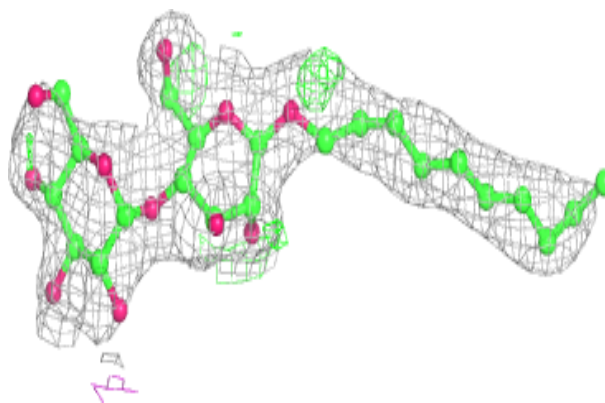
**Electron density around PGV A 610:**

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

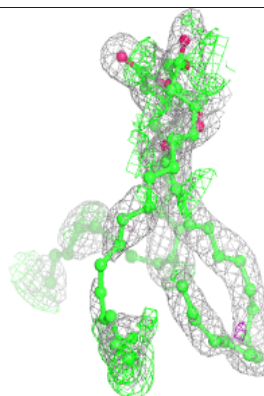
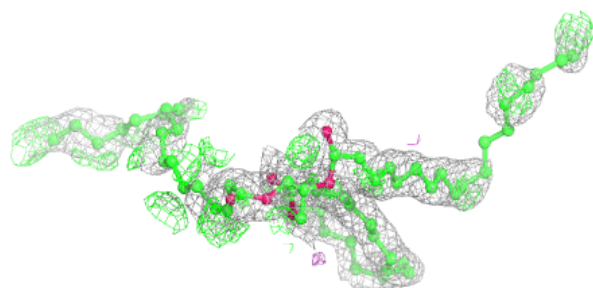
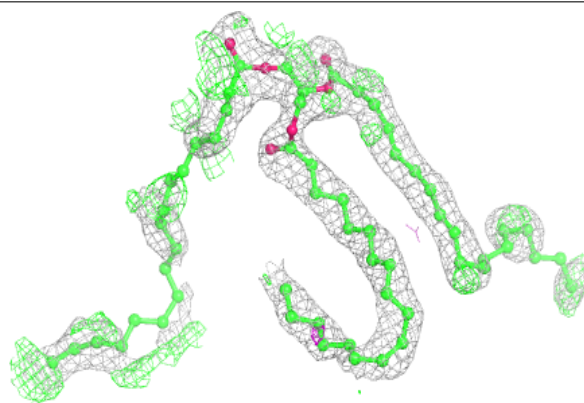


Electron density around DMU C 311:

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

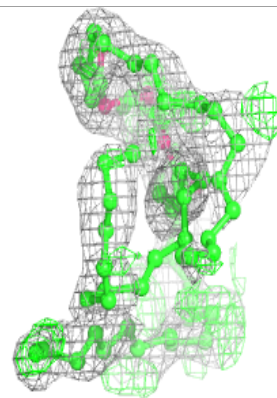
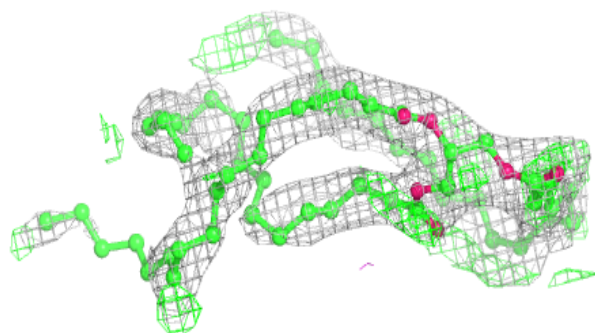
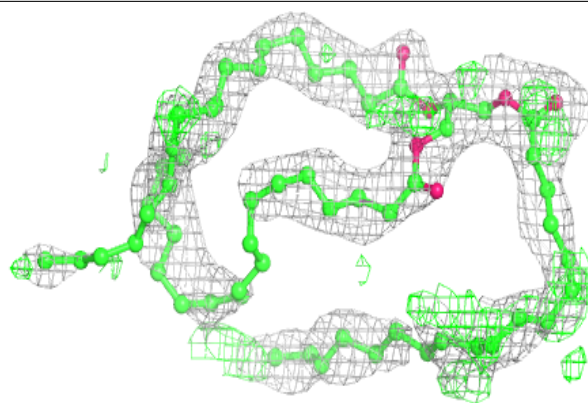
**Electron density around TGL D 201:**

