



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:04 PM JST

PDB ID : 7D5X / pdb_00007d5x
Title : Bovine heart cytochrome c oxidase in a catalytic intermediate, IO10, at 1.74 angstrom resolution
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2020-09-28
Resolution : 1.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

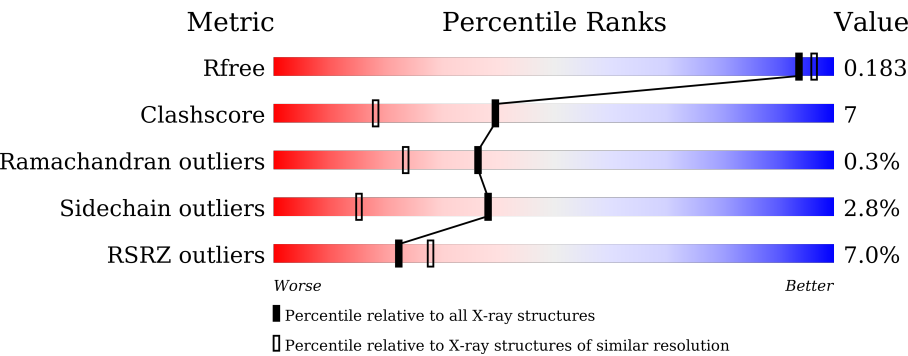
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.74 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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

Mol	Chain	Length	Quality of chain
1	A	514	2% 88% 11% .
1	N	514	2% 88% 12%
2	B	227	7% 84% 16%
2	O	227	6% 81% 17% .
3	C	259	% 90% 10%
3	P	259	% 90% 10% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	94	
6	S	94	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33923 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	34	0
			4183	2789	644	711	39			
1	N	514	Total	C	N	O	S	0	28	0
			4174	2782	645	709	38			

- 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	14	0
			1867	1214	284	349	20			
2	O	227	Total	C	N	O	S	0	9	0
			1853	1204	283	346	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	12	0
			2143	1430	341	358	14			
3	P	259	Total	C	N	O	S	0	8	0
			2131	1420	340	357	14			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	0	0
			716	444	127	140	5			
6	S	94	Total	C	N	O	S	0	0	0
			716	444	127	140	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	S	0	0	0
			672	431	129	111	1			
7	T	84	Total	C	N	O	S	0	0	0
			672	431	129	111	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	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
			461	297	78	83	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			461	297	78	83	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
			385	250	65	68	2			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

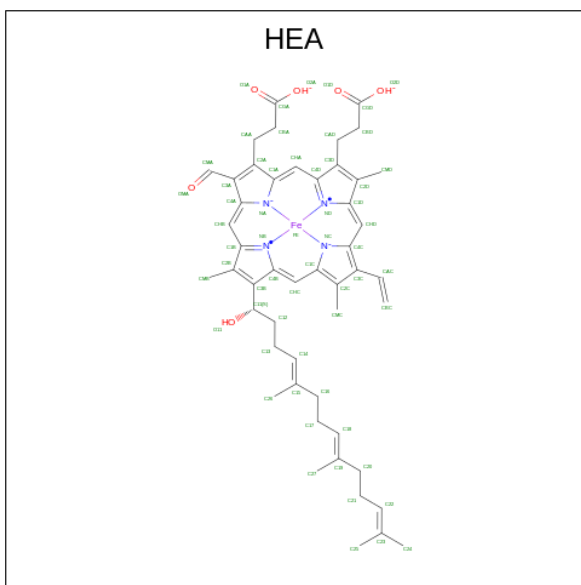
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			336	223	53	60			
13	Z	43	Total	C	N	O	0	0	0
			336	223	53	60			

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 81	C 69	Fe 1	N 4	O 7	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 81	C 69	Fe 1	N 4	O 7	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

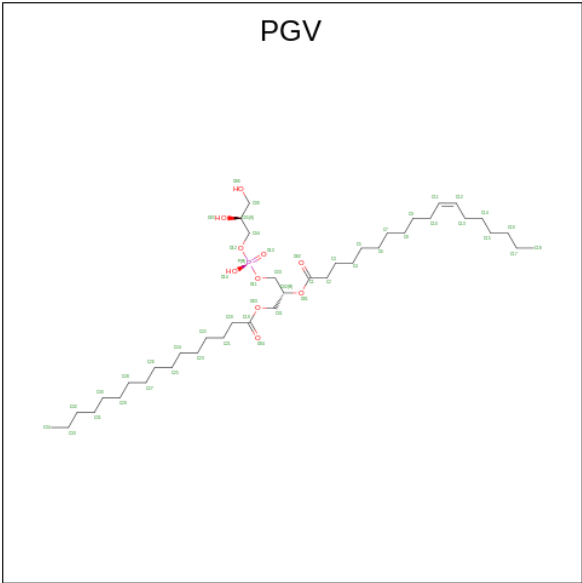
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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



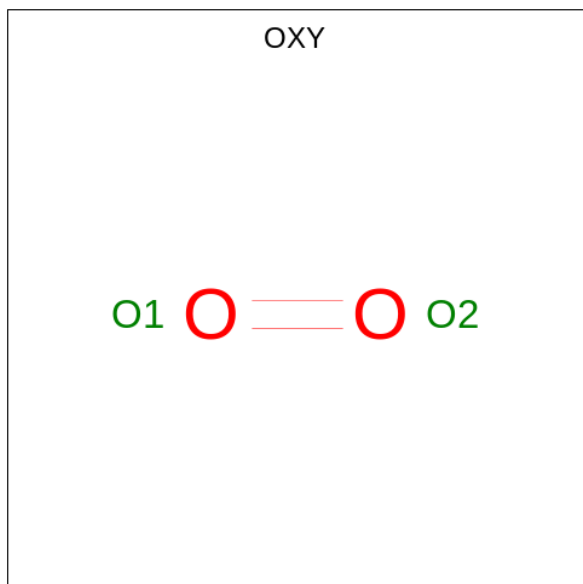
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O		0	0
			33	32	1			
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O		0	0
			37	34	3			
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O		0	0
			38	36	2			

Continued on next page...

Continued from previous page...

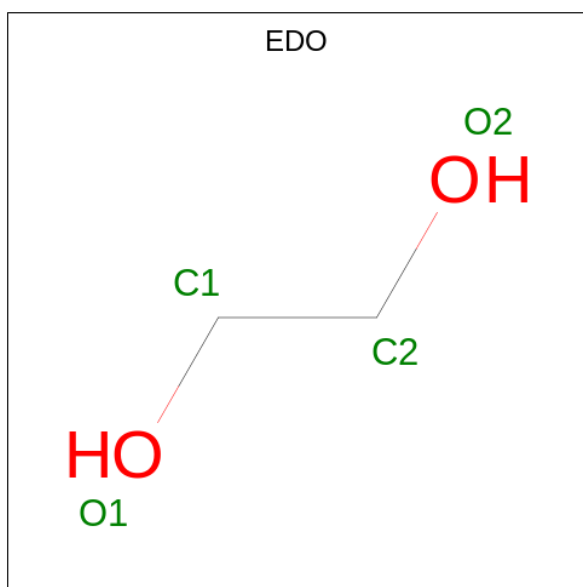
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	Q	1	Total	C	O	0	0
			37	35	2		

- Molecule 19 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 20 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total 4	C 2	O 2	0	0
20	B	1	Total 4	C 2	O 2	0	0
20	B	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	D	1	Total 4	C 2	O 2	0	0
20	D	1	Total 4	C 2	O 2	0	0
20	D	1	Total 4	C 2	O 2	0	0
20	D	1	Total 4	C 2	O 2	0	0
20	E	1	Total 4	C 2	O 2	0	0
20	E	1	Total 4	C 2	O 2	0	0
20	E	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4	C 2	O 2	0	0
20	J	1	Total 4	C 2	O 2	0	0
20	J	1	Total 4	C 2	O 2	0	0
20	L	1	Total 4	C 2	O 2	0	0
20	M	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

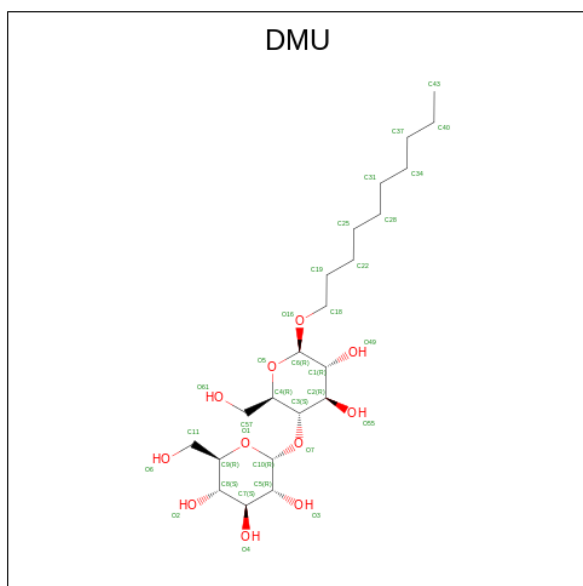
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	O	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	T	1	Total 4	C 2	O 2	0	0
20	T	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	T	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		

- Molecule 21 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



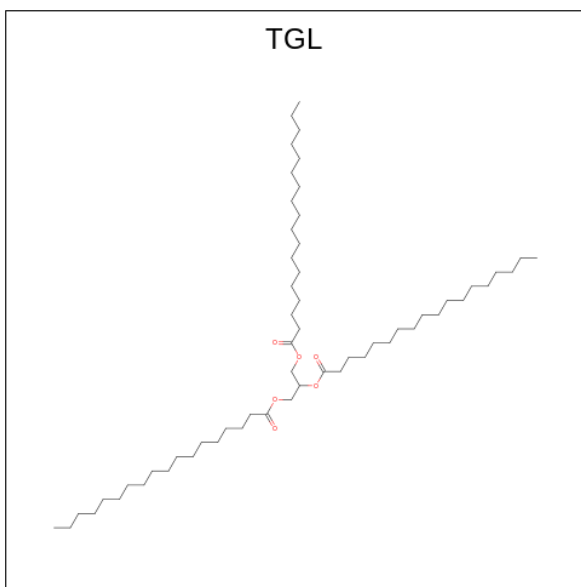
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C		0	0
			9	9			
21	A	1	Total	C		0	0
			8	8			
21	C	1	Total	C	O	0	0
			22	16	6		
21	C	1	Total	C	O	0	0
			12	11	1		
21	D	1	Total	C	O	0	0
			11	10	1		
21	D	1	Total	C		0	0
			8	8			
21	J	1	Total	C	O	0	0
			11	10	1		

Continued on next page...

Continued from previous page...

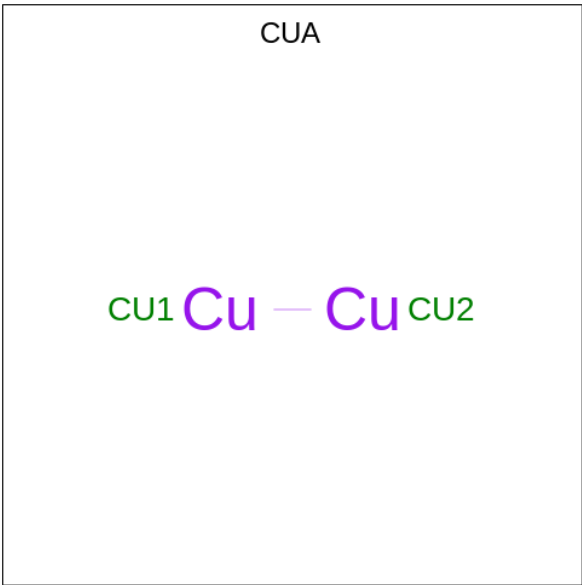
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	K	1	Total C 9 9	0	0
21	K	1	Total C 9 9	0	0
21	K	1	Total C 9 9	0	0
21	K	1	Total C 10 10	0	0
21	L	1	Total C O 21 16 5	0	0
21	M	1	Total C O 33 22 11	0	0
21	N	1	Total C 9 9	0	0
21	O	1	Total C O 11 10 1	0	0
21	P	1	Total C O 22 16 6	0	0
21	P	1	Total C O 11 10 1	0	0
21	Q	1	Total C 10 10	0	0
21	W	1	Total C O 11 10 1	0	0
21	X	1	Total C 9 9	0	0
21	X	1	Total C 8 8	0	0
21	X	1	Total C 10 10	0	0
21	Z	1	Total C O 33 22 11	0	0

- Molecule 22 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



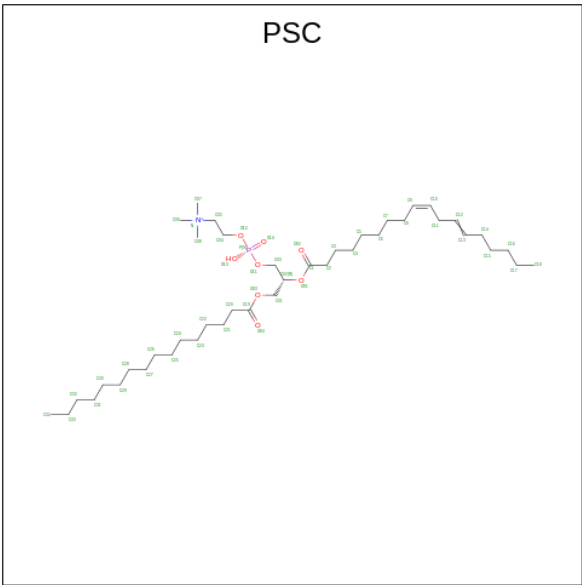
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			63	57	6		
22	D	1	Total	C	O	0	0
			63	57	6		
22	L	1	Total	C	O	0	0
			54	49	5		
22	N	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C		0	0
			43	43			
22	N	1	Total	C	O	0	0
			55	53	2		

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 24 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



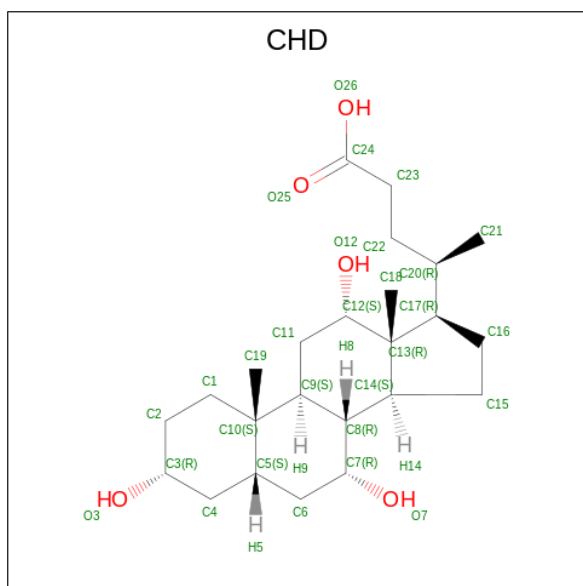
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			41	37	4		

Continued on next page...

Continued from previous page...

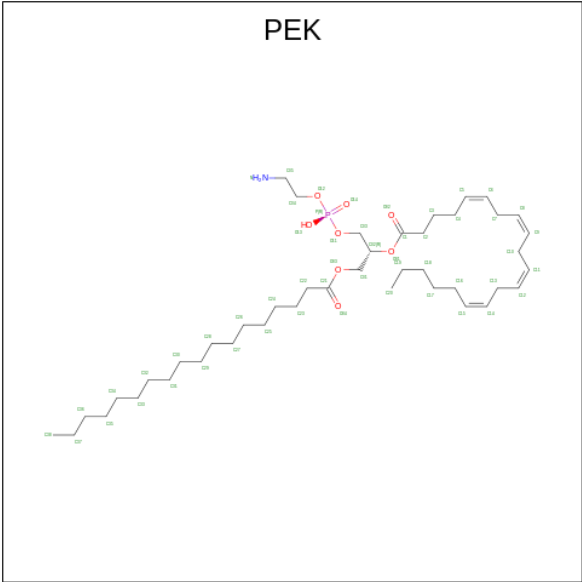
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	O	1	Total	C	O	0	0
			33	32	1		

- Molecule 25 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



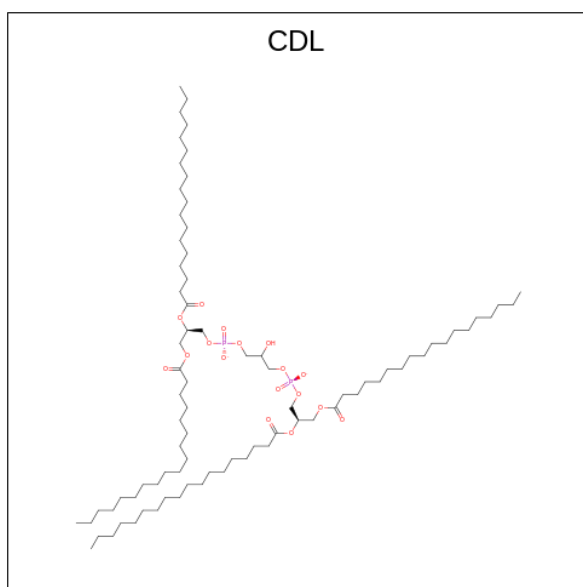
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			29	24	5		
25	C	1	Total	C	O	0	0
			29	24	5		
25	C	1	Total	C	O	0	0
			29	24	5		
25	G	1	Total	C	O	0	0
			29	24	5		
25	L	1	Total	C	O	0	0
			29	24	5		
25	P	1	Total	C	O	0	0
			29	24	5		
25	P	1	Total	C	O	0	0
			29	24	5		

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	C	1	Total C 18 18					0	0
26	C	1	Total C N O P 53 43 1 8 1					0	0
26	C	1	Total C O 40 38 2					0	0
26	P	1	Total C O 28 27 1					0	0
26	P	1	Total C N O P 53 43 1 8 1					0	0
26	P	1	Total C O 40 38 2					0	0

- Molecule 27 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).

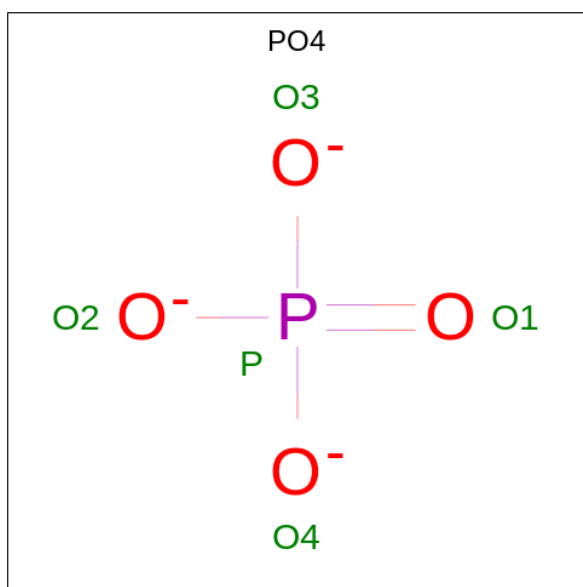


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O P 85 75 9 1	0	0
27	G	1	Total C O 69 67 2	0	0
27	P	1	Total C O 77 72 5	0	0
27	T	1	Total C O 70 66 4	0	0

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 29 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	H	1	Total	O	P	0	0
			5	4	1		
29	U	1	Total	O	P	0	0
			5	4	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	248	Total	O	0	6
			250	250		
30	B	194	Total	O	0	3
			195	195		
30	C	139	Total	O	0	0
			139	139		
30	D	182	Total	O	0	1
			183	183		
30	E	133	Total	O	0	0
			133	133		
30	F	144	Total	O	0	0
			144	144		
30	G	68	Total	O	0	0
			68	68		
30	H	87	Total	O	0	0
			87	87		
30	I	63	Total	O	0	0
			63	63		
30	J	47	Total	O	0	0
			47	47		

Continued on next page...

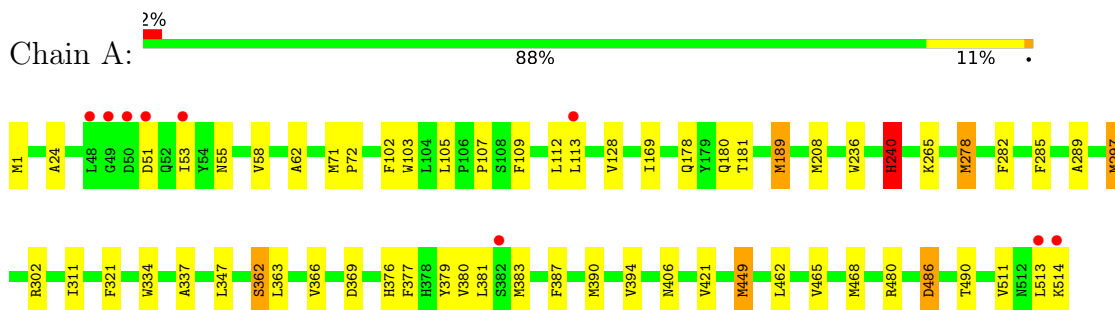
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	38	Total 38	O 38	0	0
30	L	30	Total 30	O 30	0	0
30	M	35	Total 35	O 35	0	0
30	N	247	Total 247	O 247	0	3
30	O	169	Total 169	O 169	0	1
30	P	145	Total 145	O 145	0	0
30	Q	88	Total 88	O 88	0	0
30	R	106	Total 106	O 106	0	0
30	S	133	Total 133	O 133	0	0
30	T	61	Total 61	O 61	0	0
30	U	78	Total 78	O 78	0	0
30	V	48	Total 48	O 48	0	0
30	W	46	Total 46	O 46	0	0
30	X	28	Total 28	O 28	0	0
30	Y	29	Total 29	O 29	0	0
30	Z	22	Total 22	O 22	0	0

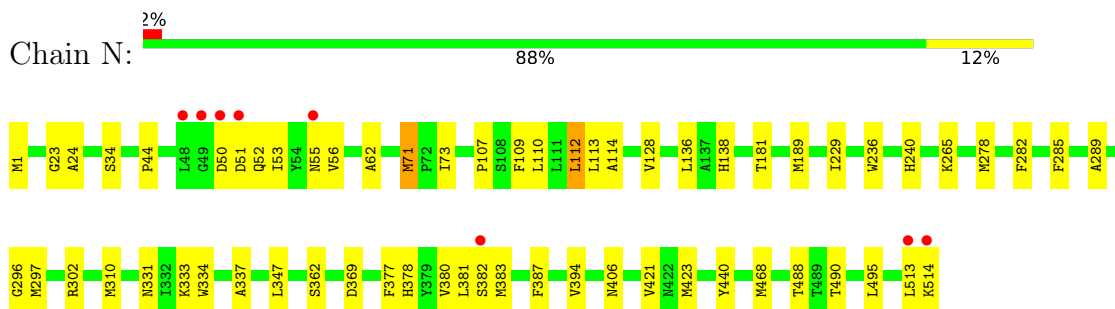
3 Residue-property plots

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

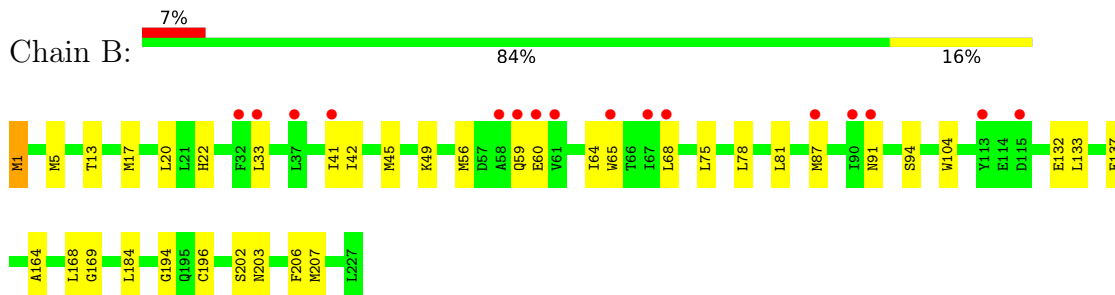
• Molecule 1: Cytochrome c oxidase subunit 1



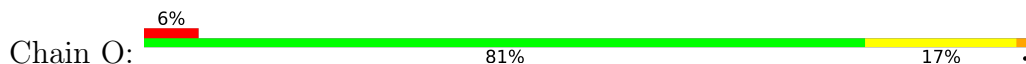
• Molecule 1: Cytochrome c oxidase subunit 1

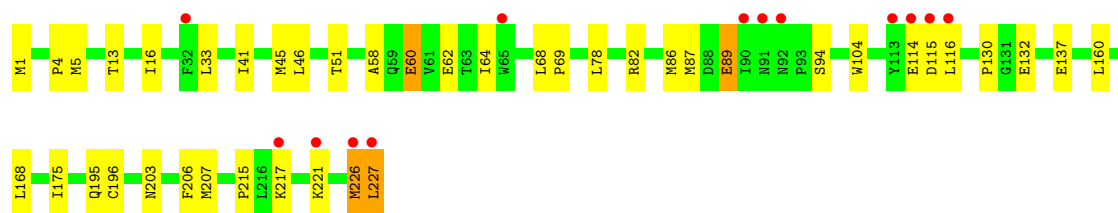


• Molecule 2: Cytochrome c oxidase subunit 2

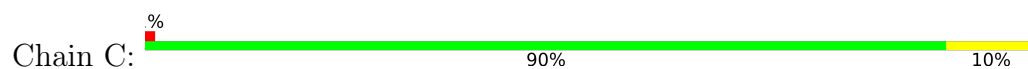


• Molecule 2: Cytochrome c oxidase subunit 2

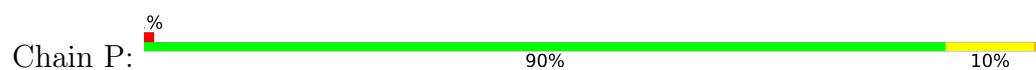




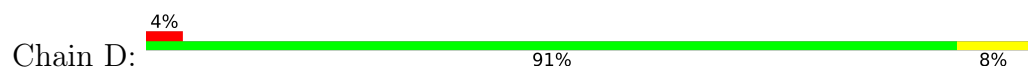
• Molecule 3: Cytochrome c oxidase subunit 3



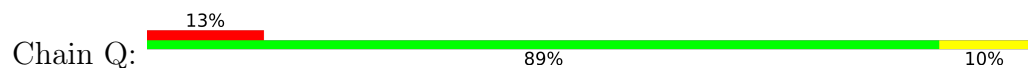
• Molecule 3: Cytochrome c oxidase subunit 3



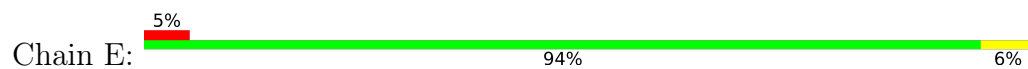
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



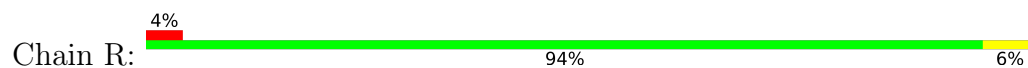
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

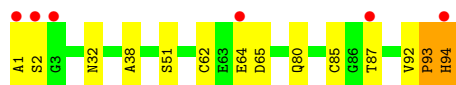
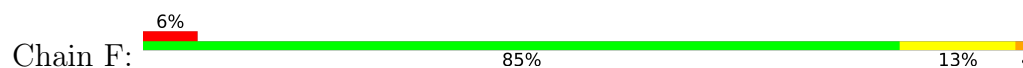


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

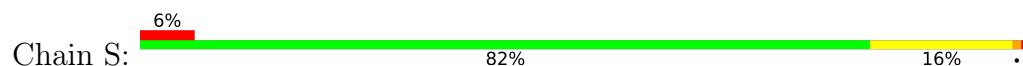




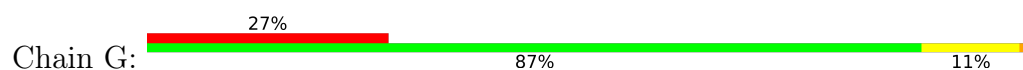
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



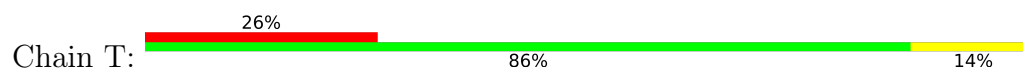
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



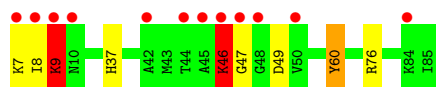
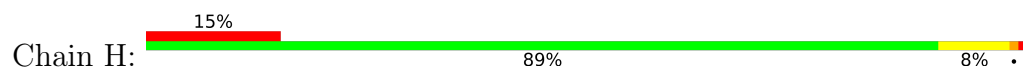
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



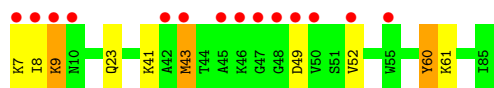
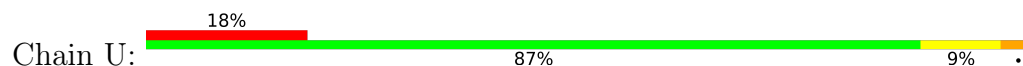
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



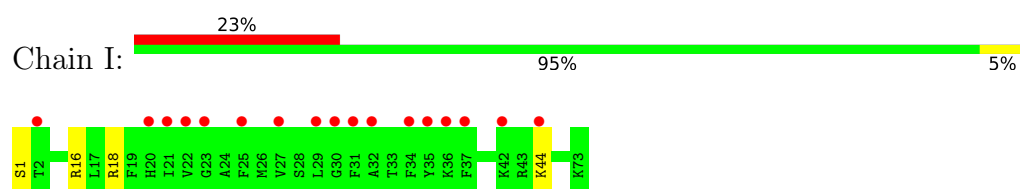
- Molecule 8: Cytochrome c oxidase subunit 6B1



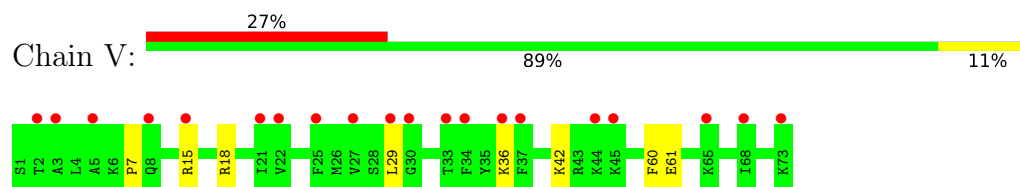
- Molecule 8: Cytochrome c oxidase subunit 6B1



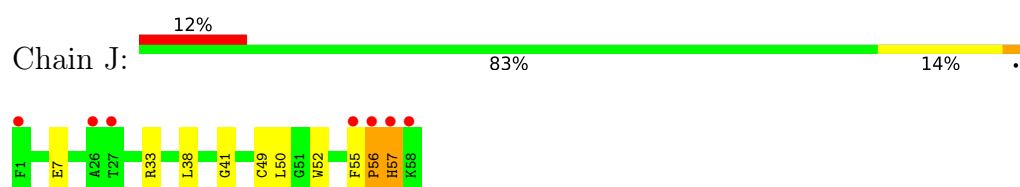
- Molecule 9: Cytochrome c oxidase subunit 6C



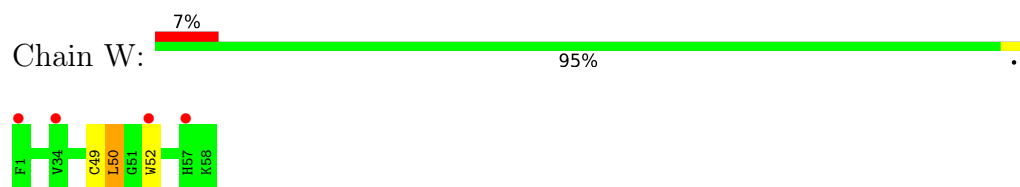
• Molecule 9: Cytochrome c oxidase subunit 6C



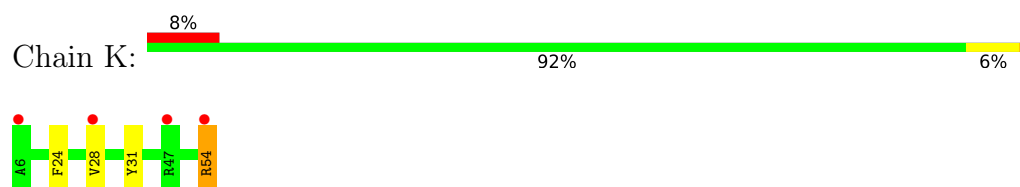
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



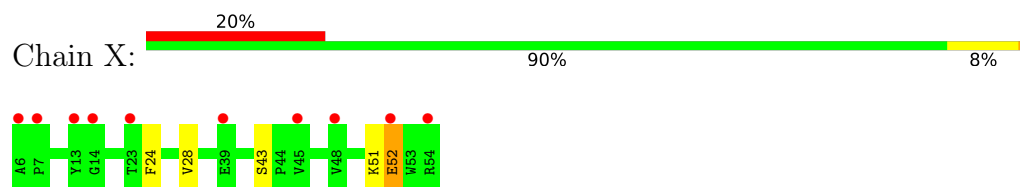
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



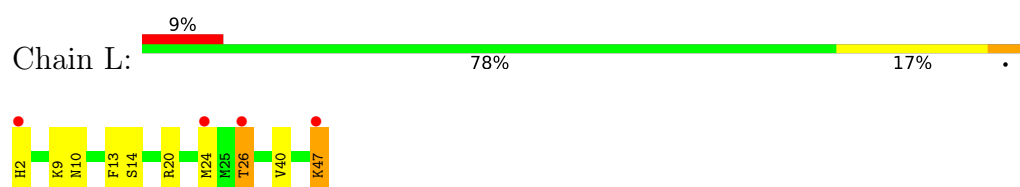
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



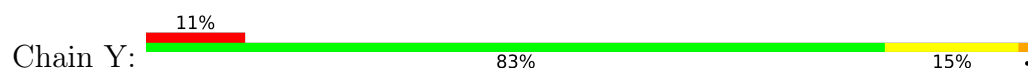
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



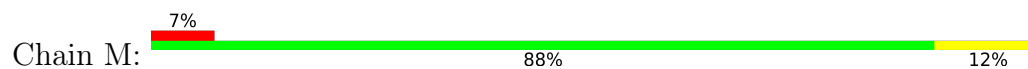
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



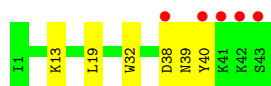
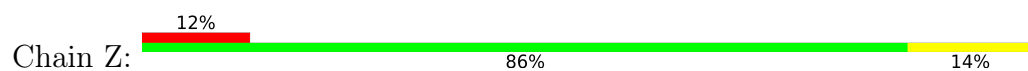
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	181.77Å 203.30Å 177.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 1.74 39.70 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.70-1.74) 99.7 (39.70-1.74)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.74Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.156 , 0.184 0.156 , 0.183	Depositor DCC
R_{free} test set	33307 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33923	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: SAC, CUA, HEA, TGL, PSC, EDO, FME, CDL, OXY, DMU, CU, NA, PGV, CHD, PEK, MG, ZN, PO4

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	1.05	1/4419 (0.0%)	1.02	10/6035 (0.2%)
1	N	0.97	2/4370 (0.0%)	0.97	4/5969 (0.1%)
2	B	0.92	0/1975	1.03	3/2689 (0.1%)
2	O	0.85	0/1937	0.97	2/2637 (0.1%)
3	C	0.92	0/2295	0.86	0/3136
3	P	0.91	0/2263	0.86	0/3092
4	D	0.87	0/1229	0.92	2/1658 (0.1%)
4	Q	0.70	0/1229	0.76	0/1658
5	E	0.84	0/871	0.80	0/1182
5	R	0.70	0/871	0.75	0/1182
6	F	0.87	0/732	0.97	2/993 (0.2%)
6	S	0.89	0/732	0.98	2/993 (0.2%)
7	G	0.86	0/699	0.89	0/950
7	T	0.82	0/699	0.87	0/950
8	H	0.85	0/682	0.94	0/921
8	U	0.76	0/682	0.84	0/921
9	I	0.76	0/605	0.81	0/802
9	V	0.64	0/605	0.78	0/802
10	J	0.75	0/472	0.85	0/636
10	W	0.67	0/472	0.83	0/636
11	K	0.81	0/399	0.84	0/546
11	X	0.70	0/399	0.72	0/546
12	L	0.94	0/393	0.87	0/526
12	Y	0.79	0/393	0.81	0/526
13	M	0.85	0/346	0.83	0/470
13	Z	0.76	0/346	0.80	0/470
All	All	0.89	3/30115 (0.0%)	0.92	25/40926 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	F	0	1
6	S	0	1
8	H	0	1
10	J	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	310	MET	SD-CE	-6.42	1.63	1.79
1	A	480	ARG	CD-NE	5.36	1.53	1.46
1	N	278	MET	SD-CE	-5.05	1.67	1.79

