



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:13 PM JST

PDB ID : 5Z84 / pdb_00005z84
Title : The structure of azide-bound cytochrome c oxidase determined using the crystals exposed to 20 mM azide solution for 4 days
Authors : Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on : 2018-01-31
Resolution : 1.85 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:

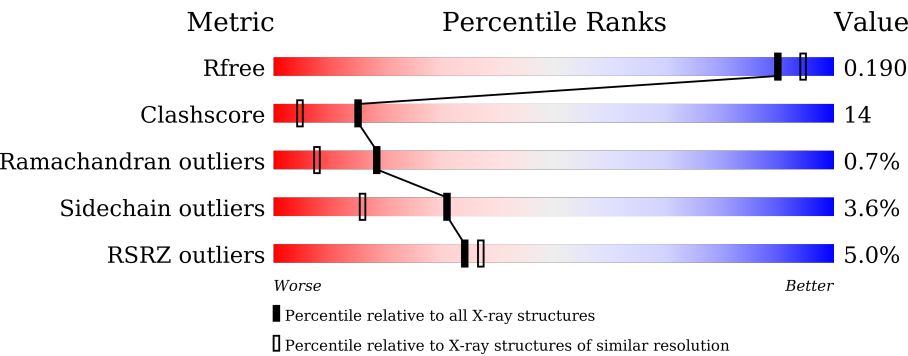
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	% 72% 24% ..
1	N	514	% 77% 20% .
2	B	227	7% 69% 24% 7%
2	O	227	5% 75% 22% .
3	C	261	% 73% 25% ..
3	P	261	2% 73% 25% ..

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AZI	A	606	-	-	X	-
18	AZI	A	607	-	-	X	-
18	AZI	N	608	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	TGL	D	201	-	-	X	-
21	EDO	A	615	-	X	X	-
21	EDO	A	621	-	-	X	-
21	EDO	D	202	-	-	X	-
21	EDO	D	203	-	-	X	-
21	EDO	N	618	-	-	X	-
21	EDO	N	621	-	-	X	-
21	EDO	N	622	-	-	X	-
24	PSC	B	303	-	-	X	-
28	CDL	C	306	-	-	X	-
28	CDL	P	304	-	-	X	-
9	SAC	V	1	-	X	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33735 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	22	0
			4193	2793	649	709	42			
1	N	514	Total	C	N	O	S	0	20	0
			4179	2786	647	704	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	10	0
			1904	1239	292	353	20			
2	O	227	Total	C	N	O	S	0	4	0
			1859	1206	287	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	9	0
			2185	1457	349	363	16			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	4	0
			1231	800	205	222	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0

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

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

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

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

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

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

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

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

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

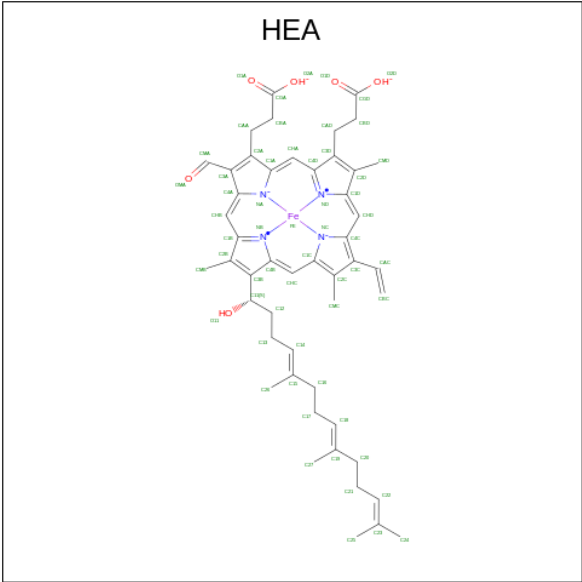
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			385	258	64	60	3			
12	Y	46	Total	C	N	O	S	0	1	0
			388	259	65	61	3			

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

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

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	1
			120	98	2	8	12		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	1
			120	98	2	8	12		

- Molecule 15 is COPPER (II) ION (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		

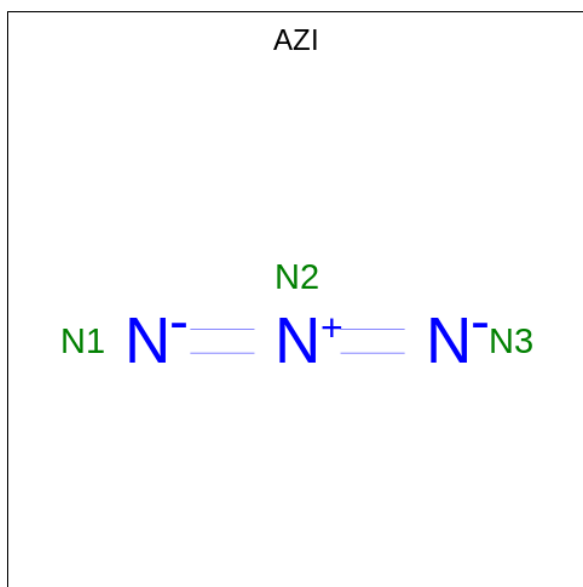
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

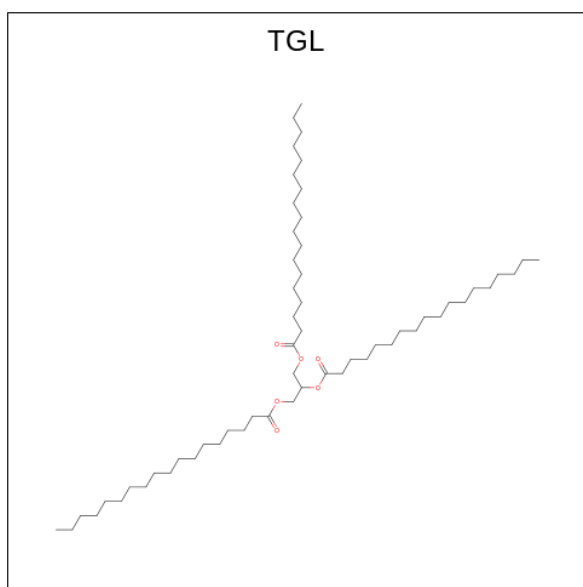
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is AZIDE ION (CCD ID: AZI) (formula: N₃).



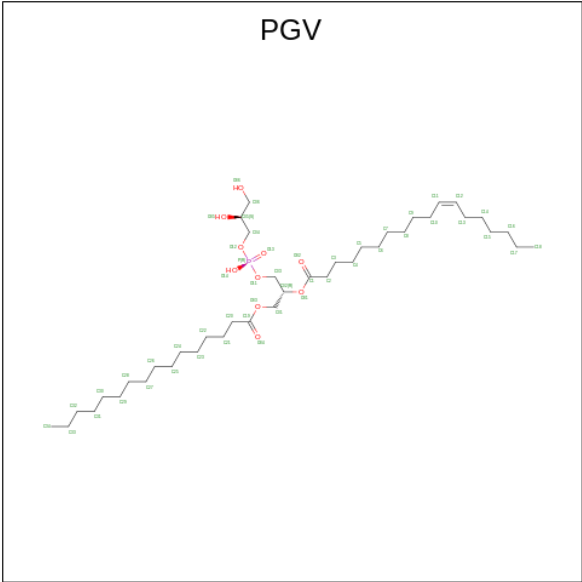
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	0
18	A	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0

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



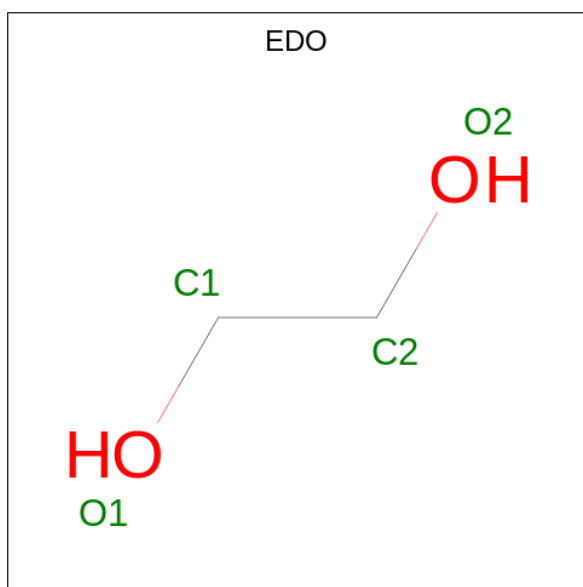
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



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

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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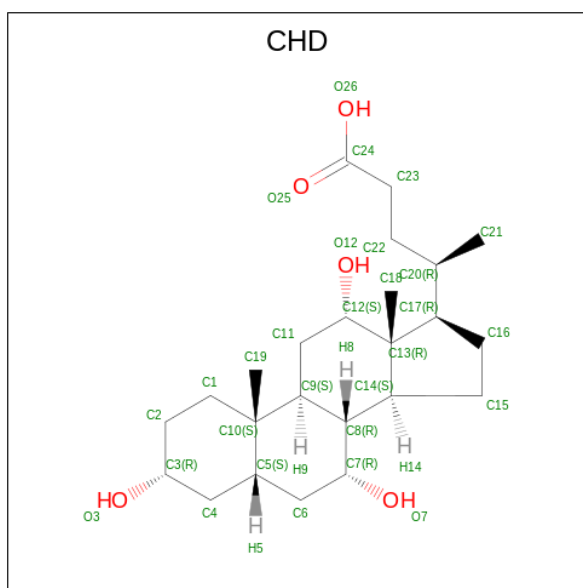
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	H	1	Total 4	C 2	O 2	0	0
21	H	1	Total 4	C 2	O 2	0	0
21	J	1	Total 4	C 2	O 2	0	0
21	L	1	Total 4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

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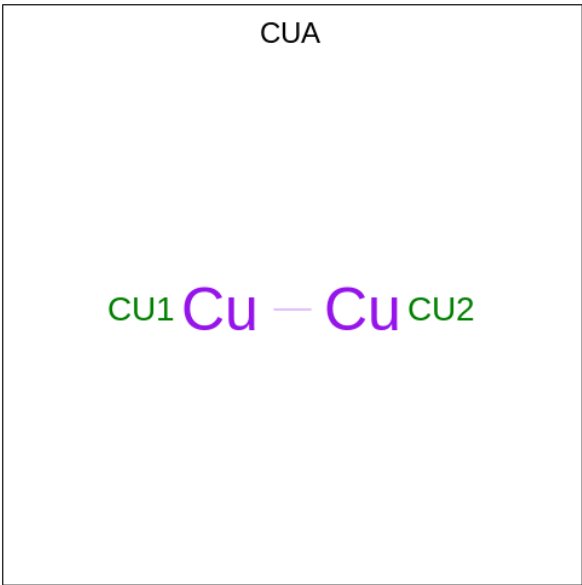
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	T	1	Total 4	C 2	O 2	0	0
21	U	1	Total 4	C 2	O 2	0	0
21	V	1	Total 4	C 2	O 2	0	0

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



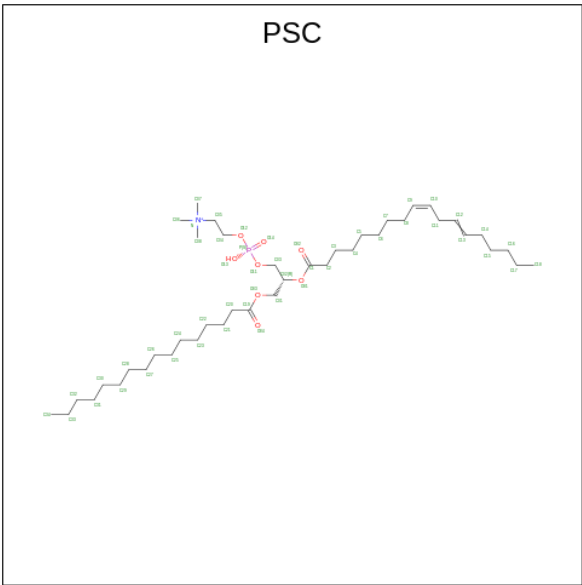
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



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).



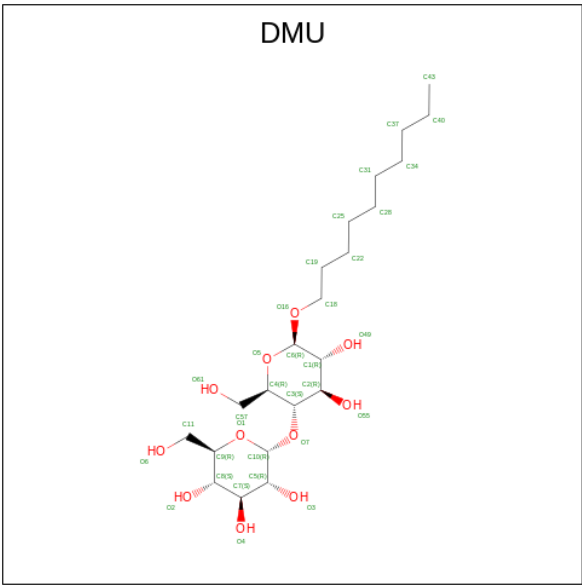
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).

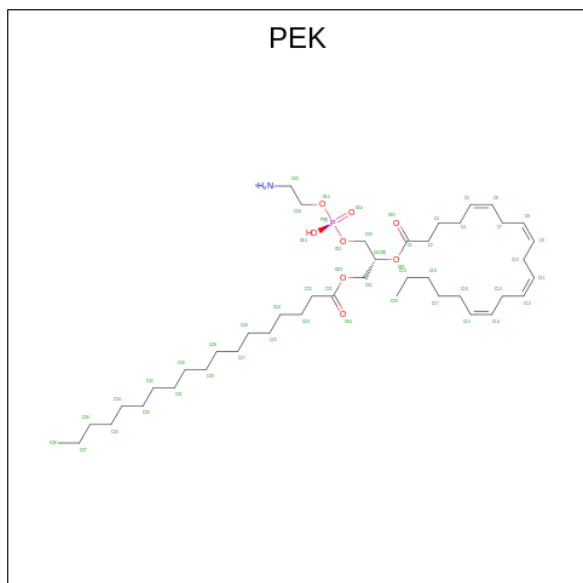


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			33	22	11		
25	L	1	Total	C	O	0	0
			33	22	11		
25	M	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total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

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

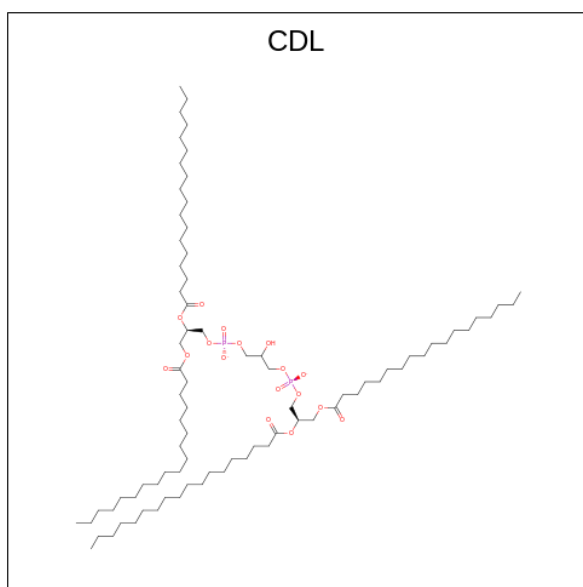
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total X 1 1	0	0
26	P	1	Total X 1 1	0	0

- Molecule 27 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYL)OXY]METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



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

- Molecule 28 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	232	Total	O	0	1
			233	233		
30	B	139	Total	O	0	1
			140	140		
30	C	101	Total	O	0	0
			101	101		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	D	110	Total 110	O 110	0	0
30	E	85	Total 85	O 85	0	0
30	F	78	Total 78	O 78	0	0
30	G	51	Total 51	O 51	0	0
30	H	45	Total 45	O 45	0	0
30	I	25	Total 25	O 25	0	0
30	J	28	Total 28	O 28	0	0
30	K	21	Total 21	O 21	0	0
30	L	29	Total 29	O 29	0	0
30	M	27	Total 27	O 27	0	0
30	N	218	Total 219	O 219	0	1
30	O	114	Total 115	O 115	0	1
30	P	90	Total 90	O 90	0	0
30	Q	36	Total 36	O 36	0	0
30	R	39	Total 39	O 39	0	0
30	S	55	Total 55	O 55	0	0
30	T	39	Total 39	O 39	0	0
30	U	33	Total 33	O 33	0	0
30	V	14	Total 14	O 14	0	0
30	W	11	Total 11	O 11	0	0
30	X	11	Total 11	O 11	0	0

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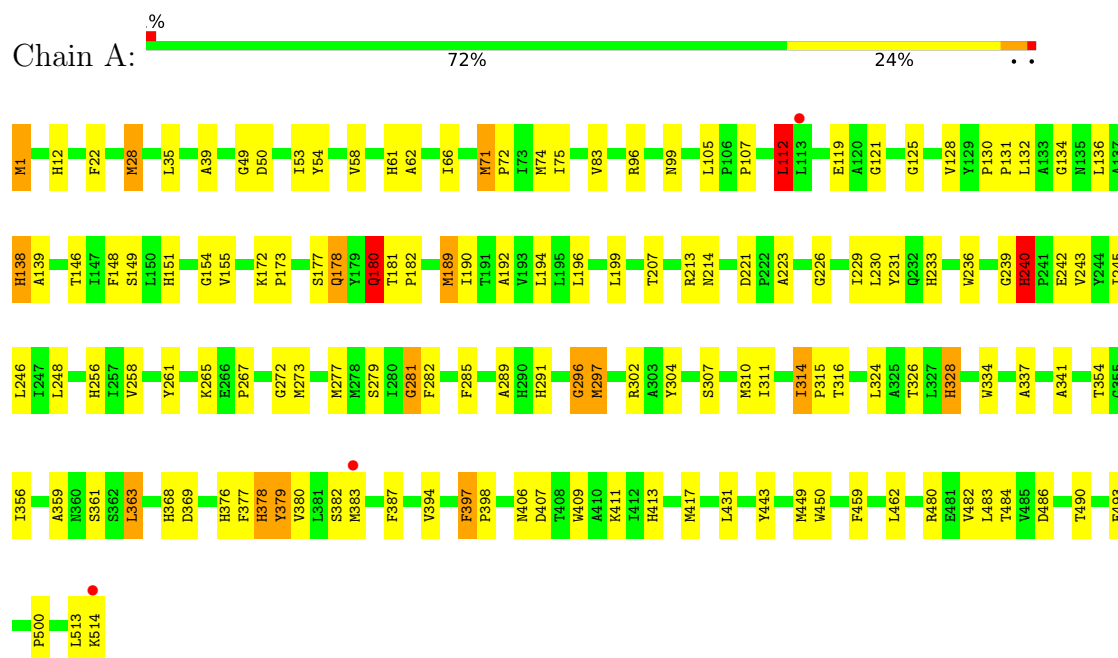
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	Y	14	Total 14	O 14	0	0
30	Z	16	Total 16	O 16	0	0

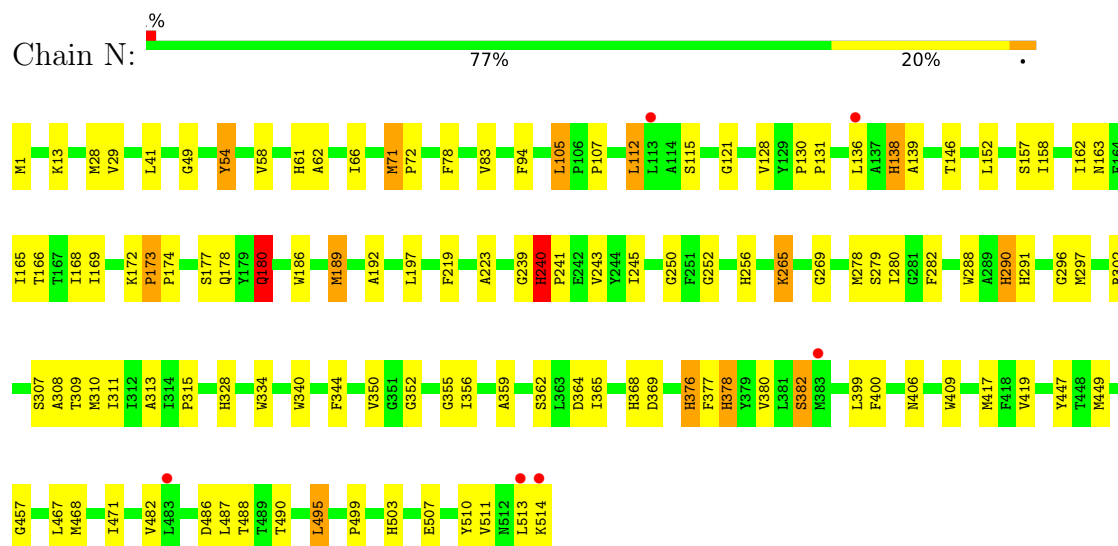
3 Residue-property plots

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.

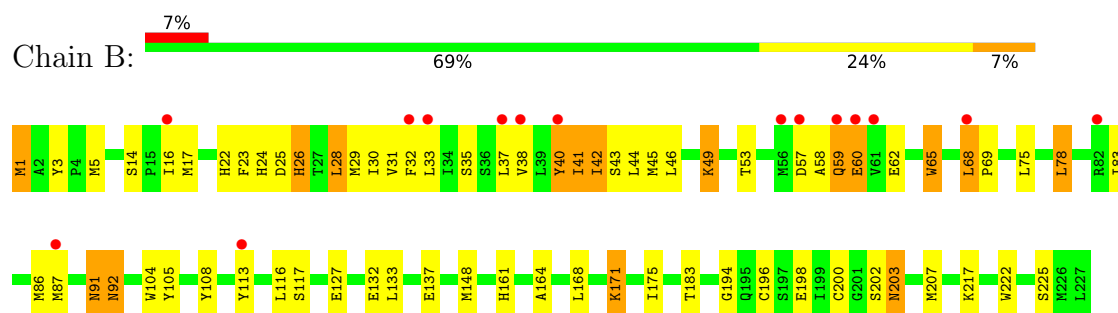
• Molecule 1: Cytochrome c oxidase subunit 1



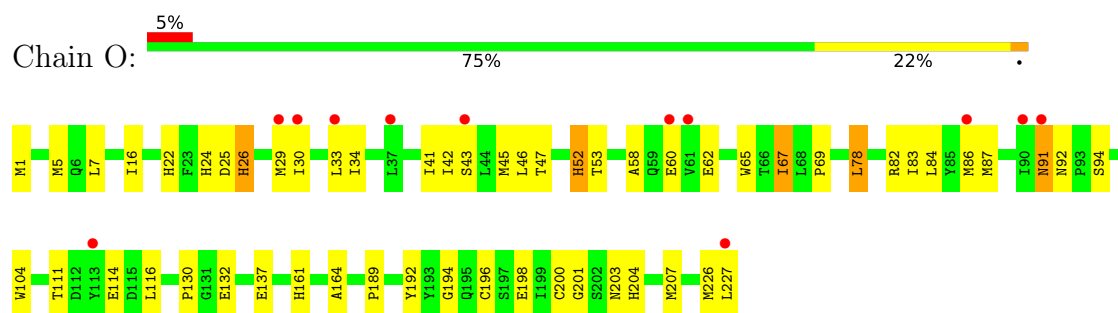
• Molecule 1: Cytochrome c oxidase subunit 1



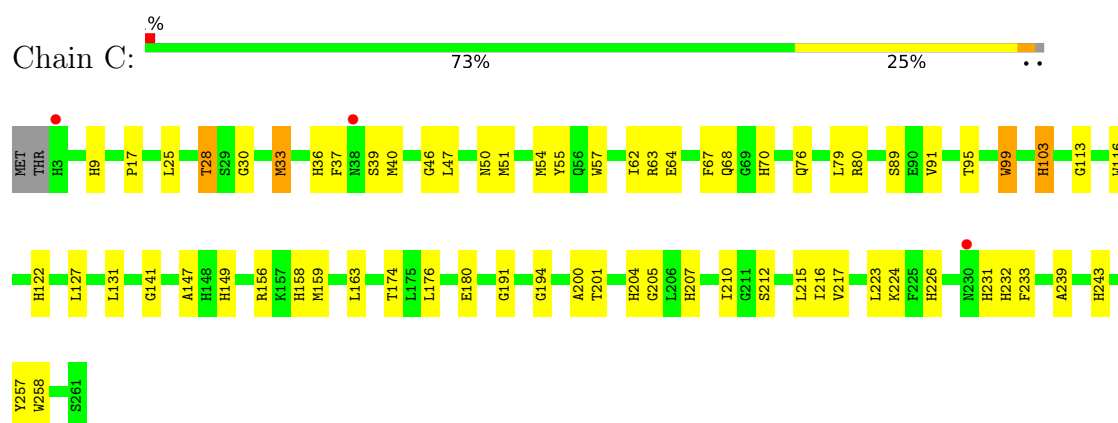
- Molecule 2: Cytochrome c oxidase subunit 2



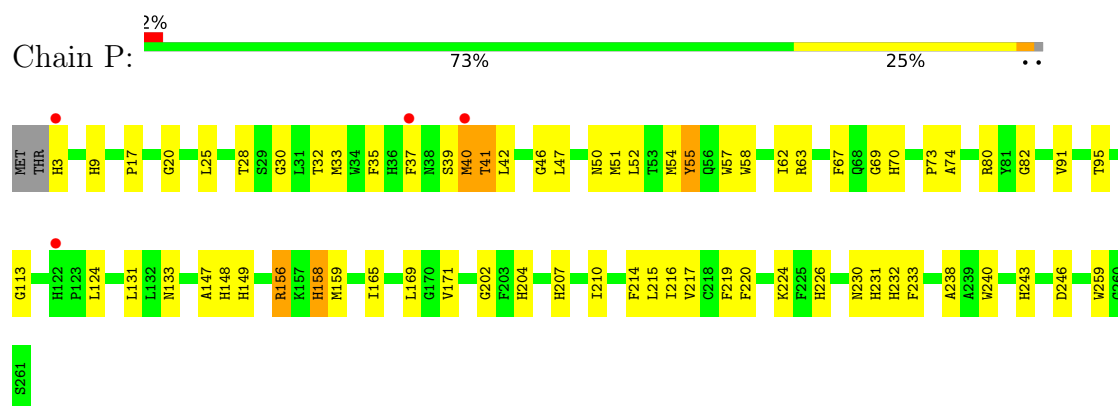
- Molecule 2: Cytochrome c oxidase subunit 2



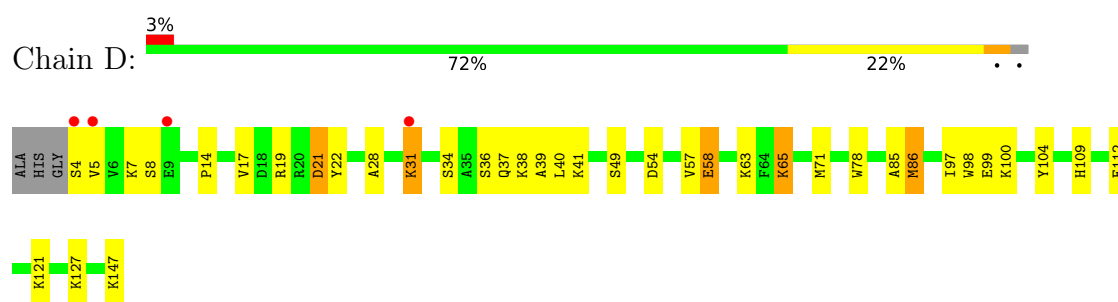
- Molecule 3: Cytochrome c oxidase subunit 3



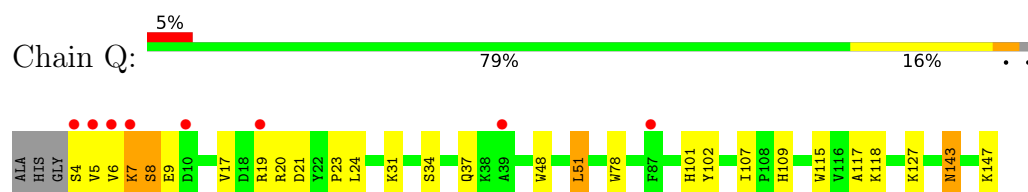
- Molecule 3: Cytochrome c oxidase subunit 3



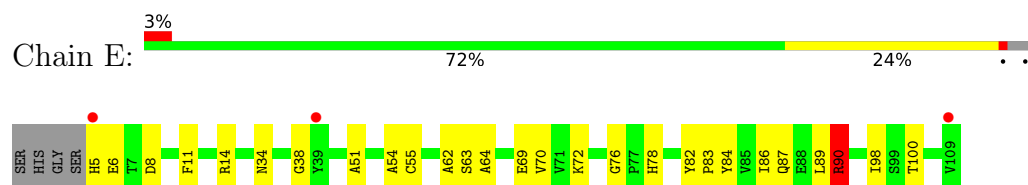
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



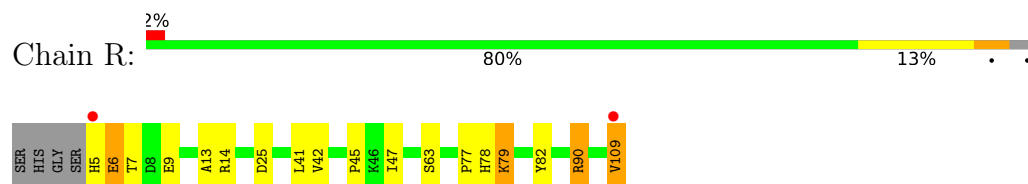
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



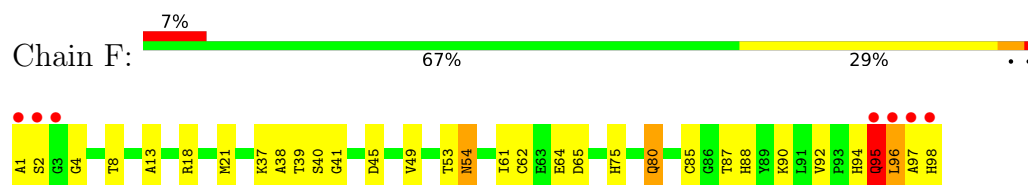
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



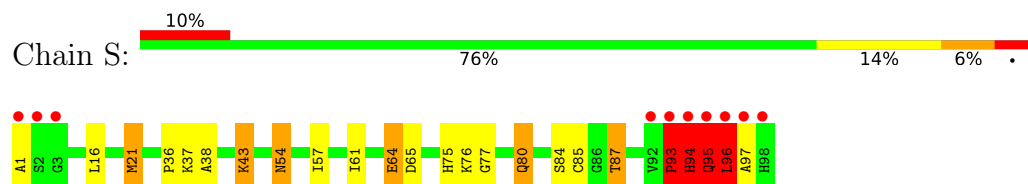
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



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

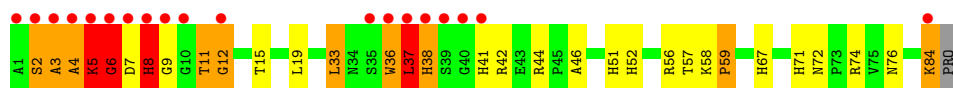


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

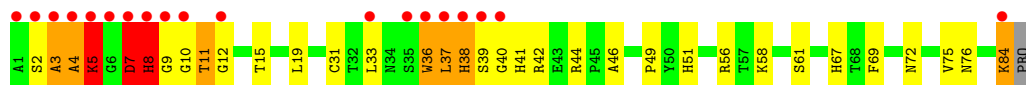


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

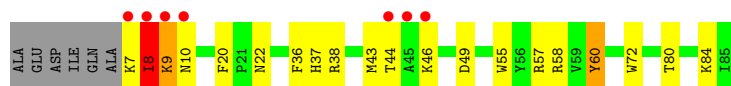




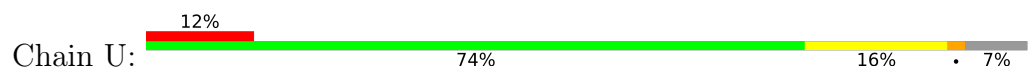
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



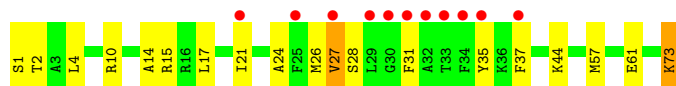
- Molecule 8: Cytochrome c oxidase subunit 6B1



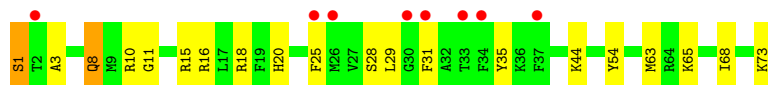
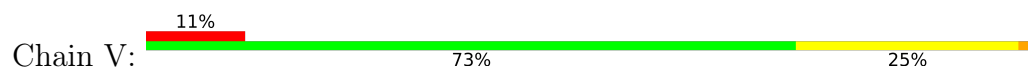
- Molecule 8: Cytochrome c oxidase subunit 6B1



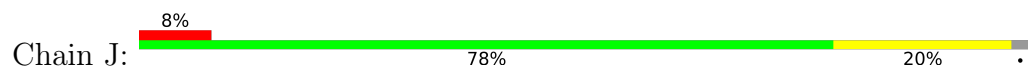
- Molecule 9: Cytochrome c oxidase subunit 6C



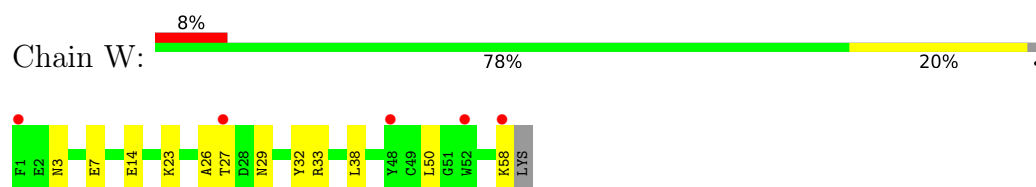
- Molecule 9: Cytochrome c oxidase subunit 6C



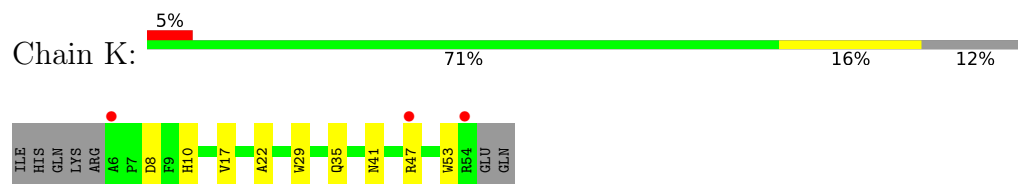
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



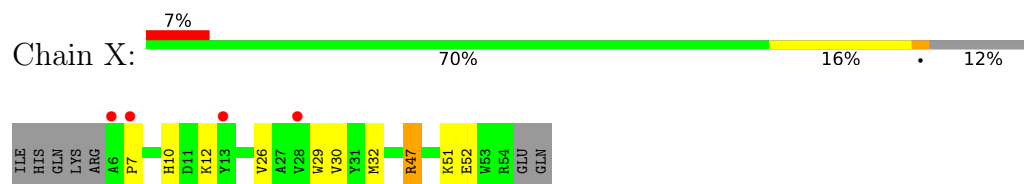
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



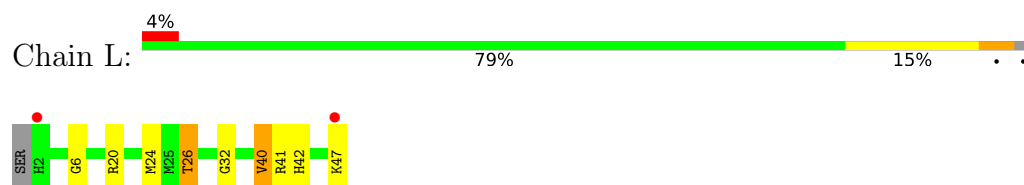
- Molecule 11: cytochrome c oxidase subunit 11, Cytochrome c oxidase subunit 7B, mitochondrial



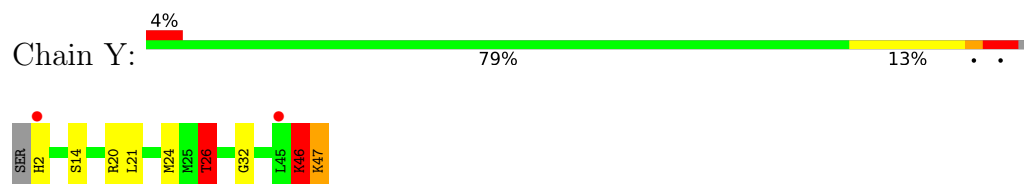
- Molecule 11: cytochrome c oxidase subunit 11, Cytochrome c oxidase subunit 7B, mitochondrial



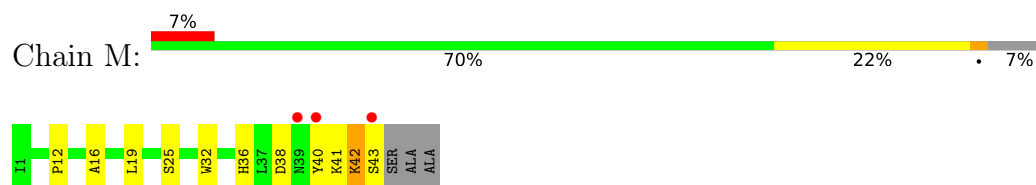
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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

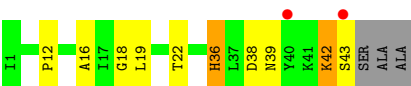


- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.41Å 206.27Å 177.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 40.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-1.85) 99.4 (40.00-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.163 , 0.189 0.165 , 0.190	Depositor DCC
R_{free} test set	28371 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33735	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: MG, CDL, PEK, EDO, DMU, CUA, FME, TGL, HEA, CU, ZN, AZI, UNX, TPO, PSC, SAC, PGV, CHD, NA

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	1.96	84/4322 (1.9%)	1.48	26/5897 (0.4%)
1	N	1.88	63/4308 (1.5%)	1.41	20/5878 (0.3%)
2	B	1.79	28/1945 (1.4%)	1.46	20/2649 (0.8%)
2	O	1.53	12/1896 (0.6%)	1.27	3/2581 (0.1%)
3	C	1.84	38/2272 (1.7%)	1.29	5/3102 (0.2%)
3	P	1.89	42/2272 (1.8%)	1.35	7/3102 (0.2%)
4	D	1.72	14/1265 (1.1%)	1.39	7/1704 (0.4%)
4	Q	1.34	3/1259 (0.2%)	1.17	6/1698 (0.4%)
5	E	1.83	14/871 (1.6%)	1.36	5/1182 (0.4%)
5	R	1.60	5/871 (0.6%)	1.29	4/1182 (0.3%)
6	F	1.65	6/795 (0.8%)	1.46	7/1079 (0.6%)
6	S	1.66	2/780 (0.3%)	1.45	5/1058 (0.5%)
7	G	1.96	12/690 (1.7%)	1.44	10/937 (1.1%)
7	T	1.92	18/702 (2.6%)	1.46	8/953 (0.8%)
8	H	1.55	4/682 (0.6%)	1.32	0/921
8	U	1.32	0/682	1.21	2/921 (0.2%)
9	I	1.48	1/605 (0.2%)	1.32	0/802
9	V	1.27	1/605 (0.2%)	1.32	0/802
10	J	1.61	4/471 (0.8%)	1.31	1/636 (0.2%)
10	W	1.52	1/480 (0.2%)	1.19	0/648
11	K	1.65	4/398 (1.0%)	1.33	2/546 (0.4%)
11	X	1.36	1/405 (0.2%)	1.16	0/556
12	L	1.61	2/401 (0.5%)	1.42	4/536 (0.7%)
12	Y	1.54	2/401 (0.5%)	1.30	2/536 (0.4%)
13	M	1.68	2/345 (0.6%)	1.24	0/470
13	Z	1.48	3/345 (0.9%)	1.21	0/470
All	All	1.75	366/30068 (1.2%)	1.37	144/40846 (0.4%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	1
6	S	0	1
7	T	0	1
12	Y	0	1
All	All	0	6

All (366) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	49	GLY	C-O	17.10	1.35	1.23
1	A	376	HIS	ND1-CE1	12.01	1.44	1.32
1	A	368	HIS	ND1-CE1	10.98	1.43	1.32
1	A	281	GLY	N-CA	10.25	1.58	1.45
3	P	20	GLY	N-CA	9.87	1.58	1.45
1	A	240	HIS	N-CA	9.80	1.53	1.46
1	A	61	HIS	ND1-CE1	9.70	1.42	1.32
1	N	310	MET	SD-CE	-9.43	1.55	1.79
1	A	310	MET	SD-CE	-9.13	1.56	1.79
5	E	78	HIS	N-CA	9.05	1.58	1.46
6	S	77	GLY	C-O	8.81	1.28	1.24
1	N	173	PRO	CA-CB	8.69	1.62	1.53
1	A	413	HIS	CG-ND1	-8.67	1.28	1.38
7	T	5	LYS	CA-C	8.62	1.64	1.52
1	A	482	VAL	CA-CB	8.58	1.63	1.54
7	G	67	HIS	ND1-CE1	8.52	1.41	1.32
2	B	161	HIS	ND1-CE1	8.42	1.41	1.32
1	N	256	HIS	ND1-CE1	8.21	1.40	1.32
1	A	376	HIS	CG-CD2	8.18	1.44	1.35
1	A	378	HIS	ND1-CE1	8.03	1.40	1.32
1	N	223	ALA	N-CA	8.02	1.56	1.46
6	S	95	GLN	CA-C	7.96	1.60	1.53
3	P	232	HIS	CG-CD2	7.95	1.44	1.35
1	N	376	HIS	ND1-CE1	7.87	1.40	1.32
3	P	243	HIS	CE1-NE2	7.84	1.40	1.32
3	C	204	HIS	CE1-NE2	7.81	1.40	1.32
1	A	199	LEU	N-CA	7.77	1.54	1.46
7	T	67	HIS	ND1-CE1	7.76	1.40	1.32
1	A	96	ARG	CZ-NH1	7.76	1.43	1.32
1	N	61	HIS	ND1-CE1	7.75	1.40	1.32
2	O	198	GLU	C-O	7.74	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	220	PHE	N-CA	7.74	1.56	1.46
1	N	376	HIS	CE1-NE2	7.69	1.40	1.32
2	O	200	CYS	N-CA	7.67	1.53	1.46
1	A	12	HIS	ND1-CE1	7.66	1.40	1.32
3	P	158	HIS	ND1-CE1	7.66	1.40	1.32
2	B	30	ILE	CA-C	-7.66	1.44	1.52
5	R	78	HIS	CE1-NE2	7.61	1.40	1.32
1	A	49	GLY	C-O	7.51	1.34	1.23
2	B	202	SER	N-CA	7.51	1.55	1.46
3	C	226	HIS	CG-CD2	7.50	1.44	1.35
3	C	141	GLY	N-CA	7.41	1.54	1.45
2	B	3	TYR	N-CA	7.38	1.51	1.45
3	C	9	HIS	CE1-NE2	7.37	1.40	1.32
2	B	53	THR	N-CA	7.37	1.55	1.46
5	E	98	ILE	N-CA	7.36	1.55	1.46
7	G	5	LYS	CA-C	7.36	1.62	1.52
5	R	47	ILE	N-CA	7.36	1.55	1.46
3	C	70	HIS	ND1-CE1	7.35	1.39	1.32
1	A	226	GLY	N-CA	7.29	1.53	1.45
3	C	231	HIS	ND1-CE1	7.29	1.39	1.32
1	N	163	ASN	CA-C	7.26	1.61	1.52
3	C	239	ALA	N-CA	7.15	1.54	1.46
1	N	162	ILE	CA-CB	7.13	1.63	1.54
2	B	203	ASN	N-CA	7.07	1.54	1.46
12	L	26	THR	CA-CB	7.07	1.64	1.53
1	N	240	HIS	N-CA	7.04	1.51	1.46
1	N	245	ILE	CA-CB	7.03	1.63	1.54
1	A	376	HIS	CE1-NE2	7.03	1.39	1.32
7	T	56	ARG	CA-CB	7.02	1.63	1.52
1	N	256	HIS	CG-CD2	6.98	1.43	1.35
9	I	4	LEU	CA-CB	6.98	1.64	1.53
2	O	24	HIS	CE1-NE2	6.97	1.39	1.32
1	N	138	HIS	ND1-CE1	6.88	1.39	1.32
12	L	32	GLY	N-CA	6.84	1.54	1.45
5	E	51	ALA	N-CA	6.83	1.54	1.46
3	P	204	HIS	CE1-NE2	6.83	1.39	1.32
4	D	97	ILE	N-CA	6.77	1.54	1.46
1	N	158	ILE	N-CA	6.74	1.54	1.46
1	N	192	ALA	N-CA	6.66	1.54	1.46
1	N	168	ILE	N-CA	6.64	1.54	1.46
1	N	290	HIS	CE1-NE2	6.63	1.39	1.32
7	T	8	HIS	N-CA	6.59	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	54	TYR	CA-C	6.57	1.61	1.52
1	A	233	HIS	CE1-NE2	6.53	1.39	1.32
1	N	368	HIS	ND1-CE1	6.49	1.39	1.32
1	N	290	HIS	CG-CD2	6.49	1.43	1.35
10	W	26	ALA	CA-CB	6.49	1.64	1.53
1	A	256	HIS	CG-CD2	6.47	1.43	1.35
1	A	12	HIS	CG-CD2	6.46	1.43	1.35
1	A	413	HIS	ND1-CE1	6.46	1.39	1.32
2	B	161	HIS	C-O	6.45	1.32	1.24
1	N	378	HIS	ND1-CE1	6.45	1.39	1.32
11	K	10	HIS	CE1-NE2	6.44	1.39	1.32
5	E	55	CYS	N-CA	6.42	1.54	1.46
3	C	200	ALA	N-CA	6.40	1.54	1.46
7	G	51	HIS	ND1-CE1	6.38	1.39	1.32
3	P	148	HIS	ND1-CE1	6.38	1.39	1.32
1	A	149	SER	CA-C	6.36	1.60	1.52
3	P	240	TRP	N-CA	6.36	1.54	1.46
1	N	482	VAL	CA-CB	6.36	1.60	1.54
3	P	57	TRP	N-CA	6.35	1.53	1.46
2	B	40	TYR	N-CA	-6.35	1.38	1.46
3	P	171	VAL	N-CA	6.33	1.54	1.46
1	N	146	THR	N-CA	6.29	1.53	1.46
2	B	30	ILE	N-CA	6.29	1.54	1.46
5	E	64	ALA	N-CA	6.29	1.53	1.46
2	B	49	LYS	N-CA	6.29	1.54	1.46
1	N	457	GLY	N-CA	6.29	1.53	1.45
7	G	8	HIS	N-CA	6.29	1.54	1.46
2	O	34	ILE	CA-CB	6.29	1.63	1.54
2	O	161	HIS	ND1-CE1	6.28	1.38	1.32
3	C	232	HIS	ND1-CE1	6.26	1.38	1.32
3	C	174	THR	N-CA	6.26	1.54	1.46
7	T	7	ASP	N-CA	6.25	1.54	1.46
3	C	243	HIS	CE1-NE2	6.25	1.38	1.32
8	H	55	TRP	N-CA	-6.25	1.38	1.46
4	D	21	ASP	CA-CB	6.24	1.64	1.53
1	A	83	VAL	CA-CB	6.24	1.57	1.54
13	M	36	HIS	CG-CD2	6.23	1.42	1.35
1	A	304	TYR	CA-C	6.21	1.60	1.52
1	N	240	HIS	CE1-NE2	6.21	1.38	1.32
3	C	103	HIS	CE1-NE2	6.20	1.38	1.32
7	G	56	ARG	CA-CB	6.20	1.62	1.53
7	G	7	ASP	N-CA	6.20	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	36	HIS	ND1-CE1	6.17	1.38	1.32
7	G	7	ASP	CA-C	6.17	1.61	1.52
1	A	387	PHE	CA-CB	6.16	1.63	1.53
3	C	158	HIS	ND1-CE1	6.16	1.38	1.32
4	D	54	ASP	N-CA	6.14	1.53	1.46
13	Z	18	GLY	N-CA	6.14	1.53	1.45
3	P	3	HIS	CE1-NE2	6.13	1.38	1.32
3	P	226	HIS	CG-CD2	6.13	1.42	1.35
3	P	214	PHE	N-CA	-6.11	1.39	1.46
4	D	58	GLU	N-CA	6.11	1.53	1.46
7	T	2	SER	CA-C	6.09	1.60	1.52
1	A	74	MET	CB-CG	6.09	1.70	1.52
5	E	38	GLY	N-CA	6.07	1.53	1.45
1	N	419	VAL	CA-CB	6.05	1.62	1.54
1	N	352	GLY	N-CA	6.04	1.53	1.45
11	K	29	TRP	CD2-CE2	6.04	1.51	1.41
1	A	462	LEU	N-CA	6.04	1.53	1.46
2	O	65	TRP	CD2-CE2	6.00	1.51	1.41
2	O	204	HIS	CG-CD2	6.00	1.42	1.35
3	C	194	GLY	N-CA	6.00	1.53	1.45
13	Z	22	THR	N-CA	6.00	1.53	1.46
5	E	76	GLY	N-CA	5.99	1.52	1.44
1	A	130	PRO	CA-C	5.99	1.57	1.52
2	B	24	HIS	CE1-NE2	5.99	1.38	1.32
3	P	147	ALA	N-CA	5.99	1.53	1.46
3	C	232	HIS	CG-CD2	5.98	1.42	1.35
1	N	173	PRO	CA-C	5.98	1.55	1.51
1	A	443	TYR	CA-CB	5.96	1.62	1.54
5	E	87	GLN	N-CA	5.95	1.53	1.46
3	P	3	HIS	CG-CD2	5.95	1.42	1.35
5	R	63	SER	CA-C	5.95	1.60	1.52
2	B	40	TYR	CA-CB	-5.95	1.44	1.53
1	N	290	HIS	N-CA	5.95	1.54	1.46
1	A	279	SER	CA-CB	5.95	1.62	1.53
1	N	49	GLY	N-CA	5.95	1.50	1.45
2	B	26	HIS	CG-CD2	5.94	1.42	1.35
3	P	216	ILE	N-CA	5.94	1.53	1.46
1	A	354	THR	N-CA	5.93	1.53	1.46
1	A	413	HIS	CG-CD2	5.90	1.42	1.35
7	T	49	PRO	CA-CB	5.89	1.57	1.53
3	P	231	HIS	CG-CD2	5.89	1.42	1.35
1	A	341	ALA	N-CA	5.88	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	165	ILE	C-O	5.87	1.31	1.24
1	N	41	LEU	CA-C	5.87	1.60	1.52
4	D	22	TYR	N-CA	5.87	1.53	1.46
2	B	44	LEU	C-O	5.86	1.30	1.24
1	A	328	HIS	CE1-NE2	5.85	1.38	1.32
7	T	51	HIS	ND1-CE1	5.83	1.38	1.32
4	D	39	ALA	CA-C	5.82	1.60	1.52
3	C	131	LEU	N-CA	5.80	1.53	1.46
1	N	166	THR	CA-CB	5.80	1.62	1.53
6	F	88	HIS	ND1-CE1	5.79	1.38	1.32
1	A	154	GLY	N-CA	5.79	1.53	1.45
7	G	59	PRO	CA-CB	5.79	1.61	1.53
8	H	20	PHE	N-CA	5.79	1.53	1.46
1	A	368	HIS	CG-CD2	5.78	1.42	1.35
1	A	326	THR	CA-CB	5.77	1.62	1.53
1	A	74	MET	CG-SD	-5.76	1.66	1.80
2	B	65	TRP	CD2-CE2	5.75	1.51	1.41
2	O	201	GLY	CA-C	5.75	1.58	1.52
3	C	46	GLY	N-CA	5.75	1.52	1.45
2	O	43	SER	CA-C	5.75	1.60	1.52
1	N	130	PRO	CA-C	5.75	1.57	1.52
3	P	204	HIS	CG-CD2	5.74	1.42	1.35
3	P	231	HIS	ND1-CE1	5.74	1.38	1.32
3	P	238	ALA	CA-CB	5.74	1.62	1.53
1	N	503	HIS	CG-CD2	5.74	1.42	1.35
1	N	61	HIS	CE1-NE2	5.73	1.38	1.32
1	A	134	GLY	C-O	5.73	1.30	1.23
5	E	62	ALA	CA-CB	5.72	1.62	1.53
3	P	226	HIS	CG-ND1	-5.70	1.31	1.38
7	G	71	HIS	CG-CD2	5.69	1.42	1.35
1	A	480	ARG	CD-NE	5.69	1.54	1.46
3	C	216	ILE	N-CA	5.69	1.53	1.46
10	J	28	ASP	N-CA	5.67	1.53	1.46
2	B	65	TRP	CA-C	-5.67	1.44	1.52
3	P	9	HIS	C-O	5.66	1.30	1.24
1	N	252	GLY	CA-C	5.66	1.58	1.52
3	C	30	GLY	N-CA	5.65	1.52	1.45
1	N	279	SER	CA-CB	5.64	1.62	1.53
1	A	397	PHE	CA-C	5.64	1.59	1.52
1	A	192	ALA	N-CA	5.63	1.53	1.46
5	R	13	ALA	CA-C	5.63	1.60	1.52
3	C	207	HIS	ND1-CE1	5.63	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	239	GLY	N-CA	5.62	1.52	1.45
1	A	50	ASP	CA-CB	5.62	1.62	1.53
1	A	493	GLU	N-CA	5.62	1.53	1.46
7	T	75	VAL	N-CA	5.61	1.51	1.46
8	H	58	ARG	CZ-NH1	5.61	1.40	1.32
3	C	149	HIS	ND1-CE1	5.60	1.38	1.32
1	N	83	VAL	CA-CB	5.59	1.56	1.54
3	P	35	PHE	CA-CB	5.59	1.62	1.53
10	J	33	ARG	CA-CB	5.59	1.62	1.53
7	T	19	LEU	CA-C	5.59	1.60	1.52
1	N	152	LEU	CA-C	5.58	1.60	1.52
2	O	52	HIS	ND1-CE1	5.58	1.38	1.32
3	C	89	SER	CB-OG	5.56	1.53	1.42
2	B	45	MET	N-CA	5.55	1.53	1.46
6	F	18	ARG	CZ-NH1	5.54	1.40	1.32
1	A	28	MET	N-CA	5.53	1.53	1.46
4	D	41	LYS	N-CA	5.52	1.53	1.46
1	A	230	LEU	N-CA	5.51	1.53	1.46
1	N	165	ILE	N-CA	5.51	1.53	1.46
3	C	116	TRP	CA-C	-5.50	1.48	1.52
4	D	63	LYS	C-O	5.50	1.30	1.24
1	N	174	PRO	N-CA	5.50	1.54	1.47
3	P	46	GLY	N-CA	5.49	1.52	1.45
1	A	138	HIS	ND1-CE1	5.49	1.38	1.32
1	N	355	GLY	N-CA	5.48	1.52	1.45
5	E	63	SER	CA-C	5.48	1.60	1.52
6	F	45	ASP	CA-C	5.47	1.59	1.52
1	A	66	ILE	CA-CB	5.47	1.60	1.54
1	A	182	PRO	N-CA	-5.47	1.40	1.47
1	A	248	LEU	CA-CB	5.46	1.60	1.53
2	B	24	HIS	CG-CD2	5.46	1.41	1.35
2	B	127	GLU	CA-C	-5.45	1.45	1.52
1	N	157	SER	N-CA	5.44	1.53	1.46
1	A	132	LEU	N-CA	5.44	1.53	1.46
3	C	163	LEU	N-CA	5.44	1.53	1.46
1	A	155	VAL	CA-CB	5.43	1.61	1.54
3	C	205	GLY	N-CA	5.43	1.52	1.45
1	N	400	PHE	C-O	5.42	1.30	1.24
1	A	379	TYR	N-CA	5.42	1.53	1.46
1	N	507	GLU	CA-CB	5.41	1.61	1.52
1	A	58	VAL	CA-CB	5.39	1.61	1.54
1	A	233	HIS	CA-CB	5.39	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	24	LEU	CA-C	5.39	1.59	1.52
1	A	151	HIS	CD2-NE2	5.39	1.43	1.37
7	T	61	SER	N-CA	5.38	1.53	1.46
2	B	171	LYS	N-CA	5.38	1.53	1.46
4	Q	23	PRO	CA-CB	5.38	1.61	1.53
1	A	324	LEU	N-CA	5.38	1.52	1.46
1	N	350	VAL	CA-C	5.38	1.59	1.52
3	P	124	LEU	N-CA	5.36	1.52	1.46
3	P	156	ARG	CA-CB	5.35	1.61	1.53
3	P	207	HIS	CG-CD2	5.35	1.41	1.35
1	A	256	HIS	ND1-CE1	5.35	1.37	1.32
4	D	36	SER	N-CA	5.35	1.53	1.46
3	C	99	TRP	N-CA	5.34	1.52	1.46
3	P	70	HIS	CG-CD2	5.34	1.41	1.35
4	D	112	GLU	N-CA	5.34	1.52	1.46
1	N	78	PHE	N-CA	5.34	1.52	1.46
2	O	26	HIS	CG-CD2	5.34	1.41	1.35
1	A	258	VAL	N-CA	5.33	1.52	1.46
12	Y	32	GLY	N-CA	5.33	1.52	1.45
1	A	190	ILE	CA-CB	5.33	1.61	1.54
3	C	55	TYR	CA-CB	5.32	1.61	1.53
2	B	25	ASP	CA-C	5.32	1.59	1.52
3	P	217	VAL	CA-CB	5.32	1.59	1.54
1	A	296	GLY	N-CA	5.31	1.52	1.45
1	N	61	HIS	CG-CD2	5.30	1.41	1.35
7	T	5	LYS	CA-CB	5.30	1.62	1.53
5	R	82	TYR	C-N	5.30	1.40	1.33
4	D	63	LYS	CA-CB	5.29	1.61	1.53
1	A	273	MET	N-CA	5.28	1.52	1.46
1	A	207	THR	N-CA	5.27	1.52	1.46
1	A	139	ALA	CA-CB	5.26	1.62	1.53
1	A	214	ASN	N-CA	5.25	1.53	1.46
2	B	198	GLU	CD-OE2	-5.24	1.15	1.25
7	T	67	HIS	CG-CD2	5.24	1.41	1.35
12	Y	26	THR	CA-CB	5.24	1.61	1.53
3	C	201	THR	N-CA	5.24	1.53	1.46
10	J	50	LEU	N-CA	5.23	1.52	1.46
11	K	35	GLN	CA-C	-5.23	1.45	1.52
1	A	285	PHE	N-CA	5.23	1.52	1.46
2	B	225	SER	CA-CB	5.23	1.62	1.53
1	A	213	ARG	CA-C	5.22	1.59	1.52
6	F	62	CYS	N-CA	5.22	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	117	ALA	CA-CB	5.22	1.61	1.53
3	C	223	LEU	N-CA	5.21	1.52	1.46
3	P	158	HIS	CG-CD2	5.21	1.41	1.35
3	P	73	PRO	CA-CB	5.21	1.61	1.53
1	A	291	HIS	CD2-NE2	-5.21	1.32	1.37
3	C	36	HIS	CA-CB	-5.20	1.47	1.54
3	C	79	LEU	CA-CB	5.20	1.61	1.53
3	C	122	HIS	CG-CD2	5.20	1.41	1.35
1	N	340	TRP	CA-CB	5.20	1.61	1.53
1	N	219	PHE	N-CA	5.20	1.52	1.46
1	A	328	HIS	ND1-CE1	5.20	1.37	1.32
3	P	215	LEU	CB-CG	5.19	1.63	1.53
1	A	194	LEU	CA-C	5.19	1.59	1.52
3	P	32	THR	CA-C	5.19	1.59	1.52
3	C	147	ALA	N-CA	5.17	1.52	1.46
6	F	8	THR	CB-CG2	5.17	1.69	1.52
7	T	8	HIS	CG-CD2	5.17	1.41	1.35
1	N	376	HIS	CG-CD2	5.17	1.41	1.35
1	A	121	GLY	N-CA	5.17	1.50	1.45
1	N	138	HIS	CG-CD2	5.16	1.41	1.35
1	A	130	PRO	CA-CB	5.16	1.61	1.54
1	A	500	PRO	CA-C	5.16	1.56	1.52
3	C	257	TYR	N-CA	5.15	1.52	1.46
1	N	409	TRP	CD2-CE2	5.15	1.50	1.41
3	P	243	HIS	ND1-CE1	5.15	1.37	1.32
3	P	55	TYR	CA-CB	5.15	1.61	1.53
8	H	80	THR	N-CA	5.15	1.52	1.46
2	B	200	CYS	N-CA	5.13	1.51	1.46
3	C	215	LEU	CB-CG	5.13	1.63	1.53
4	D	86	MET	N-CA	5.13	1.52	1.46
4	D	85	ALA	CA-C	5.13	1.59	1.52
1	N	139	ALA	CA-CB	5.13	1.62	1.53
1	A	315	PRO	CA-CB	5.12	1.61	1.53
1	N	58	VAL	CA-C	5.12	1.59	1.52
2	B	31	VAL	C-O	5.12	1.30	1.24
1	A	196	LEU	N-CA	5.12	1.52	1.46
5	E	89	LEU	CA-CB	5.12	1.62	1.53
7	G	15	THR	CA-CB	5.12	1.61	1.53
2	B	113	TYR	N-CA	5.12	1.52	1.46
1	N	94	PHE	N-CA	5.11	1.52	1.46
9	V	65	LYS	N-CA	5.10	1.52	1.46
3	P	149	HIS	ND1-CE1	5.10	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	TRP	NE1-CE2	-5.10	1.31	1.37
1	A	277	MET	N-CA	5.10	1.52	1.46
4	D	58	GLU	CD-OE1	5.10	1.35	1.25
1	A	409	TRP	CD2-CE2	5.10	1.50	1.41
2	B	222	TRP	C-O	5.09	1.30	1.24
11	K	41	ASN	C-O	5.09	1.26	1.23
1	A	231	TYR	N-CA	5.09	1.52	1.46
3	P	169	LEU	CA-CB	5.09	1.61	1.53
3	P	70	HIS	CD2-NE2	5.08	1.43	1.37
5	E	69	GLU	N-CA	5.08	1.52	1.46
3	P	82	GLY	CA-C	5.08	1.57	1.52
1	A	173	PRO	N-CA	5.08	1.52	1.46
3	P	30	GLY	N-CA	5.07	1.52	1.45
10	J	34	VAL	CA-C	5.07	1.59	1.52
1	N	13	LYS	CA-CB	5.07	1.61	1.53
1	A	99	ASN	CA-CB	5.07	1.61	1.53
3	C	28	THR	CA-CB	5.07	1.61	1.53
7	T	36	TRP	CG-CD2	5.07	1.52	1.43
7	T	46	ALA	CA-C	5.06	1.58	1.52
1	N	189	MET	SD-CE	-5.05	1.67	1.79
3	P	74	ALA	N-CA	5.05	1.52	1.46
1	A	146	THR	N-CA	5.04	1.52	1.46
6	F	39	THR	N-CA	5.04	1.52	1.45
13	Z	36	HIS	CG-CD2	5.04	1.41	1.35
3	C	57	TRP	N-CA	5.04	1.52	1.46
3	C	212	SER	CA-CB	5.04	1.61	1.53
1	N	269	GLY	CA-C	5.04	1.58	1.51
5	E	55	CYS	C-O	5.03	1.29	1.24
1	A	128	VAL	N-CA	5.03	1.52	1.46
1	N	447	TYR	N-CA	5.02	1.52	1.46
7	T	15	THR	CA-CB	5.02	1.61	1.53
5	E	34	ASN	C-O	-5.02	1.17	1.24
1	A	272	GLY	CA-C	5.02	1.58	1.52
7	T	51	HIS	CG-CD2	5.02	1.41	1.35
1	N	288	TRP	CD2-CE2	5.01	1.49	1.41
2	O	30	ILE	N-CA	5.01	1.52	1.46
7	G	51	HIS	CG-CD2	5.01	1.41	1.35
7	G	52	HIS	CG-CD2	5.01	1.41	1.35
1	A	246	LEU	CB-CG	5.00	1.63	1.53
2	B	43	SER	C-O	-5.00	1.17	1.24
11	X	10	HIS	CE1-NE2	5.00	1.37	1.32