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

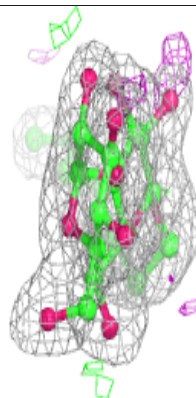
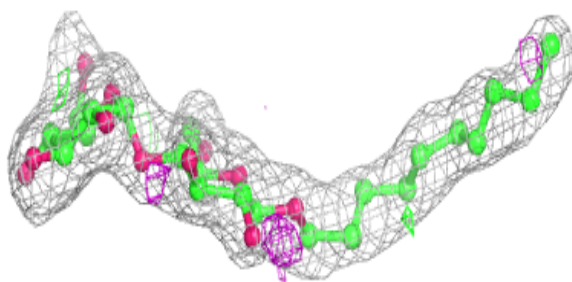
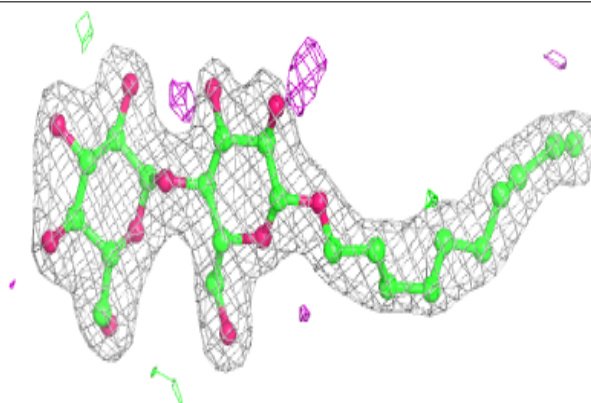


Electron density around TGL N 611:

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

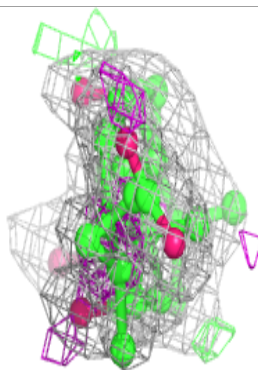
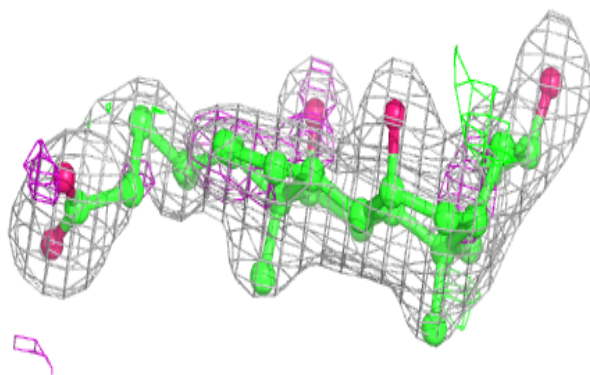
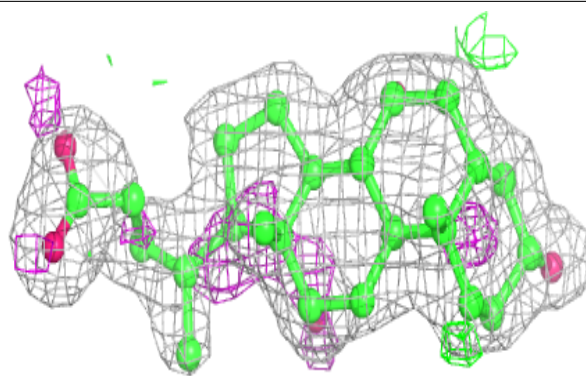
**Electron density around DMU Z 101:**

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

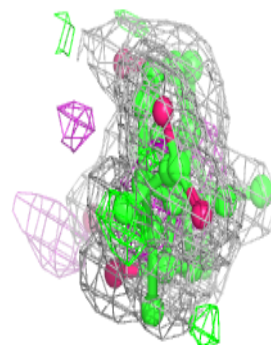
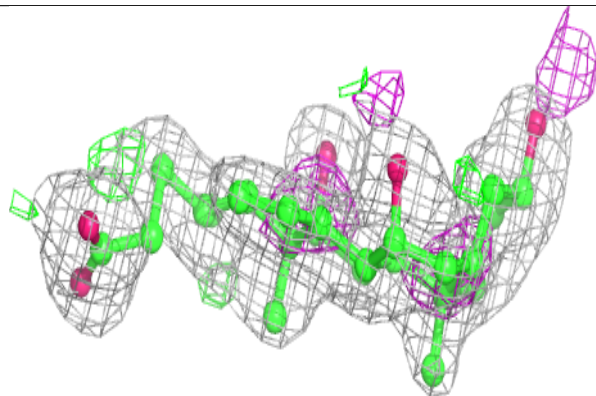
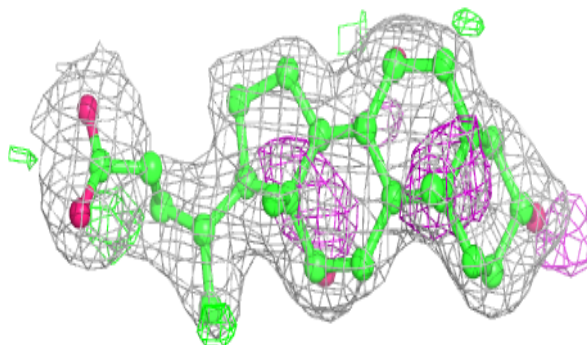