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-14.12	69.84	100.90
1	A	278	MET	CG-SD-CE	-11.93	74.65	100.90
1	N	189	MET	CG-SD-CE	-8.32	82.59	100.90
1	A	189	MET	CG-SD-CE	-7.66	84.06	100.90
1	N	240	HIS	CA-CB-CG	-7.46	106.34	113.80
1	A	240	HIS	CA-CB-CG	-7.16	106.64	113.80
1	A	102	PHE	CA-CB-CG	-6.53	107.27	113.80
1	N	310	MET	CG-SD-CE	-6.38	86.86	100.90
1	A	278	MET	CA-CB-CG	-5.97	102.16	114.10
2	O	64	ILE	CA-C-N	-5.96	113.13	122.73
2	O	64	ILE	C-N-CA	-5.96	113.13	122.73
4	D	19	ARG	NE-CZ-NH2	5.82	124.44	119.20
6	S	93	PRO	CA-C-N	5.78	132.10	121.70
6	S	93	PRO	C-N-CA	5.78	132.10	121.70
4	D	133	GLY	N-CA-C	5.74	120.11	112.77
1	A	511	VAL	CA-C-N	-5.53	113.11	122.67
1	A	511	VAL	C-N-CA	-5.53	113.11	122.67
6	F	93	PRO	CA-C-N	5.50	131.59	121.70
6	F	93	PRO	C-N-CA	5.50	131.59	121.70
1	A	376	HIS	CA-C-N	-5.46	111.58	121.14
1	A	376	HIS	C-N-CA	-5.46	111.58	121.14
2	B	64	ILE	CA-C-N	-5.34	113.37	122.56
2	B	64	ILE	C-N-CA	-5.34	113.37	122.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	TRP	CB-CA-C	5.21	119.64	110.37
1	A	513	LEU	CA-CB-CG	-5.00	98.79	116.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	F	93	PRO	Peptide
8	H	9	LYS	Peptide
10	J	56	PRO	Peptide
6	S	93	PRO	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	4183	0	4164	65	0
1	N	4174	0	4155	60	0
2	B	1867	0	1886	27	0
2	O	1853	0	1860	32	0
3	C	2143	0	2059	29	0
3	P	2131	0	2036	27	0
4	D	1195	0	1183	12	0
4	Q	1195	0	1183	15	0
5	E	852	0	845	4	0
5	R	852	0	845	5	0
6	F	716	0	697	11	0
6	S	716	0	697	16	0
7	G	672	0	645	6	0
7	T	672	0	645	10	0
8	H	662	0	623	4	0
8	U	662	0	623	9	0
9	I	601	0	613	2	0
9	V	601	0	613	5	0
10	J	461	0	459	12	0
10	W	461	0	459	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	385	0	366	3	0
11	X	385	0	366	5	0
12	L	380	0	380	12	0
12	Y	380	0	380	5	0
13	M	336	0	352	5	0
13	Z	336	0	352	2	0
14	A	141	0	115	7	0
14	N	141	0	115	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	84	0	136	8	0
18	C	88	0	138	2	0
18	N	51	0	76	1	0
18	P	89	0	140	4	0
18	Q	37	0	62	6	0
19	A	2	0	0	0	0
19	N	2	0	0	0	0
20	A	44	0	66	4	0
20	B	24	0	36	0	0
20	C	36	0	54	1	0
20	D	16	0	24	0	0
20	E	12	0	18	0	0
20	F	24	0	36	0	0
20	G	4	0	6	0	0
20	J	8	0	12	1	0
20	L	4	0	6	1	0
20	M	4	0	6	0	0
20	N	44	0	66	0	0
20	O	8	0	12	0	0
20	P	28	0	42	2	0
20	Q	8	0	12	1	0
20	R	8	0	12	2	0
20	S	28	0	41	1	0
20	T	12	0	18	0	0
20	W	8	0	12	2	0
20	Y	4	0	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	17	0	32	0	0
21	C	34	0	52	7	0
21	D	19	0	36	0	0
21	J	11	0	21	3	0
21	K	37	0	70	2	0
21	L	21	0	30	1	0
21	M	33	0	42	0	0
21	N	9	0	17	1	0
21	O	11	0	21	0	0
21	P	33	0	52	6	0
21	Q	10	0	19	1	0
21	W	11	0	21	0	0
21	X	27	0	51	0	0
21	Z	33	0	42	0	0
22	B	63	0	110	7	0
22	D	63	0	110	14	0
22	L	54	0	87	9	0
22	N	161	0	294	16	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	41	0	65	7	0
24	O	33	0	58	4	0
25	B	29	0	39	0	0
25	C	58	0	78	1	0
25	G	29	0	39	1	0
25	L	29	0	39	1	0
25	P	58	0	78	3	0
26	C	111	0	168	14	0
26	P	121	0	182	13	0
27	C	85	0	143	12	0
27	G	69	0	126	8	0
27	P	77	0	137	10	0
27	T	70	0	125	19	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	250	0	0	7	0
30	B	195	0	0	3	0
30	C	139	0	0	3	0
30	D	183	0	0	3	0
30	E	133	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	F	144	0	0	2	0
30	G	68	0	0	2	0
30	H	87	0	0	0	0
30	I	63	0	0	1	0
30	J	47	0	0	3	0
30	K	38	0	0	0	0
30	L	30	0	0	3	0
30	M	35	0	0	0	0
30	N	247	0	0	3	0
30	O	169	0	0	1	0
30	P	145	0	0	2	0
30	Q	88	0	0	2	0
30	R	106	0	0	0	0
30	S	133	0	0	4	0
30	T	61	0	0	3	0
30	U	78	0	0	3	0
30	V	48	0	0	4	0
30	W	46	0	0	1	0
30	X	28	0	0	1	0
30	Y	29	0	0	0	0
30	Z	22	0	0	1	0
All	All	33923	0	32137	425	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:161[A]:GLN:HE22	26:P:305:PEK:H41	1.27	0.97
1:N:113:LEU:HB2	22:N:607:TGL:H312	1.44	0.95
1:A:486[B]:ASP:OD2	4:D:19:ARG:HD2	1.67	0.93
12:L:20:ARG:HH21	22:L:101:TGL:HC32	1.36	0.88
1:A:113:LEU:HB2	22:L:101:TGL:H302	1.54	0.87
27:T:101:CDL:H771	27:T:101:CDL:H561	1.55	0.87
2:B:68[B]:LEU:HD12	24:B:303:PSC:H171	1.57	0.85
27:T:101:CDL:H511	27:T:101:CDL:H201	1.61	0.81
18:A:606:PGV:H311	13:M:19:LEU:HD23	1.63	0.80
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.64	0.79
1:N:53[B]:ILE:HG12	30:N:902:HOH:O	1.83	0.79
1:A:112:LEU:HD11	30:A:934:HOH:O	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:314:EDO:H21	30:C:501:HOH:O	1.84	0.77
22:N:608:TGL:H231	22:N:608:TGL:HA92	1.67	0.75
3:C:91:VAL:O	3:C:95[B]:THR:HG23	1.86	0.75
4:D:78:TRP:HB3	22:D:201:TGL:HB21	1.69	0.75
7:T:38:HIS:CE1	27:T:101:CDL:H131	2.22	0.75
3:C:48:THR:HG23	27:C:308:CDL:H402	1.69	0.74
8:H:46:LYS:HB2	8:U:52:VAL:HG12	1.70	0.74
12:L:20:ARG:NH2	22:L:101:TGL:HC32	2.01	0.73
25:P:309:CHD:H231	30:P:514:HOH:O	1.88	0.73
3:P:95[A]:THR:HG21	18:P:307:PGV:H282	1.70	0.72
20:A:609:EDO:H21	30:A:747:HOH:O	1.88	0.72
3:P:213:THR:HG23	27:P:308:CDL:H771	1.72	0.71
1:A:53[A]:ILE:HD11	12:L:40:VAL:HG13	1.71	0.71
21:C:310:DMU:H20	10:J:50:LEU:HB2	1.72	0.70
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.74	0.69
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.74	0.69
6:F:92:VAL:HG21	30:F:336:HOH:O	1.92	0.69
6:F:85:CYS:SG	6:F:87:THR:HG23	2.33	0.68
1:A:112:LEU:HD13	30:A:804:HOH:O	1.91	0.68
3:C:224:LYS:HD3	27:C:308:CDL:HB31	1.74	0.68
1:A:406:ASN:HD21	18:A:606:PGV:H22	1.59	0.67
26:P:305:PEK:H382	27:T:101:CDL:H273	1.76	0.67
22:D:201:TGL:HC42	22:D:201:TGL:OG3	1.94	0.67
3:P:91:VAL:O	3:P:95[B]:THR:HG23	1.95	0.67
3:P:33:MET:SD	21:P:310:DMU:H8	2.35	0.66
30:A:833:HOH:O	26:C:304:PEK:H382	1.95	0.66
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.76	0.66
7:T:38:HIS:NE2	27:T:101:CDL:H131	2.10	0.66
5:E:46:LYS:NZ	30:E:301:HOH:O	2.27	0.66
4:D:4:SER:HB2	30:D:326:HOH:O	1.97	0.65
27:T:101:CDL:H561	27:T:101:CDL:C77	2.27	0.64
3:P:156:ARG:HE	25:P:309:CHD:C24	2.11	0.64
3:C:40[B]:MET:HE1	21:C:320:DMU:H8	1.80	0.63
20:A:616:EDO:H22	6:F:32:ASN:HD21	1.63	0.63
3:C:127[A]:LEU:HD12	27:G:101:CDL:HB61	1.81	0.63
3:P:161[A]:GLN:HE22	26:P:305:PEK:C4	2.07	0.63
7:T:31:CYS:SG	27:T:101:CDL:H532	2.39	0.63
1:A:347:LEU:HD13	1:A:383[A]:MET:HB3	1.81	0.62
6:S:85:CYS:SG	6:S:87:THR:HG23	2.39	0.62
4:D:82:VAL:HG12	4:D:86:MET:HE2	1.82	0.62
1:A:181[B]:THR:HG21	30:A:783:HOH:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.82	0.62
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.34	0.61
4:D:78:TRP:HA	22:D:201:TGL:HB42	1.82	0.61
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.83	0.61
3:P:210:ILE:HD13	18:P:306:PGV:H301	1.82	0.60
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.83	0.60
7:T:38:HIS:HE2	27:T:101:CDL:H131	1.67	0.60
18:A:608:PGV:H343	26:C:304:PEK:H381	1.83	0.60
22:B:301:TGL:HC22	30:I:160:HOH:O	2.01	0.59
1:N:112:LEU:HD23	1:N:112:LEU:C	2.27	0.59
6:S:94:HIS:HA	30:S:294:HOH:O	2.02	0.59
4:D:77:GLU:HB3	22:D:201:TGL:HB32	1.82	0.59
1:N:347:LEU:HD13	1:N:383[A]:MET:HB3	1.84	0.59
1:N:24:ALA:HB2	14:N:601[A]:HEA:H253	1.85	0.58
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.39	0.58
26:P:305:PEK:H222	7:T:21:PHE:CD1	2.39	0.58
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.86	0.58
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.86	0.57
18:N:610:PGV:H343	26:P:304:PEK:H381	1.86	0.57
3:C:127[B]:LEU:HD22	27:G:101:CDL:HB61	1.85	0.57
20:P:311:EDO:H11	30:P:527:HOH:O	2.04	0.57
2:B:17[B]:MET:HG2	2:B:169:GLY:N	2.20	0.57
18:A:606:PGV:H312	13:M:16:ALA:HA	1.85	0.57
1:A:311:ILE:HD12	27:T:101:CDL:H221	1.86	0.57
21:C:310:DMU:H11	10:J:49:CYS:HB3	1.87	0.57
10:J:55:PHE:HE2	21:L:104:DMU:H29	1.70	0.56
6:F:64:GLU:O	6:F:65:ASP:HB2	2.06	0.56
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.41	0.56
1:N:331[B]:ASN:ND2	2:O:51:THR:HG21	2.21	0.56
2:B:42:ILE:HG21	22:D:201:TGL:H231	1.88	0.56
10:J:38:LEU:HD23	21:J:103:DMU:H22	1.87	0.56
2:B:87:MET:HE2	30:B:415:HOH:O	2.06	0.56
7:G:4:ALA:HB2	1:N:285:PHE:CD2	2.40	0.56
22:B:301:TGL:HA72	22:B:301:TGL:H101	1.88	0.55
3:C:171:VAL:HG22	27:C:308:CDL:H852	1.88	0.55
18:C:307:PGV:H161	27:T:101:CDL:H611	1.88	0.55
27:T:101:CDL:H262	27:T:101:CDL:H751	1.88	0.55
24:B:303:PSC:H241	24:B:303:PSC:H51	1.88	0.55
2:O:86:MET:O	2:O:89:GLU:HG3	2.06	0.55
1:A:390:MET:O	1:A:394[A]:VAL:HG22	2.07	0.55
3:P:3:HIS:CD2	20:P:316:EDO:H12	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:26:THR:HA	30:Z:213:HOH:O	2.05	0.55
1:A:462:LEU:O	1:A:465[B]:VAL:HG12	2.07	0.55
30:B:549:HOH:O	22:D:201:TGL:HC52	2.06	0.55
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.87	0.55
18:A:608:PGV:C34	26:C:304:PEK:H381	2.36	0.55
1:N:52[A]:GLN:O	1:N:56:VAL:HG23	2.07	0.55
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.89	0.55
2:O:41:ILE:HD13	24:O:302:PSC:H342	1.89	0.55
8:U:49:ASP:O	8:U:52:VAL:HG22	2.06	0.55
3:C:51:MET:HB2	27:C:308:CDL:H381	1.88	0.54
1:N:468:MET:HG3	30:N:932:HOH:O	2.06	0.54
1:A:169:ILE:HD11	1:A:189:MET:HE1	1.88	0.54
2:B:56:MET:HA	24:B:303:PSC:H211	1.90	0.54
8:U:41:LYS:HG3	30:U:278:HOH:O	2.06	0.54
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.90	0.54
1:A:321:PHE:CD1	24:B:303:PSC:H341	2.41	0.54
6:F:87:THR:HG21	30:F:320:HOH:O	2.07	0.54
1:N:113:LEU:HB2	22:N:607:TGL:C31	2.30	0.54
1:N:297[B]:MET:HG2	1:N:302[B]:ARG:HG2	1.89	0.54
26:C:305:PEK:H382	27:G:101:CDL:H271	1.89	0.53
1:N:112:LEU:HG	30:N:885:HOH:O	2.07	0.53
1:A:24:ALA:HB2	14:A:601[A]:HEA:H253	1.91	0.53
4:Q:94:LEU:HB3	21:Q:202:DMU:H19	1.89	0.53
22:D:201:TGL:HB22	22:D:201:TGL:OG1	2.09	0.53
3:P:33:MET:HE2	3:P:42:LEU:H	1.74	0.53
8:U:43:MET:HE3	8:U:52:VAL:HG21	1.91	0.53
26:C:305:PEK:H222	7:G:21:PHE:CD1	2.44	0.53
1:A:363[B]:LEU:HD23	2:B:20:LEU:HD22	1.91	0.52
2:B:1:FME:HE1	2:B:133[A]:LEU:HD22	1.91	0.52
3:C:180[B]:GLU:HG2	30:C:439:HOH:O	2.09	0.52
3:C:224:LYS:CD	27:C:308:CDL:HB31	2.38	0.52
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.62	0.52
3:C:180[B]:GLU:HG3	30:C:444:HOH:O	2.08	0.52
20:W:102:EDO:H12	30:W:214:HOH:O	2.09	0.52
3:C:40[A]:MET:HE3	3:C:44[A]:MET:HE3	1.90	0.52
3:P:48:THR:HG23	27:P:308:CDL:H411	1.91	0.52
1:A:105:LEU:HD11	20:A:609:EDO:H22	1.91	0.52
1:A:113:LEU:HB2	22:L:101:TGL:H323	1.91	0.52
22:N:606:TGL:HC21	30:V:145:HOH:O	2.09	0.52
1:A:347:LEU:CD1	1:A:383[A]:MET:HB3	2.40	0.51
1:N:331[B]:ASN:OD1	4:Q:20:ARG:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.45	0.51
3:P:172:TYR:CE2	26:P:305:PEK:H171	2.45	0.51
1:A:362[A]:SER:HB2	2:B:20:LEU:HD21	1.91	0.51
3:C:37:PHE:CD2	21:C:310:DMU:H13	2.46	0.51
2:O:114:GLU:HG3	2:O:227:LEU:HD23	1.93	0.51
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.93	0.51
1:A:334:TRP:CD1	22:D:201:TGL:HC41	2.46	0.51
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.51
22:B:301:TGL:CA5	22:B:301:TGL:H202	2.41	0.51
1:N:289:ALA:HB1	1:N:297[A]:MET:HE1	1.92	0.51
1:A:109:PHE:CD1	22:L:101:TGL:H301	2.46	0.51
3:C:30:GLY:HA2	3:C:42[B]:LEU:HB3	1.93	0.51
2:B:49:LYS:HE3	22:D:201:TGL:HC72	1.93	0.51
26:C:305:PEK:H382	27:G:101:CDL:C27	2.40	0.50
27:T:101:CDL:H201	27:T:101:CDL:C51	2.35	0.50
4:Q:20:ARG:HG2	30:Q:362:HOH:O	2.11	0.50
4:Q:84:ALA:CB	18:Q:201:PGV:H11	2.41	0.50
5:R:14:ARG:NH1	20:R:202:EDO:H21	2.26	0.50
2:B:13:THR:HB	2:B:168:LEU:HD23	1.94	0.50
6:S:36:PRO:HA	20:S:105:EDO:H22	1.93	0.50
18:A:608:PGV:C18	26:C:304:PEK:H322	2.42	0.49
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.95	0.49
26:P:305:PEK:H382	27:T:101:CDL:C27	2.43	0.49
5:R:14:ARG:HD2	20:R:202:EDO:O2	2.12	0.49
2:B:81:LEU:HD13	27:T:101:CDL:H141	1.95	0.49
1:N:136[B]:LEU:HD11	30:T:252:HOH:O	2.13	0.49
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.95	0.49
1:N:381[B]:LEU:HB2	14:N:602:HEA:CAC	2.42	0.49
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.48	0.49
2:B:68[B]:LEU:HD12	24:B:303:PSC:C17	2.38	0.48
4:Q:127:LYS:HD3	30:V:138:HOH:O	2.12	0.48
9:V:42:LYS:NZ	30:V:102:HOH:O	2.45	0.48
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.96	0.48
21:C:310:DMU:H4	10:J:52:TRP:CH2	2.49	0.48
6:F:92:VAL:HG23	6:F:92:VAL:O	2.13	0.48
10:J:33:ARG:HD2	30:J:226:HOH:O	2.14	0.48
22:N:606:TGL:HA62	22:N:606:TGL:H363	1.95	0.48
3:P:33:MET:CE	3:P:42:LEU:H	2.26	0.48
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.96	0.48
20:Q:203:EDO:H12	6:S:73:TRP:HD1	1.78	0.48
7:G:1:ALA:HB2	18:P:307:PGV:C34	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:38:LEU:HA	21:J:103:DMU:H22	1.96	0.48
8:U:9:LYS:HG2	30:U:265:HOH:O	2.13	0.48
3:C:161[A]:GLN:HE22	26:C:305:PEK:C2	2.27	0.48
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.43	0.48
1:N:50[B]:ASP:CG	1:N:53[B]:ILE:HG13	2.39	0.48
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.95	0.48
22:N:606:TGL:H271	22:N:606:TGL:H222	1.96	0.48
4:D:87:PHE:HE1	21:K:103:DMU:H20	1.78	0.47
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.14	0.47
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.49	0.47
1:A:383[A]:MET:HG2	1:A:421:VAL:HG21	1.95	0.47
3:C:52:LEU:HD23	27:C:308:CDL:H362	1.95	0.47
27:G:101:CDL:H473	30:G:256:HOH:O	2.14	0.47
11:K:24:PHE:O	11:K:28:VAL:HG12	2.14	0.47
22:N:607:TGL:H342	12:Y:28:PHE:HD1	1.80	0.47
1:A:285:PHE:CE2	7:T:4:ALA:HB2	2.49	0.47
3:P:116:TRP:HA	3:P:117:PRO:C	2.39	0.47
27:P:308:CDL:H852	27:P:308:CDL:H822	1.72	0.47
1:A:169:ILE:CD1	1:A:189:MET:HE1	2.45	0.47
1:A:334:TRP:CZ3	22:D:201:TGL:HA52	2.49	0.47
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.50	0.47
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.14	0.47
4:Q:118:LYS:HE3	11:X:51:LYS:HE2	1.96	0.47
6:S:94:HIS:CD2	6:S:94:HIS:OXT	2.68	0.47
1:N:488:THR:HB	1:N:495:LEU:HD13	1.97	0.47
2:O:68[B]:LEU:HD23	24:O:302:PSC:H171	1.97	0.47
21:P:310:DMU:H11	10:W:49:CYS:HB3	1.97	0.47
1:A:362[B]:SER:HB3	2:B:20:LEU:HD21	1.97	0.47
20:J:102:EDO:H12	30:J:214:HOH:O	2.14	0.47
2:O:221:LYS:HD3	30:O:560:HOH:O	2.14	0.47
6:S:43:LYS:HB3	6:S:43:LYS:HE3	1.65	0.47
11:X:51:LYS:HE3	30:X:212:HOH:O	2.13	0.47
1:N:331[B]:ASN:ND2	4:Q:21:ASP:HB3	2.30	0.46
1:N:362:SER:OG	2:O:87[A]:MET:HE2	2.15	0.46
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.50	0.46
12:L:14:SER:H	22:L:101:TGL:HC31	1.80	0.46
9:V:15:ARG:NH2	30:V:103:HOH:O	2.47	0.46
1:A:236:TRP:CH2	14:A:602:HEA:HBD1	2.51	0.46
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.51	0.46
3:P:95[B]:THR:HG22	26:P:303:PEK:H172	1.98	0.46
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:41:ILE:O	2:O:45:MET:HG2	2.16	0.46
27:P:308:CDL:H751	27:P:308:CDL:H782	1.88	0.46
1:A:113:LEU:CB	22:L:101:TGL:H302	2.37	0.46
1:A:289:ALA:HB1	1:A:297[A]:MET:HE1	1.97	0.46
3:P:62:ILE:HD12	27:P:308:CDL:H511	1.98	0.46
26:P:304:PEK:H172	26:P:304:PEK:H202	1.71	0.46
7:T:84:LYS:HB3	30:T:243:HOH:O	2.16	0.46
11:X:24:PHE:O	11:X:28:VAL:HG12	2.16	0.46
1:A:311:ILE:CD1	27:T:101:CDL:H221	2.45	0.46
3:C:51:MET:SD	27:C:308:CDL:H622	2.56	0.46
6:S:87:THR:HG22	30:S:315:HOH:O	2.16	0.46
1:A:468:MET:HG3	30:A:922:HOH:O	2.16	0.45
7:G:4:ALA:HB2	1:N:285:PHE:CE2	2.51	0.45
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.51	0.45
18:Q:201:PGV:H312	18:Q:201:PGV:H151	1.99	0.45
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.57	0.45
2:B:1:FME:HE1	2:B:133[B]:LEU:HD22	1.98	0.45
2:B:49:LYS:CE	22:D:201:TGL:HC72	2.46	0.45
1:N:114:ALA:HA	10:W:50:LEU:HD21	1.98	0.45
1:N:347:LEU:CD1	1:N:383[A]:MET:HB3	2.47	0.45
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.98	0.45
3:P:37:PHE:CE2	21:P:310:DMU:H13	2.52	0.45
27:P:308:CDL:H272	27:P:308:CDL:H651	1.99	0.45
10:J:52:TRP:O	10:J:57:HIS:HE1	1.99	0.45
27:P:308:CDL:H371	27:P:308:CDL:H642	1.99	0.45
22:N:606:TGL:H152	22:N:606:TGL:HC71	1.76	0.45
26:P:304:PEK:H161	26:P:304:PEK:H132	1.90	0.45
14:A:601[A]:HEA:H211	14:A:601[A]:HEA:H271	1.69	0.45
1:N:406:ASN:HD21	18:Q:201:PGV:H31	1.81	0.45
4:D:109:HIS:HB3	30:D:455:HOH:O	2.17	0.45
1:A:113:LEU:HB2	22:L:101:TGL:C30	2.37	0.45
26:C:304:PEK:H161	26:C:304:PEK:H132	1.64	0.45
24:O:302:PSC:C12	24:O:302:PSC:H343	2.47	0.45
2:O:5:MET:HE2	2:O:5:MET:HB3	1.61	0.44
1:A:383[A]:MET:HA	1:A:387:PHE:CD1	2.51	0.44
30:A:840:HOH:O	13:M:41:LYS:HG2	2.17	0.44
3:C:250:LEU:HD22	27:G:101:CDL:H631	1.98	0.44
12:L:24:MET:HG3	30:L:218:HOH:O	2.17	0.44
1:N:377:PHE:CD2	14:N:602:HEA:HAD1	2.52	0.44
1:A:366[B]:VAL:CG1	2:B:169:GLY:HA2	2.47	0.44
2:O:4:PRO:HB2	11:X:43:SER:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:301:TGL:H252	22:B:301:TGL:H221	1.51	0.44
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.52	0.44
25:G:102:CHD:H12	25:G:102:CHD:H212	1.99	0.44
18:Q:201:PGV:H322	13:Z:19:LEU:HD23	1.98	0.44
8:U:7:LYS:HB2	30:U:272:HOH:O	2.16	0.44
12:L:13:PHE:HA	22:L:101:TGL:OC1	2.18	0.44
1:N:109:PHE:CE1	22:N:607:TGL:H311	2.53	0.44
3:P:161[A]:GLN:NE2	26:P:305:PEK:H41	2.11	0.44
4:Q:9:GLU:O	4:Q:9:GLU:HG2	2.18	0.44
22:D:201:TGL:H342	9:I:16:ARG:HH21	1.83	0.44
2:O:16:ILE:HD12	2:O:16:ILE:HG23	1.74	0.44
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.81	0.43
2:O:13:THR:HB	2:O:168:LEU:HD23	1.99	0.43
4:Q:84:ALA:HB2	18:Q:201:PGV:H11	1.99	0.43
1:A:334:TRP:HD1	22:D:201:TGL:HC41	1.81	0.43
26:C:305:PEK:H322	30:G:256:HOH:O	2.17	0.43
1:N:423:MET:HE1	21:N:622:DMU:C43	2.48	0.43
18:Q:201:PGV:H312	18:Q:201:PGV:C15	2.49	0.43
18:A:608:PGV:H181	26:C:304:PEK:H322	1.99	0.43
27:T:101:CDL:H541	27:T:101:CDL:C75	2.48	0.43
9:V:18:ARG:HG3	9:V:18:ARG:HH11	1.83	0.43
27:C:308:CDL:H821	27:C:308:CDL:H851	1.77	0.43
22:N:606:TGL:H311	22:N:606:TGL:H141	1.62	0.43
24:O:302:PSC:H251	24:O:302:PSC:H222	1.28	0.43
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.00	0.43
4:Q:114:GLU:HB3	30:Q:303:HOH:O	2.18	0.43
5:R:81:ILE:HA	9:V:7:PRO:HG2	2.01	0.43
1:A:379:TYR:CZ	1:A:383[A]:MET:HE1	2.54	0.43
26:C:304:PEK:H221	26:C:304:PEK:H251	1.78	0.43
3:P:129:VAL:HG11	3:P:180[B]:GLU:HG2	2.00	0.43
8:U:60:TYR:CD1	8:U:60:TYR:C	2.97	0.43
14:A:602:HEA:HHA	14:A:602:HEA:HAD2	1.82	0.43
8:H:9:LYS:HD3	8:H:9:LYS:HA	1.87	0.43
11:K:31:TYR:HB2	21:K:104:DMU:H9	2.01	0.43
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG2	2.59	0.43
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.18	0.43
22:N:606:TGL:HC21	22:N:606:TGL:HC52	1.83	0.43
27:P:308:CDL:H371	27:P:308:CDL:C64	2.48	0.43
30:S:217:HOH:O	20:W:102:EDO:H11	2.19	0.43
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.48	0.43
11:X:52:GLU:H	11:X:52:GLU:HG2	1.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:513:LEU:HA	1:N:513:LEU:HD23	1.76	0.43
22:N:606:TGL:H201	22:N:606:TGL:C31	2.49	0.43
22:N:606:TGL:H291	22:N:606:TGL:H212	1.99	0.43
2:O:68[B]:LEU:HB3	2:O:69:PRO:HD3	2.00	0.43
4:Q:34:SER:O	4:Q:38:LYS:HG3	2.19	0.43
27:T:101:CDL:H541	27:T:101:CDL:H251	2.01	0.43
1:A:377:PHE:HA	1:A:380[A]:VAL:HG22	2.00	0.42
26:C:304:PEK:H42	26:C:304:PEK:H131	2.01	0.42
4:D:4:SER:N	30:D:303:HOH:O	2.51	0.42
1:A:381[B]:LEU:HB2	14:A:602:HEA:CAC	2.48	0.42
25:L:102:CHD:H112	25:L:102:CHD:H12A	1.74	0.42
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.01	0.42
1:N:297[B]:MET:CG	1:N:302[B]:ARG:HG2	2.49	0.42
22:B:301:TGL:H202	22:B:301:TGL:HA52	2.00	0.42
8:H:60:TYR:CD1	8:H:60:TYR:C	2.97	0.42
2:O:217:LYS:O	2:O:221:LYS:HG3	2.20	0.42
18:A:608:PGV:H322	26:C:304:PEK:H371	2.01	0.42
1:N:383[A]:MET:HG2	1:N:421:VAL:HG21	2.01	0.42
22:N:607:TGL:H322	12:Y:39:ILE:HD11	2.02	0.42
2:B:56:MET:CB	24:B:303:PSC:H211	2.50	0.42
21:C:310:DMU:H4	10:J:52:TRP:CZ2	2.54	0.42
1:A:55[A]:ASN:HA	1:A:58:VAL:HB	2.02	0.42
1:A:514:LYS:HA	6:F:38:ALA:CB	2.47	0.42
3:C:213:THR:HG21	27:C:308:CDL:H642	2.01	0.42
1:N:236:TRP:CH2	14:N:602:HEA:HBD1	2.54	0.42
22:N:608:TGL:H231	22:N:608:TGL:CA9	2.45	0.42
2:O:227:LEU:H	2:O:227:LEU:HG	1.69	0.42
22:B:301:TGL:HA81	22:B:301:TGL:H142	2.00	0.42
1:N:110:LEU:HG	21:P:310:DMU:H24	2.01	0.42
14:N:601[A]:HEA:H271	14:N:601[A]:HEA:H211	1.83	0.42
2:O:82:ARG:HH11	2:O:86:MET:CE	2.33	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.19	0.42
1:N:51[A]:ASP:O	1:N:55[A]:ASN:HB2	2.20	0.42
22:N:607:TGL:H222	22:N:607:TGL:HA91	1.57	0.42
3:P:59:ARG:HA	27:P:308:CDL:H512	2.00	0.42
27:T:101:CDL:H161	27:T:101:CDL:H391	2.01	0.42
8:H:37:HIS:CE1	8:H:76:ARG:NH2	2.87	0.42
12:L:13:PHE:C	20:L:103:EDO:H22	2.45	0.42
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.00	0.42
21:P:310:DMU:H4	10:W:52:TRP:CZ2	2.55	0.42
27:T:101:CDL:H201	27:T:101:CDL:CB5	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:TYR:CZ	1:A:383[B]:MET:HE1	2.54	0.42
2:B:41:ILE:O	2:B:45:MET:HG2	2.20	0.42
1:N:514:LYS:HG2	6:S:38:ALA:HB2	2.02	0.42
3:P:129:VAL:HG11	3:P:180[A]:GLU:HG3	2.02	0.42
3:C:213:THR:HG23	27:C:308:CDL:H771	2.02	0.41
10:J:55:PHE:HB3	10:J:56:PRO:HD2	2.02	0.41
1:N:53[B]:ILE:HD12	12:Y:44:LEU:HD23	2.01	0.41
2:O:58:ALA:O	2:O:62:GLU:HG3	2.20	0.41
27:P:308:CDL:H192	27:P:308:CDL:H232	2.02	0.41
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	2.02	0.41
20:A:615:EDO:H11	12:L:10:ASN:HD22	1.85	0.41
3:C:58:TRP:HB2	27:C:308:CDL:H552	2.02	0.41
6:F:51:SER:O	6:F:94:HIS:N	2.53	0.41
27:G:101:CDL:H561	27:G:101:CDL:C77	2.50	0.41
25:P:309:CHD:C23	25:P:309:CHD:H162	2.49	0.41
11:K:54:ARG:HE	11:K:54:ARG:HB3	1.55	0.41
12:L:9:LYS:HE3	30:L:221:HOH:O	2.20	0.41
12:L:9:LYS:HG3	30:L:209:HOH:O	2.19	0.41
26:P:304:PEK:H101	26:P:304:PEK:H42	2.02	0.41
1:A:103:TRP:O	1:A:107:PRO:HD2	2.20	0.41
22:B:301:TGL:H202	22:B:301:TGL:HA51	2.02	0.41
30:B:425:HOH:O	4:D:122:ARG:HB3	2.20	0.41
3:C:210:ILE:HG21	18:C:306:PGV:H281	2.02	0.41
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.82	0.41
25:C:309:CHD:H112	25:C:309:CHD:H12A	1.84	0.41
1:N:71:MET:HB3	1:N:71:MET:HE2	1.79	0.41
1:A:334:TRP:HZ3	22:D:201:TGL:HA72	1.85	0.41
24:B:303:PSC:H232	24:B:303:PSC:H201	1.79	0.41
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.03	0.41
7:G:1:ALA:HB2	18:P:307:PGV:H343	2.03	0.41
10:J:41:GLY:HA3	21:J:103:DMU:H23	2.01	0.41
1:N:383[A]:MET:HA	1:N:387:PHE:CD1	2.56	0.41
3:C:55:TYR:CE1	27:C:308:CDL:H521	2.55	0.41
12:L:26:THR:HG23	13:M:25:SER:CB	2.51	0.41
5:R:12:ASP:OD2	5:R:44:GLU:HG3	2.20	0.41
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.03	0.41
6:S:51:SER:O	6:S:94:HIS:N	2.54	0.41
1:A:240:HIS:CD2	1:A:240:HIS:C	2.98	0.41
5:E:79:LYS:HE3	30:E:354:HOH:O	2.21	0.41
5:E:94:ASN:HB3	30:E:405:HOH:O	2.21	0.41
27:G:101:CDL:H561	27:G:101:CDL:H771	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:347:LEU:HD22	1:N:383[A]:MET:SD	2.61	0.41
14:N:601[C]:HEA:H212	14:N:601[C]:HEA:H271	1.81	0.41
2:O:116:LEU:HD13	2:O:226:MET:HG2	2.03	0.41
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.73	0.41
26:P:304:PEK:H42	26:P:304:PEK:H71	1.70	0.41
3:C:37:PHE:CE2	21:C:310:DMU:H13	2.56	0.41
12:L:47:LYS:HE2	12:L:47:LYS:HB3	1.82	0.41
3:C:47:LEU:O	3:C:51:MET:HG2	2.21	0.40
2:O:160:LEU:HD22	2:O:175:ILE:HG12	2.04	0.40
1:A:51[B]:ASP:OD2	2:B:206:PHE:HE2	2.04	0.40
1:A:236:TRP:HH2	14:A:602:HEA:HBD1	1.84	0.40
10:J:7:GLU:HG3	30:J:231:HOH:O	2.20	0.40
3:P:43:LEU:HD21	21:P:318:DMU:H14	2.03	0.40
6:S:22:LEU:HD12	30:S:298:HOH:O	2.20	0.40
6:S:64:GLU:O	6:S:65:ASP:HB2	2.21	0.40
7:T:12:GLY:HA3	30:T:247:HOH:O	2.20	0.40
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.57	0.40
8:U:9:LYS:HE2	8:U:9:LYS:HB2	1.80	0.40
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.37	0.40
4:D:58:GLU:O	4:D:58:GLU:HG3	2.19	0.40
1:A:347:LEU:HD13	1:A:383[A]:MET:SD	2.61	0.40
3:C:158:HIS:HE1	6:F:1:ALA:O	2.05	0.40
1:N:51[B]:ASP:OD2	2:O:206:PHE:HE2	2.03	0.40
1:N:378:HIS:HA	1:N:382[B]:SER:HB2	2.02	0.40
1:N:380[A]:VAL:HG21	14:N:602:HEA:C3C	2.51	0.40
6:S:10:GLU:OE2	6:S:25:ARG:NH2	2.53	0.40

There are no symmetry-related clashes.

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	547/514 (106%)	531 (97%)	16 (3%)	0	100	100
1	N	540/514 (105%)	529 (98%)	11 (2%)	0	100	100
2	B	239/227 (105%)	232 (97%)	7 (3%)	0	100	100
2	O	234/227 (103%)	227 (97%)	7 (3%)	0	100	100
3	C	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
3	P	265/259 (102%)	259 (98%)	6 (2%)	0	100	100
4	D	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
5	E	103/105 (98%)	103 (100%)	0	0	100	100
5	R	103/105 (98%)	103 (100%)	0	0	100	100
6	F	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
6	S	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
7	G	82/84 (98%)	70 (85%)	8 (10%)	4 (5%)	1	0
7	T	82/84 (98%)	69 (84%)	11 (13%)	2 (2%)	4	0
8	H	77/79 (98%)	71 (92%)	3 (4%)	3 (4%)	2	0
8	U	77/79 (98%)	73 (95%)	3 (4%)	1 (1%)	9	1
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	41 (100%)	0	0	100	100
13	Z	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	3604/3550 (102%)	3492 (97%)	102 (3%)	10 (0%)	36	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	37	LEU
8	H	46	LYS
8	H	47	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	5	LYS
7	T	5	LYS
7	G	11	THR
8	H	8	ILE
8	U	43	MET
7	T	6	GLY
7	G	6	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/426 (108%)	446 (97%)	12 (3%)	40	17
1	N	451/426 (106%)	446 (99%)	5 (1%)	65	50
2	B	224/210 (107%)	213 (95%)	11 (5%)	22	4
2	O	219/210 (104%)	210 (96%)	9 (4%)	27	6
3	C	236/224 (105%)	234 (99%)	2 (1%)	73	64
3	P	232/224 (104%)	226 (97%)	6 (3%)	40	17
4	D	128/128 (100%)	127 (99%)	1 (1%)	73	64
4	Q	128/128 (100%)	123 (96%)	5 (4%)	28	7
5	E	92/92 (100%)	91 (99%)	1 (1%)	65	50
5	R	92/92 (100%)	92 (100%)	0	100	100
6	F	78/78 (100%)	75 (96%)	3 (4%)	29	8
6	S	78/78 (100%)	75 (96%)	3 (4%)	29	8
7	G	68/68 (100%)	62 (91%)	6 (9%)	9	1
7	T	68/68 (100%)	64 (94%)	4 (6%)	18	3
8	H	71/71 (100%)	66 (93%)	5 (7%)	14	2
8	U	71/71 (100%)	67 (94%)	4 (6%)	19	3
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	30
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	49/49 (100%)	48 (98%)	1 (2%)	48	26
10	W	49/49 (100%)	48 (98%)	1 (2%)	48	26
11	K	39/39 (100%)	38 (97%)	1 (3%)	40	17
11	X	39/39 (100%)	38 (97%)	1 (3%)	40	17
12	L	39/39 (100%)	36 (92%)	3 (8%)	12	1
12	Y	39/39 (100%)	36 (92%)	3 (8%)	12	1
13	M	37/37 (100%)	37 (100%)	0	100	100
13	Z	37/37 (100%)	34 (92%)	3 (8%)	11	1
All	All	3136/3036 (103%)	3042 (97%)	94 (3%)	38	12

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	A	180	GLN
1	A	278	MET
1	A	297[A]	MET
1	A	297[B]	MET
1	A	362[A]	SER
1	A	362[B]	SER
1	A	369	ASP
1	A	449[A]	MET
1	A	449[B]	MET
1	A	486[A]	ASP
1	A	486[B]	ASP
2	B	33	LEU
2	B	59[A]	GLN
2	B	59[B]	GLN
2	B	60[A]	GLU
2	B	60[B]	GLU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	94	SER
2	B	202[A]	SER
2	B	202[B]	SER
3	C	76	GLN
3	C	159	MET
4	D	31	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	90	ARG
6	F	2	SER
6	F	80	GLN
6	F	94	HIS
7	G	5	LYS
7	G	8	HIS
7	G	11	THR
7	G	33	LEU
7	G	43	GLU
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	46	LYS
8	H	49	ASP
8	H	60	TYR
9	I	18	ARG
10	J	57	HIS
11	K	54	ARG
12	L	2	HIS
12	L	26	THR
12	L	47	LYS
1	N	112	LEU
1	N	128	VAL
1	N	138	HIS
1	N	333	LYS
1	N	369	ASP
2	O	33	LEU
2	O	60[A]	GLU
2	O	60[B]	GLU
2	O	78	LEU
2	O	89	GLU
2	O	94	SER
2	O	115	ASP
2	O	226	MET
2	O	227	LEU
3	P	3	HIS
3	P	76	GLN
3	P	159	MET
3	P	180[A]	GLU
3	P	180[B]	GLU
3	P	230	ASN
4	Q	5	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Q	6	VAL
4	Q	9	GLU
4	Q	20	ARG
4	Q	58	GLU
6	S	64	GLU
6	S	80	GLN
6	S	93	PRO
7	T	8	HIS
7	T	11	THR
7	T	33	LEU
7	T	37	LEU
8	U	8	ILE
8	U	9	LYS
8	U	60	TYR
8	U	61	LYS
9	V	29	LEU
9	V	36	LYS
9	V	61	GLU
10	W	50	LEU
11	X	52	GLU
12	Y	2	HIS
12	Y	26	THR
12	Y	47	LYS
13	Z	13	LYS
13	Z	38	ASP
13	Z	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	43	GLN
1	A	170	ASN
1	A	422	ASN
1	A	503	HIS
2	B	140	ASN
2	B	181	GLN
3	C	50	ASN
4	D	109	HIS
5	E	94	ASN
6	F	32	ASN
7	G	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	41	HIS
8	H	25	GLN
8	H	28	ASN
8	H	32	ASN
8	H	37	HIS
10	J	57	HIS
11	K	35	GLN
1	N	80	ASN
1	N	98	ASN
1	N	170	ASN
1	N	422	ASN
2	O	10	GLN
3	P	50	ASN
4	Q	32	ASN
4	Q	101	HIS
4	Q	109	HIS
6	S	94	HIS
7	T	34	ASN
8	U	25	GLN
8	U	28	ASN
8	U	32	ASN
9	V	8	GLN
11	X	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	B	1	2	8,9,10	1.19	0	7,9,11	2.13	4 (57%)
1	FME	N	1	1	8,9,10	0.56	0	7,9,11	1.78	2 (28%)
2	FME	O	1	2	8,9,10	1.09	0	7,9,11	1.37	1 (14%)
9	SAC	V	1	9	7,8,9	0.60	0	8,9,11	0.97	0
9	SAC	I	1	9	7,8,9	0.62	0	8,9,11	1.25	2 (25%)
1	FME	A	1	1	8,9,10	0.67	0	7,9,11	1.74	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
2	FME	B	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-
9	SAC	I	1	9	-	2/7/8/10	-
1	FME	A	1	1	-	2/7/9/11	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.54	103.10	112.95
1	N	1	FME	O-C-CA	-3.18	116.45	124.78
1	A	1	FME	CE-SD-CG	3.11	111.10	100.40
1	N	1	FME	CE-SD-CG	3.10	111.04	100.40
2	B	1	FME	C-CA-N	-2.71	104.84	109.73
9	I	1	SAC	CA-N-C1A	-2.69	118.19	123.15
2	B	1	FME	O-C-CA	-2.26	118.84	124.78
1	A	1	FME	O-C-CA	-2.14	119.17	124.78
9	I	1	SAC	O-C-CA	-2.11	119.24	124.78
2	O	1	FME	O1-CN-N	-2.06	119.84	125.27
2	B	1	FME	O1-CN-N	-2.04	119.90	125.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	O-C-CA-CB
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 161 ligands modelled in this entry, 10 are monoatomic - leaving 151 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	$\# Z > 2$
20	EDO	N	614	-	3,3,3	0.66	0	2,2,2	0.37	0
20	EDO	A	611	-	3,3,3	0.70	0	2,2,2	0.17	0
20	EDO	B	306	-	3,3,3	0.51	0	2,2,2	0.49	0
27	CDL	T	101	-	67,67,99	1.44	10 (14%)	67,67,111	1.64	12 (17%)
21	DMU	Z	101	-	34,34,34	0.61	1 (2%)	45,45,45	1.08	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	N	615	-	3,3,3	0.55	0	2,2,2	0.35	0
20	EDO	O	304	-	3,3,3	0.32	0	2,2,2	0.17	0
25	CHD	C	301	-	32,32,32	1.19	4 (12%)	51,51,51	1.72	14 (27%)
22	TGL	D	201	-	62,62,62	1.17	3 (4%)	65,65,65	1.58	10 (15%)
20	EDO	N	613	-	3,3,3	0.89	0	2,2,2	0.32	0
20	EDO	C	314	-	3,3,3	0.34	0	2,2,2	0.46	0
21	DMU	W	103	-	10,10,34	0.31	0	9,9,45	0.88	0
29	PO4	U	101	-	4,4,4	1.18	0	6,6,6	1.04	0
21	DMU	X	103	-	9,9,34	0.51	0	8,8,45	0.35	0
20	EDO	P	314	-	3,3,3	0.82	0	2,2,2	0.24	0
20	EDO	A	613	-	3,3,3	0.59	0	2,2,2	0.16	0
27	CDL	C	308	-	79,82,99	1.27	10 (12%)	78,83,111	1.57	12 (15%)
20	EDO	N	619	-	3,3,3	0.57	0	2,2,2	0.61	0
20	EDO	A	615	-	3,3,3	0.42	0	2,2,2	0.45	0
21	DMU	C	320	-	11,11,34	0.46	0	10,10,45	0.85	0
20	EDO	C	312	-	3,3,3	0.79	0	2,2,2	0.23	0
20	EDO	N	617	-	3,3,3	0.45	0	2,2,2	0.57	0
20	EDO	P	315	-	3,3,3	0.48	0	2,2,2	0.99	0
24	PSC	O	302	-	31,31,51	0.78	1 (3%)	29,29,59	1.36	3 (10%)
20	EDO	D	204	-	3,3,3	0.43	0	2,2,2	0.52	0
18	PGV	A	608	-	50,50,50	1.08	4 (8%)	53,56,56	1.14	6 (11%)
18	PGV	P	306	-	50,50,50	0.79	2 (4%)	53,56,56	1.27	4 (7%)
20	EDO	B	307	-	3,3,3	0.35	0	2,2,2	0.83	0
21	DMU	K	104	-	9,9,34	0.35	0	8,8,45	0.53	0
20	EDO	P	311	-	3,3,3	0.27	0	2,2,2	0.80	0
14	HEA	A	602	19,1	66,67,67	1.82	19 (28%)	78,103,103	2.01	26 (33%)
20	EDO	B	309	-	3,3,3	0.77	0	2,2,2	0.22	0
27	CDL	G	101	-	65,65,99	1.28	9 (13%)	62,62,111	1.12	3 (4%)
21	DMU	D	207	-	7,7,34	0.44	0	6,6,45	0.40	0
18	PGV	A	606	-	31,31,50	0.52	0	29,29,56	0.70	1 (3%)
14	HEA	A	601[A]	-	66,67,67	1.87	21 (31%)	78,103,103	2.22	26 (33%)
20	EDO	C	319	-	3,3,3	0.46	0	2,2,2	0.43	0
26	PEK	C	303	-	17,17,52	0.47	0	15,16,57	0.97	1 (6%)
20	EDO	S	106	-	3,3,3	0.67	0	2,2,2	0.87	0
20	EDO	P	316	-	3,3,3	0.30	0	2,2,2	1.46	0
26	PEK	P	305	-	38,38,52	0.91	1 (2%)	37,37,57	1.04	3 (8%)
20	EDO	D	202	-	3,3,3	0.40	0	2,2,2	0.36	0
20	EDO	W	101	-	3,3,3	0.48	0	2,2,2	0.50	0
20	EDO	N	616	-	3,3,3	0.67	0	2,2,2	0.51	0
22	TGL	N	608	-	52,52,62	0.72	1 (1%)	50,50,65	0.80	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	C	310	-	22,22,34	1.03	1 (4%)	27,27,45	1.58	6 (22%)
20	EDO	N	621	-	3,3,3	0.22	0	2,2,2	0.96	0
20	EDO	W	102	-	3,3,3	0.22	0	2,2,2	0.77	0
20	EDO	C	317	-	3,3,3	0.29	0	2,2,2	0.16	0
18	PGV	N	610	-	50,50,50	1.04	3 (6%)	53,56,56	1.27	6 (11%)
25	CHD	B	304	-	32,32,32	0.97	0	51,51,51	1.68	13 (25%)
20	EDO	S	107	-	3,3,3	0.94	0	2,2,2	0.66	0
20	EDO	P	317	-	3,3,3	0.37	0	2,2,2	0.51	0
20	EDO	R	202	-	3,3,3	0.29	0	2,2,2	0.72	0
20	EDO	T	102	-	3,3,3	0.52	0	2,2,2	0.31	0
20	EDO	A	609	-	3,3,3	0.52	0	2,2,2	0.85	0
21	DMU	K	103	-	8,8,34	0.47	0	7,7,45	0.29	0
20	EDO	N	612	-	3,3,3	1.04	0	2,2,2	0.61	0
20	EDO	S	103	-	3,3,3	0.63	0	2,2,2	0.12	0
18	PGV	C	306	-	50,50,50	0.84	2 (4%)	53,56,56	1.02	5 (9%)
21	DMU	A	621	-	7,7,34	0.25	0	6,6,45	0.44	0
21	DMU	Q	202	-	9,9,34	0.54	0	8,8,45	0.33	0
20	EDO	T	104	-	3,3,3	0.67	0	2,2,2	1.02	0
18	PGV	C	307	-	35,35,50	0.95	1 (2%)	34,34,56	1.49	5 (14%)
20	EDO	S	108	-	3,3,3	0.30	0	2,2,2	1.01	0
20	EDO	E	202	-	3,3,3	0.63	0	2,2,2	0.24	0
14	HEA	N	602	19,1	66,67,67	1.87	19 (28%)	78,103,103	2.13	28 (35%)
20	EDO	P	313	-	3,3,3	0.44	0	2,2,2	0.23	0
14	HEA	N	601[A]	-	66,67,67	1.76	17 (25%)	78,103,103	2.17	25 (32%)
20	EDO	A	612	-	3,3,3	0.37	0	2,2,2	0.43	0
21	DMU	A	620	-	8,8,34	0.34	0	7,7,45	0.53	0
20	EDO	F	106	-	3,3,3	0.55	0	2,2,2	0.60	0
20	EDO	C	318	-	3,3,3	0.51	0	2,2,2	0.61	0
20	EDO	B	305	-	3,3,3	0.68	0	2,2,2	0.19	0
20	EDO	B	308	-	3,3,3	0.54	0	2,2,2	0.54	0
21	DMU	P	310	-	22,22,34	1.07	1 (4%)	27,27,45	1.55	4 (14%)
25	CHD	P	309	-	32,32,32	1.05	1 (3%)	51,51,51	1.90	15 (29%)
22	TGL	N	607	-	40,40,62	0.42	0	37,37,65	0.87	1 (2%)
22	TGL	N	606	-	62,62,62	1.09	3 (4%)	65,65,65	1.17	4 (6%)
20	EDO	A	619	-	3,3,3	0.45	0	2,2,2	0.55	0
18	PGV	Q	201	-	35,35,50	0.86	1 (2%)	34,34,56	1.37	3 (8%)
20	EDO	R	201	-	3,3,3	0.65	0	2,2,2	0.51	0
20	EDO	E	201	-	3,3,3	0.52	0	2,2,2	0.35	0
20	EDO	Q	203	-	3,3,3	0.40	0	2,2,2	0.18	0
20	EDO	A	616	-	3,3,3	0.16	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	X	102	-	7,7,34	0.41	0	6,6,45	0.34	0
27	CDL	P	308	-	73,73,99	1.34	11 (15%)	73,73,111	2.28	9 (12%)
20	EDO	C	311	-	3,3,3	1.10	0	2,2,2	0.46	0
20	EDO	F	103	-	3,3,3	0.86	0	2,2,2	0.49	0
21	DMU	M	101	-	34,34,34	0.51	0	45,45,45	1.20	6 (13%)
20	EDO	S	105	-	3,3,3	3.33	1 (33%)	2,2,2	2.01	1 (50%)
20	EDO	J	102	-	3,3,3	0.34	0	2,2,2	0.62	0
20	EDO	N	620	-	3,3,3	0.80	0	2,2,2	0.22	0
23	CUA	B	302	2	0,1,1	-	-	-	-	-
20	EDO	L	103	-	3,3,3	0.56	0	2,2,2	0.63	0
19	OXY	A	607	14,15	1,1,1	0.09	0	-	-	-
26	PEK	P	304	-	52,52,52	0.75	2 (3%)	55,57,57	1.11	2 (3%)
21	DMU	N	622	-	8,8,34	0.25	0	7,7,45	0.64	0
29	PO4	H	101	-	4,4,4	0.70	0	6,6,6	0.81	0
21	DMU	P	318	-	10,10,34	0.33	0	9,9,45	0.47	0
21	DMU	J	103	-	10,10,34	0.48	0	9,9,45	0.62	0
20	EDO	F	102	-	3,3,3	0.98	0	2,2,2	0.68	0
21	DMU	L	104	-	21,21,34	0.70	0	24,25,45	1.65	4 (16%)
20	EDO	Q	204	-	3,3,3	0.30	0	2,2,2	0.56	0
21	DMU	O	305	-	10,10,34	0.32	0	9,9,45	0.43	0
22	TGL	L	101	-	50,50,62	1.00	2 (4%)	48,48,65	1.33	5 (10%)
26	PEK	C	304	-	52,52,52	0.85	2 (3%)	55,57,57	1.13	2 (3%)
24	PSC	B	303	-	40,40,51	1.31	3 (7%)	42,42,59	1.91	5 (11%)
20	EDO	A	614	-	3,3,3	0.78	0	2,2,2	0.27	0
20	EDO	N	618	-	3,3,3	0.48	0	2,2,2	0.39	0
22	TGL	B	301	-	62,62,62	1.07	3 (4%)	65,65,65	1.51	5 (7%)
20	EDO	M	102	-	3,3,3	0.45	0	2,2,2	0.31	0
21	DMU	X	101	-	8,8,34	0.38	0	7,7,45	0.42	0
20	EDO	P	312	-	3,3,3	0.86	0	2,2,2	0.23	0
20	EDO	Y	101	-	3,3,3	0.38	0	2,2,2	0.22	0
25	CHD	C	309	-	32,32,32	0.80	0	51,51,51	1.32	7 (13%)
20	EDO	A	618	-	3,3,3	0.47	0	2,2,2	0.52	0
25	CHD	L	102	-	32,32,32	0.74	0	51,51,51	2.78	23 (45%)
20	EDO	O	303	-	3,3,3	0.79	0	2,2,2	0.67	0
26	PEK	C	305	-	38,38,52	0.93	1 (2%)	37,37,57	1.43	4 (10%)
20	EDO	C	315	-	3,3,3	0.56	0	2,2,2	0.18	0
20	EDO	T	103	-	3,3,3	0.62	0	2,2,2	0.29	0
25	CHD	G	102	-	32,32,32	1.14	2 (6%)	51,51,51	1.62	12 (23%)
20	EDO	A	617	-	3,3,3	1.06	0	2,2,2	0.74	0
21	DMU	K	102	-	8,8,34	0.35	0	7,7,45	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	E	203	-	3,3,3	0.48	0	2,2,2	0.59	0
20	EDO	B	310	-	3,3,3	0.48	0	2,2,2	0.72	0
20	EDO	F	107	-	3,3,3	0.62	0	2,2,2	0.08	0
20	EDO	S	102	-	3,3,3	1.04	0	2,2,2	0.74	0
23	CUA	O	301	2	0,1,1	-	-	-	-	-
20	EDO	F	104	-	3,3,3	0.39	0	2,2,2	0.58	0
19	OXY	N	609	14,15	1,1,1	0.11	0	-	-	-
25	CHD	P	301	-	32,32,32	0.89	1 (3%)	51,51,51	1.53	8 (15%)
20	EDO	A	610	-	3,3,3	0.94	0	2,2,2	0.59	0
20	EDO	D	205	-	3,3,3	0.41	0	2,2,2	0.67	0
20	EDO	S	104	-	3,3,3	0.68	0	2,2,2	0.18	0
26	PEK	P	303	-	26,26,52	0.35	0	24,24,57	0.88	1 (4%)
20	EDO	N	611	-	3,3,3	0.43	0	2,2,2	0.66	0
20	EDO	F	105	-	3,3,3	0.76	0	2,2,2	0.63	0
20	EDO	G	103	-	3,3,3	0.70	0	2,2,2	0.84	0
20	EDO	J	101	-	3,3,3	0.50	0	2,2,2	0.25	0
20	EDO	C	316	-	3,3,3	0.57	0	2,2,2	0.90	0
18	PGV	P	307	-	36,36,50	1.00	1 (2%)	35,35,56	1.32	4 (11%)
21	DMU	D	206	-	10,10,34	0.36	0	9,9,45	0.46	0
20	EDO	C	313	-	3,3,3	0.69	0	2,2,2	0.42	0
20	EDO	D	203	-	3,3,3	0.56	0	2,2,2	0.26	0
21	DMU	K	101	-	8,8,34	0.22	0	7,7,45	0.58	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
20	EDO	N	614	-	-	1/1/1/1	-
20	EDO	A	611	-	-	1/1/1/1	-
20	EDO	B	306	-	-	0/1/1/1	-
27	CDL	T	101	-	-	30/64/64/110	-
21	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
20	EDO	N	615	-	-	0/1/1/1	-
20	EDO	O	304	-	-	0/1/1/1	-
25	CHD	C	301	-	-	2/9/74/74	0/4/4/4
22	TGL	D	201	-	-	35/65/65/65	-
20	EDO	N	613	-	-	0/1/1/1	-
20	EDO	C	314	-	-	1/1/1/1	-
21	DMU	W	103	-	-	4/8/8/59	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DMU	X	103	-	-	0/7/7/59	-
20	EDO	P	314	-	-	0/1/1/1	-
20	EDO	A	613	-	-	1/1/1/1	-
27	CDL	C	308	-	-	33/76/80/110	-
20	EDO	N	619	-	-	0/1/1/1	-
20	EDO	A	615	-	-	1/1/1/1	-
21	DMU	C	320	-	-	2/9/9/59	-
20	EDO	C	312	-	-	0/1/1/1	-
20	EDO	N	617	-	-	0/1/1/1	-
20	EDO	P	315	-	-	0/1/1/1	-
24	PSC	O	302	-	-	12/26/27/55	-
20	EDO	D	204	-	-	0/1/1/1	-
18	PGV	A	608	-	-	7/55/55/55	-
18	PGV	P	306	-	-	12/55/55/55	-
20	EDO	B	307	-	-	1/1/1/1	-
21	DMU	K	104	-	-	2/7/7/59	-
20	EDO	P	311	-	-	1/1/1/1	-
14	HEA	A	602	19,1	-	6/36/76/76	-
20	EDO	B	309	-	-	1/1/1/1	-
27	CDL	G	101	-	-	17/58/58/110	-
21	DMU	D	207	-	-	1/5/5/59	-
18	PGV	A	606	-	-	10/26/27/55	-
14	HEA	A	601[A]	-	-	11/36/76/76	-
20	EDO	C	319	-	-	0/1/1/1	-
26	PEK	C	303	-	-	9/15/15/56	-
20	EDO	S	106	-	-	0/1/1/1	-
20	EDO	P	316	-	-	1/1/1/1	-
26	PEK	P	305	-	-	15/35/35/56	-
20	EDO	D	202	-	-	0/1/1/1	-
20	EDO	W	101	-	-	1/1/1/1	-
20	EDO	N	616	-	-	0/1/1/1	-
22	TGL	N	608	-	-	25/47/47/65	-
21	DMU	C	310	-	-	7/13/33/59	0/1/1/2
20	EDO	N	621	-	-	1/1/1/1	-
20	EDO	W	102	-	-	1/1/1/1	-
20	EDO	C	317	-	-	1/1/1/1	-
18	PGV	N	610	-	-	6/55/55/55	-
25	CHD	B	304	-	-	2/9/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	S	107	-	-	0/1/1/1	-
20	EDO	P	317	-	-	1/1/1/1	-
20	EDO	R	202	-	-	0/1/1/1	-
20	EDO	T	102	-	-	0/1/1/1	-
20	EDO	A	609	-	-	1/1/1/1	-
21	DMU	K	103	-	-	4/6/6/59	-
20	EDO	N	612	-	-	0/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
18	PGV	C	306	-	-	13/55/55/55	-
21	DMU	A	621	-	-	2/5/5/59	-
21	DMU	Q	202	-	-	3/7/7/59	-
20	EDO	T	104	-	-	0/1/1/1	-
18	PGV	C	307	-	-	8/32/32/55	-
20	EDO	S	108	-	-	0/1/1/1	-
20	EDO	E	202	-	-	1/1/1/1	-
14	HEA	N	602	19,1	-	6/36/76/76	-
20	EDO	P	313	-	-	1/1/1/1	-
14	HEA	N	601[A]	-	-	8/36/76/76	-
20	EDO	A	612	-	-	1/1/1/1	-
21	DMU	A	620	-	-	2/6/6/59	-
20	EDO	F	106	-	-	0/1/1/1	-
20	EDO	C	318	-	-	1/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
20	EDO	B	308	-	-	0/1/1/1	-
21	DMU	P	310	-	-	3/13/33/59	0/1/1/2
25	CHD	P	309	-	-	5/9/74/74	0/4/4/4
22	TGL	N	607	-	-	19/34/34/65	-
22	TGL	N	606	-	-	33/65/65/65	-
20	EDO	A	619	-	-	1/1/1/1	-
18	PGV	Q	201	-	-	10/32/32/55	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	Q	203	-	-	1/1/1/1	-
20	EDO	A	616	-	-	1/1/1/1	-
21	DMU	X	102	-	-	1/5/5/59	-
27	CDL	P	308	-	-	30/70/70/110	-
20	EDO	C	311	-	-	0/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
21	DMU	M	101	-	-	6/19/59/59	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	S	105	-	-	0/1/1/1	-
20	EDO	J	102	-	-	1/1/1/1	-
20	EDO	N	620	-	-	1/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
26	PEK	P	304	-	-	10/56/56/56	-
21	DMU	N	622	-	-	4/6/6/59	-
21	DMU	P	318	-	-	2/8/8/59	-
21	DMU	J	103	-	-	1/8/8/59	-
20	EDO	F	102	-	-	0/1/1/1	-
21	DMU	L	104	-	-	6/13/29/59	0/1/1/2
20	EDO	Q	204	-	-	1/1/1/1	-
21	DMU	O	305	-	-	6/8/8/59	-
22	TGL	L	101	-	-	25/43/44/65	-
26	PEK	C	304	-	-	15/56/56/56	-
24	PSC	B	303	-	-	16/41/41/55	-
20	EDO	A	614	-	-	0/1/1/1	-
20	EDO	N	618	-	-	0/1/1/1	-
22	TGL	B	301	-	-	34/65/65/65	-
20	EDO	M	102	-	-	1/1/1/1	-
21	DMU	X	101	-	-	2/6/6/59	-
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	Y	101	-	-	0/1/1/1	-
25	CHD	C	309	-	-	5/9/74/74	0/4/4/4
20	EDO	A	618	-	-	0/1/1/1	-
25	CHD	L	102	-	-	5/9/74/74	0/4/4/4
20	EDO	O	303	-	-	0/1/1/1	-
26	PEK	C	305	-	-	17/35/35/56	-
20	EDO	C	315	-	-	0/1/1/1	-
20	EDO	T	103	-	-	1/1/1/1	-
25	CHD	G	102	-	-	2/9/74/74	0/4/4/4
20	EDO	A	617	-	-	0/1/1/1	-
21	DMU	K	102	-	-	3/6/6/59	-
20	EDO	E	203	-	-	0/1/1/1	-
20	EDO	B	310	-	-	0/1/1/1	-
20	EDO	F	107	-	-	1/1/1/1	-
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
25	CHD	P	301	-	-	2/9/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	A	610	-	-	0/1/1/1	-
20	EDO	D	205	-	-	0/1/1/1	-
20	EDO	S	104	-	-	0/1/1/1	-
26	PEK	P	303	-	-	10/21/22/56	-
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	F	105	-	-	0/1/1/1	-
20	EDO	G	103	-	-	0/1/1/1	-
20	EDO	J	101	-	-	0/1/1/1	-
20	EDO	C	316	-	-	1/1/1/1	-
18	PGV	P	307	-	-	13/33/33/55	-
21	DMU	D	206	-	-	4/8/8/59	-
20	EDO	C	313	-	-	0/1/1/1	-
20	EDO	D	203	-	-	0/1/1/1	-
21	DMU	K	101	-	-	2/6/6/59	-