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-11.62	75.34	100.90
1	A	71	MET	CG-SD-CE	-11.29	76.06	100.90
1	A	112	LEU	CD1-CG-CD2	-10.36	88.00	110.80
7	T	7	ASP	N-CA-C	10.30	132.73	110.80
1	A	240	HIS	CA-CB-CG	-8.74	105.06	113.80
6	F	49	VAL	CA-C-N	-8.31	111.80	120.03
6	F	49	VAL	C-N-CA	-8.31	111.80	120.03
6	S	94	HIS	N-CA-C	8.24	128.34	110.80
1	N	240	HIS	CA-CB-CG	-7.87	105.93	113.80
1	N	83	VAL	CA-C-N	-7.84	110.88	119.19
1	N	83	VAL	C-N-CA	-7.84	110.88	119.19
12	Y	46	LYS	N-CA-C	7.75	122.30	113.01
1	N	240	HIS	N-CA-CB	7.73	117.74	110.39
7	G	7	ASP	N-CA-C	7.63	127.06	110.80
3	P	74	ALA	N-CA-C	-7.60	103.08	111.36
7	G	2	SER	N-CA-C	-7.55	102.39	114.09
1	A	125	GLY	N-CA-C	-7.52	103.38	112.48
4	Q	20	ARG	NE-CZ-NH2	-7.16	112.75	119.20
2	B	38	VAL	N-CA-C	7.09	117.86	110.62
5	R	42	VAL	N-CA-C	-6.90	99.91	108.05
1	N	105	LEU	CA-C-N	-6.82	113.36	120.38
1	N	105	LEU	C-N-CA	-6.82	113.36	120.38
1	A	189	MET	CG-SD-CE	-6.81	85.92	100.90
4	Q	107	ILE	CA-C-N	-6.78	113.32	120.03
4	Q	107	ILE	C-N-CA	-6.78	113.32	120.03
7	G	8	HIS	N-CA-C	6.71	125.09	110.80
1	A	310	MET	CA-CB-CG	-6.56	100.97	114.10
6	S	95	GLN	N-CA-C	6.55	119.15	108.08
4	Q	20	ARG	CG-CD-NE	-6.48	97.74	112.00
1	A	105	LEU	CA-C-N	-6.45	113.73	120.38
1	A	105	LEU	C-N-CA	-6.45	113.73	120.38
3	C	131	LEU	N-CA-C	-6.45	104.33	111.36
1	A	49	GLY	N-CA-C	-6.38	98.06	113.18
1	N	112	LEU	CD1-CG-CD2	-6.37	96.80	110.80
7	G	58	LYS	CA-C-N	-6.36	113.23	119.78
7	G	58	LYS	C-N-CA	-6.36	113.23	119.78
5	E	90	ARG	NE-CZ-NH1	6.32	127.82	121.50
7	G	6	GLY	N-CA-C	6.28	128.06	113.18
2	B	46	LEU	CA-C-N	-6.25	112.60	122.79
2	B	46	LEU	C-N-CA	-6.25	112.60	122.79
7	T	58	LYS	CA-C-N	-6.21	113.38	119.78
7	T	58	LYS	C-N-CA	-6.21	113.38	119.78
2	B	68[A]	LEU	CA-C-N	-6.19	112.18	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	68[A]	LEU	C-N-CA	-6.19	112.18	119.05
2	B	68[B]	LEU	CA-C-N	-6.19	112.18	119.05
2	B	68[B]	LEU	C-N-CA	-6.19	112.18	119.05
6	F	4	GLY	N-CA-C	-6.14	103.91	112.13
1	A	35	LEU	CD1-CG-CD2	-6.13	97.32	110.80
3	P	41	THR	N-CA-C	6.08	117.60	110.97
7	T	36	TRP	CB-CA-C	6.04	118.64	111.22
2	B	59	GLN	N-CA-C	6.01	117.50	111.07
1	A	173	PRO	N-CA-C	-5.92	104.78	110.47
2	B	65	TRP	N-CA-C	5.92	119.60	112.38
1	A	314	ILE	CA-C-N	-5.92	112.77	119.28
1	A	314	ILE	C-N-CA	-5.92	112.77	119.28
7	T	41	HIS	N-CA-C	5.91	119.03	110.28
12	L	20	ARG	CG-CD-NE	-5.88	99.07	112.00
3	C	159	MET	N-CA-C	-5.86	104.80	111.07
1	N	250	GLY	N-CA-C	-5.86	105.40	112.49
3	P	219	PHE	N-CA-C	-5.83	104.84	111.14
11	K	17	VAL	N-CA-C	-5.79	104.87	110.72
8	U	33	TYR	N-CA-C	-5.79	104.89	111.14
4	D	38	LYS	CB-CG-CD	-5.76	98.06	111.30
3	C	239	ALA	N-CA-C	-5.75	104.93	111.14
5	R	90	ARG	CG-CD-NE	-5.75	99.34	112.00
6	S	64	GLU	CA-C-N	-5.72	116.32	126.45
6	S	64	GLU	C-N-CA	-5.72	116.32	126.45
6	F	40	SER	N-CA-C	-5.72	105.80	112.89
3	C	194	GLY	N-CA-C	-5.72	105.71	113.37
1	A	74	MET	CB-CG-SD	-5.71	95.56	112.70
4	D	5	VAL	N-CA-C	5.70	114.95	106.85
2	B	43	SER	N-CA-C	-5.66	105.26	111.82
6	F	61	ILE	N-CA-C	-5.66	98.28	106.88
1	A	74	MET	CA-C-N	-5.65	115.91	122.63
1	A	74	MET	C-N-CA	-5.65	115.91	122.63
5	E	90	ARG	CB-CG-CD	5.65	124.29	111.30
10	J	23	LYS	CG-CD-CE	-5.63	98.34	111.30
1	N	146	THR	N-CA-C	-5.58	105.09	111.07
7	T	8	HIS	N-CA-C	5.56	122.64	110.80
7	G	44	ARG	N-CA-C	5.55	116.68	109.64
12	L	6	GLY	CA-C-N	5.55	125.82	119.83
12	L	6	GLY	C-N-CA	5.55	125.82	119.83
3	P	91	VAL	N-CA-C	-5.54	105.12	110.72
5	R	82	TYR	CA-C-N	-5.52	113.21	119.28
5	R	82	TYR	C-N-CA	-5.52	113.21	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ILE	N-CA-C	5.51	115.60	110.42
1	N	308	ALA	N-CA-C	-5.51	105.35	111.36
2	O	192	TYR	CA-CB-CG	-5.51	103.99	113.90
7	G	12	GLY	N-CA-C	5.50	129.25	113.30
2	B	28	LEU	CA-C-N	5.49	129.47	120.63
2	B	28	LEU	C-N-CA	5.49	129.47	120.63
1	A	267	PRO	CB-CA-C	-5.49	102.79	110.63
1	A	180	GLN	CA-CB-CG	-5.48	103.14	114.10
1	N	315	PRO	N-CA-C	-5.48	106.40	113.57
4	D	71	MET	N-CA-C	-5.47	106.11	112.89
4	D	58	GLU	CA-CB-CG	-5.46	103.17	114.10
5	E	87	GLN	CB-CG-CD	-5.46	103.31	112.60
1	A	75	ILE	N-CA-C	-5.42	106.52	111.67
5	E	54	ALA	N-CA-C	-5.41	105.38	111.28
2	O	67	ILE	N-CA-C	5.41	115.61	110.42
7	T	69	PHE	N-CA-C	5.41	117.17	111.28
4	Q	9	GLU	N-CA-C	5.40	120.69	112.54
2	B	41[A]	ILE	CA-C-N	-5.38	113.66	120.60
2	B	41[A]	ILE	C-N-CA	-5.38	113.66	120.60
2	B	41[B]	ILE	CA-C-N	-5.38	113.66	120.60
2	B	41[B]	ILE	C-N-CA	-5.38	113.66	120.60
1	A	310	MET	CG-SD-CE	-5.35	89.13	100.90
1	A	239	GLY	CA-C-N	-5.33	113.92	119.83
1	A	239	GLY	C-N-CA	-5.33	113.92	119.83
12	L	40	VAL	CB-CA-C	-5.32	104.96	112.14
2	B	45	MET	CG-SD-CE	5.31	112.58	100.90
3	C	113	GLY	N-CA-C	-5.31	107.78	115.27
1	N	29	VAL	N-CA-C	-5.31	105.20	110.62
1	A	240	HIS	N-CA-CB	5.30	115.42	110.39
12	Y	21	LEU	N-CA-C	-5.30	105.40	111.07
1	N	180	GLN	CA-CB-CG	-5.29	103.53	114.10
7	T	5	LYS	CB-CA-C	5.27	120.91	110.42
6	F	39	THR	N-CA-C	-5.27	101.67	109.94
1	A	119	GLU	CB-CA-C	-5.24	110.51	116.54
2	B	59	GLN	N-CA-CB	5.23	117.59	110.01
4	D	65	LYS	CB-CG-CD	-5.23	99.27	111.30
8	U	25	GLN	N-CA-C	-5.22	106.14	112.88
1	N	280	ILE	CA-C-N	-5.19	114.29	120.00
1	N	280	ILE	C-N-CA	-5.19	114.29	120.00
2	O	65	TRP	CB-CA-C	-5.19	99.58	110.17
11	K	53	TRP	N-CA-C	-5.18	107.61	114.04
3	P	113	GLY	N-CA-C	-5.17	107.98	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	66	ILE	N-CA-C	5.17	115.28	110.42
7	G	57	THR	N-CA-C	-5.15	107.02	113.72
3	P	69	GLY	N-CA-C	-5.13	108.19	115.43
3	P	82	GLY	N-CA-C	-5.13	106.58	112.73
5	E	84	TYR	N-CA-C	-5.12	105.77	111.36
1	N	310	MET	CA-CB-CG	-5.12	103.86	114.10
1	A	96	ARG	NE-CZ-NH2	-5.11	114.60	119.20
7	G	5	LYS	CB-CA-C	5.11	120.59	110.42
6	F	95	GLN	N-CA-C	5.10	120.13	112.94
2	B	92	ASN	CA-C-N	-5.09	114.71	119.85
2	B	92	ASN	C-N-CA	-5.09	114.71	119.85
4	D	57	VAL	N-CA-C	-5.08	105.59	110.72
1	N	279	SER	CA-CB-OG	-5.07	100.95	111.10
4	Q	143	ASN	CB-CA-C	-5.06	105.08	111.86
6	S	61	ILE	N-CA-C	-5.06	99.19	106.88
4	D	49	SER	CA-CB-OG	-5.02	101.06	111.10
1	N	487	LEU	N-CA-C	-5.02	106.46	112.58

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
7	T	40	GLY	Peptide
12	Y	46	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4162	98	0
1	N	4179	0	4154	92	0
2	B	1904	0	1909	60	0
2	O	1859	0	1860	41	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2185	0	2097	53	0
3	P	2185	0	2097	52	0
4	D	1231	0	1227	48	0
4	Q	1224	0	1211	25	1
5	E	852	0	845	9	0
5	R	852	0	845	7	0
6	F	778	0	754	32	0
6	S	763	0	742	33	0
7	G	675	0	643	37	0
7	T	686	0	651	31	0
8	H	662	0	623	20	0
8	U	662	0	623	9	0
9	I	601	0	613	26	0
9	V	601	0	613	17	0
10	J	460	0	459	6	0
10	W	469	0	464	14	0
11	K	384	0	366	5	0
11	X	391	0	374	6	0
12	L	385	0	389	5	0
12	Y	388	0	388	14	0
13	M	335	0	352	11	0
13	Z	335	0	352	7	0
14	A	180	0	162	22	0
14	N	180	0	162	26	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	6	0	0	7	0
18	N	6	0	0	6	0
19	A	63	0	110	3	0
19	D	63	0	110	21	0
19	L	63	0	110	4	0
19	N	63	0	110	8	0
19	Q	63	0	110	10	0
19	Y	63	0	110	13	0
20	A	102	0	152	13	0
20	C	102	0	152	11	0
20	G	51	0	76	4	0
20	N	51	0	76	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	P	51	0	76	4	0
20	Z	51	0	76	12	0
21	A	52	0	78	19	0
21	B	8	0	12	0	0
21	C	36	0	54	4	0
21	D	24	0	36	15	0
21	E	20	0	30	0	0
21	F	16	0	24	3	0
21	G	8	0	12	1	0
21	H	8	0	12	4	0
21	J	4	0	6	0	0
21	L	4	0	6	0	0
21	N	48	0	72	23	0
21	O	12	0	18	2	0
21	P	16	0	24	1	0
21	Q	8	0	12	0	0
21	R	24	0	36	2	0
21	S	8	0	12	0	0
21	T	4	0	6	0	0
21	U	4	0	6	0	0
21	V	4	0	6	0	0
22	B	29	0	39	0	0
22	C	58	0	78	8	0
22	G	29	0	39	1	0
22	J	29	0	38	2	0
22	P	58	0	78	7	0
22	W	29	0	39	9	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	23	0
24	O	52	0	80	12	0
25	C	99	0	126	18	0
25	L	33	0	42	5	0
25	M	33	0	42	1	0
25	P	99	0	126	18	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0
26	P	1	0	0	0	0
27	C	106	0	154	17	0
27	G	53	0	77	10	0
27	P	53	0	77	10	0
27	T	106	0	154	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	C	100	0	156	28	0
28	N	100	0	156	15	0
28	P	100	0	156	25	0
28	T	100	0	156	20	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	233	0	0	15	0
30	B	140	0	0	13	1
30	C	101	0	0	4	0
30	D	110	0	0	19	1
30	E	85	0	0	4	0
30	F	78	0	0	7	0
30	G	51	0	0	4	0
30	H	45	0	0	3	0
30	I	25	0	0	5	0
30	J	28	0	0	2	0
30	K	21	0	0	4	0
30	L	29	0	0	3	0
30	M	27	0	0	3	0
30	N	219	0	0	18	0
30	O	115	0	0	3	0
30	P	90	0	0	2	0
30	Q	36	0	0	3	0
30	R	39	0	0	0	0
30	S	55	0	0	6	0
30	T	39	0	0	3	0
30	U	33	0	0	0	0
30	V	14	0	0	3	0
30	W	11	0	0	2	0
30	X	11	0	0	0	0
30	Y	14	0	0	1	0
30	Z	16	0	0	1	0
All	All	33735	0	32802	890	2

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 14.

All (890) 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)
21:A:615:EDO:C2	21:A:615:EDO:C1	1.78	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:101:PGV:C2	20:Z:101:PGV:H011	1.50	1.39
21:A:615:EDO:C1	21:A:615:EDO:O2	1.71	1.36
21:C:316:EDO:H11	30:C:486:HOH:O	1.23	1.29
30:A:705:HOH:O	19:D:201:TGL:HG11	1.32	1.26
19:D:201:TGL:HG31	30:D:364:HOH:O	1.24	1.26
19:N:610:TGL:H112	30:O:424:HOH:O	1.30	1.25
4:D:31[B]:LYS:HG3	30:D:401:HOH:O	1.33	1.24
5:E:100:THR:HG21	30:E:357:HOH:O	1.09	1.23
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD2	1.44	1.17
1:A:112:LEU:HG	30:A:911:HOH:O	1.43	1.15
4:D:100[B]:LYS:HE3	30:D:310:HOH:O	1.48	1.14
1:N:302[B]:ARG:HH12	1:N:365:ILE:HD11	1.12	1.13
1:N:417[A]:MET:CE	30:N:839:HOH:O	1.94	1.13
20:Z:101:PGV:H011	20:Z:101:PGV:H22	1.26	1.12
6:S:43:LYS:HE2	6:S:43:LYS:H	1.00	1.12
21:N:621:EDO:H11	6:S:36:PRO:HD3	1.24	1.11
3:P:67:PHE:HE2	28:P:304:CDL:H1	1.01	1.10
2:B:32[A]:PHE:O	2:B:35[A]:SER:OG	1.69	1.10
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	1.92	1.09
27:C:308:PEK:H041	6:F:1:ALA:H1	0.99	1.08
24:B:303:PSC:H241	24:B:303:PSC:H202	1.35	1.08
3:P:67:PHE:CE2	28:P:304:CDL:H1	1.89	1.08
7:G:84:LYS:H	7:G:84:LYS:HD2	1.18	1.07
20:C:309:PGV:H061	8:H:22:ASN:HD22	1.09	1.07
28:P:304:CDL:H381	28:P:304:CDL:H271	1.32	1.06
20:Z:101:PGV:H011	20:Z:101:PGV:H21	1.33	1.06
1:A:39:ALA:HA	21:D:202:EDO:O1	1.52	1.06
8:H:9:LYS:HG3	8:H:10:ASN:H	1.15	1.06
1:N:486:ASP:OD2	4:Q:19[B]:ARG:HD2	1.52	1.06
21:N:618:EDO:H12	30:S:246:HOH:O	1.54	1.06
21:N:621:EDO:C1	6:S:36:PRO:HD3	1.86	1.05
21:A:615:EDO:O2	21:A:615:EDO:H12	1.53	1.04
1:N:297[B]:MET:CB	30:N:766:HOH:O	2.03	1.03
1:A:282:PHE:HA	7:T:4:ALA:CB	1.88	1.03
1:A:297[A]:MET:SD	1:A:302[A]:ARG:HG2	1.98	1.02
21:N:618:EDO:O2	30:N:701:HOH:O	1.76	1.02
1:A:513:LEU:O	1:A:514:LYS:HB2	1.59	1.01
2:B:29[A]:MET:HE2	9:I:35:TYR:HD1	1.21	1.01
1:N:297[B]:MET:HB2	30:N:766:HOH:O	1.59	1.01
3:C:33[A]:MET:HB2	25:C:302:DMU:C22	1.90	1.01
6:F:94:HIS:HD2	30:F:216:HOH:O	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19[A]:ARG:CG	4:D:21:ASP:OD1	2.10	1.00
19:D:201:TGL:H361	30:I:125:HOH:O	1.62	0.99
20:Z:101:PGV:C2	20:Z:101:PGV:C01	2.42	0.98
1:N:178[B]:GLN:HG2	1:N:186:TRP:CZ2	1.99	0.98
6:F:1:ALA:HB3	21:F:105:EDO:O1	1.64	0.97
7:G:8:HIS:CD2	7:G:9:GLY:H	1.81	0.97
7:G:84:LYS:HD2	7:G:84:LYS:N	1.79	0.97
3:C:63:ARG:HE	28:C:306:CDL:HA22	1.27	0.97
1:N:302[B]:ARG:NH1	1:N:365:ILE:HD11	1.77	0.97
27:P:307:PEK:C04	6:S:1:ALA:N	2.26	0.97
4:Q:19[A]:ARG:CD	4:Q:21:ASP:OD1	2.13	0.96
11:K:47:ARG:HD3	30:K:109:HOH:O	1.62	0.96
28:N:601:CDL:H371	2:O:78:LEU:HD12	1.48	0.96
28:P:304:CDL:H391	28:P:304:CDL:H351	1.45	0.96
27:C:308:PEK:H041	6:F:1:ALA:N	1.78	0.96
6:F:1:ALA:CB	21:F:105:EDO:O1	2.14	0.95
27:P:307:PEK:H041	6:S:1:ALA:N	1.81	0.94
30:B:533:HOH:O	19:D:201:TGL:H281	1.67	0.94
28:T:103:CDL:H641	28:T:103:CDL:H602	1.49	0.94
7:T:11:TPO:HA	7:T:11:TPO:O3P	1.66	0.94
6:S:43:LYS:HE2	6:S:43:LYS:N	1.82	0.93
7:G:12:GLY:HA3	30:G:237:HOH:O	1.67	0.92
27:C:308:PEK:C04	6:F:1:ALA:H1	1.82	0.92
1:N:513:LEU:O	1:N:514:LYS:HB2	1.68	0.92
1:A:221:ASP:OD1	21:A:621:EDO:H12	1.70	0.91
4:D:19[A]:ARG:HG2	4:D:21:ASP:OD1	1.71	0.91
4:Q:19[A]:ARG:HD3	4:Q:21:ASP:OD1	1.68	0.91
25:L:102:DMU:H26	30:L:229:HOH:O	1.71	0.91
12:Y:24[B]:MET:SD	19:Y:101:TGL:HC21	2.11	0.90
7:T:12:GLY:HA3	30:T:233:HOH:O	1.69	0.90
19:Y:101:TGL:HC41	19:Y:101:TGL:OC1	1.68	0.90
5:E:90:ARG:HD2	30:E:366:HOH:O	1.72	0.90
9:V:11:GLY:O	9:V:15:ARG:HG3	1.72	0.89
3:C:33[A]:MET:HB2	25:C:302:DMU:H11	1.52	0.89
21:D:203:EDO:H11	30:D:340:HOH:O	1.72	0.89
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.52	0.89
20:G:103:PGV:H71	20:G:103:PGV:H22	1.55	0.88
6:S:43:LYS:H	6:S:43:LYS:CE	1.87	0.88
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:CD	2.21	0.88
9:I:15:ARG:NH2	30:I:101:HOH:O	2.04	0.88
7:G:9:GLY:HA3	30:N:885:HOH:O	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PHE:HA	7:T:4:ALA:HB1	1.55	0.87
24:B:303:PSC:H202	24:B:303:PSC:C24	2.01	0.87
2:B:29[A]:MET:HE2	9:I:35:TYR:CD1	2.10	0.87
7:G:42:ARG:NH1	7:G:42:ARG:HA	1.90	0.87
30:B:533:HOH:O	19:D:201:TGL:C28	2.19	0.86
27:P:307:PEK:C04	6:S:1:ALA:H1	1.83	0.86
2:O:16:ILE:HD12	2:O:87[A]:MET:HG2	1.57	0.86
3:C:67:PHE:HE2	28:C:306:CDL:C1	1.89	0.86
24:B:303:PSC:H51	30:I:110:HOH:O	1.75	0.85
27:P:307:PEK:H041	6:S:1:ALA:H1	1.36	0.85
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.16	0.85
24:O:302:PSC:C07	9:V:10:ARG:HH21	1.90	0.85
3:C:67:PHE:HE2	28:C:306:CDL:H1	1.40	0.85
3:P:33[B]:MET:SD	25:P:306:DMU:H8	2.16	0.85
10:W:33:ARG:HG2	22:W:101:CHD:H8	1.59	0.85
7:G:72:ASN:H	7:G:76:ASN:HD22	1.24	0.84
6:S:75:HIS:H	6:S:80:GLN:HE22	1.24	0.84
7:T:72:ASN:H	7:T:76:ASN:HD22	1.24	0.84
1:N:359:ALA:HA	14:N:603[B]:HEA:OMA	1.77	0.84
4:D:100[B]:LYS:HD2	4:D:100[B]:LYS:O	1.76	0.84
28:T:103:CDL:H331	28:T:103:CDL:OA7	1.78	0.84
3:P:51[B]:MET:HE3	28:P:304:CDL:H273	1.60	0.84
27:C:304:PEK:HN2	7:G:76:ASN:HD21	1.26	0.83
3:P:63:ARG:HE	28:P:304:CDL:HA21	1.43	0.83
27:C:308:PEK:C04	6:F:1:ALA:N	2.42	0.83
1:N:178[B]:GLN:HG3	1:N:178[B]:GLN:O	1.78	0.83
7:G:42:ARG:HA	7:G:42:ARG:HH11	1.44	0.82
1:N:417[A]:MET:HE2	30:N:839:HOH:O	1.63	0.82
28:P:304:CDL:H251	28:P:304:CDL:H392	1.60	0.82
24:B:303:PSC:H081	5:E:8:ASP:OD1	1.79	0.82
24:B:303:PSC:H241	24:B:303:PSC:C20	2.05	0.82
7:G:46:ALA:HB3	30:G:247:HOH:O	1.78	0.81
3:C:51[B]:MET:CE	28:C:306:CDL:H392	2.10	0.81
27:P:307:PEK:H383	28:T:103:CDL:H273	1.63	0.81
3:C:67:PHE:CE2	28:C:306:CDL:H1	2.16	0.81
3:C:224:LYS:HE3	28:C:306:CDL:HB32	1.61	0.81
20:A:609:PGV:H343	27:C:304:PEK:H382	1.61	0.81
4:D:99:GLU:OE2	21:D:202:EDO:H22	1.81	0.81
1:A:297[A]:MET:SD	1:A:302[A]:ARG:CG	2.69	0.81
4:D:34:SER:H	4:D:37:GLN:HE21	1.26	0.80
13:M:38:ASP:OD2	13:M:42:LYS:HD3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:307:PEK:H042	6:S:1:ALA:N	1.94	0.80
4:D:31[B]:LYS:CE	30:D:401:HOH:O	2.29	0.80
22:P:305:CHD:H231	22:P:305:CHD:H162	1.63	0.80
24:O:302:PSC:H343	24:O:302:PSC:H142	1.62	0.80
22:C:307:CHD:H162	22:C:307:CHD:H231	1.62	0.80
20:C:309:PGV:H061	8:H:22:ASN:ND2	1.93	0.80
6:F:75:HIS:H	6:F:80:GLN:HE22	1.24	0.80
3:P:33[A]:MET:HE3	3:P:39:SER:OG	1.82	0.80
1:A:382[B]:SER:HB3	1:A:383[B]:MET:HE2	1.64	0.79
4:D:65:LYS:HE3	30:D:389:HOH:O	1.82	0.79
3:C:224:LYS:CD	28:C:306:CDL:HB32	2.13	0.79
21:A:615:EDO:H22	30:M:217:HOH:O	1.82	0.79
8:H:9:LYS:HG3	8:H:10:ASN:N	1.91	0.79
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.64	0.78
20:C:309:PGV:H72	20:C:309:PGV:H21	1.63	0.78
25:P:306:DMU:H35	25:P:306:DMU:H29	1.65	0.78
2:B:16[B]:ILE:HG23	30:B:502:HOH:O	1.83	0.78
2:B:41[A]:ILE:HD13	24:B:303:PSC:H342	1.66	0.78
3:P:33[A]:MET:HE1	3:P:41:THR:HB	1.66	0.78
18:A:606:AZI:N1	18:A:607:AZI:N1	2.32	0.77
1:A:359:ALA:HA	14:A:602[B]:HEA:OMA	1.83	0.77
24:B:303:PSC:C06	9:I:10:ARG:HH21	1.97	0.77
21:N:618:EDO:O1	30:N:702:HOH:O	2.01	0.77
27:P:307:PEK:C04	6:S:1:ALA:H2	1.98	0.77
21:A:618:EDO:H12	30:M:219:HOH:O	1.84	0.77
4:D:31[B]:LYS:CD	30:D:401:HOH:O	2.31	0.77
11:K:47:ARG:CD	30:K:109:HOH:O	2.28	0.77
1:N:302[B]:ARG:HH12	1:N:365:ILE:CD1	1.93	0.77
3:C:180[B]:GLU:HG2	30:C:414:HOH:O	1.83	0.77
1:A:112:LEU:C	1:A:112:LEU:HD23	2.10	0.77
7:T:37:LEU:HD23	28:T:103:CDL:H381	1.67	0.76
3:P:63:ARG:HE	28:P:304:CDL:CA2	1.98	0.76
6:F:95:GLN:C	6:F:97:ALA:H	1.93	0.76
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.76
1:A:459:PHE:CE1	21:D:202:EDO:H11	2.20	0.76
21:N:622:EDO:H11	6:S:84:SER:OG	1.86	0.76
20:Z:101:PGV:H22	20:Z:101:PGV:C01	2.13	0.76
3:C:51[B]:MET:HE3	28:C:306:CDL:H392	1.68	0.75
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.69	0.75
8:U:10:ASN:N	8:U:10:ASN:HD22	1.83	0.75
12:Y:20:ARG:HH12	19:Y:101:TGL:HC32	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ALA:CA	21:D:202:EDO:O1	2.32	0.75
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.69	0.75
3:C:33[A]:MET:HB2	25:C:302:DMU:C25	2.18	0.74
8:H:38:ARG:HH22	21:H:101:EDO:H12	1.53	0.74
3:C:224:LYS:CE	28:C:306:CDL:HB32	2.18	0.74
3:C:33[A]:MET:HB2	25:C:302:DMU:H13	1.70	0.73
8:H:9:LYS:HA	8:H:9:LYS:NZ	2.03	0.73
1:N:178[B]:GLN:O	1:N:178[B]:GLN:CG	2.36	0.73
7:T:76:ASN:HD21	27:T:102:PEK:HN2	1.34	0.73
7:G:84:LYS:H	7:G:84:LYS:CD	1.99	0.73
4:Q:78:TRP:CA	19:Q:201:TGL:HB22	2.19	0.73
28:T:103:CDL:OA7	28:T:103:CDL:H311	1.89	0.73
8:U:10:ASN:HD22	8:U:10:ASN:H	1.33	0.73
1:A:189:MET:CE	30:A:907:HOH:O	2.36	0.72
1:N:105:LEU:HD11	21:N:612:EDO:H12	1.71	0.72
20:Z:101:PGV:H21	20:Z:101:PGV:C01	2.15	0.72
7:T:44:ARG:HH22	7:T:84:LYS:NZ	1.86	0.72
28:T:103:CDL:H311	28:T:103:CDL:HA4	1.72	0.72
13:M:42:LYS:HG2	13:M:42:LYS:O	1.89	0.72
3:C:33[A]:MET:CB	25:C:302:DMU:H11	2.19	0.72
20:A:610:PGV:H311	13:M:19:LEU:HD23	1.71	0.71
19:D:201:TGL:H242	19:D:201:TGL:HA91	1.70	0.71
1:N:362[B]:SER:OG	30:N:703:HOH:O	2.08	0.71
3:C:63:ARG:HE	28:C:306:CDL:CA2	2.01	0.71
4:D:100[B]:LYS:O	4:D:100[B]:LYS:CD	2.39	0.71
21:A:613:EDO:H21	30:A:906:HOH:O	1.91	0.71
1:N:28:MET:CE	14:N:602:HEA:H271	2.21	0.71
4:D:31[B]:LYS:CG	30:D:401:HOH:O	2.06	0.70
1:N:54:TYR:HB2	30:N:866:HOH:O	1.91	0.70
9:V:18:ARG:HD3	30:V:213:HOH:O	1.90	0.70
28:T:103:CDL:H222	28:T:103:CDL:H522	1.74	0.70
3:C:51[A]:MET:HE1	20:C:305:PGV:H161	1.73	0.70
3:P:67:PHE:HE2	28:P:304:CDL:C1	1.93	0.70
7:G:46:ALA:CB	30:G:247:HOH:O	2.37	0.70
8:H:9:LYS:HA	8:H:9:LYS:HZ1	1.56	0.70
1:A:221:ASP:OD1	21:A:621:EDO:C1	2.40	0.69
4:D:19[A]:ARG:HH21	4:D:21:ASP:CG	2.00	0.69
1:N:297[B]:MET:HB3	30:N:766:HOH:O	1.75	0.69
12:L:24[B]:MET:HG2	19:L:101:TGL:HA22	1.74	0.69
2:O:29[B]:MET:HG3	9:V:35:TYR:CD1	2.27	0.69
2:O:47:THR:HB	19:Q:201:TGL:H181	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:51[B]:MET:CE	28:P:304:CDL:H273	2.22	0.68
12:Y:24[B]:MET:SD	19:Y:101:TGL:CC2	2.82	0.68
3:C:224:LYS:HE3	28:C:306:CDL:CB3	2.23	0.68
21:D:203:EDO:H21	30:F:201:HOH:O	1.94	0.68
7:T:36:TRP:CE3	7:T:39:SER:HB3	2.29	0.68
1:A:22:PHE:HA	19:L:101:TGL:HB71	1.74	0.68
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.91	0.68
7:T:31:CYS:SG	28:T:103:CDL:H532	2.33	0.68
1:N:364:ASP:OD1	14:N:603[B]:HEA:O1A	2.12	0.68
9:V:18:ARG:HG3	30:V:211:HOH:O	1.94	0.68
3:P:33[B]:MET:SD	25:P:306:DMU:C19	2.82	0.67
1:A:382[B]:SER:CB	1:A:383[B]:MET:HE2	2.24	0.67
20:A:609:PGV:H183	27:C:304:PEK:H322	1.76	0.67
24:B:303:PSC:H31	9:I:17:LEU:HD23	1.76	0.67
7:G:8:HIS:HE1	27:G:102:PEK:H042	1.60	0.67
12:Y:26:THR:OG1	30:Y:201:HOH:O	2.13	0.67
28:T:103:CDL:H252	28:T:103:CDL:H762	1.76	0.67
3:P:133:ASN:ND2	30:P:401:HOH:O	2.26	0.67
6:F:90:LYS:HD2	30:F:276:HOH:O	1.94	0.67
18:N:607:AZI:N1	18:N:608:AZI:N1	2.42	0.67
4:Q:19[A]:ARG:CG	4:Q:21:ASP:OD1	2.43	0.66
4:D:4:SER:CB	30:D:302:HOH:O	2.44	0.66
9:I:73:LYS:O	30:I:102:HOH:O	2.13	0.66
4:D:28:ALA:H	4:D:31[B]:LYS:NZ	1.93	0.66
1:A:28:MET:CE	14:A:601:HEA:H271	2.26	0.66
13:M:41:LYS:O	13:M:43:SER:N	2.25	0.66
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.31	0.66
3:C:33[A]:MET:HE3	25:C:302:DMU:H10	1.77	0.66
3:C:91:VAL:O	3:C:95:THR:HG23	1.95	0.66
6:F:64:GLU:O	6:F:65:ASP:HB2	1.96	0.66
20:G:103:PGV:H292	3:P:95:THR:HG21	1.77	0.66
4:Q:19[A]:ARG:HG2	4:Q:21:ASP:OD1	1.95	0.66
1:N:265:LYS:HE3	21:N:622:EDO:O1	1.96	0.65
25:P:306:DMU:H29	25:P:306:DMU:C9	2.25	0.65
19:N:610:TGL:HB92	19:N:610:TGL:C28	2.26	0.65
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.24	0.65
5:E:72:LYS:HE2	30:E:349:HOH:O	1.95	0.65
4:Q:78:TRP:HA	19:Q:201:TGL:HB22	1.77	0.65
1:A:378:HIS:HA	1:A:382[B]:SER:HB2	1.79	0.65
6:S:64:GLU:O	6:S:65:ASP:HB2	1.96	0.65
7:G:2:SER:OG	27:G:102:PEK:H301	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:H	1:A:180:GLN:HE21	1.45	0.65
1:A:189:MET:HE3	30:A:907:HOH:O	1.96	0.65
1:A:297[A]:MET:CG	1:A:302[A]:ARG:HG3	2.27	0.65
20:C:309:PGV:C06	8:H:22:ASN:HD22	1.98	0.65
19:A:608:TGL:HC22	30:A:918:HOH:O	1.96	0.65
6:F:87[B]:THR:HG21	30:F:258:HOH:O	1.97	0.65
2:O:114:GLU:HG3	2:O:227:LEU:HD21	1.79	0.65
4:Q:17[A]:VAL:O	4:Q:17[A]:VAL:HG23	1.97	0.64
3:P:33[B]:MET:HE3	25:P:306:DMU:H6	1.78	0.64
28:P:304:CDL:H381	28:P:304:CDL:C27	2.19	0.64
1:A:282:PHE:CA	7:T:4:ALA:HB1	2.26	0.64
3:C:180[A]:GLU:OE2	30:C:401:HOH:O	2.15	0.64
4:D:4:SER:OG	30:D:302:HOH:O	2.14	0.64
3:P:33[A]:MET:HB2	25:P:306:DMU:C19	2.27	0.64
10:W:27:THR:HB	30:W:211:HOH:O	1.97	0.64
27:C:308:PEK:H382	28:N:601:CDL:H271	1.79	0.64
22:C:307:CHD:H162	22:C:307:CHD:C23	2.27	0.64
4:D:31[B]:LYS:HE3	30:D:401:HOH:O	1.92	0.64
24:B:303:PSC:O01	9:I:14:ALA:HB2	1.97	0.64
3:C:37:PHE:CG	25:C:302:DMU:H8	2.33	0.63
3:C:224:LYS:HD3	28:C:306:CDL:HB32	1.79	0.63
3:P:224:LYS:HE3	28:P:304:CDL:HB32	1.80	0.63
13:Z:19:LEU:HD23	20:Z:101:PGV:H312	1.80	0.63
4:D:58:GLU:OE2	21:D:204:EDO:H22	1.98	0.63
4:D:34:SER:H	4:D:37:GLN:NE2	1.95	0.63
27:P:307:PEK:C38	28:T:103:CDL:H273	2.28	0.63
3:P:33[A]:MET:HB2	25:P:306:DMU:H9	1.81	0.63
8:U:10:ASN:N	8:U:10:ASN:ND2	2.47	0.63
2:B:60:GLU:H	2:B:60:GLU:CD	2.06	0.63
4:D:4:SER:HB3	30:D:302:HOH:O	1.98	0.63
7:G:59:PRO:O	21:G:104:EDO:H22	1.98	0.63
1:N:265:LYS:HD2	21:N:622:EDO:H12	1.80	0.63
6:S:85:CYS:SG	6:S:87[A]:THR:CG2	2.81	0.63
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.13	0.62
28:N:601:CDL:H161	28:N:601:CDL:OB3	1.98	0.62
19:Y:101:TGL:HC22	19:Y:101:TGL:HC81	1.81	0.62
7:T:5:LYS:HG3	27:T:101:PEK:H351	1.80	0.62
1:A:513:LEU:O	1:A:514:LYS:CB	2.38	0.62
13:Z:12:PRO:HB3	20:Z:101:PGV:H251	1.79	0.62
24:B:303:PSC:C1	9:I:14:ALA:HB2	2.29	0.62
9:I:73:LYS:HD3	9:I:73:LYS:OXT	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:TYR:OH	21:A:615:EDO:H21	1.99	0.62
7:T:7:ASP:O	7:T:9:GLY:N	2.24	0.62
7:T:44:ARG:HH22	7:T:84:LYS:HZ1	1.46	0.62
1:A:178[B]:GLN:CD	1:A:178[B]:GLN:H	2.08	0.62
28:C:306:CDL:HB21	28:C:306:CDL:OA5	1.99	0.62
1:A:177:SER:H	1:A:180:GLN:NE2	1.98	0.61
1:N:406:ASN:HD21	20:Z:101:PGV:H21	1.65	0.61
7:T:36:TRP:HE3	7:T:39:SER:HB3	1.66	0.61
4:Q:19[A]:ARG:HD3	4:Q:21:ASP:CG	2.25	0.61
28:P:304:CDL:H271	28:P:304:CDL:C38	2.21	0.61
4:D:58:GLU:OE2	21:D:204:EDO:C2	2.49	0.61
1:A:356:ILE:HD13	14:A:602[B]:HEA:HMB1	1.83	0.60
25:C:310:DMU:H32	25:C:310:DMU:H29	1.82	0.60
1:N:28:MET:CE	14:N:602:HEA:C27	2.78	0.60
2:B:68[B]:LEU:HB3	2:B:69:PRO:HD3	1.82	0.60
3:C:80[B]:ARG:HG2	3:C:233:PHE:CE1	2.37	0.60
7:G:8:HIS:CE1	27:G:102:PEK:H051	2.37	0.60
7:T:5:LYS:HG3	27:T:101:PEK:C35	2.31	0.60
1:A:223:ALA:HB2	21:A:621:EDO:H11	1.82	0.60
27:C:304:PEK:H11	27:C:304:PEK:H172	1.84	0.60
4:D:78:TRP:N	19:D:201:TGL:HB21	2.17	0.60
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.30	0.60
13:M:40:TYR:O	13:M:43:SER:HB2	2.02	0.60
1:N:177:SER:H	1:N:180:GLN:HE21	1.48	0.60
28:N:601:CDL:H761	28:N:601:CDL:H561	1.83	0.60
21:N:612:EDO:H21	30:N:798:HOH:O	2.02	0.59
1:A:328:HIS:NE2	24:B:303:PSC:H22	2.16	0.59
2:B:29[A]:MET:CE	9:I:35:TYR:HD1	2.04	0.59
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.84	0.59
1:N:177:SER:H	1:N:180:GLN:NE2	1.99	0.59
4:Q:109:HIS:HD2	30:Q:322:HOH:O	1.85	0.59
2:B:49:LYS:HD3	19:D:201:TGL:HC71	1.84	0.59
7:G:8:HIS:HE1	27:G:102:PEK:H051	1.67	0.59
28:C:306:CDL:H772	28:C:306:CDL:H212	1.84	0.59
9:I:73:LYS:HA	9:I:73:LYS:HE2	1.84	0.59
1:A:28:MET:CE	14:A:601:HEA:C27	2.80	0.59
12:L:42:HIS:ND1	25:L:102:DMU:O49	2.32	0.59
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.83	0.59
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.84	0.59
7:G:8:HIS:CD2	7:G:9:GLY:N	2.63	0.58
8:H:84:LYS:HG2	21:H:102:EDO:H11	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLY:C	7:T:4:ALA:HB1	2.29	0.58
21:A:621:EDO:C2	30:A:748:HOH:O	2.51	0.58
2:B:49:LYS:CE	30:D:394:HOH:O	2.51	0.58
4:D:19[A]:ARG:HG3	4:D:21:ASP:OD1	1.97	0.58
19:N:610:TGL:HA71	19:N:610:TGL:H121	1.84	0.58
3:C:156:ARG:HE	22:C:307:CHD:C24	2.15	0.58
28:C:306:CDL:H221	28:C:306:CDL:H632	1.85	0.58
2:O:25:ASP:O	2:O:29[B]:MET:HB2	2.03	0.58
2:B:49:LYS:HE3	30:D:394:HOH:O	2.03	0.58
6:F:94:HIS:CD2	30:F:216:HOH:O	2.31	0.58
7:G:8:HIS:CG	7:G:9:GLY:H	2.20	0.58
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.84	0.58
1:A:411:LYS:NZ	30:A:705:HOH:O	2.33	0.58
9:I:31:PHE:CD1	9:I:31:PHE:C	2.82	0.58
20:A:610:PGV:H212	13:M:12:PRO:HD3	1.86	0.58
2:O:116:LEU:HD13	2:O:226:MET:CG	2.34	0.58
3:C:33[B]:MET:HA	25:C:302:DMU:H11	1.86	0.57
19:N:610:TGL:H121	19:N:610:TGL:CA7	2.34	0.57
24:O:302:PSC:H071	9:V:10:ARG:HH21	1.66	0.57
19:D:201:TGL:C36	30:I:125:HOH:O	2.32	0.57
8:H:37:HIS:HE1	30:H:208:HOH:O	1.86	0.57
1:N:243:VAL:HB	14:N:603[B]:HEA:HAC	1.86	0.57
20:C:309:PGV:H72	20:C:309:PGV:C2	2.31	0.57
2:B:26:HIS:O	2:B:29[B]:MET:HB3	2.03	0.57
1:N:178[B]:GLN:HG2	1:N:186:TRP:CE2	2.40	0.57
1:A:486[B]:ASP:OD1	30:A:701:HOH:O	2.17	0.57
6:F:87[B]:THR:HG21	30:F:263:HOH:O	2.05	0.57
1:A:243:VAL:HB	14:A:602[B]:HEA:HAC	1.87	0.57
21:A:621:EDO:H22	30:A:748:HOH:O	2.04	0.57
2:B:68[B]:LEU:HD23	24:B:303:PSC:H172	1.86	0.57
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.87	0.57
12:Y:14:SER:H	19:Y:101:TGL:HC31	1.70	0.57
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.87	0.57
3:C:39:SER:OG	25:C:311:DMU:H2	2.04	0.57
3:P:33[B]:MET:SD	25:P:306:DMU:H6	2.44	0.57
19:Q:201:TGL:H362	9:V:20:HIS:CE1	2.39	0.57
4:D:19[A]:ARG:CD	4:D:21:ASP:OD1	2.52	0.57
3:C:62:ILE:CD1	28:C:306:CDL:H522	2.35	0.57
21:N:621:EDO:C1	6:S:36:PRO:CD	2.73	0.57
10:J:52:TRP:O	10:J:57:HIS:HE1	1.88	0.56
3:C:63:ARG:NE	28:C:306:CDL:HA22	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.03	0.56
1:N:112:LEU:HG	30:N:904:HOH:O	2.04	0.56
3:P:62:ILE:HD12	28:P:304:CDL:H522	1.86	0.56
6:F:54[A]:ASN:C	6:F:54[A]:ASN:HD22	2.13	0.56
7:T:72:ASN:H	7:T:76:ASN:ND2	2.01	0.56
12:Y:47:LYS:HE3	12:Y:47:LYS:HA	1.88	0.56
1:A:382[B]:SER:HB3	1:A:383[B]:MET:CE	2.34	0.56
21:N:621:EDO:H12	6:S:36:PRO:HD3	1.84	0.56
4:D:121:LYS:NZ	21:D:206:EDO:H22	2.21	0.56
22:W:101:CHD:O12	22:W:101:CHD:H222	2.06	0.56
3:C:51[B]:MET:HB3	28:C:306:CDL:H381	1.87	0.56
30:N:828:HOH:O	2:O:53:THR:HG21	2.06	0.56
2:B:148:MET:HE2	30:B:527:HOH:O	2.06	0.56
6:F:95:GLN:OE1	6:F:98:HIS:HB3	2.05	0.56
6:S:54:ASN:HD22	6:S:54:ASN:C	2.12	0.56
10:W:14[B]:GLU:HG2	30:W:209:HOH:O	2.06	0.56
7:T:5:LYS:HB2	27:T:101:PEK:H331	1.87	0.56
27:T:102:PEK:H71	27:T:102:PEK:H32	1.87	0.56
1:A:189:MET:HE2	30:A:907:HOH:O	2.01	0.56
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.88	0.56
24:B:303:PSC:H32	9:I:14:ALA:HA	1.88	0.55
25:L:102:DMU:C43	30:L:229:HOH:O	2.39	0.55
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.07	0.55
3:P:156:ARG:HE	22:P:305:CHD:C24	2.19	0.55
8:U:45:ALA:O	8:U:47:GLY:N	2.39	0.55
8:H:37:HIS:CE1	30:H:208:HOH:O	2.59	0.55
6:F:13:ALA:CB	6:F:21[B]:MET:HE1	2.36	0.55
1:N:309:THR:HG22	14:N:603[B]:HEA:HMB2	1.88	0.55
1:N:311[B]:ILE:CD1	28:N:601:CDL:H232	2.37	0.55
2:O:83:ILE:O	2:O:87[A]:MET:HG3	2.06	0.55
3:P:224:LYS:CE	28:P:304:CDL:HB32	2.36	0.55
3:C:67:PHE:CE2	28:C:306:CDL:C1	2.79	0.55
4:D:14:PRO:CG	21:D:203:EDO:H22	2.36	0.55
7:G:8:HIS:CE1	27:G:102:PEK:H042	2.40	0.55
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.05	0.55
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.89	0.55
3:P:33[B]:MET:CE	25:P:306:DMU:H6	2.36	0.55
3:P:80[B]:ARG:HG2	3:P:233:PHE:CE1	2.41	0.55
20:G:103:PGV:H71	20:G:103:PGV:C2	2.33	0.55
3:P:54[A]:MET:HE1	20:P:303:PGV:H131	1.89	0.55
10:W:32:TYR:OH	22:W:101:CHD:H213	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136[B]:LEU:HD11	30:A:921:HOH:O	2.06	0.55
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.72	0.55
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.41	0.55
7:T:3:ALA:O	7:T:4:ALA:CB	2.55	0.55
11:X:47:ARG:CZ	11:X:47:ARG:HB3	2.37	0.55
1:A:172:LYS:HZ2	1:A:178[A]:GLN:HE22	1.53	0.55
21:N:618:EDO:C1	30:S:246:HOH:O	2.30	0.55
3:P:62:ILE:CD1	28:P:304:CDL:H522	2.36	0.55
20:A:610:PGV:H231	20:A:610:PGV:C19	2.36	0.54
6:F:87[A]:THR:HG21	30:F:263:HOH:O	2.05	0.54
22:P:305:CHD:H212	22:P:305:CHD:H12	1.89	0.54
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.07	0.54
2:B:49:LYS:HE3	30:B:526:HOH:O	2.06	0.54
2:O:22[B]:HIS:CE1	9:V:44:LYS:NZ	2.76	0.54
24:O:302:PSC:H142	24:O:302:PSC:C34	2.34	0.54
4:D:78:TRP:CA	19:D:201:TGL:HB21	2.36	0.54
2:B:217:LYS:HG2	30:B:468:HOH:O	2.06	0.54
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.90	0.54
14:N:603[B]:HEA:HMD1	14:N:603[B]:HEA:CBD	2.38	0.54
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.07	0.54
2:B:92:ASN:N	30:B:401:HOH:O	1.91	0.54
1:N:265:LYS:CE	21:N:622:EDO:O1	2.55	0.54
4:Q:19[B]:ARG:NH1	30:Q:301:HOH:O	2.18	0.54
14:A:602[A]:HEA:NB	18:A:607:AZI:N2	2.54	0.54
27:P:307:PEK:H042	6:S:1:ALA:H1	1.62	0.53
3:C:33[B]:MET:HG2	3:C:39:SER:O	2.08	0.53
27:C:308:PEK:H292	30:O:402:HOH:O	2.07	0.53
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.27	0.53
21:A:618:EDO:H22	30:M:217:HOH:O	2.08	0.53
2:B:60:GLU:CD	2:B:60:GLU:N	2.66	0.53
7:T:36:TRP:HE3	7:T:39:SER:CB	2.22	0.53
10:W:32:TYR:HE2	22:W:101:CHD:H181	1.73	0.53
6:F:75:HIS:H	6:F:80:GLN:NE2	2.02	0.53
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.43	0.53
19:Q:201:TGL:HA91	19:Q:201:TGL:H231	1.91	0.53
2:B:14:SER:HB3	2:B:168:LEU:CD2	2.39	0.53
2:B:83:ILE:O	2:B:87[B]:MET:HB2	2.09	0.53
3:P:210:ILE:HD13	20:P:303:PGV:H301	1.90	0.53
1:N:240:HIS:CE1	18:N:608:AZI:N2	2.77	0.53
1:N:240:HIS:HE1	18:N:608:AZI:N2	2.07	0.52
24:O:302:PSC:H342	24:O:302:PSC:H12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380[A]:VAL:HG21	14:A:602[A]:HEA:C3C	2.39	0.52
21:C:316:EDO:H22	8:H:72:TRP:HZ2	1.74	0.52
9:V:25:PHE:O	9:V:28:SER:HB2	2.10	0.52
5:R:14:ARG:NH1	21:R:202:EDO:O2	2.41	0.52
10:J:7:GLU:HG3	30:J:219:HOH:O	2.10	0.52
21:N:618:EDO:H21	6:S:57:ILE:HD12	1.91	0.52
2:O:26:HIS:HA	2:O:29[B]:MET:HE3	1.91	0.52
28:P:304:CDL:H222	28:P:304:CDL:H651	1.91	0.52
4:D:28:ALA:H	4:D:31[B]:LYS:HZ3	1.58	0.52
9:I:35:TYR:CD1	9:I:35:TYR:C	2.88	0.52
1:A:307:SER:HB2	28:T:103:CDL:H192	1.92	0.52
4:D:17[A]:VAL:HG23	4:D:17[A]:VAL:O	2.09	0.52
1:N:380[A]:VAL:HG21	14:N:603[A]:HEA:C3C	2.39	0.52
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.54	0.52
13:Z:36:HIS:HD2	13:Z:39:ASN:ND2	2.06	0.52
7:G:41:HIS:HB3	7:G:74:ARG:CZ	2.40	0.52
12:Y:20:ARG:NH1	19:Y:101:TGL:HC32	2.20	0.52
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.52
3:C:50:ASN:ND2	3:C:54[A]:MET:HE2	2.25	0.52
20:N:609:PGV:H182	3:P:28:THR:HG22	1.92	0.52
6:S:94:HIS:CD2	6:S:95:GLN:N	2.78	0.52
9:V:8:GLN:HB3	9:V:15:ARG:NH2	2.24	0.52
9:V:31:PHE:C	9:V:31:PHE:CD1	2.87	0.52
10:W:32:TYR:CE2	22:W:101:CHD:H181	2.45	0.52
28:C:306:CDL:H811	28:C:306:CDL:H672	1.92	0.52
5:E:86:ILE:O	5:E:90:ARG:HG2	2.10	0.51
28:T:103:CDL:H311	28:T:103:CDL:CA4	2.39	0.51
1:A:1:FME:HE2	1:A:1:FME:HA	1.92	0.51
24:B:303:PSC:H061	9:I:10:ARG:HH21	1.75	0.51
1:N:356:ILE:HD13	14:N:603[B]:HEA:HMB1	1.92	0.51
1:N:514:LYS:HE2	30:S:227:HOH:O	2.11	0.51
9:I:27:VAL:HG12	9:I:28:SER:N	2.24	0.51
7:G:8:HIS:HE1	27:G:102:PEK:C04	2.23	0.51
11:K:47:ARG:CG	30:K:109:HOH:O	2.58	0.51
3:P:33[A]:MET:CB	25:P:306:DMU:H9	2.40	0.51
12:Y:20:ARG:NH2	19:Y:101:TGL:HC52	2.26	0.51
24:B:303:PSC:H32	9:I:14:ALA:CB	2.41	0.51
6:S:76:LYS:HD2	6:S:93:PRO:HG2	1.92	0.51
1:A:484:THR:HA	21:A:619:EDO:H12	1.92	0.51
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.93	0.51
1:N:311[B]:ILE:HD11	28:N:601:CDL:H232	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:25:ASP:HB3	21:R:205:EDO:H11	1.91	0.51
12:Y:24[B]:MET:HG2	19:Y:101:TGL:HA21	1.92	0.51
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.93	0.51
19:Q:201:TGL:H352	9:V:16:ARG:HE	1.75	0.51
21:A:613:EDO:C2	30:A:906:HOH:O	2.54	0.50
19:L:101:TGL:HC92	19:L:101:TGL:CC5	2.41	0.50
21:N:612:EDO:O2	30:N:704:HOH:O	2.19	0.50
5:R:109:VAL:HG22	5:R:109:VAL:O	2.11	0.50
8:H:37:HIS:HD2	30:H:201:HOH:O	1.93	0.50
2:B:68[B]:LEU:CD2	24:B:303:PSC:H172	2.41	0.50
3:P:33[A]:MET:HB2	25:P:306:DMU:H8	1.93	0.50
27:C:308:PEK:H42	27:C:308:PEK:O02	2.11	0.50
8:H:38:ARG:HH12	21:H:101:EDO:C2	2.23	0.50
3:P:33[A]:MET:CE	3:P:42:LEU:H	2.23	0.50
1:N:62:ALA:HB2	14:N:602:HEA:HBD1	1.94	0.50
3:P:246:ASP:HB2	30:P:481:HOH:O	2.11	0.50
1:A:289:ALA:HB1	1:A:297[B]:MET:HE1	1.93	0.50
2:B:29[A]:MET:CE	9:I:35:TYR:CD1	2.87	0.50
7:G:72:ASN:H	7:G:76:ASN:ND2	2.00	0.50
1:A:282:PHE:CA	7:T:4:ALA:CB	2.77	0.50
14:A:601:HEA:HHC	14:A:601:HEA:H122	1.93	0.50
1:N:112:LEU:HD23	1:N:112:LEU:C	2.37	0.50
7:T:36:TRP:CE3	7:T:39:SER:CB	2.94	0.50
2:B:105:TYR:CD1	30:B:404:HOH:O	2.55	0.50
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.93	0.50
7:T:44:ARG:HH22	7:T:84:LYS:HZ3	1.60	0.50
2:B:28:LEU:O	2:B:29[A]:MET:C	2.52	0.49
2:B:58:ALA:O	2:B:62:GLU:HG3	2.11	0.49
3:C:51[B]:MET:HE2	28:C:306:CDL:H392	1.92	0.49
3:C:62:ILE:HD12	28:C:306:CDL:H522	1.93	0.49
1:N:28:MET:HE2	14:N:602:HEA:C27	2.41	0.49
22:P:305:CHD:H231	22:P:305:CHD:C16	2.36	0.49
2:O:52:HIS:HE1	24:O:302:PSC:H212	1.77	0.49
1:A:297[A]:MET:CG	1:A:302[A]:ARG:CG	2.90	0.49
1:A:514:LYS:OXT	6:F:37:LYS:HE2	2.12	0.49
2:B:41[B]:ILE:HG21	24:B:303:PSC:H342	1.94	0.49
3:C:51[B]:MET:HG2	28:C:306:CDL:H611	1.93	0.49
6:F:95:GLN:HG2	6:F:98:HIS:H	1.77	0.49
14:N:602:HEA:HBC1	14:N:602:HEA:HMC3	1.94	0.49
21:O:304:EDO:H21	30:O:475:HOH:O	2.11	0.49
12:Y:47:LYS:HA	12:Y:47:LYS:CE	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HA	6:F:38:ALA:CB	2.41	0.49
2:B:91:ASN:OD1	2:B:183[B]:THR:HG21	2.13	0.49
7:G:11:TPO:O2P	7:G:12:GLY:N	2.45	0.49
4:Q:17[A]:VAL:O	4:Q:17[A]:VAL:CG2	2.60	0.49
19:Y:101:TGL:OC1	19:Y:101:TGL:CC4	2.50	0.49
4:D:100[A]:LYS:NZ	30:D:301:HOH:O	1.93	0.49
9:I:57:MET:O	9:I:61:GLU:HG2	2.13	0.49
28:T:103:CDL:H782	28:T:103:CDL:H571	1.94	0.49
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.94	0.49
3:P:224:LYS:HZ1	28:P:304:CDL:H112	1.77	0.49
22:P:305:CHD:H162	22:P:305:CHD:C23	2.37	0.49
22:C:307:CHD:C23	22:C:307:CHD:C16	2.91	0.49
4:D:78:TRP:CA	19:D:201:TGL:CB2	2.91	0.49
1:N:169:ILE:HG13	1:N:189:MET:HE1	1.95	0.49
1:A:39:ALA:HA	21:D:202:EDO:HO1	1.68	0.49
3:C:258:TRP:CZ3	25:C:310:DMU:H12	2.48	0.49
7:G:8:HIS:HE1	27:G:102:PEK:C05	2.26	0.49
1:A:240:HIS:HE1	18:A:607:AZI:N2	2.11	0.49
2:B:87[B]:MET:HB3	30:B:457:HOH:O	2.12	0.49
4:D:100[B]:LYS:O	4:D:100[B]:LYS:CE	2.61	0.49
19:A:608:TGL:HA21	19:A:608:TGL:HB21	1.95	0.48
28:P:304:CDL:H351	28:P:304:CDL:C39	2.28	0.48
13:Z:36:HIS:CD2	13:Z:39:ASN:ND2	2.80	0.48
20:C:309:PGV:H21	20:C:309:PGV:C7	2.38	0.48
3:P:33[B]:MET:CB	25:P:306:DMU:H9	2.42	0.48
4:D:78:TRP:HA	19:D:201:TGL:HB21	1.95	0.48
2:O:26:HIS:O	2:O:29[B]:MET:HB3	2.12	0.48
5:R:5:HIS:O	5:R:6:GLU:HB3	2.13	0.48
11:X:7:PRO:HB2	11:X:12:LYS:NZ	2.27	0.48
30:L:221:HOH:O	13:M:32:TRP:HH2	1.96	0.48
3:P:50:ASN:HD22	3:P:51[A]:MET:HE2	1.79	0.48
6:S:85:CYS:SG	6:S:87[B]:THR:HG22	2.53	0.48
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.49	0.48
1:N:28:MET:HE1	14:N:602:HEA:C27	2.44	0.48
14:N:602:HEA:H122	14:N:602:HEA:H262	1.96	0.48
1:A:334:TRP:CZ3	19:D:201:TGL:HA52	2.49	0.48
1:N:178[B]:GLN:HE22	1:N:189:MET:HE2	1.79	0.48
6:F:95:GLN:HG2	6:F:98:HIS:N	2.28	0.48
22:P:301:CHD:H12	22:P:301:CHD:H212	1.96	0.48
4:D:78:TRP:HB3	19:D:201:TGL:CB2	2.34	0.47
14:N:603[A]:HEA:NB	18:N:608:AZI:N2	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:50:VAL:O	8:U:51:SER:C	2.57	0.47
1:A:265:LYS:NZ	21:A:617:EDO:H22	2.29	0.47
2:B:41[B]:ILE:CD1	9:I:21:ILE:CD1	2.91	0.47
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.94	0.47
21:N:618:EDO:C2	30:S:246:HOH:O	2.61	0.47
3:P:40:MET:HE3	3:P:40:MET:HB2	1.67	0.47
3:P:63:ARG:HE	28:P:304:CDL:HA22	1.78	0.47
3:P:259:TRP:CD1	25:P:308:DMU:H30	2.49	0.47
3:C:258:TRP:CH2	25:C:310:DMU:H12	2.49	0.47
22:J:101:CHD:H222	22:J:101:CHD:H162	1.61	0.47
1:N:468:MET:HG3	30:N:910[A]:HOH:O	2.13	0.47
14:N:603[B]:HEA:HMD1	14:N:603[B]:HEA:HBD2	1.96	0.47
2:O:41:ILE:O	2:O:42:ILE:C	2.55	0.47
9:I:31:PHE:CZ	9:I:35:TYR:HB2	2.49	0.47
8:H:38:ARG:HH12	21:H:101:EDO:H21	1.80	0.47
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.95	0.47
1:A:243:VAL:HG11	18:A:606:AZI:N3	2.30	0.47
2:B:41[A]:ILE:O	2:B:42:ILE:C	2.51	0.47
2:B:49:LYS:HE2	30:D:394:HOH:O	2.14	0.47
3:C:37:PHE:CD2	25:C:302:DMU:H8	2.49	0.47
20:C:309:PGV:C2	20:C:309:PGV:C7	2.93	0.47
6:F:95:GLN:C	6:F:97:ALA:N	2.63	0.47
7:G:4:ALA:CB	1:N:282:PHE:HA	2.44	0.47
20:P:303:PGV:H11	20:P:303:PGV:H142	1.70	0.47
28:T:103:CDL:H252	28:T:103:CDL:C76	2.44	0.47
10:W:33:ARG:HE	22:W:101:CHD:H7	1.79	0.47
11:X:26:VAL:O	11:X:30:VAL:HG23	2.15	0.47
13:Z:19:LEU:HD23	20:Z:101:PGV:C31	2.45	0.47
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.97	0.47
3:C:210:ILE:HG12	20:C:305:PGV:H132	1.96	0.47
1:N:173:PRO:HB3	30:N:864:HOH:O	2.14	0.47
1:N:240:HIS:O	1:N:241:PRO:C	2.56	0.47
1:N:359:ALA:CA	14:N:603[B]:HEA:OMA	2.58	0.47
13:Z:16:ALA:HA	20:Z:101:PGV:H291	1.97	0.47
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.97	0.47
14:A:602[B]:HEA:HBD2	14:A:602[B]:HEA:HMD1	1.97	0.47
2:B:40:TYR:CE2	9:I:24:ALA:HB2	2.50	0.47
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.97	0.47
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.15	0.47
1:A:240:HIS:CE1	18:A:607:AZI:N2	2.83	0.46
3:C:176:LEU:HD23	21:C:317:EDO:H12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:201:TGL:H362	9:V:20:HIS:HE1	1.80	0.46
9:V:1:SAC:OAC	9:V:3:ALA:HB3	2.14	0.46
1:A:378:HIS:HA	1:A:382[B]:SER:CB	2.43	0.46
20:A:609:PGV:H343	27:C:304:PEK:C38	2.41	0.46
20:A:610:PGV:H132	20:A:610:PGV:H302	1.98	0.46
6:S:64:GLU:O	6:S:65:ASP:CB	2.63	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.46
1:N:362[A]:SER:OG	2:O:87[A]:MET:HE2	2.15	0.46
4:Q:78:TRP:CB	19:Q:201:TGL:HB22	2.45	0.46
4:Q:118:LYS:HE3	11:X:51:LYS:HE3	1.98	0.46
7:T:44:ARG:NH2	7:T:84:LYS:NZ	2.59	0.46
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.50	0.46
3:P:33[A]:MET:HG2	3:P:39:SER:O	2.14	0.46
6:S:96:LEU:HB3	6:S:97:ALA:H	1.56	0.46
8:U:60:TYR:CD1	8:U:60:TYR:C	2.93	0.46
10:W:32:TYR:CE2	22:W:101:CHD:C18	2.98	0.46
14:A:602[A]:HEA:C1B	18:A:607:AZI:N2	2.79	0.46
3:C:156:ARG:HH21	22:C:307:CHD:C24	2.28	0.46
9:I:26:MET:O	9:I:27:VAL:C	2.59	0.46
3:P:202:GLY:HA3	27:T:102:PEK:H21	1.98	0.46
19:Y:101:TGL:H202	19:Y:101:TGL:H231	1.78	0.46
22:J:101:CHD:O12	22:J:101:CHD:H212	2.15	0.46
8:U:9:LYS:C	8:U:9:LYS:HD2	2.41	0.46
1:A:240:HIS:C	1:A:240:HIS:CD2	2.94	0.46
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.04	0.46
7:T:12:GLY:HA3	30:T:226:HOH:O	2.15	0.46
11:X:29:TRP:CE3	11:X:32:MET:HE1	2.50	0.46
11:X:47:ARG:CZ	11:X:47:ARG:CB	2.93	0.46
27:C:304:PEK:H172	27:C:304:PEK:C11	2.46	0.46
1:N:302[B]:ARG:HE	2:O:84:LEU:HD11	1.81	0.46
28:N:601:CDL:H371	2:O:78:LEU:CD1	2.34	0.46
24:B:303:PSC:H063	9:I:10:ARG:HH21	1.76	0.45
2:O:67:ILE:HD11	21:O:305:EDO:O2	2.16	0.45
10:J:3:ASN:OD1	10:J:3:ASN:C	2.59	0.45
14:N:603[B]:HEA:HBC1	14:N:603[B]:HEA:CMC	2.47	0.45
10:W:33:ARG:HG2	22:W:101:CHD:H182	1.98	0.45
1:N:265:LYS:CD	21:N:622:EDO:H12	2.46	0.45
28:T:103:CDL:OA7	28:T:103:CDL:C33	2.58	0.45
28:T:103:CDL:OB4	28:T:103:CDL:H131	2.16	0.45
1:A:449:MET:SD	2:B:5:MET:HG2	2.57	0.45
3:P:52:LEU:HG	28:P:304:CDL:H382	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD22	2:B:23:PHE:CE2	2.51	0.45
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.51	0.45
4:D:109:HIS:HD2	30:D:359:HOH:O	1.98	0.45
27:G:102:PEK:H382	28:N:601:CDL:H861	1.99	0.45
14:N:603[A]:HEA:CMC	14:N:603[A]:HEA:HBC1	2.47	0.45
1:N:513:LEU:O	1:N:514:LYS:CB	2.44	0.45
6:S:87[A]:THR:HG21	30:S:227:HOH:O	2.17	0.45
25:C:310:DMU:H32	25:C:310:DMU:C57	2.45	0.45
19:N:610:TGL:HB92	19:N:610:TGL:H281	1.94	0.45
28:T:103:CDL:HA4	28:T:103:CDL:C31	2.43	0.45
20:Z:101:PGV:H22	20:Z:101:PGV:H202	1.99	0.45
25:C:310:DMU:H34	25:C:310:DMU:H36	1.30	0.45
28:N:601:CDL:H531	28:N:601:CDL:H261	1.97	0.45
2:O:69:PRO:HG3	24:O:302:PSC:H182	1.99	0.45
2:B:49:LYS:HD3	19:D:201:TGL:CC7	2.46	0.45
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.99	0.45
1:N:313:ALA:HB2	1:N:356:ILE:HD11	1.98	0.45
3:P:33[B]:MET:SD	25:P:306:DMU:C18	3.05	0.45
27:T:101:PEK:H361	28:T:103:CDL:C87	2.46	0.45
1:A:282:PHE:N	7:T:4:ALA:HB1	2.31	0.45
3:C:217:VAL:HG22	28:C:306:CDL:H732	1.98	0.45
21:D:203:EDO:C1	30:D:340:HOH:O	2.45	0.45
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.45	0.45
7:T:38:HIS:ND1	7:T:38:HIS:N	2.65	0.45
10:W:3:ASN:OD1	10:W:3:ASN:C	2.58	0.45
20:A:610:PGV:H312	13:M:16:ALA:HA	1.99	0.44
30:B:513:HOH:O	19:D:201:TGL:HC22	2.17	0.44
6:F:92:VAL:HG23	6:F:92:VAL:O	2.17	0.44
12:L:41:ARG:HH22	25:L:102:DMU:H30	1.82	0.44
1:N:449:MET:SD	2:O:5:MET:HG2	2.57	0.44
14:N:603[A]:HEA:C1B	18:N:608:AZI:N3	2.80	0.44
2:O:114:GLU:CG	2:O:227:LEU:HD21	2.47	0.44
1:A:172:LYS:HD2	1:A:181:THR:CG2	2.47	0.44
1:A:407:ASP:OD2	21:A:618:EDO:H11	2.18	0.44
4:D:99:GLU:OE2	21:D:202:EDO:C2	2.57	0.44
7:G:6:GLY:O	1:N:189:MET:HE3	2.17	0.44
7:G:38:HIS:CE1	28:N:601:CDL:H141	2.51	0.44
21:C:315:EDO:H12	30:C:469:HOH:O	2.17	0.44
3:P:54[A]:MET:O	3:P:55:TYR:C	2.59	0.44
28:C:306:CDL:H752	28:C:306:CDL:H191	2.00	0.44
1:N:468:MET:HE1	14:N:602:HEA:H212	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:111:THR:HA	2:O:114:GLU:O	2.18	0.44
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.99	0.44
12:Y:24[B]:MET:SD	19:Y:101:TGL:CC3	3.06	0.44
1:A:297[A]:MET:HG2	1:A:302[A]:ARG:HG3	1.99	0.44
2:B:26:HIS:HA	2:B:29[B]:MET:HE2	1.99	0.44
4:D:19[A]:ARG:HD2	4:D:21:ASP:OD1	2.18	0.44
19:N:610:TGL:HA71	19:N:610:TGL:H102	2.00	0.44
19:A:608:TGL:H242	19:A:608:TGL:H272	1.72	0.44
21:N:622:EDO:C1	6:S:84:SER:OG	2.64	0.44
24:O:302:PSC:C34	24:O:302:PSC:H12	2.48	0.44
14:A:602[A]:HEA:C1B	18:A:607:AZI:N3	2.81	0.44
20:A:609:PGV:H312	20:C:305:PGV:H321	2.00	0.44
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.99	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.17	0.44
5:R:7:THR:HB	5:R:9:GLU:OE2	2.17	0.44
12:Y:20:ARG:NH1	12:Y:24[B]:MET:SD	2.90	0.44
25:L:102:DMU:H2	25:L:102:DMU:H36	1.55	0.44
25:P:309:DMU:H22	10:W:38:LEU:HD23	1.98	0.44
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.44	0.44
28:N:601:CDL:H362	28:N:601:CDL:H121	2.00	0.44
1:A:379:TYR:CZ	1:A:383[A]:MET:HE1	2.53	0.43
1:A:382[B]:SER:C	1:A:383[B]:MET:HE2	2.43	0.43
2:B:28:LEU:HG	2:B:32[A]:PHE:CE2	2.52	0.43
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.48	0.43
4:D:121:LYS:HZ2	21:D:206:EDO:H22	1.82	0.43
1:N:311[B]:ILE:HD11	28:N:601:CDL:C23	2.48	0.43
30:N:828:HOH:O	2:O:53:THR:CG2	2.66	0.43
19:Q:201:TGL:HG32	19:Q:201:TGL:OB1	2.17	0.43
20:A:609:PGV:C18	27:C:304:PEK:H322	2.45	0.43
3:C:103:HIS:ND1	22:C:301:CHD:O26	2.51	0.43
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.47	0.43
1:N:172:LYS:HZ2	1:N:178[A]:GLN:HE22	1.67	0.43
3:P:33[A]:MET:HA	25:P:306:DMU:H9	2.00	0.43
1:A:297[A]:MET:SD	1:A:302[A]:ARG:HG3	2.56	0.43
24:B:303:PSC:H072	5:E:11:PHE:HB2	2.00	0.43
3:C:33[B]:MET:CG	3:C:39:SER:HB3	2.48	0.43
7:G:72:ASN:N	7:G:76:ASN:HD22	2.05	0.43
13:M:41:LYS:C	13:M:43:SER:N	2.76	0.43
14:A:602[A]:HEA:HBC1	14:A:602[A]:HEA:HMC3	2.00	0.43
12:L:26:THR:HG23	13:M:25:SER:CB	2.48	0.43
4:Q:78:TRP:HB3	19:Q:201:TGL:HB22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:THR:HG21	14:A:602[A]:HEA:H14	2.00	0.43
1:N:28:MET:HE1	14:N:602:HEA:H271	1.98	0.43
3:P:37:PHE:CB	25:P:306:DMU:H7	2.49	0.43
27:C:308:PEK:H382	28:N:601:CDL:C27	2.46	0.43
1:N:328:HIS:HB2	2:O:45:MET:SD	2.58	0.43
19:N:610:TGL:HC31	2:O:7:LEU:HD12	2.00	0.43
4:Q:19[A]:ARG:CD	4:Q:21:ASP:CG	2.86	0.43
1:A:28:MET:HE2	14:A:601:HEA:C27	2.47	0.43
1:A:328:HIS:NE2	24:B:303:PSC:C2	2.82	0.43
1:A:483:LEU:O	21:A:619:EDO:H12	2.19	0.43
14:A:601:HEA:HMC3	14:A:601:HEA:HBC1	2.00	0.43
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.41	0.43
4:D:17[A]:VAL:O	4:D:17[A]:VAL:CG2	2.66	0.43
22:G:101:CHD:H212	22:G:101:CHD:H12	2.01	0.43
1:N:307:SER:HB3	28:N:601:CDL:H191	1.99	0.43
2:O:82:ARG:HH11	2:O:86:MET:HE1	1.83	0.43
7:T:8:HIS:C	7:T:10:GLY:H	2.27	0.43
9:V:35:TYR:CD1	9:V:35:TYR:C	2.96	0.43
2:O:91:ASN:HD22	2:O:92:ASN:N	2.17	0.43
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.54	0.43
1:A:406:ASN:HD21	20:A:610:PGV:H22	1.82	0.43
1:N:115[A]:SER:O	1:N:121:GLY:HA2	2.18	0.43
3:P:158:HIS:NE2	27:P:307:PEK:N	2.67	0.43
1:N:467:LEU:O	1:N:471:ILE:HG13	2.19	0.42
1:A:361[B]:SER:HB3	30:A:708:HOH:O	2.18	0.42
20:A:609:PGV:C34	27:C:304:PEK:H382	2.40	0.42
28:C:306:CDL:H521	28:C:306:CDL:OB9	2.19	0.42
1:N:311[A]:ILE:CG1	28:N:601:CDL:H442	2.49	0.42
8:U:50:VAL:C	8:U:52:VAL:N	2.75	0.42
2:B:16[A]:ILE:HD13	2:B:16[A]:ILE:HA	1.87	0.42
1:N:378:HIS:HA	1:N:382[B]:SER:HB2	2.00	0.42
3:P:33[A]:MET:CE	3:P:41:THR:HB	2.41	0.42
10:W:14[A]:GLU:O	10:W:23:LYS:NZ	2.52	0.42
13:Z:38:ASP:HB2	30:Z:202:HOH:O	2.18	0.42
1:A:131:PRO:HB3	21:A:622:EDO:H22	2.01	0.42
2:B:69:PRO:HG2	30:B:437:HOH:O	2.19	0.42
25:C:302:DMU:H12	10:J:49:CYS:HB3	2.00	0.42
4:D:98:TRP:CE2	25:M:101:DMU:H11	2.54	0.42
1:N:297[B]:MET:SD	1:N:302[B]:ARG:CG	3.07	0.42
24:O:302:PSC:H221	24:O:302:PSC:H251	1.63	0.42
28:T:103:CDL:H262	28:T:103:CDL:H232	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297[A]:MET:HG2	1:A:302[A]:ARG:CG	2.50	0.42
8:H:60:TYR:CD1	8:H:60:TYR:C	2.96	0.42
14:N:602:HEA:H122	14:N:602:HEA:HHC	2.00	0.42
24:O:302:PSC:H343	24:O:302:PSC:C12	2.50	0.42
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.79	0.42
10:J:27:THR:HG22	30:J:214:HOH:O	2.18	0.42
11:K:8:ASP:HB2	30:K:110:HOH:O	2.19	0.42
21:N:622:EDO:H11	6:S:84:SER:CB	2.49	0.42
7:G:3:ALA:O	7:G:4:ALA:CB	2.66	0.42
1:N:131:PRO:HB3	21:N:613:EDO:H12	2.00	0.42
12:Y:20:ARG:HH22	19:Y:101:TGL:HC52	1.84	0.42
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.00	0.42
2:B:57:ASP:H	24:B:303:PSC:H212	1.83	0.42
19:D:201:TGL:OA1	19:D:201:TGL:HC42	2.20	0.42
1:N:488:THR:HB	1:N:495:LEU:HD13	2.02	0.42
3:P:131:LEU:HD11	28:T:103:CDL:H561	2.01	0.42
5:R:41:LEU:HA	30:V:209:HOH:O	2.20	0.42
1:A:397:PHE:HB3	1:A:398:PRO:HD3	2.01	0.42
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.01	0.42
7:G:33:LEU:O	7:G:37:LEU:HB2	2.20	0.42
1:N:344:PHE:CD1	1:N:344:PHE:C	2.98	0.42
28:P:304:CDL:OA7	28:P:304:CDL:H162	2.20	0.42
5:R:77:PRO:O	5:R:79:LYS:HD2	2.20	0.42
22:C:307:CHD:H112	22:C:307:CHD:H12A	1.86	0.42
1:A:417[A]:MET:HE1	14:A:601:HEA:H263	2.02	0.41
7:G:19:LEU:HD21	27:G:102:PEK:H372	2.02	0.41
20:G:103:PGV:H231	20:G:103:PGV:H202	1.82	0.41
8:H:8:ILE:CG2	8:H:8:ILE:O	2.68	0.41
3:P:33[A]:MET:HE2	3:P:42:LEU:H	1.85	0.41
28:P:304:CDL:OB9	28:P:304:CDL:HB4	2.20	0.41
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.20	0.41
1:A:54:TYR:HB2	30:A:744:HOH:O	2.20	0.41
1:N:377:PHE:CD2	14:N:603[A]:HEA:HAD1	2.55	0.41
14:N:603[A]:HEA:HBC1	14:N:603[A]:HEA:HMC3	2.01	0.41
4:Q:19[A]:ARG:HD2	4:Q:21:ASP:OD1	2.13	0.41
1:A:377:PHE:HB3	14:A:602[A]:HEA:C2D	2.50	0.41
2:B:32[A]:PHE:C	2:B:35[A]:SER:OG	2.53	0.41
25:C:302:DMU:H15	25:C:302:DMU:H9	1.74	0.41
25:C:302:DMU:H7	10:J:49:CYS:HB3	2.02	0.41
8:H:8:ILE:O	8:H:8:ILE:HG23	2.20	0.41
1:N:302[B]:ARG:HH21	2:O:84:LEU:CD1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:511:VAL:H	21:N:621:EDO:H22	1.84	0.41
14:N:603[A]:HEA:C1B	18:N:608:AZI:N2	2.84	0.41
24:O:302:PSC:H202	24:O:302:PSC:H231	1.51	0.41
7:G:2:SER:HB2	1:N:197:LEU:HD21	2.03	0.41
1:N:136[B]:LEU:HD21	30:T:237:HOH:O	2.19	0.41
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG3	2.60	0.41
24:O:302:PSC:H322	24:O:302:PSC:H292	1.86	0.41
3:P:54[A]:MET:HB3	3:P:58:TRP:CZ3	2.55	0.41
7:T:3:ALA:O	7:T:4:ALA:HB2	2.20	0.41
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.02	0.41
1:A:514:LYS:HG3	6:F:38:ALA:HB2	2.03	0.41
2:B:32[B]:PHE:HE1	30:B:536:HOH:O	2.03	0.41
28:P:304:CDL:H812	28:P:304:CDL:H842	1.68	0.41
22:W:101:CHD:H7	22:W:101:CHD:H191	2.02	0.41
14:A:602[A]:HEA:H243	2:B:69:PRO:HB3	2.03	0.41
1:N:514:LYS:NZ	30:N:715:HOH:O	2.52	0.41
20:N:609:PGV:H262	20:P:303:PGV:H292	2.02	0.41
14:A:602[A]:HEA:HBC1	14:A:602[A]:HEA:CMC	2.51	0.41
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.21	0.41
21:P:312:EDO:H11	6:S:16:LEU:HD13	2.02	0.41
6:S:87[A]:THR:HG22	30:S:254:HOH:O	2.21	0.41
1:A:302[B]:ARG:NE	1:A:361[B]:SER:OG	2.53	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.64	0.41
2:B:65:TRP:CD1	24:B:303:PSC:H142	2.56	0.41
2:B:108:TYR:O	2:B:117:SER:HA	2.20	0.41
3:C:67:PHE:HE2	28:C:306:CDL:O1	2.02	0.41
19:D:201:TGL:CG3	30:D:364:HOH:O	2.11	0.41
6:F:1:ALA:HB3	21:F:105:EDO:C1	2.47	0.41
7:G:6:GLY:HA2	27:G:102:PEK:H322	2.03	0.41
1:N:510:TYR:HA	21:N:621:EDO:C2	2.50	0.41
19:N:610:TGL:HC32	19:N:610:TGL:HG12	2.02	0.41
22:P:305:CHD:C16	22:P:305:CHD:C23	2.95	0.41
4:Q:109:HIS:CD2	30:Q:322:HOH:O	2.66	0.41
27:T:102:PEK:H221	27:T:102:PEK:H251	1.73	0.41
14:A:602[B]:HEA:HHC	14:A:602[B]:HEA:H122	2.03	0.41
24:B:303:PSC:H042	24:B:303:PSC:H062	1.79	0.41
19:L:101:TGL:HC92	19:L:101:TGL:HC52	2.02	0.41
28:P:304:CDL:HB21	28:P:304:CDL:OB6	2.21	0.41
2:B:37:LEU:O	2:B:41[B]:ILE:HG12	2.22	0.40
22:C:301:CHD:H212	22:C:301:CHD:H12	2.03	0.40
27:C:308:PEK:H202	7:G:36:TRP:HE1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:TYR:OH	21:D:202:EDO:H21	2.21	0.40
8:H:43:MET:CE	8:H:49:ASP:H	2.34	0.40
1:A:148:PHE:HB3	3:C:28:THR:HB	2.03	0.40
4:D:100[B]:LYS:HD2	4:D:100[B]:LYS:HA	1.87	0.40
1:N:399:LEU:O	1:N:499:PRO:HA	2.21	0.40
20:A:610:PGV:H241	13:M:12:PRO:HG3	2.03	0.40
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.83	0.40
30:B:517:HOH:O	19:D:201:TGL:H332	2.21	0.40
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.86	0.40
28:C:306:CDL:H761	28:C:306:CDL:H791	1.70	0.40
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.57	0.40
1:N:115[B]:SER:O	1:N:121:GLY:HA2	2.21	0.40
2:O:58:ALA:O	2:O:62:GLU:HG3	2.22	0.40
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.56	0.40
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.19	0.40
1:A:28:MET:HE1	14:A:601:HEA:C27	2.51	0.40
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.04	0.40
1:A:311[B]:ILE:HG13	1:A:314:ILE:HD12	2.04	0.40
2:B:42:ILE:HD13	2:B:42:ILE:HG21	1.88	0.40
3:C:76:GLN:O	3:C:80[A]:ARG:HG3	2.22	0.40
5:E:72:LYS:NZ	30:E:305:HOH:O	2.54	0.40
3:C:99:TRP:CE2	20:C:309:PGV:H232	2.57	0.40
3:C:191:GLY:HA3	30:G:218:HOH:O	2.20	0.40
3:P:33[B]:MET:CG	25:P:306:DMU:C19	2.99	0.40
10:W:29:ASN:HD22	10:W:29:ASN:H	1.70	0.40
10:W:58:LYS:HB3	10:W:58:LYS:HE2	1.88	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:226:MET:O	4:Q:5:VAL:O[2_684]	2.13	0.07
30:B:466:HOH:O	30:D:302:HOH:O[2_584]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	534/514 (104%)	519 (97%)	15 (3%)	0	100	100
1	N	532/514 (104%)	516 (97%)	16 (3%)	0	100	100
2	B	235/227 (104%)	224 (95%)	11 (5%)	0	100	100
2	O	229/227 (101%)	222 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	146/147 (99%)	141 (97%)	5 (3%)	0	100	100
4	Q	145/147 (99%)	139 (96%)	4 (3%)	2 (1%)	9	2
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	12	4
6	F	100/98 (102%)	96 (96%)	2 (2%)	2 (2%)	6	1
6	S	98/98 (100%)	89 (91%)	7 (7%)	2 (2%)	6	1
7	G	81/85 (95%)	70 (86%)	5 (6%)	6 (7%)	1	0
7	T	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	1	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	9	2
8	U	77/85 (91%)	67 (87%)	7 (9%)	3 (4%)	2	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	4	1
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	4	1
All	All	3596/3614 (100%)	3454 (96%)	119 (3%)	23 (1%)	18	10