Electron density around CHD C 306:

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

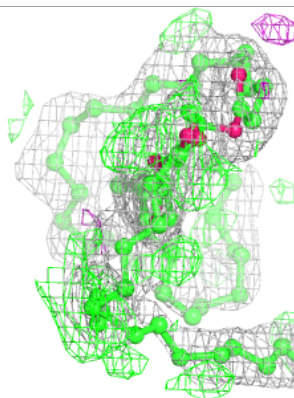
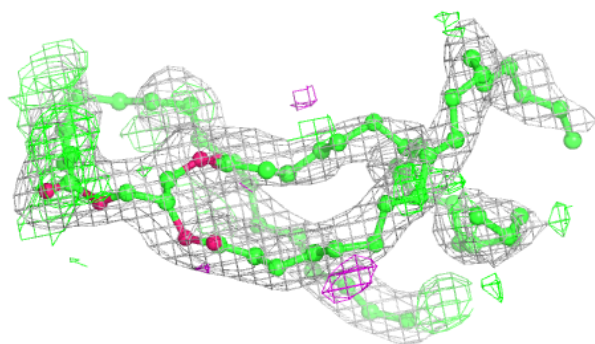
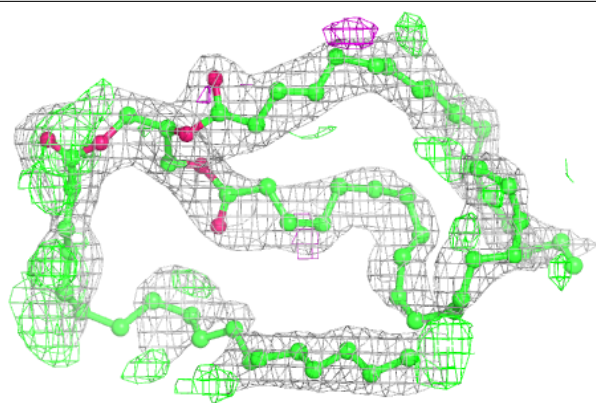
**Electron density around CHD P 306:**

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

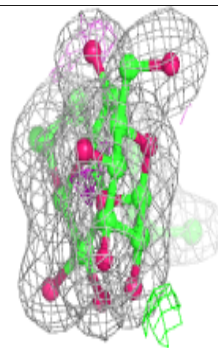
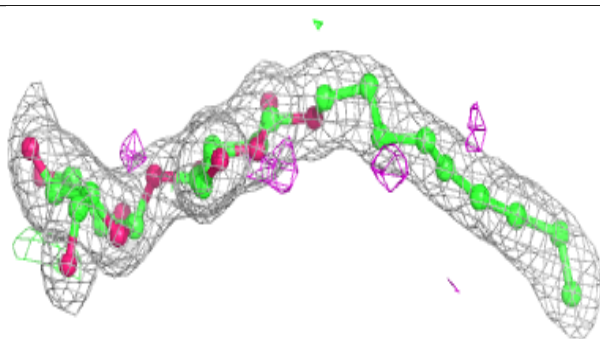
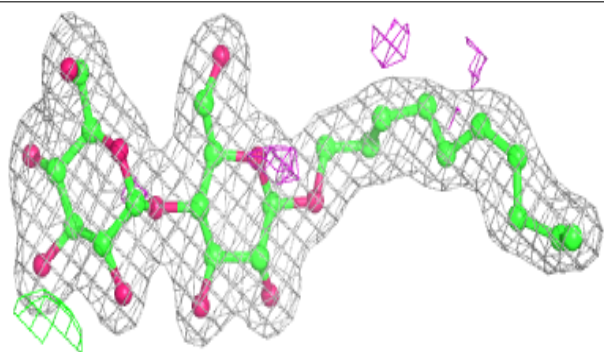


Electron density around TGL A 608:

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

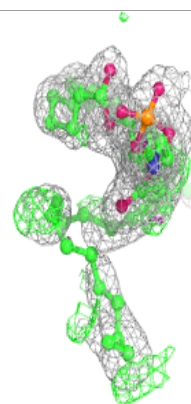
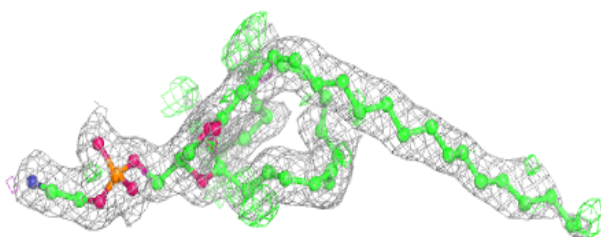
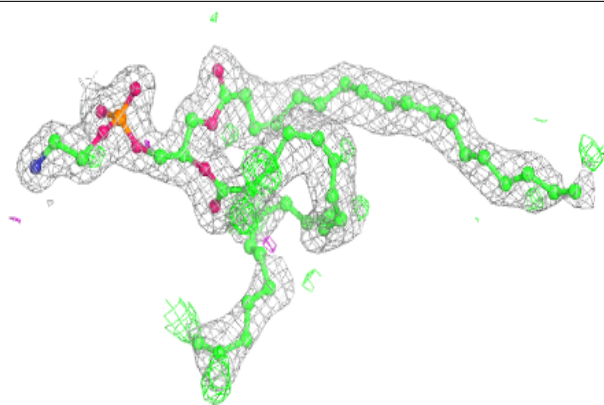
**Electron density around DMU M 101:**