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S	105	EDO	O1-C1	-5.61	1.13	1.42
18	P	307	PGV	O03-C19	5.38	1.49	1.33
22	D	201	TGL	OG2-CB1	5.32	1.49	1.34
27	G	101	CDL	OB8-CB7	5.24	1.48	1.33
27	T	101	CDL	OB8-CB7	5.21	1.48	1.33
18	C	307	PGV	O03-C19	5.11	1.48	1.33
27	T	101	CDL	OB6-CB5	5.10	1.48	1.34
24	B	303	PSC	O01-C1	5.05	1.48	1.34
22	N	606	TGL	OG2-CB1	4.96	1.48	1.34
22	D	201	TGL	OG1-CA1	4.92	1.47	1.33
14	N	601[A]	HEA	CHC-C4B	4.88	1.48	1.38
22	L	101	TGL	OG3-CC1	4.86	1.48	1.33
26	C	305	PEK	O03-C21	4.83	1.48	1.33
26	P	305	PEK	O03-C21	4.79	1.48	1.33
22	B	301	TGL	OG2-CB1	4.69	1.47	1.34
14	A	601[A]	HEA	CHA-C1A	4.64	1.47	1.38
27	P	308	CDL	OB8-CB7	4.57	1.46	1.33
22	N	606	TGL	OG1-CA1	4.55	1.46	1.33
18	Q	201	PGV	O01-C1	4.46	1.46	1.33
24	B	303	PSC	O03-C19	4.44	1.46	1.33
14	A	602	HEA	CHB-C4A	4.43	1.47	1.38
22	B	301	TGL	OG1-CA1	4.37	1.46	1.33
27	C	308	CDL	OB8-CB7	4.29	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	608	TGL	OG3-CC1	4.27	1.46	1.33
22	B	301	TGL	OG3-CC1	4.14	1.45	1.33
22	L	101	TGL	OG1-CA1	3.99	1.45	1.33
22	N	606	TGL	OG3-CC1	3.97	1.44	1.33
14	N	601[A]	HEA	C4B-NB	-3.96	1.33	1.40
24	O	302	PSC	C13-C12	3.95	1.54	1.31
22	D	201	TGL	OG3-CC1	3.91	1.44	1.33
14	A	601[A]	HEA	CHD-C1D	3.89	1.46	1.38
14	N	602	HEA	CHB-C4A	3.88	1.45	1.38
14	N	601[A]	HEA	CHB-C4A	3.85	1.45	1.38
14	N	602	HEA	C3A-C4A	-3.82	1.39	1.46
27	C	308	CDL	C59-C58	-3.81	1.30	1.51
14	A	602	HEA	CHD-C1D	3.77	1.46	1.38
24	B	303	PSC	C13-C12	3.72	1.53	1.31
14	N	601[A]	HEA	C3A-C4A	-3.67	1.39	1.46
27	P	308	CDL	OB6-CB5	3.65	1.44	1.34
14	A	601[A]	HEA	C1D-ND	-3.59	1.34	1.40
26	C	304	PEK	O03-C21	3.57	1.43	1.33
27	C	308	CDL	OB6-CB5	3.56	1.44	1.34
18	A	608	PGV	O01-C1	3.50	1.44	1.34
27	P	308	CDL	C79-C78	-3.48	1.32	1.51
21	P	310	DMU	O16-C6	3.46	1.46	1.40
14	A	601[A]	HEA	C1A-C2A	-3.42	1.39	1.45
14	A	602	HEA	C4A-NA	-3.41	1.33	1.39
14	A	601[A]	HEA	C4D-C3D	-3.40	1.39	1.45
21	C	310	DMU	O16-C6	3.40	1.46	1.40
27	C	308	CDL	C79-C78	-3.37	1.32	1.51
18	N	610	PGV	O01-C1	3.37	1.43	1.34
27	P	308	CDL	C22-C21	-3.36	1.32	1.51
14	N	602	HEA	CHA-C1A	3.32	1.44	1.38
14	N	602	HEA	C4C-NC	-3.26	1.33	1.39
27	P	308	CDL	C82-C81	-3.23	1.33	1.51
27	P	308	CDL	C62-C61	-3.21	1.33	1.51
14	A	602	HEA	FE-NC	3.21	2.06	1.95
14	N	602	HEA	CHC-C1C	3.19	1.46	1.39
27	P	308	CDL	C19-C18	-3.18	1.33	1.51
14	N	602	HEA	O11-C11	3.17	1.49	1.42
27	C	308	CDL	C39-C38	-3.17	1.33	1.51
27	T	101	CDL	C19-C18	-3.16	1.33	1.51
27	P	308	CDL	C59-C58	-3.15	1.33	1.51
27	C	308	CDL	C62-C61	-3.15	1.33	1.51
27	G	101	CDL	C79-C78	-3.14	1.34	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	101	CDL	C62-C61	-3.13	1.34	1.51
27	T	101	CDL	C59-C58	-3.13	1.34	1.51
14	N	602	HEA	CHD-C1D	3.13	1.44	1.38
14	N	601[A]	HEA	CMD-C2D	3.12	1.57	1.50
18	A	608	PGV	O03-C01	3.12	1.52	1.45
14	N	601[A]	HEA	CHA-C1A	3.12	1.44	1.38
27	P	308	CDL	C39-C38	-3.11	1.34	1.51
27	C	308	CDL	C22-C21	-3.10	1.34	1.51
27	C	308	CDL	C19-C18	-3.10	1.34	1.51
27	C	308	CDL	C82-C81	-3.07	1.34	1.51
27	G	101	CDL	C82-C81	-3.06	1.34	1.51
14	A	601[A]	HEA	C3A-C4A	-3.04	1.40	1.46
27	C	308	CDL	C42-C41	-3.03	1.34	1.51
27	T	101	CDL	C79-C78	-3.02	1.34	1.51
27	G	101	CDL	C22-C21	-3.01	1.34	1.51
27	T	101	CDL	C22-C21	-3.01	1.34	1.51
18	N	610	PGV	O03-C01	2.96	1.51	1.45
27	G	101	CDL	C19-C18	-2.94	1.35	1.51
27	T	101	CDL	C82-C81	-2.93	1.35	1.51
14	A	602	HEA	C4D-C3D	-2.92	1.40	1.45
14	A	602	HEA	C18-C19	2.92	1.40	1.33
14	A	602	HEA	CMC-C2C	2.92	1.57	1.50
14	A	602	HEA	O11-C11	2.89	1.49	1.42
14	A	601[A]	HEA	CHB-C4A	2.89	1.44	1.38
27	P	308	CDL	C42-C41	-2.88	1.35	1.51
14	A	601[A]	HEA	CBA-CGA	2.87	1.57	1.50
26	P	304	PEK	O03-C21	2.87	1.41	1.33
14	N	601[A]	HEA	FE-ND	2.83	2.03	1.94
27	T	101	CDL	C42-C41	-2.80	1.35	1.51
14	A	601[A]	HEA	C1D-C2D	-2.75	1.39	1.44
14	A	601[A]	HEA	CBD-CGD	2.74	1.57	1.50
14	A	602	HEA	CBA-CGA	2.73	1.56	1.50
27	G	101	CDL	C62-C61	-2.72	1.36	1.51
14	A	601[A]	HEA	C1C-NC	-2.71	1.34	1.39
14	N	602	HEA	C1A-C2A	-2.70	1.40	1.45
27	G	101	CDL	C42-C41	-2.70	1.36	1.51
27	G	101	CDL	C59-C58	-2.69	1.36	1.51
14	N	602	HEA	C4D-C3D	-2.69	1.40	1.45
14	N	602	HEA	C4B-C3B	-2.67	1.40	1.44
14	A	602	HEA	CHB-C1B	2.66	1.45	1.39
18	A	608	PGV	C03-C02	2.63	1.58	1.50
14	N	602	HEA	FE-NA	2.61	2.04	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601[A]	HEA	O11-C11	2.60	1.48	1.42
14	N	601[A]	HEA	CHA-C4D	2.60	1.45	1.39
25	C	301	CHD	O25-C24	2.57	1.30	1.22
14	A	601[A]	HEA	CAD-C3D	2.57	1.57	1.51
27	G	101	CDL	C39-C38	-2.56	1.37	1.51
26	C	304	PEK	O01-C1	2.55	1.41	1.34
25	C	301	CHD	C23-C24	2.54	1.56	1.50
14	A	601[A]	HEA	C1B-NB	-2.54	1.33	1.38
14	N	602	HEA	CHB-C1B	2.54	1.45	1.39
14	A	602	HEA	FE-NA	2.53	2.03	1.95
14	N	602	HEA	FE-ND	2.52	2.02	1.94
14	A	602	HEA	CHC-C1C	2.51	1.45	1.39
26	P	304	PEK	C05-C04	2.48	1.60	1.50
14	A	602	HEA	C1D-C2D	-2.47	1.39	1.44
14	N	601[A]	HEA	O1A-CGA	2.46	1.30	1.22
14	N	602	HEA	CHC-C4B	2.46	1.43	1.38
18	A	608	PGV	O01-C02	-2.46	1.40	1.46
14	N	601[A]	HEA	O2D-CGD	-2.44	1.22	1.30
14	N	602	HEA	CBA-CGA	2.41	1.56	1.50
18	N	610	PGV	O03-C19	2.40	1.40	1.33
27	T	101	CDL	CB6-CB4	2.40	1.56	1.50
27	P	308	CDL	OB6-CB4	-2.38	1.43	1.47
14	A	602	HEA	C4B-C3B	-2.35	1.40	1.44
25	G	102	CHD	O7-C7	2.34	1.48	1.43
14	N	601[A]	HEA	CHD-C4C	2.34	1.44	1.39
14	N	602	HEA	FE-NC	2.34	2.03	1.95
14	A	602	HEA	CHC-C4B	2.34	1.43	1.38
14	N	602	HEA	C12-C13	2.30	1.60	1.53
14	A	601[A]	HEA	CMB-C2B	2.29	1.55	1.50
18	C	306	PGV	O01-C02	-2.28	1.40	1.46
14	A	602	HEA	C3A-C4A	-2.27	1.42	1.46
14	A	601[A]	HEA	FE-NA	2.27	2.02	1.95
14	A	602	HEA	CBC-CAC	2.26	1.41	1.30
25	C	301	CHD	O12-C12	2.23	1.47	1.43
25	G	102	CHD	C10-C5	-2.23	1.51	1.55
14	N	602	HEA	C1D-C2D	-2.20	1.40	1.44
25	P	309	CHD	O25-C24	2.19	1.29	1.22
18	P	306	PGV	P-O14	-2.17	1.45	1.55
14	N	602	HEA	CAA-C2A	2.16	1.56	1.51
14	A	601[A]	HEA	CHC-C4B	2.15	1.42	1.38
25	C	301	CHD	C11-C9	2.13	1.57	1.53
14	A	601[A]	HEA	CAA-C2A	2.13	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[A]	HEA	C4C-NC	-2.09	1.35	1.39
14	A	601[A]	HEA	C4D-ND	-2.09	1.34	1.38
14	A	601[A]	HEA	FE-ND	2.08	2.01	1.94
14	N	601[A]	HEA	C4D-C3D	-2.06	1.41	1.45
21	Z	101	DMU	O16-C6	2.05	1.43	1.40
14	A	601[A]	HEA	CHD-C4C	2.05	1.44	1.39
14	N	601[A]	HEA	C1A-C2A	-2.05	1.41	1.45
25	P	301	CHD	C23-C24	2.04	1.55	1.50
18	C	306	PGV	P-O12	2.03	1.67	1.59
14	N	601[A]	HEA	CMB-C2B	2.03	1.55	1.50
14	A	602	HEA	C16-C17	2.02	1.60	1.53
18	P	306	PGV	O01-C02	-2.02	1.41	1.46
14	N	601[A]	HEA	CHC-C1C	2.01	1.43	1.39
14	A	602	HEA	CHA-C1A	2.01	1.42	1.38
14	N	601[A]	HEA	CBD-CGD	2.00	1.55	1.50

All (338) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	308	CDL	CB4-OB6-CB5	-14.96	98.63	117.88
22	B	301	TGL	OG2-CB1-CB2	8.53	129.88	111.50
14	N	601[A]	HEA	C13-C12-C11	-8.01	102.32	114.35
27	T	101	CDL	OB6-CB5-C51	7.54	127.76	111.50
14	N	602	HEA	C3C-C4C-NC	6.76	114.41	110.25
24	B	303	PSC	C02-O01-C1	6.74	126.55	117.88
25	L	102	CHD	C11-C12-C13	6.63	118.06	111.24
14	N	601[A]	HEA	C3C-C4C-NC	6.39	114.18	110.25
24	B	303	PSC	O01-C1-C2	6.25	124.98	111.50
25	L	102	CHD	C14-C8-C7	6.23	120.06	111.81
25	L	102	CHD	C1-C10-C5	6.08	116.76	107.77
14	A	602	HEA	C27-C19-C20	6.05	125.44	115.27
22	N	606	TGL	OG2-CB1-CB2	5.75	123.90	111.50
27	C	308	CDL	CB4-OB6-CB5	-5.74	103.67	117.79
25	P	301	CHD	C21-C20-C22	-5.66	101.49	110.36
14	A	601[A]	HEA	C13-C12-C11	-5.56	105.99	114.35
22	D	201	TGL	CG3-CG2-CG1	-5.46	98.88	111.79
14	A	601[A]	HEA	CHA-C4D-C3D	-5.44	116.84	124.84
14	N	601[A]	HEA	C3D-C4D-ND	5.42	115.61	110.36
14	A	601[A]	HEA	C2B-C1B-NB	5.31	116.24	109.88
27	P	308	CDL	OB8-CB7-C71	5.29	128.51	111.91
18	C	307	PGV	O03-C19-C20	5.24	128.36	111.91
25	P	309	CHD	C5-C4-C3	-5.17	105.17	112.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[A]	HEA	CAA-CBA-CGA	-5.13	102.56	113.60
25	P	309	CHD	C15-C14-C13	5.12	108.57	103.55
25	L	102	CHD	C13-C17-C20	5.08	125.56	119.50
25	L	102	CHD	C6-C5-C4	-4.88	105.57	111.19
27	C	308	CDL	OB6-CB5-C51	4.79	121.82	111.50
21	L	104	DMU	C6-O5-C4	4.78	118.42	113.13
27	P	308	CDL	OB6-CB5-C51	4.73	121.69	111.50
14	N	602	HEA	C4C-NC-C1C	-4.72	100.72	105.35
27	G	101	CDL	CB6-OB8-CB7	4.62	131.86	116.92
26	C	305	PEK	O03-C21-C22	4.61	130.45	112.23
22	D	201	TGL	OG3-CC1-OC1	-4.60	111.97	123.59
25	L	102	CHD	C21-C20-C17	4.58	119.94	112.92
14	N	602	HEA	C2B-C1B-NB	4.56	115.35	109.88
14	A	601[A]	HEA	C3D-C4D-ND	4.55	114.76	110.36
18	P	307	PGV	O03-C19-C20	4.51	126.05	111.91
25	C	301	CHD	C5-C4-C3	-4.40	106.30	112.76
25	L	102	CHD	C10-C9-C8	4.39	116.53	111.82
25	L	102	CHD	C15-C14-C8	4.37	124.44	118.33
24	B	303	PSC	C01-O03-C19	4.31	133.09	117.12
14	A	601[A]	HEA	C4B-NB-C1B	-4.25	100.68	105.07
14	A	601[A]	HEA	C2D-C1D-ND	4.19	114.81	109.84
27	C	308	CDL	C52-C51-CB5	-4.15	98.55	113.62
18	P	306	PGV	O01-C1-O02	-4.14	113.70	123.70
24	O	302	PSC	C28-C27-C26	-4.14	93.43	114.42
27	P	308	CDL	OB8-CB7-OB9	-4.11	113.22	123.59
14	N	601[A]	HEA	C1D-ND-C4D	-4.10	100.84	105.07
14	N	602	HEA	CBD-CAD-C3D	4.06	123.92	112.63
25	L	102	CHD	C19-C10-C1	-4.05	101.73	108.26
14	N	602	HEA	O2D-CGD-O1D	4.03	133.34	123.30
14	N	601[A]	HEA	CHA-C1A-NA	4.02	128.78	124.44
26	C	305	PEK	C01-O03-C21	4.01	129.32	116.11
14	A	602	HEA	C2D-C1D-ND	3.99	114.56	109.84
18	Q	201	PGV	O01-C1-C2	3.94	124.27	111.91
18	Q	201	PGV	C02-O01-C1	-3.94	105.28	116.73
25	B	304	CHD	C11-C9-C10	-3.92	109.68	113.73
14	N	602	HEA	C13-C12-C11	-3.91	108.48	114.35
26	C	304	PEK	O03-C21-C22	3.91	124.16	111.91
25	G	102	CHD	C6-C5-C4	-3.88	106.73	111.19
14	A	602	HEA	C13-C12-C11	-3.86	108.55	114.35
22	L	101	TGL	OG3-CC1-CC2	3.84	127.39	112.23
25	B	304	CHD	C19-C10-C1	-3.77	102.18	108.26
14	A	602	HEA	CHD-C4C-NC	3.77	130.79	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C20-C19-C18	-3.76	113.52	121.12
22	D	201	TGL	CG3-OG3-CC1	-3.72	103.33	117.12
27	P	308	CDL	C52-C51-CB5	-3.71	100.14	113.62
25	L	102	CHD	C15-C14-C13	-3.70	99.92	103.55
21	P	310	DMU	C6-O5-C4	3.70	120.94	113.69
25	L	102	CHD	C2-C1-C10	3.68	119.09	112.78
25	C	301	CHD	C22-C20-C17	-3.65	102.74	110.28
14	N	602	HEA	C16-C15-C14	-3.64	113.75	121.12
26	C	305	PEK	O03-C21-O04	-3.63	111.76	123.14
25	P	309	CHD	C19-C10-C9	-3.62	106.20	111.18
24	B	303	PSC	O01-C1-O02	-3.57	115.08	123.70
22	D	201	TGL	OG2-CG2-CG1	3.57	121.31	108.40
14	A	602	HEA	C4C-CHD-C1D	-3.56	117.89	126.34
14	A	601[A]	HEA	CHA-C4D-ND	3.50	128.22	124.42
22	D	201	TGL	OG3-CC1-CC2	3.49	122.86	111.91
18	N	610	PGV	O03-C19-O04	-3.46	114.85	123.59
27	T	101	CDL	OB6-CB4-CB3	3.46	115.84	107.93
14	A	602	HEA	CMD-C2D-C1D	3.44	130.28	125.04
25	C	301	CHD	C6-C7-C8	-3.44	107.81	111.48
14	N	601[A]	HEA	CHB-C1B-C2B	-3.42	119.63	124.98
21	C	310	DMU	C22-C19-C18	-3.42	98.32	113.49
18	C	307	PGV	C01-C02-C03	-3.42	106.50	113.95
25	L	102	CHD	C17-C13-C12	-3.42	114.55	117.67
14	A	601[A]	HEA	O2D-CGD-O1D	3.41	131.79	123.30
14	A	601[A]	HEA	C1A-CHA-C4D	-3.40	118.73	126.06
25	L	102	CHD	C11-C9-C10	-3.37	110.25	113.73
22	D	201	TGL	OG2-CB1-CB2	3.37	118.75	111.50
25	G	102	CHD	O12-C12-C13	-3.36	105.34	111.03
25	L	102	CHD	C17-C13-C14	3.35	103.47	100.09
18	P	306	PGV	C03-C02-C01	-3.33	103.91	111.79
14	N	602	HEA	C4B-NB-C1B	-3.32	101.65	105.07
27	T	101	CDL	C23-C22-C21	3.30	131.20	114.42
18	C	307	PGV	O03-C19-O04	-3.30	115.26	123.59
22	B	301	TGL	OB1-CB1-CB2	-3.28	110.92	123.73
25	P	309	CHD	C13-C17-C20	-3.28	115.58	119.50
27	C	308	CDL	OB8-CB7-C71	3.24	122.09	111.91
14	A	602	HEA	CHA-C4D-C3D	-3.24	120.08	124.84
14	N	601[A]	HEA	CHA-C4D-ND	-3.24	120.90	124.42
14	N	602	HEA	C2C-C1C-NC	3.23	115.00	110.08
14	A	601[A]	HEA	CHD-C1D-C2D	-3.21	117.82	126.73
14	N	601[A]	HEA	C4C-NC-C1C	-3.20	102.22	105.35
25	C	301	CHD	C1-C10-C5	3.19	112.49	107.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	301	CHD	C18-C13-C12	3.19	112.31	109.07
14	N	601[A]	HEA	C2D-C1D-ND	3.18	113.61	109.84
14	A	602	HEA	C1D-ND-C4D	-3.18	101.79	105.07
25	L	102	CHD	C16-C17-C13	-3.18	100.44	103.55
21	L	104	DMU	O16-C6-C1	3.16	113.24	108.30
27	T	101	CDL	CB4-OB6-CB5	-3.15	113.83	117.88
25	P	309	CHD	C23-C22-C20	-3.14	108.78	114.52
25	B	304	CHD	C1-C10-C5	3.14	112.41	107.77
18	A	608	PGV	O03-C19-C20	3.13	121.73	111.91
14	N	602	HEA	C4A-C3A-C2A	3.13	109.32	106.75
25	G	102	CHD	C11-C9-C10	-3.12	110.51	113.73
25	B	304	CHD	C6-C5-C4	-3.11	107.61	111.19
25	G	102	CHD	C13-C14-C8	-3.08	110.80	114.74
25	L	102	CHD	C9-C11-C12	3.07	118.36	114.30
22	D	201	TGL	CB3-CB2-CB1	-3.06	102.48	113.62
14	A	601[A]	HEA	C4C-CHD-C1D	-3.06	119.08	126.34
14	A	602	HEA	C26-C15-C16	3.03	120.37	115.27
18	P	307	PGV	C01-O03-C19	3.02	126.68	116.92
14	N	602	HEA	C26-C15-C16	3.00	120.31	115.27
25	P	301	CHD	O12-C12-C13	-3.00	105.97	111.03
27	C	308	CDL	C78-C77-C76	-2.99	99.24	114.42
14	A	601[A]	HEA	C1D-ND-C4D	-2.99	101.99	105.07
14	A	602	HEA	CMB-C2B-C3B	-2.99	124.65	130.34
27	T	101	CDL	OB6-CB5-OB7	-2.98	116.51	123.70
14	N	601[A]	HEA	O2A-CGA-CBA	2.97	123.58	114.03
25	P	301	CHD	C19-C10-C1	-2.96	103.50	108.26
22	D	201	TGL	OG1-CA1-CA2	2.95	121.17	111.91
27	C	308	CDL	C42-C41-C40	2.93	129.30	114.42
21	C	310	DMU	C2-C3-C4	-2.93	105.02	110.24
18	N	610	PGV	O01-C1-O02	-2.92	116.64	123.70
14	N	601[A]	HEA	CAA-CBA-CGA	-2.92	107.32	113.60
22	B	301	TGL	CG3-CG2-CG1	-2.92	104.89	111.79
22	L	101	TGL	CC4-CC3-CC2	-2.90	100.21	113.44
21	L	104	DMU	O5-C4-C57	2.90	111.48	106.83
25	C	309	CHD	C15-C14-C13	2.90	106.40	103.55
18	N	610	PGV	O03-C19-C20	2.90	120.99	111.91
21	P	310	DMU	O16-C18-C19	2.89	119.69	109.56
25	C	309	CHD	C1-C10-C5	2.89	112.04	107.77
25	C	309	CHD	C6-C5-C4	-2.88	107.88	111.19
27	C	308	CDL	C22-C21-C20	2.87	128.98	114.42
26	P	303	PEK	C8-C7-C6	-2.86	97.95	112.02
27	T	101	CDL	OB8-CB6-CB4	2.85	116.59	108.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[A]	HEA	CHB-C1B-NB	-2.85	121.32	124.42
21	M	101	DMU	O1-C9-C8	2.85	114.87	109.69
25	P	309	CHD	C22-C23-C24	-2.84	104.97	112.51
25	G	102	CHD	C18-C13-C12	-2.83	106.18	109.07
14	A	601[A]	HEA	CAD-C3D-C4D	2.83	129.61	124.66
27	T	101	CDL	C62-C61-C60	2.83	128.77	114.42
14	A	601[A]	HEA	O2A-CGA-CBA	2.82	123.08	114.03
14	A	602	HEA	CMB-C2B-C1B	2.81	129.32	125.04
25	C	301	CHD	C19-C10-C1	-2.80	103.75	108.26
14	N	601[A]	HEA	OMA-CMA-C3A	-2.80	119.36	125.69
25	B	304	CHD	C4-C3-C2	2.79	113.89	110.55
25	P	301	CHD	C22-C20-C17	-2.79	104.52	110.28
14	N	602	HEA	C1B-C2B-C3B	-2.79	103.47	106.80
14	N	601[A]	HEA	C1C-CHC-C4B	-2.79	119.72	126.34
14	N	601[A]	HEA	C2B-C1B-NB	2.78	113.22	109.88
25	L	102	CHD	C4-C3-C2	-2.78	107.23	110.55
27	C	308	CDL	C20-C19-C18	2.77	128.51	114.42
14	N	601[A]	HEA	O2D-CGD-CBD	2.77	122.94	114.03
22	N	606	TGL	OG3-CC1-CC2	2.76	120.56	111.91
14	A	601[A]	HEA	CHD-C4C-NC	2.76	128.92	123.85
14	N	601[A]	HEA	O1D-CGD-CBD	-2.76	114.22	123.08
14	A	602	HEA	CHB-C4A-C3A	-2.75	120.56	125.26
22	L	101	TGL	OG3-CC1-OC1	-2.75	114.53	123.14
14	A	601[A]	HEA	C3C-C4C-NC	-2.74	108.56	110.25
25	P	309	CHD	C13-C14-C8	-2.72	111.26	114.74
27	C	308	CDL	C21-C20-C19	-2.70	100.70	114.42
14	N	602	HEA	CHC-C4B-NB	2.69	127.69	124.37
14	A	601[A]	HEA	C1D-C2D-C3D	-2.68	104.14	106.96
22	N	606	TGL	OG1-CA1-CA2	2.68	120.31	111.91
14	A	602	HEA	C2C-C1C-NC	2.67	114.15	110.08
25	L	102	CHD	C4-C5-C10	2.66	115.49	112.66
25	B	304	CHD	O12-C12-C11	2.66	114.55	109.12
25	B	304	CHD	C13-C14-C8	-2.66	111.35	114.74
14	N	602	HEA	CHB-C1B-C2B	-2.65	120.83	124.98
27	P	308	CDL	C39-C38-C37	2.65	127.90	114.42
25	C	301	CHD	C5-C6-C7	2.65	117.38	114.46
18	N	610	PGV	C9-C10-C11	-2.63	97.39	112.43
21	Z	101	DMU	C31-C28-C25	-2.62	101.12	114.42
14	A	602	HEA	C4A-CHB-C1B	-2.62	120.42	126.06
25	G	102	CHD	C13-C17-C20	-2.61	116.38	119.50
18	P	307	PGV	O04-C19-C20	-2.61	113.56	123.73
18	P	306	PGV	C14-C13-C12	-2.60	97.51	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C4B-NB-C1B	-2.59	102.40	105.07
25	G	102	CHD	C19-C10-C5	-2.59	105.98	110.36
14	A	601[A]	HEA	C3B-C4B-NB	2.58	112.90	109.84
14	N	602	HEA	C27-C19-C20	2.58	119.61	115.27
14	A	602	HEA	C1D-C2D-C3D	-2.57	104.26	106.96
25	C	301	CHD	C1-C2-C3	-2.56	107.18	110.47
21	C	310	DMU	O7-C3-C2	2.55	116.25	110.35
25	P	309	CHD	C11-C9-C10	-2.55	111.10	113.73
26	P	305	PEK	O03-C21-C22	2.55	122.29	112.23
25	P	309	CHD	O25-C24-C23	-2.54	114.91	123.08
25	G	102	CHD	C1-C10-C5	2.54	111.52	107.77
14	N	601[A]	HEA	C1B-C2B-C3B	-2.54	103.77	106.80
14	N	601[A]	HEA	CHB-C4A-NA	-2.53	121.70	124.44
14	N	601[A]	HEA	CHB-C1B-NB	2.52	127.15	124.42
21	C	310	DMU	O16-C18-C19	2.51	118.38	109.56
18	Q	201	PGV	O01-C1-O02	-2.51	117.25	123.59
27	C	308	CDL	OB8-CB7-OB9	-2.51	117.25	123.59
22	N	608	TGL	OG3-CC1-CC2	2.51	122.16	112.23
21	P	310	DMU	O7-C3-C4	2.51	115.53	109.30
25	C	309	CHD	C5-C4-C3	-2.51	109.07	112.76
25	P	309	CHD	O7-C7-C8	2.51	115.03	109.43
25	G	102	CHD	C4-C5-C10	-2.50	110.00	112.66
14	N	602	HEA	C4A-NA-C1A	2.49	107.78	105.35
25	G	102	CHD	C19-C10-C1	-2.48	104.27	108.26
14	A	602	HEA	CHC-C4B-NB	2.47	127.41	124.37
14	N	601[A]	HEA	CHD-C1D-C2D	-2.46	119.88	126.73
25	C	309	CHD	C14-C8-C9	-2.46	106.33	109.71
27	T	101	CDL	OB8-CB7-C71	2.46	119.61	111.91
25	P	309	CHD	C14-C8-C9	-2.44	106.36	109.71
25	C	301	CHD	C18-C13-C17	-2.43	107.41	111.21
26	C	305	PEK	C24-C23-C22	2.42	121.89	113.19
25	L	102	CHD	O7-C7-C8	2.42	114.83	109.43
25	P	301	CHD	C16-C17-C20	-2.41	108.41	112.15
25	C	309	CHD	C4-C5-C10	2.41	115.22	112.66
21	M	101	DMU	C22-C19-C18	-2.41	102.83	113.49
20	S	105	EDO	O1-C1-C2	2.40	129.19	111.91
18	A	608	PGV	O03-C19-O04	-2.40	117.53	123.59
14	A	602	HEA	CHA-C4D-ND	2.40	127.03	124.42
25	C	301	CHD	O3-C3-C2	-2.39	104.07	110.16
14	N	601[A]	HEA	CHA-C1A-C2A	-2.39	121.06	124.94
25	L	102	CHD	C5-C4-C3	-2.39	109.25	112.76
14	N	602	HEA	C2D-C1D-ND	2.39	112.67	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	C1D-ND-C4D	-2.38	102.62	105.07
22	N	606	TGL	CG1-OG1-CA1	2.37	125.91	117.12
27	G	101	CDL	C60-C59-C58	2.37	126.47	114.42
14	A	601[A]	HEA	C4A-C3A-C2A	2.37	108.70	106.75
22	D	201	TGL	OB1-CB1-CB2	-2.37	114.49	123.73
14	A	602	HEA	C3B-C4B-NB	2.36	112.63	109.84
21	Z	101	DMU	O4-C7-C8	2.36	115.80	110.35
14	A	602	HEA	C3C-C2C-C1C	-2.35	104.32	107.16
24	O	302	PSC	C25-C24-C23	-2.35	102.50	114.42
14	A	602	HEA	CHB-C4A-NA	2.34	126.97	124.44
18	C	307	PGV	C9-C10-C11	-2.34	99.05	112.43
14	N	602	HEA	CHD-C4C-C3C	-2.33	117.34	127.71
21	Z	101	DMU	O61-C57-C4	-2.33	103.31	111.29
14	N	602	HEA	CHC-C4B-C3B	-2.32	119.82	125.80
14	N	602	HEA	C4C-CHD-C1D	-2.32	120.83	126.34
18	C	307	PGV	C01-O03-C19	2.31	124.40	116.92
18	A	608	PGV	O01-C1-O02	-2.30	118.14	123.70
26	C	303	PEK	C11-C10-C9	2.30	123.35	112.02
25	B	304	CHD	O3-C3-C4	-2.30	105.28	109.85
25	P	301	CHD	C6-C7-C8	-2.29	109.03	111.48
14	N	602	HEA	C3A-C2A-C1A	-2.29	104.89	107.08
22	B	301	TGL	CG1-OG1-CA1	2.29	125.59	117.12
14	A	601[A]	HEA	CBA-CAA-C2A	-2.28	106.28	112.63
14	A	602	HEA	CHC-C4B-C3B	-2.28	119.92	125.80
25	P	301	CHD	C5-C4-C3	-2.28	109.42	112.76
26	P	304	PEK	O03-C21-C22	2.26	119.02	111.91
14	N	602	HEA	CHD-C4C-NC	2.26	128.00	123.85
18	C	306	PGV	O01-C1-C2	2.26	116.36	111.50
21	M	101	DMU	O7-C3-C2	-2.26	101.28	107.28
14	A	602	HEA	C2B-C1B-NB	2.25	112.58	109.88
18	A	608	PGV	O01-C02-C01	-2.24	100.29	108.40
18	N	610	PGV	O01-C02-C01	-2.24	100.29	108.40
25	L	102	CHD	O25-C24-C23	-2.24	115.89	123.08
24	B	303	PSC	O03-C01-C02	-2.23	101.94	108.38
22	L	101	TGL	C20-CA9-CA8	-2.23	103.09	114.42
14	N	602	HEA	C3B-C4B-NB	2.23	112.48	109.84
18	C	306	PGV	O03-C01-C02	-2.23	101.94	108.43
18	C	306	PGV	O03-C19-C20	2.21	118.83	111.91
27	P	308	CDL	C81-C80-C79	-2.21	103.22	114.42
25	P	309	CHD	C21-C20-C22	-2.21	106.91	110.36
27	P	308	CDL	C43-C42-C41	2.20	125.59	114.42
22	B	301	TGL	CB3-CB2-CB1	-2.20	105.62	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	301	CHD	C16-C17-C20	-2.20	108.74	112.15
27	P	308	CDL	C80-C79-C78	2.20	125.59	114.42
18	N	610	PGV	O01-C1-C2	2.20	116.23	111.50
21	M	101	DMU	C31-C28-C25	-2.19	103.30	114.42
25	P	301	CHD	C11-C9-C10	-2.19	111.47	113.73
25	P	309	CHD	C1-C2-C3	2.19	113.27	110.47
25	B	304	CHD	C9-C11-C12	-2.18	111.42	114.30
18	A	608	PGV	C9-C8-C7	-2.18	103.36	114.42
27	G	101	CDL	C39-C38-C37	2.18	125.49	114.42
14	N	602	HEA	CHA-C4D-C3D	-2.18	121.64	124.84
14	N	601[A]	HEA	C17-C18-C19	2.17	132.89	127.66
21	M	101	DMU	O2-C8-C9	-2.17	103.91	109.30
27	T	101	CDL	CB6-OB8-CB7	2.17	125.14	117.12
26	P	305	PEK	C01-O03-C21	2.16	123.22	116.11
25	G	102	CHD	C16-C17-C20	-2.16	108.81	112.15
26	C	304	PEK	C02-O01-C1	-2.15	112.49	117.79
25	B	304	CHD	C18-C13-C12	-2.15	106.88	109.07
21	L	104	DMU	C18-O16-C6	2.15	117.40	113.84
27	T	101	CDL	C81-C80-C79	-2.15	103.53	114.42
24	O	302	PSC	C21-C20-C19	-2.15	104.72	114.26
14	A	601[A]	HEA	CHD-C1D-ND	2.14	127.02	124.37
14	N	601[A]	HEA	C13-C14-C15	-2.14	122.51	127.66
27	C	308	CDL	C61-C60-C59	-2.14	103.58	114.42
18	P	306	PGV	O01-C1-C2	2.13	116.10	111.50
21	P	310	DMU	O55-C2-C1	-2.13	105.42	110.35
25	G	102	CHD	O7-C7-C6	2.13	115.22	109.94
25	B	304	CHD	O26-C24-O25	-2.12	118.01	123.30
22	N	607	TGL	CA7-CA6-CA5	-2.11	103.69	114.42
25	C	301	CHD	C18-C13-C14	-2.11	107.90	111.21
25	C	301	CHD	C10-C9-C8	-2.11	109.56	111.82
21	C	310	DMU	O5-C6-C1	-2.10	105.91	110.35
18	P	307	PGV	C27-C26-C25	-2.10	103.78	114.42
14	N	601[A]	HEA	C4D-C3D-C2D	-2.09	103.85	106.90
25	L	102	CHD	O26-C24-C23	2.09	120.75	114.03
14	A	602	HEA	CAD-CBD-CGD	-2.09	109.11	113.60
25	C	309	CHD	C11-C9-C10	-2.09	111.57	113.73
25	C	301	CHD	C14-C8-C7	-2.09	109.04	111.81
27	T	101	CDL	OB7-CB5-C51	-2.08	115.62	123.73
22	L	101	TGL	CA7-CA6-CA5	-2.07	103.90	114.42
14	N	602	HEA	C21-C20-C19	2.07	119.80	112.98
27	T	101	CDL	C24-C23-C22	-2.07	103.92	114.42
14	A	601[A]	HEA	O1D-CGD-CBD	-2.07	116.44	123.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	M	101	DMU	O1-C9-C11	2.07	111.57	106.44
25	L	102	CHD	C22-C23-C24	-2.06	107.03	112.51
14	N	602	HEA	O1A-CGA-CBA	-2.06	116.47	123.08
26	P	305	PEK	O03-C21-O04	-2.06	116.69	123.14
14	N	602	HEA	CMD-C2D-C1D	2.06	128.17	125.04
18	C	306	PGV	O01-C1-O02	-2.06	118.73	123.70
26	P	304	PEK	O03-C21-O04	-2.05	118.41	123.59
14	A	602	HEA	CBA-CAA-C2A	-2.05	106.94	112.63
14	A	601[A]	HEA	C26-C15-C16	2.05	118.72	115.27
25	P	309	CHD	C1-C10-C9	2.05	114.57	111.35
18	A	608	PGV	C03-C02-C01	-2.04	106.96	111.79
18	C	306	PGV	O12-P-O13	-2.04	101.11	109.07
18	A	606	PGV	O02-C1-C2	-2.03	113.55	126.89
14	A	601[A]	HEA	C17-C16-C15	-2.03	106.29	112.98
25	P	309	CHD	C4-C3-C2	-2.03	108.13	110.55
27	C	308	CDL	OB6-CB5-OB7	-2.03	118.80	123.70
21	C	310	DMU	O5-C4-C3	2.02	113.37	109.69
22	D	201	TGL	CB4-CB3-CB2	-2.02	105.92	113.19
25	B	304	CHD	C4-C5-C10	-2.02	110.51	112.66
14	N	601[A]	HEA	C21-C22-C23	-2.01	120.89	127.75
25	B	304	CHD	C16-C17-C13	2.01	105.52	103.55

There are no chirality outliers.