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
7	G	4	ALA
7	G	5	LYS
7	G	8	HIS
13	M	42	LYS
4	Q	7	LYS
4	Q	8	SER
5	R	6	GLU
6	S	94	HIS
7	T	5	LYS
7	T	8	HIS
8	U	46	LYS
7	G	37	LEU
6	S	96	LEU
7	T	3	ALA
7	T	4	ALA
7	G	6	GLY
8	U	45	ALA
13	Z	42	LYS
6	F	96	LEU
7	G	3	ALA
8	U	11	TYR
8	H	8	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/426 (105%)	438 (98%)	9 (2%)	48	36
1	N	445/426 (104%)	437 (98%)	8 (2%)	51	40
2	B	220/210 (105%)	211 (96%)	9 (4%)	27	12
2	O	214/210 (102%)	209 (98%)	5 (2%)	44	30
3	C	233/226 (103%)	228 (98%)	5 (2%)	47	33
3	P	233/226 (103%)	229 (98%)	4 (2%)	53	42
4	D	132/129 (102%)	126 (96%)	6 (4%)	24	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	131/129 (102%)	122 (93%)	9 (7%)	14	3
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	18
5	R	92/95 (97%)	88 (96%)	4 (4%)	26	11
6	F	85/81 (105%)	80 (94%)	5 (6%)	18	5
6	S	83/81 (102%)	72 (87%)	11 (13%)	4	0
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	1
7	T	68/68 (100%)	62 (91%)	6 (9%)	9	1
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	2
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	6
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	3
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	7
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	36
10	W	50/50 (100%)	48 (96%)	2 (4%)	28	13
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	38 (95%)	2 (5%)	22	8
12	L	40/40 (100%)	39 (98%)	1 (2%)	42	27
12	Y	40/40 (100%)	37 (92%)	3 (8%)	12	3
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	7
All	All	3130/3082 (102%)	3012 (96%)	118 (4%)	31	14

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	138	HIS
1	A	178[A]	GLN
1	A	178[B]	GLN
1	A	180	GLN
1	A	297[A]	MET
1	A	297[B]	MET
1	A	363	LEU
1	A	369	ASP
2	B	42	ILE
2	B	59	GLN

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Mol	Chain	Res	Type
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	91	ASN
2	B	116	LEU
2	B	171	LYS
3	C	17	PRO
3	C	33[A]	MET
3	C	33[B]	MET
3	C	40	MET
3	C	127	LEU
4	D	7	LYS
4	D	8	SER
4	D	31[A]	LYS
4	D	31[B]	LYS
4	D	127	LYS
4	D	147	LYS
5	E	5	HIS
5	E	70	VAL
5	E	90	ARG
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	80	GLN
6	F	95	GLN
6	F	96	LEU
7	G	5	LYS
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	38	HIS
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	44	THR
8	H	46	LYS
8	H	60	TYR
9	I	2	THR
9	I	27	VAL
9	I	37	PHE
9	I	73	LYS

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Mol	Chain	Res	Type
10	J	58	LYS
12	L	47	LYS
1	N	128	VAL
1	N	138	HIS
1	N	180	GLN
1	N	265	LYS
1	N	369	ASP
1	N	382[A]	SER
1	N	382[B]	SER
1	N	495	LEU
2	O	33	LEU
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
3	P	17	PRO
3	P	40	MET
3	P	159	MET
3	P	230	ASN
4	Q	4	SER
4	Q	6	VAL
4	Q	7	LYS
4	Q	8	SER
4	Q	31	LYS
4	Q	51	LEU
4	Q	127	LYS
4	Q	143	ASN
4	Q	147	LYS
5	R	45	PRO
5	R	79	LYS
5	R	90	ARG
5	R	109	VAL
6	S	21[A]	MET
6	S	21[B]	MET
6	S	37	LYS
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
6	S	87[A]	THR
6	S	87[B]	THR
6	S	93	PRO
6	S	95	GLN

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Mol	Chain	Res	Type
6	S	96	LEU
7	T	7	ASP
7	T	33	LEU
7	T	37	LEU
7	T	38	HIS
7	T	42	ARG
7	T	84	LYS
8	U	7	LYS
8	U	8	ILE
8	U	10	ASN
8	U	29	CYS
9	V	8	GLN
9	V	29	LEU
9	V	73	LYS
10	W	7	GLU
10	W	50	LEU
11	X	47	ARG
11	X	52	GLU
12	Y	2	HIS
12	Y	26	THR
12	Y	47	LYS
13	Z	42	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	422	ASN
2	B	59	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	29	HIS
4	D	32	ASN
4	D	37	GLN
4	D	119	GLN
4	D	143	ASN
5	E	94	ASN
6	F	80	GLN
7	G	8	HIS
7	G	38	HIS

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Mol	Chain	Res	Type
7	G	76	ASN
8	H	22	ASN
8	H	28	ASN
8	H	32	ASN
9	I	53	ASN
10	J	57	HIS
11	K	35	GLN
1	N	180	GLN
1	N	422	ASN
2	O	52	HIS
2	O	181	GLN
3	P	38	ASN
3	P	50	ASN
3	P	68	GLN
4	Q	32	ASN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	76	ASN
8	U	10	ASN
8	U	25	GLN
8	U	28	ASN
8	U	31	GLN
8	U	32	ASN
8	U	37	HIS
9	V	20	HIS
9	V	53	ASN
10	W	57	HIS
13	Z	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	SAC	I	1	9	7,8,9	1.12	1 (14%)	8,9,11	1.97	2 (25%)
7	TPO	G	11	7	8,10,11	2.02	2 (25%)	10,14,16	1.39	2 (20%)
1	FME	A	1	1	8,9,10	0.87	0	7,9,11	2.27	3 (42%)
7	TPO	T	11	7	8,10,11	1.82	2 (25%)	10,14,16	1.67	2 (20%)
2	FME	B	1	2	8,9,10	1.97	2 (25%)	7,9,11	2.29	2 (28%)
1	FME	N	1	1	8,9,10	1.52	1 (12%)	7,9,11	1.61	2 (28%)
2	FME	O	1	2	8,9,10	1.21	1 (12%)	7,9,11	1.88	2 (28%)
9	SAC	V	1	9	7,8,9	1.64	1 (14%)	8,9,11	1.54	3 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SAC	I	1	9	-	4/7/8/10	-
7	TPO	G	11	7	-	5/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
9	SAC	V	1	9	-	7/7/8/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.17	1.52	1.46
2	B	1	FME	CA-N	3.89	1.51	1.46
1	N	1	FME	CA-N	3.78	1.51	1.46
7	G	11	TPO	P-OG1	3.43	1.65	1.59
7	T	11	TPO	P-O1P	3.08	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	3.06	1.60	1.50
9	I	1	SAC	CA-N	2.63	1.50	1.46
2	B	1	FME	CB-CG	2.38	1.60	1.51
7	T	11	TPO	P-OG1	2.34	1.63	1.59
2	O	1	FME	CA-N	2.11	1.49	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	C-CA-N	-4.23	102.11	109.73
9	I	1	SAC	OG-CB-CA	-4.10	100.50	110.97
7	T	11	TPO	CG2-CB-CA	3.72	120.51	113.16
2	B	1	FME	CG-CB-CA	-3.71	102.63	112.95
2	O	1	FME	CG-CB-CA	-3.32	103.72	112.95
1	A	1	FME	CE-SD-CG	3.13	111.16	100.40
1	N	1	FME	CG-CB-CA	2.92	121.07	112.95
1	A	1	FME	C-CA-N	2.90	114.97	109.73
1	A	1	FME	CA-N-CN	2.81	127.14	122.82
9	I	1	SAC	C-CA-N	2.70	114.61	109.73
7	G	11	TPO	CG2-CB-CA	2.63	118.36	113.16
2	O	1	FME	CA-N-CN	2.53	126.71	122.82
9	V	1	SAC	CA-N-C1A	2.46	127.68	123.15
9	V	1	SAC	O-C-CA	-2.23	118.94	124.78
9	V	1	SAC	OG-CB-CA	-2.23	105.28	110.97
7	T	11	TPO	O3P-P-O1P	-2.09	102.50	110.68
7	G	11	TPO	O3P-P-OG1	2.07	115.26	105.99
1	N	1	FME	O-C-CA	-2.05	119.39	124.78

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
9	I	1	SAC	N-CA-CB-OG
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	C-CA-CB-CG

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

There are no ring outliers.

5 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 142 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 132 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
22	CHD	B	301	-	32,32,32	2.05	10 (31%)	51,51,51	1.93	17 (33%)
21	EDO	N	617	-	3,3,3	1.05	0	2,2,2	0.14	0
25	DMU	P	309	-	34,34,34	0.89	1 (2%)	45,45,45	1.26	3 (6%)
14	HEA	A	601	1	66,67,67	1.94	25 (37%)	78,103,103	2.48	32 (41%)
21	EDO	L	103	-	3,3,3	0.26	0	2,2,2	1.08	0
22	CHD	P	301	-	32,32,32	1.61	8 (25%)	51,51,51	2.01	16 (31%)
21	EDO	A	623	-	3,3,3	0.53	0	2,2,2	0.80	0
22	CHD	W	101	-	32,32,32	1.02	0	51,51,51	3.27	20 (39%)
21	EDO	N	622	-	3,3,3	0.51	0	2,2,2	0.70	0
21	EDO	E	201	-	3,3,3	0.84	0	2,2,2	0.44	0
21	EDO	A	614	-	3,3,3	0.39	0	2,2,2	1.18	0
21	EDO	E	204	-	3,3,3	0.79	0	2,2,2	0.39	0
22	CHD	C	307	-	32,32,32	1.19	3 (9%)	51,51,51	3.02	21 (41%)
25	DMU	L	102	-	34,34,34	0.96	1 (2%)	45,45,45	1.73	11 (24%)
21	EDO	H	102	-	3,3,3	0.59	0	2,2,2	1.26	0
22	CHD	C	301	-	32,32,32	1.72	6 (18%)	51,51,51	2.40	21 (41%)
21	EDO	D	202	-	3,3,3	0.55	0	2,2,2	0.74	0
19	TGL	N	610	-	62,62,62	1.16	4 (6%)	65,65,65	1.77	12 (18%)
21	EDO	N	618	-	3,3,3	0.45	0	2,2,2	1.46	0
18	AZI	N	608	14	0,2,2	-	-	0,1,1	-	-
21	EDO	R	203	-	3,3,3	0.54	0	2,2,2	0.82	0
21	EDO	C	314	-	3,3,3	0.54	0	2,2,2	0.77	0
21	EDO	N	620	-	3,3,3	0.43	0	2,2,2	0.73	0
21	EDO	E	205	-	3,3,3	0.38	0	2,2,2	0.80	0
21	EDO	C	319	-	3,3,3	0.68	0	2,2,2	0.26	0
22	CHD	G	101	-	32,32,32	1.66	7 (21%)	51,51,51	1.74	10 (19%)
18	AZI	N	607	15	0,2,2	-	-	0,1,1	-	-
20	PGV	P	303	-	50,50,50	0.80	1 (2%)	53,56,56	1.25	8 (15%)
21	EDO	N	616	-	3,3,3	0.56	0	2,2,2	1.11	0
21	EDO	R	205	-	3,3,3	0.32	0	2,2,2	1.05	0
21	EDO	D	205	-	3,3,3	0.50	0	2,2,2	0.71	0
21	EDO	A	613	-	3,3,3	1.64	1 (33%)	2,2,2	0.92	0
21	EDO	R	206	-	3,3,3	1.02	0	2,2,2	0.48	0
21	EDO	H	101	-	3,3,3	0.24	0	2,2,2	2.63	2 (100%)
21	EDO	N	619	-	3,3,3	0.55	0	2,2,2	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	P	313	-	3,3,3	0.60	0	2,2,2	0.70	0
21	EDO	A	616	-	3,3,3	1.02	0	2,2,2	0.33	0
21	EDO	F	105	-	3,3,3	0.66	0	2,2,2	0.42	0
28	CDL	T	103	-	99,99,99	1.51	14 (14%)	105,111,111	1.72	25 (23%)
14	HEA	A	602[B]	1,18	66,67,67	2.02	21 (31%)	78,103,103	1.98	23 (29%)
21	EDO	T	104	-	3,3,3	1.06	0	2,2,2	0.46	0
27	PEK	C	308	-	52,52,52	1.27	3 (5%)	55,57,57	1.59	9 (16%)
19	TGL	L	101	-	62,62,62	2.03	8 (12%)	65,65,65	2.34	17 (26%)
20	PGV	C	309	-	50,50,50	1.41	3 (6%)	53,56,56	1.48	8 (15%)
21	EDO	A	611	-	3,3,3	0.37	0	2,2,2	1.14	0
20	PGV	A	609	-	50,50,50	1.11	5 (10%)	53,56,56	1.19	5 (9%)
21	EDO	S	102	-	3,3,3	1.13	0	2,2,2	0.39	0
21	EDO	C	320	-	3,3,3	0.79	0	2,2,2	1.30	0
14	HEA	A	602[A]	1,18	66,67,67	1.87	19 (28%)	78,103,103	2.23	27 (34%)
20	PGV	G	103	-	50,50,50	1.25	2 (4%)	53,56,56	1.69	6 (11%)
21	EDO	Q	203	-	3,3,3	0.58	0	2,2,2	0.16	0
21	EDO	A	622	-	3,3,3	0.30	0	2,2,2	0.48	0
21	EDO	F	104	-	3,3,3	0.33	0	2,2,2	0.47	0
21	EDO	B	304	-	3,3,3	0.50	0	2,2,2	0.23	0
20	PGV	N	609	-	50,50,50	1.13	5 (10%)	53,56,56	1.32	5 (9%)
21	EDO	B	305	-	3,3,3	1.73	1 (33%)	2,2,2	0.11	0
22	CHD	J	101	-	32,32,32	0.74	0	51,51,51	3.22	28 (54%)
19	TGL	Q	201	-	62,62,62	1.49	4 (6%)	65,65,65	1.64	8 (12%)
27	PEK	P	307	-	52,52,52	1.21	2 (3%)	55,57,57	1.32	6 (10%)
21	EDO	D	204	-	3,3,3	0.61	0	2,2,2	0.98	0
21	EDO	G	105	-	3,3,3	0.91	0	2,2,2	0.20	0
21	EDO	R	204	-	3,3,3	0.88	0	2,2,2	0.42	0
25	DMU	C	310	-	34,34,34	0.87	1 (2%)	45,45,45	2.11	9 (20%)
25	DMU	P	308	-	34,34,34	0.75	0	45,45,45	2.19	13 (28%)
21	EDO	A	621	-	3,3,3	0.80	0	2,2,2	0.23	0
21	EDO	A	620	-	3,3,3	0.68	0	2,2,2	0.65	0
21	EDO	Q	202	-	3,3,3	0.36	0	2,2,2	1.09	0
21	EDO	G	104	-	3,3,3	0.58	0	2,2,2	0.47	0
20	PGV	Z	101	-	50,50,50	1.15	2 (4%)	53,56,56	1.36	7 (13%)
27	PEK	G	102	-	52,52,52	1.12	2 (3%)	55,57,57	1.49	5 (9%)
22	CHD	P	305	-	32,32,32	1.32	4 (12%)	51,51,51	3.13	22 (43%)
25	DMU	Z	102	-	34,34,34	0.75	1 (2%)	45,45,45	1.33	5 (11%)
27	PEK	T	102	-	52,52,52	1.18	6 (11%)	55,57,57	2.57	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DMU	P	306	-	34,34,34	1.02	1 (2%)	45,45,45	1.38	3 (6%)
21	EDO	U	101	-	3,3,3	0.36	0	2,2,2	0.82	0
20	PGV	A	610	-	50,50,50	1.42	4 (8%)	53,56,56	1.63	8 (15%)
21	EDO	A	617	-	3,3,3	1.21	0	2,2,2	1.28	0
28	CDL	P	304	-	99,99,99	1.61	18 (18%)	105,111,111	1.60	19 (18%)
14	HEA	N	603[B]	1,18	66,67,67	2.05	21 (31%)	78,103,103	1.73	18 (23%)
21	EDO	C	317	-	3,3,3	0.47	0	2,2,2	0.37	0
28	CDL	N	601	-	99,99,99	1.54	14 (14%)	105,111,111	1.60	20 (19%)
21	EDO	O	303	-	3,3,3	0.68	0	2,2,2	0.78	0
20	PGV	C	305	-	50,50,50	1.06	1 (2%)	53,56,56	1.36	7 (13%)
21	EDO	E	203	-	3,3,3	0.31	0	2,2,2	1.26	0
21	EDO	J	102	-	3,3,3	0.39	0	2,2,2	1.78	0
21	EDO	D	206	-	3,3,3	0.26	0	2,2,2	1.32	0
21	EDO	O	304	-	3,3,3	0.35	0	2,2,2	0.92	0
21	EDO	C	315	-	3,3,3	0.68	0	2,2,2	0.51	0
27	PEK	T	101	-	52,52,52	1.30	2 (3%)	55,57,57	1.43	7 (12%)
21	EDO	C	312	-	3,3,3	1.23	0	2,2,2	0.14	0
21	EDO	S	103	-	3,3,3	0.68	0	2,2,2	1.76	1 (50%)
21	EDO	C	313	-	3,3,3	0.36	0	2,2,2	0.80	0
21	EDO	C	318	-	3,3,3	0.66	0	2,2,2	0.39	0
25	DMU	M	101	-	34,34,34	0.71	0	45,45,45	1.41	6 (13%)
21	EDO	N	614	-	3,3,3	0.40	0	2,2,2	1.22	0
21	EDO	N	611	-	3,3,3	0.36	0	2,2,2	1.12	0
21	EDO	N	612	-	3,3,3	1.36	0	2,2,2	1.62	0
21	EDO	V	101	-	3,3,3	0.39	0	2,2,2	0.90	0
14	HEA	N	602	1	66,67,67	1.90	23 (34%)	78,103,103	2.33	32 (41%)
21	EDO	C	316	-	3,3,3	0.52	0	2,2,2	1.52	0
21	EDO	D	207	-	3,3,3	0.62	0	2,2,2	0.56	0
19	TGL	Y	101	-	62,62,62	1.45	5 (8%)	65,65,65	1.88	11 (16%)
21	EDO	E	202	-	3,3,3	0.53	0	2,2,2	0.84	0
21	EDO	F	103	-	3,3,3	0.64	0	2,2,2	0.54	0
21	EDO	R	201	-	3,3,3	1.14	0	2,2,2	1.17	0
18	AZI	A	606	15	0,2,2	-	-	0,1,1	-	-
18	AZI	A	607	14	0,2,2	-	-	0,1,1	-	-
19	TGL	D	201	-	62,62,62	1.66	5 (8%)	65,65,65	2.26	11 (16%)
21	EDO	P	311	-	3,3,3	0.84	0	2,2,2	0.14	0
21	EDO	P	310	-	3,3,3	0.67	0	2,2,2	2.16	1 (50%)
27	PEK	C	304	-	52,52,52	1.06	5 (9%)	55,57,57	1.28	8 (14%)
21	EDO	O	305	-	3,3,3	0.39	0	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	A	615	-	3,3,3	2.67	1 (33%)	2,2,2	4.78	1 (50%)
21	EDO	F	102	-	3,3,3	1.06	0	2,2,2	0.29	0
21	EDO	R	202	-	3,3,3	0.18	0	2,2,2	1.29	0
21	EDO	P	312	-	3,3,3	0.59	0	2,2,2	0.63	0
21	EDO	A	618	-	3,3,3	0.23	0	2,2,2	1.43	0
14	HEA	N	603[A]	1,18	66,67,67	2.12	22 (33%)	78,103,103	2.24	25 (32%)
21	EDO	N	615	-	3,3,3	1.57	1 (33%)	2,2,2	0.65	0
25	DMU	C	311	-	34,34,34	1.43	3 (8%)	45,45,45	2.32	11 (24%)
21	EDO	N	613	-	3,3,3	0.54	0	2,2,2	0.44	0
23	CUA	O	301	2	0,1,1	-	-	-	-	-
24	PSC	O	302	-	51,51,51	1.29	3 (5%)	57,59,59	1.34	4 (7%)
21	EDO	D	203	-	3,3,3	0.45	0	2,2,2	0.71	0
21	EDO	A	619	-	3,3,3	1.55	0	2,2,2	1.69	0
19	TGL	A	608	-	62,62,62	1.37	5 (8%)	65,65,65	2.18	11 (16%)
21	EDO	N	621	-	3,3,3	0.33	0	2,2,2	0.89	0
28	CDL	C	306	-	99,99,99	1.58	17 (17%)	105,111,111	1.66	20 (19%)
21	EDO	A	612	-	3,3,3	0.51	0	2,2,2	1.15	0
25	DMU	C	302	-	34,34,34	0.94	0	45,45,45	1.73	14 (31%)
24	PSC	B	303	-	51,51,51	1.46	4 (7%)	57,59,59	1.46	7 (12%)
23	CUA	B	302	2	0,1,1	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	B	301	-	-	2/9/74/74	0/4/4/4
21	EDO	N	617	-	-	0/1/1/1	-
25	DMU	P	309	-	-	7/19/59/59	0/2/2/2
14	HEA	A	601	1	-	5/36/76/76	-
21	EDO	L	103	-	-	1/1/1/1	-
22	CHD	P	301	-	-	2/9/74/74	0/4/4/4
21	EDO	A	623	-	-	0/1/1/1	-
22	CHD	W	101	-	-	7/9/74/74	0/4/4/4
21	EDO	N	622	-	-	1/1/1/1	-
21	EDO	E	201	-	-	1/1/1/1	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	E	204	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	C	307	-	-	8/9/74/74	0/4/4/4
25	DMU	L	102	-	-	12/19/59/59	0/2/2/2
21	EDO	H	102	-	-	1/1/1/1	-
22	CHD	C	301	-	-	3/9/74/74	0/4/4/4
21	EDO	D	202	-	-	1/1/1/1	-
19	TGL	N	610	-	-	39/65/65/65	-
21	EDO	N	618	-	-	0/1/1/1	-
21	EDO	R	203	-	-	1/1/1/1	-
21	EDO	C	314	-	-	0/1/1/1	-
21	EDO	N	620	-	-	0/1/1/1	-
21	EDO	E	205	-	-	0/1/1/1	-
21	EDO	C	319	-	-	1/1/1/1	-
22	CHD	G	101	-	-	2/9/74/74	0/4/4/4
20	PGV	P	303	-	-	11/55/55/55	-
21	EDO	N	616	-	-	1/1/1/1	-
21	EDO	R	205	-	-	1/1/1/1	-
21	EDO	D	205	-	-	1/1/1/1	-
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	R	206	-	-	1/1/1/1	-
21	EDO	H	101	-	-	0/1/1/1	-
21	EDO	N	619	-	-	0/1/1/1	-
21	EDO	P	313	-	-	1/1/1/1	-
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	F	105	-	-	0/1/1/1	-
28	CDL	T	103	-	-	63/110/110/110	-
14	HEA	A	602[B]	1,18	-	6/36/76/76	-
21	EDO	T	104	-	-	0/1/1/1	-
27	PEK	C	308	-	-	28/56/56/56	-
19	TGL	L	101	-	-	38/65/65/65	-
20	PGV	C	309	-	-	27/55/55/55	-
21	EDO	A	611	-	-	1/1/1/1	-
20	PGV	A	609	-	-	8/55/55/55	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	C	320	-	-	1/1/1/1	-
14	HEA	A	602[A]	1,18	-	8/36/76/76	-
20	PGV	G	103	-	-	33/55/55/55	-
21	EDO	Q	203	-	-	1/1/1/1	-
21	EDO	A	622	-	-	1/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	B	304	-	-	0/1/1/1	-
20	PGV	N	609	-	-	13/55/55/55	-
21	EDO	B	305	-	-	1/1/1/1	-
22	CHD	J	101	-	-	7/9/74/74	0/4/4/4
19	TGL	Q	201	-	-	37/65/65/65	-
27	PEK	P	307	-	-	27/56/56/56	-
21	EDO	D	204	-	-	1/1/1/1	-
21	EDO	G	105	-	-	1/1/1/1	-
21	EDO	R	204	-	-	0/1/1/1	-
25	DMU	C	310	-	-	6/19/59/59	0/2/2/2
25	DMU	P	308	-	-	7/19/59/59	0/2/2/2
21	EDO	A	621	-	-	1/1/1/1	-
21	EDO	A	620	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	0/1/1/1	-
21	EDO	G	104	-	-	1/1/1/1	-
20	PGV	Z	101	-	-	31/55/55/55	-
27	PEK	G	102	-	-	34/56/56/56	-
22	CHD	P	305	-	-	6/9/74/74	0/4/4/4
25	DMU	Z	102	-	-	5/19/59/59	0/2/2/2
27	PEK	T	102	-	-	23/56/56/56	-
25	DMU	P	306	-	-	6/19/59/59	0/2/2/2
21	EDO	U	101	-	-	1/1/1/1	-
20	PGV	A	610	-	-	26/55/55/55	-
21	EDO	A	617	-	-	1/1/1/1	-
28	CDL	P	304	-	-	56/110/110/110	-
14	HEA	N	603[B]	1,18	-	7/36/76/76	-
21	EDO	C	317	-	-	1/1/1/1	-
28	CDL	N	601	-	-	53/110/110/110	-
21	EDO	O	303	-	-	0/1/1/1	-
20	PGV	C	305	-	-	14/55/55/55	-
21	EDO	E	203	-	-	1/1/1/1	-
21	EDO	J	102	-	-	1/1/1/1	-
21	EDO	D	206	-	-	1/1/1/1	-
21	EDO	O	304	-	-	1/1/1/1	-
21	EDO	C	315	-	-	1/1/1/1	-
27	PEK	T	101	-	-	29/56/56/56	-
21	EDO	C	312	-	-	0/1/1/1	-
21	EDO	S	103	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	C	313	-	-	1/1/1/1	-
21	EDO	C	318	-	-	1/1/1/1	-
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
21	EDO	N	614	-	-	1/1/1/1	-
21	EDO	N	611	-	-	1/1/1/1	-
21	EDO	N	612	-	-	1/1/1/1	-
21	EDO	V	101	-	-	0/1/1/1	-
14	HEA	N	602	1	-	7/36/76/76	-
21	EDO	C	316	-	-	0/1/1/1	-
21	EDO	D	207	-	-	0/1/1/1	-
19	TGL	Y	101	-	-	34/65/65/65	-
21	EDO	E	202	-	-	0/1/1/1	-
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	R	201	-	-	0/1/1/1	-
19	TGL	D	201	-	-	40/65/65/65	-
21	EDO	P	311	-	-	0/1/1/1	-
21	EDO	P	310	-	-	1/1/1/1	-
27	PEK	C	304	-	-	12/56/56/56	-
21	EDO	O	305	-	-	0/1/1/1	-
21	EDO	A	615	-	-	1/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	R	202	-	-	1/1/1/1	-
21	EDO	P	312	-	-	0/1/1/1	-
21	EDO	A	618	-	-	1/1/1/1	-
14	HEA	N	603[A]	1,18	-	6/36/76/76	-
21	EDO	N	615	-	-	0/1/1/1	-
25	DMU	C	311	-	-	8/19/59/59	0/2/2/2
21	EDO	N	613	-	-	1/1/1/1	-
24	PSC	O	302	-	-	33/55/55/55	-
21	EDO	D	203	-	-	1/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
19	TGL	A	608	-	-	36/65/65/65	-
21	EDO	N	621	-	-	0/1/1/1	-
28	CDL	C	306	-	-	70/110/110/110	-
21	EDO	A	612	-	-	1/1/1/1	-
25	DMU	C	302	-	-	7/19/59/59	0/2/2/2
24	PSC	B	303	-	-	28/55/55/55	-