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

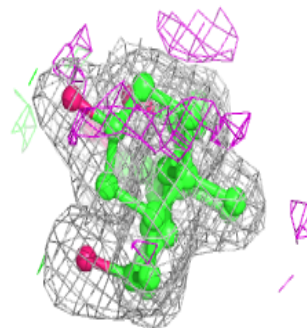
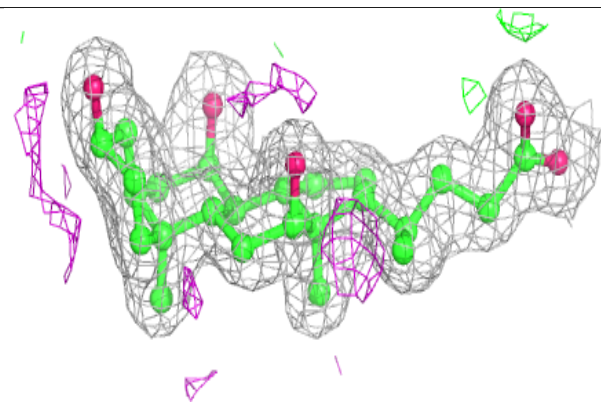
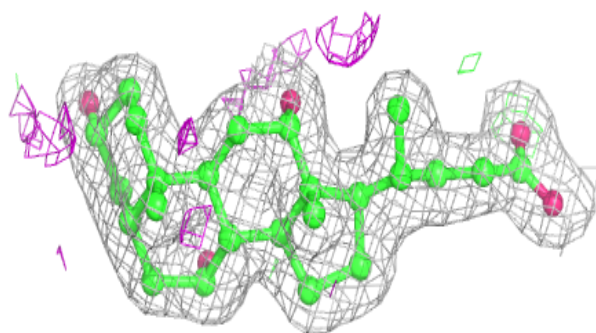


Electron density around PEK T 101:

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

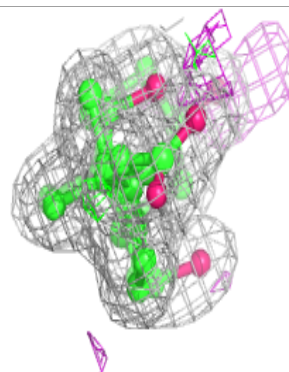
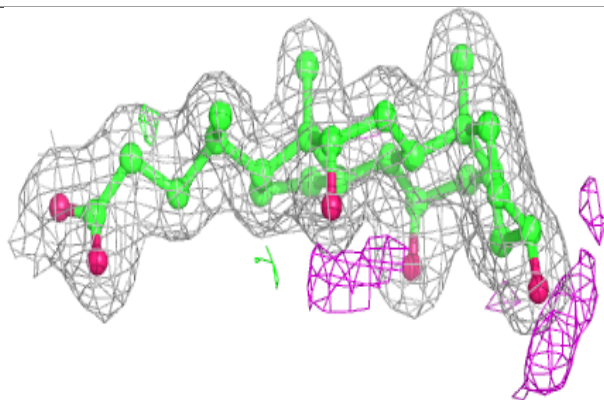
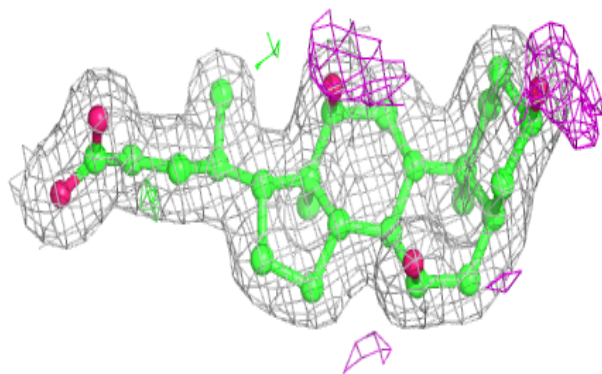
**Electron density around CHD P 301:**