All (620) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602	HEA	C4D-C3D-CAD-CBD
18	A	606	PGV	C1-C2-C3-C4
20	A	615	EDO	O1-C1-C2-O2
21	L	104	DMU	O5-C6-O16-C18
21	L	104	DMU	C19-C18-O16-C6
22	D	201	TGL	CB2-CB1-OG2-CG2
22	D	201	TGL	OB1-CB1-OG2-CG2
22	N	608	TGL	CC2-CC1-OG3-CG3
24	B	303	PSC	O02-C1-O01-C02
24	B	303	PSC	C2-C1-O01-C02
26	C	303	PEK	C3-C4-C5-C6
26	C	303	PEK	C9-C10-C11-C12
26	C	305	PEK	C22-C21-O03-C01
26	C	305	PEK	C6-C7-C8-C9
26	P	303	PEK	C6-C7-C8-C9
27	T	101	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	T	101	CDL	OB6-CB4-CB6-OB8
22	N	608	TGL	OC1-CC1-OG3-CG3
26	C	305	PEK	O04-C21-O03-C01
22	D	201	TGL	CG2-CG1-OG1-CA1
27	C	308	CDL	OB9-CB7-OB8-CB6
25	L	102	CHD	C13-C17-C20-C21
27	C	308	CDL	C71-CB7-OB8-CB6
25	P	309	CHD	C20-C22-C23-C24
22	B	301	TGL	CC2-CC1-OG3-CG3
24	B	303	PSC	C11-C10-C9-C8
26	C	304	PEK	C10-C11-C12-C13
26	C	305	PEK	C13-C14-C15-C16
26	P	305	PEK	C10-C11-C12-C13
22	B	301	TGL	OC1-CC1-OG3-CG3
27	C	308	CDL	C51-CB5-OB6-CB4
27	P	308	CDL	C51-CB5-OB6-CB4
22	L	101	TGL	CC2-CC1-OG3-CG3
22	N	607	TGL	CB7-CB8-CB9-C10
25	P	309	CHD	C17-C20-C22-C23
27	T	101	CDL	C17-C18-C19-C20
27	G	101	CDL	C17-C18-C19-C20
18	P	307	PGV	O04-C19-O03-C01
18	C	307	PGV	C20-C19-O03-C01
18	P	307	PGV	C20-C19-O03-C01
25	C	309	CHD	C17-C20-C22-C23
14	A	602	HEA	C2D-C3D-CAD-CBD
24	O	302	PSC	C22-C23-C24-C25
25	P	309	CHD	C21-C20-C22-C23
21	L	104	DMU	C1-C6-O16-C18
22	N	606	TGL	CB9-C10-C11-C12
27	C	308	CDL	OB7-CB5-OB6-CB4
26	P	305	PEK	C21-C22-C23-C24
18	C	307	PGV	O04-C19-O03-C01
22	L	101	TGL	CA2-CA1-OG1-CG1
27	G	101	CDL	C71-CB7-OB8-CB6
27	P	308	CDL	CB5-C51-C52-C53
25	L	102	CHD	C16-C17-C20-C22
22	N	606	TGL	CB1-CB2-CB3-CB4
27	G	101	CDL	CB7-C71-C72-C73
22	D	201	TGL	CC2-CC1-OG3-CG3
21	P	310	DMU	O16-C18-C19-C22
22	N	607	TGL	CA9-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	N	608	TGL	CB9-C10-C11-C12
25	C	309	CHD	C21-C20-C22-C23
21	L	104	DMU	O16-C18-C19-C22
20	P	316	EDO	O1-C1-C2-O2
27	G	101	CDL	OB9-CB7-OB8-CB6
22	L	101	TGL	OC1-CC1-OG3-CG3
18	P	306	PGV	C12-C13-C14-C15
24	O	302	PSC	C11-C10-C9-C8
22	B	301	TGL	CB1-CB2-CB3-CB4
27	P	308	CDL	OB7-CB5-OB6-CB4
18	P	307	PGV	C22-C23-C24-C25
21	C	310	DMU	O16-C18-C19-C22
24	B	303	PSC	C20-C21-C22-C23
22	B	301	TGL	C17-C18-C19-C33
18	C	306	PGV	C7-C8-C9-C10
18	P	306	PGV	C7-C8-C9-C10
22	D	201	TGL	CA7-CA8-CA9-C20
22	D	201	TGL	C16-C15-CC9-CC8
22	L	101	TGL	C21-C20-CA9-CA8
22	N	606	TGL	C24-C25-C26-C27
27	C	308	CDL	C11-C12-C13-C14
18	N	610	PGV	C29-C30-C31-C32
18	P	306	PGV	C13-C14-C15-C16
21	N	622	DMU	C25-C28-C31-C34
22	N	607	TGL	C17-C18-C19-C33
22	N	608	TGL	C11-C10-CB9-CB8
27	T	101	CDL	C61-C62-C63-C64
22	N	606	TGL	CB4-CB5-CB6-CB7
22	N	606	TGL	C10-C11-C12-C13
26	P	305	PEK	C13-C14-C15-C16
22	B	301	TGL	C13-C14-C29-C30
22	N	608	TGL	CC4-CC5-CC6-CC7
18	A	606	PGV	C7-C8-C9-C10
22	L	101	TGL	C11-C10-CB9-CB8
22	B	301	TGL	CA1-CA2-CA3-CA4
22	N	608	TGL	CC1-CC2-CC3-CC4
22	N	606	TGL	C14-C29-C30-C31
27	T	101	CDL	C79-C80-C81-C82
22	B	301	TGL	CA6-CA7-CA8-CA9
22	D	201	TGL	C19-C33-C34-C35
22	L	101	TGL	CA3-CA4-CA5-CA6
27	P	308	CDL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	P	308	CDL	C58-C59-C60-C61
21	A	621	DMU	C28-C31-C34-C37
22	D	201	TGL	C14-C29-C30-C31
22	N	607	TGL	CB5-CB6-CB7-CB8
24	B	303	PSC	C22-C23-C24-C25
24	B	303	PSC	C23-C24-C25-C26
27	C	308	CDL	C19-C20-C21-C22
27	C	308	CDL	C21-C22-C23-C24
21	N	622	DMU	C22-C25-C28-C31
22	N	608	TGL	CA4-CA5-CA6-CA7
22	N	608	TGL	C20-C21-C22-C23
27	P	308	CDL	C57-C58-C59-C60
21	C	310	DMU	C31-C34-C37-C40
21	L	104	DMU	C28-C31-C34-C37
21	Q	202	DMU	C28-C31-C34-C37
21	X	101	DMU	C22-C25-C28-C31
22	B	301	TGL	CC7-CC8-CC9-C15
22	D	201	TGL	CA9-C20-C21-C22
26	C	304	PEK	C26-C27-C28-C29
27	C	308	CDL	C40-C41-C42-C43
27	P	308	CDL	C17-C18-C19-C20
27	P	308	CDL	C59-C60-C61-C62
27	T	101	CDL	C13-C14-C15-C16
21	O	305	DMU	C19-C22-C25-C28
22	N	607	TGL	CB9-C10-C11-C12
27	C	308	CDL	C34-C35-C36-C37
18	C	306	PGV	C22-C23-C24-C25
21	K	103	DMU	C25-C28-C31-C34
22	L	101	TGL	C24-C25-C26-C27
22	N	606	TGL	CB7-CB8-CB9-C10
22	N	608	TGL	CA7-CA8-CA9-C20
27	T	101	CDL	C78-C79-C80-C81
22	D	201	TGL	OC1-CC1-OG3-CG3
26	P	305	PEK	C2-C3-C4-C5
22	L	101	TGL	CB5-CB6-CB7-CB8
22	L	101	TGL	C11-C12-C13-C14
22	N	607	TGL	C18-C19-C33-C34
26	P	304	PEK	C22-C23-C24-C25
27	P	308	CDL	C19-C20-C21-C22
27	P	308	CDL	C42-C43-C44-C45
27	P	308	CDL	C51-C52-C53-C54
26	C	303	PEK	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	B	301	TGL	C21-C22-C23-C24
22	D	201	TGL	CA1-CA2-CA3-CA4
22	B	301	TGL	C10-C11-C12-C13
21	M	101	DMU	O6-C11-C9-C8
25	L	102	CHD	C16-C17-C20-C21
18	C	306	PGV	C28-C29-C30-C31
22	N	606	TGL	CB3-CB4-CB5-CB6
26	C	305	PEK	C30-C31-C32-C33
22	D	201	TGL	CC9-C15-C16-C17
24	O	302	PSC	C5-C6-C7-C8
21	A	621	DMU	C31-C34-C37-C40
27	P	308	CDL	C37-C38-C39-C40
22	N	606	TGL	OB1-CB1-OG2-CG2
22	N	607	TGL	C11-C12-C13-C14
27	P	308	CDL	C60-C61-C62-C63
22	L	101	TGL	OA1-CA1-OG1-CG1
20	A	619	EDO	O1-C1-C2-O2
20	N	621	EDO	O1-C1-C2-O2
20	P	317	EDO	O1-C1-C2-O2
21	Z	101	DMU	C25-C28-C31-C34
26	C	304	PEK	C28-C29-C30-C31
22	N	608	TGL	CA5-CA6-CA7-CA8
27	T	101	CDL	C71-CB7-OB8-CB6
18	P	307	PGV	C2-C3-C4-C5
22	N	607	TGL	C21-C20-CA9-CA8
21	Z	101	DMU	C28-C31-C34-C37
22	D	201	TGL	CB4-CB5-CB6-CB7
22	N	606	TGL	C17-C18-C19-C33
18	P	307	PGV	C13-C14-C15-C16
27	C	308	CDL	C55-C56-C57-C58
18	A	608	PGV	C29-C30-C31-C32
22	N	606	TGL	C20-C21-C22-C23
27	G	101	CDL	C72-C73-C74-C75
27	T	101	CDL	OB9-CB7-OB8-CB6
18	Q	201	PGV	C7-C8-C9-C10
22	N	608	TGL	CB5-CB6-CB7-CB8
22	N	606	TGL	CB2-CB1-OG2-CG2
27	T	101	CDL	C51-CB5-OB6-CB4
18	C	307	PGV	C27-C28-C29-C30
22	B	301	TGL	CB4-CB5-CB6-CB7
22	D	201	TGL	C24-C25-C26-C27
27	T	101	CDL	OB7-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	P	306	PGV	C24-C25-C26-C27
22	D	201	TGL	C11-C12-C13-C14
27	T	101	CDL	C20-C21-C22-C23
22	L	101	TGL	C21-C22-C23-C24
27	C	308	CDL	C41-C42-C43-C44
21	J	103	DMU	C18-C19-C22-C25
22	N	606	TGL	CA2-CA3-CA4-CA5
26	P	304	PEK	C7-C8-C9-C10
22	N	606	TGL	C13-C14-C29-C30
26	C	304	PEK	C23-C24-C25-C26
22	B	301	TGL	CB5-CB6-CB7-CB8
22	B	301	TGL	C16-C17-C18-C19
22	N	608	TGL	CC3-CC4-CC5-CC6
27	T	101	CDL	C12-C13-C14-C15
27	T	101	CDL	C19-C20-C21-C22
22	L	101	TGL	C20-C21-C22-C23
24	B	303	PSC	C19-C20-C21-C22
22	B	301	TGL	C12-C13-C14-C29
22	N	606	TGL	CA4-CA5-CA6-CA7
27	G	101	CDL	C60-C61-C62-C63
18	P	306	PGV	C20-C21-C22-C23
27	G	101	CDL	C43-C44-C45-C46
18	A	606	PGV	C11-C10-C9-C8
18	Q	201	PGV	C30-C31-C32-C33
22	D	201	TGL	CC5-CC6-CC7-CC8
22	N	606	TGL	CB6-CB7-CB8-CB9
22	B	301	TGL	C18-C19-C33-C34
22	D	201	TGL	CA3-CA4-CA5-CA6
22	L	101	TGL	C12-C13-C14-C29
18	C	306	PGV	C24-C25-C26-C27
21	K	103	DMU	C28-C31-C34-C37
22	D	201	TGL	CG1-CG2-CG3-OG3
27	P	308	CDL	C13-C14-C15-C16
26	P	305	PEK	C7-C8-C9-C10
24	B	303	PSC	C21-C22-C23-C24
27	C	308	CDL	C78-C79-C80-C81
27	P	308	CDL	C12-C13-C14-C15
27	P	308	CDL	C54-C55-C56-C57
14	N	602	HEA	C4D-C3D-CAD-CBD
22	B	301	TGL	CA7-CA8-CA9-C20
22	N	606	TGL	CA7-CA8-CA9-C20
18	A	606	PGV	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	O	305	DMU	C22-C25-C28-C31
27	C	308	CDL	C64-C65-C66-C67
18	C	307	PGV	C31-C32-C33-C34
22	N	608	TGL	C13-C14-C29-C30
22	D	201	TGL	CB1-CB2-CB3-CB4
21	Z	101	DMU	C22-C25-C28-C31
22	D	201	TGL	C20-C21-C22-C23
21	Q	202	DMU	C18-C19-C22-C25
18	C	306	PGV	C19-C20-C21-C22
21	C	310	DMU	C18-C19-C22-C25
21	Z	101	DMU	C34-C37-C40-C43
26	C	305	PEK	C4-C5-C6-C7
26	P	304	PEK	C4-C5-C6-C7
22	N	608	TGL	CC6-CC7-CC8-CC9
24	O	302	PSC	C25-C26-C27-C28
20	Q	204	EDO	O1-C1-C2-O2
22	B	301	TGL	C29-C30-C31-C32
22	B	301	TGL	OG1-CG1-CG2-OG2
21	D	206	DMU	C34-C37-C40-C43
22	N	606	TGL	CC6-CC7-CC8-CC9
21	O	305	DMU	C18-C19-C22-C25
18	A	608	PGV	C26-C27-C28-C29
18	P	307	PGV	C14-C15-C16-C17
22	N	606	TGL	CC5-CC6-CC7-CC8
26	P	305	PEK	C33-C34-C35-C36
22	B	301	TGL	C24-C25-C26-C27
21	X	101	DMU	C19-C22-C25-C28
27	T	101	CDL	C64-C65-C66-C67
26	P	303	PEK	C25-C26-C27-C28
21	O	305	DMU	C31-C34-C37-C40
18	C	306	PGV	C10-C11-C12-C13
18	P	306	PGV	C10-C11-C12-C13
26	P	304	PEK	C13-C14-C15-C16
22	B	301	TGL	C15-C16-C17-C18
22	L	101	TGL	CA5-CA6-CA7-CA8
24	B	303	PSC	C24-C25-C26-C27
21	C	320	DMU	C31-C34-C37-C40
18	C	306	PGV	C1-C2-C3-C4
22	D	201	TGL	CC1-CC2-CC3-CC4
22	N	607	TGL	C22-C23-C24-C25
27	P	308	CDL	CB7-C71-C72-C73
27	C	308	CDL	C51-C52-C53-C54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	G	101	CDL	C19-C20-C21-C22
22	N	607	TGL	C16-C17-C18-C19
27	C	308	CDL	C18-C19-C20-C21
26	P	305	PEK	C29-C30-C31-C32
27	C	308	CDL	C36-C37-C38-C39
27	T	101	CDL	C53-C54-C55-C56
27	C	308	CDL	C58-C59-C60-C61
27	P	308	CDL	C53-C54-C55-C56
27	T	101	CDL	C80-C81-C82-C83
18	P	307	PGV	C7-C8-C9-C10
21	P	310	DMU	C34-C37-C40-C43
22	N	608	TGL	C21-C22-C23-C24
21	W	103	DMU	O16-C18-C19-C22
22	N	606	TGL	C19-C33-C34-C35
22	D	201	TGL	OG1-CG1-CG2-CG3
27	T	101	CDL	C11-C12-C13-C14
27	T	101	CDL	C84-C85-C86-C87
21	C	320	DMU	O16-C18-C19-C22
21	M	101	DMU	C25-C28-C31-C34
21	P	318	DMU	C34-C37-C40-C43
21	X	102	DMU	C28-C31-C34-C37
21	P	310	DMU	C18-C19-C22-C25
22	N	608	TGL	CC2-CC3-CC4-CC5
24	O	302	PSC	C20-C21-C22-C23
22	N	607	TGL	CA3-CA4-CA5-CA6
26	C	305	PEK	C26-C27-C28-C29
22	N	607	TGL	C24-C25-C26-C27
14	A	601[A]	HEA	C2A-C3A-CMA-OMA
14	N	601[A]	HEA	C2A-C3A-CMA-OMA
24	B	303	PSC	C9-C10-C11-C12
26	C	303	PEK	C5-C6-C7-C8
26	C	303	PEK	C6-C7-C8-C9
26	C	303	PEK	C11-C10-C9-C8
26	C	303	PEK	C11-C12-C13-C14
26	C	303	PEK	C12-C13-C14-C15
26	C	304	PEK	C11-C10-C9-C8
26	C	304	PEK	C11-C12-C13-C14
26	C	305	PEK	C5-C6-C7-C8
26	C	305	PEK	C9-C10-C11-C12
26	C	305	PEK	C11-C12-C13-C14
26	C	305	PEK	C12-C13-C14-C15
26	P	303	PEK	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	303	PEK	C11-C10-C9-C8
26	P	303	PEK	C9-C10-C11-C12
26	P	303	PEK	C11-C12-C13-C14
26	P	303	PEK	C12-C13-C14-C15
26	P	304	PEK	C9-C10-C11-C12
26	P	304	PEK	C11-C12-C13-C14
26	P	305	PEK	C9-C10-C11-C12
26	P	305	PEK	C11-C12-C13-C14
26	P	305	PEK	C12-C13-C14-C15
21	Z	101	DMU	O16-C18-C19-C22
27	P	308	CDL	C43-C44-C45-C46
21	C	310	DMU	C34-C37-C40-C43
22	N	606	TGL	C23-C24-C25-C26
22	L	101	TGL	C10-C11-C12-C13
18	Q	201	PGV	C2-C1-O01-C02
22	N	606	TGL	CC2-CC1-OG3-CG3
22	L	101	TGL	CB3-CB4-CB5-CB6
27	C	308	CDL	C35-C36-C37-C38
22	B	301	TGL	OB1-CB1-OG2-CG2
21	O	305	DMU	C34-C37-C40-C43
18	Q	201	PGV	C29-C30-C31-C32
22	N	606	TGL	C11-C10-CB9-CB8
20	A	609	EDO	O1-C1-C2-O2
20	A	611	EDO	O1-C1-C2-O2
20	A	612	EDO	O1-C1-C2-O2
20	J	102	EDO	O1-C1-C2-O2
20	N	620	EDO	O1-C1-C2-O2
20	W	102	EDO	O1-C1-C2-O2
21	M	101	DMU	O16-C18-C19-C22
27	T	101	CDL	C74-C75-C76-C77
27	C	308	CDL	C56-C57-C58-C59
27	T	101	CDL	C57-C58-C59-C60
18	P	307	PGV	C27-C28-C29-C30
22	D	201	TGL	C22-C23-C24-C25
18	A	606	PGV	C15-C16-C17-C18
22	B	301	TGL	CA9-C20-C21-C22
22	N	608	TGL	C21-C20-CA9-CA8
27	G	101	CDL	C22-C23-C24-C25
21	K	102	DMU	C28-C31-C34-C37
21	C	310	DMU	C28-C31-C34-C37
27	P	308	CDL	C76-C77-C78-C79
27	P	308	CDL	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	B	301	TGL	C21-C20-CA9-CA8
27	G	101	CDL	C81-C82-C83-C84
26	P	305	PEK	C26-C27-C28-C29
22	D	201	TGL	CB3-CB4-CB5-CB6
22	L	101	TGL	CC2-CC3-CC4-CC5
26	P	305	PEK	C32-C33-C34-C35
18	Q	201	PGV	O02-C1-O01-C02
27	T	101	CDL	C18-C19-C20-C21
21	D	206	DMU	C22-C25-C28-C31
22	D	201	TGL	OG2-CG2-CG3-OG3
21	K	102	DMU	C19-C22-C25-C28
27	C	308	CDL	C82-C83-C84-C85
21	Z	101	DMU	O6-C11-C9-C8
21	M	101	DMU	C28-C31-C34-C37
27	C	308	CDL	C61-C62-C63-C64
22	N	608	TGL	CB3-CB4-CB5-CB6
21	K	104	DMU	C28-C31-C34-C37
21	M	101	DMU	C22-C25-C28-C31
27	G	101	CDL	C34-C35-C36-C37
25	C	309	CHD	C20-C22-C23-C24
22	L	101	TGL	C33-C34-C35-C36
21	Q	202	DMU	C31-C34-C37-C40
27	C	308	CDL	C24-C25-C26-C27
27	P	308	CDL	C38-C39-C40-C41
21	W	103	DMU	C18-C19-C22-C25
24	O	302	PSC	C24-C25-C26-C27
18	C	306	PGV	C02-C03-O11-P
18	P	306	PGV	C02-C03-O11-P
21	W	103	DMU	C34-C37-C40-C43
22	B	301	TGL	C22-C23-C24-C25
25	L	102	CHD	C13-C17-C20-C22
22	N	606	TGL	OC1-CC1-OG3-CG3
14	A	601[A]	HEA	C16-C17-C18-C19
18	A	606	PGV	C4-C5-C6-C7
18	A	608	PGV	C11-C10-C9-C8
22	N	607	TGL	C11-C10-CB9-CB8
27	C	308	CDL	C54-C55-C56-C57
24	O	302	PSC	C29-C30-C31-C32
22	D	201	TGL	C16-C17-C18-C19
27	P	308	CDL	C40-C41-C42-C43
26	C	304	PEK	O03-C21-C22-C23
24	B	303	PSC	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	304	PEK	C26-C27-C28-C29
14	N	602	HEA	C2D-C3D-CAD-CBD
21	A	620	DMU	C22-C25-C28-C31
22	N	608	TGL	CC9-C15-C16-C17
14	A	601[A]	HEA	C4A-C3A-CMA-OMA
22	B	301	TGL	OG1-CG1-CG2-CG3
22	N	606	TGL	CG1-CG2-CG3-OG3
22	D	201	TGL	OG1-CG1-CG2-OG2
22	N	606	TGL	OG2-CG2-CG3-OG3
21	N	622	DMU	C31-C34-C37-C40
27	C	308	CDL	C59-C60-C61-C62
22	N	606	TGL	C21-C20-CA9-CA8
26	C	305	PEK	C35-C36-C37-C38
22	D	201	TGL	CB9-C10-C11-C12
22	N	606	TGL	CA3-CA4-CA5-CA6
27	T	101	CDL	C71-C72-C73-C74
26	C	304	PEK	C13-C14-C15-C16
22	D	201	TGL	CC7-CC8-CC9-C15
18	P	307	PGV	C28-C29-C30-C31
27	P	308	CDL	C62-C63-C64-C65
18	C	306	PGV	C27-C28-C29-C30
22	N	607	TGL	C33-C34-C35-C36
21	K	101	DMU	C34-C37-C40-C43
22	N	608	TGL	C29-C30-C31-C32
22	D	201	TGL	C18-C19-C33-C34
18	Q	201	PGV	C2-C3-C4-C5
21	A	620	DMU	C25-C28-C31-C34
14	A	601[A]	HEA	C27-C19-C20-C21
27	G	101	CDL	C21-C22-C23-C24
20	F	107	EDO	O1-C1-C2-O2
20	N	614	EDO	O1-C1-C2-O2
20	P	313	EDO	O1-C1-C2-O2
22	D	201	TGL	C23-C24-C25-C26
18	N	610	PGV	C11-C12-C13-C14
27	C	308	CDL	C17-C18-C19-C20
27	G	101	CDL	C59-C60-C61-C62
18	C	307	PGV	C14-C15-C16-C17
27	G	101	CDL	C61-C62-C63-C64
18	C	306	PGV	C20-C21-C22-C23
22	N	606	TGL	CA9-C20-C21-C22
21	K	102	DMU	C31-C34-C37-C40
27	P	308	CDL	C41-C42-C43-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	304	PEK	C14-C15-C16-C17
22	B	301	TGL	CC4-CC5-CC6-CC7
21	K	104	DMU	C19-C22-C25-C28
22	N	608	TGL	C15-C16-C17-C18
18	P	306	PGV	C31-C32-C33-C34
22	L	101	TGL	CB7-CB8-CB9-C10
24	O	302	PSC	C12-C13-C14-C15
26	C	305	PEK	C3-C4-C5-C6
14	N	601[A]	HEA	C16-C17-C18-C19
18	P	306	PGV	C1-C2-C3-C4
22	N	606	TGL	CA6-CA7-CA8-CA9
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
22	N	606	TGL	C15-C16-C17-C18
27	G	101	CDL	C80-C81-C82-C83
14	N	602	HEA	CAA-CBA-CGA-O1A
21	D	206	DMU	C28-C31-C34-C37
26	C	304	PEK	C16-C17-C18-C19
21	N	622	DMU	C28-C31-C34-C37
27	P	308	CDL	C23-C24-C25-C26
14	A	602	HEA	CAA-CBA-CGA-O1A
25	L	102	CHD	C20-C22-C23-C24
22	D	201	TGL	C29-C30-C31-C32
22	L	101	TGL	CA6-CA7-CA8-CA9
21	P	318	DMU	C22-C25-C28-C31
22	N	607	TGL	C12-C13-C14-C29
25	B	304	CHD	C22-C23-C24-O26
20	E	202	EDO	O1-C1-C2-O2
18	P	307	PGV	C3-C4-C5-C6
21	K	103	DMU	C31-C34-C37-C40
27	C	308	CDL	C71-C72-C73-C74
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
25	G	102	CHD	C22-C23-C24-O25
21	L	104	DMU	C18-C19-C22-C25
21	K	101	DMU	C28-C31-C34-C37
27	C	308	CDL	C62-C63-C64-C65
14	N	602	HEA	CAD-CBD-CGD-O1D
24	B	303	PSC	C10-C11-C12-C13
24	O	302	PSC	C9-C10-C11-C12
24	O	302	PSC	C10-C11-C12-C13
26	C	304	PEK	C6-C7-C8-C9
26	C	305	PEK	C11-C10-C9-C8
26	P	304	PEK	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	304	PEK	C6-C7-C8-C9
14	A	602	HEA	CAA-CBA-CGA-O2A
25	G	102	CHD	C22-C23-C24-O26
27	T	101	CDL	C52-C53-C54-C55
18	N	610	PGV	C31-C32-C33-C34
18	A	608	PGV	C10-C11-C12-C13
26	C	304	PEK	C4-C5-C6-C7
25	B	304	CHD	C22-C23-C24-O25
27	T	101	CDL	C60-C61-C62-C63
18	C	306	PGV	C9-C10-C11-C12
18	C	307	PGV	C9-C10-C11-C12
24	B	303	PSC	C7-C8-C9-C10
22	B	301	TGL	C11-C12-C13-C14
22	N	607	TGL	C25-C26-C27-C28
18	C	306	PGV	C23-C24-C25-C26
27	P	308	CDL	OB6-CB4-CB6-OB8
22	B	301	TGL	C19-C33-C34-C35
22	N	608	TGL	CC7-CC8-CC9-C15
22	L	101	TGL	CA1-CA2-CA3-CA4
27	C	308	CDL	C37-C38-C39-C40
26	P	303	PEK	C10-C11-C12-C13
14	N	602	HEA	CAA-CBA-CGA-O2A
25	C	309	CHD	C22-C23-C24-O26
18	A	606	PGV	C22-C23-C24-C25
14	N	601[A]	HEA	CAD-CBD-CGD-O1D
26	C	305	PEK	C14-C15-C16-C17
22	N	606	TGL	CC7-CC8-CC9-C15
20	A	613	EDO	O1-C1-C2-O2
20	A	616	EDO	O1-C1-C2-O2
20	B	309	EDO	O1-C1-C2-O2
20	C	318	EDO	O1-C1-C2-O2
20	P	311	EDO	O1-C1-C2-O2
20	Q	203	EDO	O1-C1-C2-O2
18	A	608	PGV	C31-C32-C33-C34
21	O	305	DMU	O16-C18-C19-C22
26	C	305	PEK	C31-C32-C33-C34
26	P	305	PEK	C28-C29-C30-C31
27	T	101	CDL	C22-C23-C24-C25
21	D	206	DMU	C18-C19-C22-C25
18	A	608	PGV	C11-C12-C13-C14
18	Q	201	PGV	C9-C10-C11-C12
14	N	602	HEA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	608	PGV	O03-C19-C20-C21
18	P	307	PGV	C4-C5-C6-C7
26	P	305	PEK	C3-C4-C5-C6
18	Q	201	PGV	C27-C28-C29-C30
18	N	610	PGV	O03-C19-C20-C21
26	P	305	PEK	C30-C31-C32-C33
18	P	307	PGV	O03-C01-C02-C03
27	C	308	CDL	C60-C61-C62-C63
22	B	301	TGL	CB2-CB1-OG2-CG2
14	A	602	HEA	CAD-CBD-CGD-O2D
25	P	309	CHD	C22-C23-C24-O26
24	O	302	PSC	C23-C24-C25-C26
22	D	201	TGL	OG1-CA1-CA2-CA3
27	T	101	CDL	C72-C71-CB7-OB8
24	B	303	PSC	C26-C27-C28-C29
26	C	303	PEK	C10-C11-C12-C13
22	B	301	TGL	CC9-C15-C16-C17
22	N	606	TGL	CC3-CC4-CC5-CC6
27	T	101	CDL	C75-C76-C77-C78
18	A	606	PGV	C9-C10-C11-C12
24	B	303	PSC	C12-C13-C14-C15
27	T	101	CDL	C55-C56-C57-C58
22	N	608	TGL	CA2-CA3-CA4-CA5
25	C	301	CHD	C22-C23-C24-O26
18	P	306	PGV	C9-C10-C11-C12
18	P	306	PGV	C11-C12-C13-C14
24	O	302	PSC	C7-C8-C9-C10
18	Q	201	PGV	C11-C10-C9-C8
14	A	601[A]	HEA	C12-C11-C3B-C2B
14	N	601[A]	HEA	C12-C11-C3B-C2B
25	C	309	CHD	C22-C23-C24-O25
22	N	608	TGL	CB4-CB5-CB6-CB7
26	C	304	PEK	C17-C18-C19-C20
21	W	103	DMU	C28-C31-C34-C37
22	B	301	TGL	CB9-C10-C11-C12
21	C	310	DMU	C3-C4-C57-O61
22	N	607	TGL	CA2-CA3-CA4-CA5
20	B	307	EDO	O1-C1-C2-O2
20	C	317	EDO	O1-C1-C2-O2
20	M	102	EDO	O1-C1-C2-O2
20	W	101	EDO	O1-C1-C2-O2
26	P	303	PEK	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	304	PEK	C14-C15-C16-C17
25	C	301	CHD	C22-C23-C24-O25
25	P	301	CHD	C22-C23-C24-O25
26	C	304	PEK	C15-C16-C17-C18
14	A	602	HEA	CAD-CBD-CGD-O1D
27	C	308	CDL	C16-C17-C18-C19
27	C	308	CDL	C44-C45-C46-C47
22	B	301	TGL	OG3-CC1-CC2-CC3
18	C	307	PGV	C24-C25-C26-C27
14	A	601[A]	HEA	C18-C19-C20-C21
26	C	305	PEK	C23-C24-C25-C26
27	P	308	CDL	C35-C36-C37-C38
14	N	601[A]	HEA	C2C-C3C-CAC-CBC
18	A	606	PGV	C31-C32-C33-C34
18	N	610	PGV	C26-C27-C28-C29
27	C	308	CDL	C15-C16-C17-C18
18	P	307	PGV	C5-C6-C7-C8
22	L	101	TGL	C25-C26-C27-C28
14	A	601[A]	HEA	C12-C13-C14-C15
21	D	207	DMU	C31-C34-C37-C40
22	L	101	TGL	C18-C19-C33-C34
22	N	608	TGL	C25-C26-C27-C28
26	P	303	PEK	C3-C4-C5-C6
14	N	601[A]	HEA	CAD-CBD-CGD-O2D
21	C	310	DMU	C22-C25-C28-C31
25	P	309	CHD	C22-C23-C24-O25
27	G	101	CDL	C31-C32-C33-C34
27	T	101	CDL	C72-C71-CB7-OB9
22	N	607	TGL	CB4-CB5-CB6-CB7
18	C	306	PGV	C11-C12-C13-C14
18	N	610	PGV	C10-C11-C12-C13
22	D	201	TGL	OA1-CA1-CA2-CA3
27	C	308	CDL	C83-C84-C85-C86
22	D	201	TGL	OB1-CB1-CB2-CB3
22	B	301	TGL	CA5-CA6-CA7-CA8
22	B	301	TGL	CC5-CC6-CC7-CC8
27	P	308	CDL	C18-C19-C20-C21
14	A	601[A]	HEA	CAA-CBA-CGA-O2A
27	G	101	CDL	C63-C64-C65-C66
20	C	314	EDO	O1-C1-C2-O2
20	C	316	EDO	O1-C1-C2-O2
20	T	103	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	K	103	DMU	C22-C25-C28-C31
14	N	601[A]	HEA	CAA-CBA-CGA-O2A
25	P	301	CHD	C22-C23-C24-O26
18	P	306	PGV	C29-C30-C31-C32
14	N	601[A]	HEA	C26-C15-C16-C17
14	A	601[A]	HEA	CAA-CBA-CGA-O1A
18	A	606	PGV	C14-C15-C16-C17
22	N	607	TGL	C21-C22-C23-C24
26	C	304	PEK	C7-C8-C9-C10
24	B	303	PSC	O03-C19-C20-C21
18	C	307	PGV	O03-C01-C02-C03
21	M	101	DMU	C19-C22-C25-C28
27	P	308	CDL	C82-C83-C84-C85
22	L	101	TGL	C22-C23-C24-C25
18	Q	201	PGV	O01-C1-C2-C3
22	L	101	TGL	OG1-CA1-CA2-CA3

There are no ring outliers.

55 monomers are involved in 199 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	T	101	CDL	19	0
22	D	201	TGL	14	0
20	C	314	EDO	1	0
27	C	308	CDL	12	0
20	A	615	EDO	1	0
21	C	320	DMU	1	0
24	O	302	PSC	4	0
18	A	608	PGV	5	0
18	P	306	PGV	1	0
21	K	104	DMU	1	0
20	P	311	EDO	1	0
14	A	602	HEA	4	0
27	G	101	CDL	8	0
18	A	606	PGV	3	0
14	A	601[A]	HEA	3	0
20	P	316	EDO	1	0
26	P	305	PEK	7	0
22	N	608	TGL	2	0
21	C	310	DMU	6	0
20	W	102	EDO	2	0
18	N	610	PGV	1	0

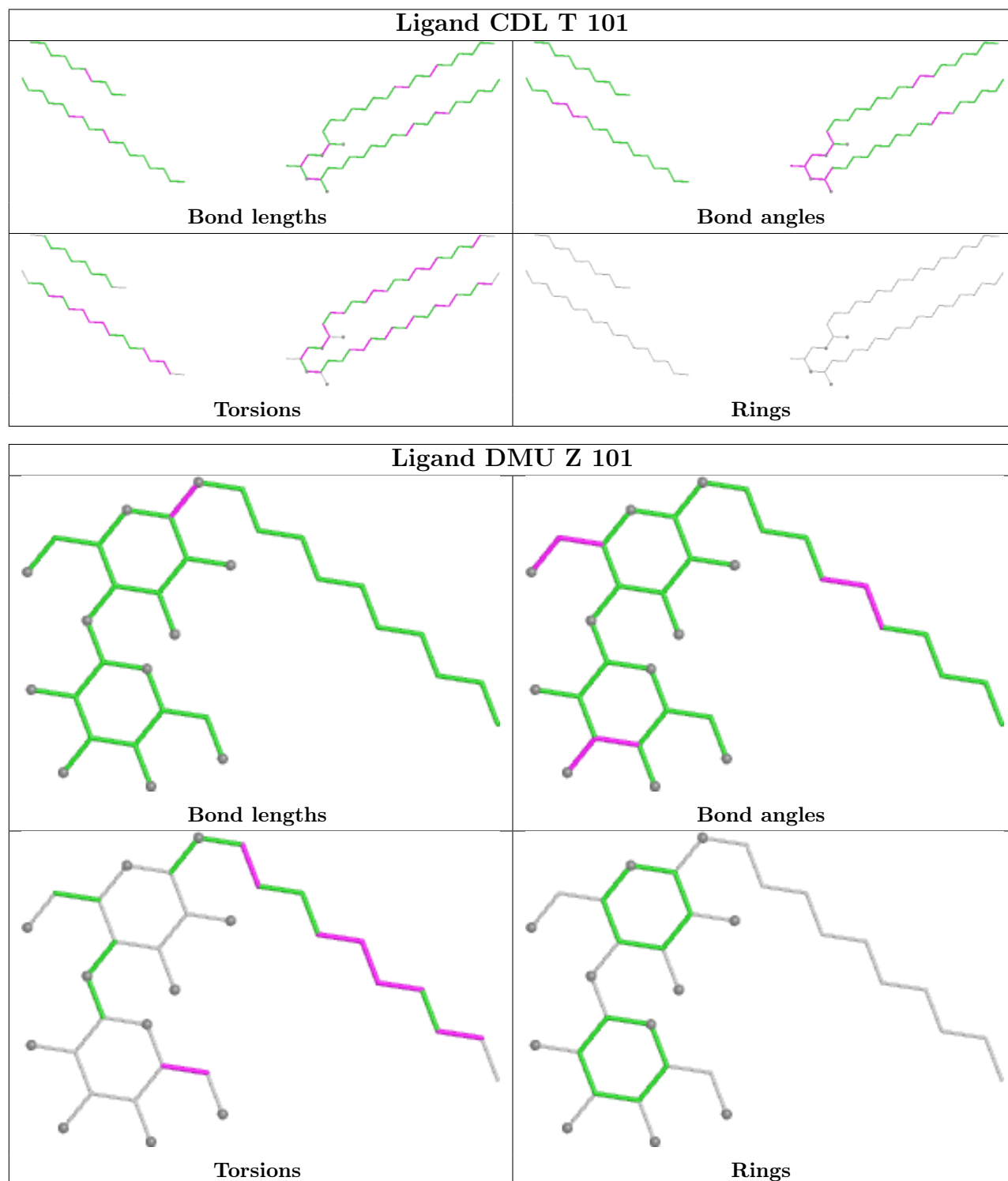
Continued on next page...

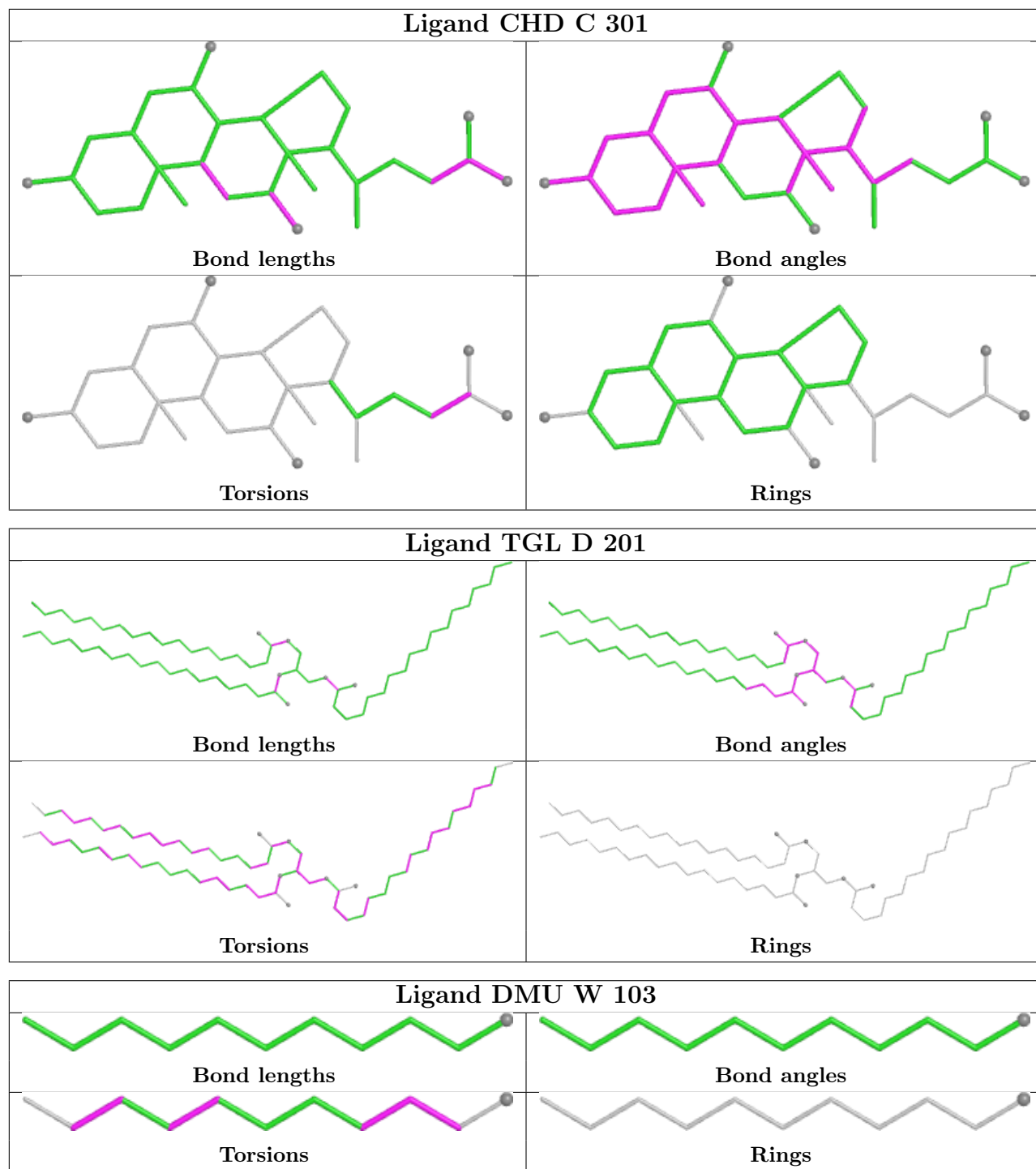
Continued from previous page...

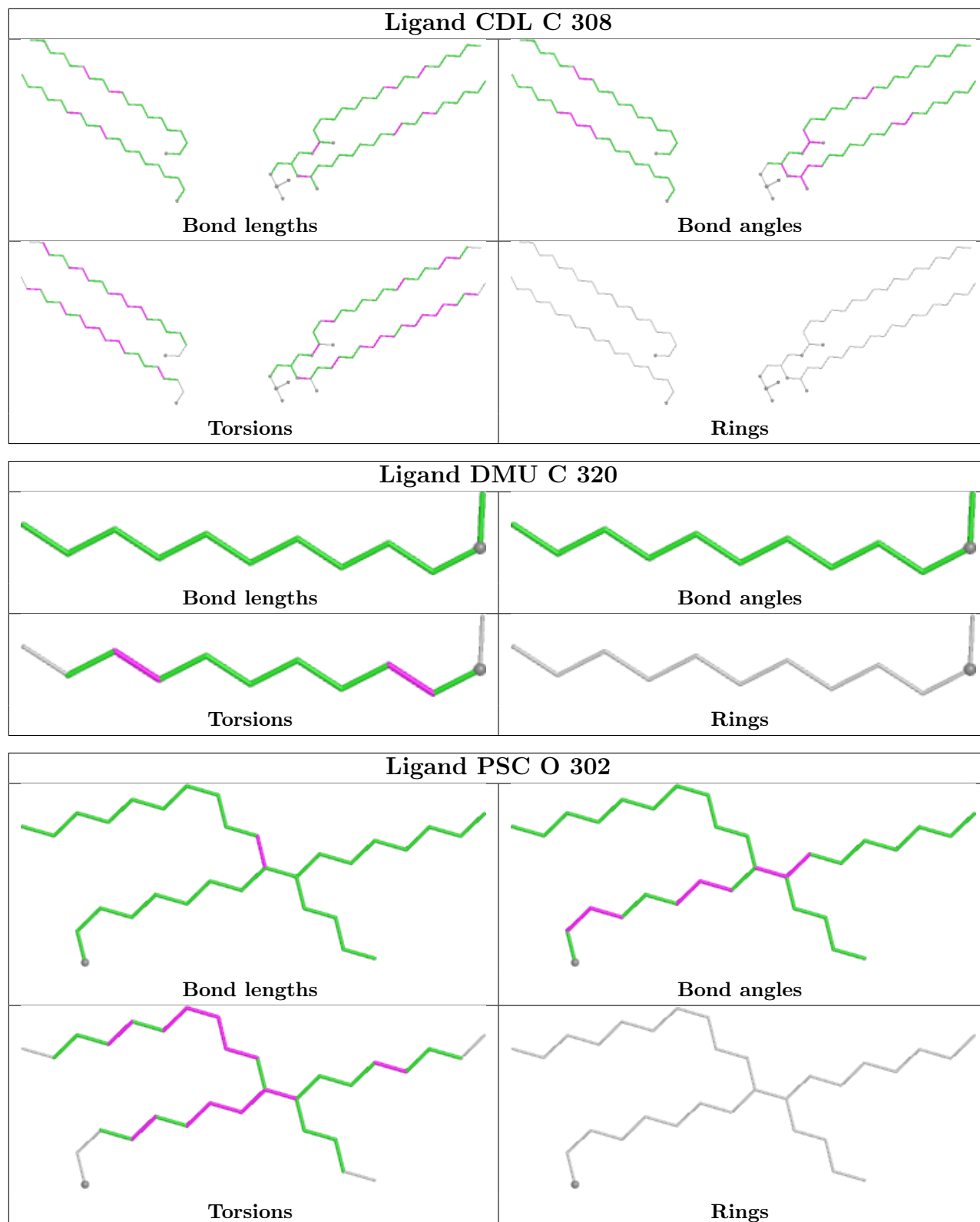
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	R	202	EDO	2	0
20	A	609	EDO	2	0
21	K	103	DMU	1	0
18	C	306	PGV	1	0
21	Q	202	DMU	1	0
18	C	307	PGV	1	0
14	N	602	HEA	4	0
14	N	601[A]	HEA	3	0
21	P	310	DMU	5	0
25	P	309	CHD	3	0
22	N	607	TGL	6	0
22	N	606	TGL	8	0
18	Q	201	PGV	6	0
20	Q	203	EDO	1	0
20	A	616	EDO	1	0
27	P	308	CDL	10	0
20	S	105	EDO	1	0
20	J	102	EDO	1	0
20	L	103	EDO	1	0
26	P	304	PEK	5	0
21	N	622	DMU	1	0
21	P	318	DMU	1	0
21	J	103	DMU	3	0
21	L	104	DMU	1	0
22	L	101	TGL	9	0
26	C	304	PEK	9	0
24	B	303	PSC	7	0
22	B	301	TGL	7	0
25	C	309	CHD	1	0
25	L	102	CHD	1	0
26	C	305	PEK	5	0
25	G	102	CHD	1	0
26	P	303	PEK	1	0
18	P	307	PGV	3	0

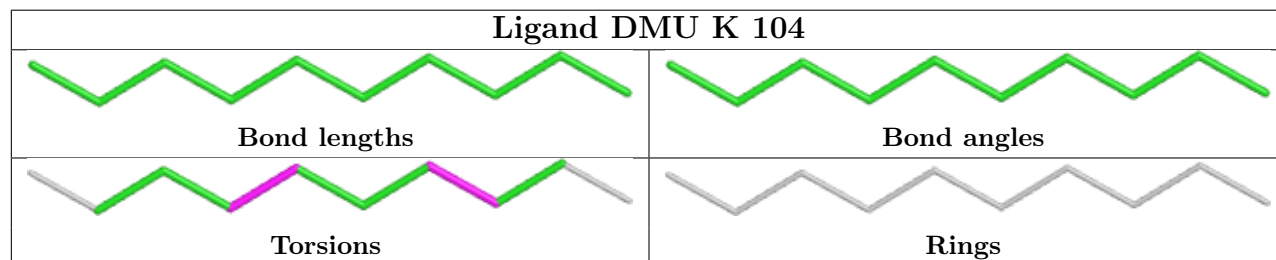
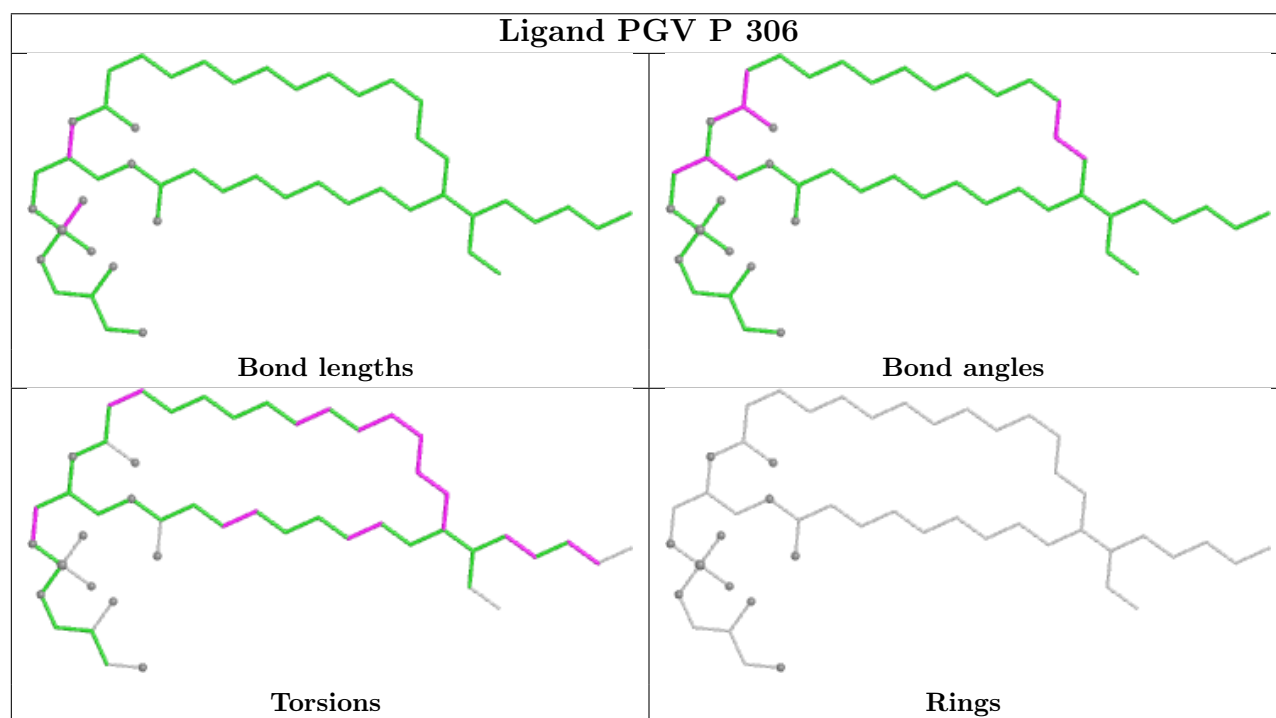
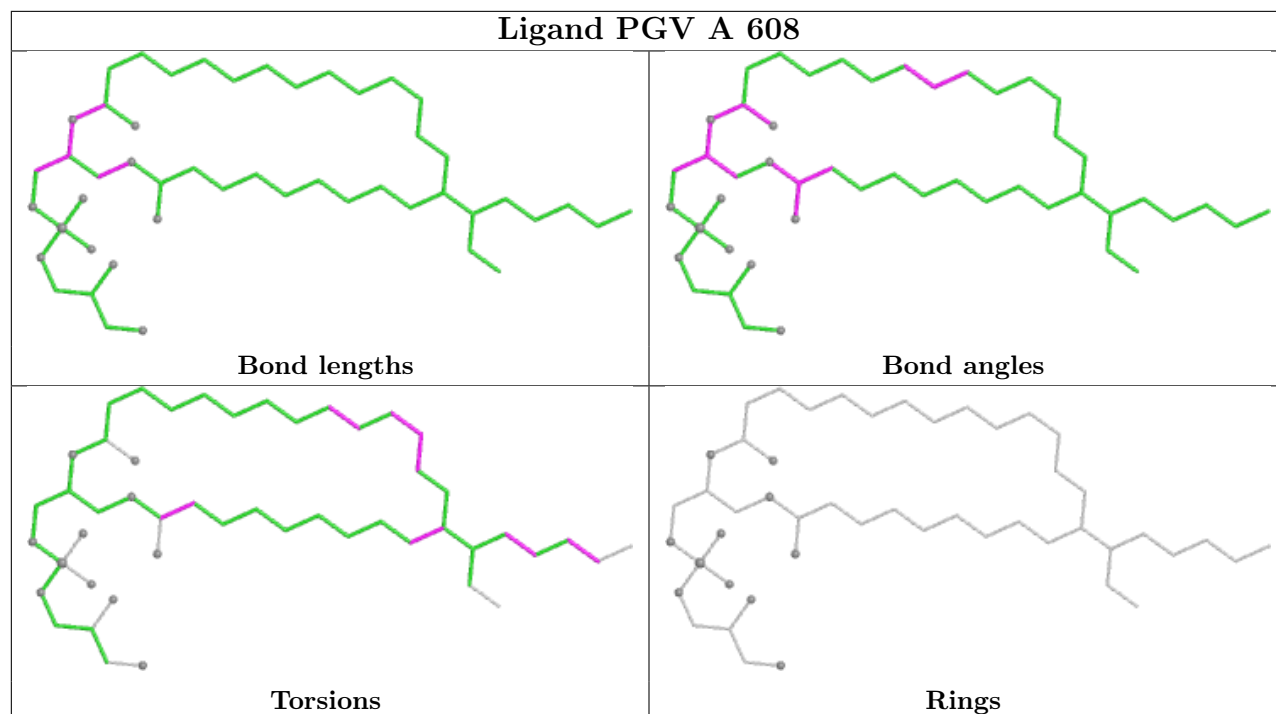
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