All (325) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG3-CC1	9.15	1.60	1.33
19	L	101	TGL	OG2-CB1	9.01	1.59	1.34
19	D	201	TGL	OB1-CB1	7.45	1.44	1.22
19	Y	101	TGL	OG2-CB1	6.77	1.53	1.34
20	C	309	PGV	O01-C1	6.53	1.52	1.34
19	Q	201	TGL	OB1-CB1	6.41	1.41	1.22
14	N	603[B]	HEA	FE-NB	6.39	2.14	1.94
19	D	201	TGL	OG1-CA1	6.22	1.51	1.33
28	N	601	CDL	OB6-CB5	6.20	1.51	1.34
24	B	303	PSC	O01-C1	6.11	1.51	1.34
28	T	103	CDL	OB6-CB5	6.08	1.51	1.34
19	Y	101	TGL	OG3-CC1	5.82	1.50	1.33
19	Q	201	TGL	OG2-CB1	5.80	1.50	1.34
28	P	304	CDL	OA8-CA7	5.77	1.50	1.33
28	P	304	CDL	OB8-CB7	5.75	1.50	1.33
20	G	103	PGV	O01-C1	5.71	1.50	1.34
19	A	608	TGL	OG1-CA1	5.68	1.49	1.33
28	C	306	CDL	OA8-CA7	5.63	1.49	1.33
20	A	610	PGV	O03-C19	5.62	1.49	1.33
14	N	603[A]	HEA	FE-NB	5.60	2.12	1.94
27	T	101	PEK	O01-C1	5.58	1.50	1.34
28	N	601	CDL	OB8-CB7	5.52	1.49	1.33
28	C	306	CDL	OB8-CB7	5.52	1.49	1.33
27	T	101	PEK	O03-C21	5.41	1.49	1.33
27	C	308	PEK	O03-C21	5.40	1.49	1.33
20	Z	101	PGV	O03-C19	5.37	1.49	1.33
14	N	603[B]	HEA	FE-ND	5.35	2.11	1.94
19	D	201	TGL	OG2-CB1	5.35	1.49	1.34
20	A	610	PGV	O01-C1	5.34	1.49	1.34
19	A	608	TGL	OG2-CB1	5.27	1.49	1.34
28	T	103	CDL	OB8-CB7	5.23	1.48	1.33
24	O	302	PSC	O01-C1	5.21	1.49	1.34
27	C	308	PEK	O01-C1	5.20	1.49	1.34
20	C	309	PGV	O03-C19	5.19	1.48	1.33
27	P	307	PEK	O01-C1	5.17	1.48	1.34
28	P	304	CDL	OA6-CA5	5.11	1.48	1.34
28	T	103	CDL	OA6-CA5	5.05	1.48	1.34
27	G	102	PEK	O01-C1	4.98	1.48	1.34
28	N	601	CDL	OA6-CA5	4.94	1.48	1.34
24	O	302	PSC	O03-C19	4.87	1.47	1.33
27	T	102	PEK	C2-C1	4.84	1.64	1.50
19	N	610	TGL	OG1-CA1	4.82	1.47	1.33
14	N	603[A]	HEA	FE-NA	4.80	2.11	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	103	CDL	OA8-CA7	4.79	1.47	1.33
14	N	603[A]	HEA	CHB-C4A	4.78	1.47	1.38
28	C	306	CDL	PB2-OB3	4.76	1.67	1.50
19	Q	201	TGL	OG1-CA1	4.75	1.47	1.33
20	G	103	PGV	O03-C19	4.75	1.47	1.33
27	P	307	PEK	O03-C21	4.74	1.47	1.33
25	C	311	DMU	O16-C6	4.72	1.48	1.40
27	G	102	PEK	O03-C21	4.68	1.47	1.33
20	Z	101	PGV	O01-C1	4.68	1.47	1.34
14	A	602[B]	HEA	FE-NB	4.57	2.09	1.94
19	L	101	TGL	OG1-CA1	4.56	1.46	1.33
19	N	610	TGL	OG2-CB1	4.56	1.47	1.34
19	Y	101	TGL	OG1-CA1	4.54	1.46	1.33
14	A	602[B]	HEA	FE-ND	4.53	2.08	1.94
14	N	603[B]	HEA	C1D-ND	-4.47	1.32	1.40
28	N	601	CDL	OA8-CA7	4.45	1.46	1.33
14	A	602[B]	HEA	CHB-C4A	4.43	1.47	1.38
28	C	306	CDL	OA6-CA5	4.41	1.46	1.34
22	C	301	CHD	C11-C12	4.37	1.60	1.53
14	N	603[B]	HEA	CHB-C4A	4.37	1.46	1.38
21	A	615	EDO	C2-C1	4.36	1.78	1.48
24	B	303	PSC	O03-C19	4.36	1.46	1.33
25	P	306	DMU	O16-C6	4.31	1.47	1.40
19	N	610	TGL	OG3-CC1	4.24	1.45	1.33
24	O	302	PSC	C13-C12	4.16	1.55	1.31
14	A	601	HEA	CHD-C1D	4.16	1.47	1.38
14	A	601	HEA	C3A-C4A	-4.14	1.38	1.46
19	L	101	TGL	OG3-CG3	4.13	1.54	1.45
14	N	603[A]	HEA	O11-C11	4.13	1.51	1.42
22	G	101	CHD	C4-C5	4.12	1.60	1.53
24	B	303	PSC	C13-C12	4.06	1.55	1.31
19	Q	201	TGL	OG3-CC1	4.04	1.45	1.33
22	B	301	CHD	C19-C10	4.04	1.61	1.54
14	A	602[A]	HEA	CHB-C4A	4.04	1.46	1.38
19	L	101	TGL	CG3-CG2	4.03	1.63	1.50
28	P	304	CDL	PB2-OB3	4.02	1.65	1.50
14	A	601	HEA	CHB-C4A	4.02	1.46	1.38
20	C	305	PGV	O01-C02	-4.00	1.36	1.46
14	A	602[B]	HEA	CHC-C4B	3.99	1.46	1.38
14	A	602[B]	HEA	C4D-ND	-3.93	1.30	1.38
14	N	603[A]	HEA	C4D-C3D	-3.81	1.38	1.45
28	C	306	CDL	OB6-CB5	3.80	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	301	CHD	C8-C7	3.77	1.59	1.53
14	A	601	HEA	C4B-C3B	-3.76	1.38	1.44
28	P	304	CDL	OB6-CB5	3.75	1.44	1.34
14	A	602[A]	HEA	C4D-C3D	-3.75	1.38	1.45
24	B	303	PSC	C2-C1	3.70	1.61	1.50
19	D	201	TGL	OG3-CC1	3.66	1.44	1.33
19	A	608	TGL	OG3-CC1	3.63	1.43	1.33
19	A	608	TGL	OC1-CC1	-3.62	1.11	1.22
14	N	602	HEA	CHC-C4B	3.58	1.45	1.38
14	A	601	HEA	CMB-C2B	3.58	1.58	1.50
14	N	603[A]	HEA	C4B-NB	-3.57	1.34	1.40
14	N	602	HEA	O11-C11	3.46	1.50	1.42
22	B	301	CHD	C20-C17	3.42	1.60	1.54
14	A	602[B]	HEA	FE-NC	3.39	2.06	1.95
14	N	602	HEA	CHB-C4A	3.38	1.45	1.38
20	A	610	PGV	O02-C1	3.38	1.32	1.22
14	A	602[B]	HEA	CMA-C3A	3.38	1.52	1.45
14	N	603[B]	HEA	C1A-C2A	-3.36	1.39	1.45
25	C	310	DMU	O16-C6	3.35	1.45	1.40
14	A	602[B]	HEA	C4B-C3B	-3.35	1.39	1.44
14	A	602[A]	HEA	C1A-C2A	-3.34	1.39	1.45
22	B	301	CHD	C1-C2	3.33	1.60	1.53
25	P	309	DMU	O16-C6	3.33	1.45	1.40
28	C	306	CDL	PB2-OB2	3.33	1.72	1.59
14	N	602	HEA	CMC-C2C	3.32	1.57	1.50
14	A	602[A]	HEA	FE-NA	3.31	2.06	1.95
28	C	306	CDL	C79-C78	-3.30	1.33	1.51
22	G	101	CHD	C1-C2	3.30	1.60	1.53
25	C	311	DMU	C10-C5	3.28	1.61	1.52
14	A	601	HEA	CHC-C4B	3.27	1.45	1.38
14	N	603[A]	HEA	CHC-C1C	3.27	1.46	1.39
14	A	602[B]	HEA	C4A-NA	-3.26	1.33	1.39
14	A	602[B]	HEA	C3A-C4A	-3.22	1.40	1.46
14	N	602	HEA	C3A-C4A	-3.22	1.40	1.46
28	C	306	CDL	C59-C58	-3.22	1.33	1.51
14	N	603[B]	HEA	C4B-NB	-3.21	1.34	1.40
14	A	602[A]	HEA	CHD-C1D	3.21	1.45	1.38
27	C	304	PEK	P-O14	3.20	1.62	1.50
14	N	603[B]	HEA	C4B-C3B	-3.18	1.39	1.44
27	T	102	PEK	P-O14	3.14	1.62	1.50
14	N	603[B]	HEA	C3A-C4A	-3.14	1.40	1.46
19	L	101	TGL	OG2-CG2	3.12	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602[B]	HEA	CHD-C1D	3.12	1.44	1.38
14	N	603[A]	HEA	CHB-C1B	3.11	1.46	1.39
14	N	602	HEA	CHA-C1A	3.08	1.44	1.38
22	C	301	CHD	C23-C24	3.08	1.57	1.50
28	N	601	CDL	C22-C21	-3.03	1.34	1.51
28	T	103	CDL	C59-C58	-3.03	1.34	1.51
14	N	602	HEA	CHC-C1C	3.02	1.46	1.39
14	A	601	HEA	C1A-NA	-3.02	1.33	1.39
14	A	602[A]	HEA	C3A-C4A	-3.02	1.40	1.46
28	C	306	CDL	C19-C18	-3.01	1.34	1.51
14	N	603[B]	HEA	C1A-NA	-3.00	1.33	1.39
28	C	306	CDL	C82-C81	-3.00	1.34	1.51
14	A	602[B]	HEA	CHD-C4C	2.99	1.46	1.39
14	A	602[B]	HEA	C1A-C2A	-2.99	1.39	1.45
14	A	602[A]	HEA	FE-ND	2.98	2.04	1.94
20	N	609	PGV	O03-C19	2.98	1.42	1.33
20	A	609	PGV	O03-C19	2.97	1.42	1.33
20	N	609	PGV	O03-C01	2.97	1.51	1.45
28	T	103	CDL	C79-C78	-2.96	1.35	1.51
28	P	304	CDL	C42-C41	-2.96	1.35	1.51
22	P	301	CHD	C16-C15	2.95	1.62	1.54
22	B	301	CHD	C4-C3	2.95	1.57	1.51
22	P	305	CHD	C16-C17	2.95	1.60	1.54
14	A	602[A]	HEA	C4A-NA	-2.95	1.34	1.39
28	C	306	CDL	C22-C21	-2.95	1.35	1.51
28	C	306	CDL	C62-C61	-2.95	1.35	1.51
14	N	603[B]	HEA	CHA-C1A	2.94	1.44	1.38
28	P	304	CDL	PA1-OA5	2.93	1.71	1.59
27	C	304	PEK	O01-C1	2.93	1.42	1.34
14	N	602	HEA	C4B-NB	-2.93	1.35	1.40
22	G	101	CHD	C20-C17	2.93	1.59	1.54
14	N	602	HEA	CBD-CGD	2.91	1.57	1.50
14	A	602[B]	HEA	C1B-NB	-2.91	1.32	1.38
14	A	601	HEA	C12-C13	2.90	1.62	1.53
14	A	602[A]	HEA	FE-NC	2.90	2.04	1.95
28	P	304	CDL	C79-C78	-2.89	1.35	1.51
22	B	301	CHD	O7-C7	2.88	1.49	1.43
20	N	609	PGV	C01-C02	2.87	1.59	1.50
14	N	602	HEA	C4D-C3D	-2.87	1.40	1.45
28	P	304	CDL	C22-C21	-2.86	1.35	1.51
14	N	602	HEA	CMD-C2D	2.86	1.56	1.50
28	N	601	CDL	C19-C18	-2.86	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	301	CHD	C10-C5	2.85	1.60	1.55
14	A	601	HEA	C1D-ND	-2.85	1.35	1.40
28	N	601	CDL	C62-C61	-2.85	1.35	1.51
14	N	603[A]	HEA	FE-ND	2.85	2.03	1.94
28	P	304	CDL	C19-C18	-2.84	1.35	1.51
28	P	304	CDL	C82-C81	-2.84	1.35	1.51
14	A	602[A]	HEA	CHC-C1C	2.83	1.45	1.39
27	C	304	PEK	O03-C21	2.83	1.41	1.33
22	P	301	CHD	C23-C24	2.81	1.57	1.50
28	T	103	CDL	C19-C18	-2.81	1.35	1.51
14	N	602	HEA	C1A-NA	-2.81	1.34	1.39
28	N	601	CDL	C59-C58	-2.80	1.35	1.51
28	N	601	CDL	C79-C78	-2.80	1.35	1.51
28	P	304	CDL	C62-C61	-2.78	1.35	1.51
28	N	601	CDL	C82-C81	-2.78	1.36	1.51
22	P	301	CHD	C11-C12	2.77	1.57	1.53
14	N	603[A]	HEA	CHC-C4B	2.77	1.44	1.38
14	N	603[B]	HEA	CHC-C4B	2.76	1.44	1.38
14	N	602	HEA	C12-C11	-2.76	1.48	1.52
28	N	601	CDL	C42-C41	-2.75	1.36	1.51
28	T	103	CDL	C22-C21	-2.75	1.36	1.51
20	C	309	PGV	C01-C02	2.75	1.59	1.50
22	B	301	CHD	C13-C17	-2.74	1.50	1.55
14	N	603[A]	HEA	CHD-C4C	2.73	1.45	1.39
14	N	603[A]	HEA	C4C-NC	-2.71	1.34	1.39
22	G	101	CHD	C8-C7	2.71	1.58	1.53
27	C	304	PEK	O01-C02	2.71	1.53	1.46
14	A	601	HEA	CHA-C1A	2.70	1.43	1.38
28	T	103	CDL	C39-C38	-2.70	1.36	1.51
22	P	301	CHD	C8-C14	2.70	1.59	1.53
28	T	103	CDL	C82-C81	-2.70	1.36	1.51
14	N	602	HEA	CHD-C1D	2.70	1.44	1.38
28	C	306	CDL	CB2-C1	2.69	1.60	1.51
22	B	301	CHD	C2-C3	2.67	1.58	1.51
14	A	602[A]	HEA	C4B-C3B	-2.66	1.40	1.44
25	C	311	DMU	O3-C5	2.66	1.49	1.43
28	T	103	CDL	C62-C61	-2.63	1.36	1.51
28	P	304	CDL	C59-C58	-2.63	1.36	1.51
19	A	608	TGL	OG2-CG2	2.62	1.53	1.46
14	A	602[A]	HEA	C1D-C2D	-2.62	1.39	1.44
14	N	603[A]	HEA	C1A-C2A	-2.61	1.40	1.45
28	C	306	CDL	C42-C41	-2.61	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P	304	CDL	CB2-C1	2.61	1.60	1.51
22	G	101	CHD	O7-C7	2.60	1.48	1.43
22	P	305	CHD	C8-C9	2.60	1.58	1.53
28	T	103	CDL	C42-C41	-2.59	1.37	1.51
14	A	602[A]	HEA	C4D-ND	-2.59	1.33	1.38
28	C	306	CDL	C39-C38	-2.59	1.37	1.51
14	A	602[A]	HEA	O11-C11	2.59	1.48	1.42
14	A	602[B]	HEA	CHC-C1C	2.58	1.45	1.39
28	N	601	CDL	CB3-CB4	2.58	1.58	1.50
28	N	601	CDL	C39-C38	-2.57	1.37	1.51
22	G	101	CHD	C11-C9	2.57	1.58	1.53
14	N	603[B]	HEA	C1B-C2B	-2.56	1.39	1.44
22	B	301	CHD	C11-C9	2.56	1.58	1.53
22	C	301	CHD	C11-C9	2.55	1.58	1.53
28	P	304	CDL	C39-C38	-2.54	1.37	1.51
14	A	601	HEA	CBD-CAD	2.53	1.60	1.52
14	A	602[A]	HEA	C4C-NC	-2.53	1.34	1.39
22	P	301	CHD	C11-C9	2.52	1.57	1.53
14	A	602[A]	HEA	CHC-C4B	2.52	1.43	1.38
28	T	103	CDL	CB3-CB4	2.52	1.58	1.50
14	N	603[A]	HEA	C1D-C2D	-2.52	1.39	1.44
14	N	603[B]	HEA	C4C-NC	-2.51	1.34	1.39
22	P	301	CHD	C10-C9	2.50	1.60	1.56
22	C	307	CHD	C16-C17	2.48	1.59	1.54
28	P	304	CDL	PB2-OB2	2.48	1.69	1.59
14	A	602[B]	HEA	CHA-C1A	2.47	1.43	1.38
14	N	603[A]	HEA	C4B-C3B	-2.46	1.40	1.44
14	N	603[A]	HEA	CHD-C1D	2.44	1.43	1.38
28	P	304	CDL	O1-C1	2.44	1.50	1.43
20	A	609	PGV	C01-C02	2.43	1.58	1.50
14	A	601	HEA	CAD-C3D	2.43	1.57	1.51
14	N	602	HEA	FE-NA	2.43	2.03	1.95
14	N	603[B]	HEA	CMA-C3A	2.42	1.50	1.45
14	A	602[A]	HEA	CHD-C4C	2.42	1.44	1.39
20	P	303	PGV	O03-C19	2.41	1.40	1.33
14	N	602	HEA	O1A-CGA	2.40	1.30	1.22
14	N	602	HEA	FE-NB	2.40	2.02	1.94
14	N	603[A]	HEA	C4A-NA	-2.38	1.35	1.39
25	Z	102	DMU	O16-C6	2.38	1.44	1.40
14	A	601	HEA	O1D-CGD	2.38	1.30	1.22
14	A	601	HEA	C1A-C2A	-2.37	1.41	1.45
14	A	601	HEA	CMA-C3A	2.36	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	CBA-CGA	2.35	1.56	1.50
27	T	102	PEK	C3-C2	2.35	1.60	1.52
22	P	301	CHD	C8-C7	2.34	1.57	1.53
14	N	602	HEA	CBD-CAD	2.34	1.59	1.52
19	L	101	TGL	OC1-CC1	2.34	1.29	1.22
14	N	603[A]	HEA	C3B-C2B	2.33	1.40	1.34
14	A	602[B]	HEA	C1A-NA	-2.33	1.35	1.39
14	N	602	HEA	C1D-C2D	-2.33	1.40	1.44
22	P	305	CHD	C20-C17	2.33	1.58	1.54
14	N	603[B]	HEA	FE-NA	2.33	2.03	1.95
14	A	601	HEA	CMD-C2D	2.33	1.55	1.50
28	T	103	CDL	CB6-CB4	2.31	1.57	1.50
14	A	602[A]	HEA	FE-NB	2.31	2.02	1.94
21	B	305	EDO	O1-C1	2.30	1.54	1.42
14	A	601	HEA	CMC-C2C	2.30	1.55	1.50
14	N	603[A]	HEA	O1D-CGD	2.29	1.29	1.22
14	A	602[B]	HEA	C4C-NC	-2.29	1.35	1.39
21	A	613	EDO	O2-C2	2.28	1.53	1.42
14	A	601	HEA	C4D-C3D	-2.26	1.41	1.45
14	A	601	HEA	CHB-C1B	2.26	1.44	1.39
14	N	603[A]	HEA	C1A-NA	-2.26	1.35	1.39
28	N	601	CDL	PB2-OB5	2.26	1.68	1.59
14	N	603[B]	HEA	C4D-C3D	-2.26	1.41	1.45
14	N	602	HEA	CBA-CAA	2.25	1.59	1.52
22	C	307	CHD	C4-C3	2.24	1.56	1.51
14	A	601	HEA	O1A-CGA	2.24	1.29	1.22
22	C	301	CHD	C13-C12	-2.24	1.51	1.54
22	C	301	CHD	C8-C7	2.22	1.57	1.53
14	A	602[B]	HEA	C1D-ND	-2.21	1.36	1.40
20	A	609	PGV	O01-C1	2.21	1.40	1.34
20	A	610	PGV	P-O13	2.21	1.58	1.50
22	G	101	CHD	C2-C3	2.21	1.56	1.51
28	C	306	CDL	OB2-CB2	2.21	1.53	1.44
27	T	102	PEK	C3-C4	2.20	1.61	1.52
14	N	603[A]	HEA	C3A-C4A	-2.18	1.42	1.46
22	P	305	CHD	C11-C9	2.18	1.57	1.53
14	N	603[B]	HEA	FE-NC	2.18	2.02	1.95
21	N	615	EDO	O2-C2	2.17	1.53	1.42
14	N	603[B]	HEA	C4A-NA	-2.17	1.35	1.39
19	N	610	TGL	OC1-CC1	-2.17	1.16	1.22
28	P	304	CDL	CA3-CA4	2.17	1.57	1.50
14	A	601	HEA	C16-C17	-2.14	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	CMA-C3A	2.14	1.49	1.45
20	N	609	PGV	O01-C1	2.13	1.40	1.34
19	Y	101	TGL	CG3-CG2	2.13	1.57	1.50
14	N	603[B]	HEA	CHD-C1D	2.12	1.42	1.38
14	A	601	HEA	C12-C11	-2.12	1.49	1.52
19	Y	101	TGL	CB2-CB1	2.12	1.56	1.50
28	C	306	CDL	OB6-CB4	-2.12	1.41	1.46
14	A	602[B]	HEA	FE-NA	2.11	2.02	1.95
14	A	601	HEA	C1C-NC	-2.11	1.35	1.39
14	A	601	HEA	CHA-C4D	2.10	1.44	1.39
25	L	102	DMU	O16-C6	2.09	1.43	1.40
20	A	609	PGV	O03-C01	2.09	1.49	1.45
14	N	603[A]	HEA	CHA-C4D	2.08	1.44	1.39
14	A	601	HEA	CBD-CGD	2.08	1.55	1.50
20	A	609	PGV	C3-C2	2.08	1.59	1.52
27	T	102	PEK	C05-C04	2.07	1.58	1.50
22	C	307	CHD	C20-C17	2.07	1.58	1.54
22	P	301	CHD	C16-C17	2.07	1.58	1.54
22	C	301	CHD	C2-C3	2.07	1.56	1.51
20	N	609	PGV	O06-C06	2.07	1.51	1.42
14	N	603[B]	HEA	C1C-NC	-2.06	1.35	1.39
27	C	308	PEK	C01-C02	2.06	1.57	1.50
27	T	102	PEK	O01-C1	2.05	1.40	1.34
19	D	201	TGL	OC1-CC1	2.05	1.28	1.22
14	A	602[A]	HEA	C20-C19	2.04	1.55	1.51
27	C	304	PEK	P-O13	-2.03	1.45	1.55
14	N	603[B]	HEA	CHD-C4C	2.01	1.43	1.39
19	L	101	TGL	CB2-CB1	2.01	1.56	1.50
14	A	602[B]	HEA	CHB-C1B	2.01	1.43	1.39
14	N	602	HEA	C1B-C2B	-2.00	1.40	1.44

All (653) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	102	PEK	C2-C3-C4	14.82	139.64	113.23
22	P	305	CHD	C23-C22-C20	-12.78	91.17	114.52
22	C	307	CHD	C23-C22-C20	-11.42	93.65	114.52
19	D	201	TGL	OG2-CB1-CB2	-10.77	88.29	111.50
22	J	101	CHD	C14-C8-C9	-10.23	95.67	109.71
19	A	608	TGL	OG2-CB1-CB2	9.81	132.64	111.50
22	W	101	CHD	C17-C13-C12	9.42	126.27	117.67
19	N	610	TGL	OG2-CB1-CB2	8.76	130.37	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	T	103	CDL	OB6-CB5-C51	8.68	130.21	111.50
22	W	101	CHD	C11-C12-C13	8.51	119.98	111.24
19	L	101	TGL	OG2-CB1-CB2	8.36	129.52	111.50
19	Q	201	TGL	OG2-CB1-CB2	-8.17	93.89	111.50
22	W	101	CHD	C18-C13-C12	-8.00	100.92	109.07
19	D	201	TGL	OG2-CB1-OB1	7.97	142.97	123.70
25	C	311	DMU	O16-C6-C1	7.86	120.58	108.30
14	N	603[A]	HEA	C13-C12-C11	-7.79	102.65	114.35
19	Y	101	TGL	OG2-CB1-CB2	7.63	127.94	111.50
14	N	603[A]	HEA	OMA-CMA-C3A	-7.60	108.50	125.69
19	L	101	TGL	CG2-OG2-CB1	7.54	136.35	117.79
19	A	608	TGL	OG3-CC1-OC1	-7.48	104.71	123.59
25	C	311	DMU	O7-C10-C5	7.48	127.48	108.10
28	N	601	CDL	OB6-CB5-C51	7.30	127.23	111.50
27	T	102	PEK	O01-C1-O02	-7.16	106.40	123.70
27	G	102	PEK	O01-C1-C2	7.15	126.91	111.50
20	G	103	PGV	O01-C1-C2	6.92	126.41	111.50
19	L	101	TGL	OG3-CG3-CG2	6.90	128.53	108.43
22	W	101	CHD	C13-C17-C20	6.80	127.61	119.50
22	P	305	CHD	C16-C17-C20	6.74	122.58	112.15
21	A	615	EDO	O2-C2-C1	-6.74	63.40	111.91
22	J	101	CHD	C15-C14-C8	6.64	127.61	118.33
27	C	308	PEK	O01-C1-C2	6.62	125.77	111.50
22	C	301	CHD	C23-C22-C20	-6.55	102.56	114.52
25	C	310	DMU	O16-C6-C1	6.47	118.40	108.30
22	W	101	CHD	C14-C13-C12	6.46	113.42	107.40
14	A	601	HEA	C3C-C4C-NC	6.45	114.22	110.25
14	N	602	HEA	C13-C14-C15	-6.38	112.30	127.66
22	C	307	CHD	C21-C20-C17	6.36	122.65	112.92
27	T	101	PEK	O01-C1-C2	6.14	124.74	111.50
24	O	302	PSC	O01-C1-C2	6.06	124.57	111.50
20	G	103	PGV	O03-C19-C20	6.05	130.89	111.91
22	J	101	CHD	C18-C13-C12	-6.01	102.95	109.07
14	N	603[A]	HEA	CAD-CBD-CGD	-6.00	100.69	113.60
14	A	602[A]	HEA	CHA-C4D-ND	5.83	130.75	124.42
19	D	201	TGL	CB3-CB2-CB1	5.81	134.75	113.62
25	P	308	DMU	O16-C6-C1	5.80	117.35	108.30
14	A	601	HEA	C3D-C4D-ND	5.76	115.94	110.36
28	C	306	CDL	OA6-CA5-C11	5.75	123.90	111.50
27	P	307	PEK	O01-C1-C2	5.71	123.82	111.50
25	P	308	DMU	O7-C10-C5	5.71	122.89	108.10
14	A	601	HEA	C13-C12-C11	-5.68	105.82	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C13-C14-C15	-5.58	114.23	127.66
25	C	310	DMU	C10-O1-C9	-5.54	102.82	113.69
14	A	602[A]	HEA	OMA-CMA-C3A	-5.53	113.19	125.69
22	J	101	CHD	C11-C12-C13	5.53	116.92	111.24
19	A	608	TGL	OG2-CG2-CG3	5.52	128.40	108.40
22	P	305	CHD	C14-C13-C12	5.48	112.50	107.40
14	A	601	HEA	C4B-NB-C1B	-5.47	99.42	105.07
25	P	308	DMU	C18-O16-C6	-5.46	104.78	113.84
24	B	303	PSC	O01-C1-C2	5.45	123.25	111.50
22	W	101	CHD	C14-C8-C7	5.38	118.94	111.81
19	Y	101	TGL	CG2-OG2-CB1	5.35	130.97	117.79
14	A	602[B]	HEA	C27-C19-C20	5.35	124.28	115.27
22	P	305	CHD	C6-C7-C8	5.35	117.19	111.48
22	C	307	CHD	C6-C7-C8	5.33	117.17	111.48
14	A	602[B]	HEA	CAA-CBA-CGA	-5.27	102.27	113.60
19	A	608	TGL	OG3-CC1-CC2	5.17	128.15	111.91
22	C	301	CHD	C22-C20-C17	-5.17	99.60	110.28
22	C	307	CHD	C16-C17-C20	5.16	120.13	112.15
28	P	304	CDL	OA6-CA5-C11	5.12	122.54	111.50
22	C	307	CHD	C22-C23-C24	-5.12	98.92	112.51
14	N	602	HEA	C3C-C4C-NC	5.10	113.38	110.25
25	C	310	DMU	O7-C10-C5	5.10	121.31	108.10
28	T	103	CDL	OA6-CA5-C11	5.09	122.48	111.50
20	Z	101	PGV	O01-C1-C2	5.09	122.48	111.50
24	B	303	PSC	O01-C1-O02	-5.08	111.44	123.70
14	A	601	HEA	CAD-CBD-CGD	-5.07	102.69	113.60
22	W	101	CHD	C17-C13-C14	-5.05	95.00	100.09
25	C	311	DMU	O3-C5-C10	5.05	122.31	110.05
20	C	309	PGV	O03-C19-C20	5.05	127.74	111.91
22	P	305	CHD	C13-C17-C20	-5.03	113.49	119.50
22	C	307	CHD	C15-C14-C13	5.02	108.48	103.55
22	B	301	CHD	C16-C17-C20	-4.99	104.42	112.15
14	A	601	HEA	C4C-NC-C1C	-4.97	100.48	105.35
25	P	306	DMU	O16-C6-C1	4.92	115.99	108.30
22	J	101	CHD	C11-C9-C10	4.91	118.80	113.73
22	P	301	CHD	C22-C20-C17	-4.90	100.17	110.28
19	N	610	TGL	OG3-CC1-CC2	4.85	127.14	111.91
14	A	602[A]	HEA	C27-C19-C20	4.85	123.42	115.27
22	J	101	CHD	C15-C14-C13	4.82	108.28	103.55
14	N	603[B]	HEA	CAA-CBA-CGA	-4.82	103.24	113.60
22	P	305	CHD	C15-C14-C8	4.82	125.06	118.33
20	A	610	PGV	C02-O01-C1	4.81	129.63	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C14-C8-C7	4.79	118.16	111.81
28	C	306	CDL	OA2-PA1-OA3	4.77	127.70	109.07
14	A	602[A]	HEA	CHA-C4D-C3D	-4.74	117.88	124.84
20	A	610	PGV	C3-C2-C1	4.66	130.57	113.62
25	C	302	DMU	C10-C5-C7	-4.65	100.31	110.00
14	A	602[A]	HEA	C3A-C2A-C1A	-4.63	102.65	107.08
22	J	101	CHD	C17-C13-C14	-4.60	95.45	100.09
22	G	101	CHD	C11-C12-C13	4.59	115.95	111.24
14	A	602[A]	HEA	C13-C12-C11	-4.57	107.48	114.35
28	P	304	CDL	OB8-CB7-C71	4.56	126.22	111.91
25	P	309	DMU	O16-C6-C1	4.56	115.42	108.30
28	N	601	CDL	CB4-OB6-CB5	4.55	129.00	117.79
25	P	308	DMU	C10-O1-C9	-4.50	104.86	113.69
14	A	602[B]	HEA	C13-C12-C11	-4.49	107.60	114.35
22	P	301	CHD	C21-C20-C22	-4.48	103.34	110.36
25	C	310	DMU	C10-C5-C7	-4.47	100.69	110.00
19	Q	201	TGL	CG2-OG2-CB1	-4.46	106.80	117.79
22	C	301	CHD	C5-C4-C3	-4.46	106.20	112.76
22	C	301	CHD	C1-C2-C3	-4.45	104.76	110.47
19	Q	201	TGL	OG2-CB1-OB1	4.40	134.33	123.70
19	D	201	TGL	OG1-CA1-CA2	4.39	125.69	111.91
19	A	608	TGL	CG3-OG3-CC1	4.39	133.37	117.12
20	C	309	PGV	C02-O01-C1	4.37	128.54	117.79
25	L	102	DMU	O5-C4-C3	4.36	118.95	109.75
22	C	307	CHD	C5-C6-C7	4.36	119.28	114.46
22	W	101	CHD	C6-C5-C4	-4.35	106.18	111.19
22	J	101	CHD	C16-C17-C13	4.34	107.81	103.55
22	C	307	CHD	C15-C14-C8	4.33	124.39	118.33
19	L	101	TGL	OC1-CC1-CC2	-4.33	106.84	123.73
19	Y	101	TGL	OG3-CG3-CG2	4.31	120.98	108.43
14	A	602[B]	HEA	CMB-C2B-C3B	-4.31	122.13	130.34
22	P	305	CHD	C19-C10-C9	-4.29	105.27	111.18
22	W	101	CHD	C9-C11-C12	4.29	119.97	114.30
14	N	602	HEA	C25-C23-C24	-4.29	105.13	114.60
27	G	102	PEK	O03-C21-C22	4.29	125.36	111.91
22	P	301	CHD	C23-C22-C20	-4.27	106.72	114.52
25	M	101	DMU	C18-O16-C6	-4.24	106.80	113.84
14	N	603[A]	HEA	C26-C15-C16	4.24	122.41	115.27
25	P	308	DMU	O49-C1-C2	-4.24	100.55	110.35
14	N	602	HEA	C12-C13-C14	4.22	123.38	112.23
27	C	304	PEK	C24-C23-C22	-4.21	98.04	113.19
28	N	601	CDL	CB6-OB8-CB7	4.20	132.68	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	102	PEK	O03-C21-C22	4.20	125.08	111.91
20	A	610	PGV	O01-C1-O02	4.19	133.82	123.70
27	T	102	PEK	O02-C1-C2	4.18	140.05	123.73
22	C	307	CHD	C17-C13-C12	-4.17	113.86	117.67
22	J	101	CHD	C17-C13-C12	4.15	121.46	117.67
22	J	101	CHD	C21-C20-C22	4.13	116.83	110.36
19	N	610	TGL	OG1-CA1-CA2	4.12	124.85	111.91
14	A	601	HEA	C2B-C1B-NB	4.10	114.79	109.88
22	J	101	CHD	C16-C15-C14	-4.09	97.02	105.13
22	P	301	CHD	C9-C11-C12	-4.08	108.91	114.30
14	N	603[B]	HEA	CHB-C4A-NA	4.07	128.85	124.44
14	A	601	HEA	C4A-NA-C1A	-4.04	101.39	105.35
19	Y	101	TGL	OG3-CC1-CC2	4.03	124.56	111.91
22	C	307	CHD	C4-C5-C10	4.02	116.92	112.66
14	N	603[B]	HEA	OMA-CMA-C3A	-4.02	116.60	125.69
22	C	307	CHD	C14-C13-C12	4.01	111.14	107.40
22	J	101	CHD	C14-C13-C12	4.01	111.14	107.40
14	N	602	HEA	C2D-C1D-ND	4.00	114.58	109.84
14	A	601	HEA	C1D-ND-C4D	-3.99	100.95	105.07
19	Y	101	TGL	OG2-CB1-OB1	-3.98	114.09	123.70
19	L	101	TGL	CG3-OG3-CC1	3.97	131.84	117.12
20	N	609	PGV	O03-C19-O04	-3.96	113.59	123.59
25	L	102	DMU	O3-C5-C10	3.92	119.58	110.05
22	B	301	CHD	C19-C10-C1	-3.92	101.95	108.26
25	Z	102	DMU	C6-O5-C4	3.92	121.37	113.69
27	C	308	PEK	O03-C21-C22	3.91	124.19	111.91
14	N	602	HEA	C27-C19-C20	3.90	121.83	115.27
14	N	602	HEA	C2B-C1B-NB	3.88	114.53	109.88
19	D	201	TGL	CG1-OG1-CA1	3.88	131.48	117.12
20	A	610	PGV	C4-C3-C2	-3.87	99.26	113.19
22	P	305	CHD	C17-C13-C12	-3.86	114.14	117.67
20	C	309	PGV	C01-O03-C19	3.85	131.39	117.12
14	N	603[B]	HEA	C3D-C4D-ND	3.85	114.09	110.36
24	B	303	PSC	O03-C19-C20	3.85	123.98	111.91
25	C	302	DMU	O2-C8-C7	-3.83	101.49	110.35
14	A	602[B]	HEA	C26-C15-C16	3.82	121.70	115.27
14	N	602	HEA	C1D-ND-C4D	-3.82	101.13	105.07
14	N	603[A]	HEA	CAA-CBA-CGA	-3.82	105.39	113.60
28	C	306	CDL	PA1-OA2-CA2	3.81	143.99	121.68
28	T	103	CDL	OB6-CB4-CB3	3.79	122.12	108.40
14	A	602[B]	HEA	CBA-CAA-C2A	-3.78	102.11	112.63
22	W	101	CHD	C22-C20-C17	3.78	118.09	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	102	PEK	O01-C1-O02	-3.78	114.57	123.70
19	L	101	TGL	OG2-CG2-CG3	3.76	122.02	108.40
22	C	301	CHD	C16-C17-C13	-3.75	99.87	103.55
14	A	602[B]	HEA	CAD-C3D-C2D	3.74	134.84	127.88
19	A	608	TGL	OG2-CB1-OB1	-3.74	114.67	123.70
14	N	603[B]	HEA	C13-C12-C11	-3.73	108.74	114.35
19	N	610	TGL	OG3-CC1-OC1	-3.73	114.17	123.59
20	A	610	PGV	O03-C19-C20	3.72	123.60	111.91
22	P	301	CHD	C10-C9-C8	-3.72	107.82	111.82
14	N	603[B]	HEA	CMB-C2B-C1B	3.72	130.70	125.04
22	C	307	CHD	C13-C17-C20	-3.71	115.06	119.50
14	A	601	HEA	C17-C18-C19	-3.71	118.73	127.66
22	P	305	CHD	C11-C9-C8	3.71	116.30	110.88
22	J	101	CHD	C10-C9-C8	3.70	115.79	111.82
14	N	602	HEA	C1B-C2B-C3B	-3.69	102.39	106.80
14	N	603[B]	HEA	CMB-C2B-C3B	-3.68	123.33	130.34
20	G	103	PGV	O04-C19-C20	-3.67	109.40	123.73
14	N	602	HEA	C3D-C4D-ND	3.66	113.90	110.36
19	Q	201	TGL	OG1-CA1-CA2	3.65	123.36	111.91
22	P	305	CHD	O7-C7-C6	-3.65	100.89	109.94
14	N	602	HEA	CAA-CBA-CGA	-3.64	105.77	113.60
28	N	601	CDL	OA6-CA5-C11	3.64	119.35	111.50
14	N	603[A]	HEA	CHD-C4C-NC	3.64	130.54	123.85
19	L	101	TGL	OB1-CB1-CB2	-3.62	109.59	123.73
20	N	609	PGV	O03-C19-C20	3.61	123.25	111.91
14	N	603[A]	HEA	C3A-C2A-C1A	-3.61	103.63	107.08
19	A	608	TGL	CG3-CG2-CG1	-3.60	103.27	111.79
14	A	602[A]	HEA	CAD-CBD-CGD	-3.59	105.88	113.60
14	A	602[A]	HEA	C12-C13-C14	-3.59	102.77	112.23
19	L	101	TGL	OG3-CC1-OC1	3.56	132.59	123.59
28	P	304	CDL	PA1-OA2-CA2	3.56	142.57	121.68
28	T	103	CDL	OA8-CA7-C31	3.56	123.07	111.91
28	N	601	CDL	OA8-CA7-C31	3.56	123.07	111.91
19	Y	101	TGL	CA4-CA3-CA2	-3.55	100.42	113.19
14	A	601	HEA	OMA-CMA-C3A	-3.55	117.66	125.69
22	P	305	CHD	C21-C20-C17	3.55	118.35	112.92
20	C	305	PGV	C30-C29-C28	-3.54	96.45	114.42
19	D	201	TGL	CC3-CC2-CC1	-3.54	100.75	113.62
22	C	301	CHD	C11-C9-C10	-3.53	110.08	113.73
20	C	305	PGV	O03-C19-O04	-3.52	114.70	123.59
14	N	602	HEA	OMA-CMA-C3A	-3.52	117.72	125.69
22	G	101	CHD	C1-C2-C3	-3.52	105.95	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C6-C5-C10	3.52	116.39	112.66
28	P	304	CDL	OA8-CA7-C31	3.51	122.92	111.91
19	N	610	TGL	OG2-CB1-OB1	-3.49	115.27	123.70
25	C	310	DMU	C7-C8-C9	3.49	116.46	110.24
25	L	102	DMU	O16-C6-C1	-3.49	102.86	108.30
20	C	309	PGV	O01-C1-C2	3.48	119.01	111.50
25	C	311	DMU	C18-O16-C6	3.48	119.60	113.84
27	P	307	PEK	O03-C21-O04	-3.47	114.84	123.59
14	A	602[A]	HEA	C3C-C2C-C1C	-3.46	102.98	107.16
22	J	101	CHD	C5-C4-C3	3.45	117.83	112.76
28	C	306	CDL	PB2-OB2-CB2	3.44	141.85	121.68
20	P	303	PGV	O01-C1-O02	-3.43	115.41	123.70
14	A	602[B]	HEA	CMB-C2B-C1B	3.43	130.26	125.04
19	D	201	TGL	CG3-OG3-CC1	3.42	129.78	117.12
22	P	301	CHD	C1-C10-C5	3.41	112.81	107.77
19	Q	201	TGL	OG3-CC1-OC1	-3.40	115.00	123.59
14	N	602	HEA	C4C-NC-C1C	-3.40	102.02	105.35
14	N	603[A]	HEA	C4C-CHD-C1D	-3.39	118.30	126.34
14	A	602[A]	HEA	C2A-C1A-NA	3.38	113.61	110.32
22	P	305	CHD	C5-C4-C3	-3.37	107.81	112.76
28	P	304	CDL	OA8-CA6-CA4	3.36	118.23	108.43
27	C	308	PEK	O03-C21-O04	-3.36	115.12	123.59
28	C	306	CDL	O1-C1-CA2	-3.35	97.79	109.56
22	C	301	CHD	O3-C3-C2	-3.35	101.64	110.16
27	T	101	PEK	O03-C21-C22	3.35	122.41	111.91
22	C	301	CHD	C5-C6-C7	3.34	118.15	114.46
22	W	101	CHD	C4-C5-C10	3.34	116.20	112.66
27	C	308	PEK	O01-C1-O02	-3.34	115.64	123.70
25	M	101	DMU	C22-C19-C18	-3.33	98.72	113.49
22	W	101	CHD	C1-C10-C5	3.32	112.68	107.77
14	A	602[A]	HEA	C4C-CHD-C1D	-3.32	118.46	126.34
22	P	301	CHD	C9-C8-C7	3.32	115.84	111.88
22	W	101	CHD	C11-C9-C10	3.30	117.13	113.73
22	P	305	CHD	C15-C14-C13	3.30	106.79	103.55
19	L	101	TGL	OG1-CA1-CA2	3.29	122.25	111.91
28	P	304	CDL	C54-C53-C52	-3.29	97.74	114.42
25	P	308	DMU	O3-C5-C10	3.28	118.02	110.05
14	A	601	HEA	CHA-C4D-C3D	-3.28	120.02	124.84
22	B	301	CHD	C18-C13-C12	-3.27	105.73	109.07
25	C	311	DMU	O16-C18-C19	3.27	121.02	109.56
20	Z	101	PGV	O01-C1-O02	-3.27	115.81	123.70
28	P	304	CDL	OA2-PA1-OA3	3.26	121.80	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	303	PGV	C22-C21-C20	-3.26	101.49	113.19
20	N	609	PGV	O01-C1-O02	-3.25	115.85	123.70
14	A	602[B]	HEA	C20-C19-C18	-3.24	114.56	121.12
28	T	103	CDL	OB6-CB5-OB7	-3.24	115.87	123.70
20	Z	101	PGV	O03-C19-C20	3.24	122.07	111.91
22	J	101	CHD	C9-C8-C7	3.24	115.75	111.88
19	L	101	TGL	C26-C25-C24	-3.24	98.00	114.42
14	N	602	HEA	CHA-C1A-NA	3.22	127.92	124.44
20	C	309	PGV	O04-C19-C20	-3.22	111.17	123.73
25	C	302	DMU	C7-C8-C9	3.22	115.98	110.24
25	L	102	DMU	O7-C10-C5	3.22	116.43	108.10
20	A	610	PGV	C03-C02-C01	-3.21	104.18	111.79
22	G	101	CHD	C16-C17-C20	-3.21	107.18	112.15
14	N	602	HEA	O2D-CGD-O1D	-3.21	115.30	123.30
27	T	102	PEK	O03-C21-O04	-3.21	115.50	123.59
14	A	601	HEA	C2C-C1C-NC	3.19	114.94	110.08
22	C	301	CHD	C22-C23-C24	-3.19	104.05	112.51
14	A	602[A]	HEA	CHD-C4C-NC	3.18	129.70	123.85
14	A	602[A]	HEA	CAD-C3D-C2D	3.18	133.80	127.88
14	N	602	HEA	C20-C21-C22	-3.17	101.47	111.88
25	L	102	DMU	C57-C4-C3	-3.16	104.12	113.33
22	W	101	CHD	C19-C10-C1	-3.16	103.16	108.26
20	A	609	PGV	O03-C19-C20	3.16	121.83	111.91
22	B	301	CHD	C1-C10-C9	3.16	116.31	111.35
20	G	103	PGV	C03-C02-C01	-3.15	104.33	111.79
22	C	301	CHD	C6-C7-C8	-3.14	108.12	111.48
28	N	601	CDL	OA8-CA7-OA9	-3.14	115.68	123.59
14	A	602[A]	HEA	C3C-C4C-NC	-3.13	108.32	110.25
28	C	306	CDL	CA6-OA8-CA7	3.12	128.69	117.12
14	N	602	HEA	C16-C15-C14	3.11	127.41	121.12
22	C	301	CHD	C21-C20-C17	-3.10	108.17	112.92
14	A	602[A]	HEA	CHA-C1A-C2A	-3.10	119.92	124.94
14	N	602	HEA	CAD-CBD-CGD	-3.07	106.99	113.60
14	N	602	HEA	O2A-CGA-CBA	3.06	123.87	114.03
22	G	101	CHD	C23-C22-C20	-3.06	108.94	114.52
14	A	601	HEA	C2D-C1D-ND	3.05	113.46	109.84
22	W	101	CHD	C15-C14-C8	3.04	122.58	118.33
14	N	603[A]	HEA	CHC-C1C-NC	3.04	129.43	123.85
22	C	301	CHD	C2-C1-C10	3.03	117.98	112.78
25	P	306	DMU	O16-C18-C19	3.03	120.18	109.56
20	Z	101	PGV	C01-O03-C19	3.02	128.32	117.12
14	N	602	HEA	CMC-C2C-C1C	3.02	129.97	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602[B]	HEA	C17-C18-C19	-3.02	120.39	127.66
28	C	306	CDL	OB8-CB7-C71	3.02	121.38	111.91
14	A	602[A]	HEA	C4A-C3A-C2A	3.01	109.23	106.75
22	C	307	CHD	C14-C8-C9	-3.01	105.58	109.71
20	A	609	PGV	O01-C02-C01	-2.99	97.59	108.40
24	B	303	PSC	O03-C19-O04	-2.98	116.06	123.59
14	N	603[B]	HEA	C4D-C3D-C2D	-2.97	102.57	106.90
28	T	103	CDL	OB8-CB7-C71	2.96	121.21	111.91
22	C	307	CHD	C1-C10-C5	2.96	112.15	107.77
28	C	306	CDL	CB4-OB6-CB5	-2.96	110.50	117.79
27	C	308	PEK	C01-O03-C21	2.96	128.07	117.12
22	J	101	CHD	C1-C2-C3	2.95	114.26	110.47
21	H	101	EDO	O1-C1-C2	-2.95	90.72	111.91
20	Z	101	PGV	C4-C3-C2	2.94	123.78	113.19
22	P	305	CHD	C6-C5-C4	-2.94	107.80	111.19
22	J	101	CHD	C18-C13-C14	2.94	115.82	111.21
14	A	602[A]	HEA	CMB-C2B-C1B	2.94	129.52	125.04
28	C	306	CDL	C73-C72-C71	-2.94	102.62	113.19
19	A	608	TGL	OB1-CB1-CB2	-2.94	112.28	123.73
22	P	305	CHD	C6-C5-C10	2.93	115.77	112.66
22	C	307	CHD	O26-C24-O25	2.93	130.61	123.30
27	T	101	PEK	O01-C1-O02	-2.93	116.62	123.70
22	C	307	CHD	O7-C7-C6	-2.92	102.69	109.94
22	G	101	CHD	C5-C4-C3	-2.92	108.47	112.76
28	T	103	CDL	C83-C82-C81	2.92	129.24	114.42
19	Q	201	TGL	OG3-CC1-CC2	2.92	121.06	111.91
28	C	306	CDL	CB2-C1-CA2	2.91	121.36	112.79
28	P	304	CDL	OB8-CB7-OB9	-2.90	116.28	123.59
22	P	301	CHD	C14-C13-C12	2.89	110.09	107.40
25	L	102	DMU	O5-C6-O16	2.88	116.81	109.97
20	A	610	PGV	C01-O03-C19	2.88	127.78	117.12
25	C	311	DMU	O5-C6-O16	2.87	116.77	109.97
22	B	301	CHD	C22-C20-C17	2.87	116.21	110.28
19	L	101	TGL	CB6-CB5-CB4	-2.86	99.91	114.42
22	B	301	CHD	O12-C12-C13	-2.86	106.20	111.03
14	N	603[A]	HEA	C12-C13-C14	-2.85	104.69	112.23
25	C	310	DMU	O55-C2-C1	2.85	116.94	110.35
22	W	101	CHD	C6-C7-C8	2.85	114.53	111.48
14	N	602	HEA	C1D-C2D-C3D	-2.85	103.96	106.96
27	G	102	PEK	O03-C21-O04	-2.84	116.41	123.59
22	G	101	CHD	C11-C9-C8	2.84	115.04	110.88
14	A	602[B]	HEA	CAD-C3D-C4D	-2.84	119.69	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602[A]	HEA	CAD-C3D-C4D	-2.83	119.71	124.66
25	C	311	DMU	O3-C5-C7	2.83	116.89	110.35
14	N	603[B]	HEA	CHC-C1C-C2C	-2.83	119.25	127.24
22	P	301	CHD	C19-C10-C1	-2.82	103.72	108.26
27	G	102	PEK	O03-C01-C02	2.82	116.64	108.43
19	Q	201	TGL	OG1-CA1-OA1	-2.82	116.48	123.59
25	P	308	DMU	O7-C3-C4	-2.81	101.75	109.45
22	W	101	CHD	C19-C10-C5	-2.80	105.61	110.36
14	A	601	HEA	C4D-C3D-C2D	-2.79	102.83	106.90
25	P	308	DMU	C10-C5-C7	-2.79	104.19	110.00
20	A	609	PGV	O03-C19-O04	-2.79	116.56	123.59
28	C	306	CDL	C39-C38-C37	2.78	128.56	114.42
14	N	603[B]	HEA	C3C-C4C-NC	2.78	111.96	110.25
14	N	603[A]	HEA	O2A-CGA-CBA	2.78	122.95	114.03
28	N	601	CDL	C80-C79-C78	2.77	128.51	114.42
27	T	102	PEK	C24-C23-C22	-2.77	103.23	113.19
14	A	601	HEA	O2A-CGA-CBA	2.77	122.93	114.03
22	B	301	CHD	C23-C22-C20	-2.77	109.46	114.52
28	T	103	CDL	CB6-OB8-CB7	2.77	127.37	117.12
28	P	304	CDL	OA6-CA5-OA7	-2.77	117.01	123.70
25	C	302	DMU	C10-O1-C9	2.76	119.11	113.69
22	B	301	CHD	C11-C9-C10	-2.76	110.88	113.73
22	P	305	CHD	C1-C10-C9	2.76	115.70	111.35
28	T	103	CDL	C23-C22-C21	2.76	128.44	114.42
22	C	301	CHD	C9-C11-C12	-2.75	110.66	114.30
14	A	601	HEA	CBD-CAD-C3D	-2.75	104.99	112.63
19	L	101	TGL	C25-C24-C23	-2.74	100.50	114.42
20	C	305	PGV	C21-C20-C19	-2.74	103.65	113.62
22	C	307	CHD	C11-C9-C10	-2.74	110.91	113.73
14	A	601	HEA	CHB-C4A-NA	-2.73	121.48	124.44
25	C	302	DMU	C18-O16-C6	-2.73	109.31	113.84
25	P	308	DMU	O4-C7-C8	2.73	116.66	110.35
25	P	308	DMU	O5-C6-O16	-2.73	103.51	109.97
22	W	101	CHD	C2-C1-C10	2.73	117.45	112.78
25	C	310	DMU	O5-C4-C57	2.72	113.21	106.44
14	N	603[A]	HEA	C17-C18-C19	2.72	134.22	127.66
28	P	304	CDL	CB4-OB6-CB5	-2.72	111.09	117.79
14	N	602	HEA	C2C-C1C-NC	2.71	114.21	110.08
28	N	601	CDL	OB7-CB5-C51	-2.71	113.15	123.73
28	C	306	CDL	OA4-PA1-OA2	-2.71	95.17	107.75
14	A	602[A]	HEA	CMB-C2B-C3B	-2.70	125.19	130.34
28	P	304	CDL	OB2-PB2-OB3	2.69	119.60	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	O	302	PSC	O01-C1-O02	-2.69	117.20	123.70
22	B	301	CHD	C2-C1-C10	-2.69	108.17	112.78
19	L	101	TGL	OG3-CC1-CC2	2.69	120.33	111.91
22	J	101	CHD	C9-C10-C5	2.68	112.35	108.58
22	C	301	CHD	C21-C20-C22	-2.68	106.16	110.36
28	T	103	CDL	OB8-CB6-CB4	2.68	116.23	108.43
14	N	603[A]	HEA	C3D-C4D-ND	2.67	112.94	110.36
20	N	609	PGV	O12-P-O13	2.67	119.49	109.07
28	C	306	CDL	OA8-CA7-C31	2.67	120.28	111.91
22	G	101	CHD	C19-C10-C1	-2.66	103.97	108.26
19	D	201	TGL	OG1-CA1-OA1	-2.66	116.88	123.59
25	Z	102	DMU	O49-C1-C2	-2.65	104.21	110.35
27	T	101	PEK	C01-O03-C21	2.65	126.95	117.12
22	B	301	CHD	C22-C23-C24	-2.65	105.47	112.51
14	A	601	HEA	O2D-CGD-O1D	-2.65	116.69	123.30
22	P	305	CHD	O3-C3-C4	-2.65	104.57	109.85
27	C	304	PEK	C2-C3-C4	-2.64	108.52	113.23
20	P	303	PGV	C27-C26-C25	-2.64	101.04	114.42
25	C	302	DMU	C57-C4-C3	2.63	120.99	113.33
22	P	305	CHD	C16-C17-C13	2.63	106.14	103.55
27	T	101	PEK	C02-O01-C1	2.63	124.27	117.79
14	N	602	HEA	CHD-C1D-C2D	-2.63	119.42	126.73
14	N	603[B]	HEA	CHC-C1C-NC	2.63	128.69	123.85
22	C	301	CHD	C16-C17-C20	-2.63	108.08	112.15
14	A	601	HEA	C2A-C1A-NA	2.62	112.88	110.32
22	G	101	CHD	C21-C20-C17	-2.62	108.91	112.92
19	N	610	TGL	CG3-OG3-CC1	2.62	126.83	117.12
28	T	103	CDL	C80-C79-C78	2.62	127.72	114.42
14	A	601	HEA	C20-C21-C22	-2.61	103.29	111.88
22	P	305	CHD	C19-C10-C1	-2.61	104.05	108.26
14	N	603[A]	HEA	CHC-C1C-C2C	-2.61	119.86	127.24
14	N	603[B]	HEA	C27-C19-C20	2.61	119.66	115.27
22	C	301	CHD	C15-C14-C8	-2.61	114.69	118.33
28	C	306	CDL	C13-C12-C11	-2.59	103.87	113.19
22	P	305	CHD	O26-C24-O25	2.58	129.73	123.30
28	N	601	CDL	C62-C61-C60	2.58	127.51	114.42
14	A	602[A]	HEA	C3B-C4B-NB	2.57	112.89	109.84
19	N	610	TGL	OG1-CA1-OA1	-2.57	117.10	123.59
14	N	603[A]	HEA	CHA-C4D-C3D	-2.57	121.06	124.84
28	C	306	CDL	C42-C41-C40	2.57	127.47	114.42
14	N	603[A]	HEA	C20-C21-C22	-2.56	103.47	111.88
27	C	308	PEK	P-O12-C04	-2.56	109.00	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	302	DMU	O55-C2-C3	2.55	116.71	109.94
14	N	602	HEA	CHB-C1B-C2B	-2.55	121.00	124.98
14	A	602[A]	HEA	C26-C15-C16	2.54	119.54	115.27
14	N	603[A]	HEA	C3C-C4C-NC	-2.54	108.69	110.25
14	A	601	HEA	CAD-C3D-C4D	2.54	129.09	124.66
14	N	603[A]	HEA	C1B-C2B-C3B	-2.54	103.77	106.80
14	A	601	HEA	C4A-C3A-C2A	-2.53	104.67	106.75
28	T	103	CDL	OB7-CB5-C51	-2.53	113.88	123.73
22	B	301	CHD	O26-C24-O25	-2.53	117.00	123.30
19	Y	101	TGL	C26-C25-C24	-2.52	101.65	114.42
27	C	304	PEK	O03-C21-O04	-2.51	117.26	123.59
19	Y	101	TGL	C20-CA9-CA8	-2.51	101.70	114.42
27	C	304	PEK	O11-P-O14	-2.51	99.28	109.07
20	G	103	PGV	C21-C20-C19	-2.50	104.51	113.62
14	N	603[A]	HEA	CBA-CAA-C2A	-2.50	105.67	112.63
22	C	301	CHD	C15-C16-C17	2.50	110.09	105.13
27	C	308	PEK	O01-C02-C01	2.50	117.45	108.40
28	N	601	CDL	O1-C1-CA2	-2.50	100.81	109.56
25	M	101	DMU	C10-O1-C9	2.49	118.58	113.69
25	Z	102	DMU	O4-C7-C5	-2.49	104.58	110.35
25	Z	102	DMU	C10-O7-C3	-2.49	111.80	117.96
14	A	601	HEA	CHC-C4B-NB	-2.49	121.30	124.37
28	T	103	CDL	CB4-OB6-CB5	2.48	123.91	117.79
14	A	602[B]	HEA	C1D-C2D-C3D	-2.48	104.35	106.96
28	C	306	CDL	C76-C75-C74	-2.48	101.86	114.42
25	P	308	DMU	C7-C8-C9	2.47	114.65	110.24
20	A	609	PGV	C30-C29-C28	2.47	126.96	114.42
14	N	603[A]	HEA	CHC-C4B-NB	2.47	127.42	124.37
22	B	301	CHD	O3-C3-C4	-2.46	104.94	109.85
25	C	302	DMU	C25-C22-C19	-2.46	101.93	114.42
22	P	305	CHD	C19-C10-C5	2.46	114.54	110.36
21	P	310	EDO	O2-C2-C1	2.44	129.49	111.91
25	L	102	DMU	C1-C2-C3	2.44	115.26	109.68
25	M	101	DMU	C28-C25-C22	-2.44	102.03	114.42
22	P	301	CHD	O3-C3-C2	-2.44	103.95	110.16
22	C	307	CHD	C19-C10-C5	-2.44	106.22	110.36
20	G	103	PGV	O02-C1-C2	-2.44	114.21	123.73
22	W	101	CHD	O26-C24-C23	2.44	121.86	114.03
28	P	304	CDL	C83-C82-C81	2.44	126.79	114.42
22	B	301	CHD	C16-C17-C13	2.43	105.94	103.55
27	T	102	PEK	C02-O01-C1	2.43	123.78	117.79
19	A	608	TGL	OG1-CA1-CA2	2.43	119.54	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	601	CDL	C60-C59-C58	2.43	126.77	114.42
22	B	301	CHD	C13-C17-C20	-2.42	116.61	119.50
22	B	301	CHD	O26-C24-C23	2.42	121.80	114.03
27	C	304	PEK	O03-C01-C02	-2.42	101.40	108.43
19	N	610	TGL	OB1-CB1-CB2	-2.41	114.31	123.73
14	A	602[B]	HEA	CMD-C2D-C3D	2.41	132.66	126.12
19	A	608	TGL	CG1-OG1-CA1	2.41	126.03	117.12
20	C	305	PGV	O01-C1-O02	-2.40	117.89	123.70
14	N	603[B]	HEA	CHA-C4D-ND	-2.40	121.81	124.42
28	N	601	CDL	OB8-CB7-C71	2.40	119.44	111.91
28	P	304	CDL	C39-C38-C37	2.40	126.61	114.42
14	A	602[B]	HEA	CHA-C4D-C3D	-2.40	121.32	124.84
24	O	302	PSC	C29-C28-C27	-2.39	102.27	114.42
25	L	102	DMU	C8-C7-C5	-2.39	106.65	110.82
25	C	311	DMU	C8-C7-C5	-2.39	106.66	110.82
14	A	602[A]	HEA	C2B-C1B-NB	2.38	112.74	109.88
19	N	610	TGL	CG3-CG2-CG1	-2.38	106.15	111.79
28	T	103	CDL	C19-C18-C17	2.38	126.51	114.42
25	C	310	DMU	O7-C10-O1	2.38	117.32	110.67
14	A	602[A]	HEA	CAA-C2A-C1A	2.38	129.38	124.89
25	M	101	DMU	O49-C1-C6	-2.37	104.28	110.05
19	N	610	TGL	CB3-CB2-CB1	-2.37	105.00	113.62
19	Y	101	TGL	CB4-CB3-CB2	2.37	121.70	113.19
27	C	304	PEK	O01-C02-C01	-2.37	99.83	108.40
28	T	103	CDL	OA8-CA7-OA9	-2.37	117.62	123.59
19	L	101	TGL	C20-CA9-CA8	-2.36	102.42	114.42
28	P	304	CDL	C57-C56-C55	-2.36	102.42	114.42
27	P	307	PEK	C03-C02-C01	-2.36	106.20	111.79
22	P	305	CHD	C14-C8-C9	-2.36	106.47	109.71
14	N	602	HEA	O2D-CGD-CBD	2.36	121.61	114.03
22	J	101	CHD	C2-C1-C10	2.36	116.83	112.78
19	N	610	TGL	OG1-CG1-CG2	2.36	115.29	108.43
14	N	602	HEA	CBD-CAD-C3D	-2.35	106.08	112.63
28	T	103	CDL	C43-C42-C41	2.34	126.31	114.42
14	N	602	HEA	CMD-C2D-C1D	2.34	128.60	125.04
25	L	102	DMU	C2-C3-C4	2.34	116.28	110.93
14	A	602[A]	HEA	C4B-NB-C1B	-2.33	102.66	105.07
27	C	304	PEK	O04-C21-C22	2.33	132.83	123.73
28	P	304	CDL	C40-C39-C38	2.33	126.25	114.42
25	C	311	DMU	O5-C4-C3	2.33	114.66	109.75
14	N	603[A]	HEA	C1C-CHC-C4B	-2.33	120.82	126.34
22	B	301	CHD	O7-C7-C6	2.33	115.72	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	309	DMU	C1-C2-C3	2.32	114.97	109.68
14	A	601	HEA	C12-C13-C14	2.32	118.35	112.23
28	N	601	CDL	C23-C22-C21	2.32	126.18	114.42
27	P	307	PEK	O03-C21-C22	2.32	119.17	111.91
28	N	601	CDL	CA6-OA8-CA7	2.31	125.66	117.12
20	C	305	PGV	O01-C1-C2	2.31	116.47	111.50
28	P	304	CDL	C19-C18-C17	2.30	126.12	114.42
25	C	310	DMU	O4-C7-C5	-2.30	105.02	110.35
27	T	101	PEK	O03-C01-C02	2.30	115.13	108.43
14	N	602	HEA	CHC-C1C-C2C	-2.30	120.75	127.24
27	P	307	PEK	C35-C34-C33	2.30	126.08	114.42
28	N	601	CDL	OB8-CB7-OB9	-2.29	117.80	123.59
20	C	305	PGV	O14-P-O13	2.29	123.58	112.24
27	P	307	PEK	O01-C1-O02	-2.29	118.16	123.70
28	N	601	CDL	C72-C71-CB7	2.29	121.94	113.62
25	C	302	DMU	O1-C9-C8	2.28	113.84	109.69
24	B	303	PSC	O03-C01-C02	2.28	115.08	108.43
22	C	301	CHD	C19-C10-C9	-2.28	108.04	111.18
28	T	103	CDL	CB6-CB4-CB3	-2.27	106.42	111.79
14	A	601	HEA	C20-C19-C18	2.27	125.71	121.12
20	C	309	PGV	C21-C20-C19	-2.27	105.36	113.62
25	L	102	DMU	O1-C9-C11	2.27	112.08	106.44
19	L	101	TGL	CB5-CB4-CB3	2.27	125.94	114.42
20	P	303	PGV	O14-P-O13	2.27	123.45	112.24
22	B	301	CHD	C14-C8-C9	2.26	112.82	109.71
24	O	302	PSC	C28-C27-C26	-2.26	102.94	114.42
21	H	101	EDO	O2-C2-C1	-2.26	95.63	111.91
20	N	609	PGV	O02-C1-C2	2.26	132.54	123.73
22	C	307	CHD	C16-C17-C13	2.26	105.77	103.55
25	P	306	DMU	C8-C7-C5	2.25	114.76	110.82
14	A	602[B]	HEA	C3D-C4D-ND	2.24	112.53	110.36
22	C	307	CHD	C22-C20-C17	-2.23	105.68	110.28
24	B	303	PSC	C4-C3-C2	2.23	121.19	113.19
25	C	311	DMU	C10-C5-C7	2.23	114.63	110.00
22	C	301	CHD	C11-C12-C13	2.22	113.53	111.24
28	C	306	CDL	OA6-CA5-OA7	-2.22	118.33	123.70
28	N	601	CDL	C83-C82-C81	2.22	125.70	114.42
19	D	201	TGL	CB5-CB4-CB3	2.22	125.69	114.42
22	P	301	CHD	C14-C8-C7	-2.22	108.86	111.81
20	C	309	PGV	O01-C02-C01	2.22	116.43	108.40
14	A	602[A]	HEA	O2A-CGA-CBA	2.21	121.13	114.03
14	A	602[B]	HEA	O11-C11-C12	-2.21	103.24	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	306	CDL	OA6-CA4-CA6	2.20	116.38	108.40
28	N	601	CDL	C82-C81-C80	2.20	125.59	114.42
14	A	602[B]	HEA	C26-C15-C14	-2.20	118.04	123.68
14	A	601	HEA	CHC-C1C-C2C	-2.20	121.03	127.24
25	M	101	DMU	O2-C8-C7	-2.20	105.27	110.35
22	J	101	CHD	C19-C10-C5	-2.20	106.64	110.36
14	A	601	HEA	C27-C19-C18	-2.19	118.05	123.68
24	B	303	PSC	C01-O03-C19	2.19	125.23	117.12
20	A	609	PGV	C34-C33-C32	-2.19	96.81	113.42
28	N	601	CDL	C43-C42-C41	2.19	125.52	114.42
20	P	303	PGV	O03-C19-O04	-2.19	118.08	123.59
22	J	101	CHD	C6-C5-C4	-2.18	108.68	111.19
14	A	602[B]	HEA	CHD-C4C-NC	2.18	127.86	123.85
25	C	302	DMU	O1-C9-C11	2.18	111.86	106.44
19	L	101	TGL	CA4-CA3-CA2	-2.18	105.35	113.19
14	A	601	HEA	CAA-CBA-CGA	-2.18	108.92	113.60
14	A	601	HEA	O2D-CGD-CBD	2.18	121.02	114.03
14	N	602	HEA	C27-C19-C18	-2.18	118.10	123.68
28	P	304	CDL	OB8-CB6-CB4	2.17	114.76	108.43
14	N	603[B]	HEA	CHB-C4A-C3A	-2.17	121.55	125.26
28	T	103	CDL	CB2-C1-CA2	-2.17	106.41	112.79
28	P	304	CDL	C56-C55-C54	2.16	125.41	114.42
27	C	308	PEK	C02-O01-C1	2.16	123.12	117.79
14	N	603[A]	HEA	C2A-C1A-NA	2.16	112.43	110.32
25	P	308	DMU	O5-C4-C57	2.16	111.80	106.44
25	C	302	DMU	O4-C7-C8	2.16	115.33	110.35
14	A	602[B]	HEA	C4C-CHD-C1D	-2.16	121.23	126.34
21	S	103	EDO	O1-C1-C2	-2.15	96.40	111.91
14	N	602	HEA	C1C-CHC-C4B	-2.15	121.23	126.34
20	C	305	PGV	C4-C3-C2	-2.15	105.45	113.19
14	A	602[B]	HEA	O2D-CGD-CBD	2.15	120.94	114.03
28	T	103	CDL	C59-C58-C57	2.15	125.34	114.42
14	A	602[A]	HEA	C20-C19-C18	-2.15	116.77	121.12
25	P	308	DMU	C10-O7-C3	2.15	123.27	117.96
28	T	103	CDL	OB8-CB7-OB9	-2.15	118.18	123.59
20	C	309	PGV	O03-C01-C02	2.15	114.68	108.43
22	C	301	CHD	C16-C15-C14	-2.14	100.89	105.13
14	A	602[B]	HEA	OMA-CMA-C3A	-2.14	120.85	125.69
22	P	301	CHD	C2-C1-C10	-2.14	109.12	112.78
28	N	601	CDL	OA6-CA5-OA7	-2.14	118.54	123.70
27	C	308	PEK	O03-C01-C02	2.13	114.63	108.43
27	T	101	PEK	O03-C21-O04	-2.13	118.22	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603[A]	HEA	O11-C11-C12	2.13	115.36	109.42
28	T	103	CDL	C58-C57-C56	-2.13	103.63	114.42
27	C	304	PEK	C02-O01-C1	-2.12	112.57	117.79
20	Z	101	PGV	O01-C02-C01	2.12	116.07	108.40
22	J	101	CHD	C23-C22-C20	2.12	118.38	114.52
14	N	602	HEA	C4A-C3A-C2A	-2.11	105.02	106.75
28	T	103	CDL	C42-C41-C40	2.11	125.16	114.42
14	N	603[A]	HEA	C26-C15-C14	-2.11	118.26	123.68
19	L	101	TGL	C22-C21-C20	-2.11	103.70	114.42
20	Z	101	PGV	O03-C19-O04	-2.11	118.26	123.59
14	A	601	HEA	C4C-CHD-C1D	-2.11	121.34	126.34
28	T	103	CDL	C63-C62-C61	2.11	125.12	114.42
20	A	610	PGV	O02-C1-C2	-2.10	115.53	123.73
22	W	101	CHD	O12-C12-C13	2.10	114.58	111.03
14	N	603[B]	HEA	C20-C19-C18	-2.10	116.87	121.12
25	C	311	DMU	C10-O7-C3	-2.10	112.77	117.96
14	A	602[B]	HEA	CHB-C4A-C3A	-2.10	121.67	125.26
25	C	302	DMU	O3-C5-C10	2.10	115.14	110.05
19	D	201	TGL	OG3-CC1-OC1	-2.10	118.30	123.59
19	A	608	TGL	C33-C19-C18	2.10	125.06	114.42
20	P	303	PGV	C03-C02-C01	-2.09	106.83	111.79
28	C	306	CDL	C43-C42-C41	2.09	125.04	114.42
22	J	101	CHD	C1-C10-C5	2.09	110.85	107.77
25	P	309	DMU	C6-C1-C2	2.08	114.34	110.00
19	N	610	TGL	CC4-CC3-CC2	2.08	120.68	113.19
22	J	101	CHD	C4-C3-C2	2.08	113.04	110.55
22	P	301	CHD	C11-C9-C10	-2.08	111.58	113.73
14	N	602	HEA	C1A-CHA-C4D	-2.07	121.58	126.06
22	P	301	CHD	C5-C4-C3	-2.07	109.72	112.76
22	G	101	CHD	C21-C20-C22	2.07	113.61	110.36
28	T	103	CDL	C62-C61-C60	2.07	124.92	114.42
22	J	101	CHD	C4-C5-C10	2.06	114.85	112.66
19	D	201	TGL	OC1-CC1-CC2	2.06	131.78	123.73
19	Q	201	TGL	OB1-CB1-CB2	2.06	131.75	123.73
22	C	301	CHD	C18-C13-C12	2.06	111.16	109.07
14	A	602[B]	HEA	CAD-CBD-CGD	-2.06	109.18	113.60
25	Z	102	DMU	C18-O16-C6	-2.06	110.43	113.84
28	P	304	CDL	C23-C22-C21	2.05	124.84	114.42
14	N	603[B]	HEA	CBA-CAA-C2A	-2.05	106.94	112.63
25	C	302	DMU	O1-C10-C5	-2.05	106.02	110.35
28	T	103	CDL	C40-C39-C38	2.04	124.80	114.42
22	G	101	CHD	C13-C17-C20	-2.04	117.06	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C5-C6-C7	-2.04	112.21	114.46
22	P	301	CHD	C6-C5-C10	2.04	114.82	112.66
14	N	603[A]	HEA	C4A-C3A-C2A	2.04	108.42	106.75
25	C	302	DMU	O55-C2-C1	-2.04	105.64	110.35
20	P	303	PGV	O02-C1-C2	2.03	131.67	123.73
19	Y	101	TGL	CA7-CA6-CA5	-2.03	104.11	114.42
19	Y	101	TGL	CG3-OG3-CC1	2.02	124.59	117.12
28	C	306	CDL	C40-C39-C38	2.02	124.66	114.42
20	P	303	PGV	C3-C2-C1	-2.01	106.30	113.62
14	N	603[B]	HEA	C17-C18-C19	2.01	132.51	127.66
25	L	102	DMU	C6-C1-C2	2.01	114.18	110.00
22	C	307	CHD	C11-C9-C8	2.01	113.81	110.88
14	A	602[A]	HEA	C1A-CHA-C4D	-2.01	121.73	126.06
14	N	603[B]	HEA	C13-C14-C15	2.01	132.49	127.66
22	P	301	CHD	C5-C6-C7	2.00	116.67	114.46