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

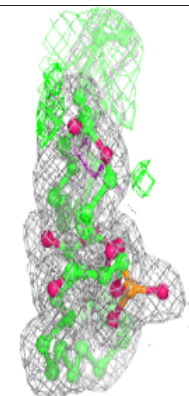
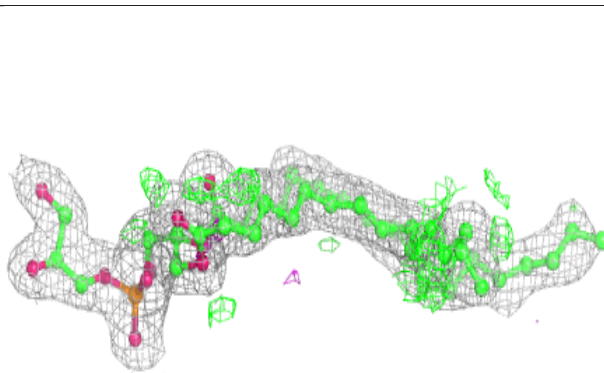
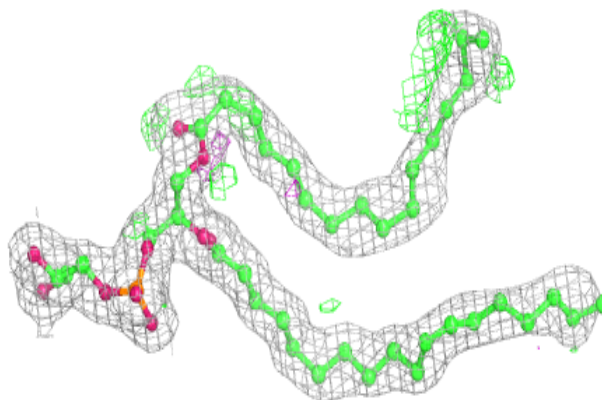


Electron density around CHD C 301:

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

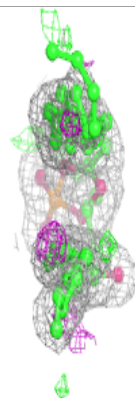
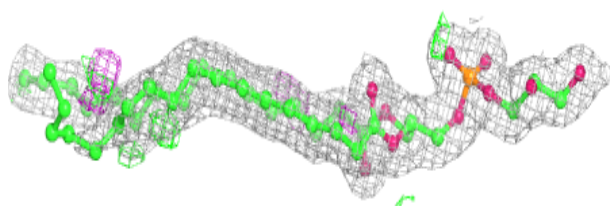
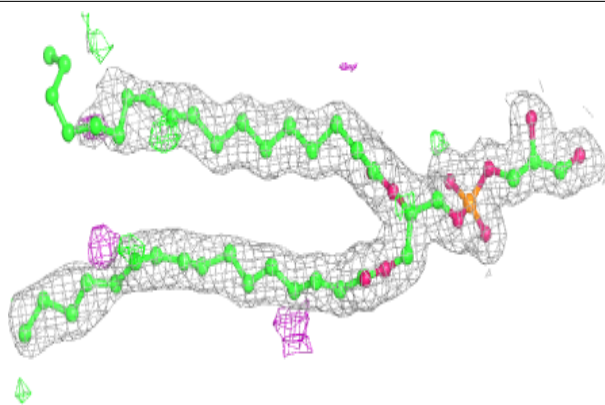
**Electron density around PGV N 610:**

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

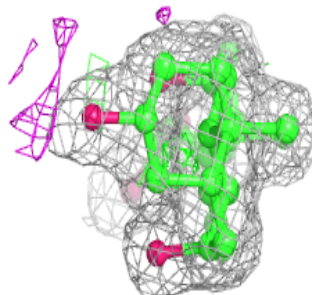
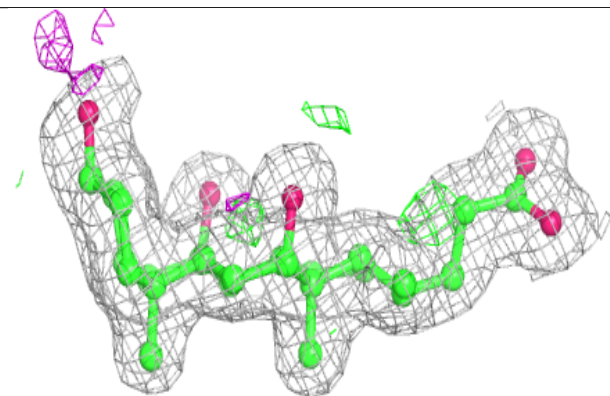
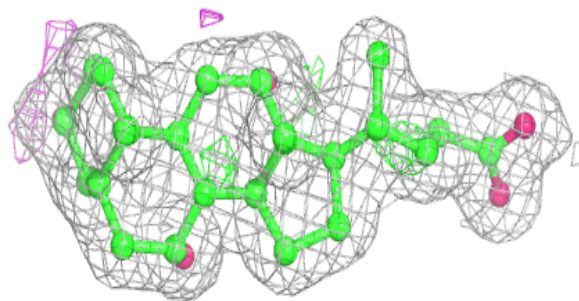


Electron density around PGV C 304:

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

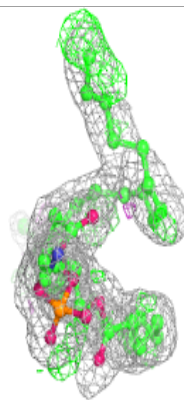
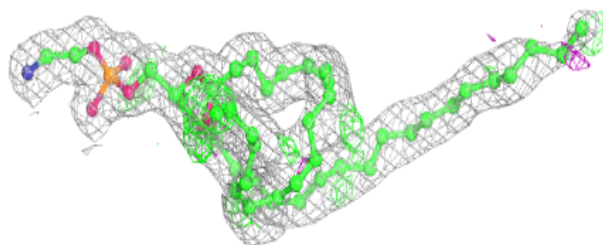
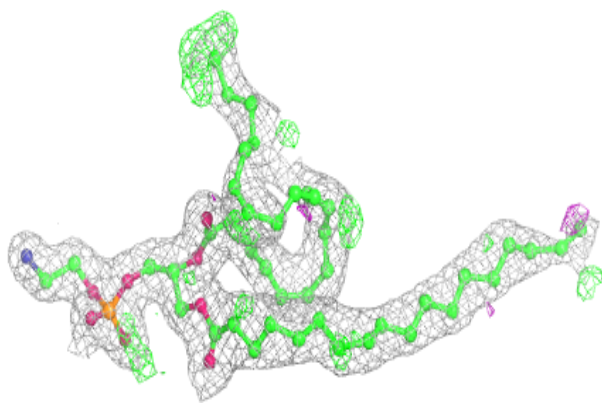
**Electron density around CHD B 301:**

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

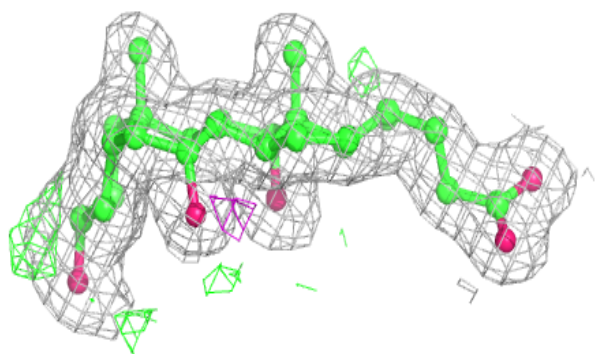
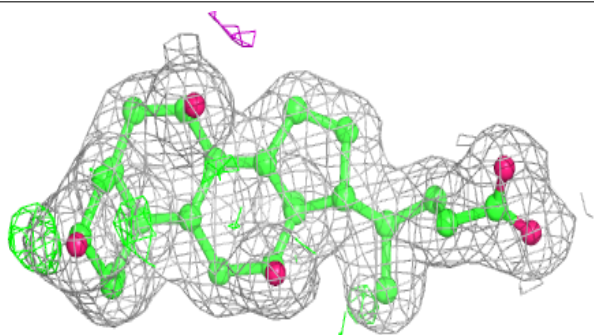


Electron density around PEK G 101:

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

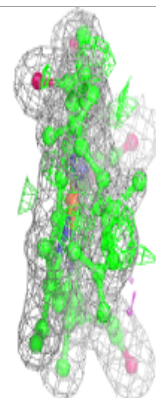
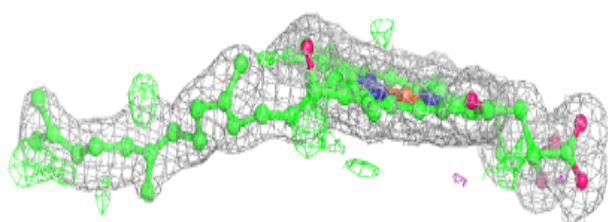
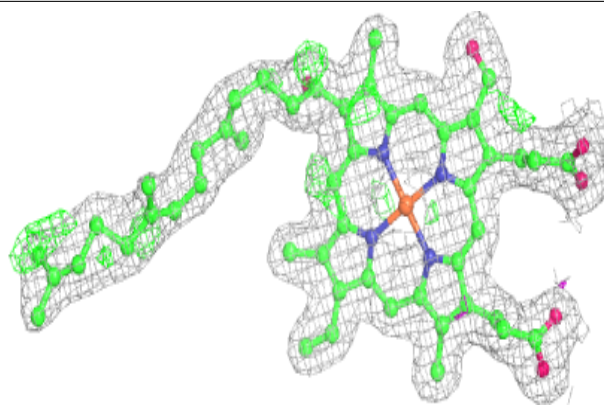
**Electron density around CHD G 102:**

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

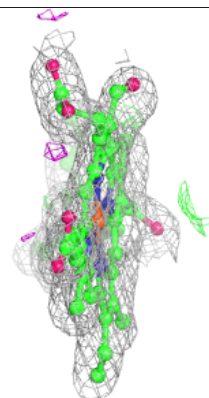
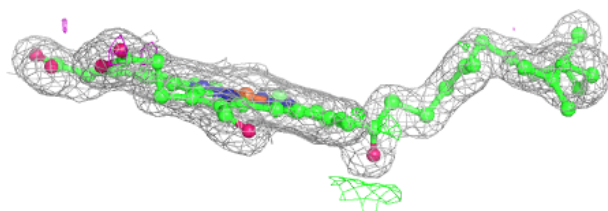
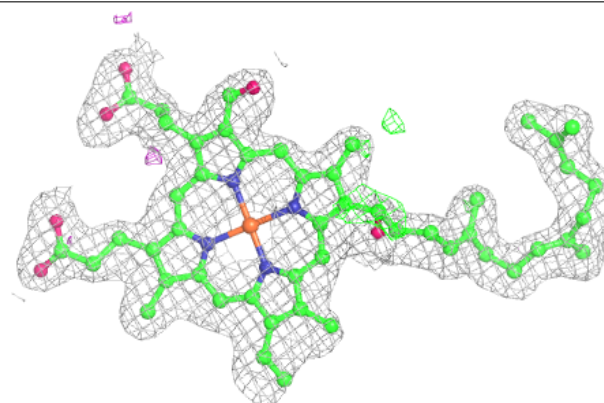