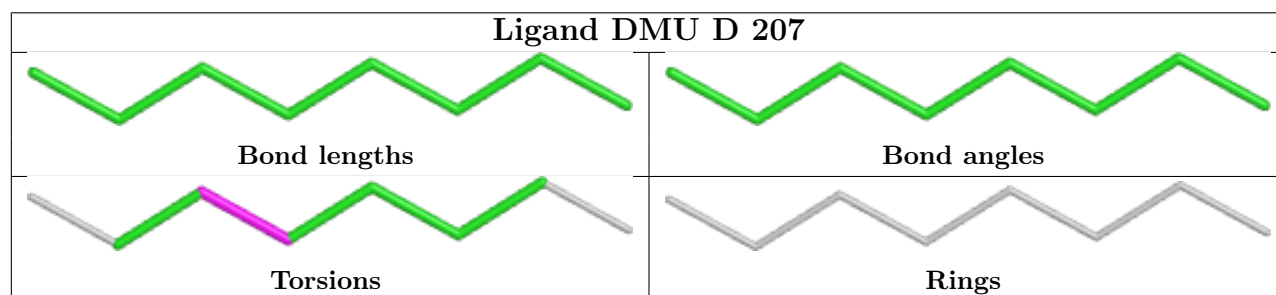
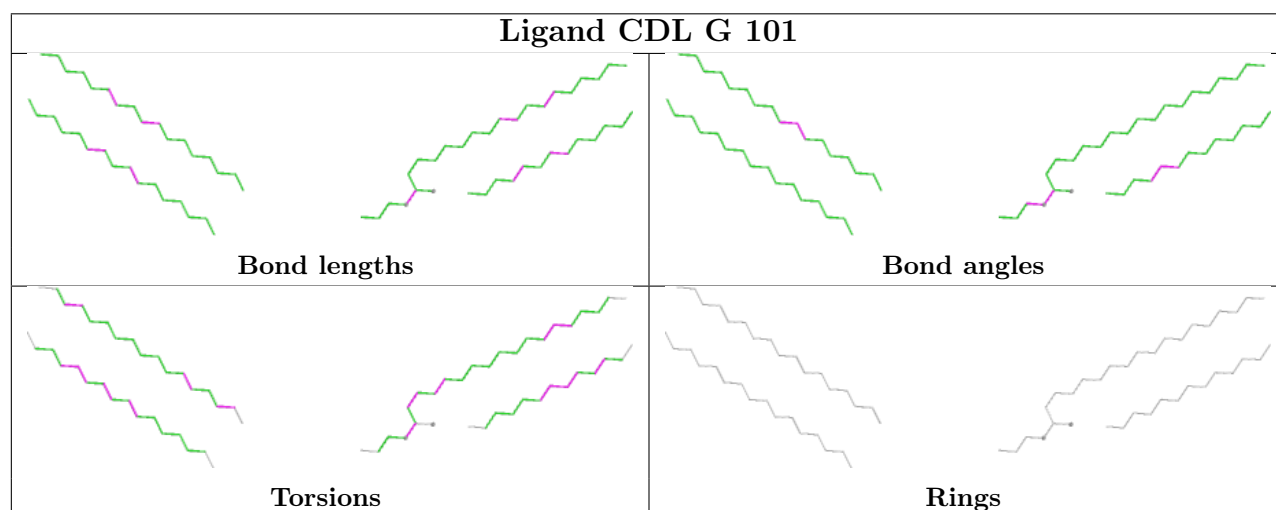
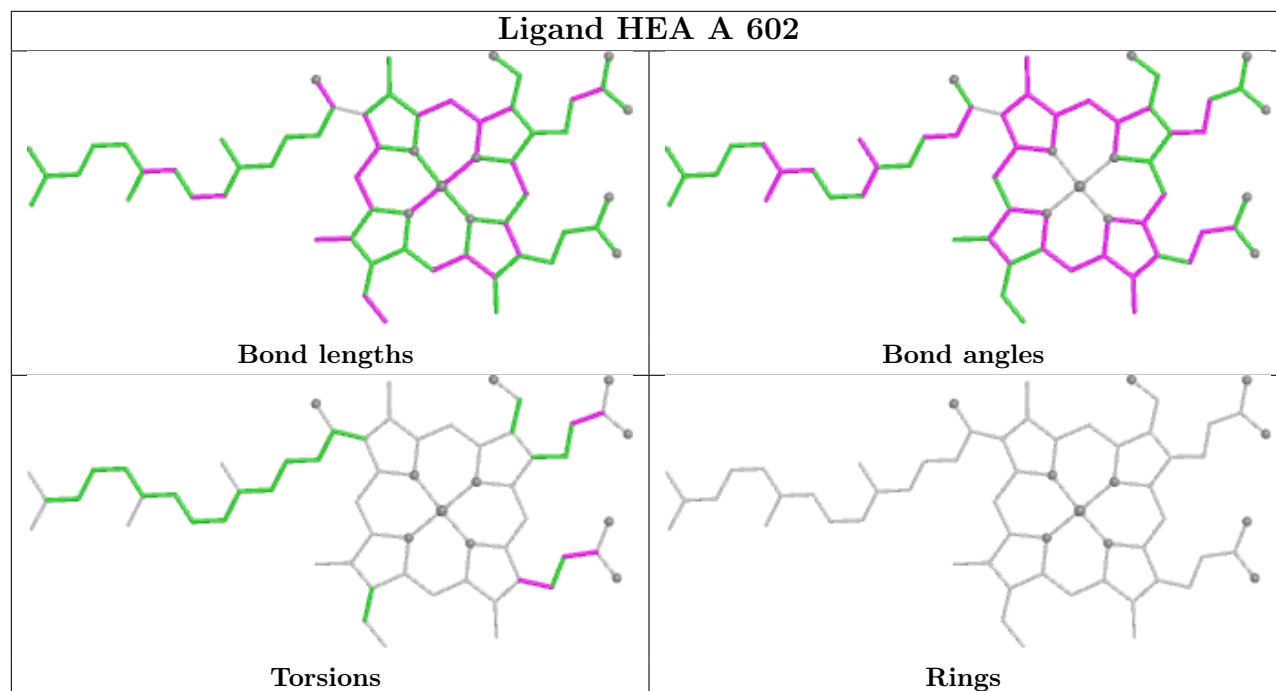
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

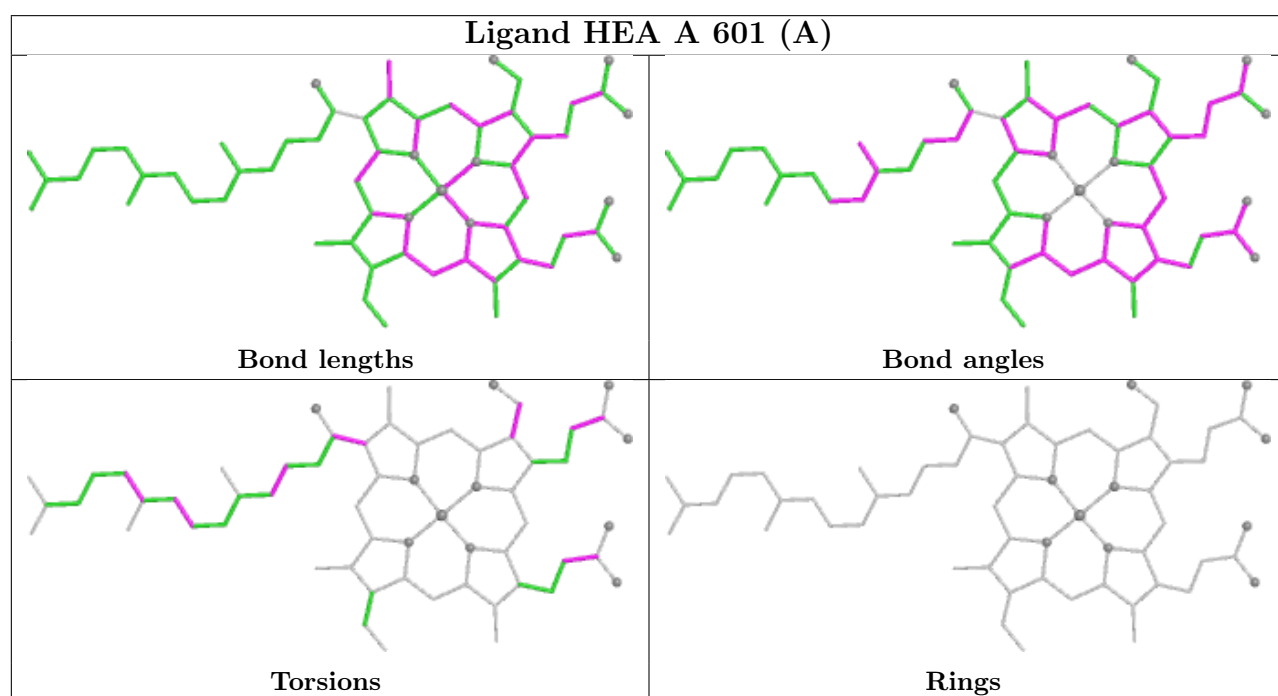
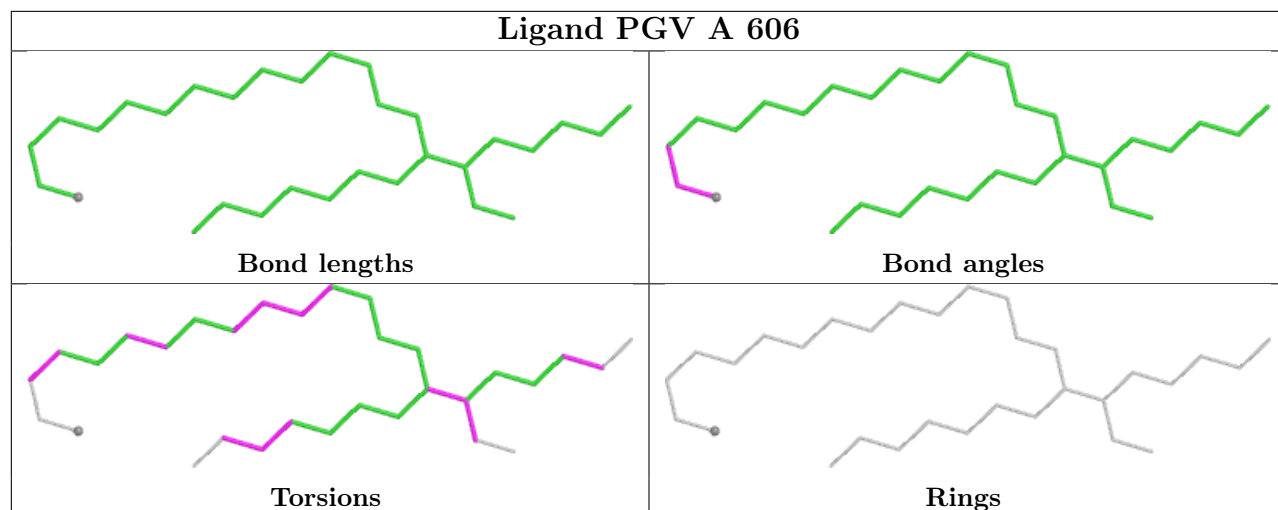


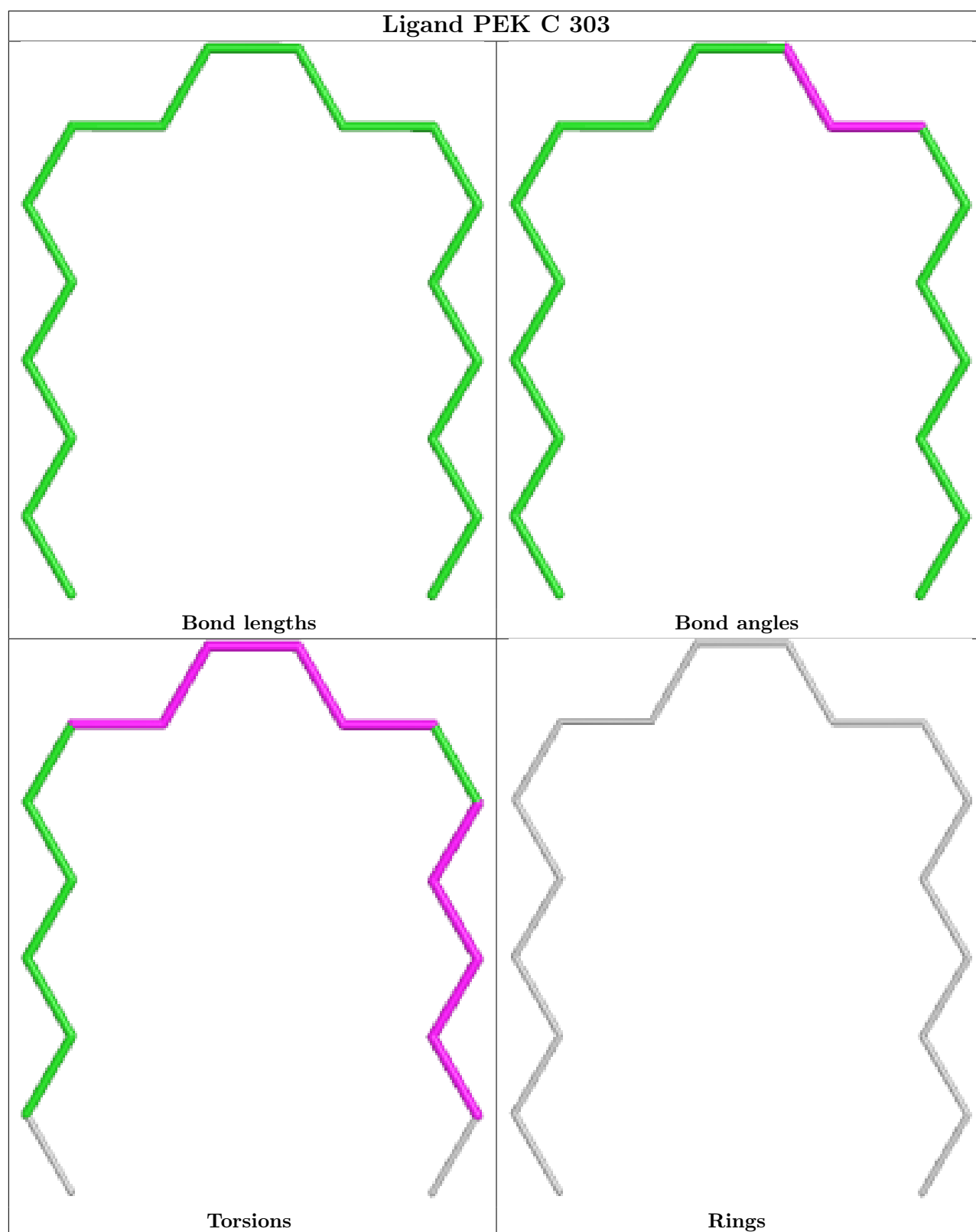


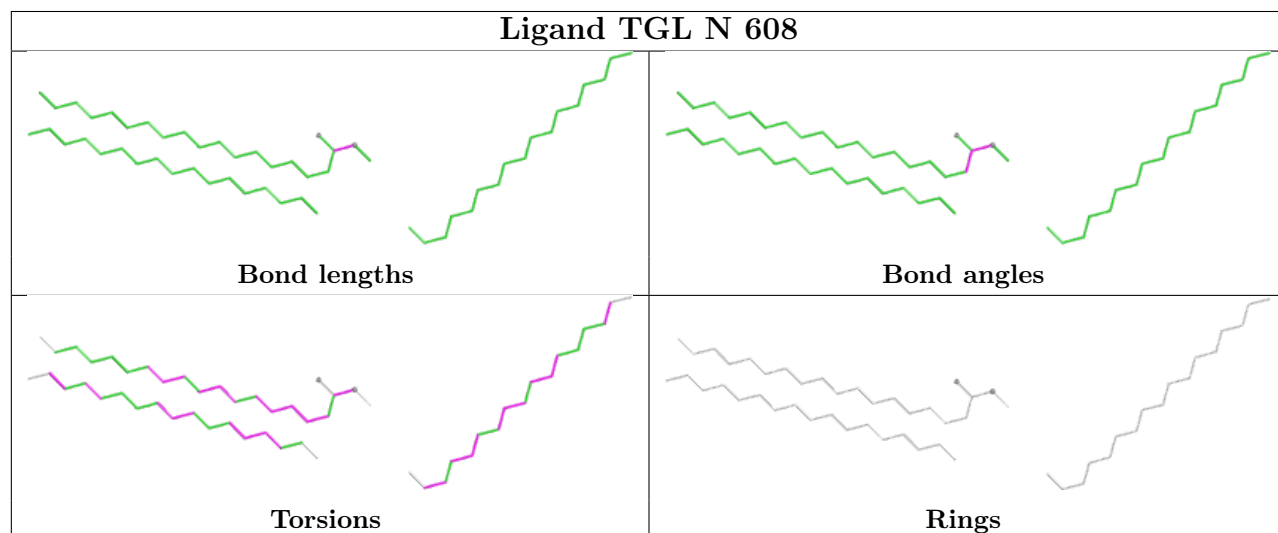
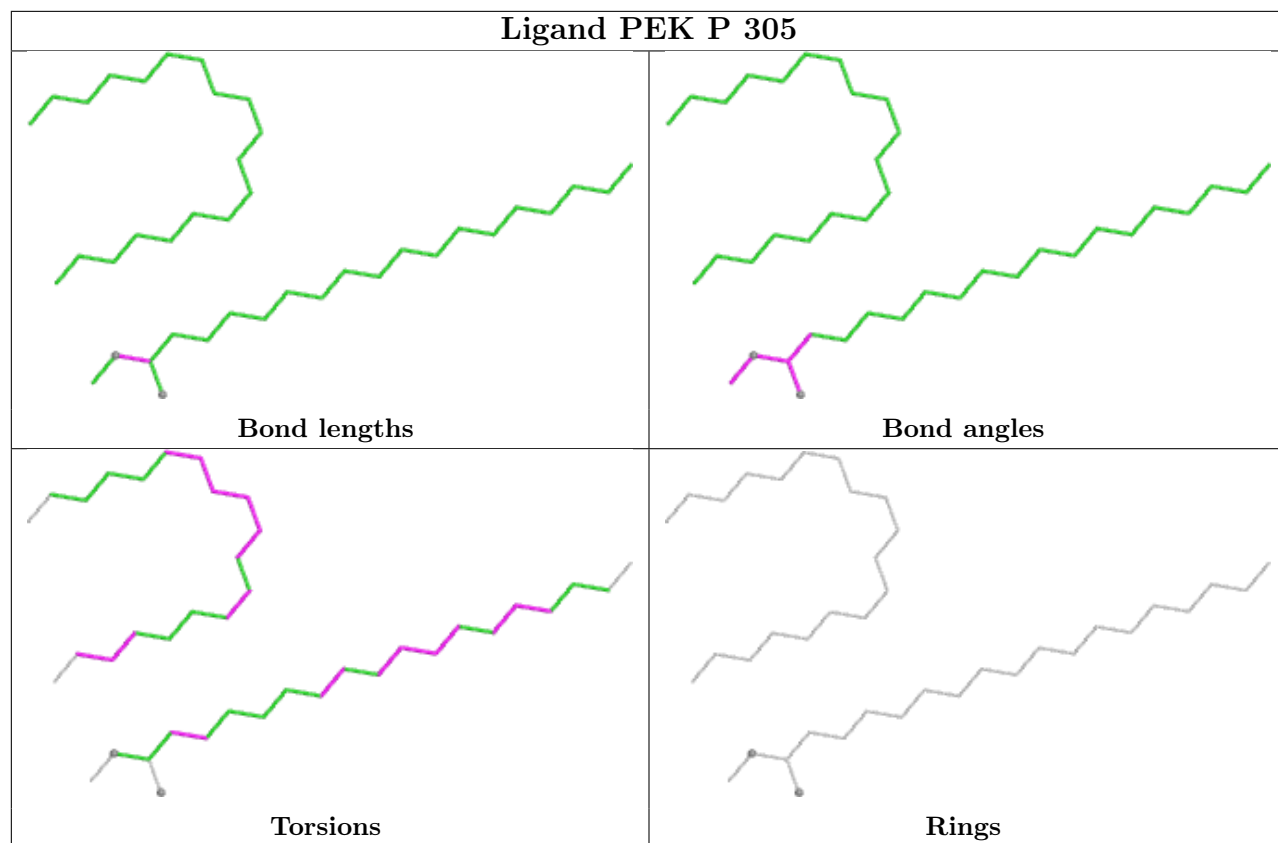


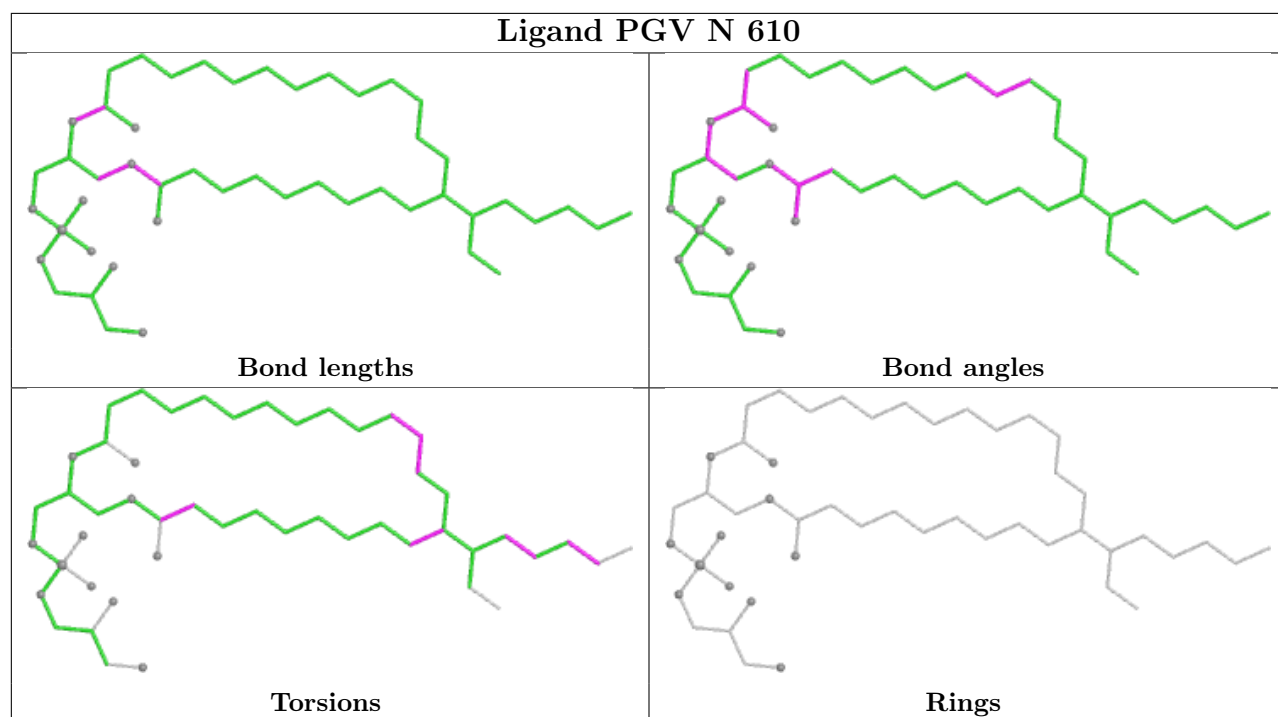
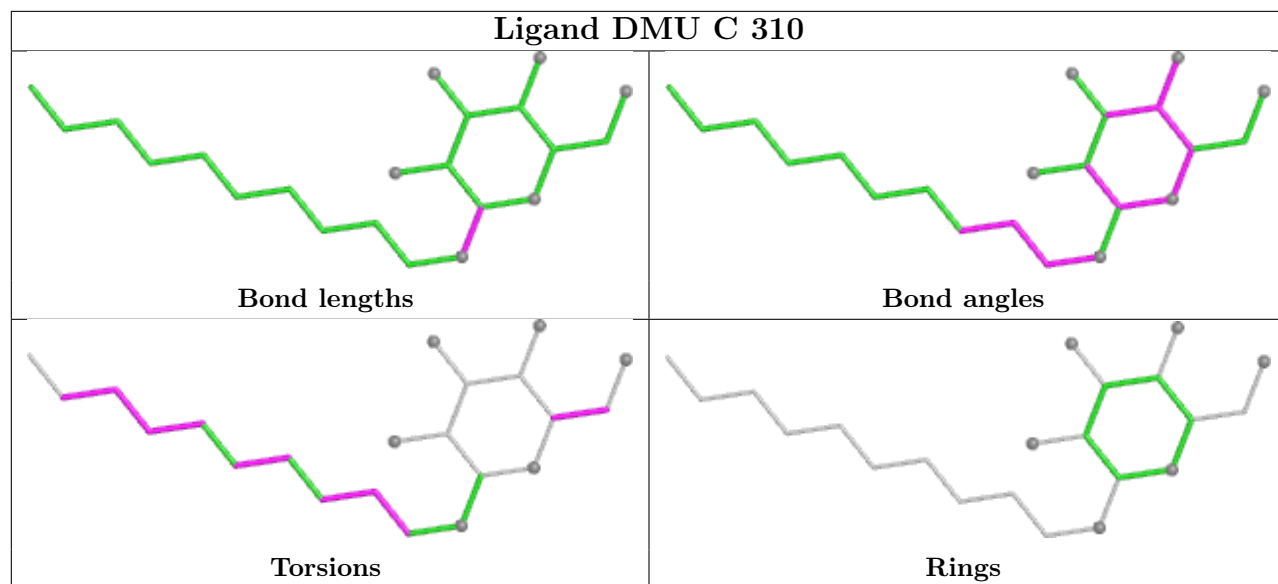


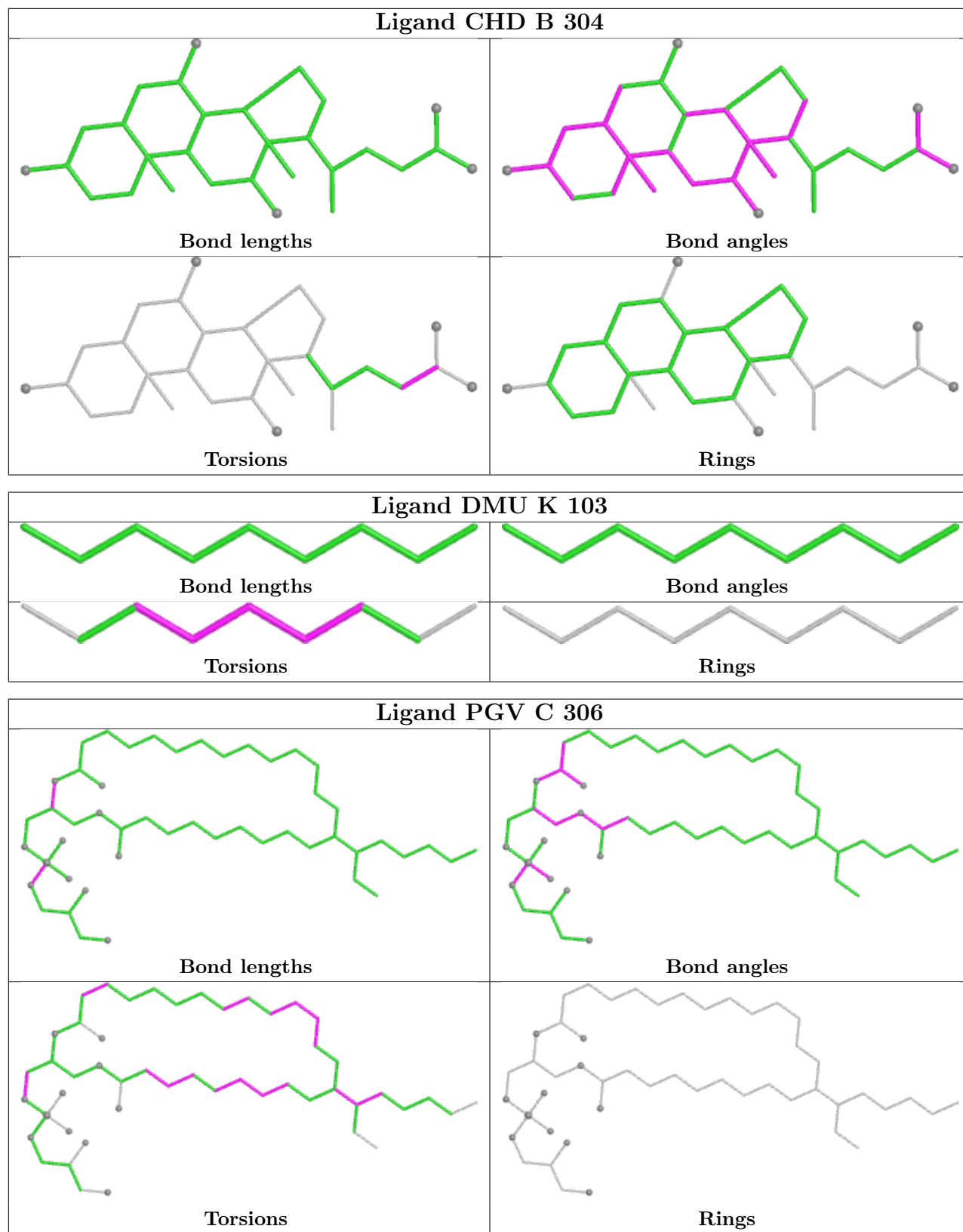


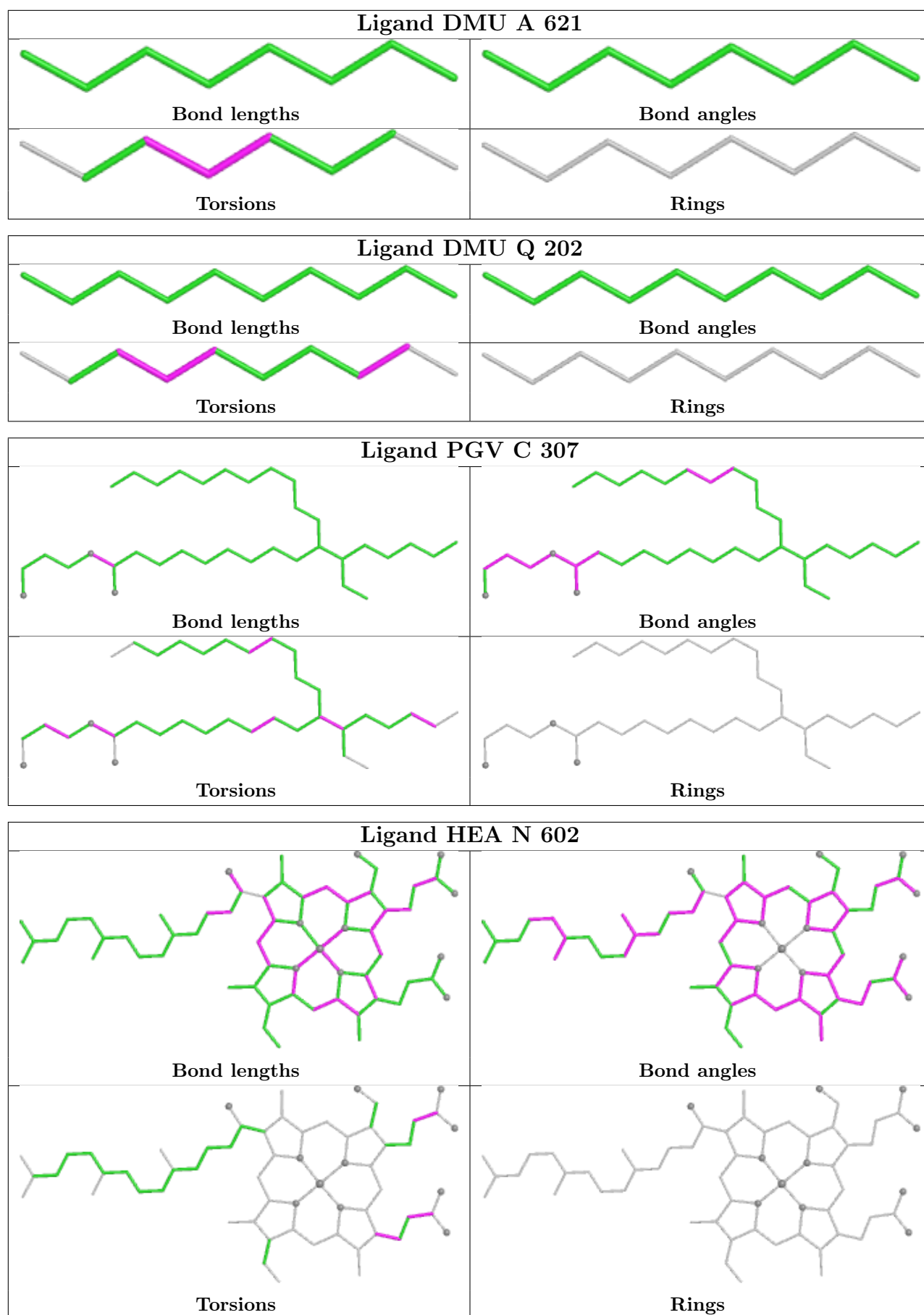


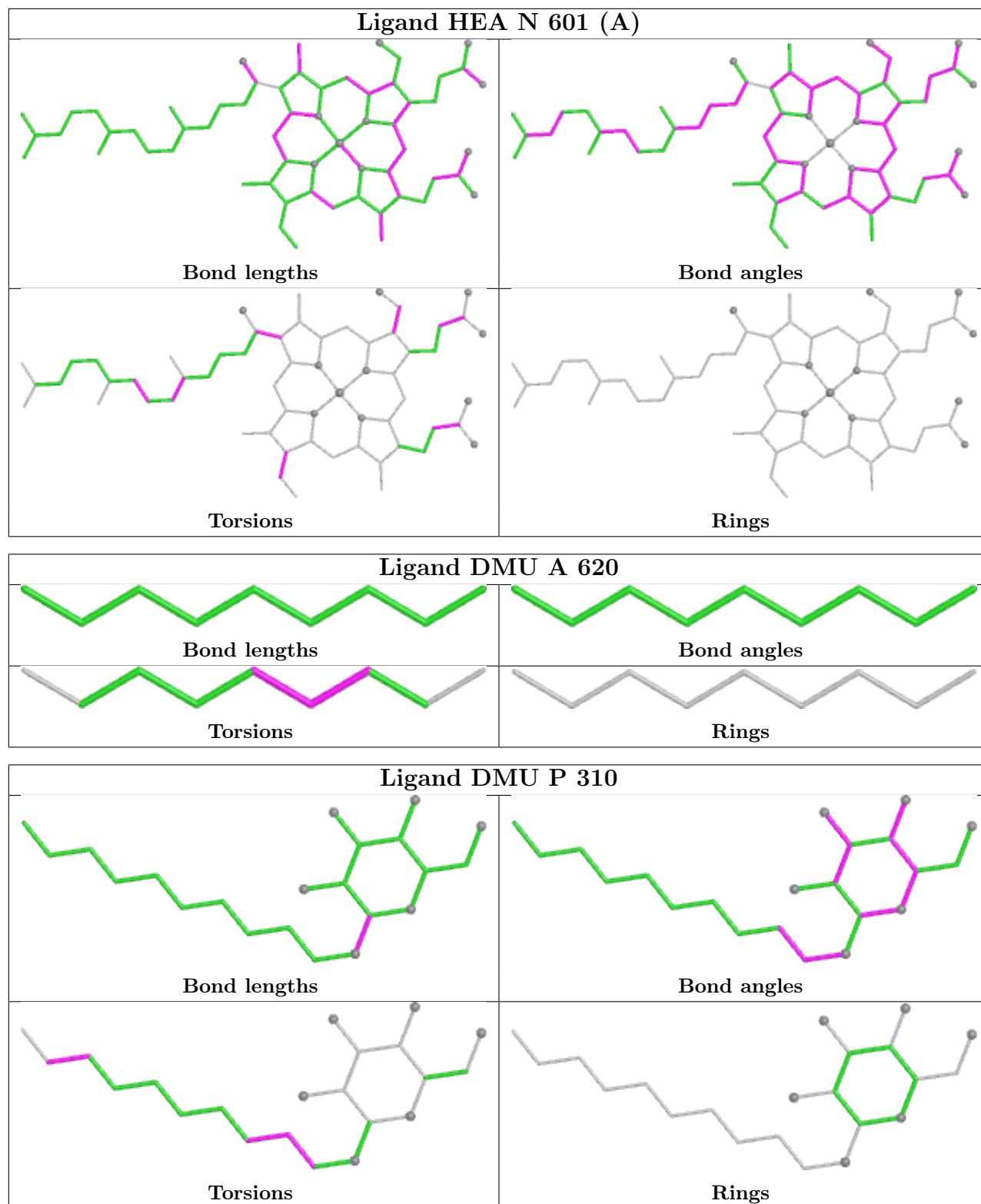


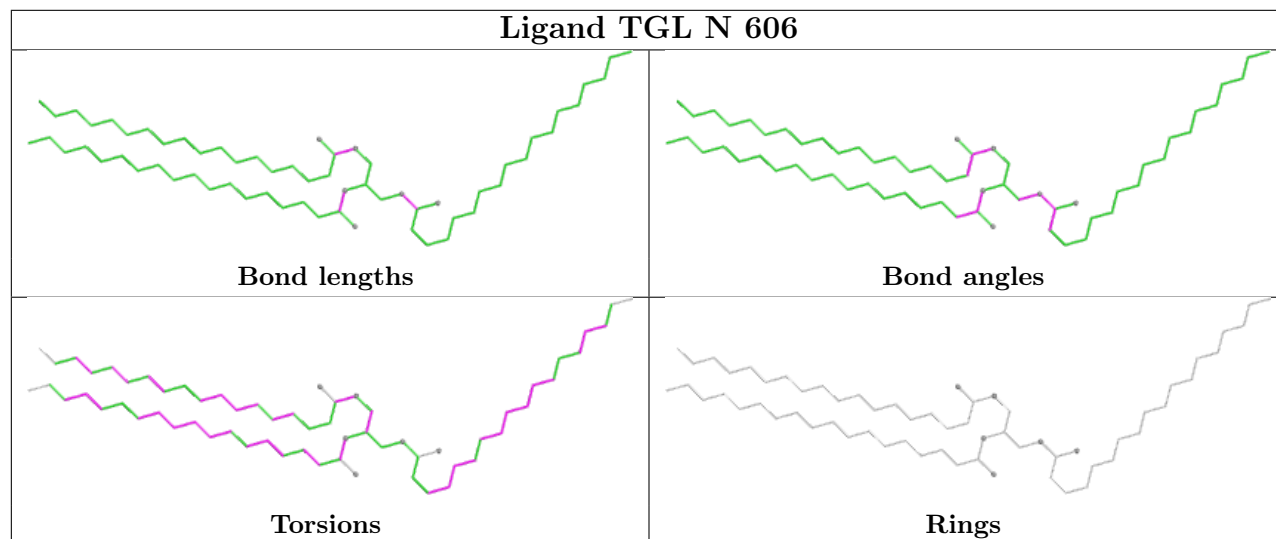
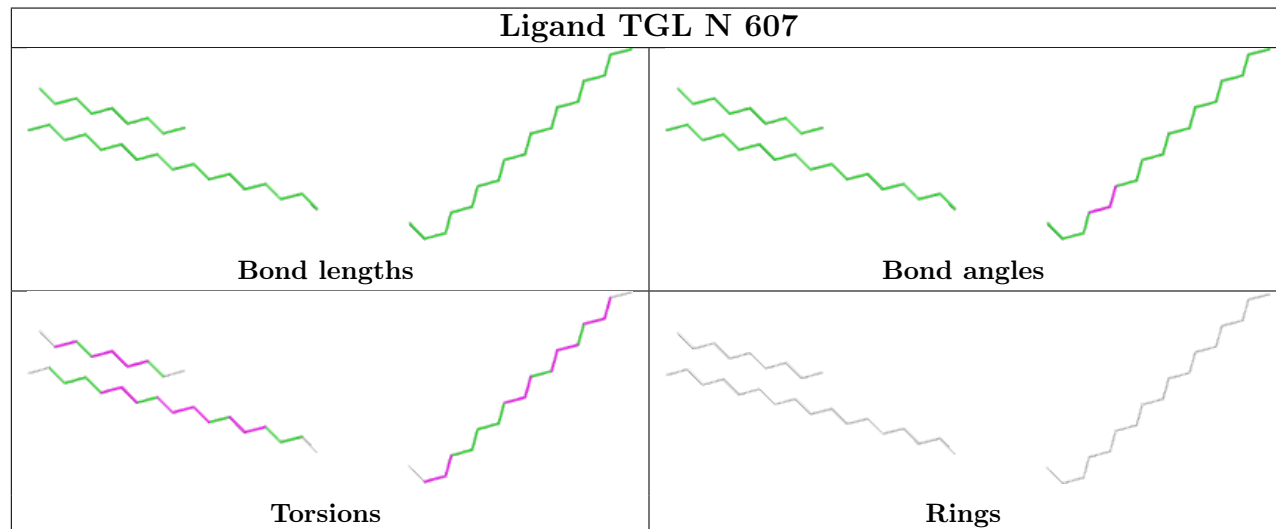
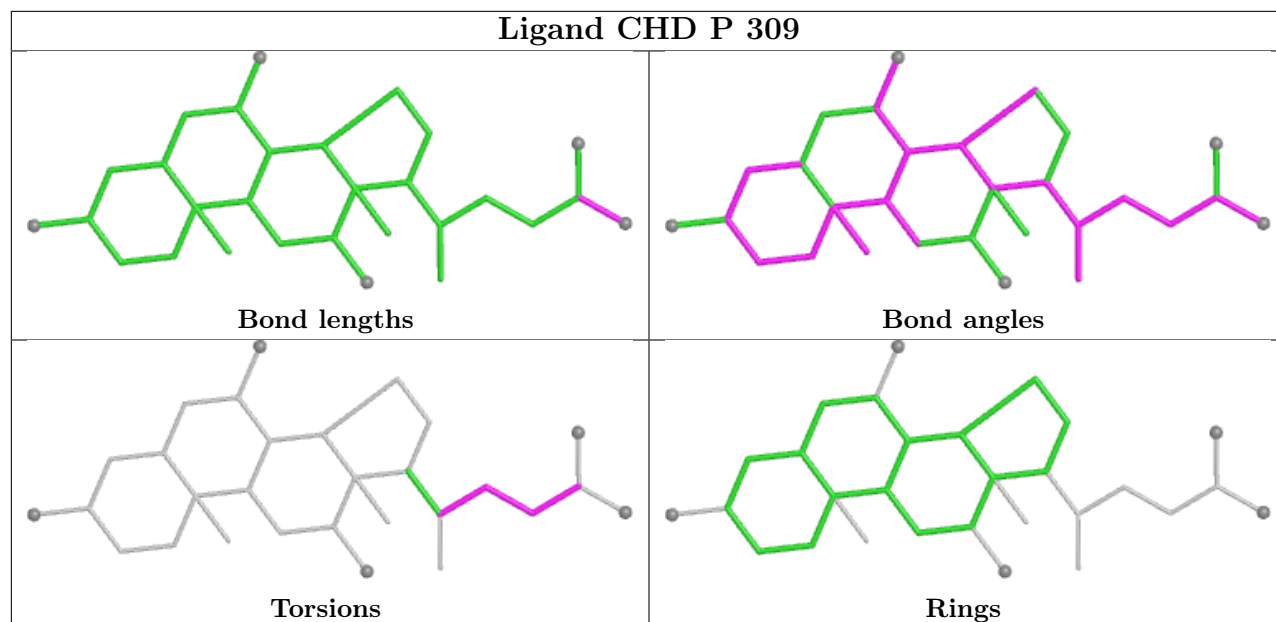


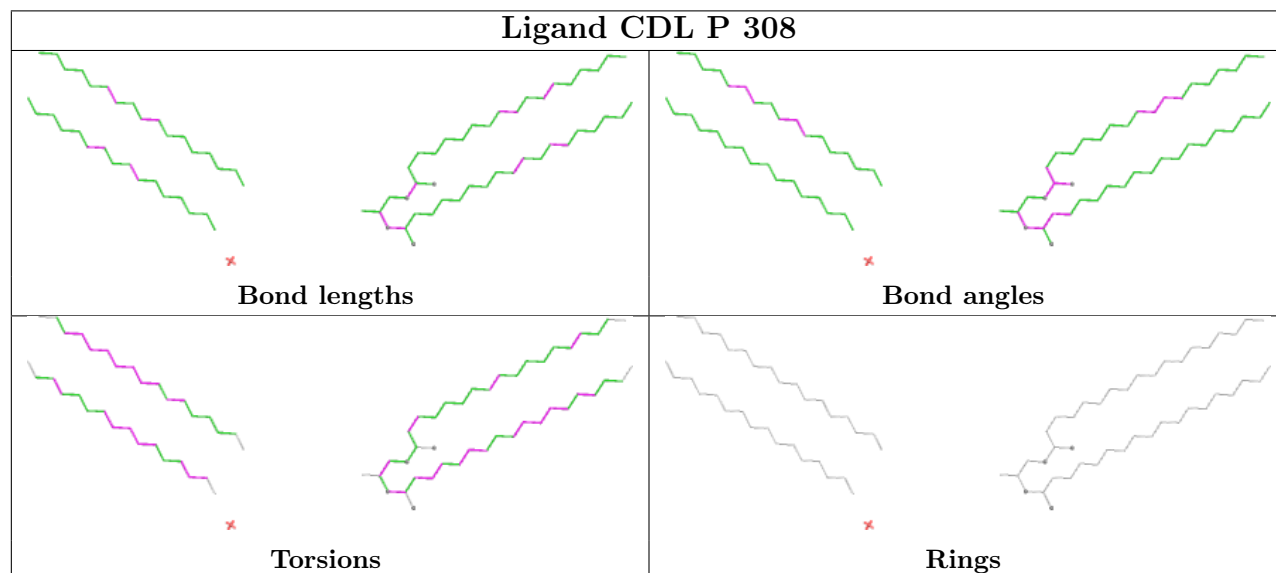
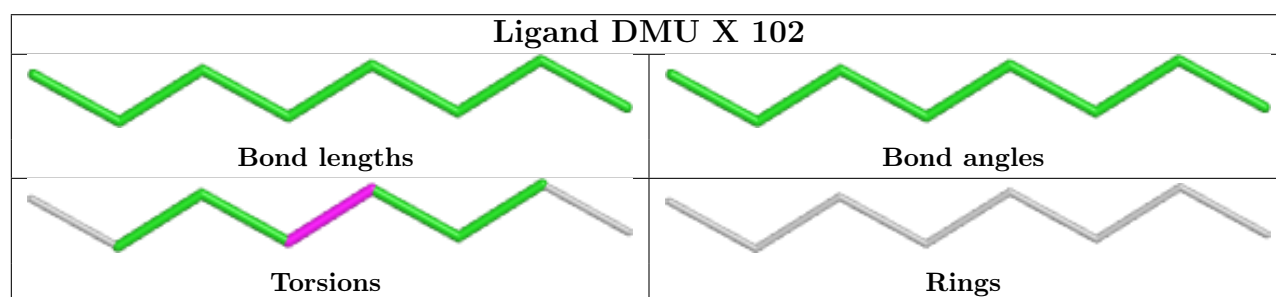
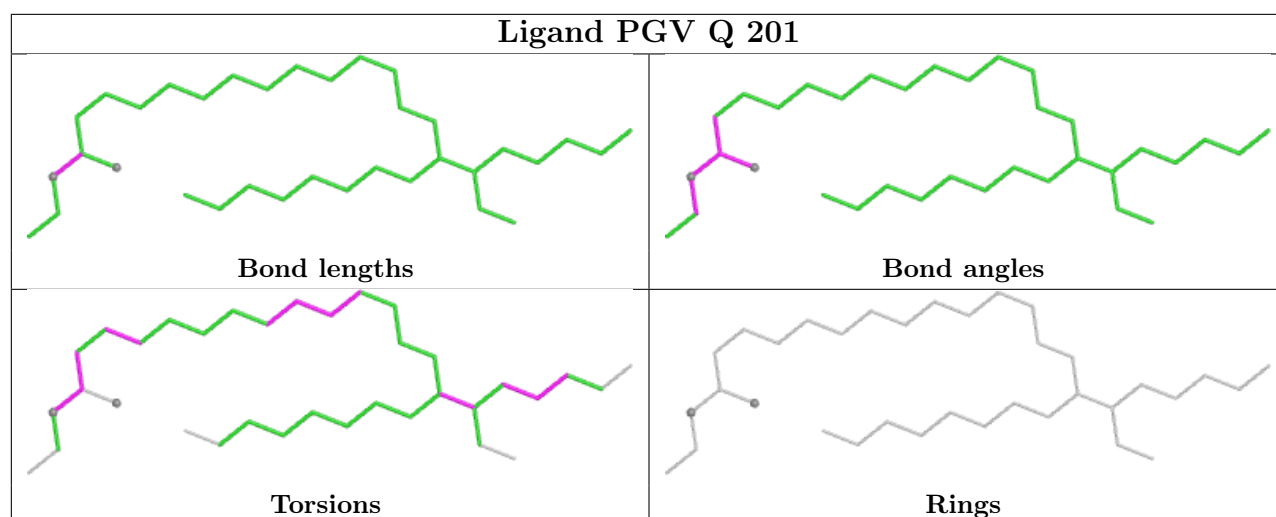