There are no chirality outliers.

All (1025) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[A]	HEA	C2A-C3A-CMA-OMA
14	A	602[A]	HEA	C4A-C3A-CMA-OMA
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	603[A]	HEA	C2A-C3A-CMA-OMA
14	N	603[A]	HEA	C4A-C3A-CMA-OMA
14	N	603[B]	HEA	C2A-C3A-CMA-OMA
14	N	603[B]	HEA	C4D-C3D-CAD-CBD
19	D	201	TGL	CG2-CG1-OG1-CA1
19	L	101	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	OB1-CB1-OG2-CG2
19	L	101	TGL	CC2-CC1-OG3-CG3
19	L	101	TGL	OC1-CC1-OG3-CG3
19	Y	101	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	OB1-CB1-OG2-CG2
20	A	610	PGV	C03-O11-P-O13
20	A	610	PGV	C03-O11-P-O14
20	A	610	PGV	O01-C02-C03-O11
20	A	610	PGV	C04-C05-C06-O06
20	A	610	PGV	C2-C1-O01-C02
20	C	309	PGV	C03-O11-P-O13
20	C	309	PGV	C03-O11-P-O14
20	C	309	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
20	G	103	PGV	C03-O11-P-O14
20	G	103	PGV	C04-O12-P-O11
20	G	103	PGV	C04-O12-P-O13
20	G	103	PGV	C04-O12-P-O14
20	G	103	PGV	O03-C01-C02-O01
20	G	103	PGV	O12-C04-C05-C06
20	G	103	PGV	O12-C04-C05-O05
20	Z	101	PGV	O02-C1-O01-C02
20	Z	101	PGV	C2-C1-O01-C02
20	Z	101	PGV	C20-C19-O03-C01
20	Z	101	PGV	C10-C11-C12-C13
22	W	101	CHD	C13-C17-C20-C22
24	B	303	PSC	C03-O11-P-O13
24	B	303	PSC	C04-O12-P-O13
24	B	303	PSC	O12-C04-C05-N
24	B	303	PSC	O04-C19-O03-C01
24	B	303	PSC	C20-C19-O03-C01
24	O	302	PSC	C03-O11-P-O12
24	O	302	PSC	O12-C04-C05-N
24	O	302	PSC	C2-C1-O01-C02
24	O	302	PSC	O04-C19-O03-C01
24	O	302	PSC	C20-C19-O03-C01
25	C	302	DMU	C19-C18-O16-C6
25	C	311	DMU	C1-C6-O16-C18
25	C	311	DMU	O5-C6-O16-C18
25	C	311	DMU	C19-C18-O16-C6
25	P	306	DMU	C1-C6-O16-C18
25	P	306	DMU	O5-C6-O16-C18
25	P	309	DMU	O5-C6-O16-C18
27	C	304	PEK	C10-C11-C12-C13
27	C	308	PEK	C04-O12-P-O14
27	C	308	PEK	O12-C04-C05-N
27	C	308	PEK	O02-C1-O01-C02
27	C	308	PEK	C2-C1-O01-C02
27	C	308	PEK	C12-C13-C14-C15
27	C	308	PEK	C13-C14-C15-C16
27	G	102	PEK	C03-O11-P-O14
27	G	102	PEK	O12-C04-C05-N
27	G	102	PEK	O02-C1-O01-C02
27	G	102	PEK	C2-C1-O01-C02
27	P	307	PEK	C03-O11-P-O13
27	P	307	PEK	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
27	P	307	PEK	C04-O12-P-O14
27	P	307	PEK	C2-C1-O01-C02
27	P	307	PEK	C13-C14-C15-C16
27	T	101	PEK	O03-C01-C02-O01
27	T	101	PEK	C2-C1-O01-C02
27	T	101	PEK	C12-C13-C14-C15
27	T	102	PEK	C9-C10-C11-C12
28	C	306	CDL	CA3-OA5-PA1-OA2
28	C	306	CDL	OA7-CA5-OA6-CA4
28	C	306	CDL	C11-CA5-OA6-CA4
28	C	306	CDL	C1-CB2-OB2-PB2
28	N	601	CDL	CA2-OA2-PA1-OA3
28	N	601	CDL	CA3-OA5-PA1-OA3
28	N	601	CDL	C11-CA5-OA6-CA4
28	N	601	CDL	CB2-OB2-PB2-OB3
28	N	601	CDL	CB3-OB5-PB2-OB4
28	N	601	CDL	OB6-CB4-CB6-OB8
28	P	304	CDL	CB2-OB2-PB2-OB3
28	P	304	CDL	CB2-OB2-PB2-OB4
28	P	304	CDL	CB2-OB2-PB2-OB5
28	P	304	CDL	CB3-OB5-PB2-OB3
28	P	304	CDL	CB3-OB5-PB2-OB4
28	T	103	CDL	O1-C1-CA2-OA2
28	T	103	CDL	CA2-OA2-PA1-OA3
28	T	103	CDL	CA3-OA5-PA1-OA3
28	T	103	CDL	CA3-OA5-PA1-OA4
28	T	103	CDL	C1-CB2-OB2-PB2
25	C	310	DMU	C5-C10-O7-C3
25	L	102	DMU	C2-C3-O7-C10
20	Z	101	PGV	O04-C19-O03-C01
28	T	103	CDL	OA9-CA7-OA8-CA6
25	P	308	DMU	C5-C10-O7-C3
28	T	103	CDL	C31-CA7-OA8-CA6
19	A	608	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	OA1-CA1-OG1-CG1
19	D	201	TGL	OC1-CC1-OG3-CG3
19	Q	201	TGL	OC1-CC1-OG3-CG3
28	N	601	CDL	OA9-CA7-OA8-CA6
22	W	101	CHD	C13-C17-C20-C21
20	A	610	PGV	O02-C1-O01-C02
24	O	302	PSC	O02-C1-O01-C02
27	P	307	PEK	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
27	T	101	PEK	O02-C1-O01-C02
28	C	306	CDL	OB7-CB5-OB6-CB4
28	N	601	CDL	OA7-CA5-OA6-CA4
28	P	304	CDL	OB7-CB5-OB6-CB4
19	A	608	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	CA2-CA1-OG1-CG1
19	Q	201	TGL	CC2-CC1-OG3-CG3
22	W	101	CHD	C16-C17-C20-C21
14	A	602[B]	HEA	C2D-C3D-CAD-CBD
14	N	603[B]	HEA	C2D-C3D-CAD-CBD
25	L	102	DMU	O6-C11-C9-O1
28	T	103	CDL	C42-C43-C44-C45
19	D	201	TGL	CC2-CC1-OG3-CG3
27	G	102	PEK	C22-C21-O03-C01
28	N	601	CDL	C31-CA7-OA8-CA6
25	L	102	DMU	O6-C11-C9-C8
24	O	302	PSC	C11-C12-C13-C14
27	C	304	PEK	C13-C14-C15-C16
27	C	308	PEK	C4-C5-C6-C7
27	T	102	PEK	C4-C5-C6-C7
27	T	102	PEK	C10-C11-C12-C13
28	C	306	CDL	C76-C77-C78-C79
27	G	102	PEK	O04-C21-O03-C01
28	T	103	CDL	C79-C80-C81-C82
19	A	608	TGL	C21-C20-CA9-CA8
20	A	610	PGV	C20-C21-C22-C23
19	Y	101	TGL	CA2-CA1-OG1-CG1
27	T	101	PEK	C22-C21-O03-C01
28	C	306	CDL	C51-CB5-OB6-CB4
28	P	304	CDL	C51-CB5-OB6-CB4
28	T	103	CDL	C11-CA5-OA6-CA4
25	L	102	DMU	C3-C4-C57-O61
19	Y	101	TGL	OA1-CA1-OG1-CG1
19	D	201	TGL	C21-C22-C23-C24
19	L	101	TGL	CA9-C20-C21-C22
24	B	303	PSC	C21-C22-C23-C24
24	O	302	PSC	C29-C30-C31-C32
25	C	302	DMU	C25-C28-C31-C34
25	L	102	DMU	O5-C4-C57-O61
22	W	101	CHD	C16-C17-C20-C22
28	N	601	CDL	C81-C82-C83-C84
19	N	610	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	OB1-CB1-OG2-CG2
28	T	103	CDL	OA7-CA5-OA6-CA4
28	T	103	CDL	C60-C61-C62-C63
27	T	101	PEK	O04-C21-O03-C01
14	A	601	HEA	C15-C16-C17-C18
28	P	304	CDL	C81-C82-C83-C84
20	A	610	PGV	C20-C19-O03-C01
19	N	610	TGL	OC1-CC1-OG3-CG3
19	N	610	TGL	CB2-CB1-OG2-CG2
24	O	302	PSC	C20-C21-C22-C23
28	C	306	CDL	CB2-C1-CA2-OA2
28	P	304	CDL	CB2-C1-CA2-OA2
28	P	304	CDL	CA2-C1-CB2-OB2
22	P	305	CHD	C21-C20-C22-C23
19	A	608	TGL	CA2-CA1-OG1-CG1
19	N	610	TGL	CA2-CA1-OG1-CG1
28	T	103	CDL	C23-C24-C25-C26
22	C	307	CHD	C17-C20-C22-C23
28	C	306	CDL	O1-C1-CA2-OA2
28	P	304	CDL	O1-C1-CB2-OB2
28	T	103	CDL	O1-C1-CB2-OB2
19	A	608	TGL	CA1-CA2-CA3-CA4
19	N	610	TGL	CC1-CC2-CC3-CC4
25	P	309	DMU	C1-C6-O16-C18
27	P	307	PEK	O03-C01-C02-O01
28	T	103	CDL	OB6-CB4-CB6-OB8
19	N	610	TGL	OB1-CB1-OG2-CG2
28	N	601	CDL	CA5-C11-C12-C13
19	A	608	TGL	OA1-CA1-OG1-CG1
24	O	302	PSC	C22-C23-C24-C25
22	C	307	CHD	C21-C20-C22-C23
19	Y	101	TGL	C20-C21-C22-C23
24	O	302	PSC	C11-C10-C9-C8
27	T	101	PEK	C13-C14-C15-C16
20	A	609	PGV	C26-C27-C28-C29
19	A	608	TGL	CB1-CB2-CB3-CB4
19	D	201	TGL	CA1-CA2-CA3-CA4
19	D	201	TGL	CB1-CB2-CB3-CB4
19	N	610	TGL	CA1-CA2-CA3-CA4
20	C	309	PGV	C1-C2-C3-C4
20	Z	101	PGV	C19-C20-C21-C22
27	P	307	PEK	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
27	T	101	PEK	C21-C22-C23-C24
27	T	102	PEK	C1-C2-C3-C4
28	C	306	CDL	CA7-C31-C32-C33
28	C	306	CDL	CB5-C51-C52-C53
25	P	309	DMU	O16-C18-C19-C22
28	C	306	CDL	CB4-CB6-OB8-CB7
19	A	608	TGL	C24-C25-C26-C27
28	T	103	CDL	CA7-C31-C32-C33
28	T	103	CDL	CB5-C51-C52-C53
21	C	318	EDO	O1-C1-C2-O2
21	H	102	EDO	O1-C1-C2-O2
21	J	102	EDO	O1-C1-C2-O2
21	N	613	EDO	O1-C1-C2-O2
19	N	610	TGL	OA1-CA1-OG1-CG1
20	A	610	PGV	O04-C19-O03-C01
19	Y	101	TGL	CC1-CC2-CC3-CC4
28	C	306	CDL	O1-C1-CB2-OB2
28	P	304	CDL	O1-C1-CA2-OA2
28	P	304	CDL	CB4-CB6-OB8-CB7
25	L	102	DMU	O16-C18-C19-C22
20	P	303	PGV	C10-C11-C12-C13
27	C	308	PEK	C7-C8-C9-C10
27	P	307	PEK	C4-C5-C6-C7
27	T	102	PEK	C13-C14-C15-C16
19	A	608	TGL	CB2-CB1-OG2-CG2
25	Z	102	DMU	O16-C18-C19-C22
20	A	610	PGV	C03-O11-P-O12
20	C	309	PGV	C03-O11-P-O12
20	G	103	PGV	C03-O11-P-O12
20	Z	101	PGV	C03-O11-P-O12
20	Z	101	PGV	C04-O12-P-O11
24	B	303	PSC	C03-O11-P-O12
24	B	303	PSC	C04-O12-P-O11
27	C	308	PEK	C03-O11-P-O12
27	C	308	PEK	C04-O12-P-O11
27	G	102	PEK	C04-O12-P-O11
27	P	307	PEK	C03-O11-P-O12
27	T	101	PEK	C03-O11-P-O12
27	T	101	PEK	C04-O12-P-O11
28	C	306	CDL	CB2-OB2-PB2-OB5
28	C	306	CDL	CB3-OB5-PB2-OB2
28	N	601	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
28	P	304	CDL	CB3-OB5-PB2-OB2
28	T	103	CDL	CA3-OA5-PA1-OA2
28	T	103	CDL	CB2-OB2-PB2-OB5
19	L	101	TGL	CA2-CA1-OG1-CG1
25	P	308	DMU	O6-C11-C9-O1
19	L	101	TGL	CC2-CC3-CC4-CC5
19	Y	101	TGL	CA2-CA3-CA4-CA5
20	Z	101	PGV	C24-C25-C26-C27
27	G	102	PEK	C29-C30-C31-C32
28	T	103	CDL	C34-C35-C36-C37
24	B	303	PSC	C2-C1-O01-C02
19	D	201	TGL	C17-C18-C19-C33
19	D	201	TGL	C18-C19-C33-C34
19	L	101	TGL	CA3-CA4-CA5-CA6
19	N	610	TGL	CB7-CB8-CB9-C10
19	Q	201	TGL	CC9-C15-C16-C17
19	Q	201	TGL	C19-C33-C34-C35
19	Y	101	TGL	CA3-CA4-CA5-CA6
19	Y	101	TGL	CB6-CB7-CB8-CB9
20	A	610	PGV	C14-C15-C16-C17
20	C	309	PGV	C13-C14-C15-C16
24	B	303	PSC	C20-C21-C22-C23
27	T	102	PEK	C26-C27-C28-C29
28	C	306	CDL	C57-C58-C59-C60
28	N	601	CDL	C60-C61-C62-C63
28	T	103	CDL	C13-C14-C15-C16
19	A	608	TGL	CB4-CB5-CB6-CB7
19	A	608	TGL	C23-C24-C25-C26
19	N	610	TGL	CB6-CB7-CB8-CB9
19	N	610	TGL	CA9-C20-C21-C22
19	Q	201	TGL	C11-C10-CB9-CB8
19	Y	101	TGL	CB3-CB4-CB5-CB6
20	C	309	PGV	C23-C24-C25-C26
25	M	101	DMU	C19-C22-C25-C28
20	Z	101	PGV	C01-C02-O01-C1
24	B	303	PSC	O02-C1-O01-C02
28	T	103	CDL	OB7-CB5-OB6-CB4
19	Q	201	TGL	CB4-CB5-CB6-CB7
24	O	302	PSC	C24-C25-C26-C27
27	P	307	PEK	C33-C34-C35-C36
20	Z	101	PGV	C02-C03-O11-P
27	T	101	PEK	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	C12-C13-C14-C29
20	A	610	PGV	C21-C22-C23-C24
20	C	305	PGV	C14-C15-C16-C17
20	G	103	PGV	C24-C25-C26-C27
24	O	302	PSC	C25-C26-C27-C28
27	G	102	PEK	C24-C25-C26-C27
28	T	103	CDL	C21-C22-C23-C24
19	L	101	TGL	C12-C13-C14-C29
19	N	610	TGL	CA6-CA7-CA8-CA9
25	C	310	DMU	O16-C18-C19-C22
28	P	304	CDL	C61-C62-C63-C64
28	T	103	CDL	C71-C72-C73-C74
27	P	307	PEK	C21-C22-C23-C24
25	C	302	DMU	C1-C6-O16-C18
19	D	201	TGL	CC5-CC6-CC7-CC8
19	N	610	TGL	CA4-CA5-CA6-CA7
19	Q	201	TGL	CA6-CA7-CA8-CA9
19	Y	101	TGL	CB5-CB6-CB7-CB8
19	Y	101	TGL	CA9-C20-C21-C22
20	C	305	PGV	C7-C8-C9-C10
28	P	304	CDL	C43-C44-C45-C46
28	T	103	CDL	C22-C23-C24-C25
28	T	103	CDL	C51-C52-C53-C54
19	A	608	TGL	CA4-CA5-CA6-CA7
19	L	101	TGL	CB3-CB4-CB5-CB6
19	Q	201	TGL	C10-C11-C12-C13
20	C	309	PGV	C6-C7-C8-C9
20	G	103	PGV	C13-C14-C15-C16
28	N	601	CDL	C14-C15-C16-C17
28	P	304	CDL	CB5-C51-C52-C53
19	A	608	TGL	CA2-CA3-CA4-CA5
19	A	608	TGL	C10-C11-C12-C13
19	A	608	TGL	C20-C21-C22-C23
19	Y	101	TGL	CA5-CA6-CA7-CA8
19	Y	101	TGL	CC4-CC5-CC6-CC7
27	C	308	PEK	C28-C29-C30-C31
28	N	601	CDL	C35-C36-C37-C38
28	T	103	CDL	C41-C42-C43-C44
22	C	307	CHD	C20-C22-C23-C24
19	A	608	TGL	CA3-CA4-CA5-CA6
19	N	610	TGL	C16-C15-CC9-CC8
25	P	308	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
27	C	304	PEK	C26-C27-C28-C29
27	C	308	PEK	C25-C26-C27-C28
20	C	309	PGV	C04-C05-C06-O06
20	G	103	PGV	C04-C05-C06-O06
25	C	302	DMU	C18-C19-C22-C25
28	T	103	CDL	C51-CB5-OB6-CB4
20	Z	101	PGV	C2-C3-C4-C5
24	O	302	PSC	C5-C6-C7-C8
27	G	102	PEK	C30-C31-C32-C33
27	T	101	PEK	C22-C23-C24-C25
28	T	103	CDL	C17-C18-C19-C20
20	C	305	PGV	C12-C13-C14-C15
20	G	103	PGV	C12-C13-C14-C15
19	A	608	TGL	CB9-C10-C11-C12
19	D	201	TGL	C16-C15-CC9-CC8
25	L	102	DMU	C31-C34-C37-C40
28	C	306	CDL	C42-C43-C44-C45
28	N	601	CDL	C42-C43-C44-C45
28	N	601	CDL	C59-C60-C61-C62
28	P	304	CDL	C40-C41-C42-C43
25	C	302	DMU	O5-C6-O16-C18
22	P	305	CHD	C17-C20-C22-C23
19	Q	201	TGL	CC5-CC6-CC7-CC8
28	N	601	CDL	C21-C22-C23-C24
28	N	601	CDL	C41-C42-C43-C44
28	P	304	CDL	C22-C23-C24-C25
28	P	304	CDL	C23-C24-C25-C26
28	P	304	CDL	C57-C58-C59-C60
19	N	610	TGL	CA3-CA4-CA5-CA6
19	D	201	TGL	CC6-CC7-CC8-CC9
19	N	610	TGL	CB9-C10-C11-C12
19	N	610	TGL	C13-C14-C29-C30
19	Q	201	TGL	C12-C13-C14-C29
28	P	304	CDL	C77-C78-C79-C80
19	A	608	TGL	CC6-CC7-CC8-CC9
19	N	610	TGL	CC9-C15-C16-C17
25	C	311	DMU	C31-C34-C37-C40
27	C	304	PEK	C16-C17-C18-C19
28	C	306	CDL	C11-C12-C13-C14
28	C	306	CDL	C72-C73-C74-C75
28	N	601	CDL	C79-C80-C81-C82
19	A	608	TGL	CA5-CA6-CA7-CA8

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	CA7-CA8-CA9-C20
19	Y	101	TGL	CC3-CC4-CC5-CC6
20	A	610	PGV	C10-C11-C12-C13
20	C	305	PGV	C10-C11-C12-C13
19	N	610	TGL	CC4-CC5-CC6-CC7
20	Z	101	PGV	C4-C5-C6-C7
27	C	304	PEK	C34-C35-C36-C37
27	T	102	PEK	C30-C31-C32-C33
27	T	102	PEK	C33-C34-C35-C36
28	C	306	CDL	C23-C24-C25-C26
28	C	306	CDL	C61-C62-C63-C64
28	N	601	CDL	C13-C14-C15-C16
25	C	310	DMU	C19-C22-C25-C28
28	C	306	CDL	C59-C60-C61-C62
20	A	610	PGV	O05-C05-C06-O06
20	C	309	PGV	O05-C05-C06-O06
19	D	201	TGL	C10-C11-C12-C13
20	G	103	PGV	C7-C8-C9-C10
20	P	303	PGV	C7-C8-C9-C10
27	G	102	PEK	C25-C26-C27-C28
28	N	601	CDL	C18-C19-C20-C21
28	N	601	CDL	C62-C63-C64-C65
28	P	304	CDL	C31-C32-C33-C34
28	T	103	CDL	C19-C20-C21-C22
20	C	309	PGV	C12-C13-C14-C15
20	Z	101	PGV	C12-C13-C14-C15
27	T	102	PEK	C15-C16-C17-C18
19	Q	201	TGL	CA2-CA3-CA4-CA5
28	P	304	CDL	C82-C83-C84-C85
25	C	311	DMU	C18-C19-C22-C25
28	C	306	CDL	C62-C63-C64-C65
20	P	303	PGV	C11-C12-C13-C14
20	C	309	PGV	C30-C31-C32-C33
28	P	304	CDL	C11-C12-C13-C14
19	L	101	TGL	OA1-CA1-OG1-CG1
28	T	103	CDL	CA2-C1-CB2-OB2
24	B	303	PSC	C22-C23-C24-C25
25	Z	102	DMU	C25-C28-C31-C34
28	T	103	CDL	C18-C19-C20-C21
28	T	103	CDL	C73-C74-C75-C76
27	G	102	PEK	C22-C23-C24-C25
28	C	306	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
28	C	306	CDL	C53-C54-C55-C56
28	T	103	CDL	C14-C15-C16-C17
21	A	615	EDO	O1-C1-C2-O2
21	C	317	EDO	O1-C1-C2-O2
21	C	319	EDO	O1-C1-C2-O2
21	D	203	EDO	O1-C1-C2-O2
21	D	204	EDO	O1-C1-C2-O2
21	D	206	EDO	O1-C1-C2-O2
21	N	611	EDO	O1-C1-C2-O2
21	N	614	EDO	O1-C1-C2-O2
21	N	622	EDO	O1-C1-C2-O2
21	P	310	EDO	O1-C1-C2-O2
21	P	313	EDO	O1-C1-C2-O2
21	R	202	EDO	O1-C1-C2-O2
19	N	610	TGL	C11-C10-CB9-CB8
19	Q	201	TGL	C13-C14-C29-C30
19	Y	101	TGL	C10-C11-C12-C13
27	G	102	PEK	C32-C33-C34-C35
27	G	102	PEK	C33-C34-C35-C36
28	N	601	CDL	C31-C32-C33-C34
28	T	103	CDL	C81-C82-C83-C84
28	C	306	CDL	C12-C13-C14-C15
28	P	304	CDL	C20-C21-C22-C23
28	P	304	CDL	C60-C61-C62-C63
19	L	101	TGL	CA6-CA7-CA8-CA9
19	Q	201	TGL	CB2-CB3-CB4-CB5
20	Z	101	PGV	C27-C28-C29-C30
28	N	601	CDL	C71-C72-C73-C74
20	C	309	PGV	C28-C29-C30-C31
28	C	306	CDL	C64-C65-C66-C67
24	B	303	PSC	C11-C10-C9-C8
27	P	307	PEK	C10-C11-C12-C13
20	G	103	PGV	C22-C23-C24-C25
27	G	102	PEK	C23-C24-C25-C26
20	P	303	PGV	C12-C13-C14-C15
27	C	308	PEK	C2-C3-C4-C5
19	Q	201	TGL	OB1-CB1-OG2-CG2
28	N	601	CDL	OB7-CB5-OB6-CB4
19	N	610	TGL	CA7-CA8-CA9-C20
20	A	609	PGV	C28-C29-C30-C31
20	N	609	PGV	C27-C28-C29-C30
28	P	304	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	T	103	CDL	C59-C60-C61-C62
19	L	101	TGL	C10-C11-C12-C13
19	N	610	TGL	CC6-CC7-CC8-CC9
19	Q	201	TGL	CB9-C10-C11-C12
19	Y	101	TGL	C11-C12-C13-C14
28	T	103	CDL	C12-C13-C14-C15
25	P	309	DMU	C19-C22-C25-C28
24	O	302	PSC	C2-C3-C4-C5
24	O	302	PSC	C3-C4-C5-C6
27	P	307	PEK	C29-C30-C31-C32
27	T	101	PEK	C27-C28-C29-C30
19	Q	201	TGL	CB2-CB1-OG2-CG2
28	N	601	CDL	C51-CB5-OB6-CB4
27	C	308	PEK	O01-C02-C03-O11
28	C	306	CDL	OB5-CB3-CB4-OB6
19	D	201	TGL	C16-C17-C18-C19
20	P	303	PGV	C24-C25-C26-C27
28	C	306	CDL	C58-C59-C60-C61
28	C	306	CDL	C73-C74-C75-C76
28	N	601	CDL	C34-C35-C36-C37
27	T	102	PEK	C3-C4-C5-C6
25	Z	102	DMU	C28-C31-C34-C37
27	P	307	PEK	C26-C27-C28-C29
20	G	103	PGV	C29-C30-C31-C32
19	D	201	TGL	C21-C20-CA9-CA8
19	N	610	TGL	C21-C20-CA9-CA8
20	N	609	PGV	C29-C30-C31-C32
25	Z	102	DMU	C19-C22-C25-C28
28	N	601	CDL	C77-C78-C79-C80
28	T	103	CDL	C16-C17-C18-C19
20	Z	101	PGV	C11-C10-C9-C8
25	P	306	DMU	O6-C11-C9-C8
19	D	201	TGL	CA6-CA7-CA8-CA9
19	Y	101	TGL	C16-C17-C18-C19
20	A	609	PGV	C10-C11-C12-C13
24	B	303	PSC	C3-C4-C5-C6
28	C	306	CDL	C82-C83-C84-C85
19	Q	201	TGL	C17-C18-C19-C33
20	N	609	PGV	C30-C31-C32-C33
19	Q	201	TGL	C22-C23-C24-C25
20	N	609	PGV	C14-C15-C16-C17
25	L	102	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
28	N	601	CDL	C43-C44-C45-C46
27	G	102	PEK	C03-O11-P-O12
28	N	601	CDL	CA3-OA5-PA1-OA2
20	A	610	PGV	C13-C14-C15-C16
19	Y	101	TGL	CA1-CA2-CA3-CA4
28	C	306	CDL	C22-C23-C24-C25
20	A	610	PGV	C01-C02-C03-O11
20	C	309	PGV	C01-C02-C03-O11
20	Z	101	PGV	C01-C02-C03-O11
27	T	101	PEK	C01-C02-C03-O11
25	M	101	DMU	C28-C31-C34-C37
19	L	101	TGL	C21-C22-C23-C24
24	B	303	PSC	C4-C5-C6-C7
19	Y	101	TGL	C12-C13-C14-C29
20	C	305	PGV	C20-C21-C22-C23
20	C	309	PGV	C7-C8-C9-C10
20	N	609	PGV	C23-C24-C25-C26
27	T	102	PEK	C2-C3-C4-C5
28	C	306	CDL	CA5-C11-C12-C13
19	D	201	TGL	C11-C10-CB9-CB8
19	Y	101	TGL	C21-C20-CA9-CA8
28	P	304	CDL	C80-C81-C82-C83
28	T	103	CDL	C80-C81-C82-C83
19	L	101	TGL	C11-C10-CB9-CB8
24	B	303	PSC	C25-C26-C27-C28
19	D	201	TGL	OG1-CG1-CG2-CG3
19	Y	101	TGL	OG1-CG1-CG2-CG3
20	Z	101	PGV	O03-C01-C02-C03
24	O	302	PSC	O03-C01-C02-C03
27	P	307	PEK	O03-C01-C02-C03
28	N	601	CDL	CA3-CA4-CA6-OA8
28	N	601	CDL	C54-C55-C56-C57
28	N	601	CDL	C64-C65-C66-C67
28	P	304	CDL	CA3-CA4-CA6-OA8
28	T	103	CDL	CB3-CB4-CB6-OB8
27	C	304	PEK	C4-C5-C6-C7
27	C	308	PEK	C35-C36-C37-C38
28	C	306	CDL	C36-C37-C38-C39
20	A	610	PGV	C15-C16-C17-C18
20	A	609	PGV	C31-C32-C33-C34
20	G	103	PGV	C3-C4-C5-C6
20	Z	101	PGV	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	B	303	PSC	C15-C16-C17-C18
20	G	103	PGV	O05-C05-C06-O06
22	J	101	CHD	C16-C17-C20-C22
20	G	103	PGV	C11-C10-C9-C8
20	N	609	PGV	C12-C13-C14-C15
24	O	302	PSC	C31-C32-C33-C34
27	C	304	PEK	C17-C18-C19-C20
25	C	311	DMU	C34-C37-C40-C43
20	G	103	PGV	C31-C32-C33-C34
19	L	101	TGL	CG1-CG2-OG2-CB1
19	L	101	TGL	C11-C12-C13-C14
24	O	302	PSC	C23-C24-C25-C26
19	D	201	TGL	CA4-CA5-CA6-CA7
19	Q	201	TGL	CA4-CA5-CA6-CA7
25	L	102	DMU	C34-C37-C40-C43
27	T	102	PEK	C34-C35-C36-C37
28	N	601	CDL	C72-C73-C74-C75
19	Y	101	TGL	C18-C19-C33-C34
14	A	602[A]	HEA	C4D-C3D-CAD-CBD
21	A	617	EDO	O1-C1-C2-O2
21	L	103	EDO	O1-C1-C2-O2
21	O	304	EDO	O1-C1-C2-O2
20	P	303	PGV	C1-C2-C3-C4
28	T	103	CDL	C58-C59-C60-C61
20	C	309	PGV	O03-C01-C02-O01
28	T	103	CDL	C75-C76-C77-C78
19	L	101	TGL	CC6-CC7-CC8-CC9
20	C	305	PGV	C15-C16-C17-C18
27	P	307	PEK	C35-C36-C37-C38
27	T	101	PEK	C17-C18-C19-C20
28	N	601	CDL	C20-C21-C22-C23
27	C	308	PEK	C26-C27-C28-C29
19	L	101	TGL	C25-C26-C27-C28
22	C	307	CHD	C16-C17-C20-C22
19	A	608	TGL	C25-C26-C27-C28
25	L	102	DMU	C25-C28-C31-C34
27	C	304	PEK	C7-C8-C9-C10
27	C	308	PEK	C10-C11-C12-C13
28	P	304	CDL	C39-C40-C41-C42
28	P	304	CDL	C74-C75-C76-C77
19	A	608	TGL	CB5-CB6-CB7-CB8
28	T	103	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
28	C	306	CDL	OB5-CB3-CB4-CB6
28	P	304	CDL	OA5-CA3-CA4-CA6
28	N	601	CDL	C11-C12-C13-C14
28	P	304	CDL	C51-C52-C53-C54
27	T	101	PEK	O12-C04-C05-N
19	Q	201	TGL	C20-C21-C22-C23
25	P	309	DMU	C22-C25-C28-C31
27	C	304	PEK	C23-C24-C25-C26
28	C	306	CDL	C77-C78-C79-C80
24	O	302	PSC	C26-C27-C28-C29
25	C	302	DMU	C19-C22-C25-C28
28	C	306	CDL	C63-C64-C65-C66
20	C	305	PGV	C1-C2-C3-C4
20	N	609	PGV	C13-C14-C15-C16
27	T	101	PEK	C26-C27-C28-C29
19	D	201	TGL	CC7-CC8-CC9-C15
27	C	308	PEK	C32-C33-C34-C35
20	G	103	PGV	C19-C20-C21-C22
19	Y	101	TGL	C29-C30-C31-C32
20	Z	101	PGV	C05-C04-O12-P
25	L	102	DMU	C19-C18-O16-C6
19	Q	201	TGL	C16-C17-C18-C19
24	O	302	PSC	C27-C28-C29-C30
28	T	103	CDL	C64-C65-C66-C67
19	N	610	TGL	CB1-CB2-CB3-CB4
20	C	309	PGV	C22-C23-C24-C25
27	T	102	PEK	C23-C24-C25-C26
19	Q	201	TGL	OG1-CG1-CG2-CG3
20	C	309	PGV	O03-C01-C02-C03
28	C	306	CDL	CB3-CB4-CB6-OB8
28	P	304	CDL	CB3-CB4-CB6-OB8
28	T	103	CDL	CA3-CA4-CA6-OA8
28	C	306	CDL	C37-C38-C39-C40
19	L	101	TGL	C20-C21-C22-C23
25	C	311	DMU	O1-C10-O7-C3
20	N	609	PGV	C31-C32-C33-C34
19	L	101	TGL	CB7-CB8-CB9-C10
19	Y	101	TGL	C11-C10-CB9-CB8
28	N	601	CDL	C33-C34-C35-C36
14	A	602[B]	HEA	C2A-C3A-CMA-OMA
24	B	303	PSC	C9-C10-C11-C12
24	B	303	PSC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	C	308	PEK	C11-C12-C13-C14
27	G	102	PEK	C6-C7-C8-C9
27	G	102	PEK	C11-C10-C9-C8
27	G	102	PEK	C11-C12-C13-C14
27	G	102	PEK	C12-C13-C14-C15
27	P	307	PEK	C04-O12-P-O11
27	P	307	PEK	C9-C10-C11-C12
27	P	307	PEK	C12-C13-C14-C15
27	T	101	PEK	C11-C10-C9-C8
27	T	101	PEK	C9-C10-C11-C12
27	T	102	PEK	C12-C13-C14-C15
20	C	309	PGV	C21-C22-C23-C24
20	N	609	PGV	C28-C29-C30-C31
28	C	306	CDL	OA5-CA3-CA4-OA6
28	P	304	CDL	OA5-CA3-CA4-OA6
20	A	609	PGV	C11-C10-C9-C8
20	A	610	PGV	C11-C10-C9-C8
20	N	609	PGV	C11-C10-C9-C8
19	L	101	TGL	CC1-CC2-CC3-CC4
19	L	101	TGL	C29-C30-C31-C32
19	A	608	TGL	CA6-CA7-CA8-CA9
28	N	601	CDL	C17-C18-C19-C20
27	G	102	PEK	C28-C29-C30-C31
20	Z	101	PGV	O03-C01-C02-O01
27	G	102	PEK	O03-C01-C02-O01
28	C	306	CDL	OA6-CA4-CA6-OA8
19	Q	201	TGL	CB5-CB6-CB7-CB8
27	P	307	PEK	C30-C31-C32-C33
22	J	101	CHD	C13-C17-C20-C22
25	P	306	DMU	C22-C25-C28-C31
28	C	306	CDL	C84-C85-C86-C87
28	N	601	CDL	C58-C59-C60-C61
19	A	608	TGL	C29-C30-C31-C32
25	M	101	DMU	C31-C34-C37-C40
22	P	305	CHD	C16-C17-C20-C22
24	O	302	PSC	C13-C14-C15-C16
20	C	309	PGV	C5-C6-C7-C8
19	A	608	TGL	C13-C14-C29-C30
20	C	305	PGV	C24-C25-C26-C27
21	A	611	EDO	O1-C1-C2-O2
21	G	104	EDO	O1-C1-C2-O2
19	Y	101	TGL	CC5-CC6-CC7-CC8

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Mol	Chain	Res	Type	Atoms
20	A	609	PGV	C23-C24-C25-C26
25	P	309	DMU	C28-C31-C34-C37
14	A	602[A]	HEA	C2D-C3D-CAD-CBD
19	Q	201	TGL	CC2-CC3-CC4-CC5
19	N	610	TGL	C20-C21-C22-C23
27	G	102	PEK	O03-C21-C22-C23
19	L	101	TGL	C14-C29-C30-C31
19	Y	101	TGL	CA6-CA7-CA8-CA9
20	Z	101	PGV	C29-C30-C31-C32
27	P	307	PEK	C7-C8-C9-C10
27	G	102	PEK	C3-C4-C5-C6
27	T	102	PEK	C17-C18-C19-C20
22	P	305	CHD	C20-C22-C23-C24
25	P	308	DMU	C25-C28-C31-C34
27	C	304	PEK	C35-C36-C37-C38
19	Y	101	TGL	C22-C23-C24-C25
19	D	201	TGL	CG3-CG2-OG2-CB1
24	O	302	PSC	C01-C02-O01-C1
19	Q	201	TGL	C15-C16-C17-C18
20	A	610	PGV	C29-C30-C31-C32
19	L	101	TGL	C15-C16-C17-C18
25	C	311	DMU	O16-C18-C19-C22
24	B	303	PSC	C6-C7-C8-C9
28	P	304	CDL	CA5-C11-C12-C13
19	D	201	TGL	CG1-CG2-CG3-OG3
19	L	101	TGL	OG1-CG1-CG2-CG3
20	C	309	PGV	C02-C03-O11-P
20	G	103	PGV	O03-C01-C02-C03
20	P	303	PGV	C02-C03-O11-P
27	T	101	PEK	O03-C01-C02-C03
28	C	306	CDL	C1-CA2-OA2-PA1
28	C	306	CDL	CA4-CA3-OA5-PA1
28	C	306	CDL	CA3-CA4-CA6-OA8
28	N	601	CDL	CB3-CB4-CB6-OB8
28	P	304	CDL	C56-C57-C58-C59
20	C	305	PGV	C27-C28-C29-C30
20	A	609	PGV	C30-C31-C32-C33
25	C	310	DMU	C25-C28-C31-C34
27	T	101	PEK	C30-C31-C32-C33
19	A	608	TGL	OG1-CG1-CG2-OG2
19	D	201	TGL	OG2-CG2-CG3-OG3
19	N	610	TGL	OG2-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
28	C	306	CDL	OB6-CB4-CB6-OB8
28	N	601	CDL	OA6-CA4-CA6-OA8
28	P	304	CDL	OB6-CB4-CB6-OB8
19	L	101	TGL	C22-C23-C24-C25
20	G	103	PGV	C23-C24-C25-C26
25	C	310	DMU	C28-C31-C34-C37
20	P	303	PGV	C11-C10-C9-C8
27	C	308	PEK	C29-C30-C31-C32
22	J	101	CHD	C21-C20-C22-C23
19	L	101	TGL	C21-C20-CA9-CA8
28	T	103	CDL	C24-C25-C26-C27
24	O	302	PSC	C15-C16-C17-C18
19	A	608	TGL	CC9-C15-C16-C17
20	C	309	PGV	C04-O12-P-O11
28	N	601	CDL	CA2-OA2-PA1-OA5
28	N	601	CDL	CB2-OB2-PB2-OB5
28	P	304	CDL	CA3-OA5-PA1-OA2
28	T	103	CDL	CA2-OA2-PA1-OA5
28	C	306	CDL	C17-C18-C19-C20
20	A	610	PGV	C05-C04-O12-P
20	G	103	PGV	C02-C03-O11-P
19	D	201	TGL	C12-C13-C14-C29
20	Z	101	PGV	C03-O11-P-O13
20	Z	101	PGV	C04-O12-P-O14
24	O	302	PSC	C03-O11-P-O13
27	C	308	PEK	C03-O11-P-O14
27	G	102	PEK	C03-O11-P-O13
27	G	102	PEK	C04-O12-P-O14
27	T	101	PEK	C03-O11-P-O14
27	T	101	PEK	C04-O12-P-O14
28	C	306	CDL	CA3-OA5-PA1-OA3
28	C	306	CDL	CB2-OB2-PB2-OB3
28	C	306	CDL	CB2-OB2-PB2-OB4
28	C	306	CDL	CB3-OB5-PB2-OB3
28	T	103	CDL	CA2-OA2-PA1-OA4
28	T	103	CDL	CB2-OB2-PB2-OB4
20	A	610	PGV	C31-C32-C33-C34
20	C	305	PGV	C28-C29-C30-C31
25	P	308	DMU	C28-C31-C34-C37
28	T	103	CDL	C71-CB7-OB8-CB6
27	C	308	PEK	C01-C02-C03-O11
28	C	306	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	CB5-CB6-CB7-CB8
19	Y	101	TGL	C15-C16-C17-C18
27	C	304	PEK	C28-C29-C30-C31
21	R	205	EDO	O1-C1-C2-O2
19	Q	201	TGL	CC4-CC5-CC6-CC7
27	G	102	PEK	C7-C8-C9-C10
20	N	609	PGV	C15-C16-C17-C18
24	B	303	PSC	C05-C04-O12-P
19	D	201	TGL	OG2-CB1-CB2-CB3
20	C	309	PGV	C31-C32-C33-C34
24	O	302	PSC	C28-C29-C30-C31
22	W	101	CHD	C17-C20-C22-C23
28	C	306	CDL	C35-C36-C37-C38
28	N	601	CDL	CB7-C71-C72-C73
28	N	601	CDL	C55-C56-C57-C58
28	C	306	CDL	CA2-C1-CB2-OB2
20	G	103	PGV	C2-C3-C4-C5
28	C	306	CDL	C74-C75-C76-C77
28	N	601	CDL	C16-C17-C18-C19
20	C	309	PGV	O01-C02-C03-O11
20	Z	101	PGV	O01-C02-C03-O11
27	T	101	PEK	O01-C02-C03-O11
28	T	103	CDL	OB9-CB7-OB8-CB6
20	G	103	PGV	C4-C5-C6-C7
20	G	103	PGV	C1-C2-C3-C4
28	T	103	CDL	C11-C12-C13-C14
14	A	602[B]	HEA	C4A-C3A-CMA-OMA
14	N	603[B]	HEA	C4A-C3A-CMA-OMA
19	A	608	TGL	OG1-CG1-CG2-CG3
19	D	201	TGL	OG1-CG1-CG2-OG2
19	L	101	TGL	OG1-CG1-CG2-OG2
19	Q	201	TGL	OG2-CG2-CG3-OG3
19	Y	101	TGL	OG1-CG1-CG2-OG2
24	O	302	PSC	O03-C01-C02-O01
28	P	304	CDL	OA6-CA4-CA6-OA8
28	T	103	CDL	C74-C75-C76-C77
19	D	201	TGL	C25-C26-C27-C28
27	C	308	PEK	C34-C35-C36-C37
20	C	305	PGV	C02-C03-O11-P
24	O	302	PSC	C02-C03-O11-P
28	C	306	CDL	C31-CA7-OA8-CA6
27	G	102	PEK	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
28	C	306	CDL	C40-C41-C42-C43
28	N	601	CDL	C57-C58-C59-C60
28	T	103	CDL	C38-C39-C40-C41
22	J	101	CHD	C16-C17-C20-C21
27	G	102	PEK	C35-C36-C37-C38
19	L	101	TGL	C24-C25-C26-C27
28	C	306	CDL	OA9-CA7-OA8-CA6
27	T	102	PEK	C16-C17-C18-C19
25	P	308	DMU	O16-C18-C19-C22
19	D	201	TGL	C11-C12-C13-C14
19	Y	101	TGL	CC2-CC3-CC4-CC5
27	C	304	PEK	C29-C30-C31-C32
21	A	614	EDO	O1-C1-C2-O2
21	R	203	EDO	O1-C1-C2-O2
21	U	101	EDO	O1-C1-C2-O2
28	C	306	CDL	C56-C57-C58-C59
27	P	307	PEK	O01-C1-C2-C3
22	C	307	CHD	C16-C17-C20-C21
28	T	103	CDL	OA6-CA4-CA6-OA8
19	L	101	TGL	CC7-CC8-CC9-C15
19	Q	201	TGL	C29-C30-C31-C32
20	A	610	PGV	C04-O12-P-O11
24	O	302	PSC	C04-O12-P-O11
28	P	304	CDL	CA2-OA2-PA1-OA5
19	L	101	TGL	CG1-CG2-CG3-OG3
27	G	102	PEK	O03-C01-C02-C03
19	A	608	TGL	C11-C10-CB9-CB8
19	N	610	TGL	C24-C25-C26-C27
28	P	304	CDL	C72-C73-C74-C75
19	Q	201	TGL	OG1-CA1-CA2-CA3
28	T	103	CDL	C52-C51-CB5-OB6
24	B	303	PSC	C31-C32-C33-C34
28	P	304	CDL	CA4-CA3-OA5-PA1
20	Z	101	PGV	C5-C6-C7-C8
27	C	308	PEK	C14-C15-C16-C17
28	T	103	CDL	C56-C57-C58-C59
27	G	102	PEK	C4-C5-C6-C7
28	C	306	CDL	C51-C52-C53-C54
28	N	601	CDL	C83-C84-C85-C86
14	N	602	HEA	CAD-CBD-CGD-O1D
19	Q	201	TGL	CC7-CC8-CC9-C15
28	N	601	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
19	N	610	TGL	CC5-CC6-CC7-CC8
28	P	304	CDL	OB9-CB7-OB8-CB6
19	N	610	TGL	CA2-CA3-CA4-CA5
19	N	610	TGL	C12-C13-C14-C29
20	G	103	PGV	C6-C7-C8-C9
14	N	603[A]	HEA	CAA-CBA-CGA-O1A
28	C	306	CDL	C31-C32-C33-C34
19	L	101	TGL	OG1-CA1-CA2-CA3
19	Y	101	TGL	C24-C25-C26-C27
20	P	303	PGV	C05-C04-O12-P
14	A	602[B]	HEA	CAA-CBA-CGA-O1A
22	G	101	CHD	C22-C23-C24-O26
22	W	101	CHD	C22-C23-C24-O25
25	C	302	DMU	C22-C25-C28-C31
19	D	201	TGL	CB7-CB8-CB9-C10
27	T	101	PEK	C24-C25-C26-C27
14	A	602[A]	HEA	CAA-CBA-CGA-O1A
14	N	603[A]	HEA	CAD-CBD-CGD-O1D
21	A	619	EDO	O1-C1-C2-O2
21	C	320	EDO	O1-C1-C2-O2
20	Z	101	PGV	C13-C14-C15-C16
27	C	308	PEK	C24-C25-C26-C27
14	N	603[B]	HEA	CAA-CBA-CGA-O1A
25	P	309	DMU	C31-C34-C37-C40
19	D	201	TGL	CC9-C15-C16-C17
24	O	302	PSC	C14-C15-C16-C17
14	A	601	HEA	CAD-CBD-CGD-O1D
22	G	101	CHD	C22-C23-C24-O25
14	A	602[B]	HEA	CAA-CBA-CGA-O2A
19	L	101	TGL	C16-C15-CC9-CC8
22	B	301	CHD	C22-C23-C24-O26
25	L	102	DMU	C4-C3-O7-C10
27	C	308	PEK	C6-C7-C8-C9
27	P	307	PEK	C11-C10-C9-C8
27	T	102	PEK	C5-C6-C7-C8
27	G	102	PEK	C31-C32-C33-C34
19	N	610	TGL	CB2-CB3-CB4-CB5
20	Z	101	PGV	C20-C21-C22-C23
14	N	602	HEA	CAD-CBD-CGD-O2D
14	N	603[A]	HEA	CAA-CBA-CGA-O2A
22	B	301	CHD	C22-C23-C24-O25
19	D	201	TGL	CB2-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
22	J	101	CHD	C13-C17-C20-C21
22	J	101	CHD	C22-C23-C24-O26
14	N	602	HEA	C26-C15-C16-C17
27	C	308	PEK	C1-C2-C3-C4
22	P	305	CHD	C22-C23-C24-O26
28	C	306	CDL	C21-C22-C23-C24
28	T	103	CDL	C76-C77-C78-C79
19	D	201	TGL	OB1-CB1-OG2-CG2
28	P	304	CDL	C78-C79-C80-C81
14	A	602[A]	HEA	CAA-CBA-CGA-O2A
22	J	101	CHD	C22-C23-C24-O25
19	Q	201	TGL	CB1-CB2-CB3-CB4
22	W	101	CHD	C22-C23-C24-O26
27	P	307	PEK	C2-C3-C4-C5
19	N	610	TGL	CC2-CC3-CC4-CC5
20	C	309	PGV	C4-C5-C6-C7
19	N	610	TGL	C33-C34-C35-C36
22	C	307	CHD	C22-C23-C24-O26
19	D	201	TGL	CB3-CB4-CB5-CB6
19	L	101	TGL	CC3-CC4-CC5-CC6
20	C	309	PGV	C24-C25-C26-C27
19	Q	201	TGL	OG2-CB1-CB2-CB3
27	T	102	PEK	O03-C21-C22-C23
19	N	610	TGL	CG1-CG2-CG3-OG3
21	A	622	EDO	O1-C1-C2-O2
21	D	205	EDO	O1-C1-C2-O2
21	E	204	EDO	O1-C1-C2-O2
21	N	612	EDO	O1-C1-C2-O2
21	Q	203	EDO	O1-C1-C2-O2
21	R	206	EDO	O1-C1-C2-O2
21	S	103	EDO	O1-C1-C2-O2
22	C	301	CHD	C16-C17-C20-C22
28	P	304	CDL	C38-C39-C40-C41
14	N	603[B]	HEA	C26-C15-C16-C17
19	N	610	TGL	OG3-CC1-CC2-CC3
27	T	102	PEK	C2-C1-O01-C02
19	A	608	TGL	CC4-CC5-CC6-CC7
19	N	610	TGL	C22-C23-C24-C25
28	T	103	CDL	C72-C73-C74-C75
28	P	304	CDL	C13-C14-C15-C16
28	P	304	CDL	C42-C43-C44-C45
14	N	603[A]	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	N	603[B]	HEA	CAA-CBA-CGA-O2A
20	A	609	PGV	O03-C19-C20-C21
27	P	307	PEK	C27-C28-C29-C30
22	C	307	CHD	C13-C17-C20-C22
25	C	310	DMU	C18-C19-C22-C25
14	A	602[A]	HEA	CAD-CBD-CGD-O1D
28	C	306	CDL	C44-C45-C46-C47
19	Y	101	TGL	OG1-CA1-CA2-CA3
24	B	303	PSC	O01-C1-C2-C3
20	Z	101	PGV	C15-C16-C17-C18
27	T	102	PEK	C25-C26-C27-C28
14	A	602[A]	HEA	CAD-CBD-CGD-O2D
22	P	305	CHD	C22-C23-C24-O25
20	P	303	PGV	C22-C23-C24-C25
28	P	304	CDL	C71-CB7-OB8-CB6
28	T	103	CDL	CB2-C1-CA2-OA2
20	A	610	PGV	C24-C25-C26-C27
28	P	304	CDL	C35-C36-C37-C38
28	C	306	CDL	OB9-CB7-OB8-CB6
19	Y	101	TGL	CC7-CC8-CC9-C15
20	C	305	PGV	C13-C14-C15-C16
24	O	302	PSC	C7-C8-C9-C10
19	Q	201	TGL	OG3-CC1-CC2-CC3
14	A	601	HEA	C26-C15-C16-C17
28	N	601	CDL	C44-C45-C46-C47
25	P	306	DMU	O6-C11-C9-O1
28	P	304	CDL	C76-C77-C78-C79
20	P	303	PGV	C21-C22-C23-C24
28	P	304	CDL	C84-C85-C86-C87
20	G	103	PGV	C25-C26-C27-C28
19	A	608	TGL	OG3-CC1-CC2-CC3
24	B	303	PSC	C12-C13-C14-C15
14	A	601	HEA	CAD-CBD-CGD-O2D
28	P	304	CDL	C44-C45-C46-C47
22	P	301	CHD	C22-C23-C24-O26
19	N	610	TGL	OG1-CA1-CA2-CA3
27	T	101	PEK	O03-C21-C22-C23
28	T	103	CDL	C55-C56-C57-C58
19	D	201	TGL	OG1-CA1-CA2-CA3
20	G	103	PGV	C9-C10-C11-C12
20	Z	101	PGV	C9-C10-C11-C12
27	T	101	PEK	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
20	A	610	PGV	O03-C01-C02-C03
22	C	307	CHD	C22-C23-C24-O25
20	G	103	PGV	O01-C02-C03-O11
28	P	304	CDL	OB5-CB3-CB4-OB6
28	T	103	CDL	OB5-CB3-CB4-OB6
28	C	306	CDL	C71-CB7-OB8-CB6
19	A	608	TGL	C14-C29-C30-C31
21	A	612	EDO	O1-C1-C2-O2
21	A	621	EDO	O1-C1-C2-O2
21	C	313	EDO	O1-C1-C2-O2
21	C	315	EDO	O1-C1-C2-O2
21	E	203	EDO	O1-C1-C2-O2
27	T	102	PEK	O01-C1-C2-C3
27	C	308	PEK	C17-C18-C19-C20
25	P	308	DMU	O6-C11-C9-C8
22	C	301	CHD	C22-C23-C24-O25
20	G	103	PGV	C14-C15-C16-C17
20	N	609	PGV	O03-C19-C20-C21
24	B	303	PSC	O03-C19-C20-C21
19	N	610	TGL	C21-C22-C23-C24
19	Q	201	TGL	C24-C25-C26-C27
24	B	303	PSC	C14-C15-C16-C17
19	D	201	TGL	OG3-CC1-CC2-CC3
22	P	301	CHD	C22-C23-C24-O25
19	D	201	TGL	C20-C21-C22-C23
14	N	602	HEA	CAA-CBA-CGA-O1A
14	A	601	HEA	CAA-CBA-CGA-O1A
24	O	302	PSC	O03-C19-C20-C21
20	C	305	PGV	C9-C10-C11-C12
20	C	305	PGV	C11-C12-C13-C14
20	N	609	PGV	C11-C12-C13-C14
24	B	303	PSC	C7-C8-C9-C10
14	N	602	HEA	C14-C15-C16-C17
19	D	201	TGL	OA1-CA1-CA2-CA3
20	A	610	PGV	C28-C29-C30-C31
19	Q	201	TGL	OC1-CC1-CC2-CC3
19	D	201	TGL	OC1-CC1-CC2-CC3
19	Q	201	TGL	CG1-CG2-CG3-OG3
19	N	610	TGL	C10-C11-C12-C13
25	P	306	DMU	C19-C22-C25-C28
28	C	306	CDL	C79-C80-C81-C82
27	T	102	PEK	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
20	C	309	PGV	C19-C20-C21-C22
19	A	608	TGL	OC1-CC1-CC2-CC3
20	G	103	PGV	C30-C31-C32-C33
25	Z	102	DMU	C31-C34-C37-C40
20	A	610	PGV	C04-O12-P-O13
28	P	304	CDL	CA3-OA5-PA1-OA3
20	G	103	PGV	C26-C27-C28-C29
27	T	101	PEK	O04-C21-C22-C23
27	T	102	PEK	O02-C1-C2-C3
27	P	307	PEK	C01-C02-C03-O11
24	O	302	PSC	O04-C19-C20-C21
21	A	618	EDO	O1-C1-C2-O2
21	B	305	EDO	O1-C1-C2-O2
21	D	202	EDO	O1-C1-C2-O2
21	E	201	EDO	O1-C1-C2-O2
21	G	105	EDO	O1-C1-C2-O2
21	N	616	EDO	O1-C1-C2-O2
28	N	601	CDL	C73-C74-C75-C76
27	G	102	PEK	O04-C21-C22-C23
19	A	608	TGL	CA9-C20-C21-C22
19	L	101	TGL	C13-C14-C29-C30
19	D	201	TGL	CG1-CG2-OG2-CB1
19	Q	201	TGL	CG3-CG2-OG2-CB1
27	T	101	PEK	C03-C02-O01-C1
27	G	102	PEK	C21-C22-C23-C24
28	T	103	CDL	C32-C33-C34-C35
28	C	306	CDL	C12-C11-CA5-OA6
19	L	101	TGL	C23-C24-C25-C26
22	C	301	CHD	C22-C23-C24-O26
28	C	306	CDL	C78-C79-C80-C81
28	N	601	CDL	C36-C37-C38-C39
24	B	303	PSC	O04-C19-C20-C21
14	N	602	HEA	C27-C19-C20-C21
28	C	306	CDL	C12-C11-CA5-OA7
14	N	602	HEA	CAA-CBA-CGA-O2A
28	C	306	CDL	C52-C51-CB5-OB6
20	Z	101	PGV	O03-C19-C20-C21