Electron density around HEA N 602:

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

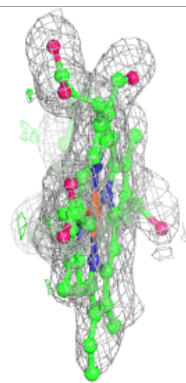
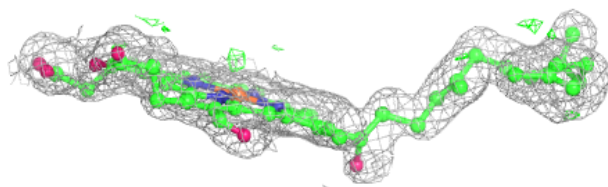
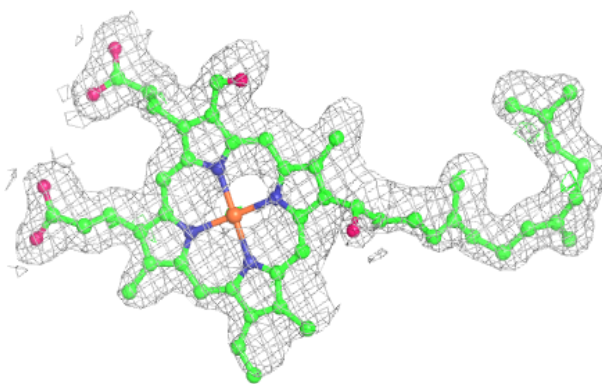
**Electron density around HEA N 603 (B):**

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

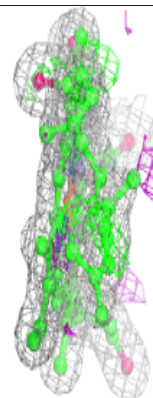
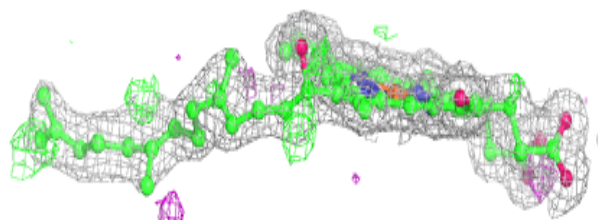
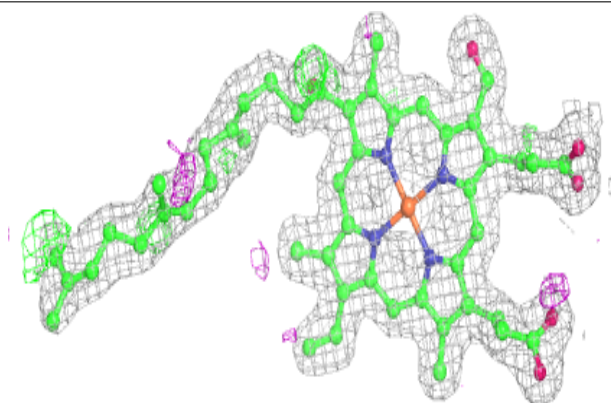


Electron density around HEA A 602 (A):

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

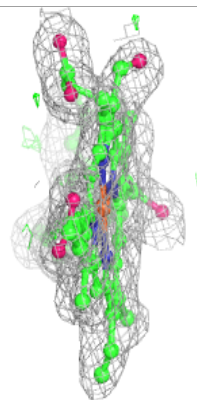
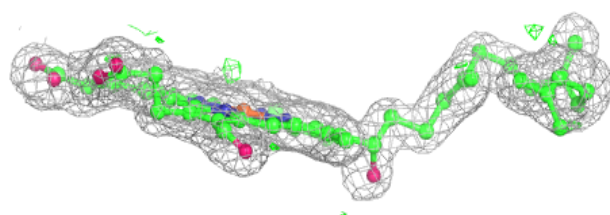
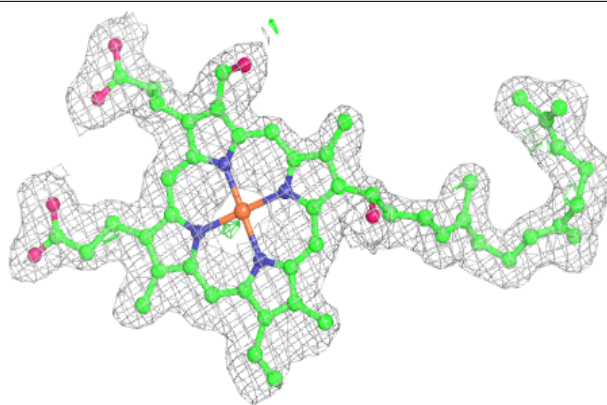
**Electron density around HEA A 601:**