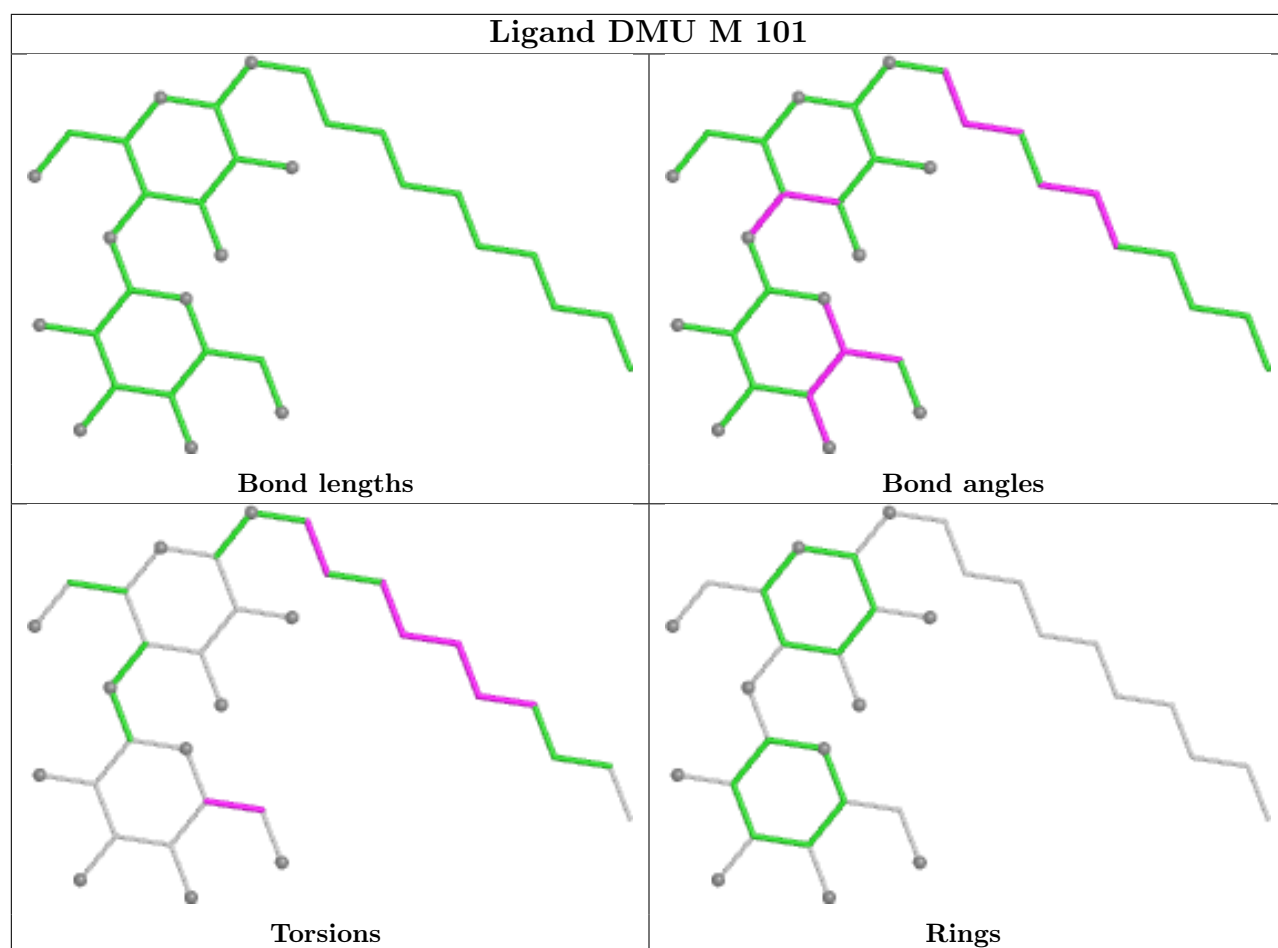


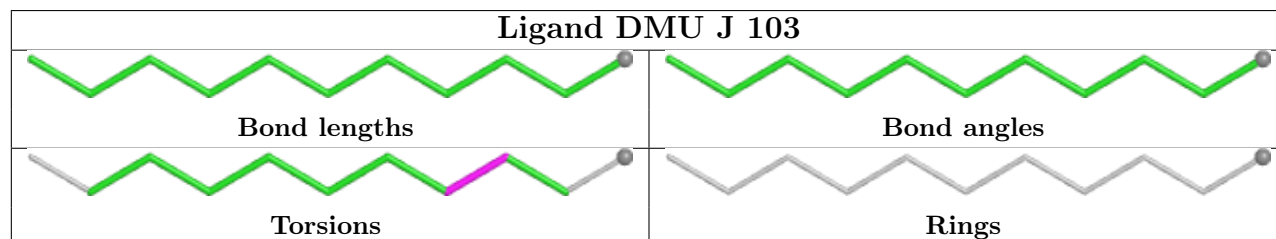
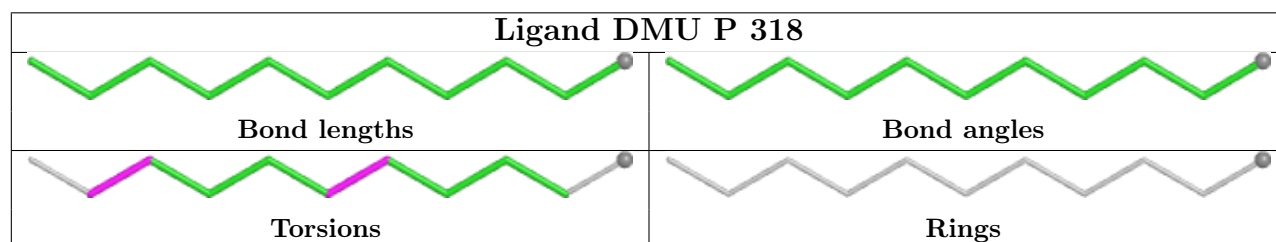
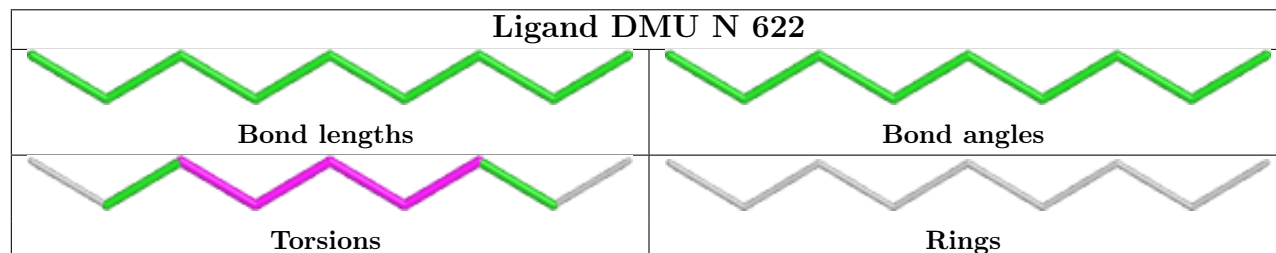
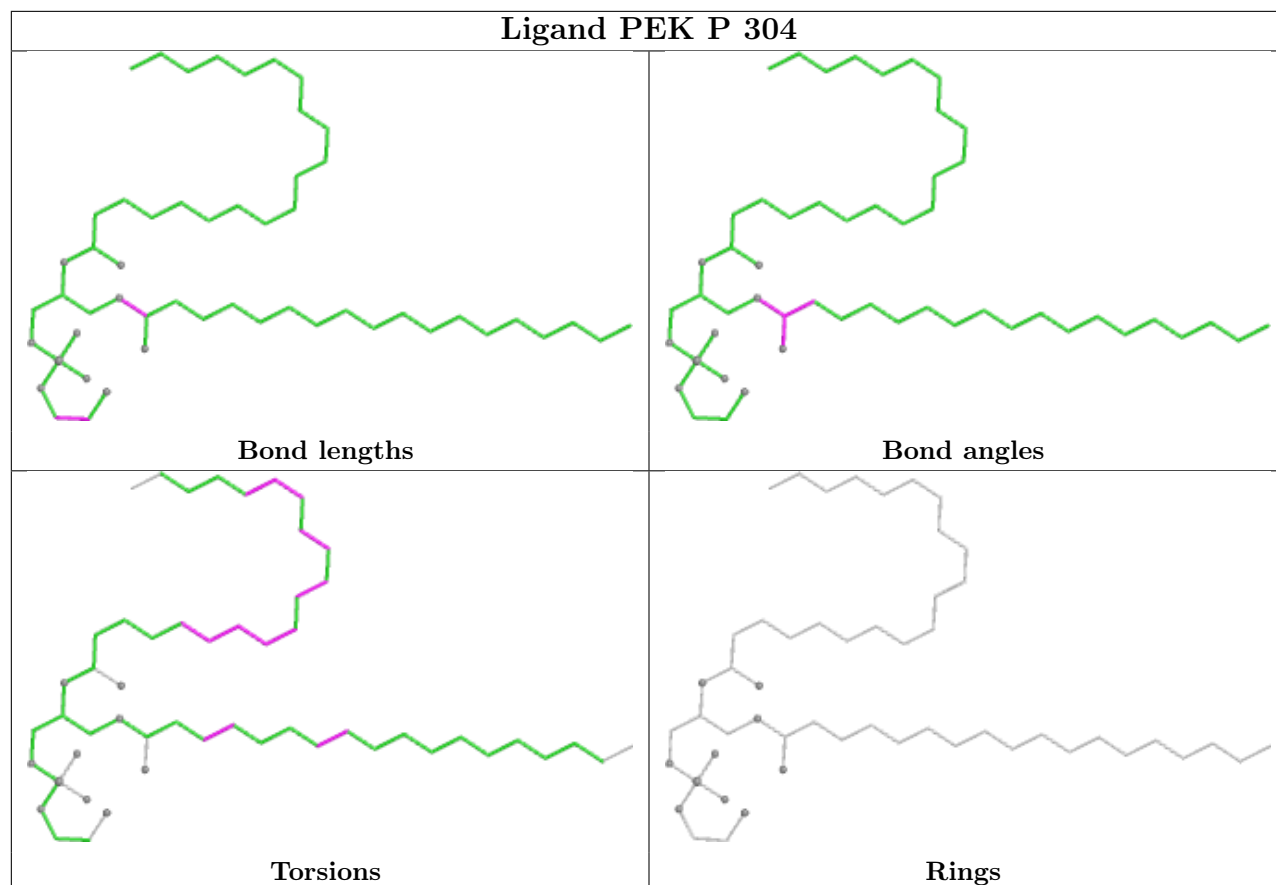


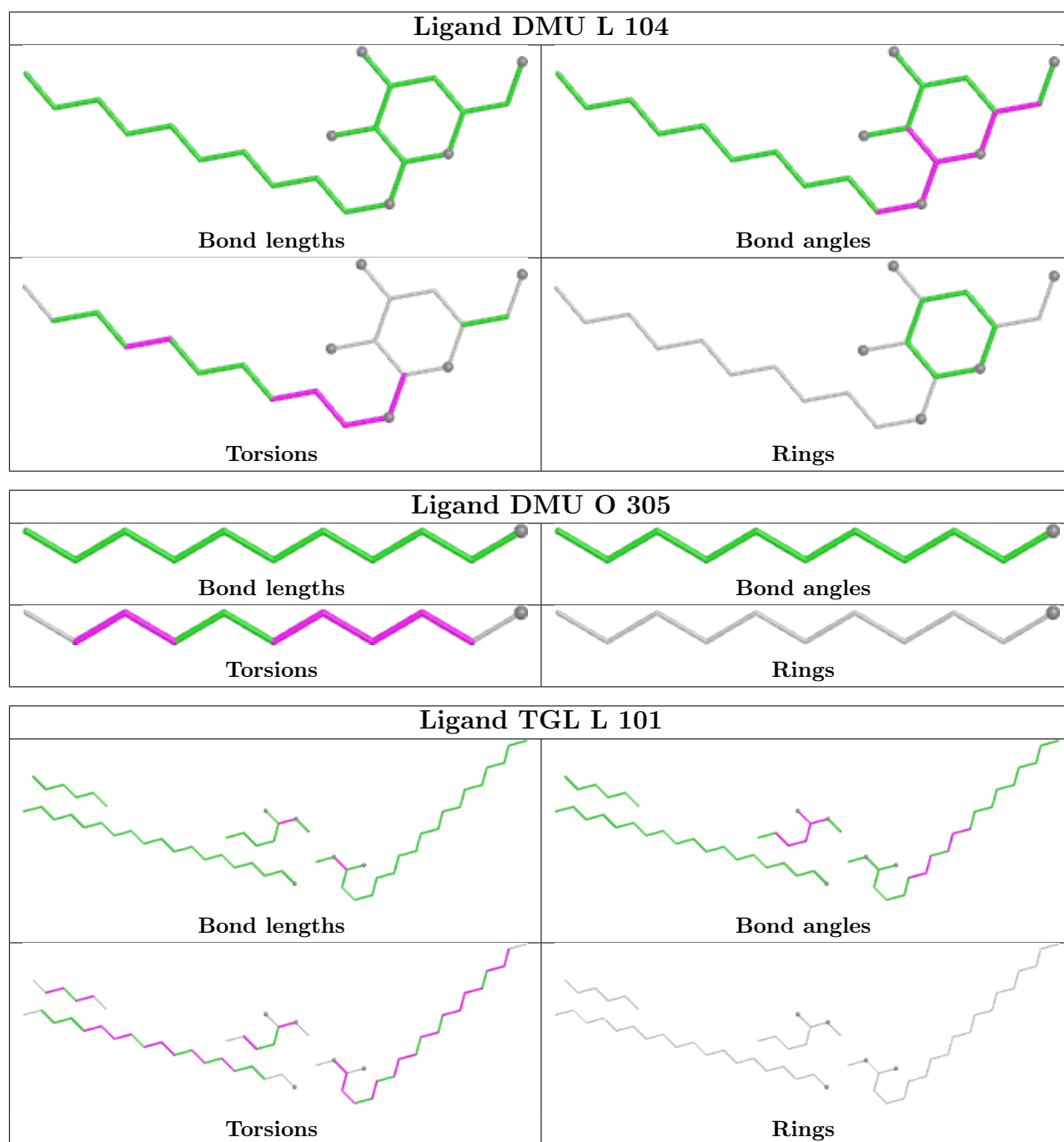




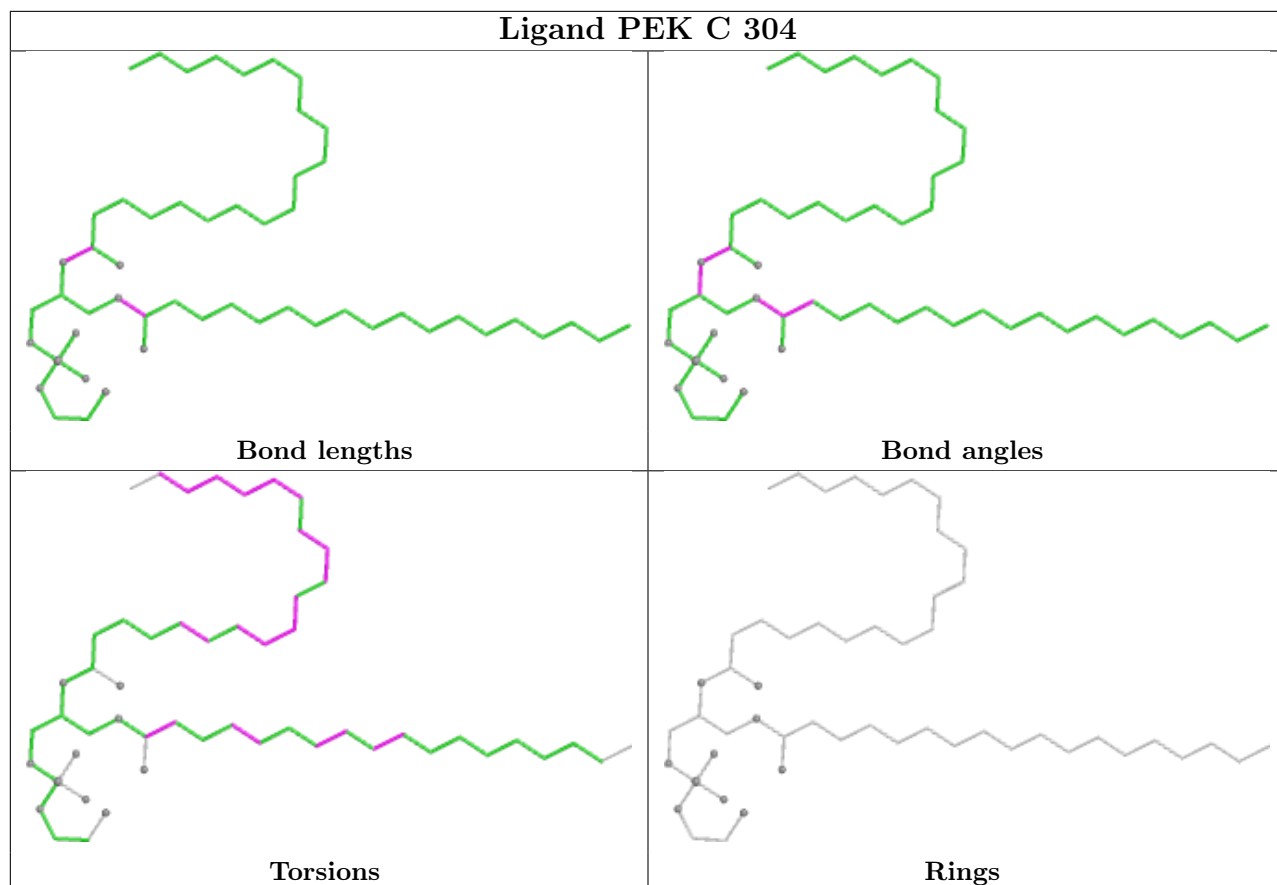




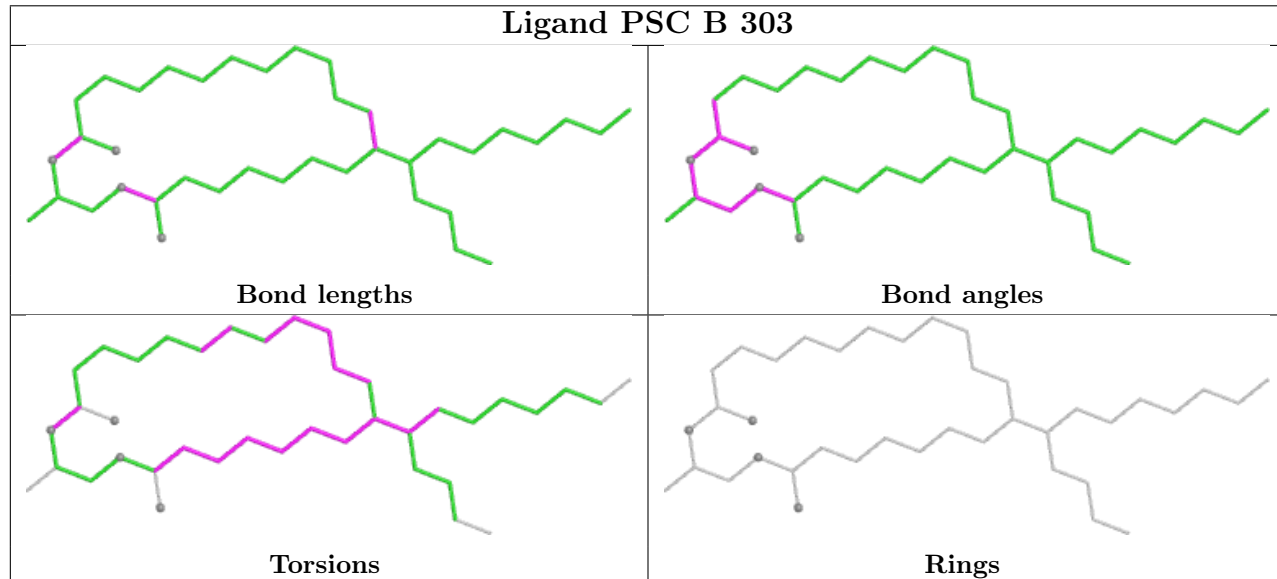


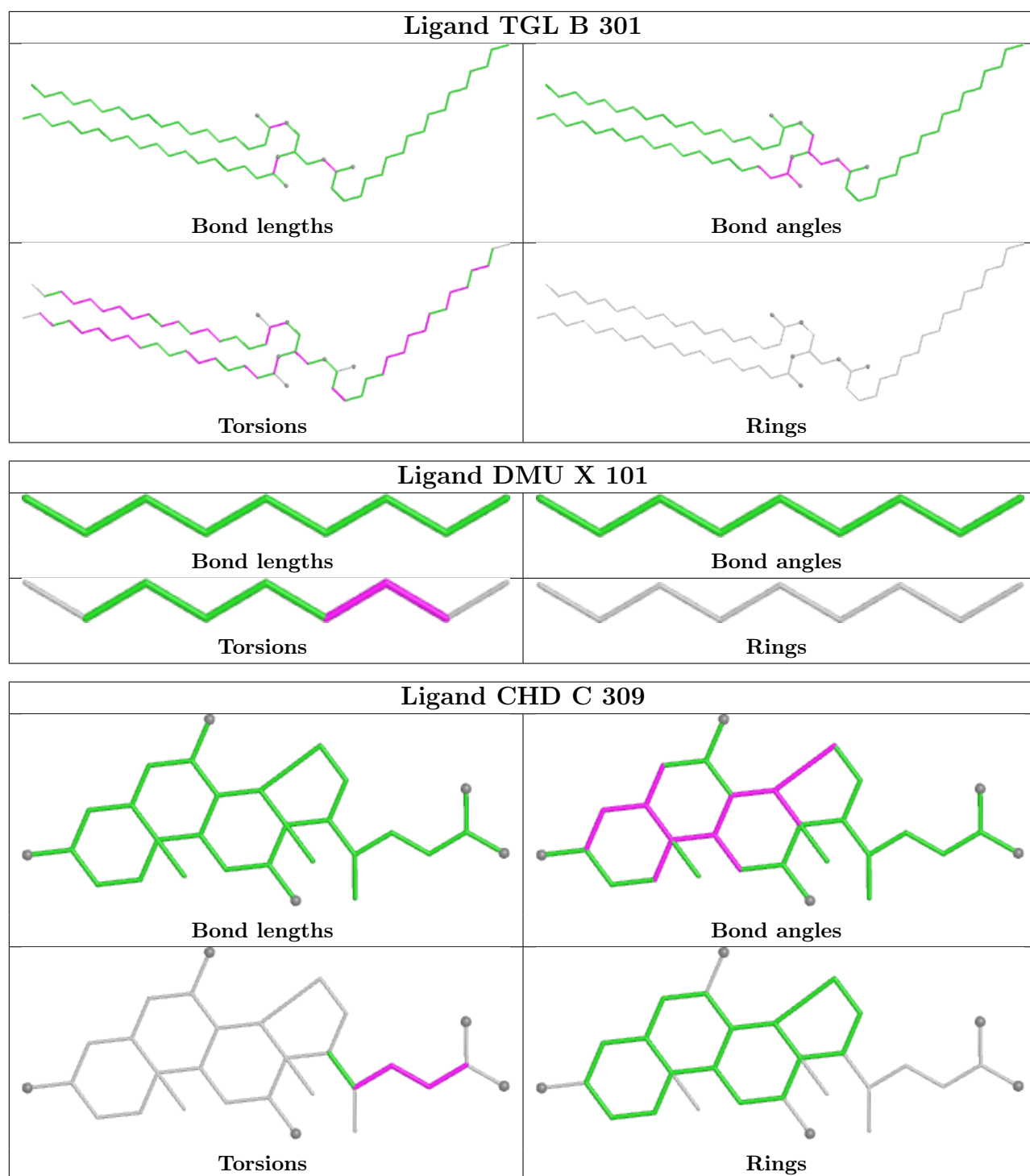


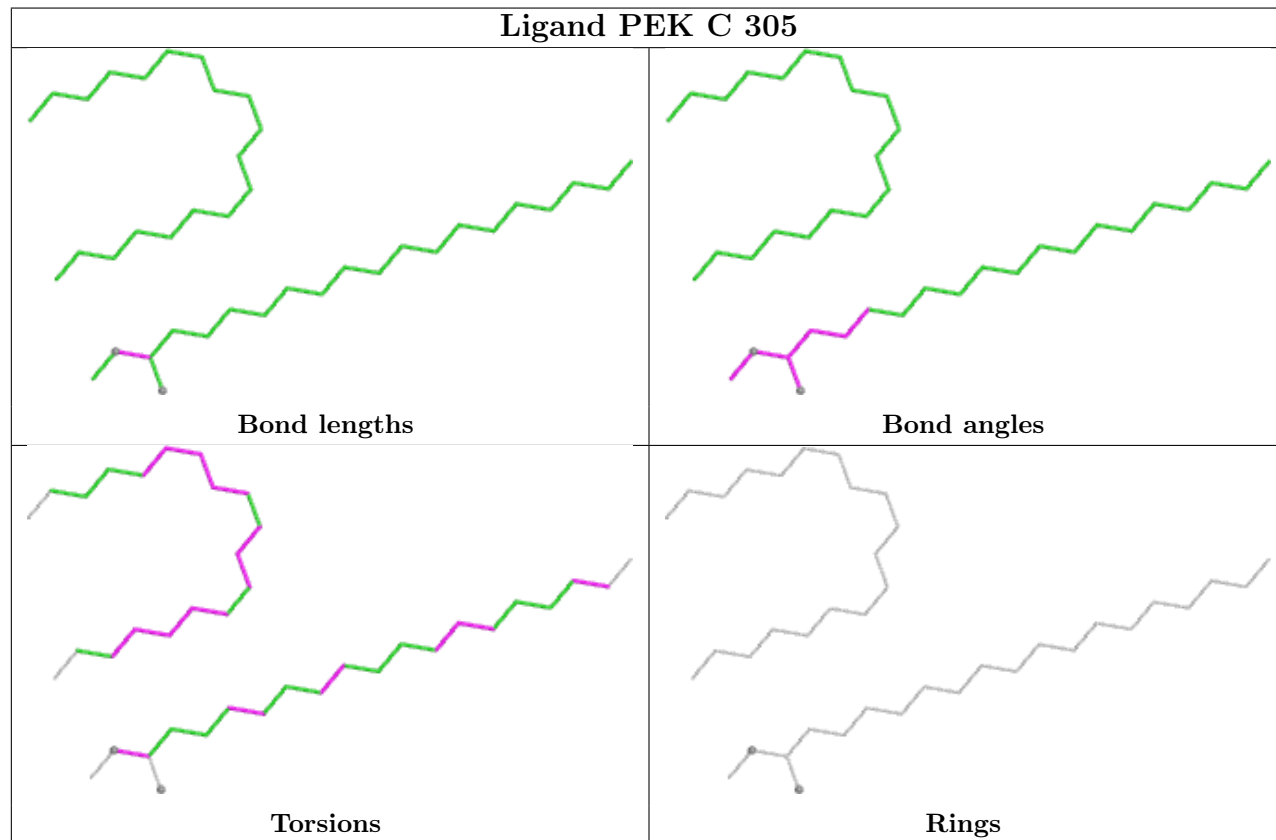
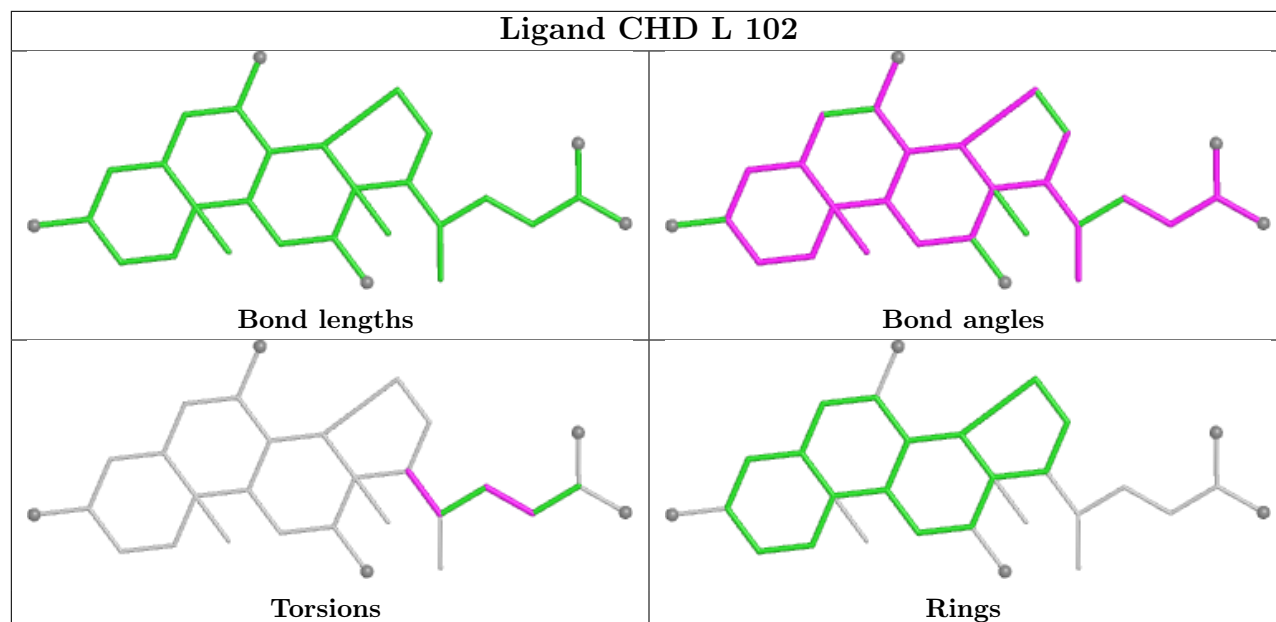
Ligand PEK C 304

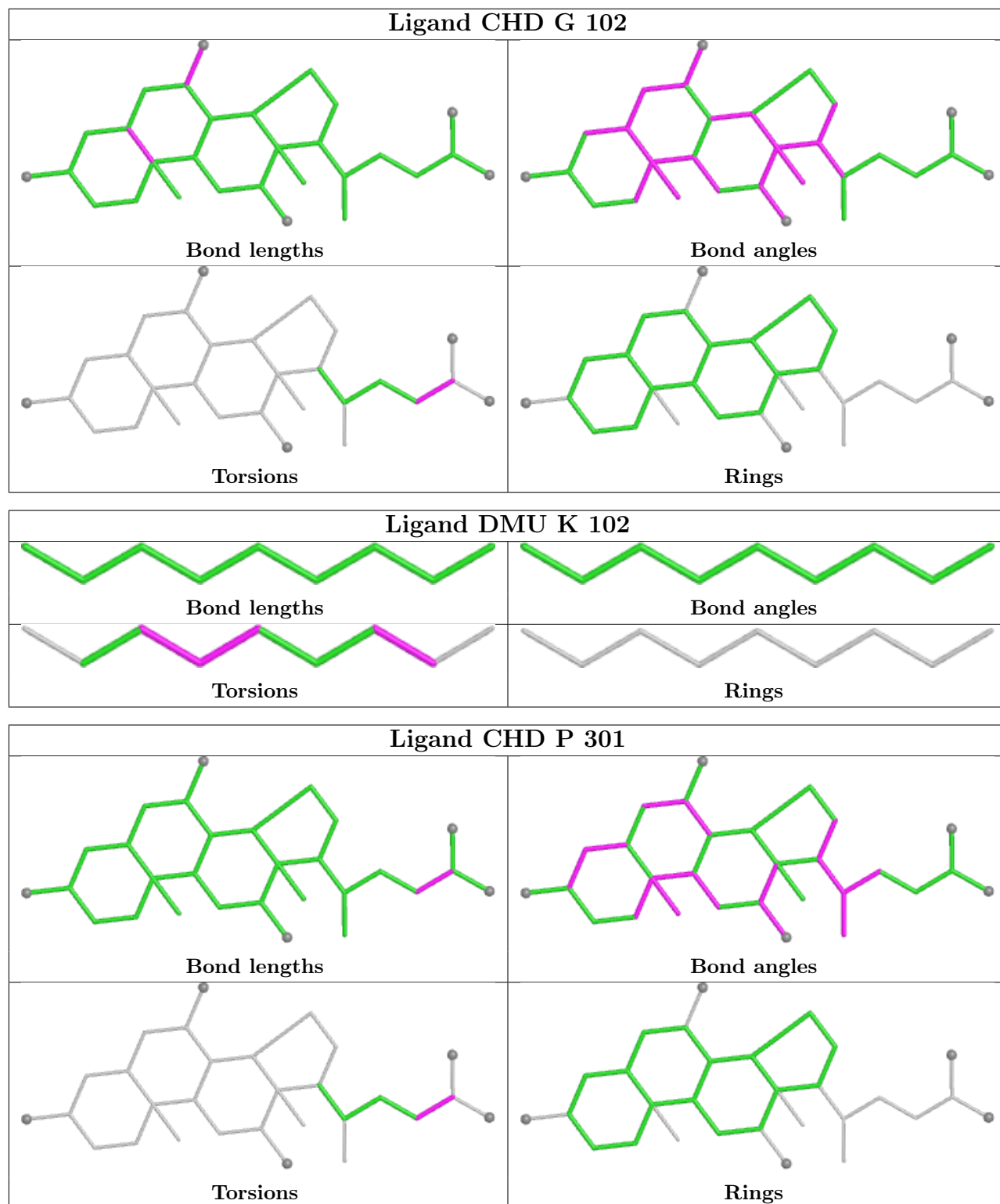


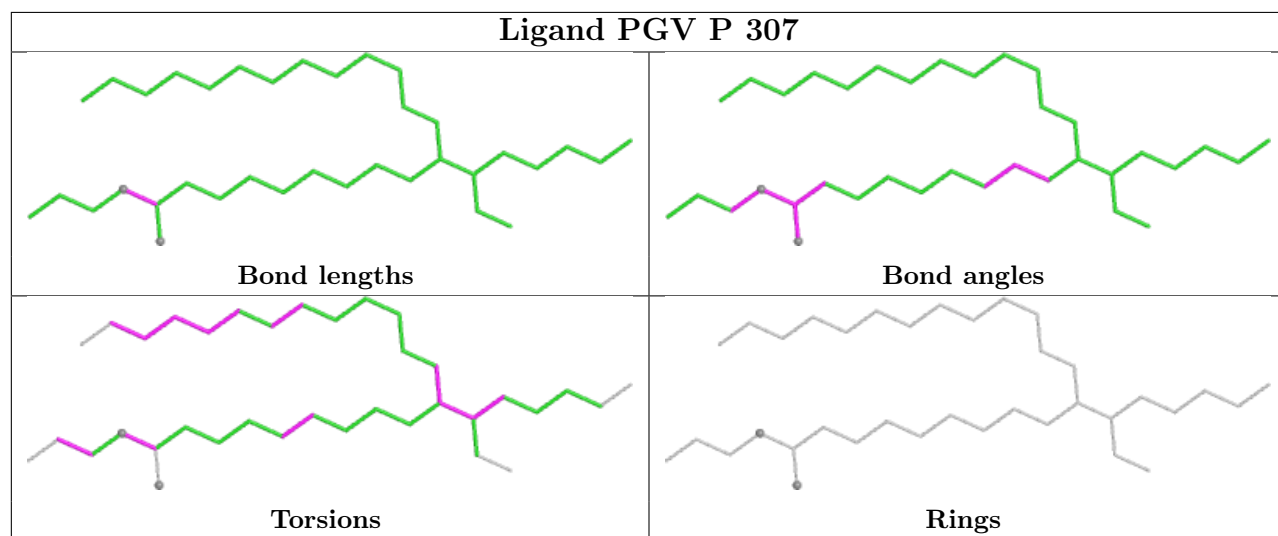
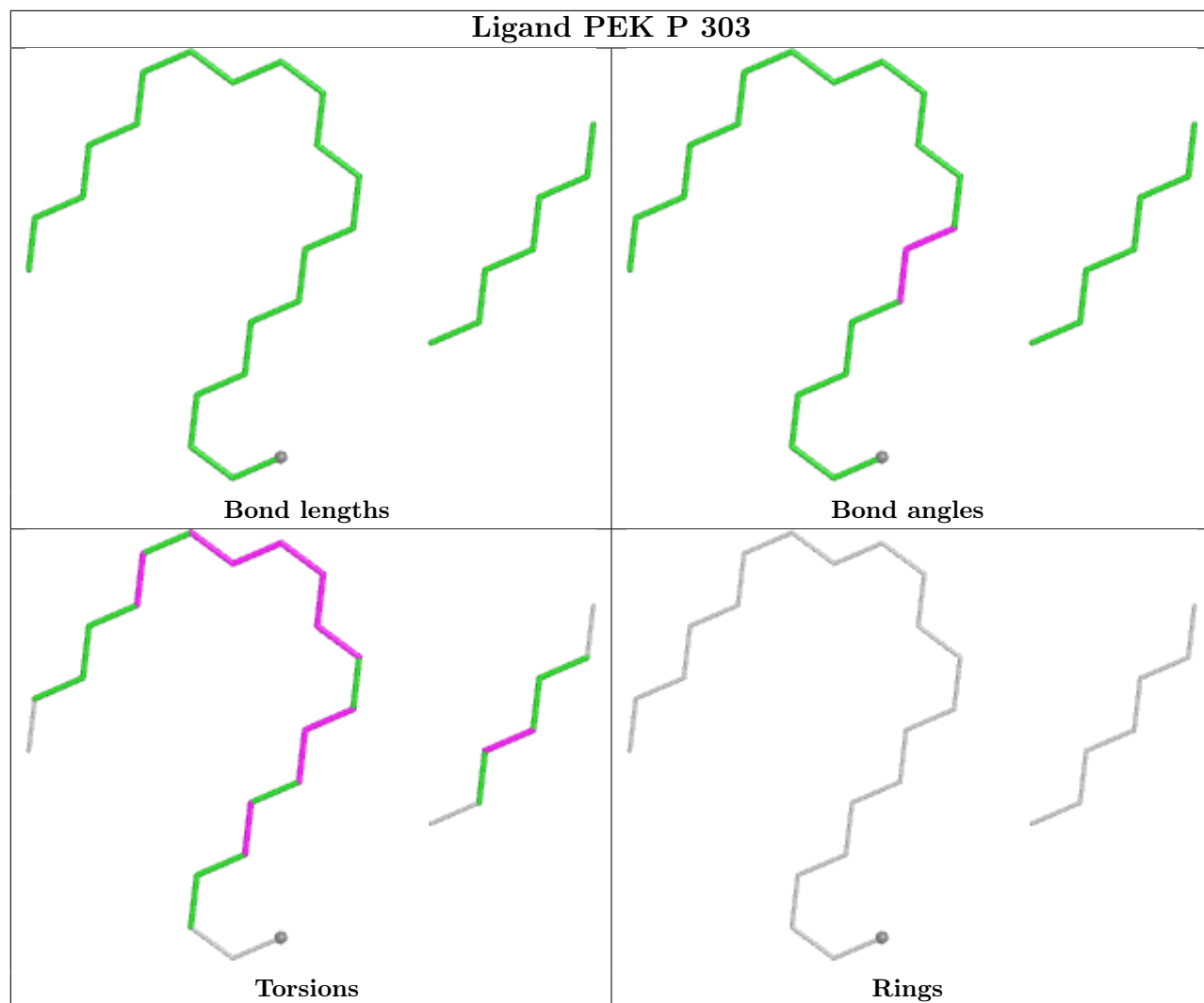
Ligand PSC B 303

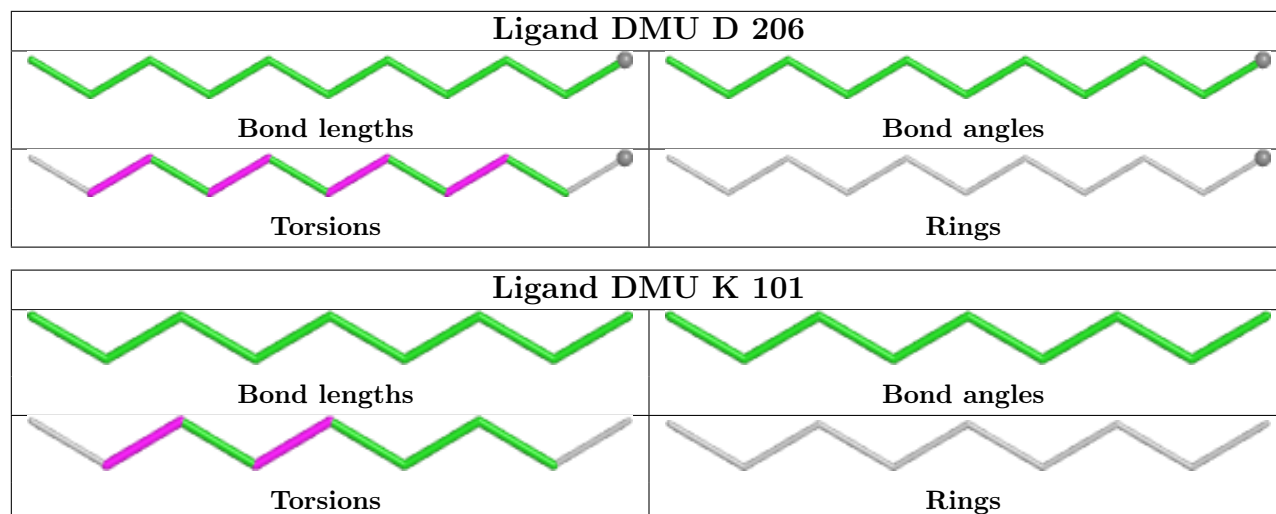












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.18	9 (1%) 67 74	11, 24, 32, 89	34 (6%)
1	N	513/514 (99%)	-0.10	8 (1%) 70 77	13, 27, 36, 76	28 (5%)
2	B	226/227 (99%)	0.32	16 (7%) 22 27	21, 32, 56, 112	14 (6%)
2	O	226/227 (99%)	0.37	13 (5%) 29 35	24, 36, 68, 130	9 (3%)
3	C	259/259 (100%)	-0.03	3 (1%) 76 83	18, 27, 40, 91	12 (4%)
3	P	259/259 (100%)	-0.04	3 (1%) 76 83	18, 28, 41, 91	8 (3%)
4	D	144/144 (100%)	0.26	6 (4%) 40 49	26, 34, 62, 94	0
4	Q	144/144 (100%)	0.96	19 (13%) 7 9	32, 48, 89, 218	0
5	E	105/105 (100%)	0.25	5 (4%) 35 43	26, 33, 62, 155	0
5	R	105/105 (100%)	0.38	4 (3%) 44 53	28, 40, 75, 159	0
6	F	94/94 (100%)	0.34	6 (6%) 25 31	23, 35, 61, 166	0
6	S	94/94 (100%)	0.48	6 (6%) 25 31	23, 32, 64, 131	0
7	G	84/84 (100%)	1.73	23 (27%) 1 1	26, 37, 140, 219	0
7	T	84/84 (100%)	1.62	22 (26%) 1 2	25, 39, 146, 232	0
8	H	79/79 (100%)	1.00	12 (15%) 5 7	29, 39, 117, 155	0
8	U	79/79 (100%)	1.04	14 (17%) 4 4	32, 43, 133, 164	0
9	I	72/73 (98%)	1.20	17 (23%) 2 2	28, 46, 78, 102	0
9	V	72/73 (98%)	1.42	20 (27%) 1 1	29, 53, 91, 134	0
10	J	58/58 (100%)	0.76	7 (12%) 8 11	27, 38, 86, 149	0
10	W	58/58 (100%)	0.60	4 (6%) 23 28	28, 40, 79, 154	0
11	K	49/49 (100%)	0.73	4 (8%) 17 23	31, 40, 58, 69	0
11	X	49/49 (100%)	1.23	10 (20%) 3 3	38, 47, 84, 101	0
12	L	46/46 (100%)	0.27	4 (8%) 16 21	26, 30, 53, 113	0
12	Y	46/46 (100%)	0.59	5 (10%) 10 14	29, 36, 71, 131	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	0.31	3 (6%)	22 28	26, 31, 87, 146	0
13	Z	43/43 (100%)	0.83	5 (11%)	9 12	34, 39, 103, 174	0
All	All	3544/3550 (99%)	0.34	248 (6%)	22 28	11, 32, 74, 232	105 (2%)