There are no ring outliers.

79 monomers are involved in 458 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	309	DMU	1	0
14	A	601	HEA	8	0
22	P	301	CHD	1	0
22	W	101	CHD	9	0
21	N	622	EDO	7	0
22	C	307	CHD	6	0
25	L	102	DMU	5	0
21	H	102	EDO	1	0
22	C	301	CHD	2	0
21	D	202	EDO	7	0
19	N	610	TGL	8	0
21	N	618	EDO	6	0
18	N	608	AZI	6	0
22	G	101	CHD	1	0
18	N	607	AZI	1	0
20	P	303	PGV	4	0
21	R	205	EDO	1	0
21	A	613	EDO	2	0
21	H	101	EDO	3	0
21	F	105	EDO	3	0
28	T	103	CDL	20	0
14	A	602[B]	HEA	5	0
27	C	308	PEK	9	0
19	L	101	TGL	4	0
20	C	309	PGV	8	0
20	A	609	PGV	6	0
14	A	602[A]	HEA	9	0
20	G	103	PGV	4	0
21	A	622	EDO	1	0
20	N	609	PGV	2	0
22	J	101	CHD	2	0
19	Q	201	TGL	10	0
27	P	307	PEK	10	0
21	D	204	EDO	2	0
25	C	310	DMU	5	0
25	P	308	DMU	1	0
21	A	621	EDO	5	0
21	G	104	EDO	1	0
20	Z	101	PGV	12	0
27	G	102	PEK	10	0
22	P	305	CHD	6	0
27	T	102	PEK	4	0
25	P	306	DMU	16	0

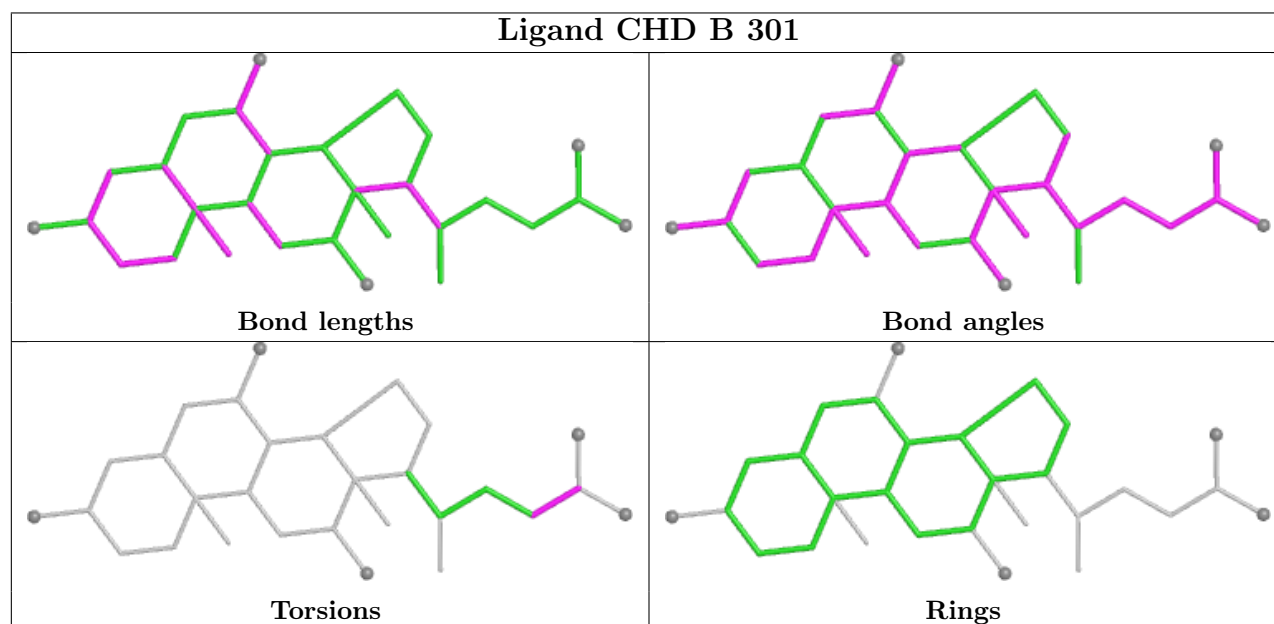
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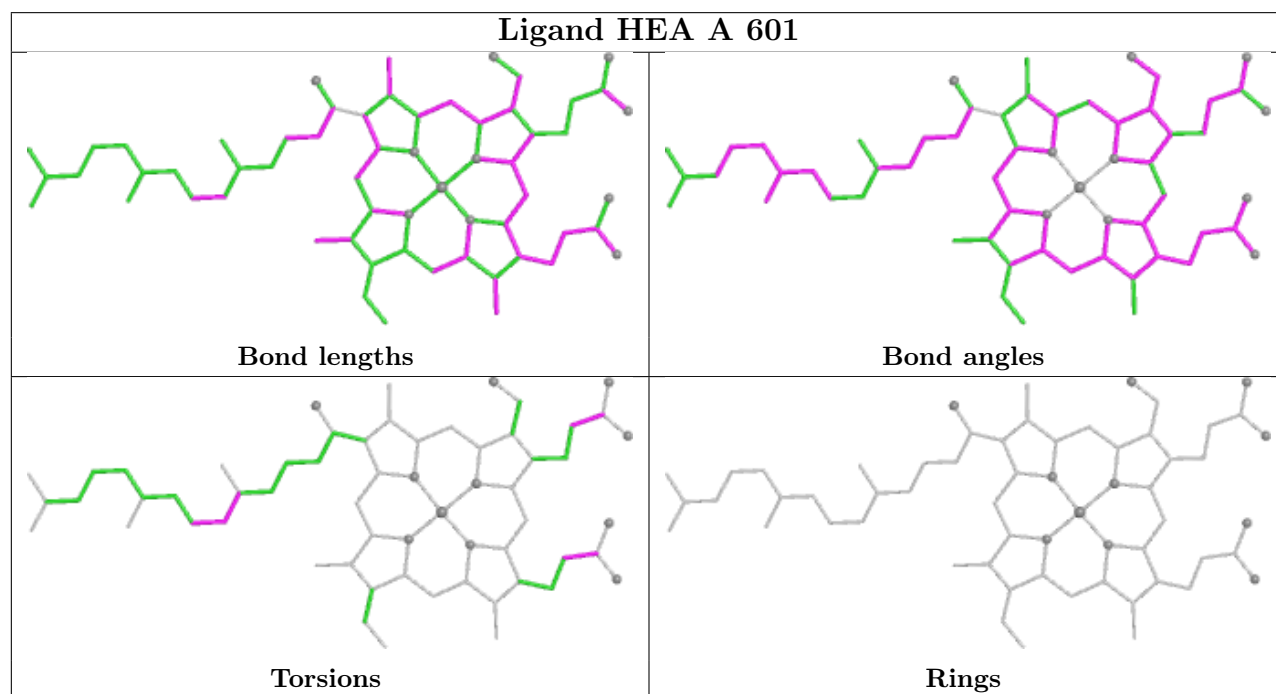
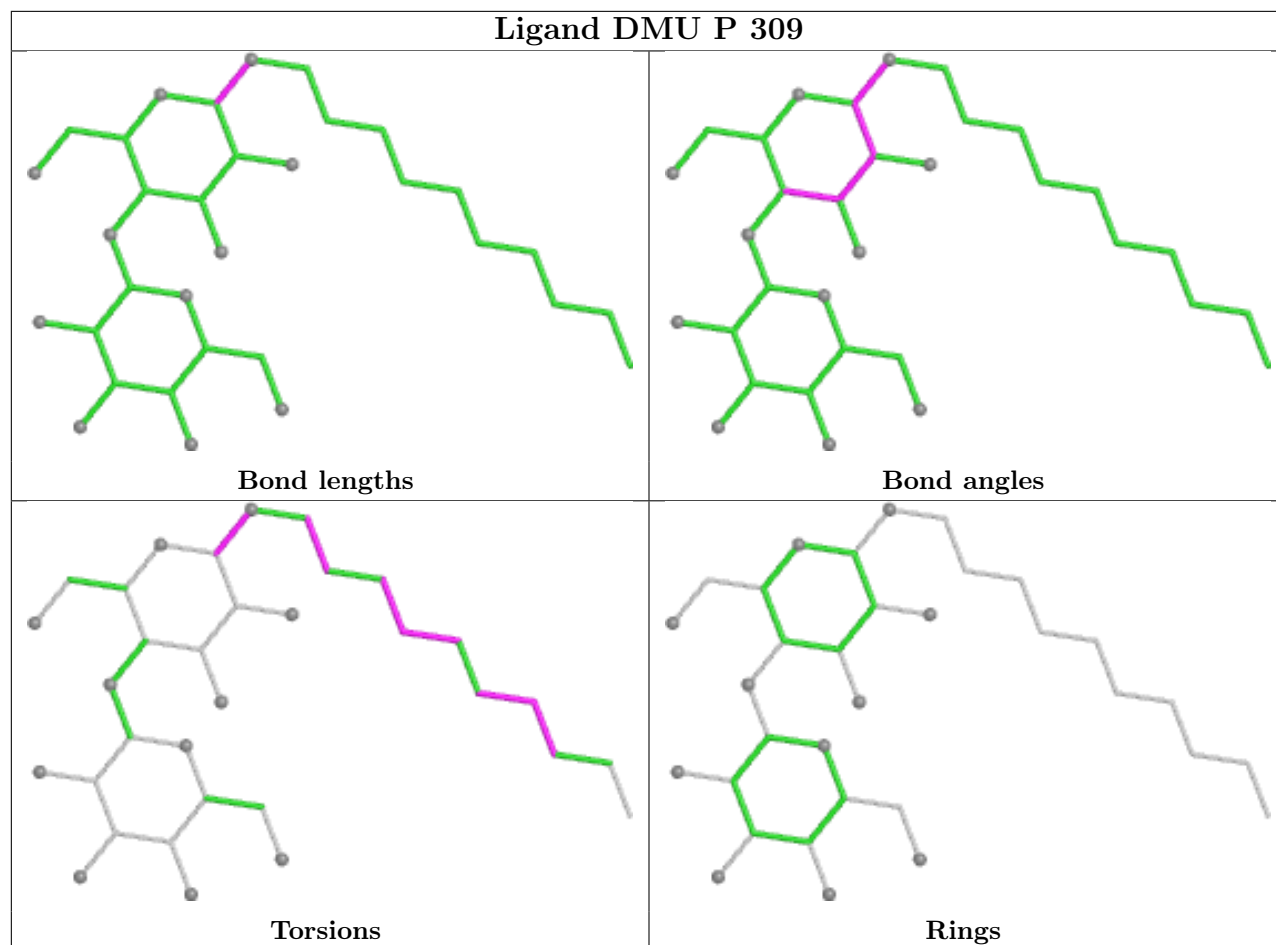
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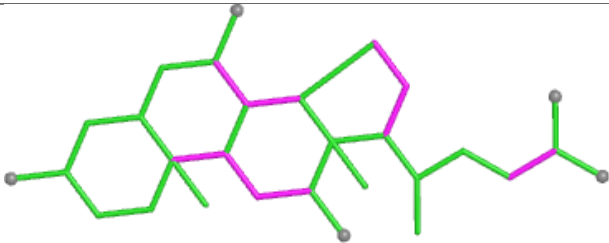
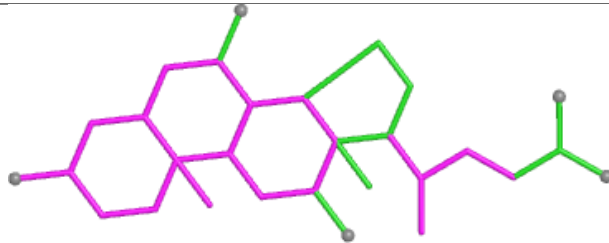
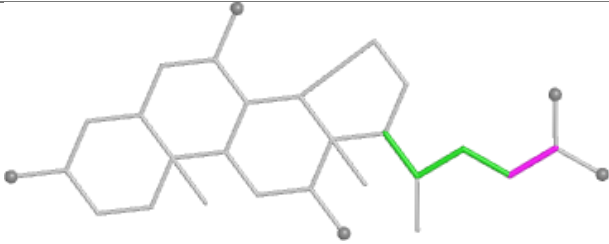
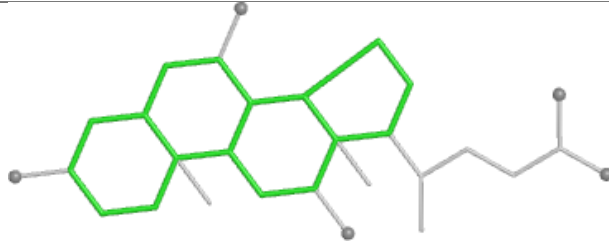
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	610	PGV	7	0
21	A	617	EDO	1	0
28	P	304	CDL	25	0
14	N	603[B]	HEA	9	0
21	C	317	EDO	1	0
28	N	601	CDL	15	0
20	C	305	PGV	3	0
21	D	206	EDO	2	0
21	O	304	EDO	1	0
21	C	315	EDO	1	0
27	T	101	PEK	4	0
25	M	101	DMU	1	0
21	N	612	EDO	3	0
14	N	602	HEA	10	0
21	C	316	EDO	2	0
19	Y	101	TGL	13	0
18	A	606	AZI	2	0
18	A	607	AZI	6	0
19	D	201	TGL	21	0
27	C	304	PEK	8	0
21	O	305	EDO	1	0
21	A	615	EDO	5	0
21	R	202	EDO	1	0
21	P	312	EDO	1	0
21	A	618	EDO	3	0
14	N	603[A]	HEA	7	0
25	C	311	DMU	1	0
21	N	613	EDO	1	0
24	O	302	PSC	12	0
21	D	203	EDO	4	0
21	A	619	EDO	2	0
19	A	608	TGL	3	0
21	N	621	EDO	6	0
28	C	306	CDL	28	0
25	C	302	DMU	12	0
24	B	303	PSC	23	0

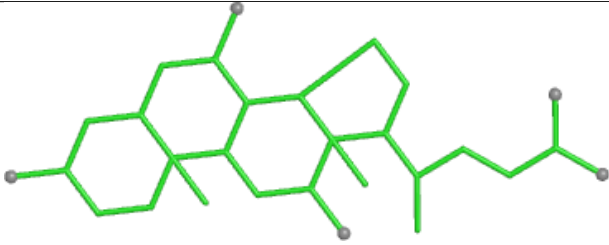
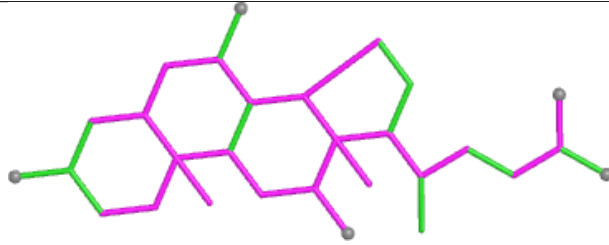
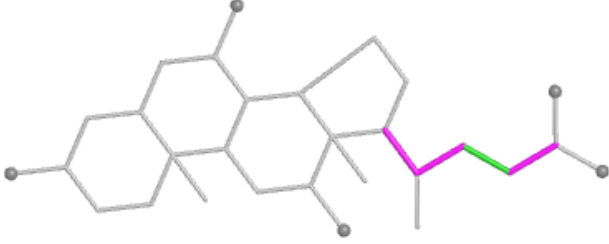
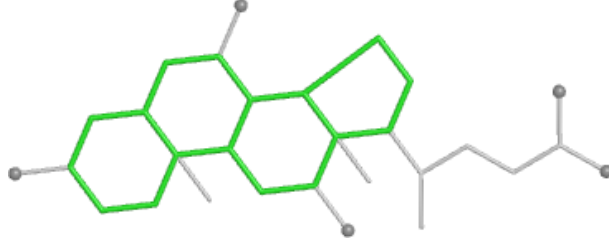
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

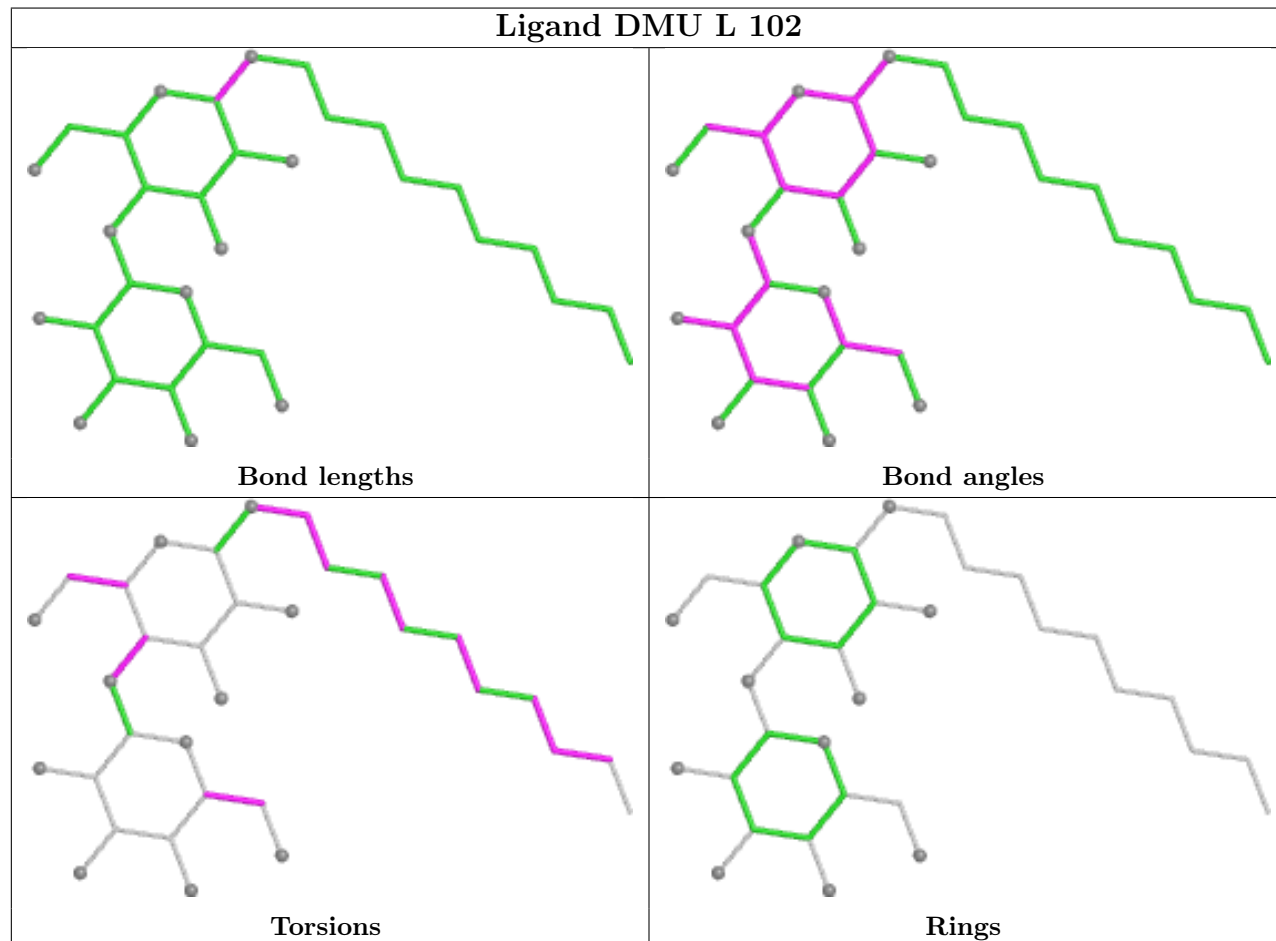
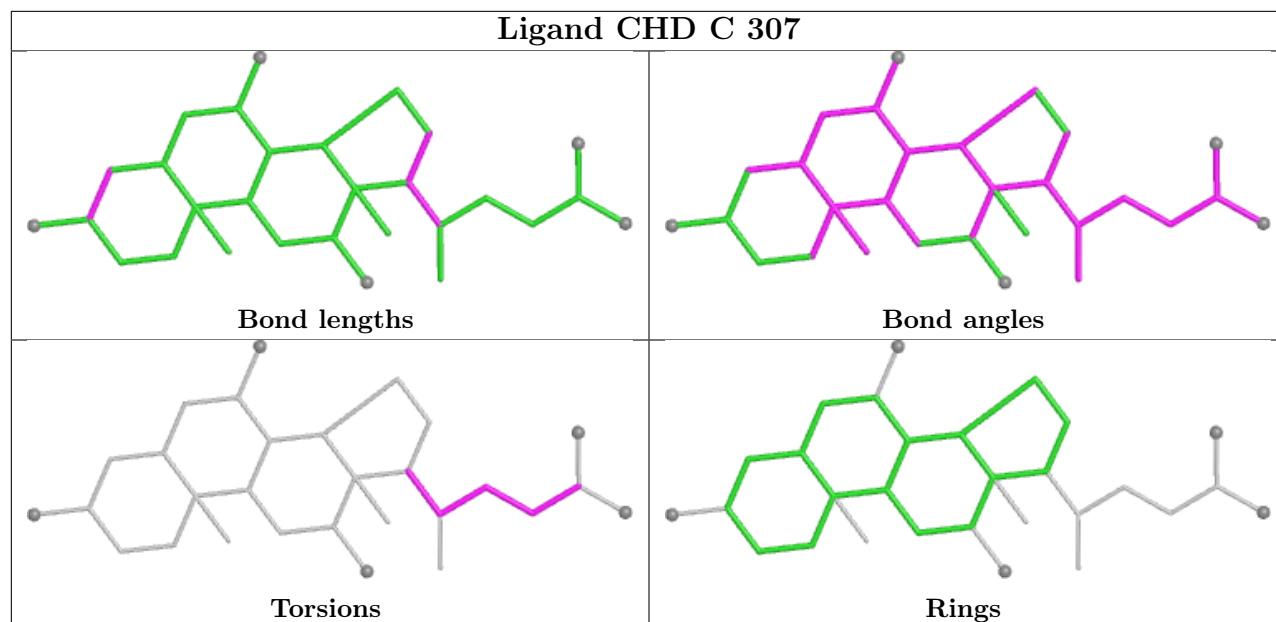
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

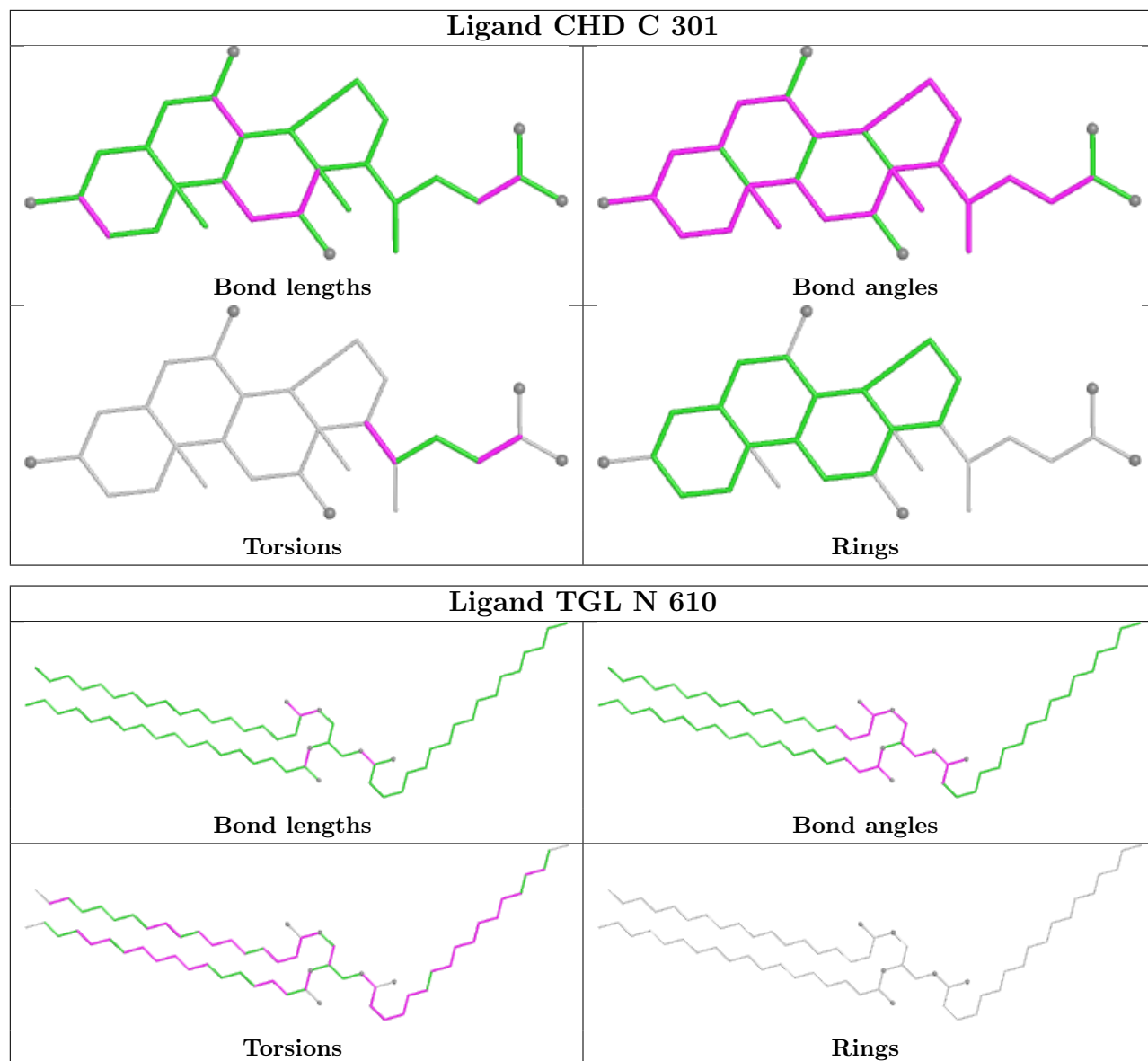


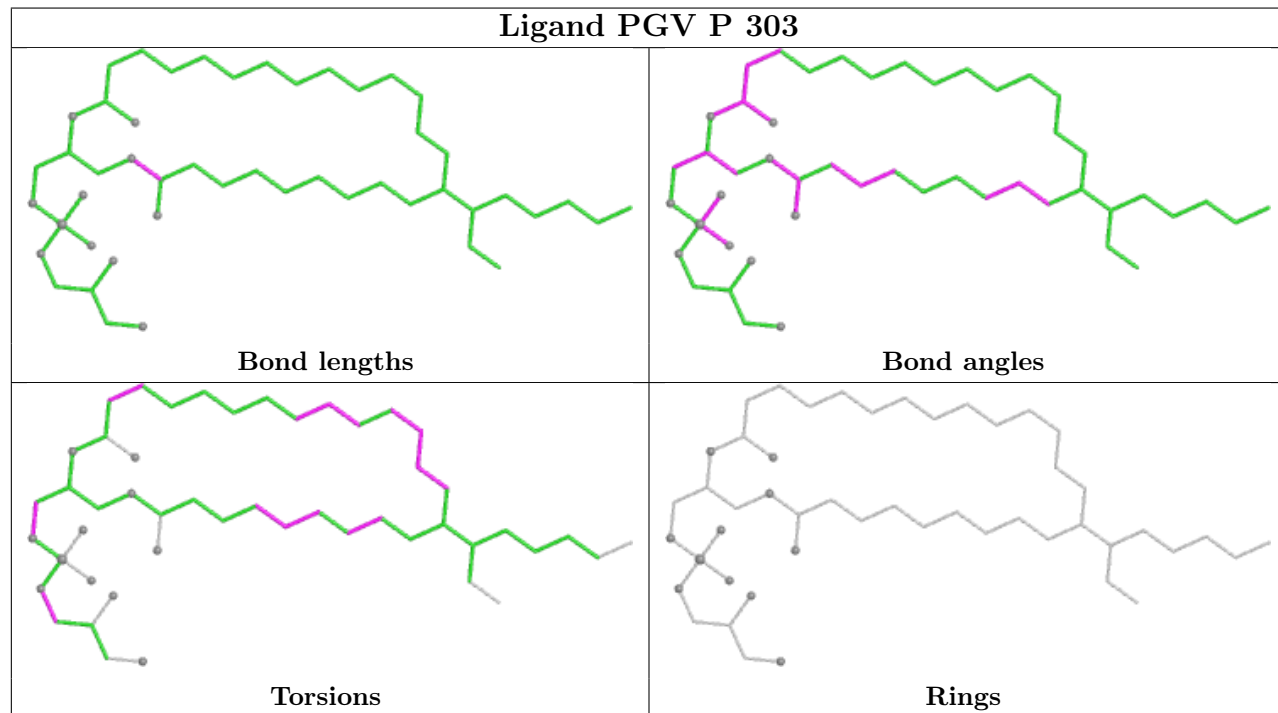
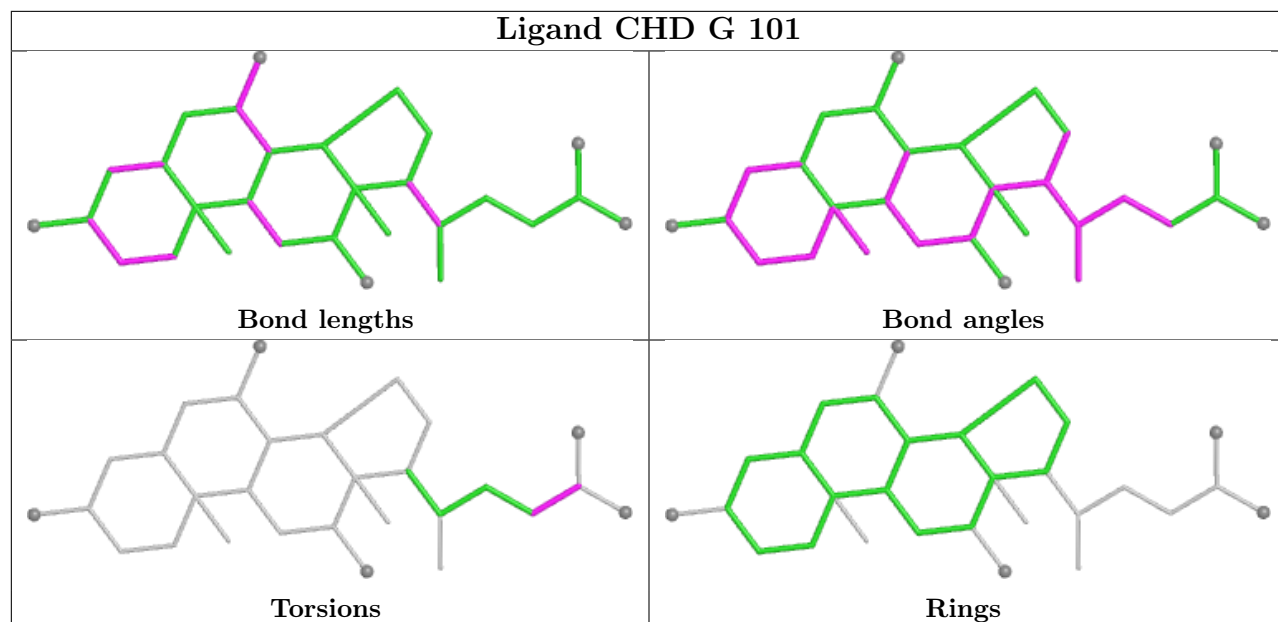


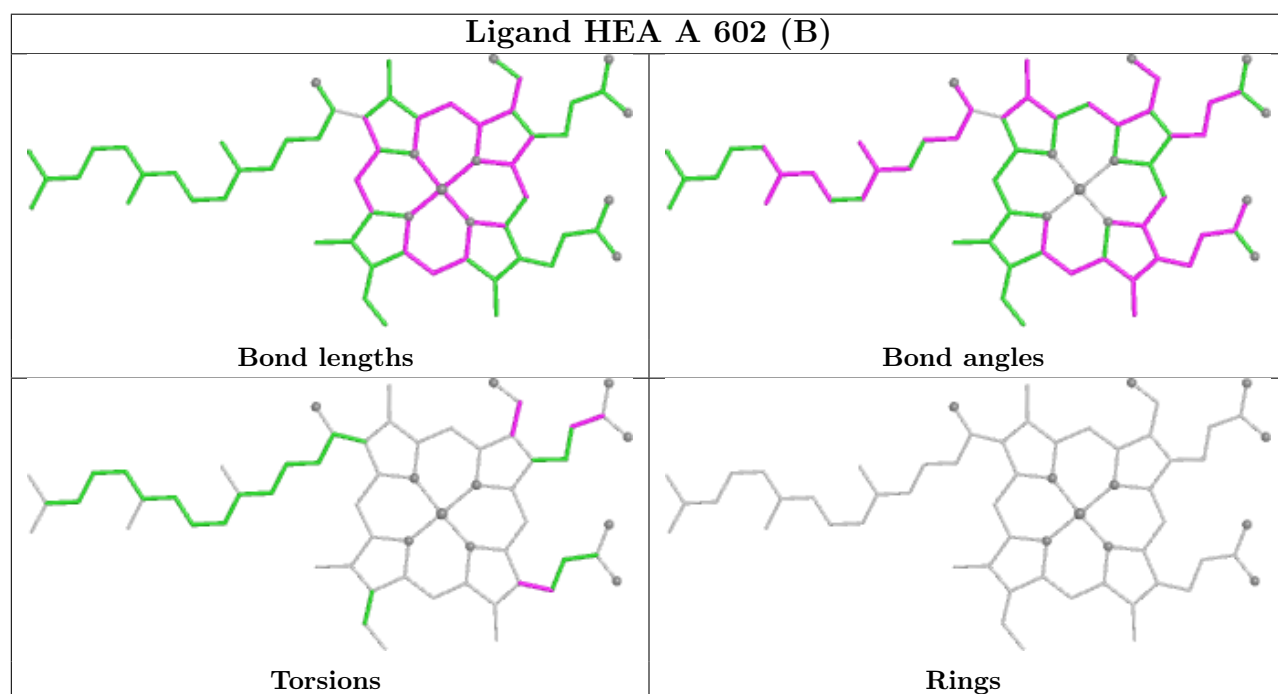
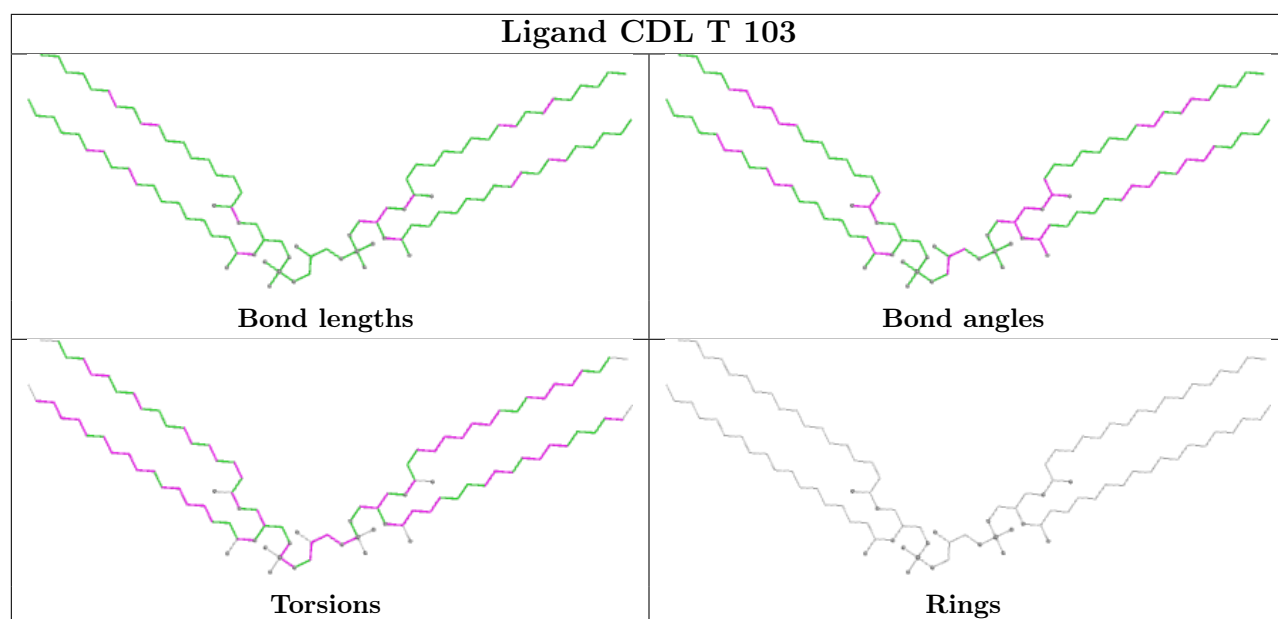
Ligand CHD P 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

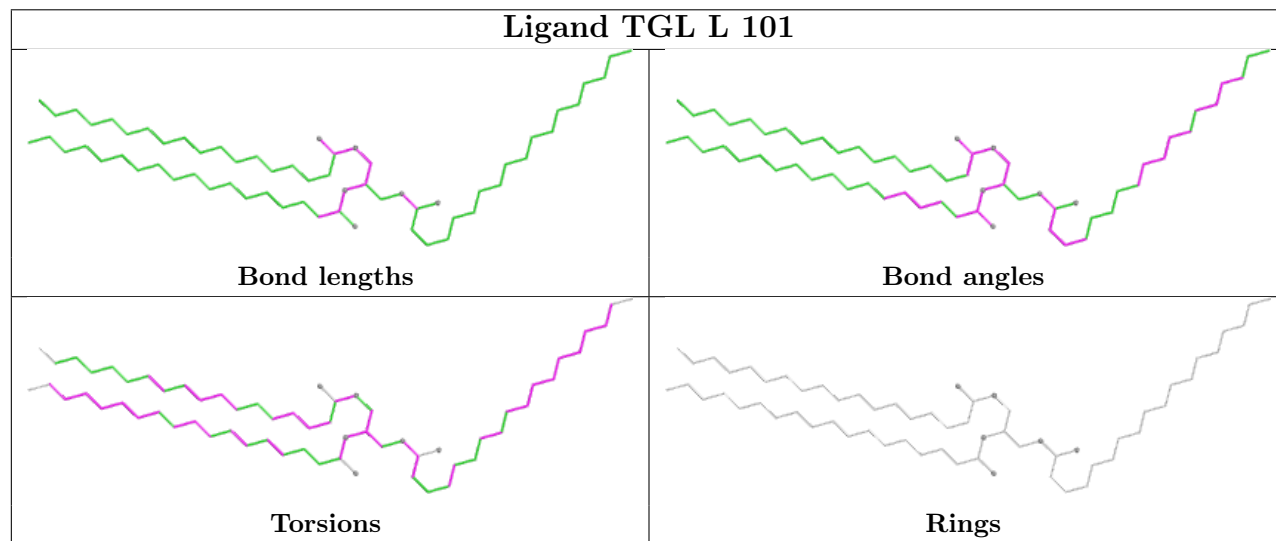
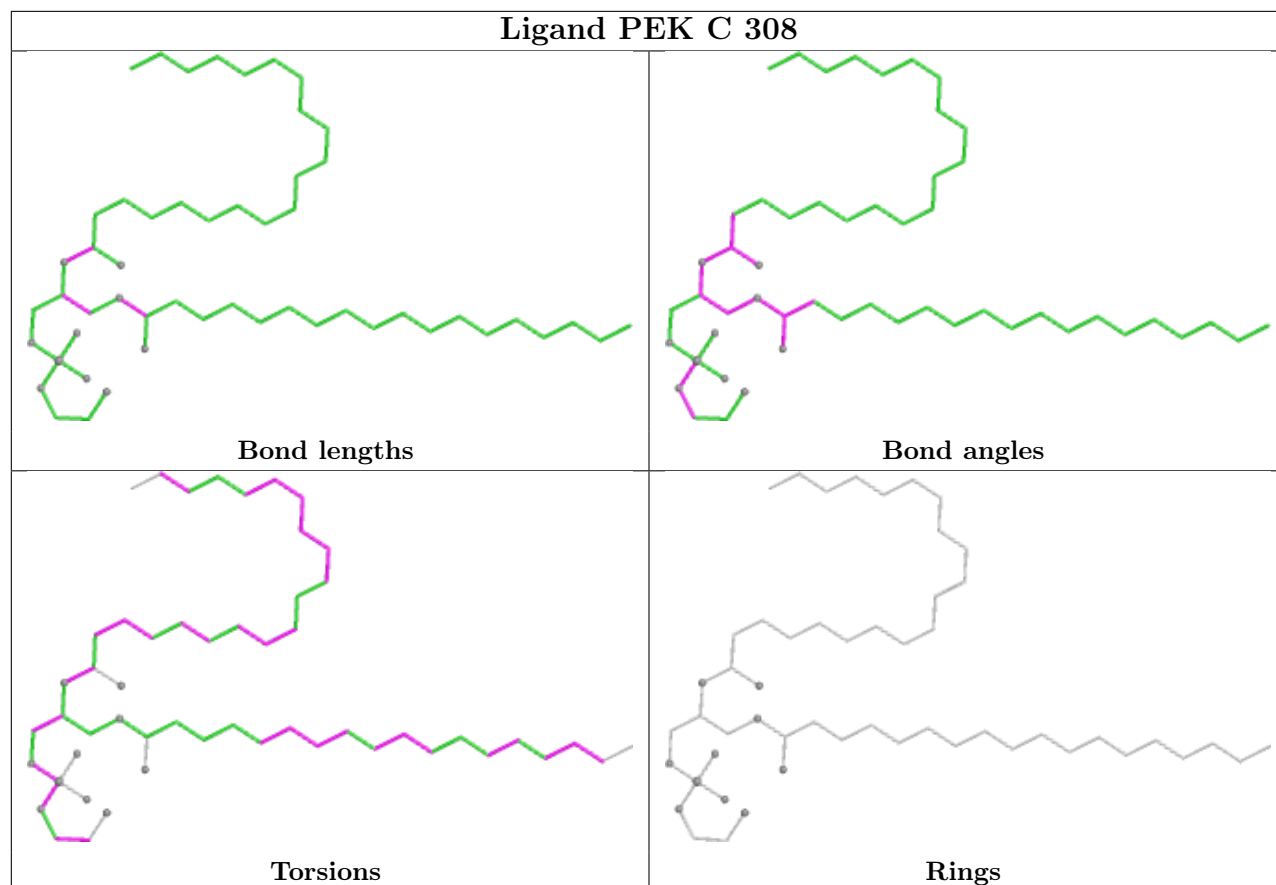
Ligand CHD W 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

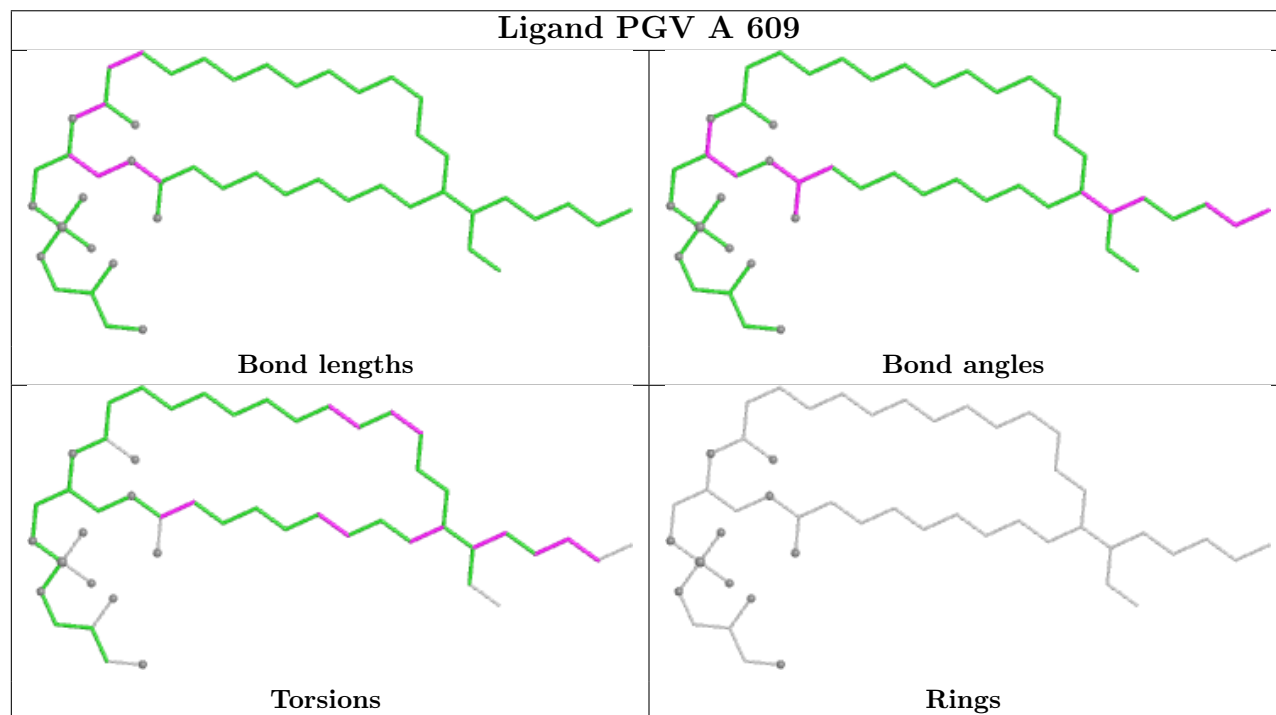
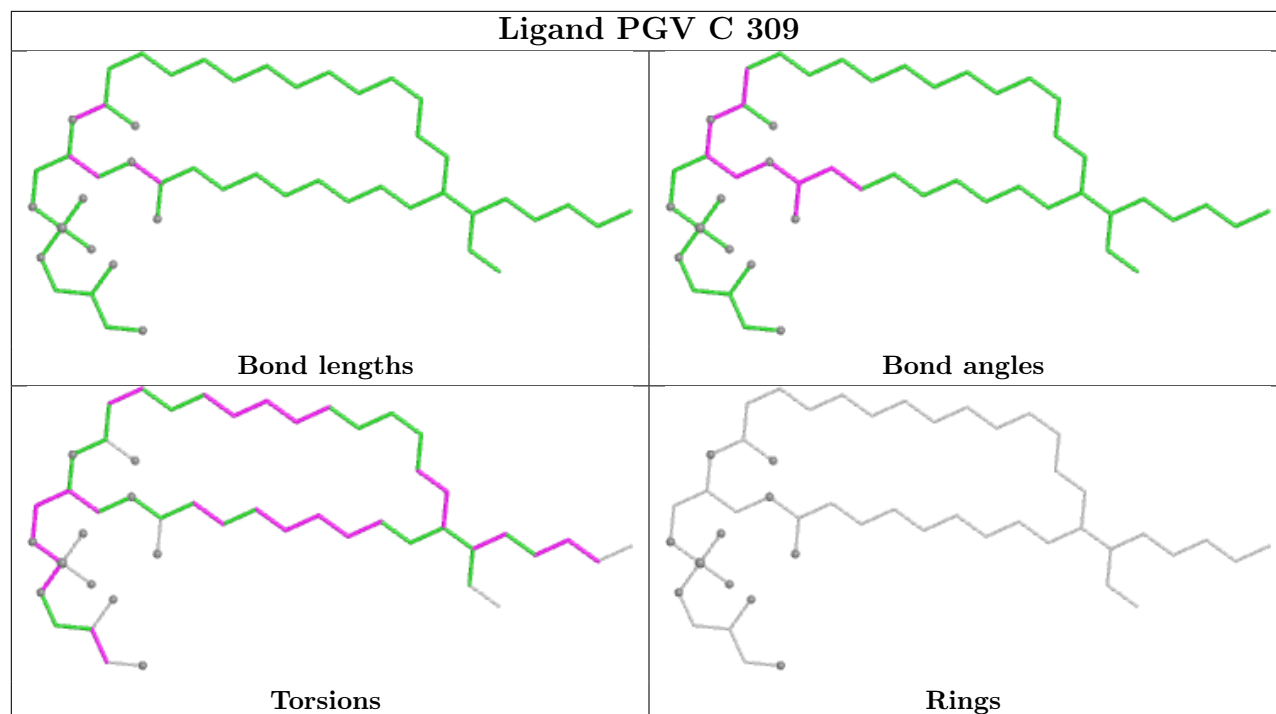