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

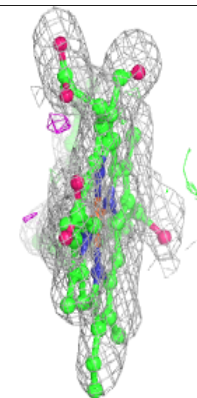
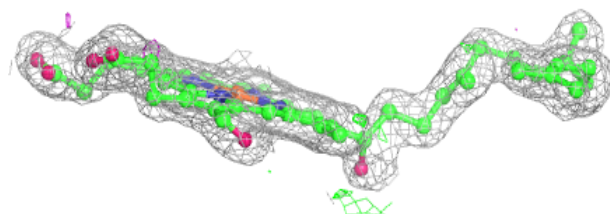
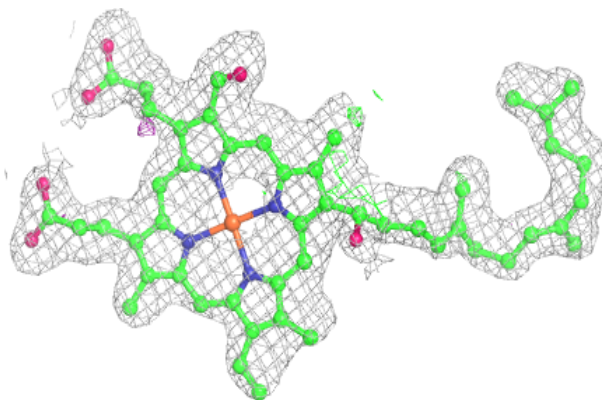


Electron density around HEA A 602 (B):

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

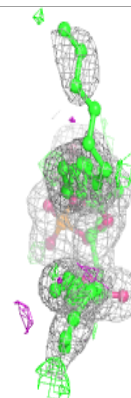
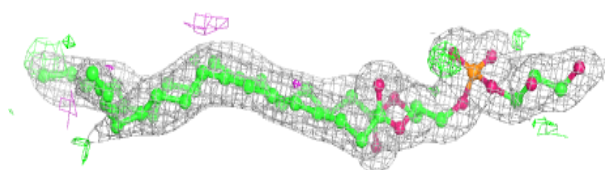
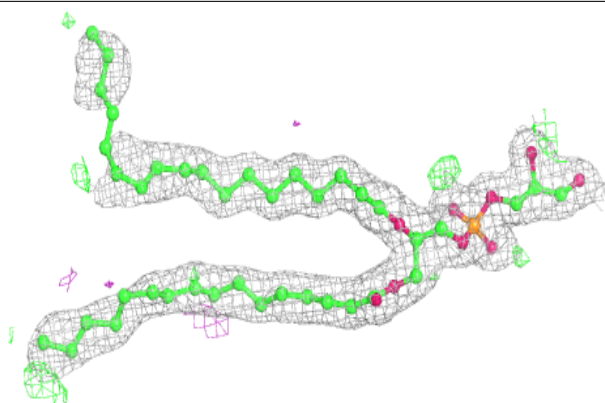
**Electron density around HEA N 603 (A):**

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

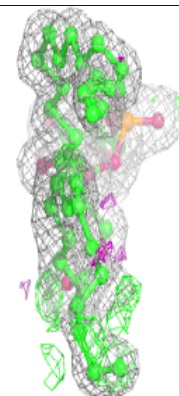
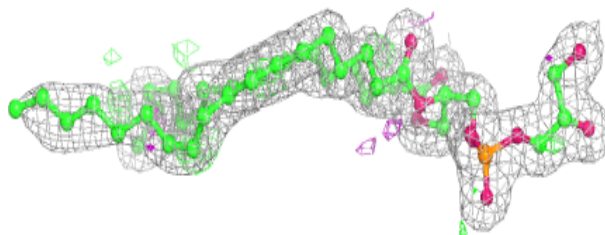
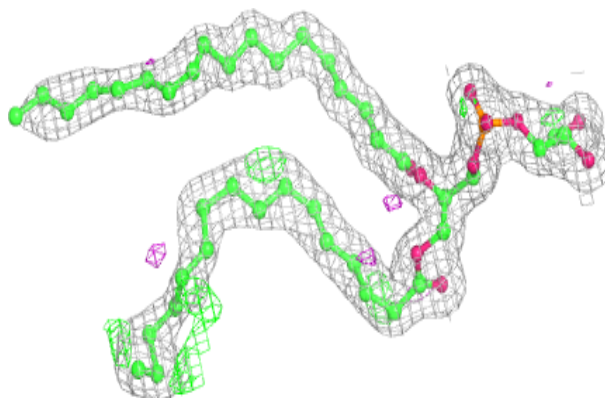


Electron density around PGV P 304:

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

**Electron density around PGV 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.