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	6	GLY	13.4
7	T	6	GLY	12.9
7	T	3	ALA	12.5
1	N	50[A]	ASP	12.3
6	F	1	ALA	10.0
1	A	50[A]	ASP	9.4
7	G	3	ALA	9.4
8	U	8	ILE	9.4
7	G	11	THR	9.1
1	A	49[A]	GLY	9.0
7	T	8	HIS	8.8
4	Q	6	VAL	8.7
7	G	36	TRP	8.6
7	T	36	TRP	8.5
7	G	7	ASP	8.0
7	T	9	GLY	7.9
7	G	8	HIS	7.7
8	H	8	ILE	7.7
6	S	94	HIS	7.5
6	S	1	ALA	7.1
7	T	11	THR	7.0
4	Q	5	VAL	7.0
4	D	4	SER	6.8
7	G	1	ALA	6.7
7	T	5	LYS	6.5
7	T	2	SER	6.5
7	T	7	ASP	6.2
7	T	1	ALA	6.1
8	H	46	LYS	6.1
6	S	3	GLY	6.0
7	G	2	SER	5.9
7	G	5	LYS	5.7
9	I	29	LEU	5.7
1	N	49[A]	GLY	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	J	58	LYS	5.7
6	S	2	SER	5.6
8	H	45	ALA	5.6
7	T	38	HIS	5.5
7	G	4	ALA	5.4
9	I	37	PHE	5.2
4	D	5	VAL	5.2
2	O	113	TYR	5.1
3	P	3	HIS	5.1
7	G	9	GLY	5.0
9	V	2	THR	5.0
7	G	10	GLY	4.9
6	F	2	SER	4.9
11	K	6	ALA	4.9
2	O	90	ILE	4.8
2	O	91	ASN	4.8
2	O	227	LEU	4.7
7	G	37	LEU	4.7
6	F	94	HIS	4.7
6	S	93	PRO	4.6
8	U	9	LYS	4.6
7	G	35	SER	4.5
2	B	90	ILE	4.5
8	H	44	THR	4.4
2	B	59[A]	GLN	4.3
9	V	37	PHE	4.3
8	U	50	VAL	4.3
12	Y	47	LYS	4.3
11	X	6	ALA	4.2
12	Y	2	HIS	4.2
9	I	2	THR	4.2
5	R	109	VAL	4.2
7	T	4	ALA	4.2
10	J	1	PHE	4.1
7	T	10	GLY	4.1
13	Z	42	LYS	4.1
13	Z	43	SER	4.1
7	G	38	HIS	4.1
8	U	48	GLY	4.0
8	U	45	ALA	4.0
8	H	7	LYS	4.0
8	U	42	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	Q	73	ARG	3.9
1	N	51[A]	ASP	3.9
8	U	46	LYS	3.9
4	Q	8	SER	3.8
12	L	47	LYS	3.8
11	K	47	ARG	3.8
4	Q	72	ASN	3.8
2	B	91	ASN	3.7
1	A	514	LYS	3.7
8	U	7	LYS	3.7
11	X	7	PRO	3.7
7	G	41	HIS	3.7
12	L	2	HIS	3.6
5	R	5	HIS	3.6
10	J	56	PRO	3.6
8	H	47	GLY	3.6
3	C	3	HIS	3.6
8	H	9	LYS	3.5
8	U	10	ASN	3.5
1	A	382[A]	SER	3.5
6	F	3	GLY	3.5
7	T	37	LEU	3.5
4	Q	39	ALA	3.5
1	A	53[A]	ILE	3.5
9	V	25	PHE	3.5
1	A	113	LEU	3.5
9	V	33	THR	3.5
2	B	61	VAL	3.4
8	U	47	GLY	3.4
2	O	65	TRP	3.4
9	I	25	PHE	3.3
2	B	65	TRP	3.3
2	B	113	TYR	3.2
4	Q	4	SER	3.2
4	Q	35	ALA	3.2
2	B	68[A]	LEU	3.2
1	N	55[A]	ASN	3.2
13	Z	38	ASP	3.2
10	W	57	HIS	3.2
8	U	52	VAL	3.2
2	O	217	LYS	3.1
4	Q	51	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	31	LYS	3.1
9	V	3	ALA	3.1
9	V	21	ILE	3.0
4	Q	9	GLU	3.0
11	X	39	GLU	3.0
8	H	10	ASN	3.0
11	X	48	VAL	3.0
1	N	513	LEU	3.0
7	G	84	LYS	3.0
9	V	44	LYS	3.0
5	E	109	VAL	2.9
7	G	33	LEU	2.9
2	O	92	ASN	2.9
5	E	5	HIS	2.9
5	R	108	LYS	2.9
4	Q	17	VAL	2.9
7	T	40	GLY	2.9
5	E	6	GLU	2.9
7	G	39	SER	2.8
7	T	33	LEU	2.8
9	V	65	LYS	2.8
7	T	12	GLY	2.8
9	I	35	TYR	2.8
9	V	45	LYS	2.8
1	A	51[A]	ASP	2.8
9	I	23	GLY	2.8
7	T	39	SER	2.8
12	Y	24	MET	2.8
6	F	87	THR	2.8
9	V	30	GLY	2.8
9	I	20	HIS	2.7
11	X	23	THR	2.7
9	I	34	PHE	2.7
13	M	40	TYR	2.7
13	Z	40	TYR	2.7
10	J	57	HIS	2.7
9	V	27	VAL	2.7
13	M	42	LYS	2.7
9	I	22	VAL	2.6
3	C	258	TRP	2.6
4	Q	40	LEU	2.6
4	D	7	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	48	GLY	2.6
10	J	55	PHE	2.6
2	B	33	LEU	2.6
2	B	37	LEU	2.6
1	N	382[A]	SER	2.6
1	N	514	LYS	2.6
9	V	36	LYS	2.6
12	L	24	MET	2.6
6	F	64	GLU	2.6
11	X	52	GLU	2.6
2	O	32[A]	PHE	2.5
9	V	34	PHE	2.5
2	O	116	LEU	2.5
9	V	73	LYS	2.5
9	I	32	ALA	2.5
13	Z	41	LYS	2.5
7	G	42	ARG	2.5
8	H	50	VAL	2.5
2	B	41	ILE	2.5
11	X	54	ARG	2.5
1	N	48[A]	LEU	2.5
2	B	58	ALA	2.5
2	B	60[A]	GLU	2.5
6	S	64	GLU	2.5
8	U	49	ASP	2.4
9	V	22	VAL	2.4
2	O	221	LYS	2.4
9	I	30	GLY	2.4
8	U	55	TRP	2.4
10	W	52	TRP	2.4
7	T	43	GLU	2.4
5	R	90	ARG	2.4
2	B	87	MET	2.4
1	A	513	LEU	2.3
4	Q	143	ASN	2.3
4	Q	19	ARG	2.3
2	O	115	ASP	2.3
4	Q	147	LYS	2.3
9	I	36	LYS	2.3
5	E	39	TYR	2.3
11	X	13	TYR	2.3
4	Q	74	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	27	VAL	2.3
11	X	14	GLY	2.3
4	Q	7	LYS	2.3
8	H	42	ALA	2.3
9	V	5	ALA	2.3
9	V	29	LEU	2.3
4	Q	36	SER	2.3
9	V	15	ARG	2.3
11	X	45	VAL	2.3
12	Y	44	LEU	2.2
8	U	43	MET	2.2
12	L	26	THR	2.2
10	W	1	PHE	2.2
7	T	42	ARG	2.2
4	D	147	LYS	2.2
9	I	42	LYS	2.2
7	T	41	HIS	2.2
9	I	31	PHE	2.2
9	I	21	ILE	2.2
9	V	68	ILE	2.2
9	V	8	GLN	2.1
10	J	26	ALA	2.1
1	A	48[A]	LEU	2.1
2	O	226	MET	2.1
7	T	35	SER	2.1
13	M	43	SER	2.1
2	O	114	GLU	2.1
2	B	67	ILE	2.1
9	I	44	LYS	2.1
10	J	27	THR	2.1
12	Y	26	THR	2.1
2	B	32[A]	PHE	2.1
3	P	122	HIS	2.1
5	E	108	LYS	2.1
8	H	84	LYS	2.1
11	K	28	VAL	2.1
2	B	115	ASP	2.1
11	K	54	ARG	2.1
7	G	45	PRO	2.1
3	C	37	PHE	2.1
4	Q	87	PHE	2.1
7	G	12	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	40	GLY	2.0
3	P	37	PHE	2.0
4	D	87	PHE	2.0
10	W	34	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.32	0.21	180,189,197,198	0
9	SAC	I	1	9/10	0.68	0.22	99,114,130,131	0
1	FME	N	1	10/11	0.91	0.15	34,43,83,105	0
1	FME	A	1	10/11	0.94	0.09	35,49,83,99	0
2	FME	B	1	10/11	0.96	0.12	27,31,39,120	0
2	FME	O	1	10/11	0.97	0.10	35,36,43,78	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	P	311	4/4	0.71	0.22	55,58,66,107	0
20	EDO	N	621	4/4	0.72	0.22	43,55,64,70	0
21	DMU	A	620	9/33	0.72	0.25	69,78,97,104	0
18	PGV	P	307	38/51	0.74	0.27	41,74,97,111	0
27	CDL	G	101	69/100	0.74	0.27	43,74,103,114	0
20	EDO	C	317	4/4	0.75	0.21	43,69,73,74	0
21	DMU	D	207	8/33	0.76	0.25	59,75,89,97	0
20	EDO	C	319	4/4	0.76	0.16	70,70,71,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	DMU	K	103	9/33	0.77	0.28	61,87,107,112	0
20	EDO	C	318	4/4	0.77	0.20	57,74,80,83	0
25	CHD	L	102	29/29	0.78	0.24	52,97,132,158	0
21	DMU	X	103	10/33	0.78	0.26	63,81,89,91	0
27	CDL	T	101	70/100	0.78	0.23	46,72,109,137	0
21	DMU	X	101	9/33	0.79	0.21	60,74,88,88	0
22	TGL	B	301	63/63	0.80	0.21	33,71,116,127	0
22	TGL	N	608	55/63	0.80	0.23	49,72,120,127	0
21	DMU	Q	202	10/33	0.80	0.25	58,61,87,98	0
26	PEK	P	303	28/53	0.80	0.22	45,58,92,106	0
18	PGV	C	307	37/51	0.80	0.25	41,72,107,115	0
20	EDO	C	314	4/4	0.80	0.24	57,60,86,89	0
21	DMU	P	310	22/33	0.81	0.18	40,68,94,112	0
22	TGL	D	201	63/63	0.81	0.23	33,67,134,153	0
26	PEK	C	303	18/53	0.81	0.19	44,52,87,92	0
20	EDO	F	107	4/4	0.82	0.23	46,49,61,109	0
26	PEK	P	305	40/53	0.82	0.23	38,75,101,126	0
18	PGV	A	606	33/51	0.82	0.22	32,56,99,123	0
18	PGV	Q	201	37/51	0.82	0.23	43,65,110,121	0
26	PEK	C	305	40/53	0.83	0.21	42,70,103,122	0
21	DMU	K	102	9/33	0.83	0.23	61,71,95,102	0
20	EDO	S	105	4/4	0.83	0.18	60,74,77,87	0
25	CHD	P	309	29/29	0.83	0.18	40,77,135,146	0
21	DMU	K	104	10/33	0.83	0.25	52,65,87,94	0
24	PSC	B	303	41/52	0.84	0.19	46,78,116,162	0
25	CHD	C	309	29/29	0.84	0.15	46,58,110,165	0
20	EDO	J	101	4/4	0.84	0.20	50,51,84,98	0
22	TGL	N	606	63/63	0.84	0.22	45,77,110,145	0
21	DMU	X	102	8/33	0.84	0.17	65,71,83,84	0
27	CDL	P	308	77/100	0.85	0.21	41,75,129,151	0
20	EDO	C	311	4/4	0.86	0.16	33,39,42,42	0
20	EDO	N	620	4/4	0.86	0.22	49,53,55,64	0
21	DMU	C	320	12/33	0.86	0.20	60,63,88,92	0
20	EDO	D	205	4/4	0.86	0.17	56,60,62,71	0
20	EDO	A	619	4/4	0.86	0.14	53,62,70,73	0
20	EDO	P	312	4/4	0.86	0.15	39,40,47,54	0
20	EDO	P	317	4/4	0.86	0.17	54,59,60,67	0
27	CDL	C	308	85/100	0.86	0.18	42,72,133,153	0
22	TGL	N	607	43/63	0.86	0.23	41,60,99,125	0
21	DMU	L	104	21/33	0.86	0.20	51,77,98,107	0
20	EDO	S	104	4/4	0.86	0.17	55,60,61,83	0
21	DMU	C	310	22/33	0.87	0.16	29,59,107,121	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	EDO	D	204	4/4	0.87	0.14	45,49,58,58	0
21	DMU	D	206	11/33	0.87	0.17	46,70,82,83	0
20	EDO	Y	101	4/4	0.87	0.15	46,54,58,61	0
20	EDO	M	102	4/4	0.87	0.14	58,60,82,86	0
24	PSC	O	302	33/52	0.88	0.20	29,62,99,125	0
20	EDO	J	102	4/4	0.88	0.16	53,56,56,70	0
20	EDO	L	103	4/4	0.88	0.21	38,75,81,126	0
20	EDO	Q	204	4/4	0.88	0.15	47,50,53,61	0
20	EDO	A	611	4/4	0.88	0.20	47,55,63,109	0
20	EDO	F	105	4/4	0.88	0.15	33,39,68,69	0
20	EDO	T	102	4/4	0.88	0.20	40,74,80,92	0
22	TGL	L	101	54/63	0.88	0.21	30,56,125,171	0
20	EDO	W	101	4/4	0.88	0.19	49,73,83,132	0
20	EDO	D	203	4/4	0.88	0.19	37,47,73,80	0
21	DMU	O	305	11/33	0.88	0.18	60,66,96,97	0
20	EDO	B	309	4/4	0.88	0.17	31,46,47,64	0
20	EDO	C	315	4/4	0.89	0.16	49,58,68,72	0
21	DMU	W	103	11/33	0.89	0.17	52,63,72,91	0
20	EDO	S	106	4/4	0.89	0.11	37,42,58,59	0
20	EDO	T	103	4/4	0.90	0.15	39,45,60,65	0
20	EDO	A	614	4/4	0.90	0.18	39,40,43,47	0
20	EDO	W	102	4/4	0.90	0.16	50,64,72,81	0
20	EDO	R	202	4/4	0.90	0.14	47,62,63,78	0
20	EDO	A	616	4/4	0.90	0.17	42,49,58,67	0
21	DMU	P	318	11/33	0.90	0.18	45,62,80,85	0
29	PO4	U	101	5/5	0.90	0.12	53,54,120,187	0
20	EDO	B	307	4/4	0.91	0.14	41,50,54,81	0
20	EDO	P	315	4/4	0.91	0.12	28,39,40,52	0
20	EDO	F	106	4/4	0.91	0.18	37,38,45,101	0
29	PO4	H	101	5/5	0.91	0.12	59,71,91,156	0
21	DMU	J	103	11/33	0.91	0.16	49,59,88,96	0
21	DMU	Z	101	33/33	0.92	0.10	37,47,69,80	0
21	DMU	M	101	33/33	0.92	0.10	34,43,60,77	0
21	DMU	N	622	9/33	0.92	0.16	48,68,78,80	0
20	EDO	A	613	4/4	0.92	0.19	43,53,63,82	0
20	EDO	E	203	4/4	0.92	0.12	44,44,48,70	0
20	EDO	P	313	4/4	0.92	0.11	55,57,62,74	0
21	DMU	K	101	9/33	0.92	0.17	54,62,82,91	0
20	EDO	F	104	4/4	0.92	0.14	39,40,59,88	0
20	EDO	P	316	4/4	0.92	0.11	49,57,59,62	0
20	EDO	S	108	4/4	0.92	0.18	38,50,60,72	0
20	EDO	B	310	4/4	0.92	0.13	41,47,48,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	EDO	B	305	4/4	0.93	0.13	37,44,49,54	0
17	NA	P	302	1/1	0.93	0.09	39,39,39,39	0
20	EDO	N	614	4/4	0.93	0.20	33,36,50,107	0
20	EDO	N	617	4/4	0.93	0.16	32,42,45,66	0
20	EDO	C	316	4/4	0.93	0.14	29,34,40,52	0
20	EDO	B	308	4/4	0.93	0.18	34,38,47,113	0
20	EDO	A	609	4/4	0.94	0.13	29,33,44,92	0
20	EDO	E	202	4/4	0.94	0.09	36,38,40,45	0
20	EDO	A	617	4/4	0.94	0.10	28,29,31,34	0
20	EDO	N	618	4/4	0.94	0.12	29,45,62,64	0
19	OXY	N	609	2/2	0.94	0.19	16,16,16,25	2
21	DMU	A	621	8/33	0.94	0.12	46,50,67,77	0
20	EDO	C	313	4/4	0.94	0.14	35,56,64,109	0
20	EDO	Q	203	4/4	0.94	0.12	29,47,51,73	0
20	EDO	B	306	4/4	0.95	0.08	25,27,30,33	0
20	EDO	O	304	4/4	0.95	0.09	42,47,54,57	0
20	EDO	N	611	4/4	0.95	0.08	22,27,29,32	0
20	EDO	A	612	4/4	0.95	0.15	28,40,76,100	0
20	EDO	N	615	4/4	0.95	0.10	41,41,42,50	0
26	PEK	P	304	53/53	0.95	0.13	27,44,94,113	0
20	EDO	P	314	4/4	0.95	0.14	35,36,37,44	0
20	EDO	N	616	4/4	0.95	0.11	36,41,42,47	0
19	OXY	A	607	2/2	0.95	0.18	14,14,14,29	2
20	EDO	T	104	4/4	0.95	0.10	29,32,38,43	0
17	NA	C	302	1/1	0.95	0.08	40,40,40,40	0
25	CHD	C	301	29/29	0.95	0.07	25,28,35,38	0
20	EDO	A	615	4/4	0.95	0.17	32,39,39,119	0
20	EDO	N	612	4/4	0.96	0.08	26,27,28,29	0
20	EDO	S	107	4/4	0.96	0.10	28,30,33,33	0
20	EDO	N	613	4/4	0.96	0.08	38,39,42,47	0
18	PGV	P	306	51/51	0.96	0.11	22,30,82,104	0
20	EDO	R	201	4/4	0.96	0.08	41,41,42,44	0
18	PGV	A	608	51/51	0.96	0.11	22,28,70,89	0
20	EDO	S	103	4/4	0.96	0.09	35,37,40,45	0
20	EDO	O	303	4/4	0.96	0.09	30,32,32,33	0
18	PGV	N	610	51/51	0.96	0.11	24,31,69,80	0
26	PEK	C	304	53/53	0.96	0.12	25,43,94,114	0
20	EDO	G	103	4/4	0.97	0.07	29,32,37,37	0
20	EDO	A	618	4/4	0.97	0.12	30,37,45,51	0
20	EDO	F	103	4/4	0.97	0.09	31,31,31,33	0
20	EDO	C	312	4/4	0.97	0.07	32,34,35,36	0
18	PGV	C	306	51/51	0.97	0.10	23,29,83,100	0

Continued on next page...

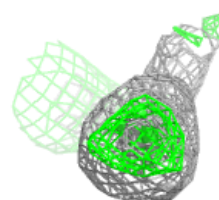
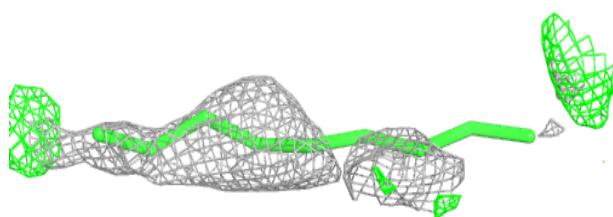
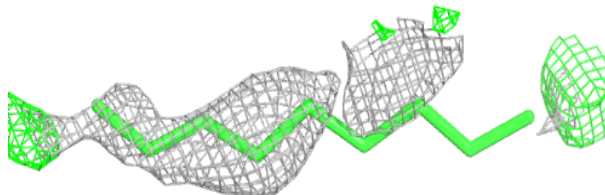
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CHD	B	304	29/29	0.97	0.06	23,27,32,43	0
20	EDO	E	201	4/4	0.97	0.09	38,40,43,43	0
20	EDO	S	102	4/4	0.97	0.08	23,24,25,25	0
25	CHD	G	102	29/29	0.97	0.06	22,26,30,39	0
20	EDO	N	619	4/4	0.97	0.09	30,38,39,43	0
25	CHD	P	301	29/29	0.97	0.07	25,29,37,39	0
20	EDO	D	202	4/4	0.97	0.08	33,35,56,63	0
16	MG	A	604	1/1	0.98	0.05	20,20,20,20	0
14	HEA	A	602	60/60	0.98	0.06	19,23,29,36	0
20	EDO	F	102	4/4	0.98	0.05	24,24,24,26	0
20	EDO	A	610	4/4	0.98	0.06	21,23,26,29	0
14	HEA	N	602	60/60	0.98	0.06	20,24,30,35	0
23	CUA	O	301	2/2	0.99	0.03	27,27,27,27	0
14	HEA	N	601[B]	54/60	0.99	0.07	20,25,38,41	12
14	HEA	N	601[C]	51/60	0.99	0.07	20,25,36,42	9
14	HEA	A	601[B]	54/60	0.99	0.07	17,21,31,38	12
15	CU	N	603	1/1	0.99	0.03	24,24,24,24	0
14	HEA	A	601[C]	51/60	0.99	0.07	17,21,28,36	9
16	MG	N	604	1/1	0.99	0.04	23,23,23,23	0
17	NA	A	605	1/1	0.99	0.06	27,27,27,27	0
14	HEA	A	601[A]	60/60	0.99	0.07	15,21,41,52	18
28	ZN	S	101	1/1	0.99	0.03	27,27,27,27	0
17	NA	N	605	1/1	0.99	0.03	31,31,31,31	0
14	HEA	N	601[A]	60/60	0.99	0.07	17,26,42,50	18
15	CU	A	603	1/1	1.00	0.02	22,22,22,22	0
23	CUA	B	302	2/2	1.00	0.02	24,24,24,24	0
28	ZN	F	101	1/1	1.00	0.03	26,26,26,26	0

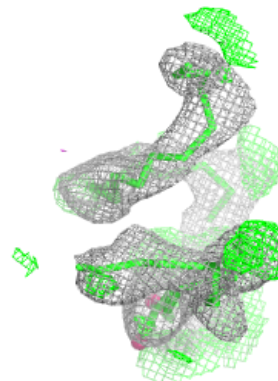
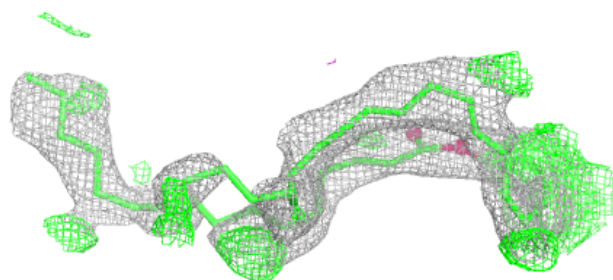
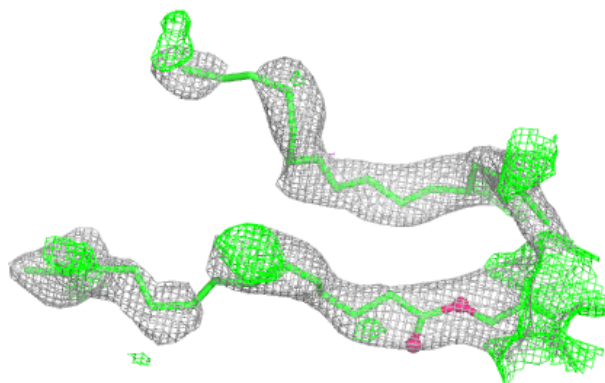
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU A 620:

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

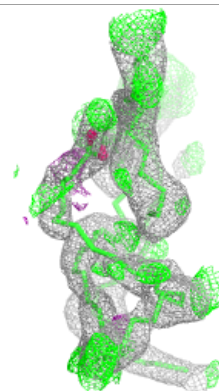
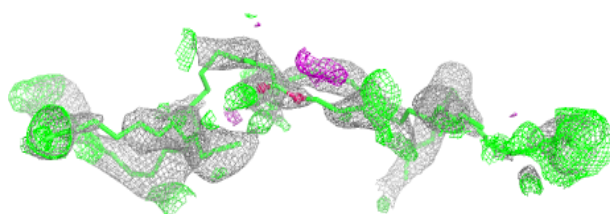
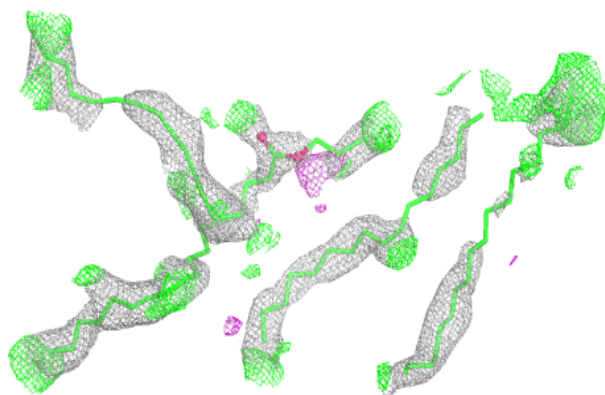
**Electron density around PGV P 307:**

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

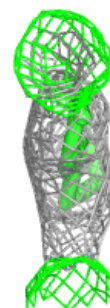
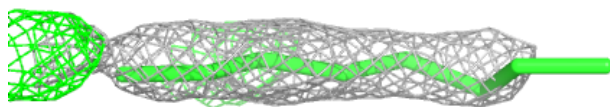
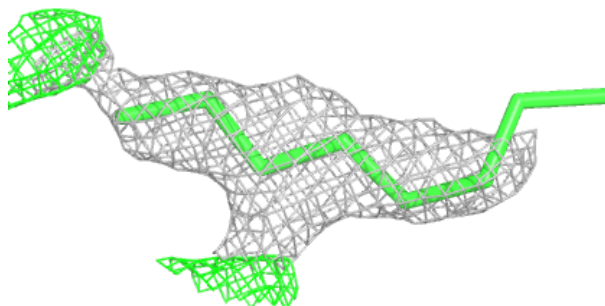


Electron density around CDL G 101:

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

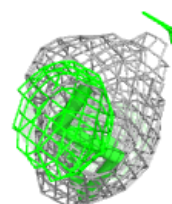
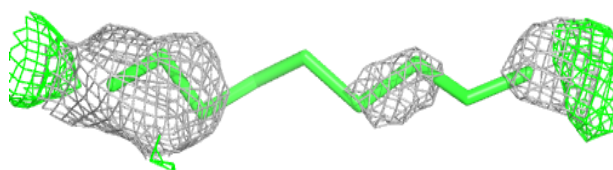
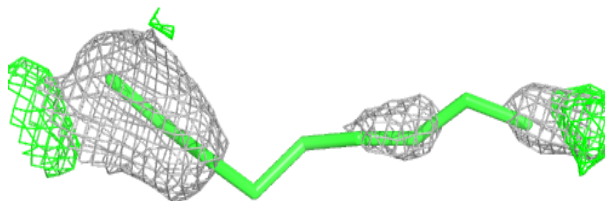
**Electron density around DMU D 207:**

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

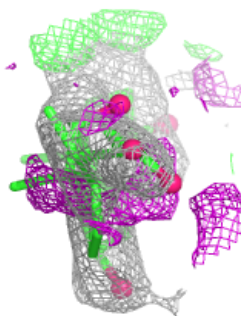
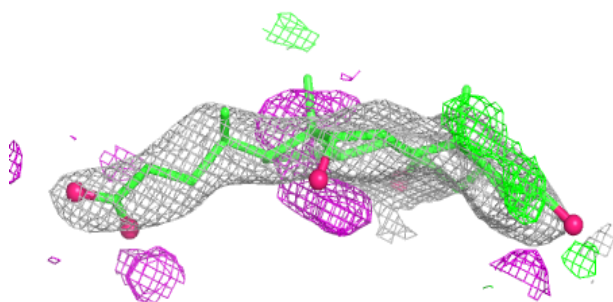
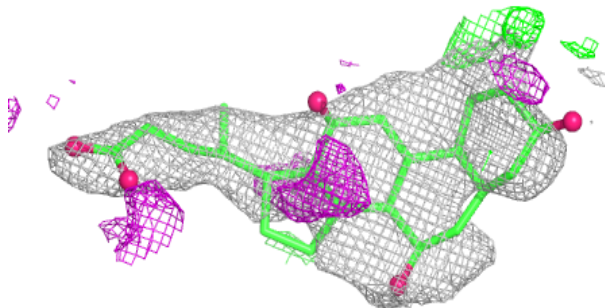


Electron density around DMU K 103:

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

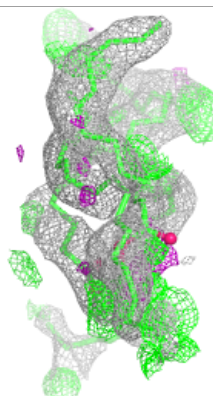
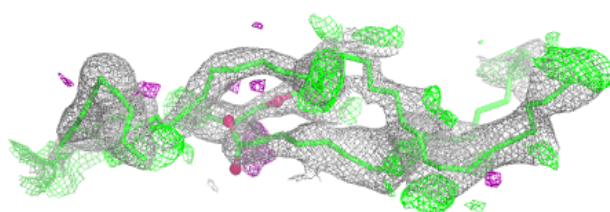
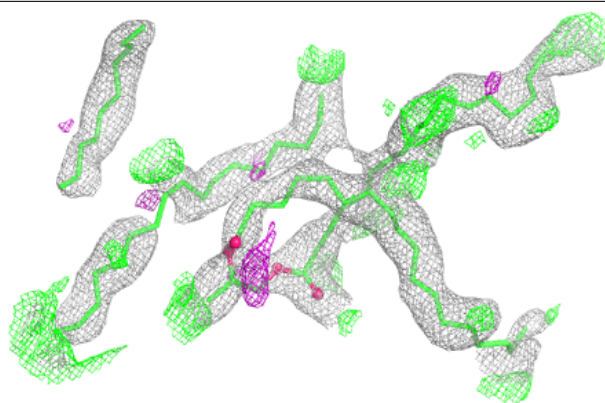
**Electron density around CHD L 102:**

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

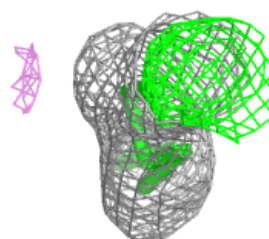
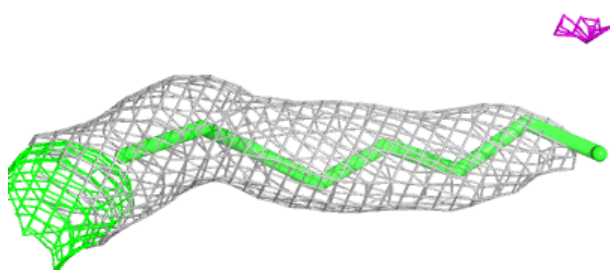
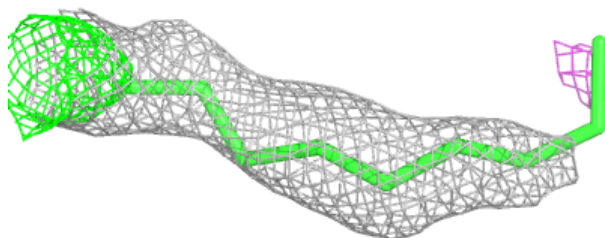


Electron density around CDL T 101:

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

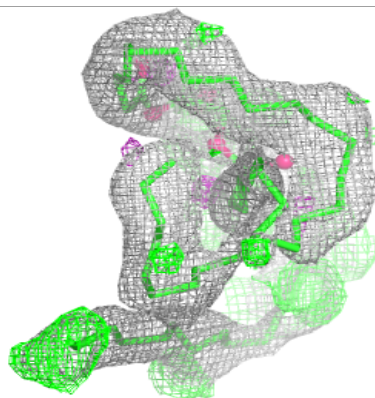
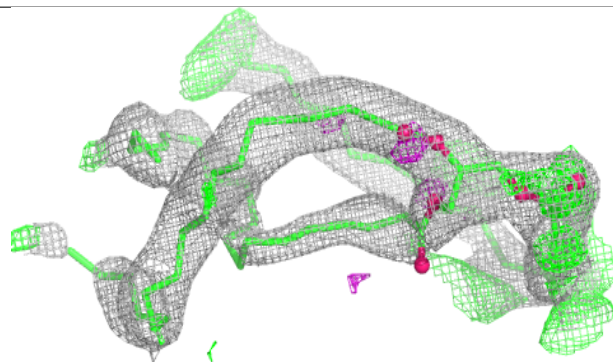
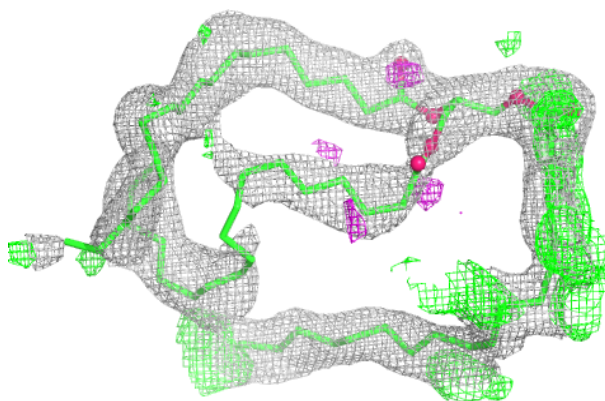
**Electron density around DMU X 101:**

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

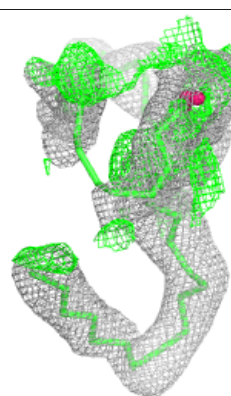
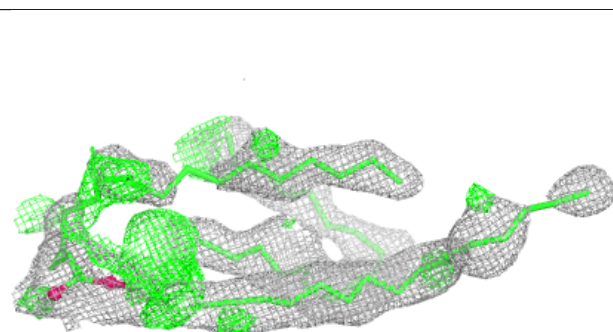
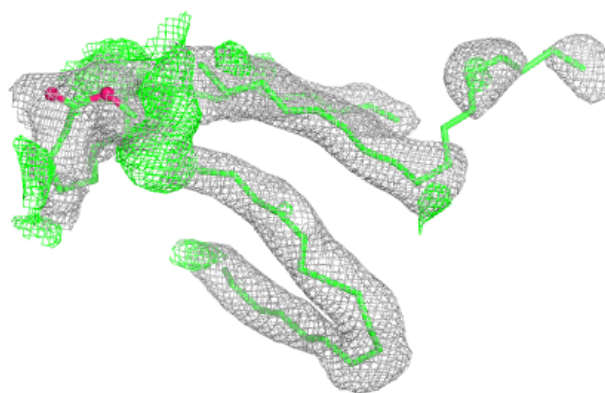


Electron density around TGL B 301:

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

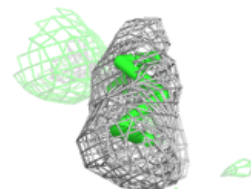
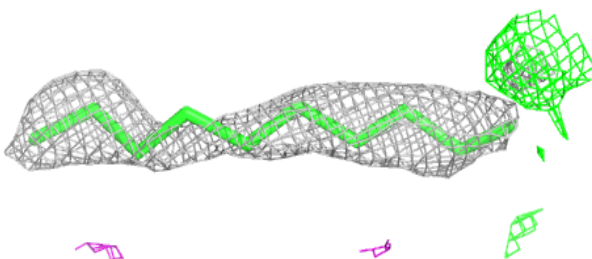
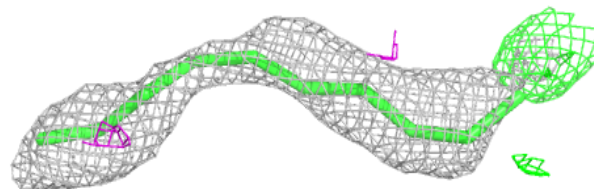
**Electron density around TGL N 608:**

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

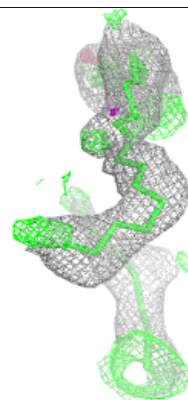
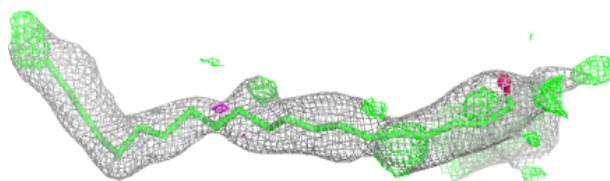
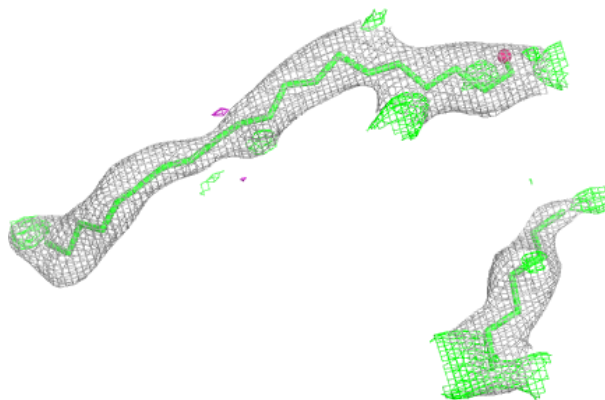


Electron density around DMU Q 202:

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

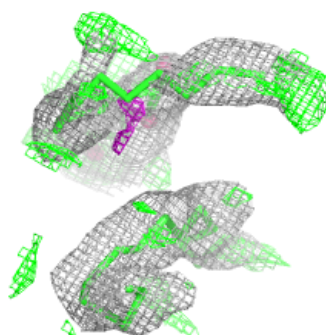
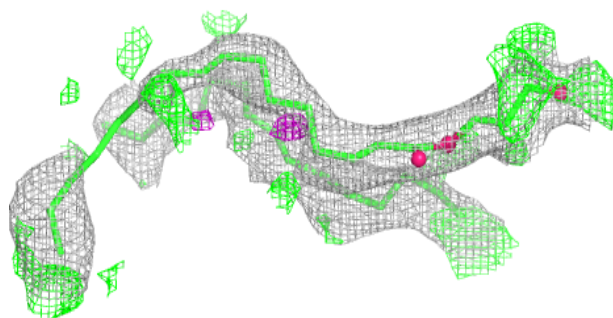
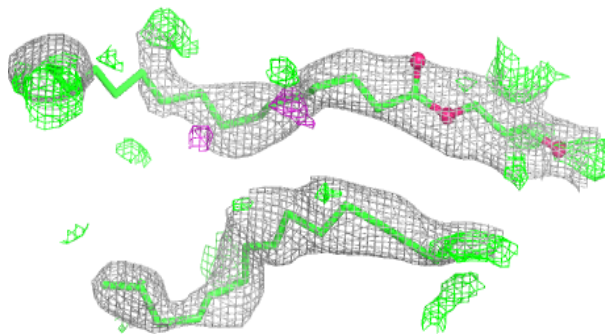
**Electron density around PEK P 303:**

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

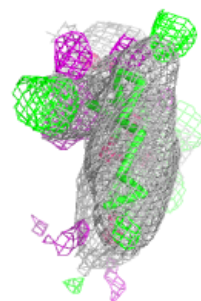
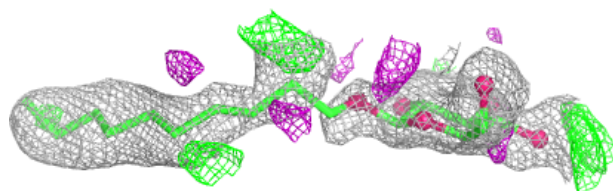
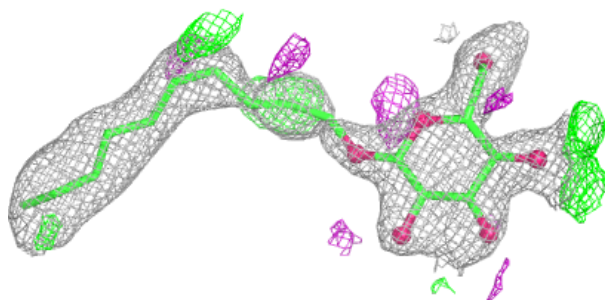


Electron density around PGV C 307:

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

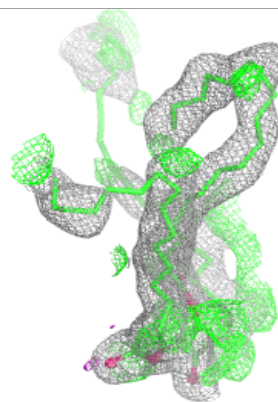
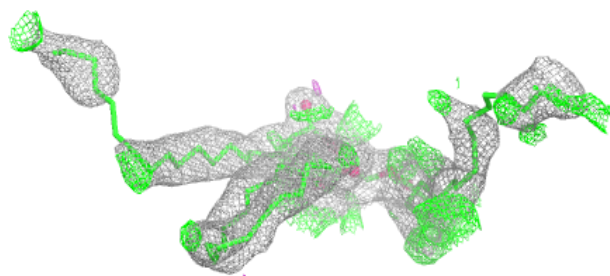
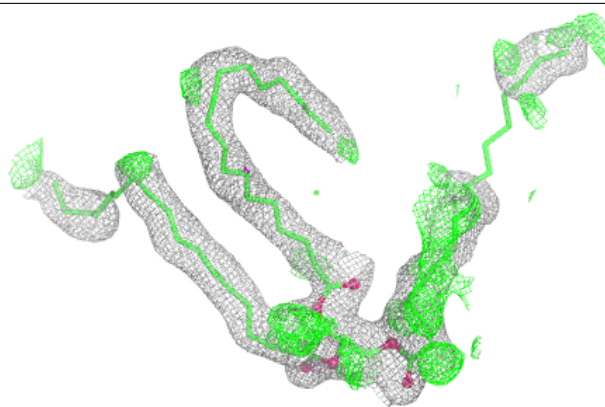
**Electron density around DMU P 310:**

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

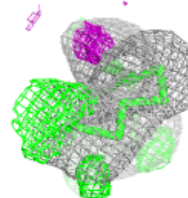
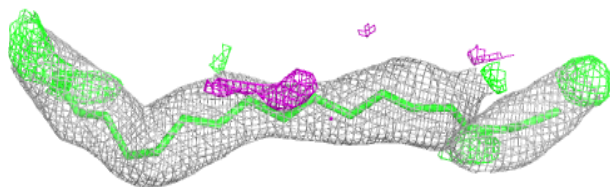
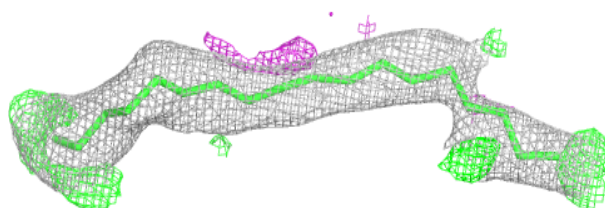


Electron density around TGL D 201:

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

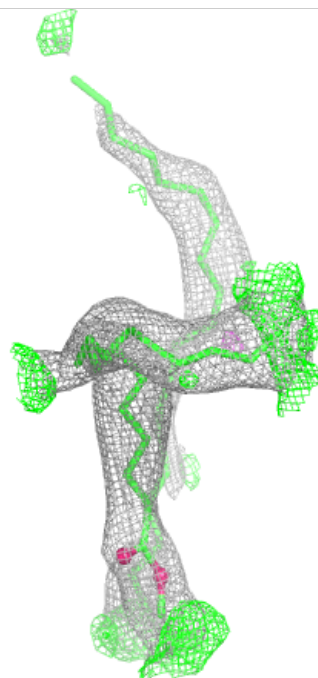
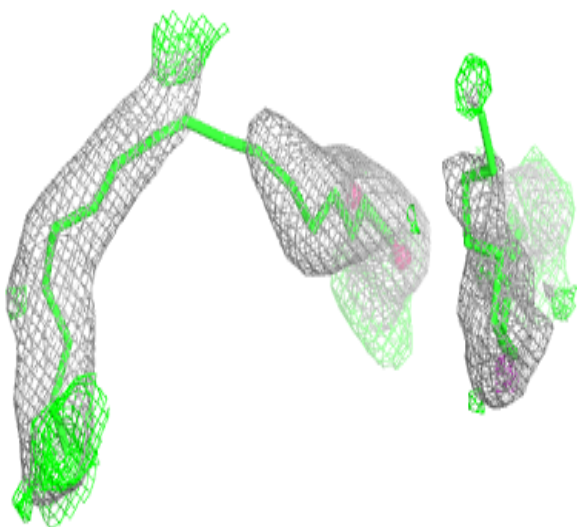
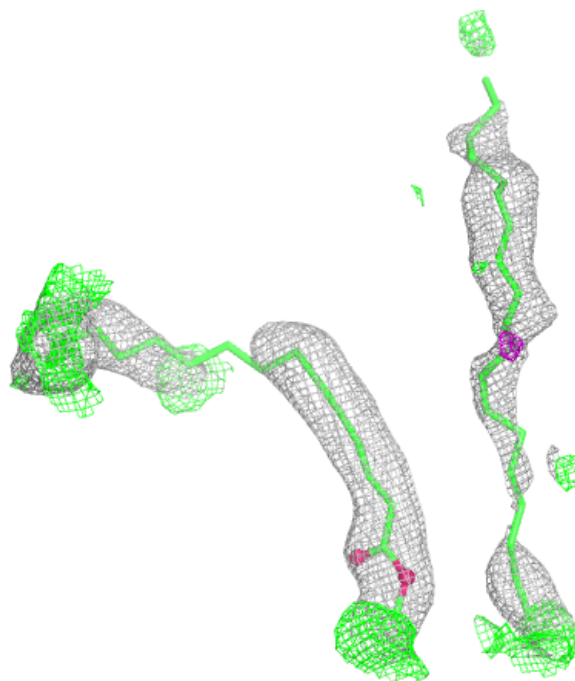
**Electron density around PEK C 303:**

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



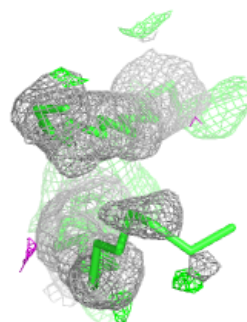
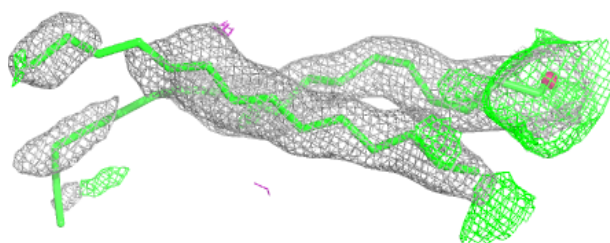
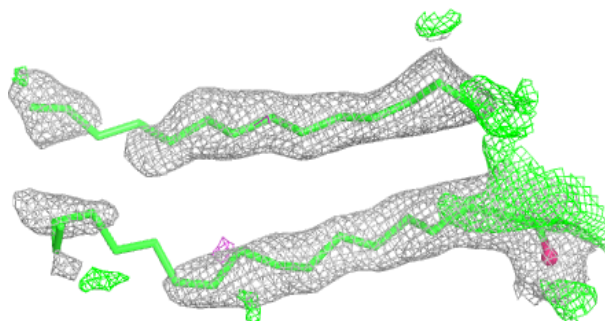
Electron density around PEK P 305:

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

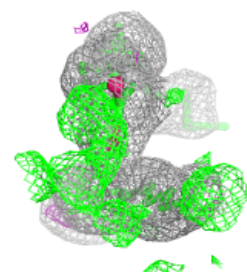
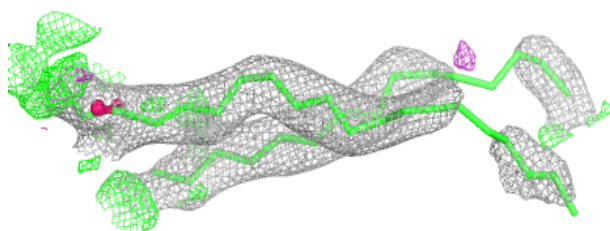
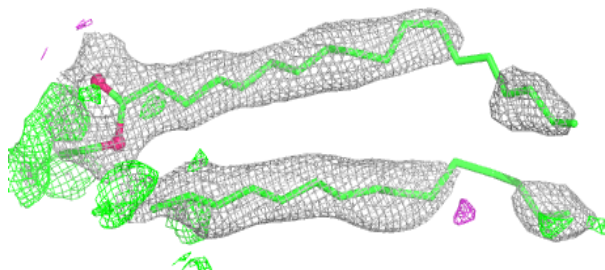


Electron density around PGV A 606:

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

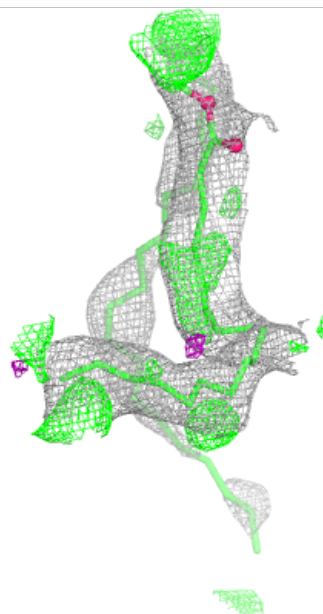
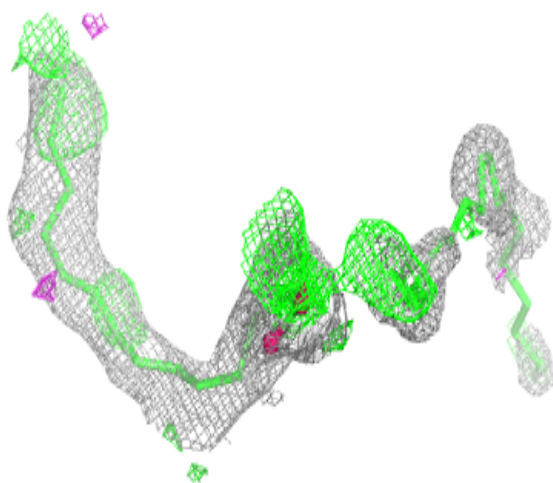
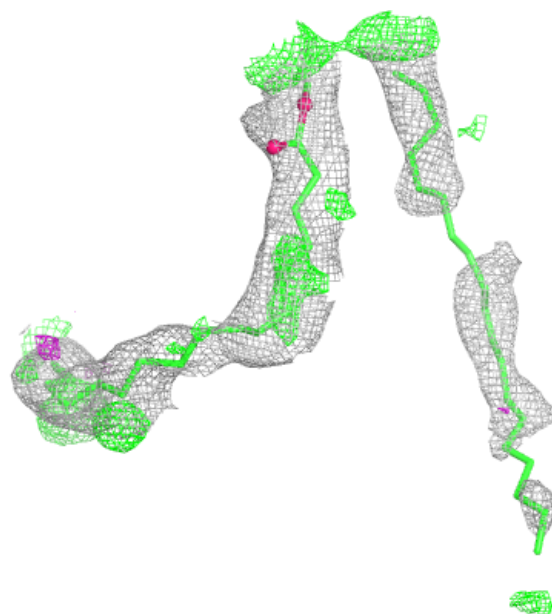
**Electron density around PGV Q 201:**

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



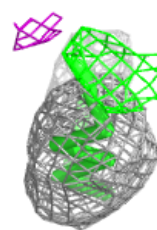
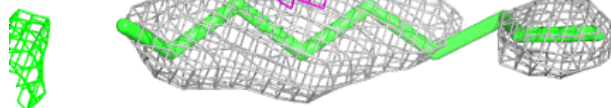
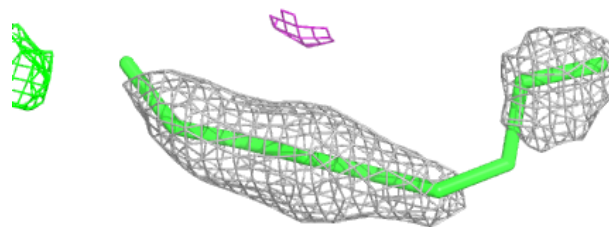
Electron density around PEK C 305:

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

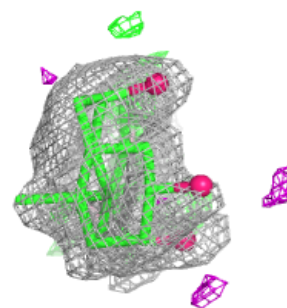
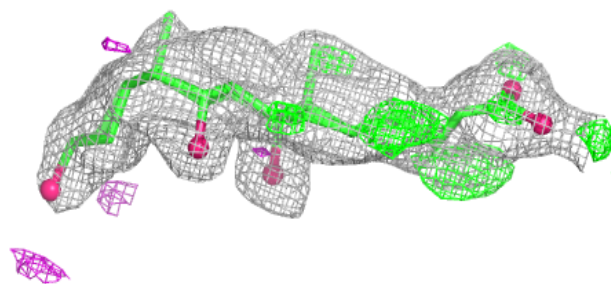
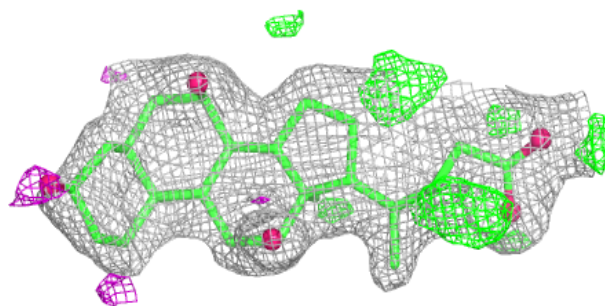


Electron density around DMU K 102:

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

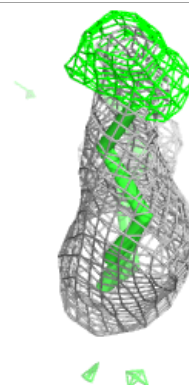
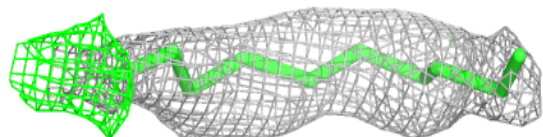
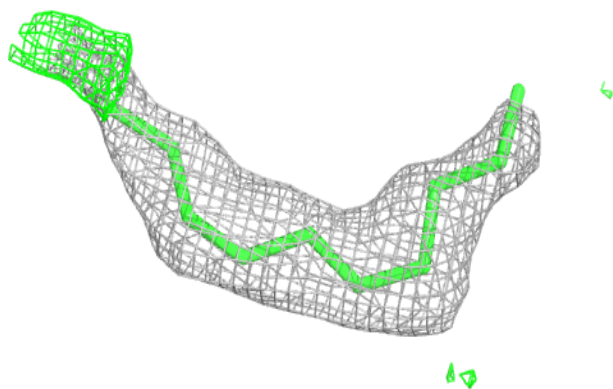
**Electron density around CHD P 309:**

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

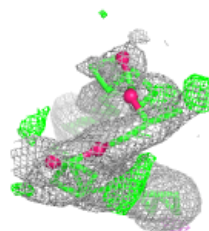
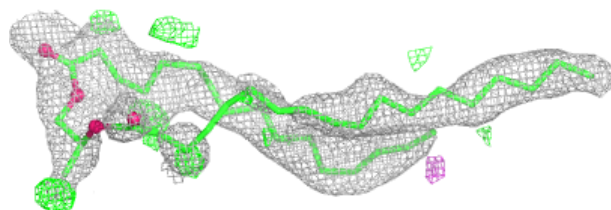
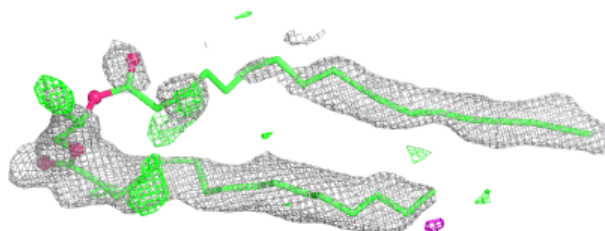


Electron density around DMU K 104:

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

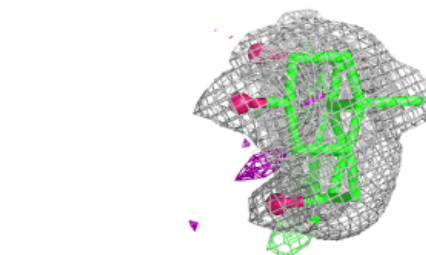
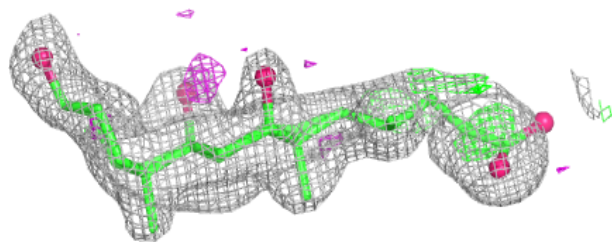
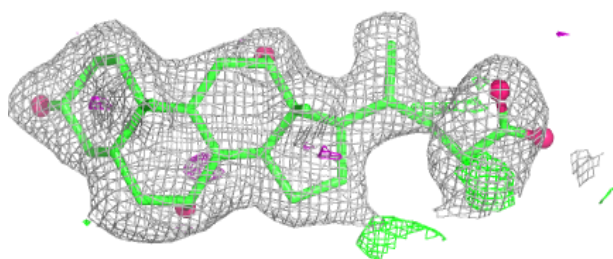
**Electron density around PSC B 303:**

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

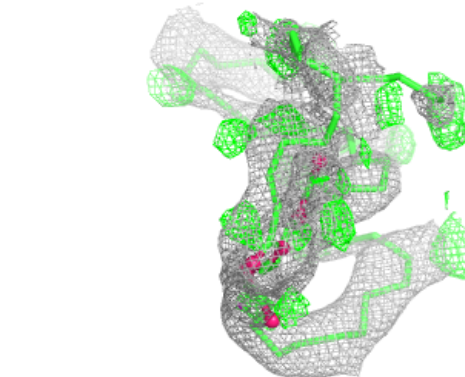
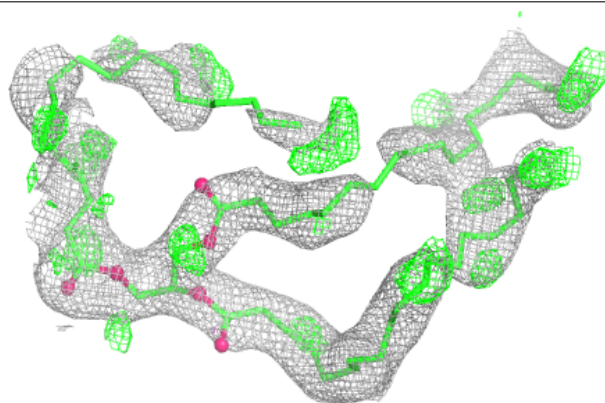


Electron density around CHD C 309:

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

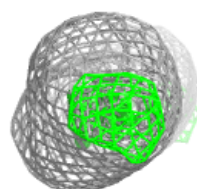
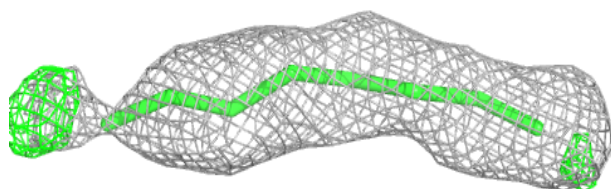
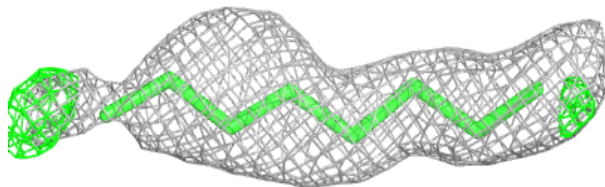
**Electron density around TGL N 606:**

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



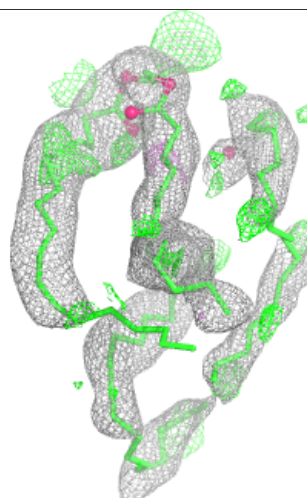
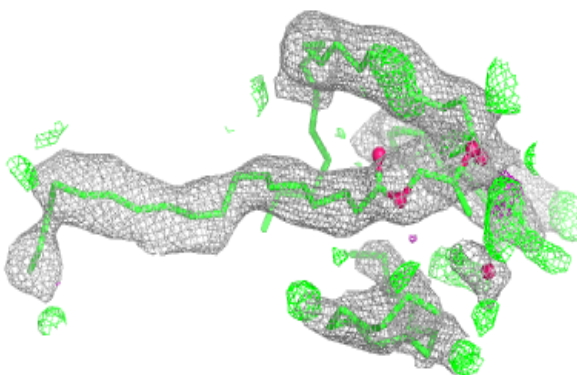
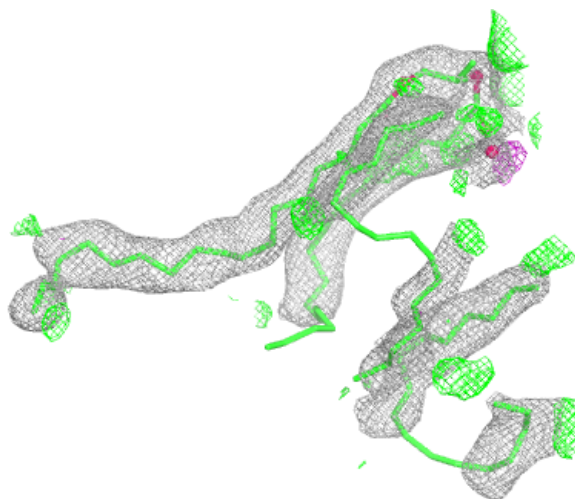
Electron density around DMU X 102:

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



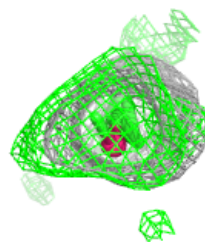
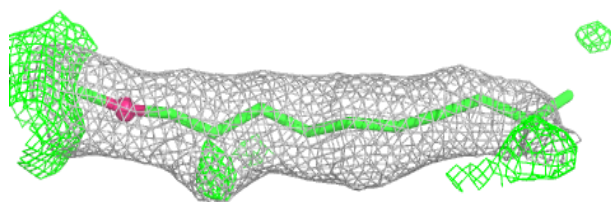
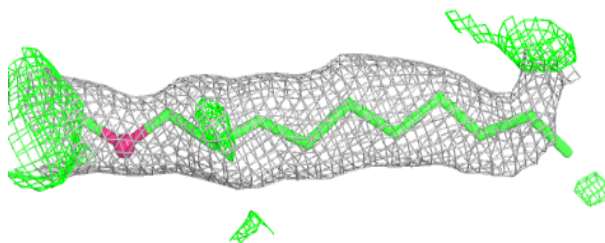
Electron density around CDL P 308:

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



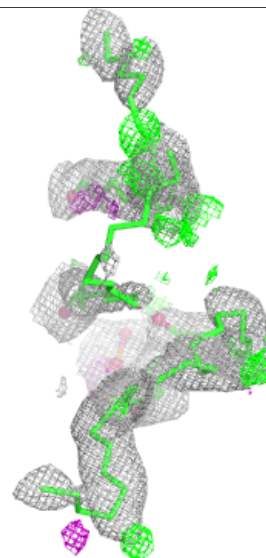
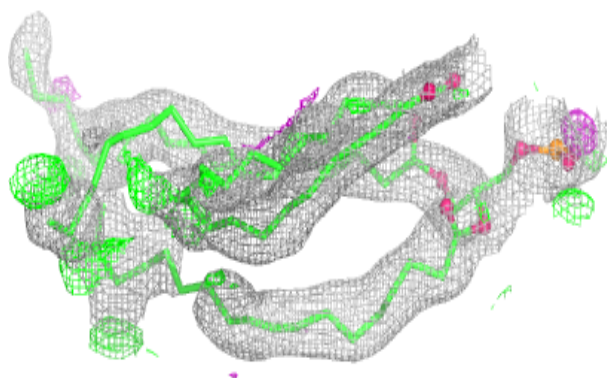
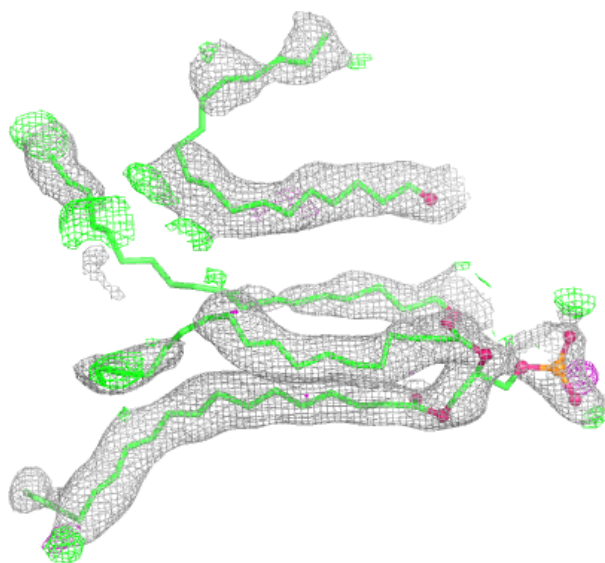
Electron density around DMU C 320:

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



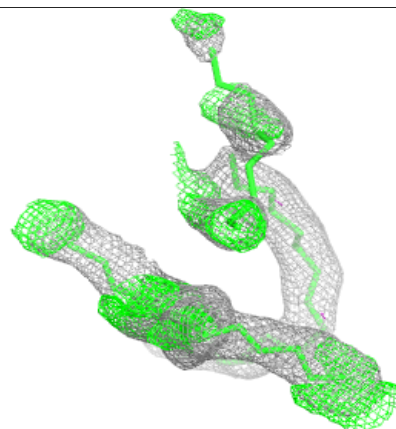
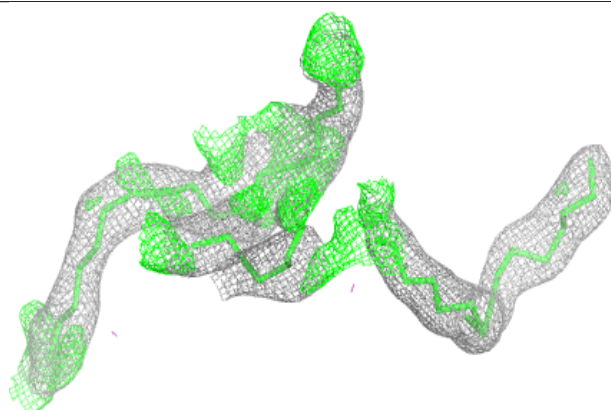
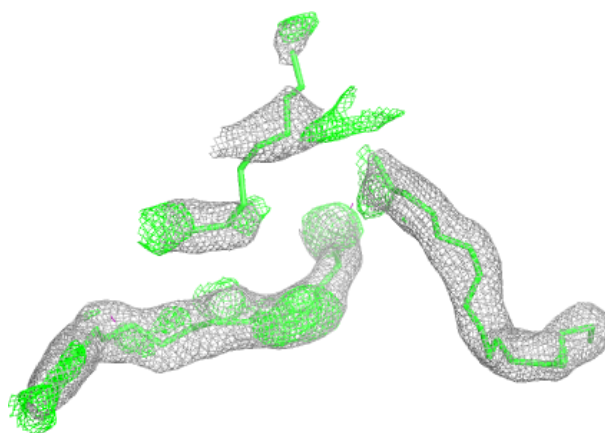
Electron density around CDL C 308:

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

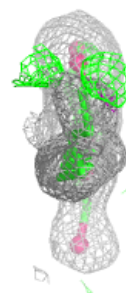
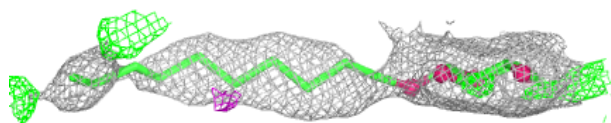
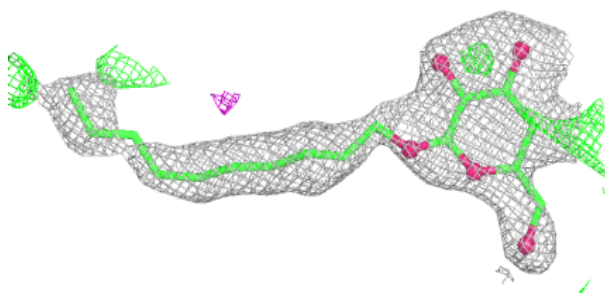


Electron density around TGL N 607:

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

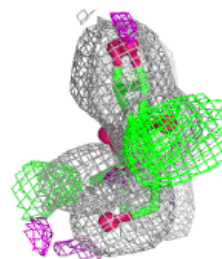
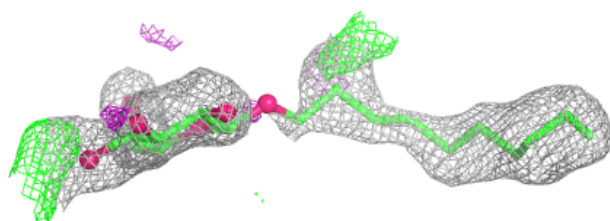
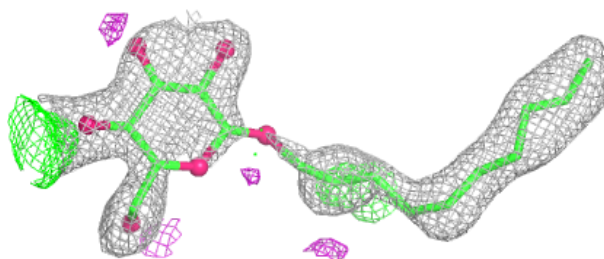
**Electron density around DMU L 104:**

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

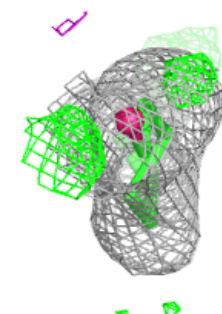
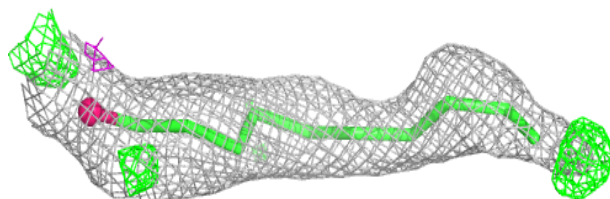
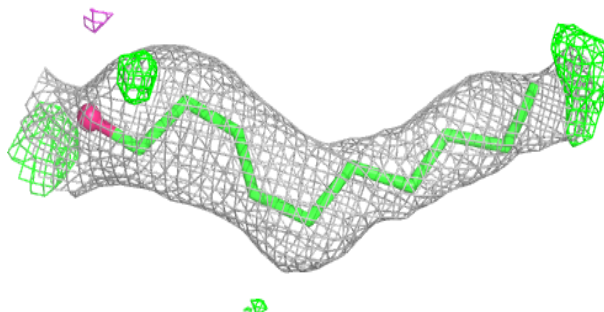


Electron density around DMU C 310:

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

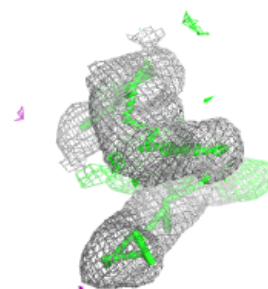
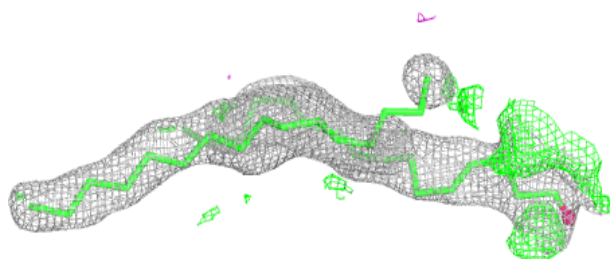
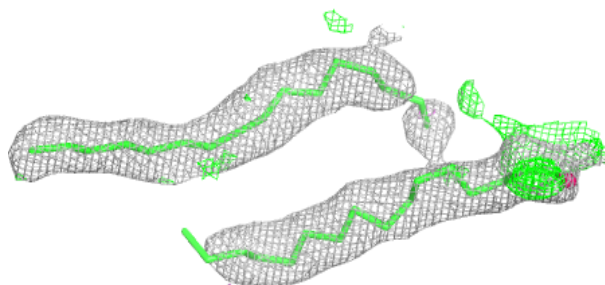
**Electron density around DMU D 206:**

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

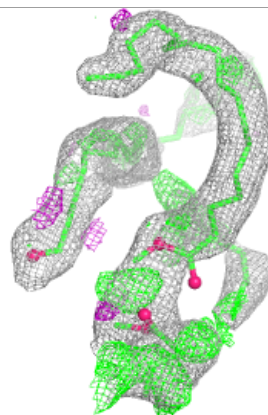
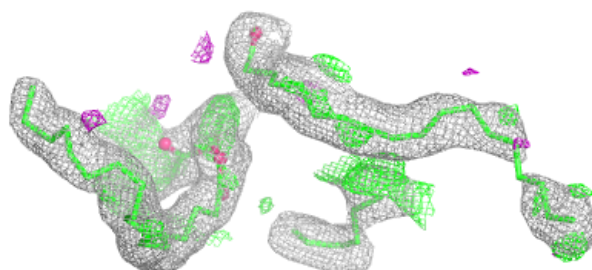
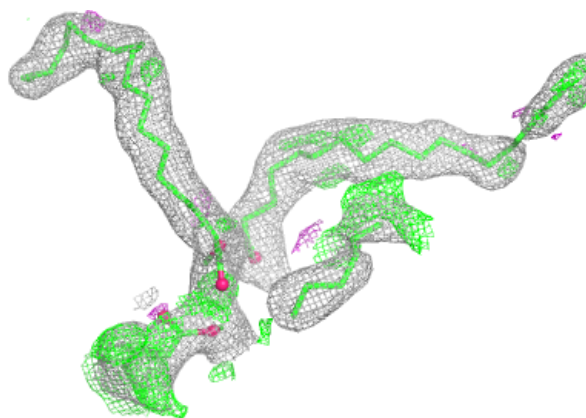


Electron density around PSC O 302:

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

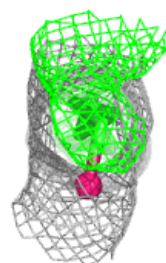
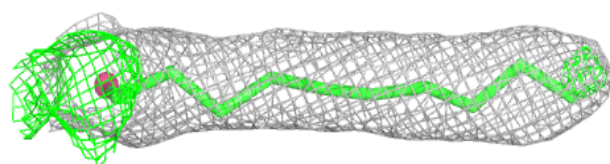
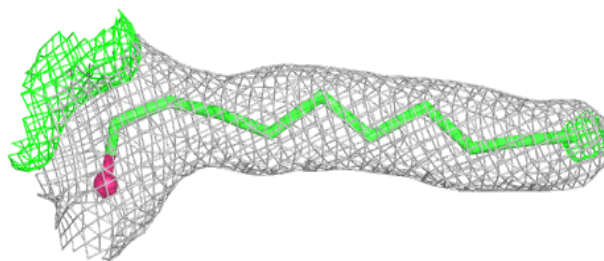
**Electron density around TGL L 101:**

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

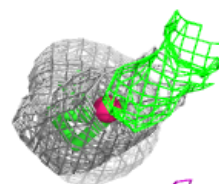
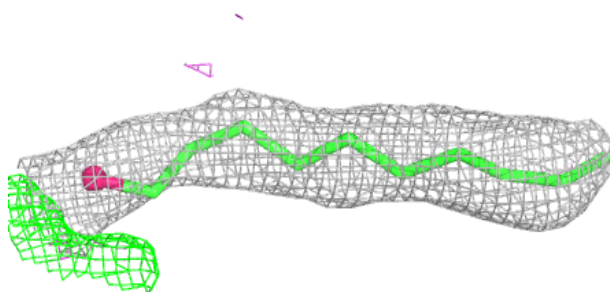
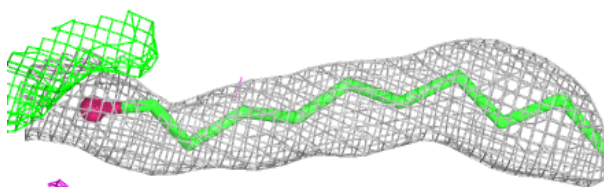


Electron density around DMU O 305:

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

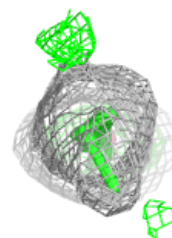
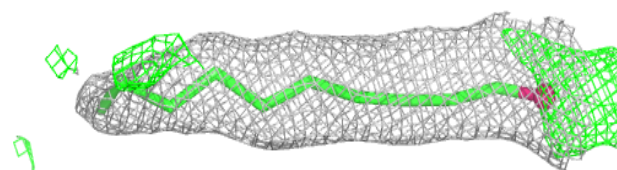
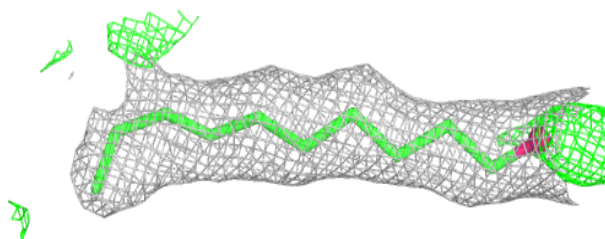
**Electron density around DMU W 103:**

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

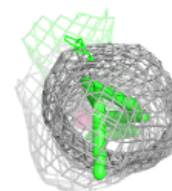
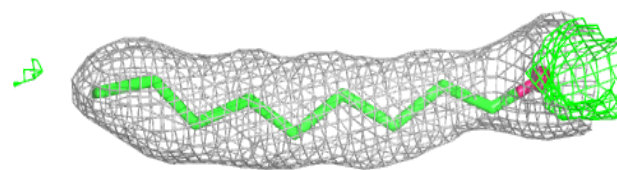
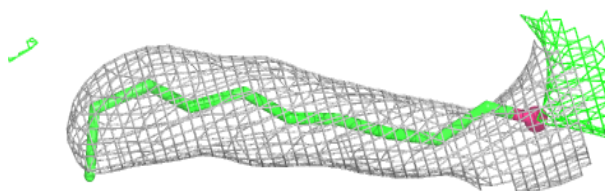


Electron density around DMU P 318:

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

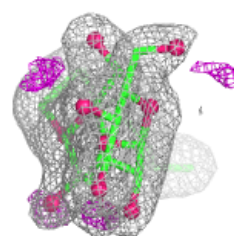
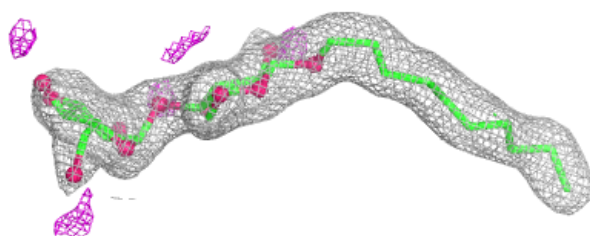
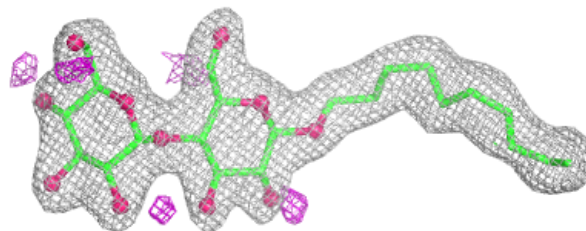
**Electron density around DMU J 103:**

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

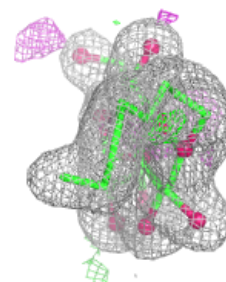
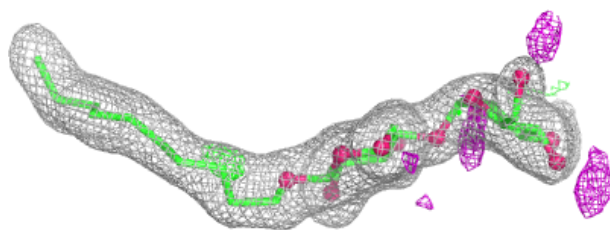
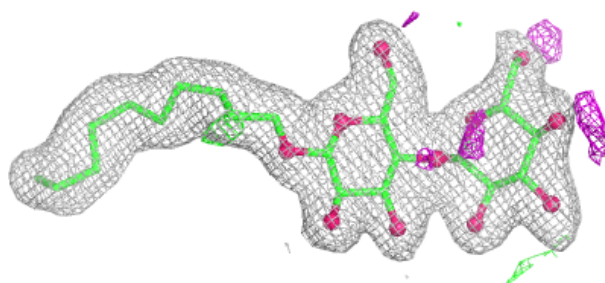


Electron density around DMU Z 101:

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

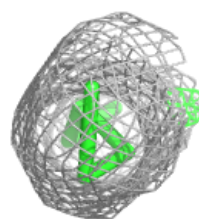
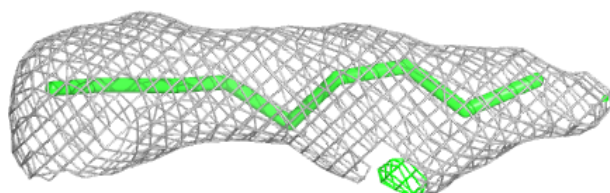
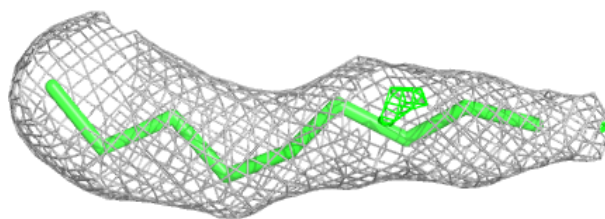
**Electron density around DMU M 101:**

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

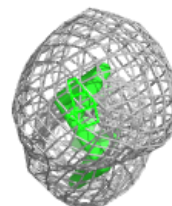
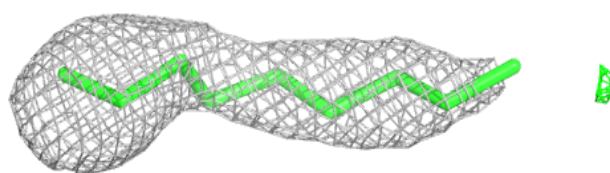
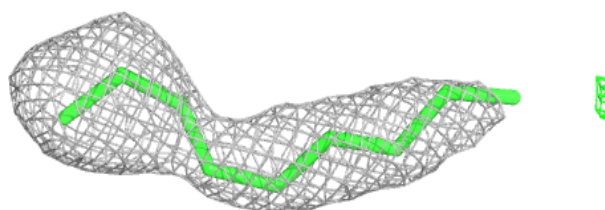


Electron density around DMU N 622:

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

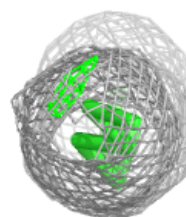
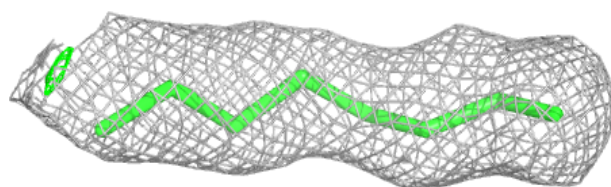
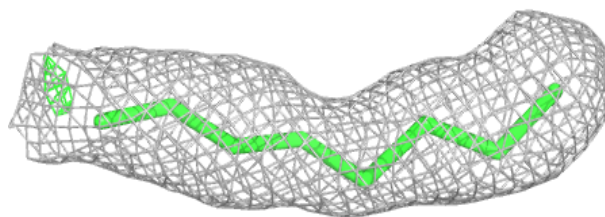
**Electron density around DMU K 101:**

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

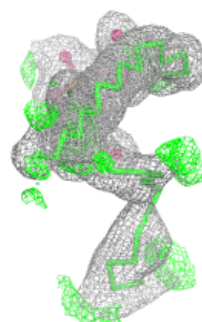
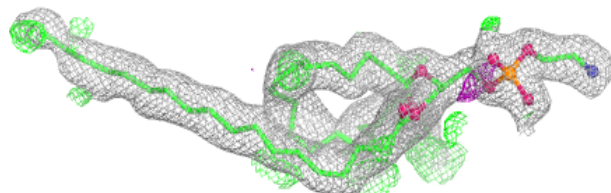
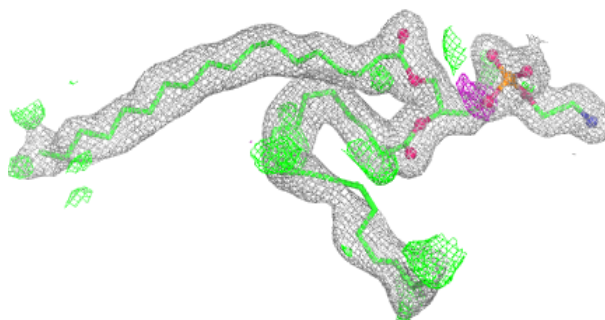


Electron density around DMU A 621:

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

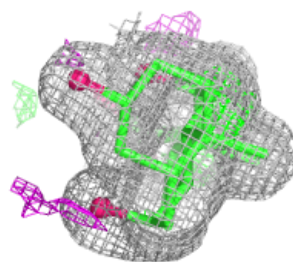
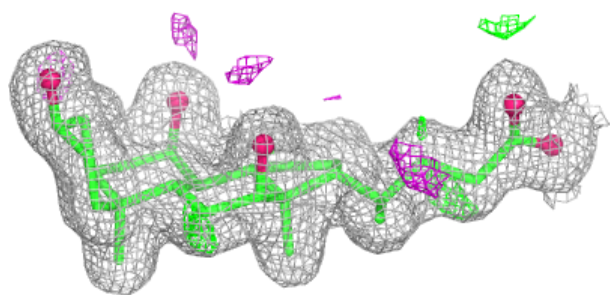
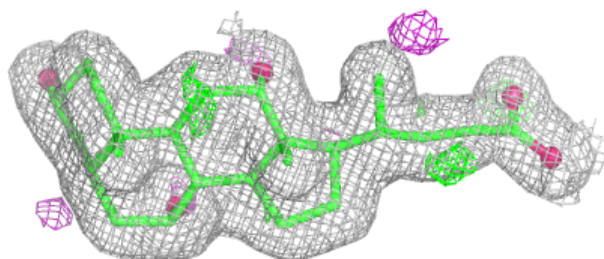
**Electron density around PEK P 304:**

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

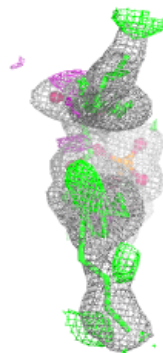
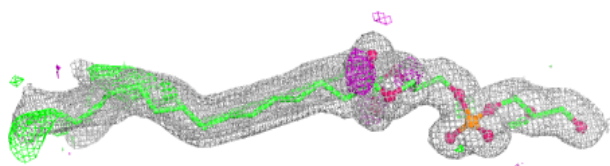
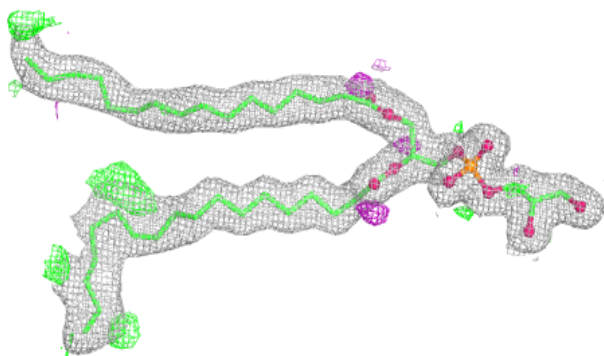


Electron density around CHD C 301:

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

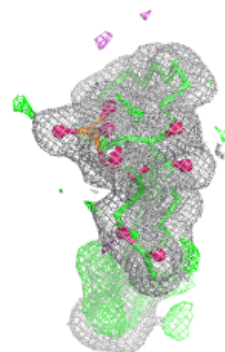
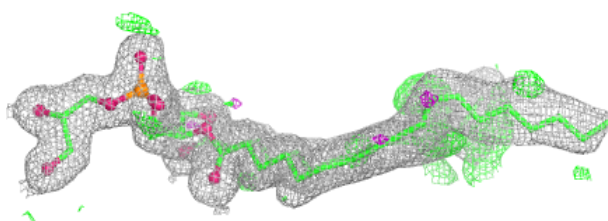
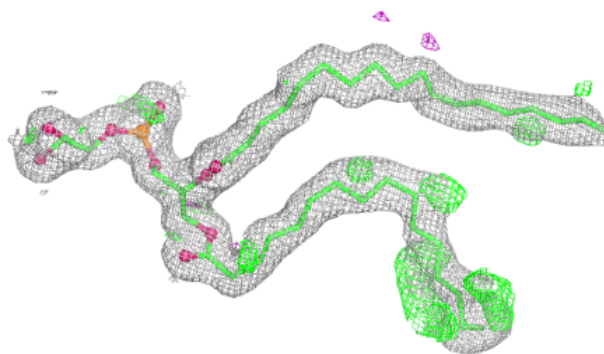
**Electron density around PGV P 306:**

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

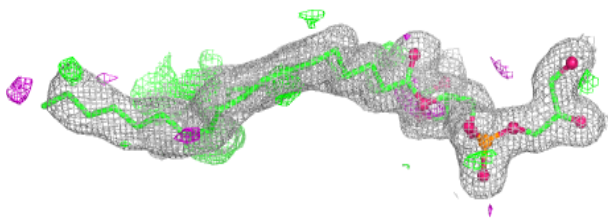
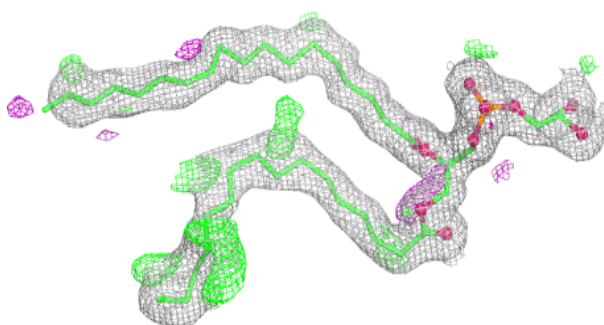


Electron density around PGV A 608:

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

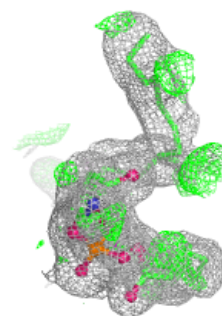
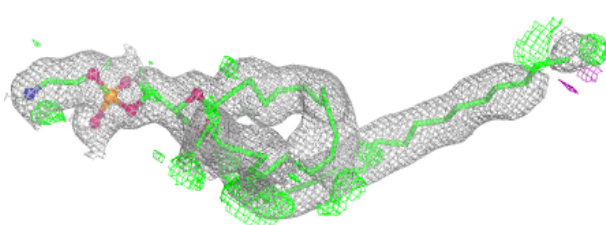
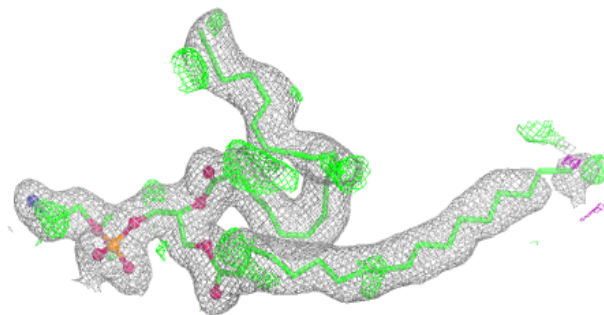
**Electron density around PGV N 610:**

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

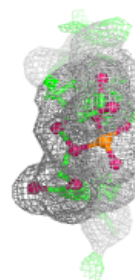
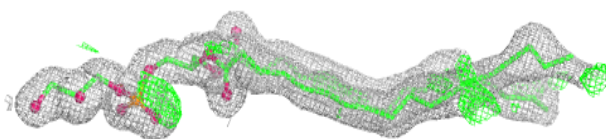
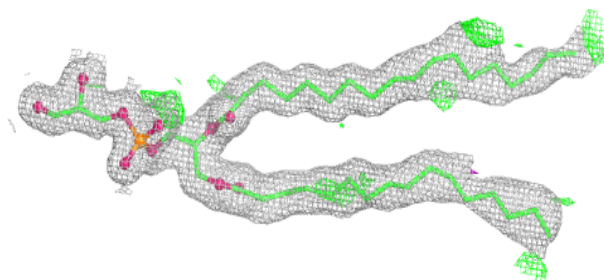


Electron density around PEK C 304:

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

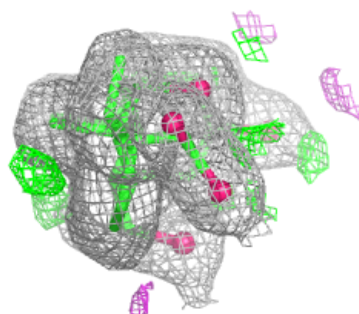
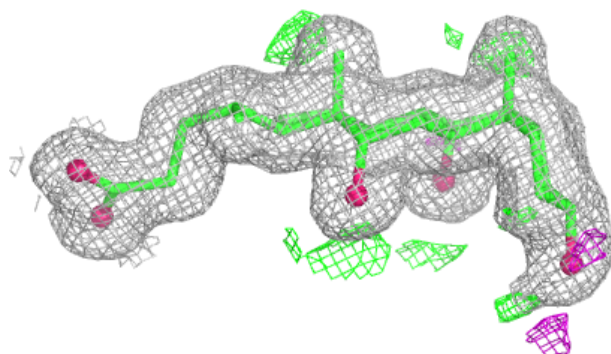
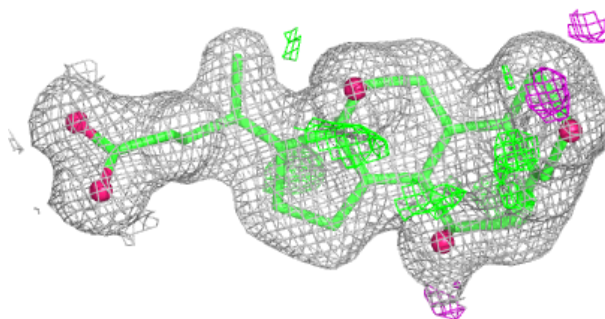
**Electron density around PGV C 306:**

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

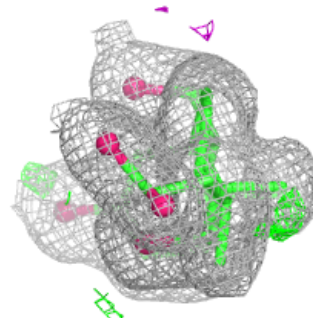
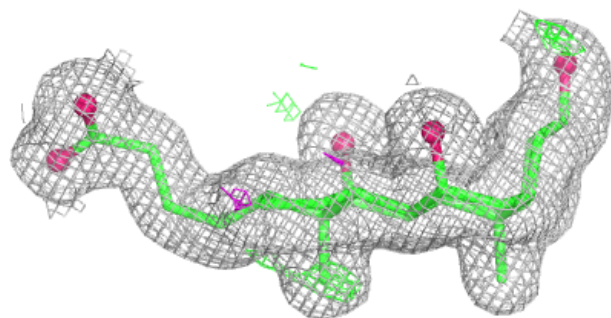
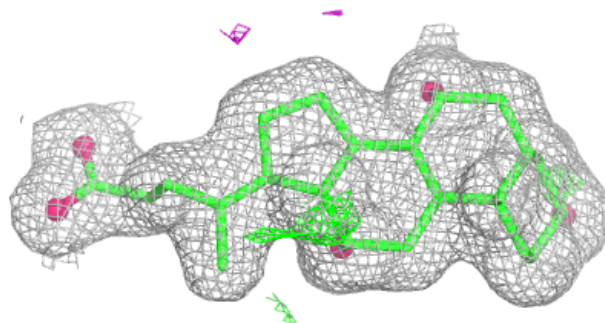


Electron density around CHD B 304:

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

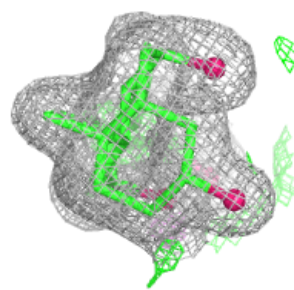
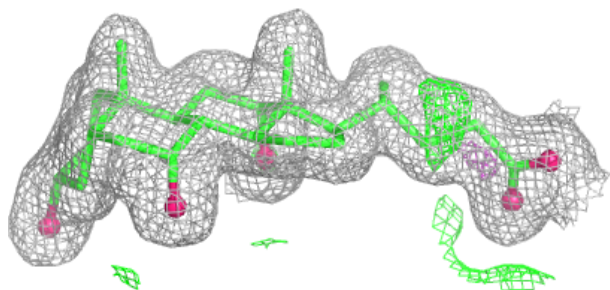
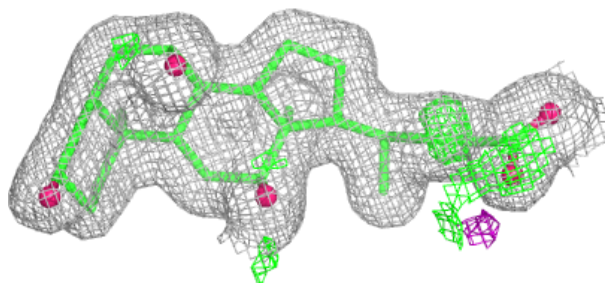
**Electron density around CHD G 102:**

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

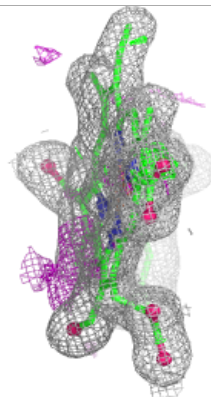
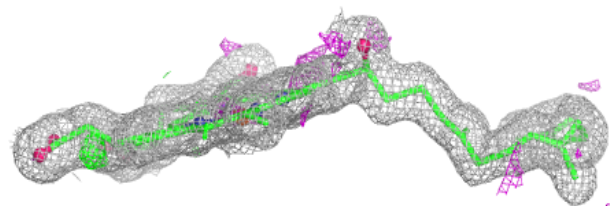
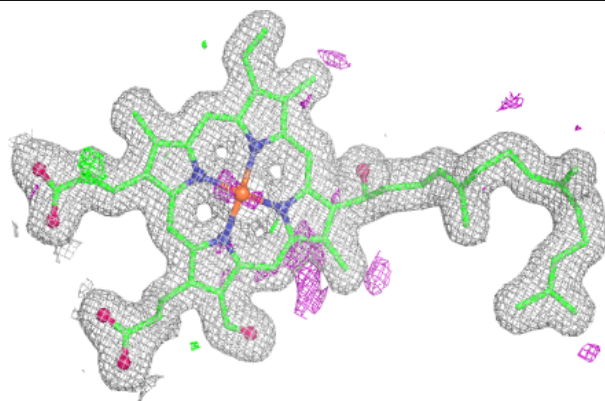


Electron density around CHD P 301:

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

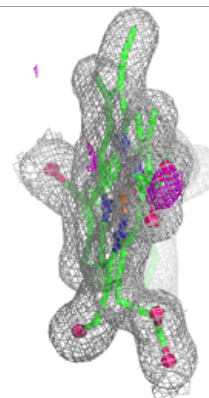
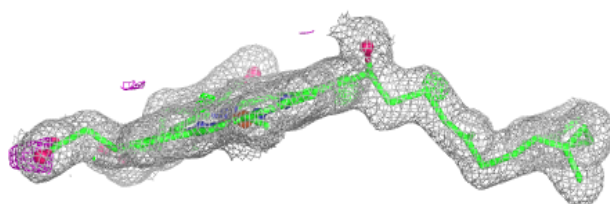
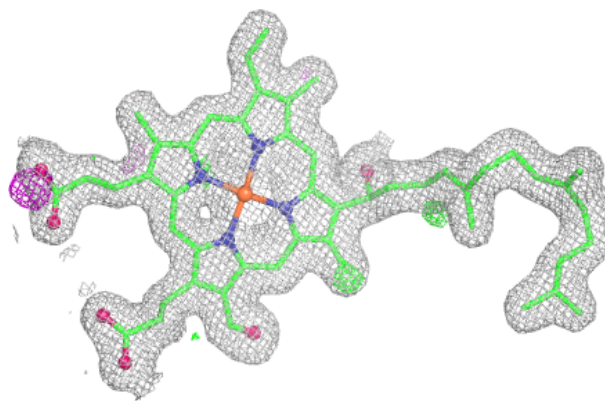
**Electron density around HEA A 602:**

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

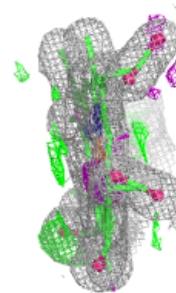
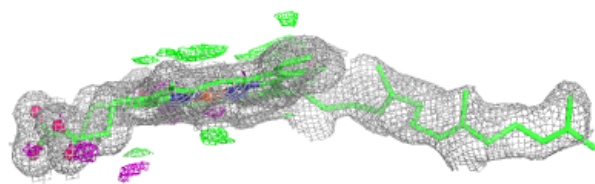
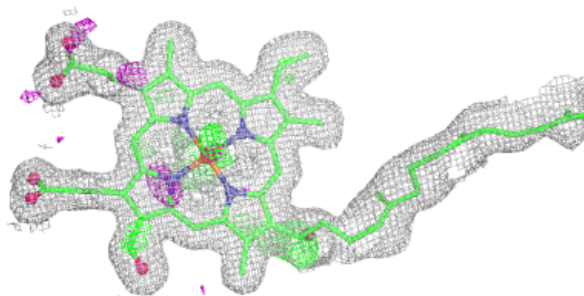


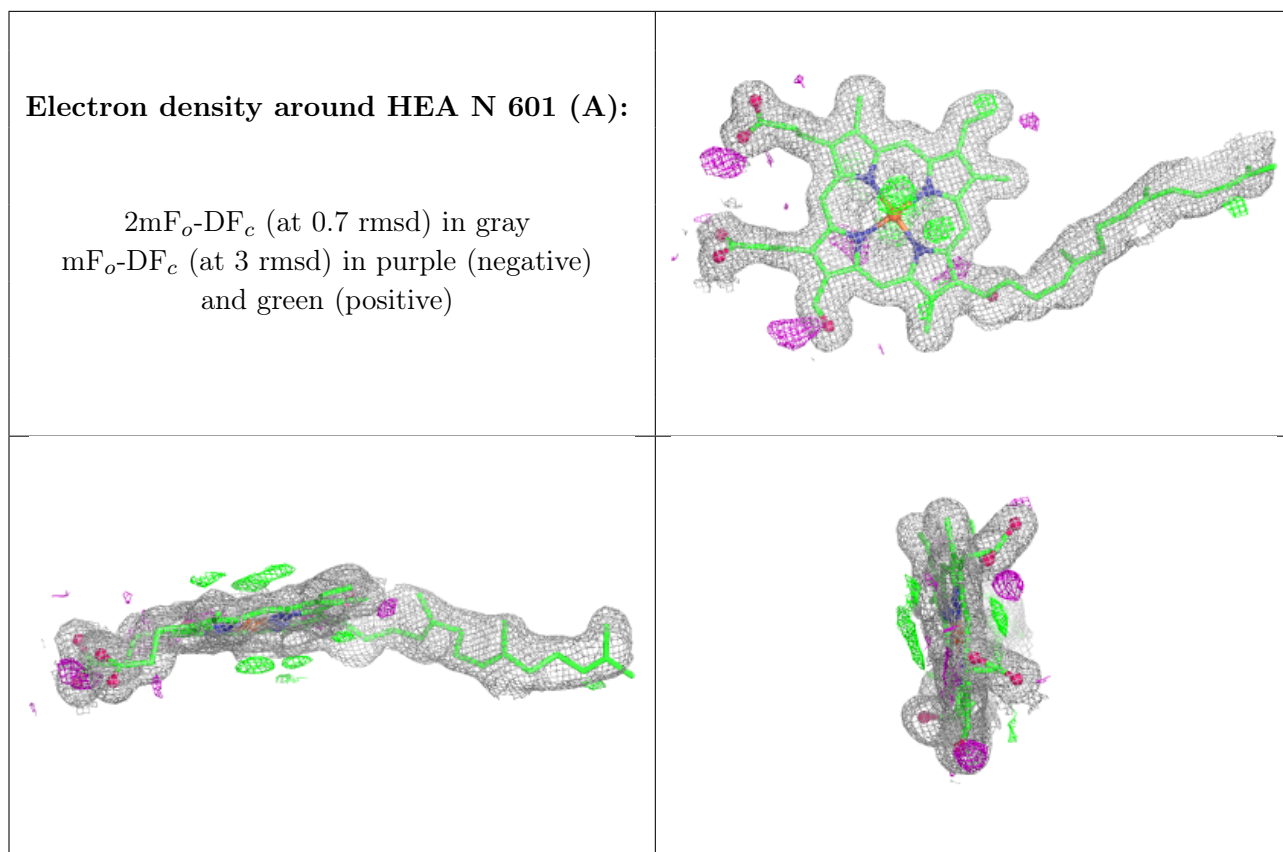
Electron density around HEA N 602:

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

**Electron density around HEA A 601 (A):**

$2mF_o-DF_c$ (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.