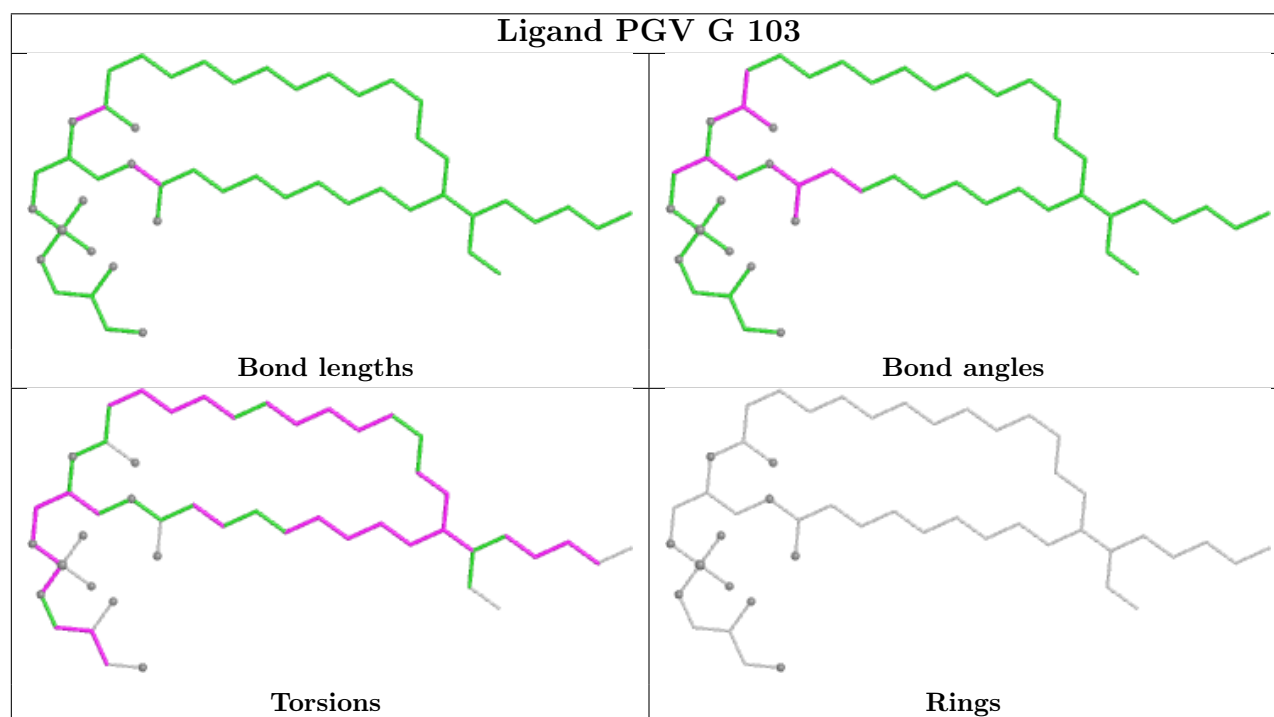
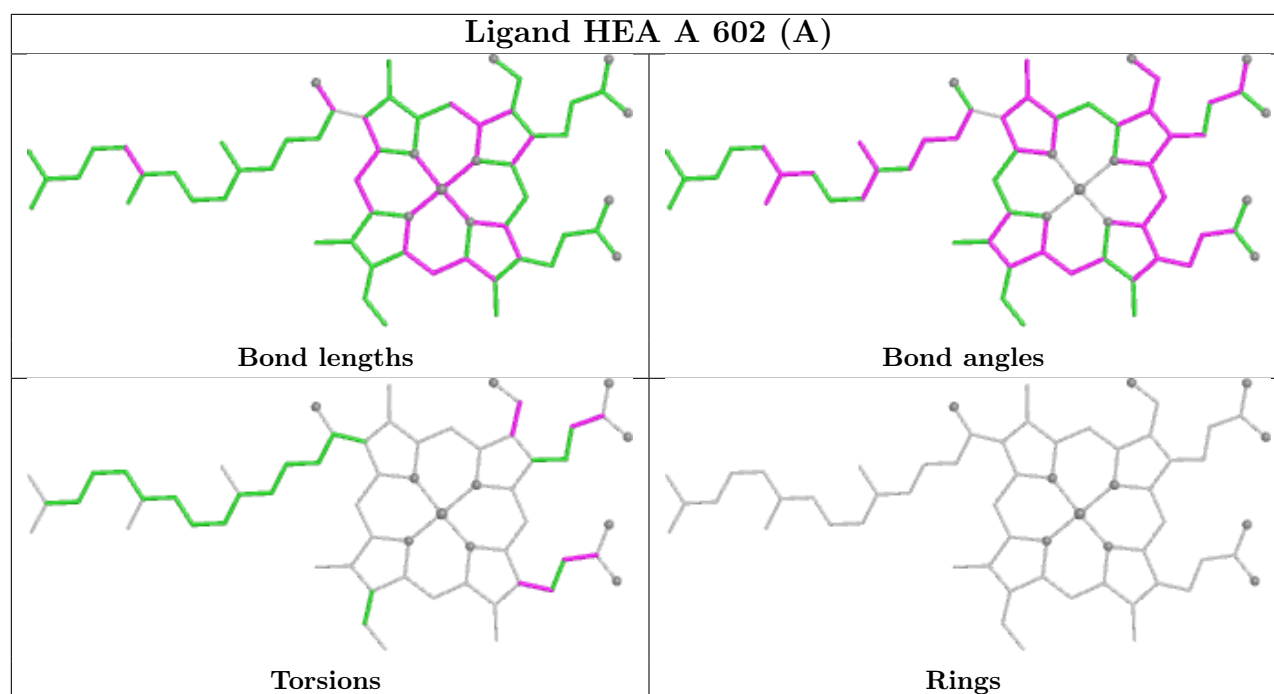


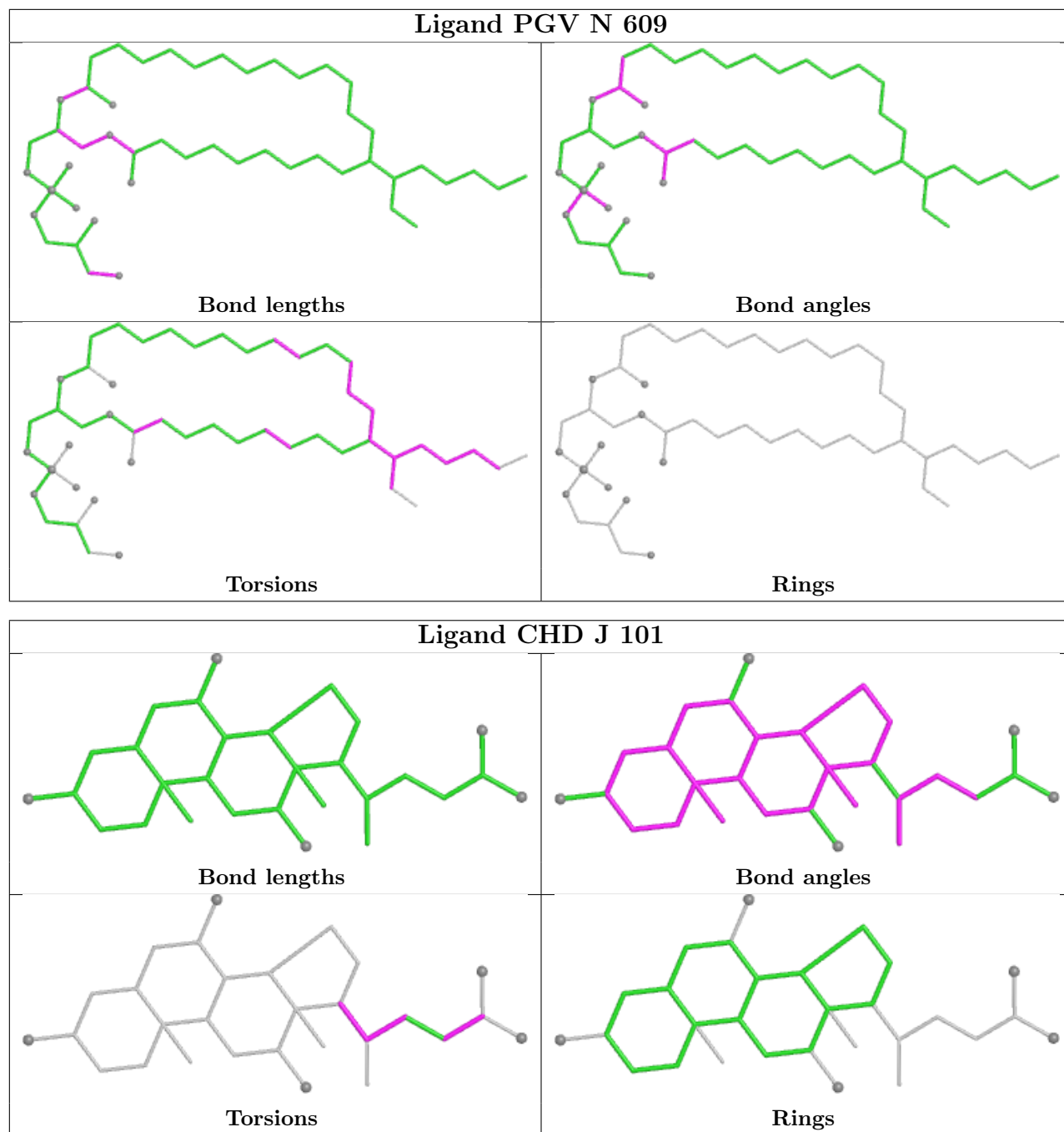


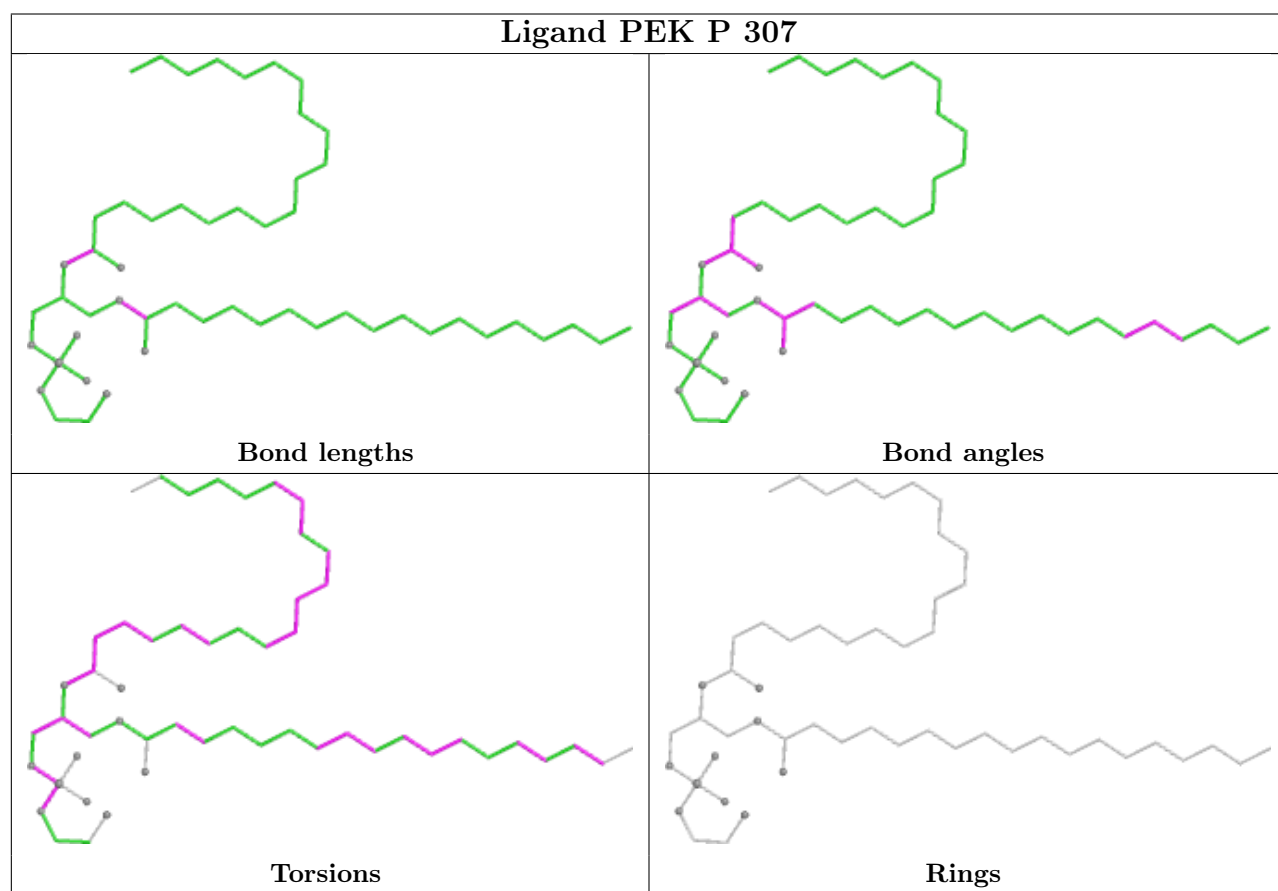
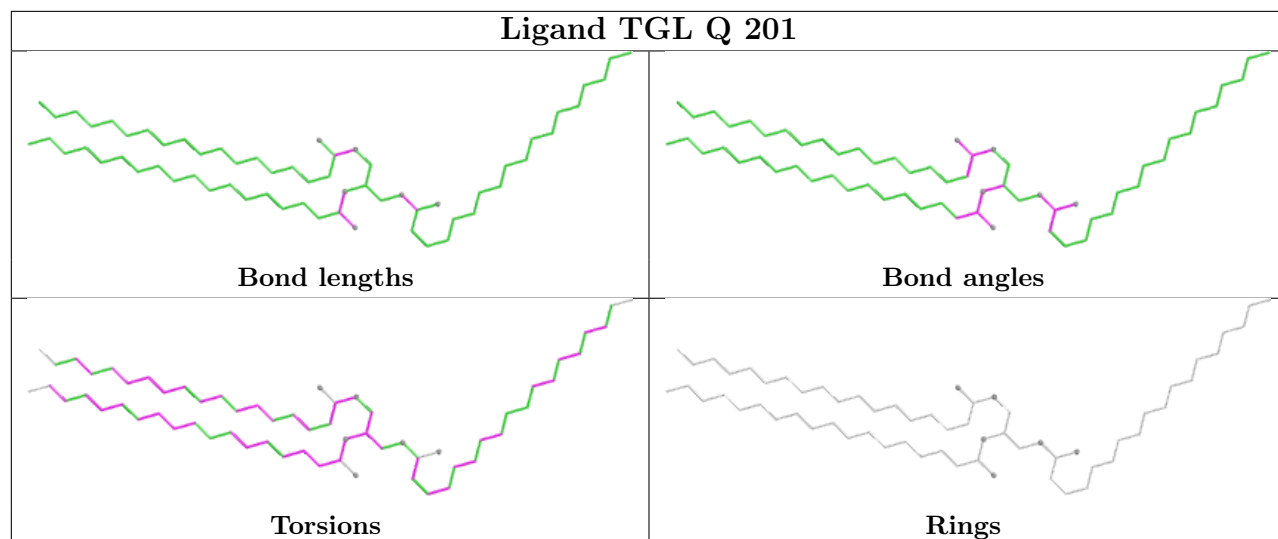


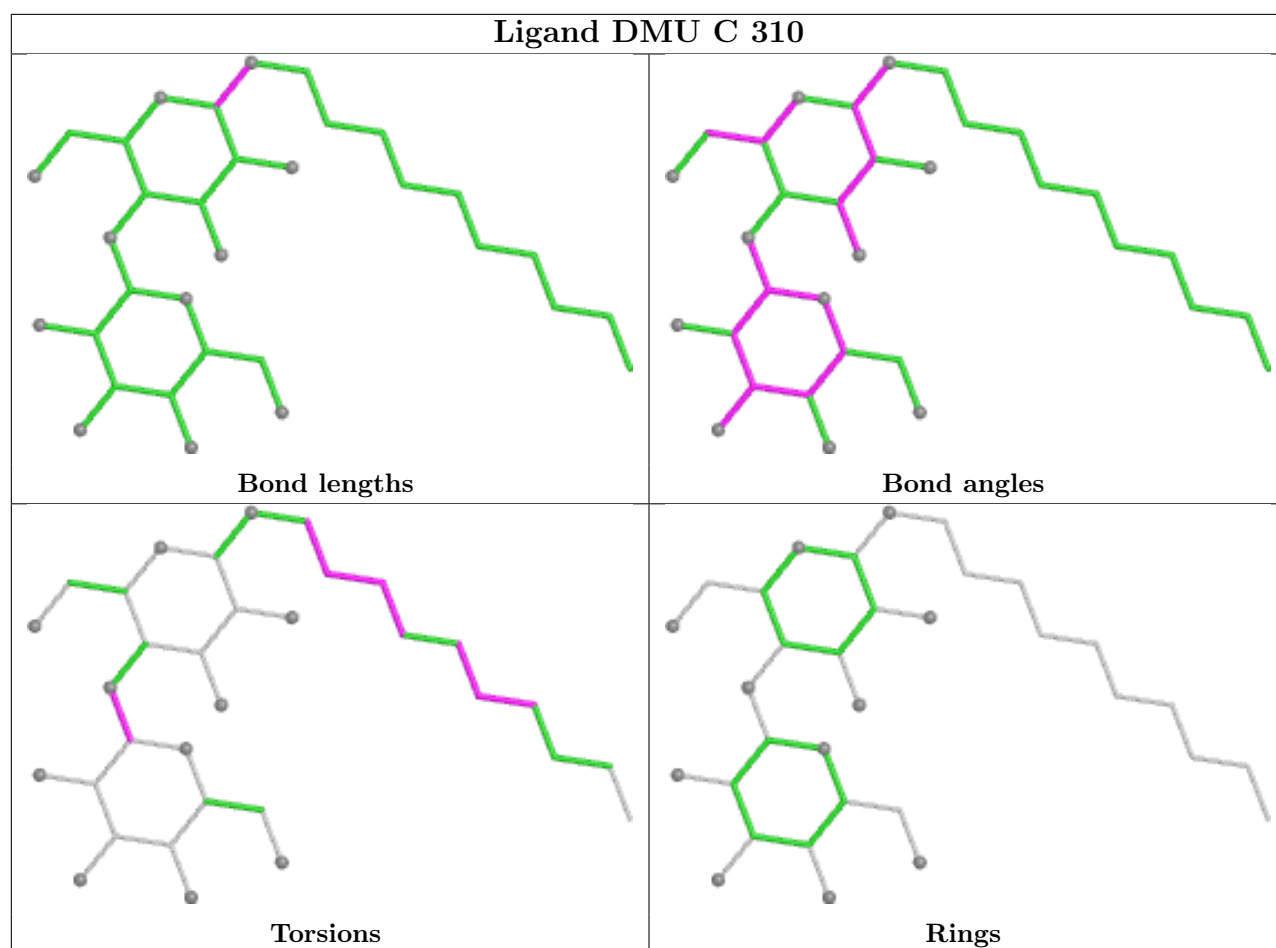


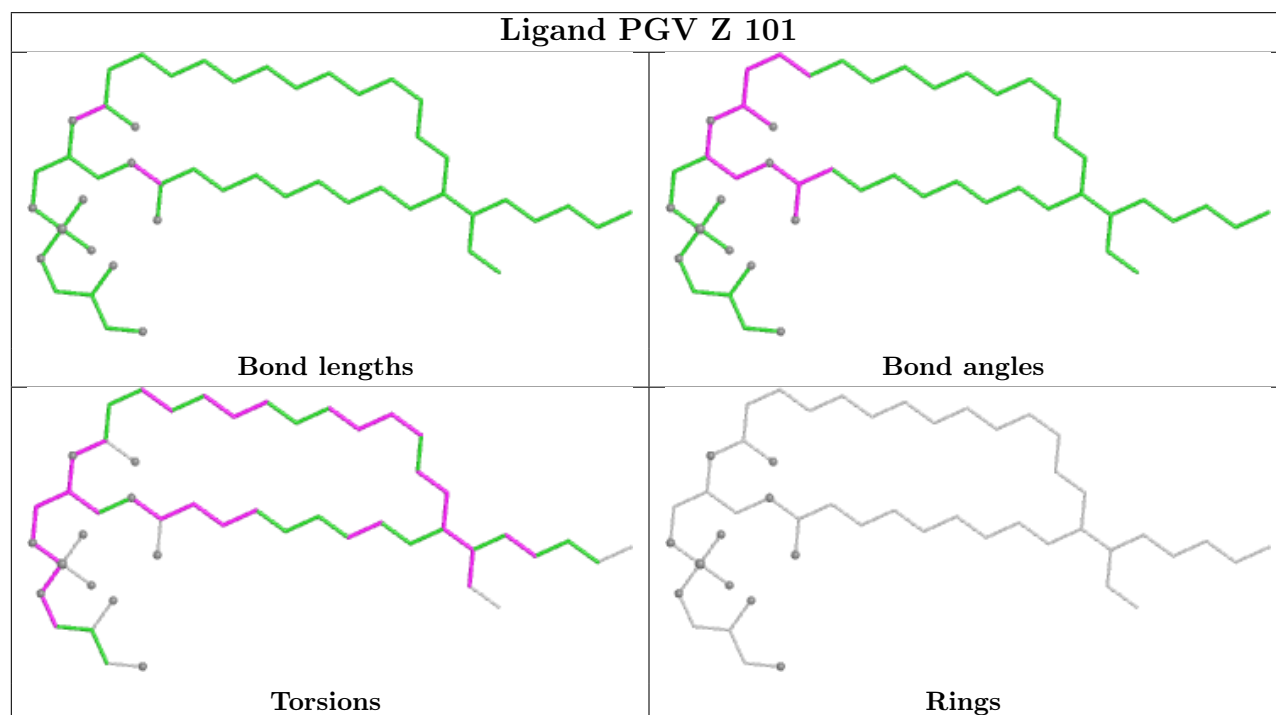
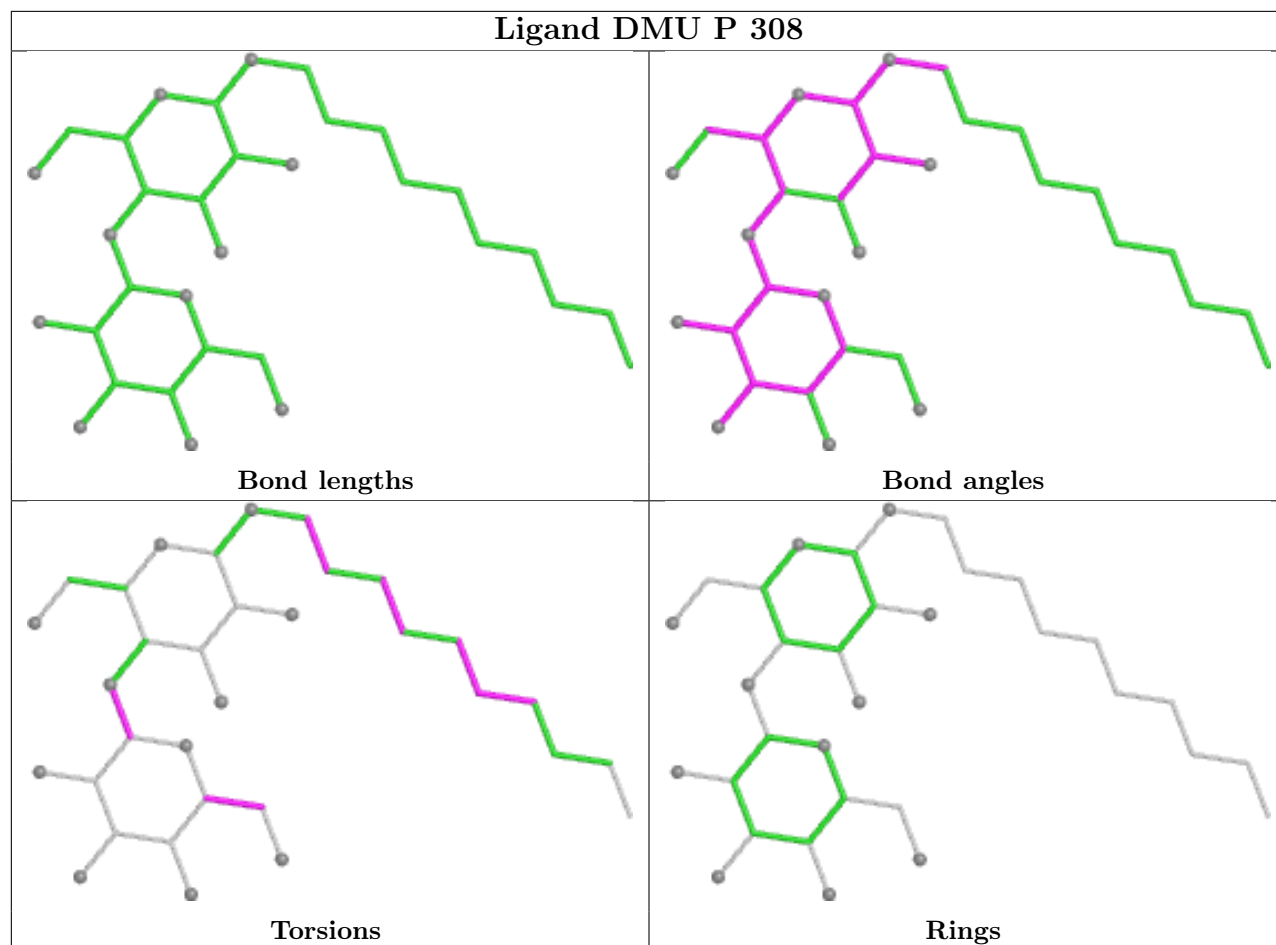


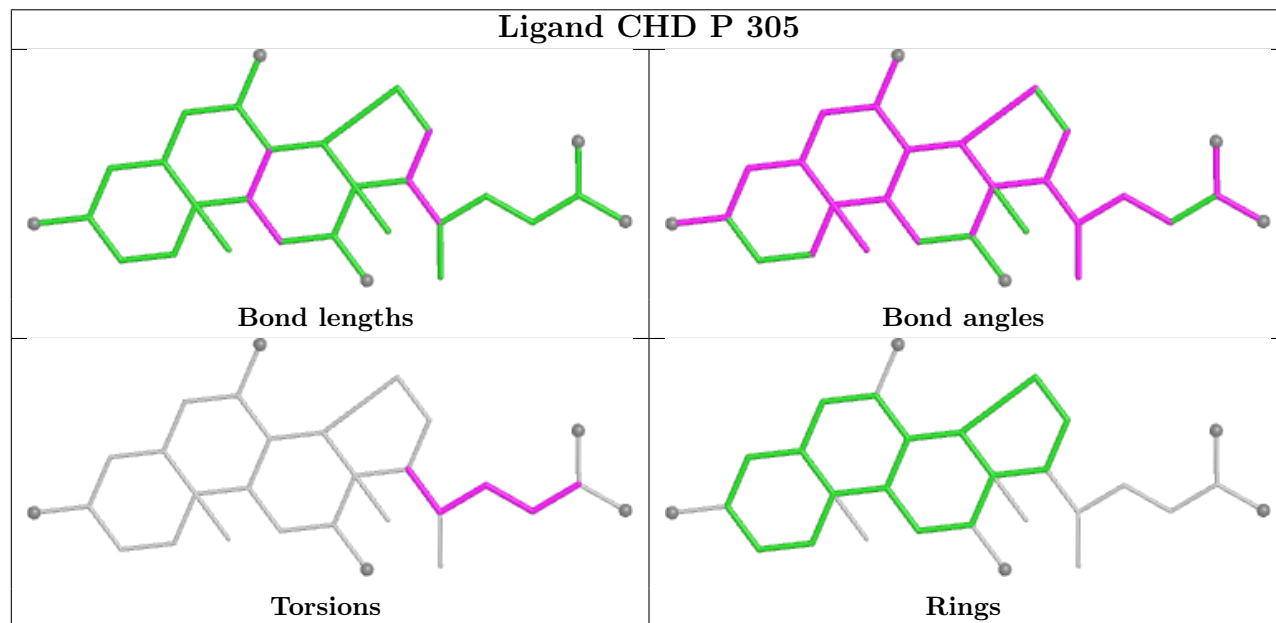
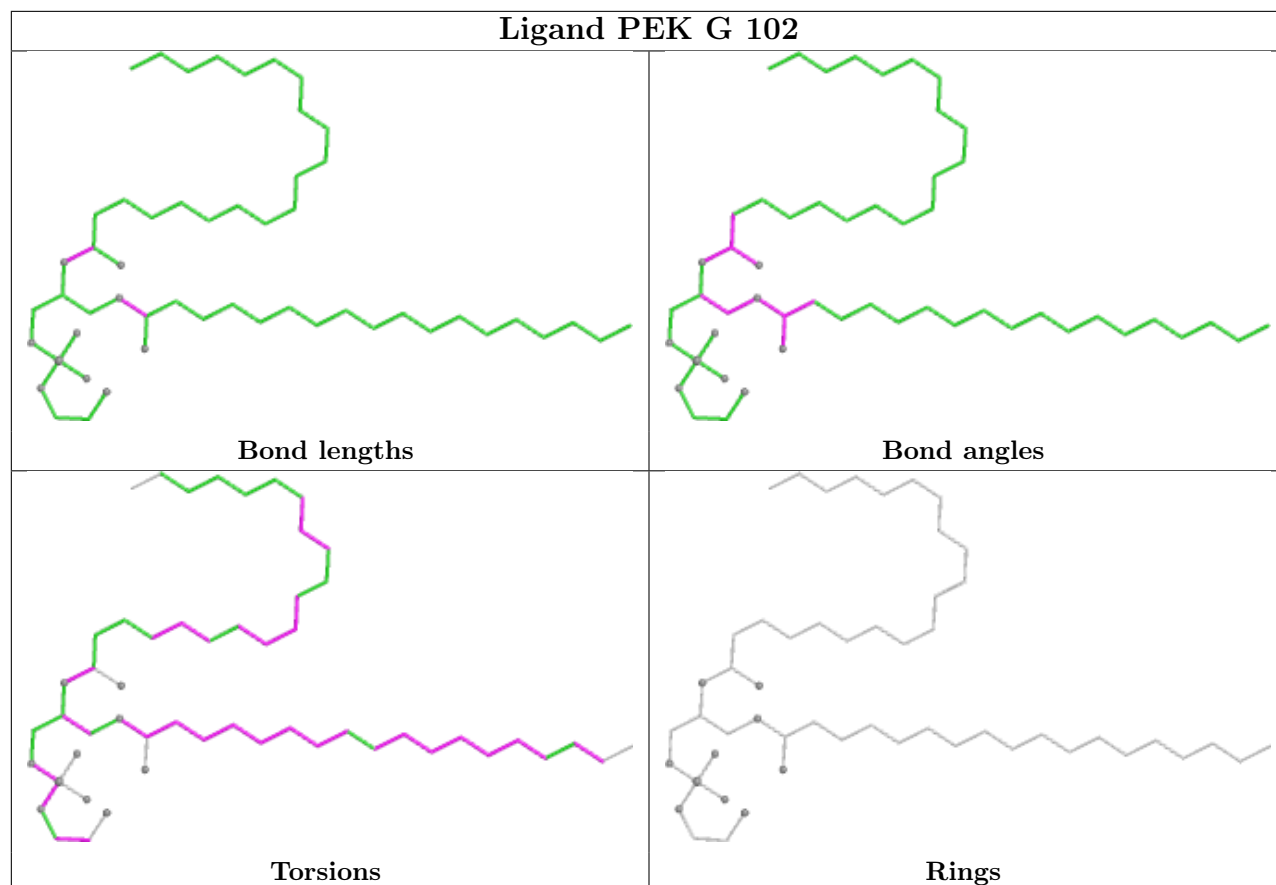


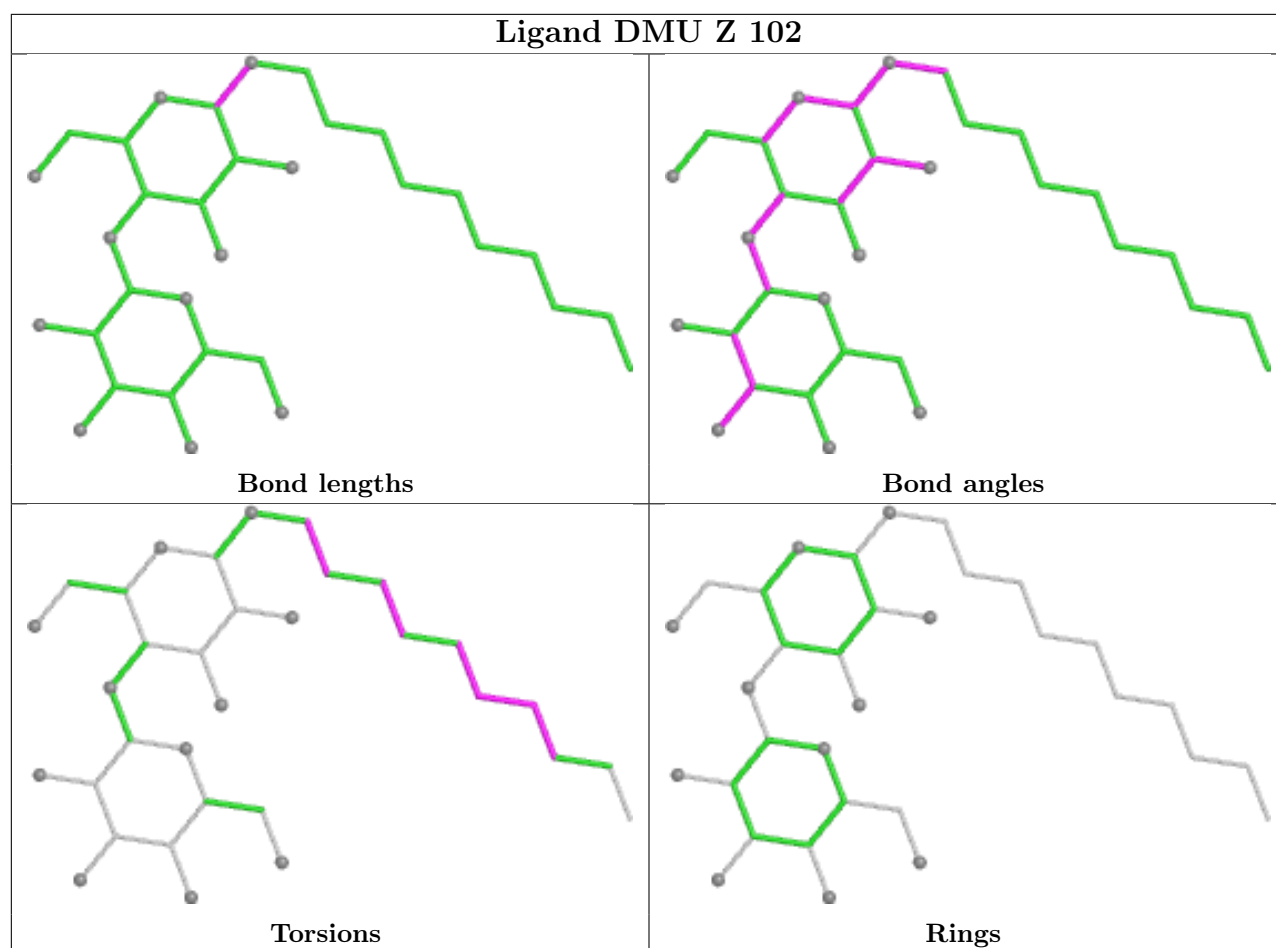


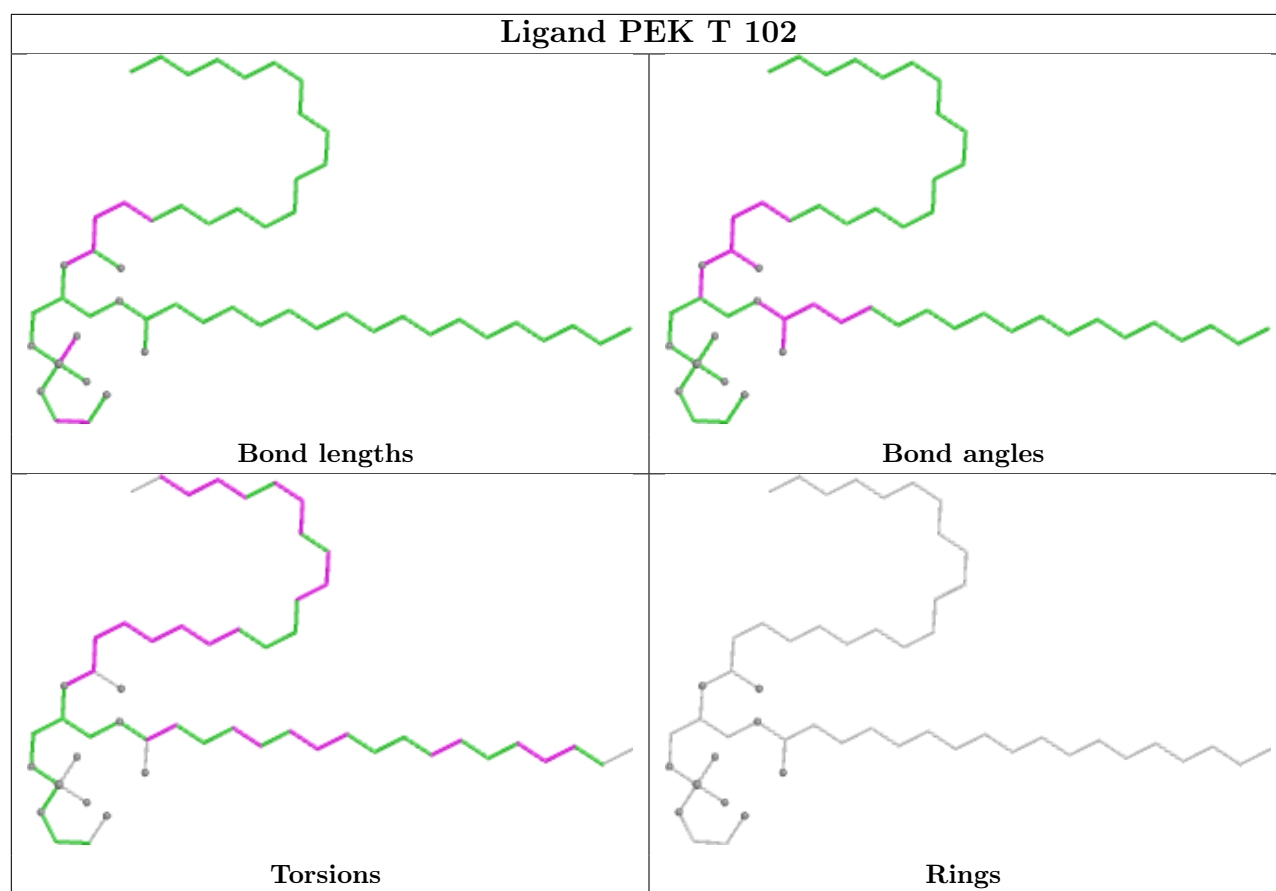


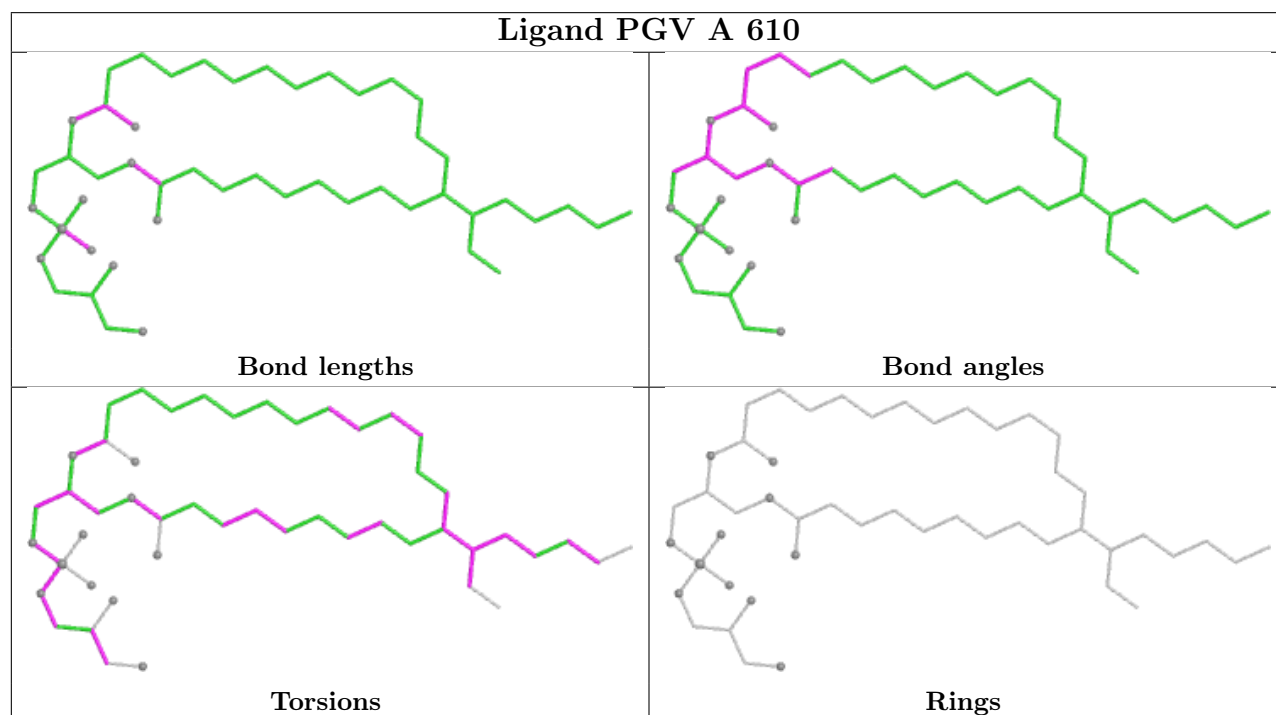
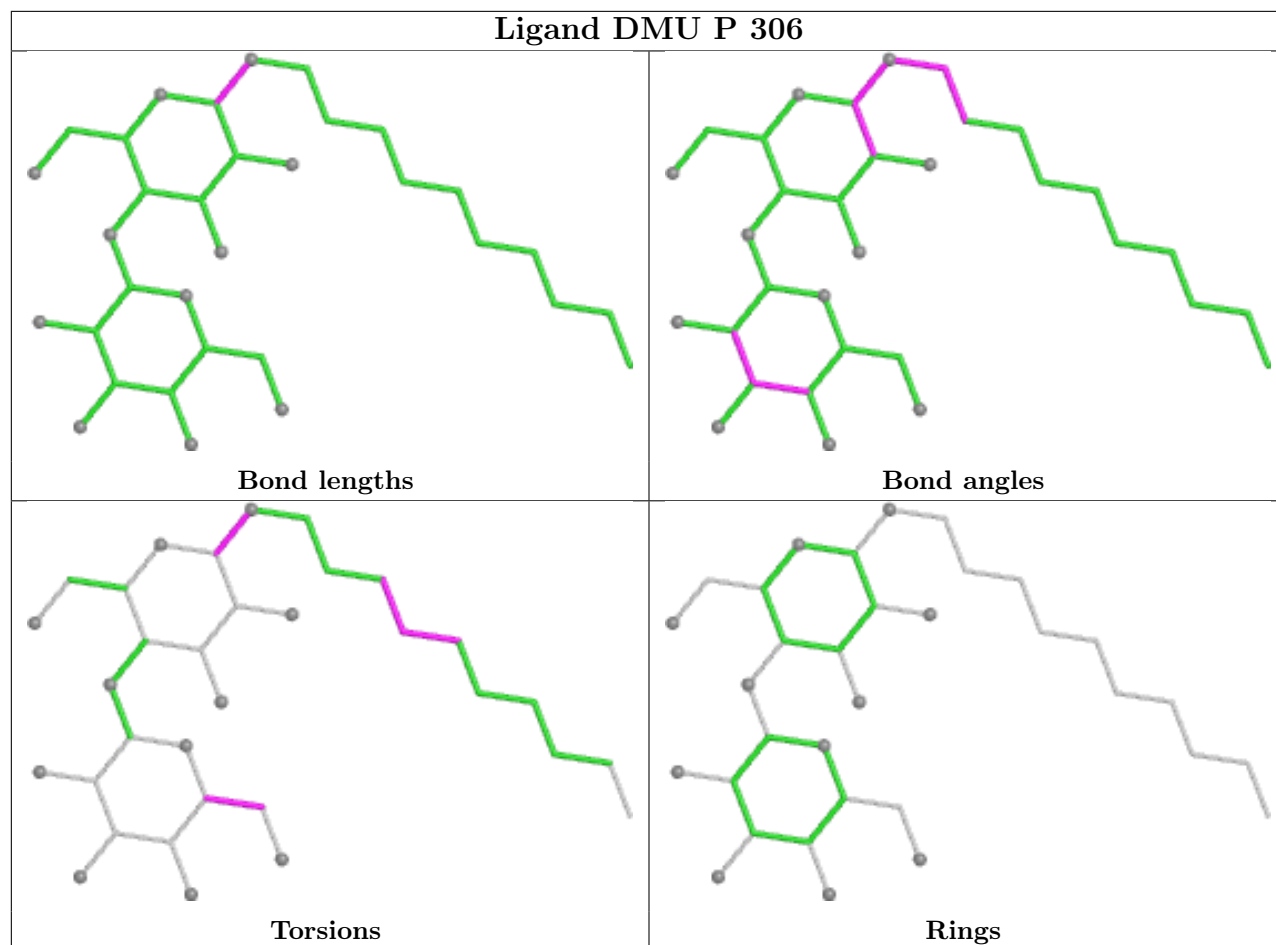


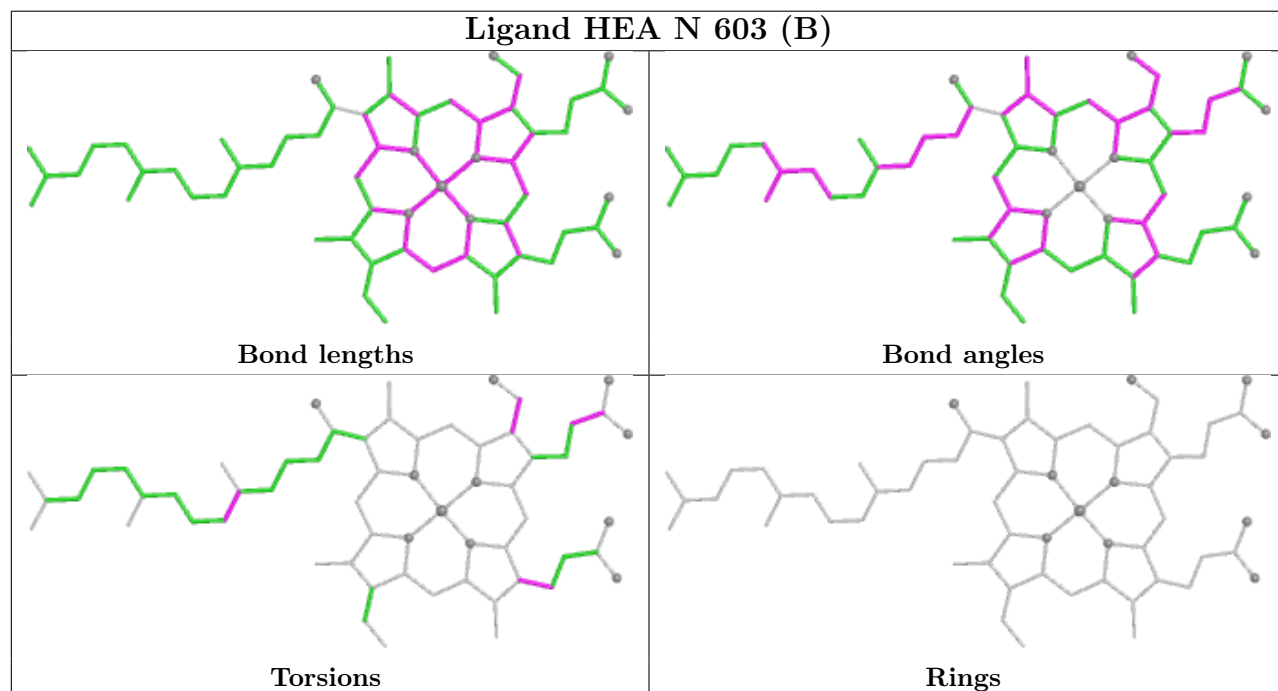
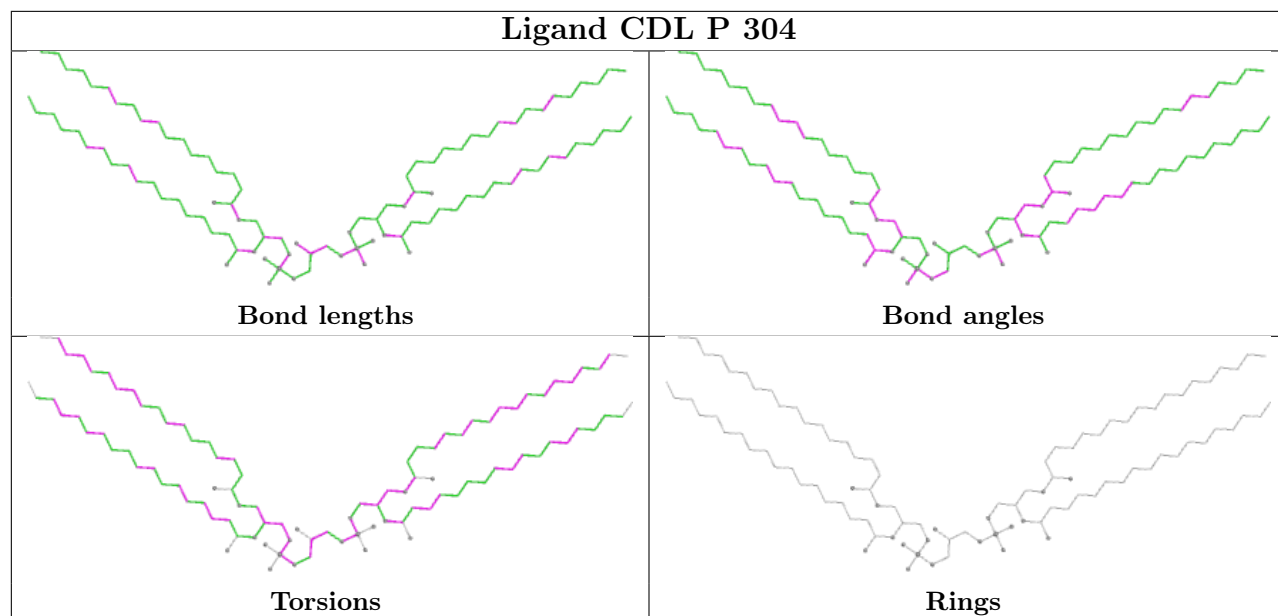


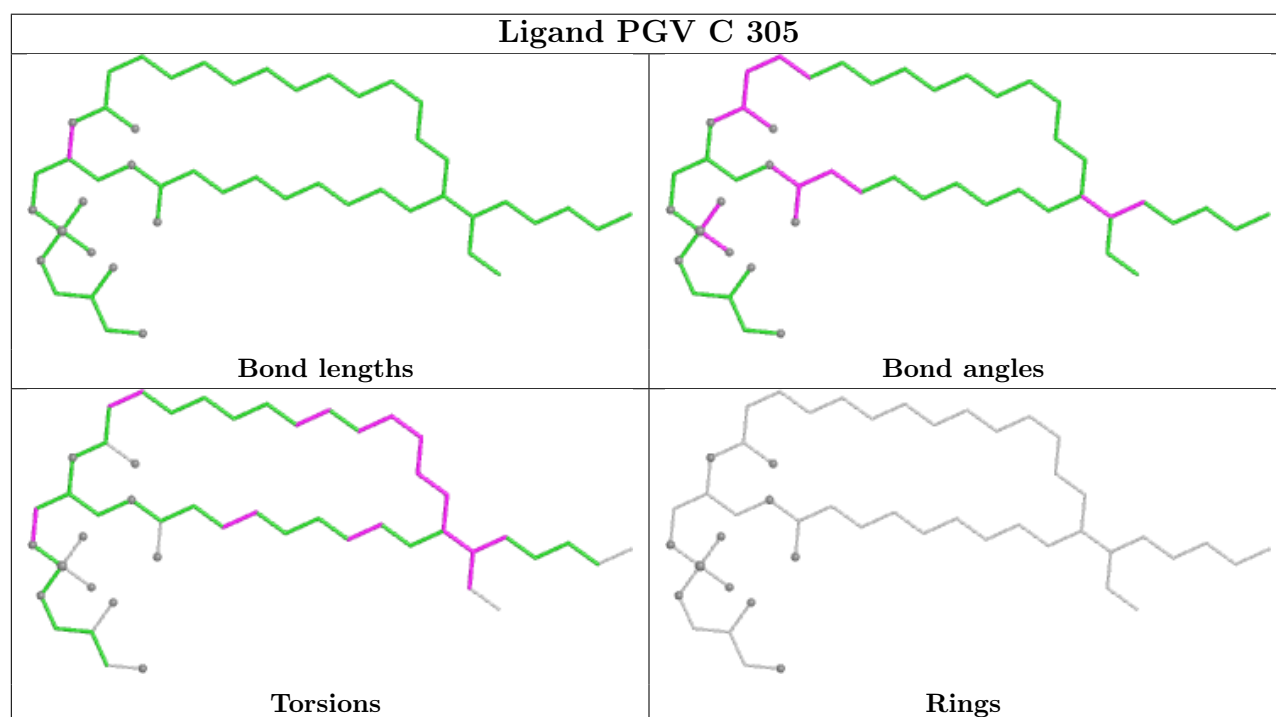
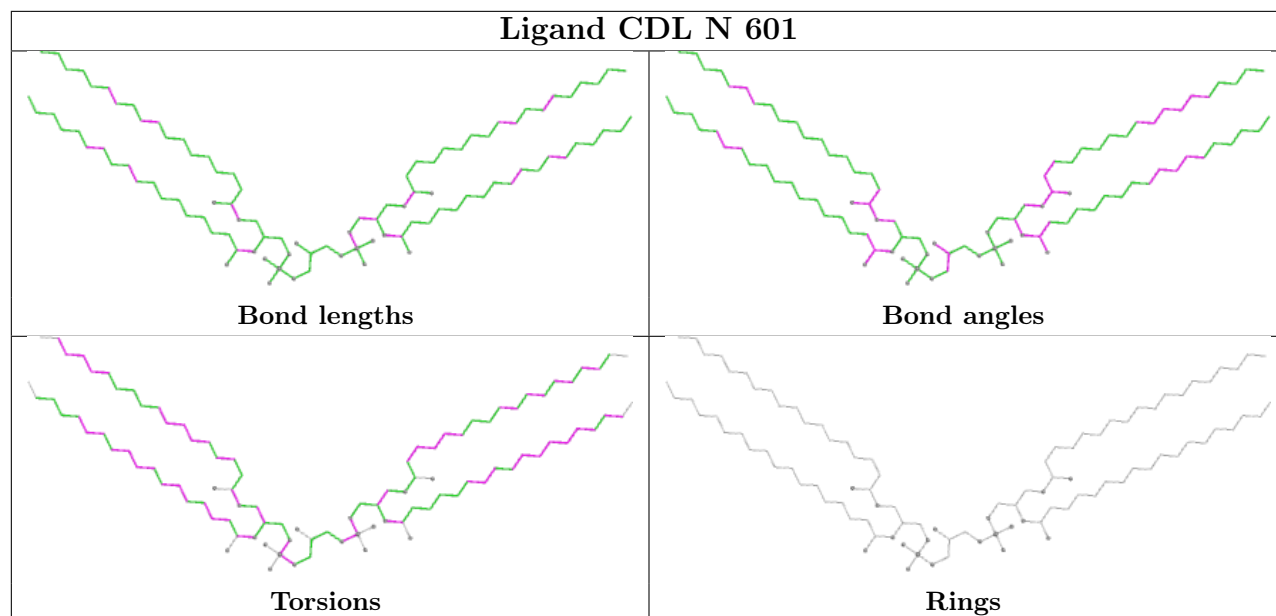


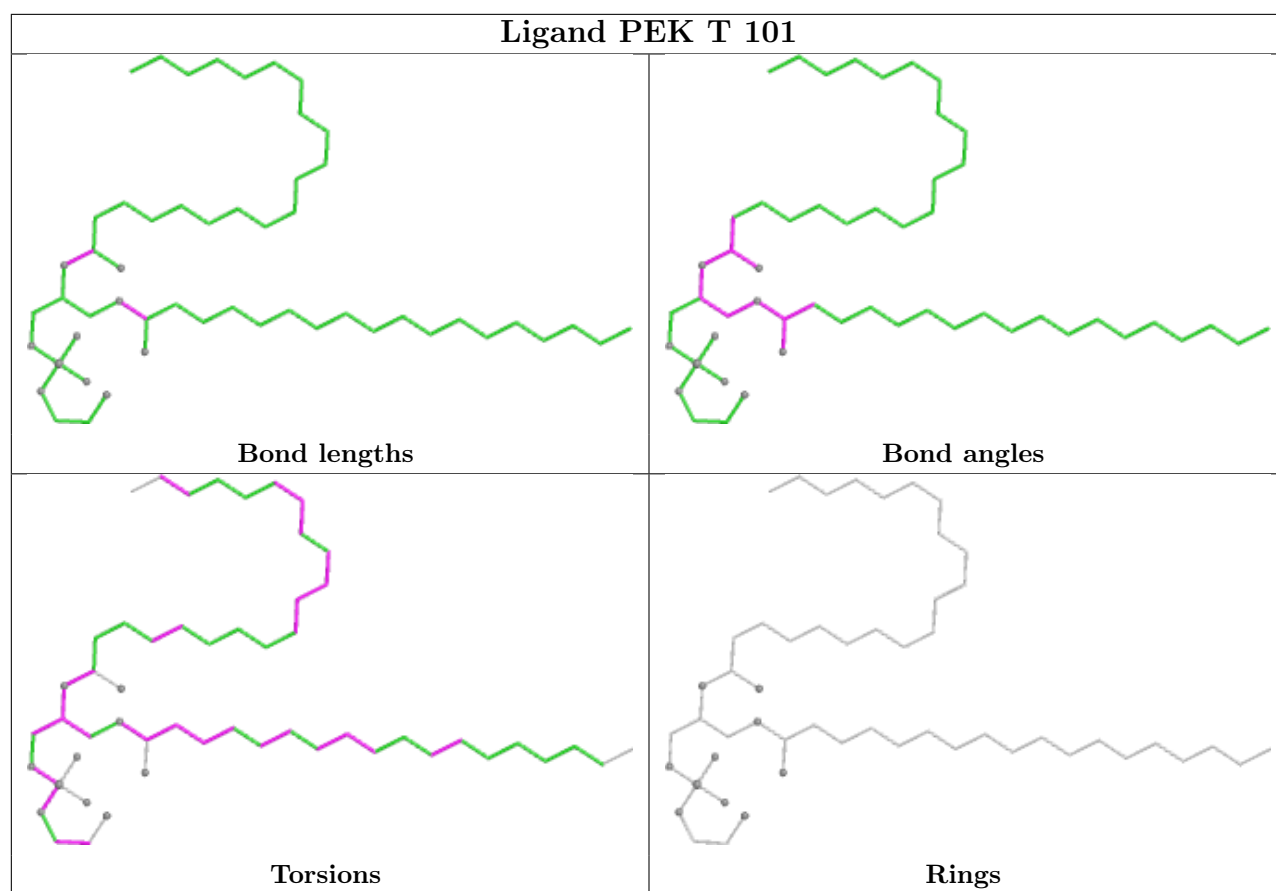


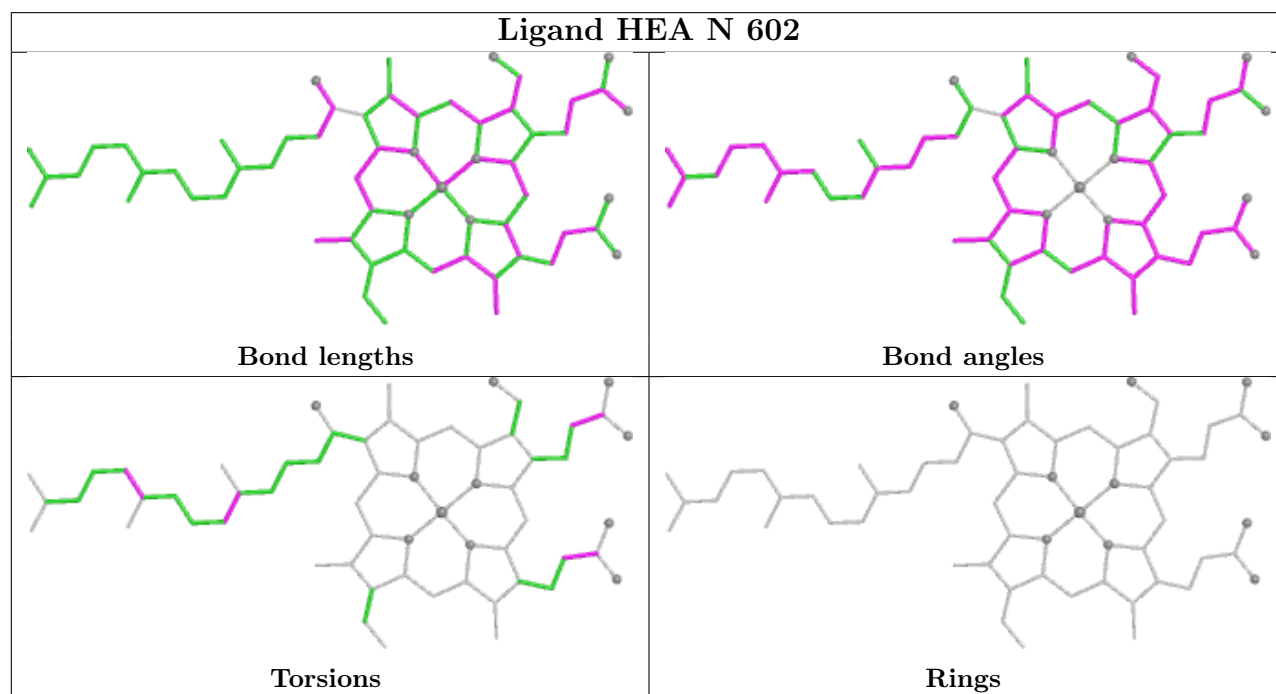
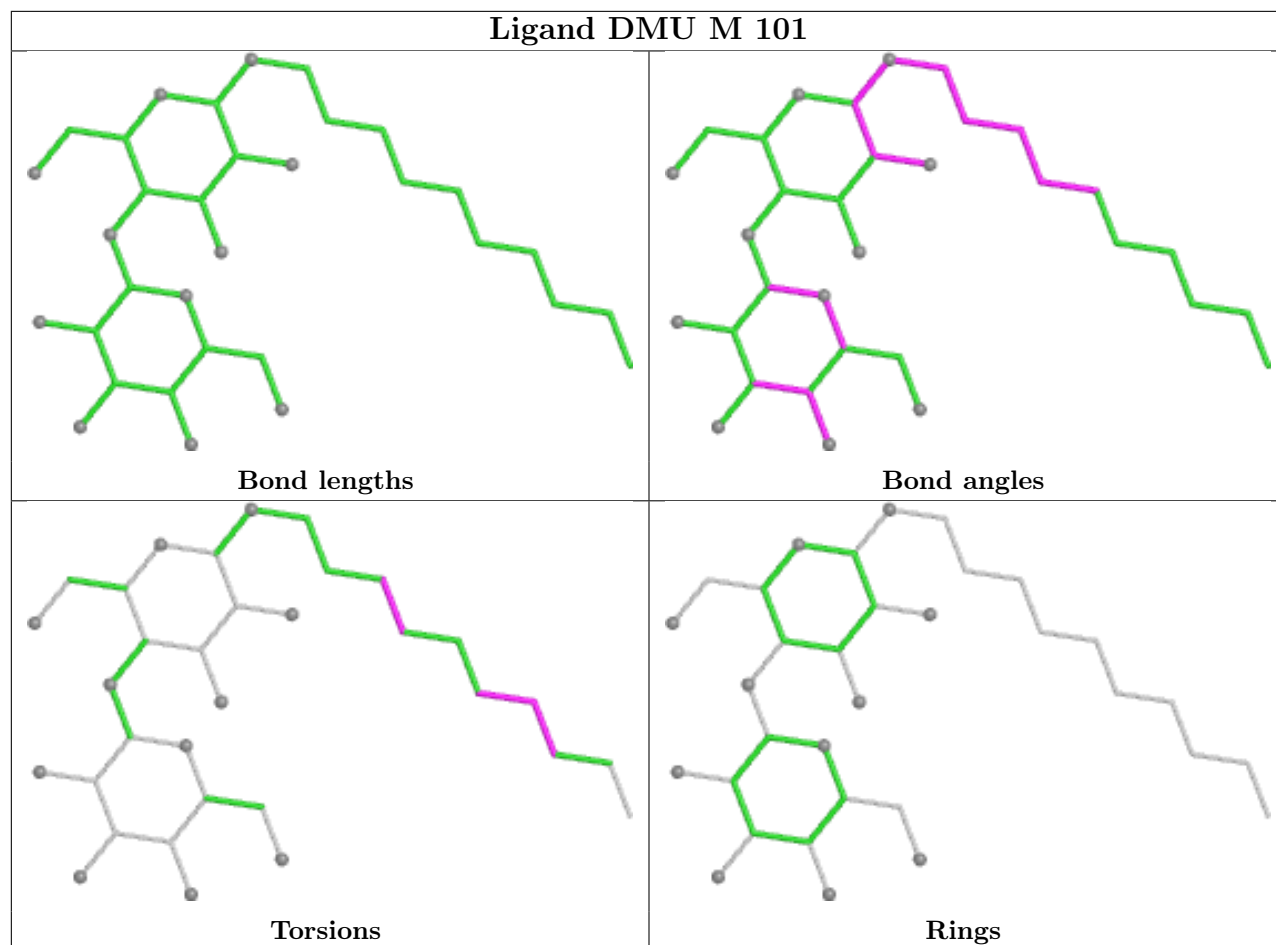


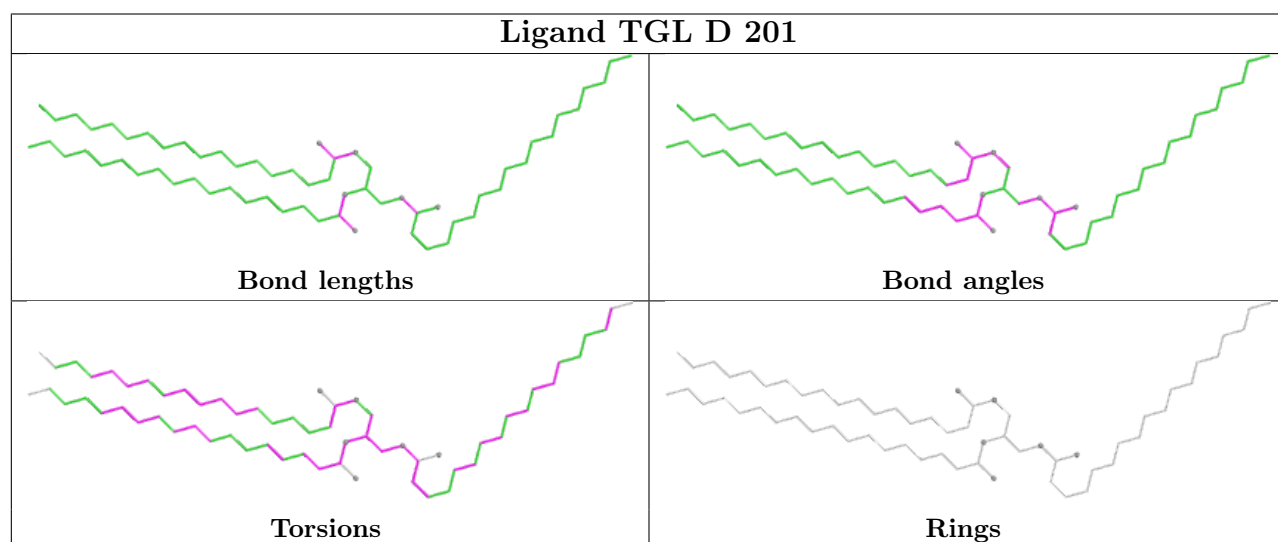
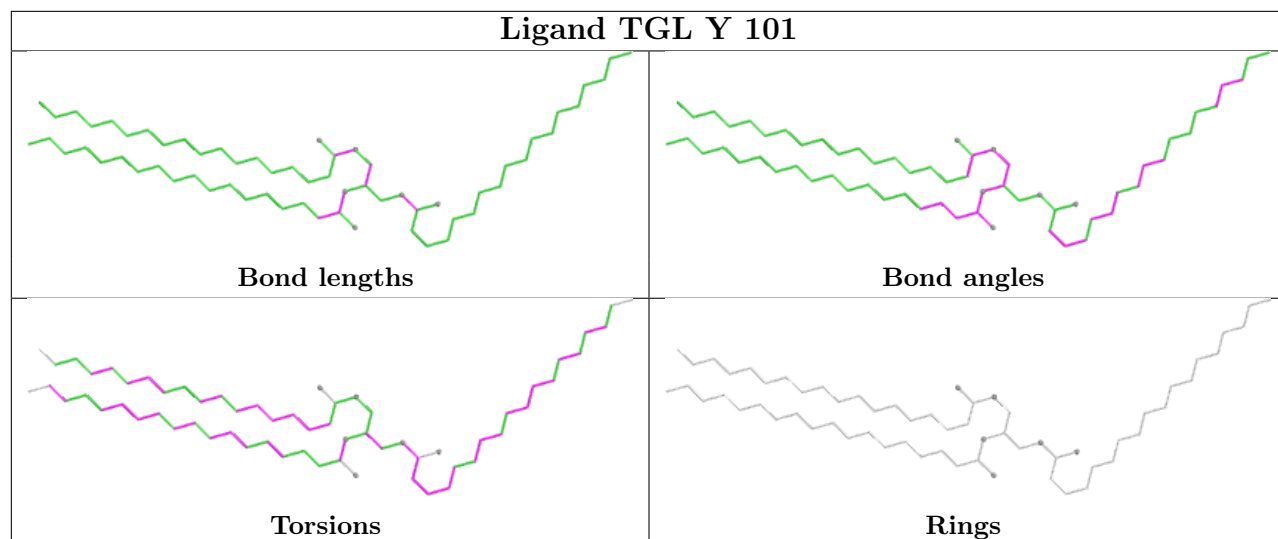


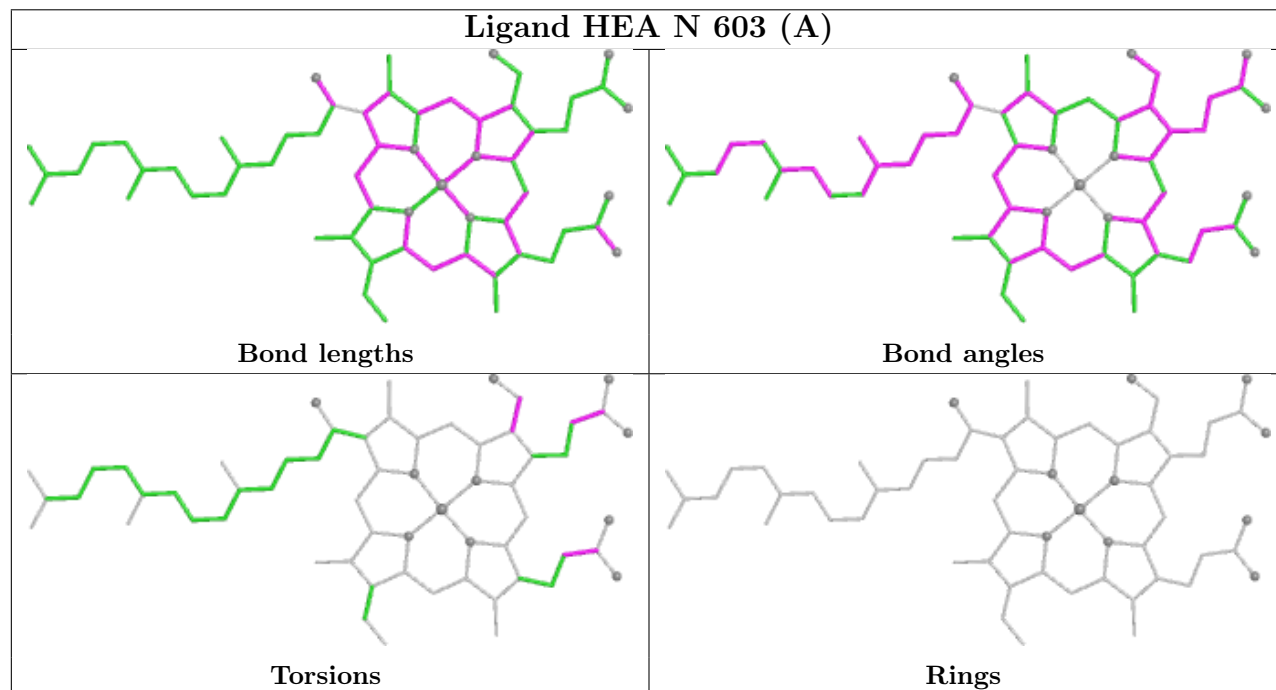
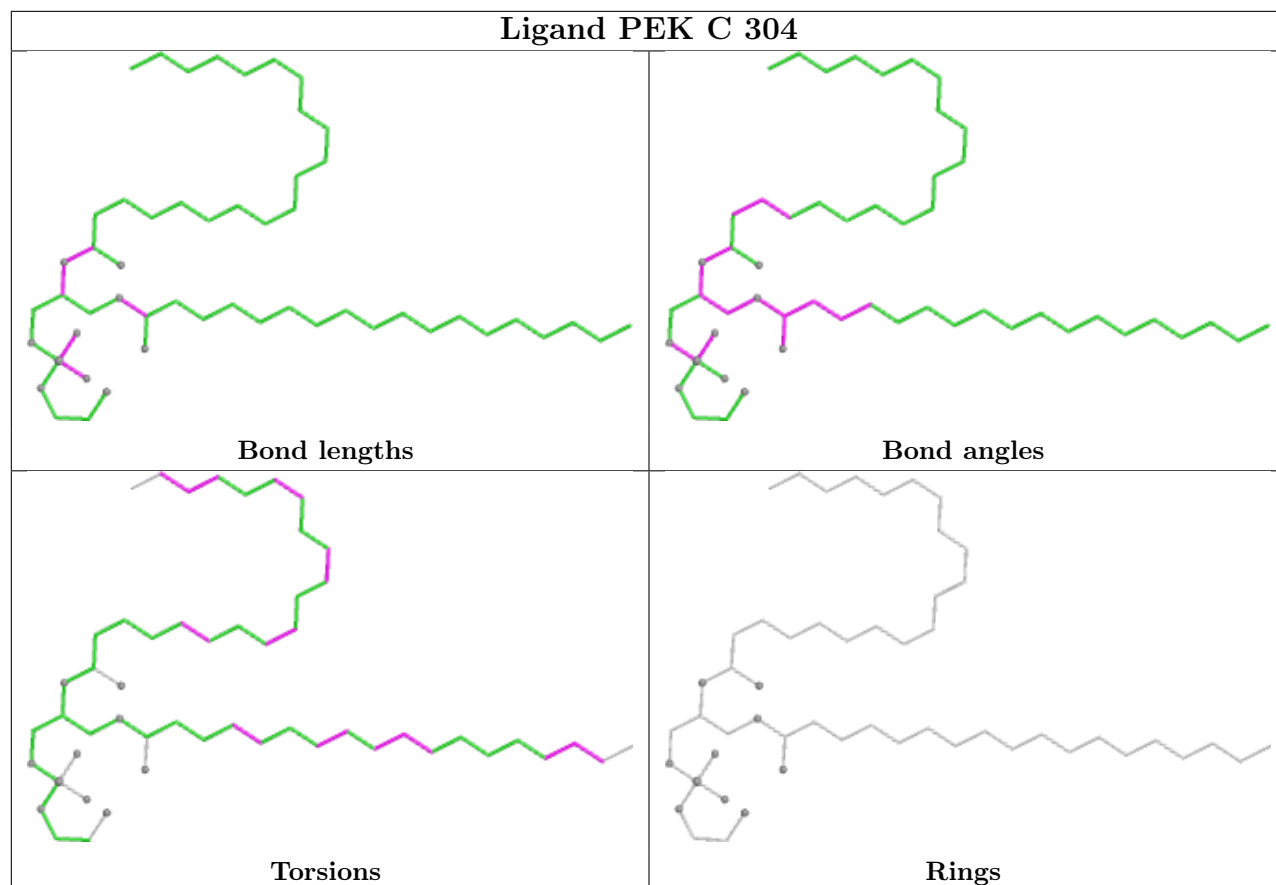


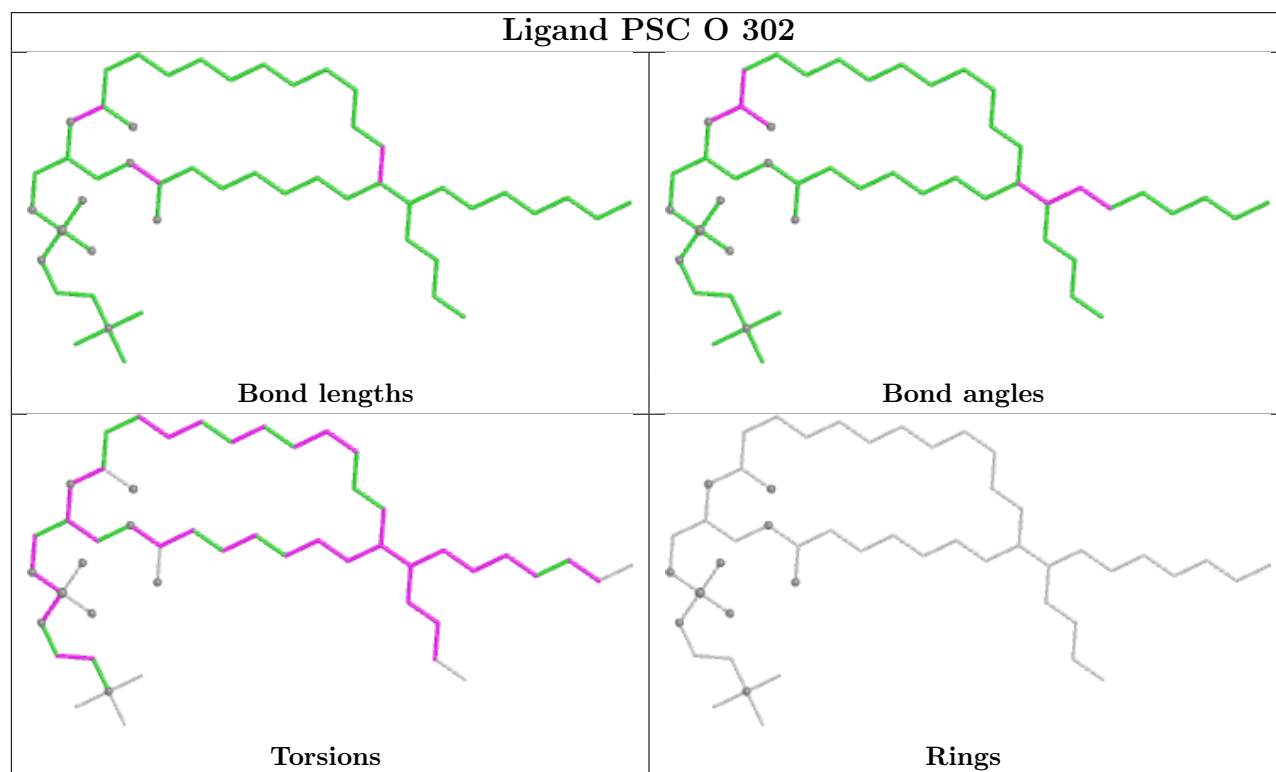
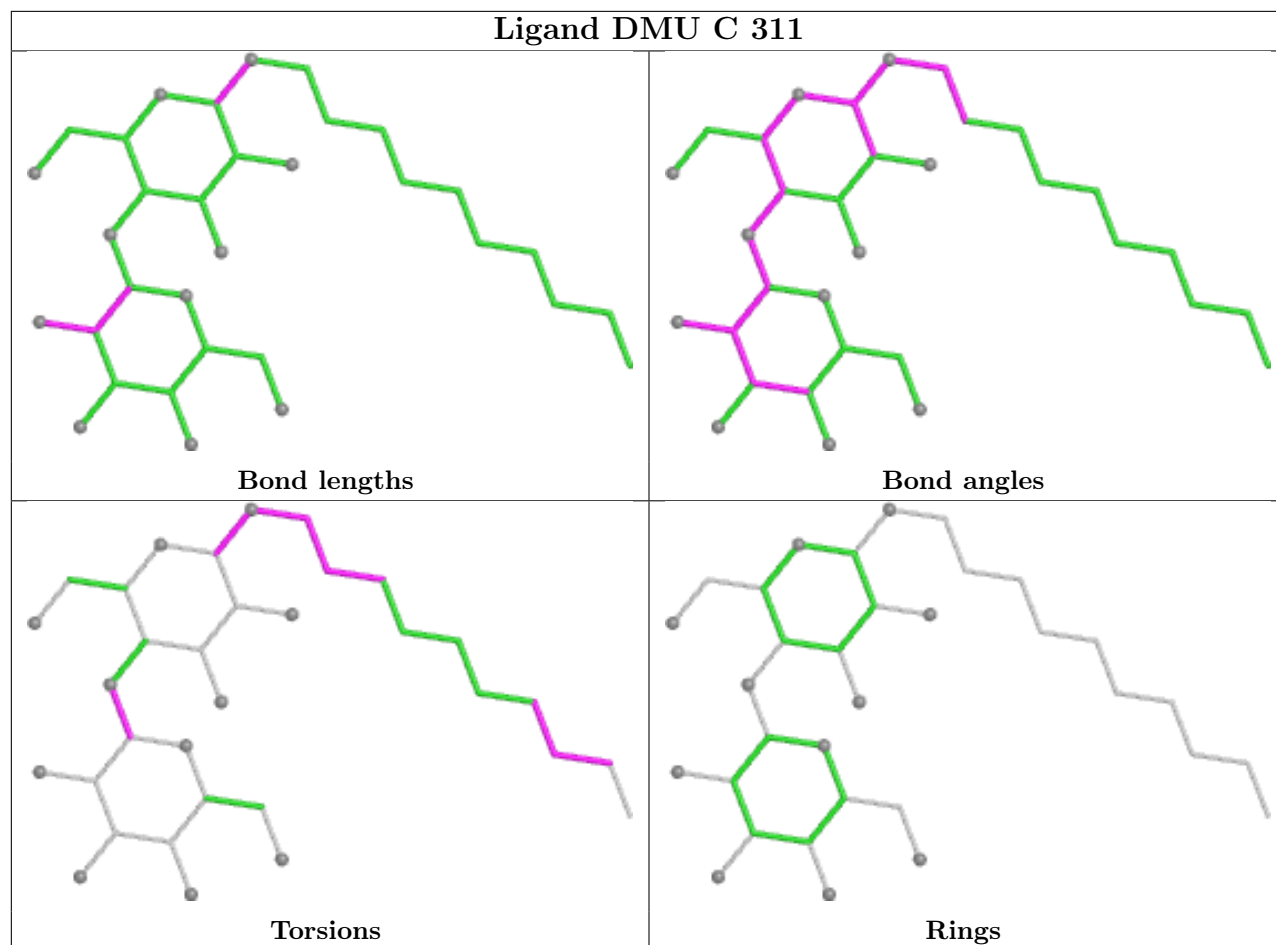


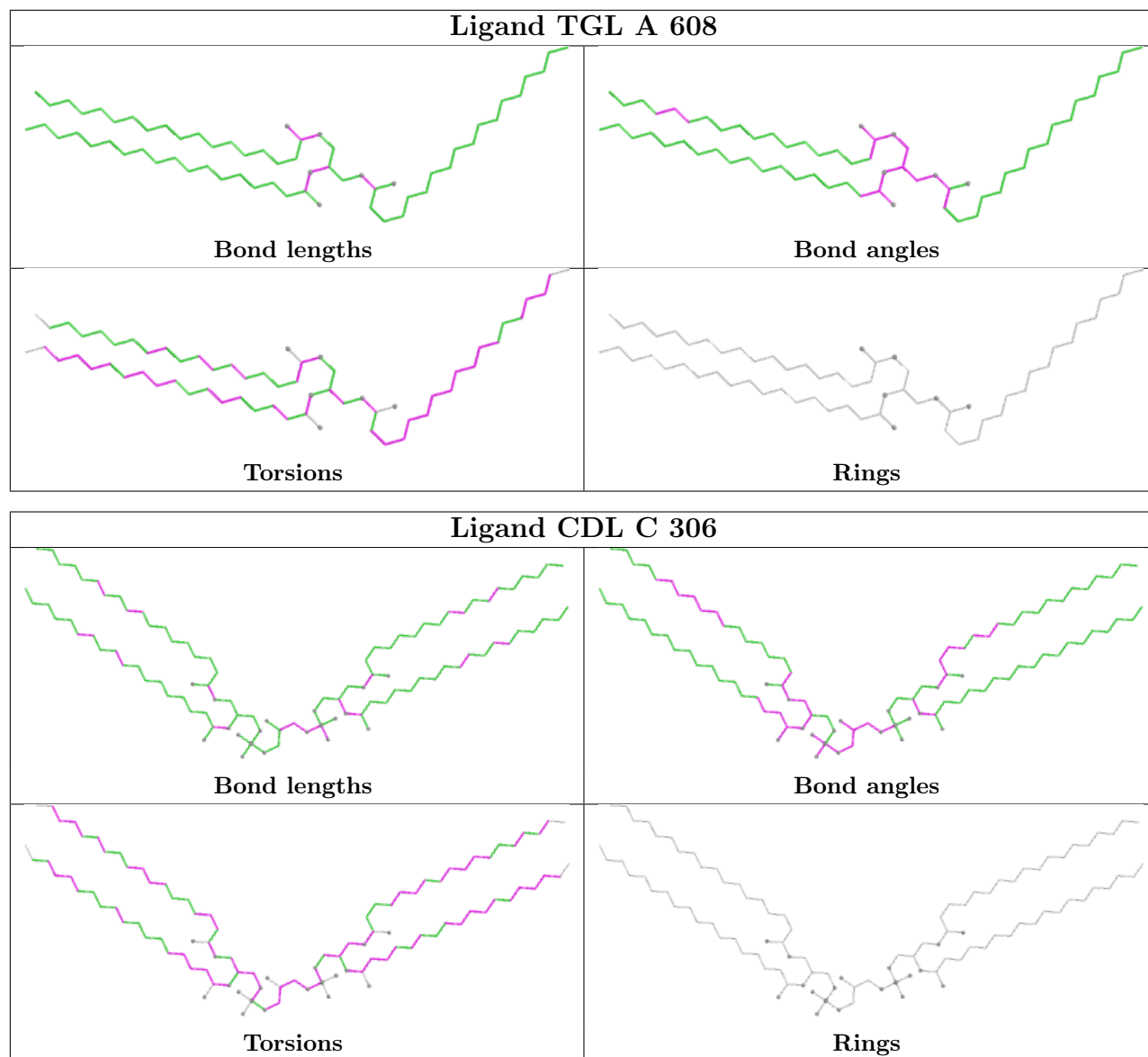


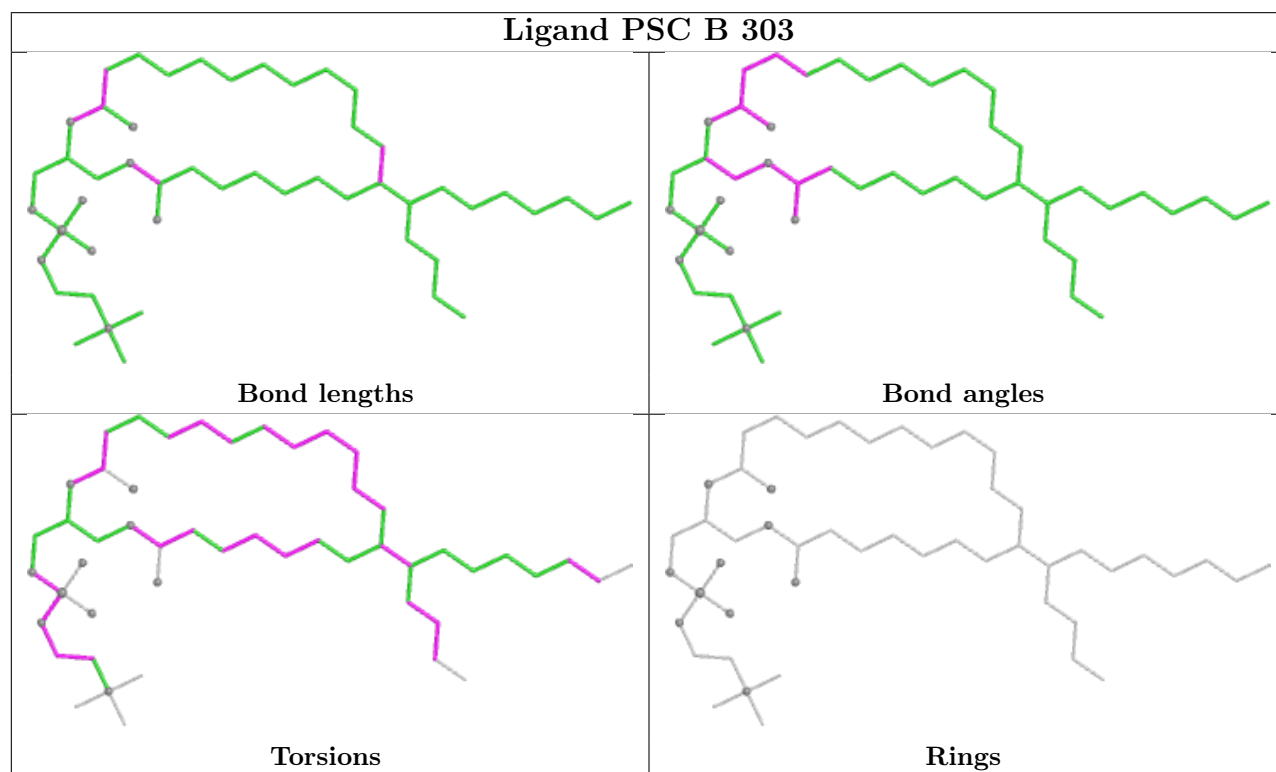
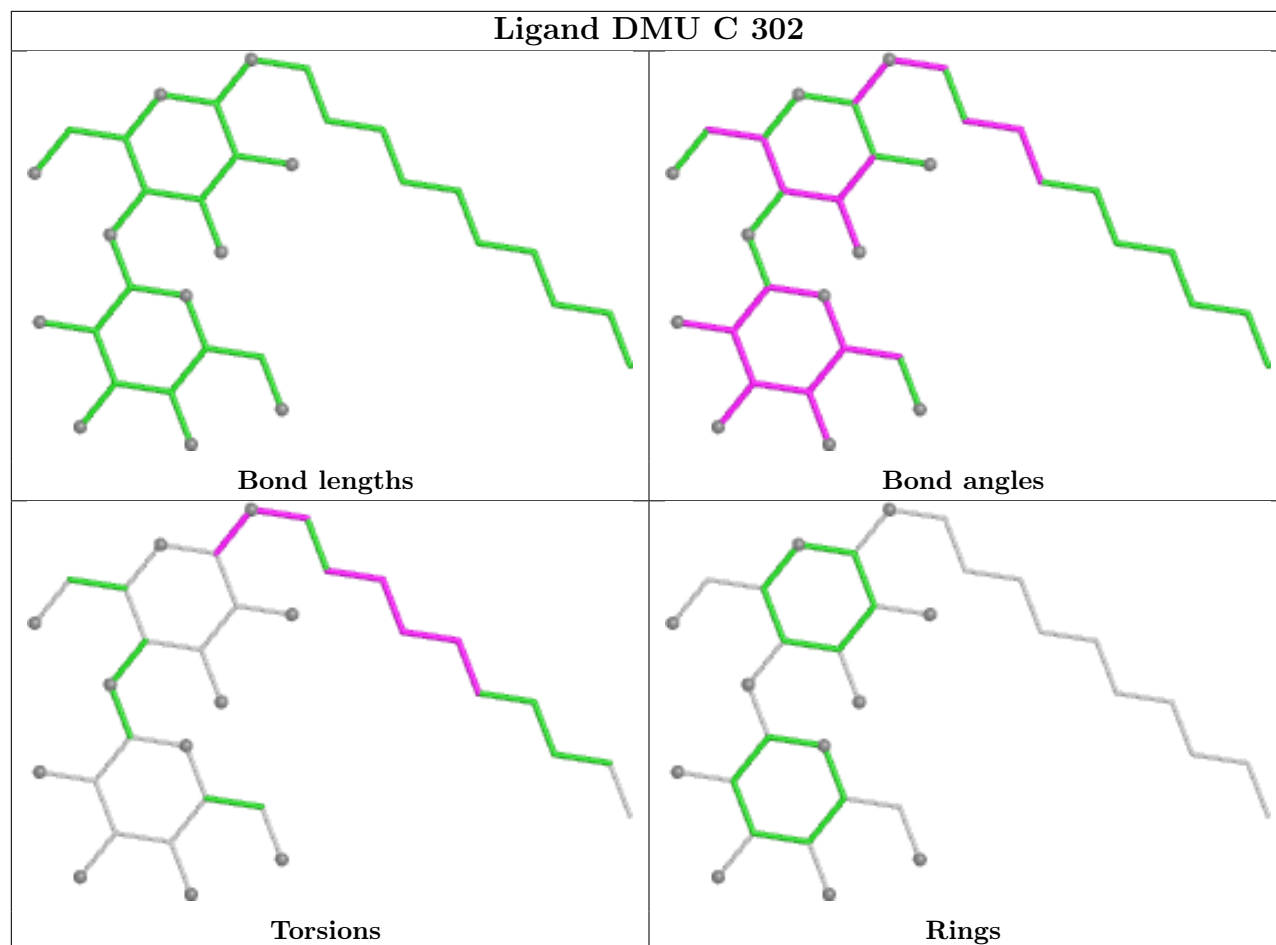












5.7 Other polymers [i](#)

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%)	-0.52	3 (0%) 85 88	13, 30, 38, 76	22 (4%)
1	N	513/514 (99%)	-0.29	6 (1%) 76 80	16, 34, 44, 77	20 (3%)
2	B	226/227 (99%)	0.10	15 (6%) 24 26	20, 37, 57, 78	10 (4%)
2	O	226/227 (99%)	0.32	12 (5%) 32 35	23, 45, 69, 89	4 (1%)
3	C	259/261 (99%)	-0.30	3 (1%) 76 80	14, 33, 45, 84	9 (3%)
3	P	259/261 (99%)	-0.23	4 (1%) 72 76	14, 35, 46, 72	9 (3%)
4	D	144/147 (97%)	0.04	4 (2%) 55 58	18, 39, 60, 82	4 (2%)
4	Q	144/147 (97%)	0.71	8 (5%) 30 33	22, 53, 78, 152	3 (2%)
5	E	105/109 (96%)	-0.03	3 (2%) 53 57	31, 38, 63, 113	0
5	R	105/109 (96%)	0.14	2 (1%) 66 70	38, 46, 65, 120	0
6	F	98/98 (100%)	0.38	7 (7%) 22 24	19, 41, 95, 147	4 (4%)
6	S	98/98 (100%)	0.75	10 (10%) 12 12	20, 42, 104, 148	2 (2%)
7	G	83/85 (97%)	0.92	19 (22%) 2 2	32, 43, 113, 127	0
7	T	83/85 (97%)	1.04	19 (22%) 2 2	21, 43, 101, 133	1 (1%)
8	H	79/85 (92%)	0.52	7 (8%) 15 15	35, 45, 91, 104	0
8	U	79/85 (92%)	0.59	10 (12%) 8 7	39, 50, 102, 116	0
9	I	72/73 (98%)	0.81	11 (15%) 5 5	35, 49, 85, 92	0
9	V	72/73 (98%)	0.85	8 (11%) 10 10	36, 58, 83, 102	0
10	J	58/59 (98%)	0.51	5 (8%) 16 16	34, 44, 70, 107	0
10	W	58/59 (98%)	0.55	5 (8%) 16 16	25, 47, 72, 125	1 (1%)
11	K	49/56 (87%)	0.31	3 (6%) 27 29	38, 45, 59, 65	0
11	X	49/56 (87%)	0.62	4 (8%) 17 18	25, 55, 77, 82	1 (2%)
12	L	46/47 (97%)	-0.02	2 (4%) 40 43	25, 36, 56, 86	1 (2%)
12	Y	46/47 (97%)	0.45	2 (4%) 40 43	25, 45, 68, 107	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.16	3 (6%) 22 24	32, 36, 71, 103	0
13	Z	43/46 (93%)	0.44	2 (4%) 36 39	43, 50, 83, 142	0
All	All	3550/3614 (98%)	0.08	177 (4%) 34 37	13, 38, 71, 152	92 (2%)

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	10.4
4	Q	6	VAL	9.2
4	Q	5	VAL	8.4
6	S	96	LEU	7.7
6	F	1	ALA	7.6
7	T	3	ALA	7.1
7	G	3	ALA	7.0
6	S	94	HIS	7.0
8	H	8	ILE	6.7
7	G	36	TRP	6.7
7	G	5	LYS	6.6
7	T	36	TRP	6.6
6	F	97	ALA	6.5
6	S	1	ALA	6.5
1	N	113[A]	LEU	6.4
6	S	93	PRO	6.4
7	T	5	LYS	6.3
4	Q	7	LYS	6.2
6	F	96	LEU	6.1
7	T	6	GLY	6.1
6	S	98	HIS	6.0
6	S	3	GLY	5.9
7	T	9	GLY	5.8
7	G	1	ALA	5.8
7	T	2	SER	5.8
4	D	31[A]	LYS	5.6
9	I	37	PHE	5.5
2	O	113	TYR	5.4
7	T	1	ALA	5.4
9	V	37	PHE	5.3
5	R	109	VAL	5.1
7	G	2	SER	5.1
5	E	109	VAL	5.0
7	G	4	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
6	F	98	HIS	4.7
8	U	8	ILE	4.6
7	G	6	GLY	4.5
7	T	4	ALA	4.4
9	I	27	VAL	4.3
7	T	8	HIS	4.3
4	Q	87[A]	PHE	4.3
12	Y	2	HIS	4.3
2	B	59	GLN	4.2
6	S	95	GLN	4.2
7	T	84	LYS	4.2
1	N	136[A]	LEU	4.2
4	D	5	VAL	4.2
4	Q	4	SER	4.2
9	I	30	GLY	4.1
7	G	8	HIS	4.1
12	L	2	HIS	4.0
8	H	44	THR	4.0
1	A	113[A]	LEU	4.0
2	B	16[A]	ILE	4.0
6	S	2	SER	4.0
9	V	2	THR	4.0
7	G	7	ASP	3.9
3	C	3	HIS	3.9
7	T	7	ASP	3.9
3	P	3	HIS	3.8
7	G	9	GLY	3.8
4	D	4	SER	3.8
8	U	44	THR	3.7
11	K	6	ALA	3.7
8	U	45	ALA	3.6
2	B	32[A]	PHE	3.6
7	G	10	GLY	3.5
7	G	37	LEU	3.5
11	X	6	ALA	3.5
9	I	33	THR	3.4
6	F	2	SER	3.4
7	G	38	HIS	3.4
7	T	38	HIS	3.4
8	H	7	LYS	3.4
9	I	29	LEU	3.4
10	J	58	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
5	R	5	HIS	3.3
2	B	113	TYR	3.2
2	O	33	LEU	3.2
9	I	25	PHE	3.2
10	W	58	LYS	3.2
4	Q	10	ASP	3.2
7	T	37	LEU	3.2
6	F	3	GLY	3.2
8	U	9	LYS	3.1
9	V	33	THR	3.1
8	U	47	GLY	3.1
7	G	84	LYS	3.1
13	M	40	TYR	3.1
8	U	10	ASN	3.1
9	I	21	ILE	3.1
11	K	47	ARG	3.1
7	T	10	GLY	3.1
1	A	514	LYS	3.0
2	O	86	MET	3.0
2	B	60	GLU	3.0
5	E	5	HIS	2.9
8	U	46	LYS	2.9
2	B	33	LEU	2.9
9	V	31	PHE	2.9
10	J	1	PHE	2.8
1	A	383[A]	MET	2.8
7	G	40	GLY	2.8
9	I	34	PHE	2.8
1	N	513	LEU	2.8
2	B	57	ASP	2.8
9	I	31	PHE	2.7
2	O	227	LEU	2.7
6	S	92	VAL	2.7
10	J	48	TYR	2.7
3	P	40	MET	2.6
10	J	52	TRP	2.6
3	P	37	PHE	2.6
2	B	68[A]	LEU	2.6
7	T	33	LEU	2.6
9	V	30	GLY	2.6
9	I	32	ALA	2.6
7	T	39	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	N	383[A]	MET	2.6
8	H	9	LYS	2.6
3	C	230	ASN	2.6
10	J	57	HIS	2.5
6	F	95	GLN	2.5
11	X	7	PRO	2.5
5	E	39	TYR	2.5
3	C	38	ASN	2.5
7	G	41	HIS	2.5
13	Z	40	TYR	2.5
7	G	12	GLY	2.5
2	O	91	ASN	2.5
8	H	45	ALA	2.5
7	T	40	GLY	2.4
2	O	37	LEU	2.4
2	O	29[A]	MET	2.4
12	L	47	LYS	2.4
8	U	11	TYR	2.4
9	V	25	PHE	2.4
9	V	34	PHE	2.4
7	T	35	SER	2.4
8	H	10	ASN	2.4
11	X	28[A]	VAL	2.4
2	B	56	MET	2.4
2	B	40	TYR	2.3
9	I	35	TYR	2.3
4	Q	19[A]	ARG	2.3
8	U	55	TRP	2.3
4	D	9	GLU	2.3
2	B	87[A]	MET	2.3
2	O	90	ILE	2.3
2	O	43	SER	2.3
9	V	26	MET	2.3
2	O	30	ILE	2.3
7	G	35	SER	2.3
2	B	38	VAL	2.3
10	W	27	THR	2.3
4	Q	39	ALA	2.2
10	W	48	TYR	2.2
13	Z	43	SER	2.2
10	W	52	TRP	2.2
11	X	13	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	37	LEU	2.2
13	M	39	ASN	2.2
2	O	60	GLU	2.1
10	W	1	PHE	2.1
3	P	122	HIS	2.1
1	N	514	LYS	2.1
8	U	42	ALA	2.1
7	G	39	SER	2.1
11	K	54	ARG	2.1
13	M	43	SER	2.1
7	T	12	GLY	2.1
1	N	483	LEU	2.1
2	B	61	VAL	2.0
12	Y	45	LEU	2.0
2	B	82	ARG	2.0
8	H	46	LYS	2.0
2	O	61	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.60	0.19	101,116,124,132	0
7	TPO	T	11	11/12	0.62	0.23	109,118,139,142	0
7	TPO	G	11	11/12	0.69	0.26	92,121,130,132	0
9	SAC	I	1	9/10	0.72	0.18	70,80,87,89	0
1	FME	N	1	10/11	0.91	0.13	47,56,74,79	0
1	FME	A	1	10/11	0.92	0.12	41,50,81,95	0
2	FME	O	1	10/11	0.96	0.09	41,42,54,65	0
2	FME	B	1	10/11	0.97	0.08	33,35,45,66	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CHD	J	101	29/29	0.59	0.24	99,135,149,150	0
21	EDO	C	319	4/4	0.69	0.21	81,98,105,107	0
27	PEK	T	101	53/53	0.72	0.26	51,87,154,155	0
22	CHD	W	101	29/29	0.73	0.24	69,124,145,148	0
25	DMU	C	310	33/33	0.77	0.16	56,82,112,121	0
25	DMU	L	102	33/33	0.77	0.19	54,93,139,139	0
27	PEK	G	102	53/53	0.77	0.23	52,95,154,154	0
21	EDO	R	205	4/4	0.77	0.18	57,58,61,75	0
21	EDO	D	204	4/4	0.78	0.23	65,69,81,85	0
21	EDO	A	619	4/4	0.78	0.21	50,57,58,83	0
25	DMU	C	311	33/33	0.79	0.19	56,82,119,129	0
25	DMU	P	306	33/33	0.79	0.16	47,79,120,123	0
28	CDL	P	304	100/100	0.79	0.27	43,87,119,134	0
28	CDL	T	103	100/100	0.79	0.25	54,88,145,159	0
25	DMU	P	308	33/33	0.80	0.16	55,78,101,105	0
21	EDO	C	318	4/4	0.80	0.21	58,86,90,94	0
21	EDO	A	612	4/4	0.80	0.22	52,61,65,67	0
28	CDL	N	601	100/100	0.80	0.27	57,90,140,159	0
20	PGV	G	103	51/51	0.80	0.23	53,83,119,139	0
25	DMU	C	302	33/33	0.80	0.18	35,79,111,124	0
19	TGL	A	608	63/63	0.81	0.24	43,79,109,121	0
25	DMU	P	309	33/33	0.81	0.14	65,87,106,112	0
27	PEK	C	308	53/53	0.81	0.22	49,80,136,148	0
19	TGL	Q	201	63/63	0.81	0.25	52,76,98,109	0
21	EDO	H	101	4/4	0.81	0.21	54,57,67,73	0
21	EDO	Q	203	4/4	0.81	0.21	81,81,88,91	0
19	TGL	Y	101	63/63	0.81	0.26	48,78,110,148	0
20	PGV	C	309	51/51	0.81	0.22	45,78,121,151	0
27	PEK	P	307	53/53	0.82	0.22	45,78,128,145	0
21	EDO	N	622	4/4	0.82	0.21	55,58,81,101	0
24	PSC	B	303	52/52	0.82	0.23	42,85,156,156	0
24	PSC	O	302	52/52	0.82	0.24	48,84,160,160	0
20	PGV	A	610	51/51	0.82	0.23	36,72,112,121	0
21	EDO	C	315	4/4	0.83	0.21	60,75,77,79	0
19	TGL	N	610	63/63	0.83	0.23	52,82,110,122	0
21	EDO	V	101	4/4	0.83	0.19	62,68,74,75	0
28	CDL	C	306	100/100	0.84	0.20	40,80,115,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CHD	P	305	29/29	0.84	0.14	53,65,71,76	0
20	PGV	Z	101	51/51	0.84	0.22	51,83,138,144	0
21	EDO	F	105	4/4	0.84	0.23	69,74,77,78	0
19	TGL	L	101	63/63	0.85	0.26	36,64,99,119	0
21	EDO	D	203	4/4	0.85	0.18	55,61,73,93	0
21	EDO	H	102	4/4	0.85	0.20	68,73,79,94	0
22	CHD	C	307	29/29	0.85	0.14	52,65,72,75	0
21	EDO	C	313	4/4	0.85	0.15	77,84,85,95	0
21	EDO	P	313	4/4	0.85	0.19	54,62,70,73	0
21	EDO	R	201	4/4	0.86	0.20	57,61,66,72	0
19	TGL	D	201	63/63	0.86	0.22	37,67,90,97	0
21	EDO	A	616	4/4	0.87	0.16	46,47,50,50	0
21	EDO	R	202	4/4	0.88	0.17	61,67,72,78	0
21	EDO	A	617	4/4	0.88	0.17	49,53,56,62	0
21	EDO	L	103	4/4	0.88	0.22	71,75,76,99	0
21	EDO	A	614	4/4	0.88	0.21	59,69,74,83	0
21	EDO	R	203	4/4	0.89	0.14	53,63,69,73	0
21	EDO	N	619	4/4	0.89	0.16	50,53,59,62	0
21	EDO	U	101	4/4	0.89	0.17	66,70,70,84	0
21	EDO	G	104	4/4	0.89	0.18	56,67,71,89	0
21	EDO	C	317	4/4	0.89	0.17	68,69,71,84	0
21	EDO	A	621	4/4	0.90	0.15	38,52,62,68	0
21	EDO	D	206	4/4	0.90	0.21	54,62,67,73	0
21	EDO	N	614	4/4	0.90	0.15	56,59,66,69	0
21	EDO	S	103	4/4	0.90	0.13	44,56,72,72	0
25	DMU	Z	102	33/33	0.90	0.12	50,60,75,78	0
26	UNX	C	303	1/1	0.90	0.14	28,28,28,28	0
21	EDO	E	203	4/4	0.90	0.12	50,59,66,70	0
21	EDO	D	202	4/4	0.91	0.13	44,51,52,68	0
21	EDO	E	205	4/4	0.91	0.16	60,63,68,78	0
21	EDO	A	620	4/4	0.91	0.16	64,64,67,70	0
21	EDO	R	206	4/4	0.91	0.13	47,52,58,63	0
21	EDO	D	207	4/4	0.91	0.19	62,66,70,75	0
21	EDO	N	618	4/4	0.91	0.14	60,63,67,70	0
21	EDO	E	201	4/4	0.92	0.12	43,46,56,58	0
21	EDO	C	314	4/4	0.92	0.12	60,64,67,85	0
21	EDO	A	618	4/4	0.92	0.15	43,68,78,83	0
21	EDO	N	617	4/4	0.93	0.13	50,53,53,57	0
21	EDO	A	615	4/4	0.93	0.12	25,30,31,46	0
26	UNX	P	302	1/1	0.93	0.19	28,28,28,28	0
21	EDO	F	104	4/4	0.93	0.12	50,52,62,64	0
21	EDO	J	102	4/4	0.93	0.17	52,75,78,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	O	305	4/4	0.93	0.10	67,74,79,79	0
21	EDO	P	310	4/4	0.93	0.15	36,42,48,59	0
21	EDO	P	312	4/4	0.93	0.14	52,60,72,75	0
21	EDO	A	623	4/4	0.93	0.14	55,57,62,63	0
21	EDO	N	611	4/4	0.93	0.16	72,73,74,76	0
21	EDO	A	613	4/4	0.93	0.12	35,37,39,41	0
21	EDO	T	104	4/4	0.94	0.13	39,41,42,49	0
21	EDO	O	304	4/4	0.94	0.12	63,67,67,83	0
21	EDO	N	613	4/4	0.94	0.13	42,49,49,54	0
25	DMU	M	101	33/33	0.94	0.10	43,50,62,73	0
21	EDO	N	621	4/4	0.94	0.12	48,51,51,71	0
21	EDO	N	612	4/4	0.94	0.18	36,41,53,64	0
18	AZI	N	608	3/3	0.95	0.10	39,39,39,41	0
18	AZI	A	607	3/3	0.95	0.18	34,34,37,37	0
21	EDO	N	615	4/4	0.95	0.12	38,39,43,47	0
27	PEK	T	102	53/53	0.95	0.14	34,51,84,97	0
21	EDO	N	616	4/4	0.95	0.09	34,37,38,39	0
21	EDO	B	305	4/4	0.95	0.12	35,45,53,55	0
27	PEK	C	304	53/53	0.95	0.12	32,49,84,106	0
21	EDO	C	316	4/4	0.95	0.13	41,61,67,70	0
21	EDO	F	103	4/4	0.96	0.10	40,41,42,45	0
22	CHD	C	301	29/29	0.96	0.07	30,33,37,40	0
21	EDO	A	611	4/4	0.96	0.14	39,44,46,56	0
21	EDO	C	312	4/4	0.96	0.12	42,42,45,45	0
22	CHD	P	301	29/29	0.96	0.07	31,36,39,46	0
20	PGV	N	609	51/51	0.96	0.11	30,40,71,77	0
21	EDO	E	204	4/4	0.96	0.07	43,44,47,50	0
21	EDO	N	620	4/4	0.96	0.11	49,59,67,73	0
21	EDO	Q	202	4/4	0.96	0.12	62,66,69,69	0
21	EDO	C	320	4/4	0.96	0.12	37,45,48,63	0
20	PGV	C	305	51/51	0.97	0.11	29,38,92,108	0
21	EDO	B	304	4/4	0.97	0.08	32,33,38,40	0
21	EDO	P	311	4/4	0.97	0.09	44,44,47,48	0
16	MG	N	605	1/1	0.97	0.05	35,35,35,35	0
21	EDO	D	205	4/4	0.97	0.08	40,41,58,58	0
20	PGV	A	609	51/51	0.97	0.10	27,38,69,73	0
22	CHD	B	301	29/29	0.97	0.07	29,33,36,44	0
18	AZI	N	607	3/3	0.97	0.08	39,39,40,42	0
21	EDO	A	622	4/4	0.97	0.10	37,45,60,64	0
21	EDO	O	303	4/4	0.97	0.11	41,41,42,44	0
21	EDO	E	202	4/4	0.97	0.09	44,46,46,48	0
21	EDO	R	204	4/4	0.97	0.09	45,49,49,50	0

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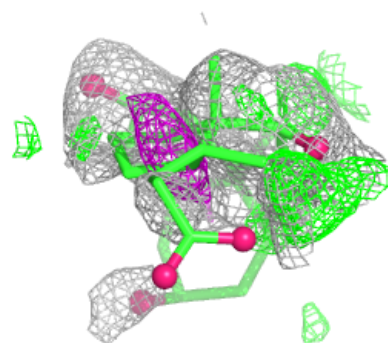
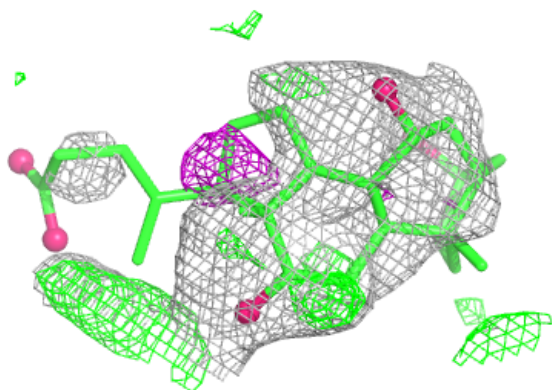
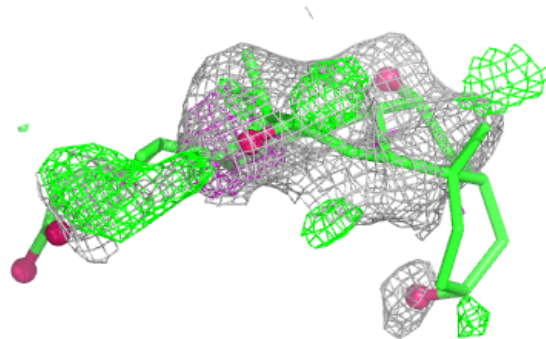
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	S	102	4/4	0.98	0.08	33,34,36,36	0
14	HEA	N	603[A]	60/60	0.98	0.06	24,27,33,35	60
14	HEA	N	603[B]	60/60	0.98	0.06	26,33,45,47	60
14	HEA	A	602[A]	60/60	0.98	0.06	21,27,31,36	60
21	EDO	G	105	4/4	0.98	0.06	35,38,42,44	0
18	AZI	A	606	3/3	0.98	0.10	33,33,36,36	0
20	PGV	P	303	51/51	0.98	0.09	31,40,77,86	0
14	HEA	A	602[B]	60/60	0.98	0.06	21,26,35,39	60
22	CHD	G	101	29/29	0.98	0.05	32,34,38,43	0
17	NA	A	605	1/1	0.99	0.03	32,32,32,32	0
17	NA	N	606	1/1	0.99	0.05	39,39,39,39	0
14	HEA	N	602	60/60	0.99	0.07	28,34,56,65	0
16	MG	A	604	1/1	0.99	0.03	28,28,28,28	0
14	HEA	A	601	60/60	0.99	0.06	23,28,49,51	0
21	EDO	F	102	4/4	0.99	0.06	29,31,31,33	0
23	CUA	O	301	2/2	1.00	0.02	36,36,36,36	0
15	CU	N	604	1/1	1.00	0.01	33,33,33,33	0
15	CU	A	603	1/1	1.00	0.01	30,30,30,30	0
23	CUA	B	302	2/2	1.00	0.02	30,30,30,31	0
29	ZN	F	101	1/1	1.00	0.02	36,36,36,36	0
29	ZN	S	101	1/1	1.00	0.03	38,38,38,38	0

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

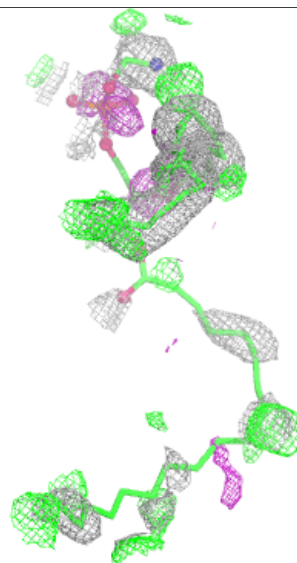
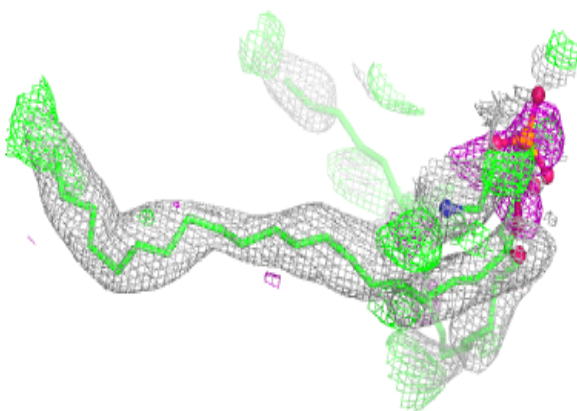
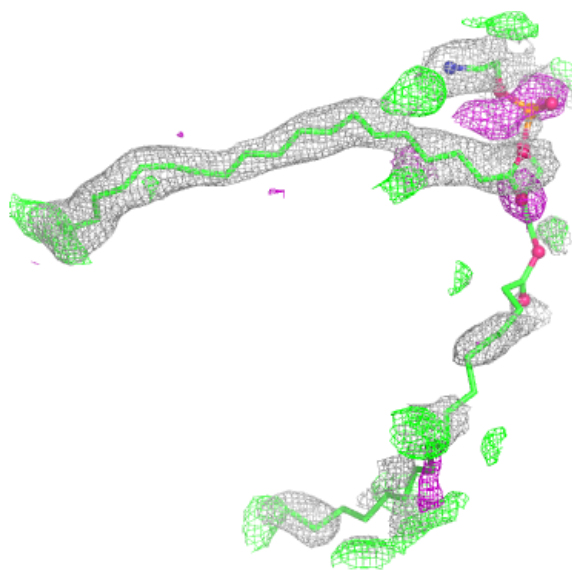
Electron density around CHD J 101:

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



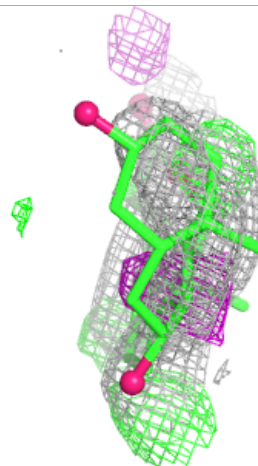
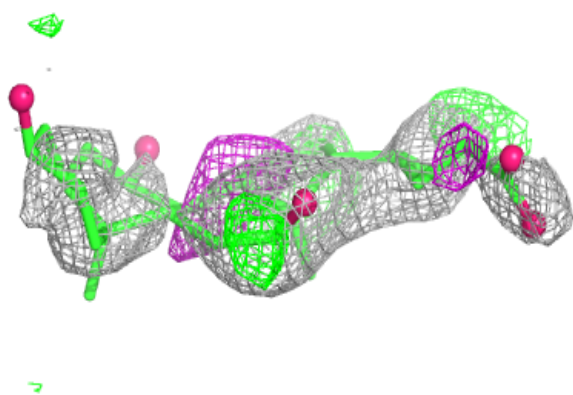
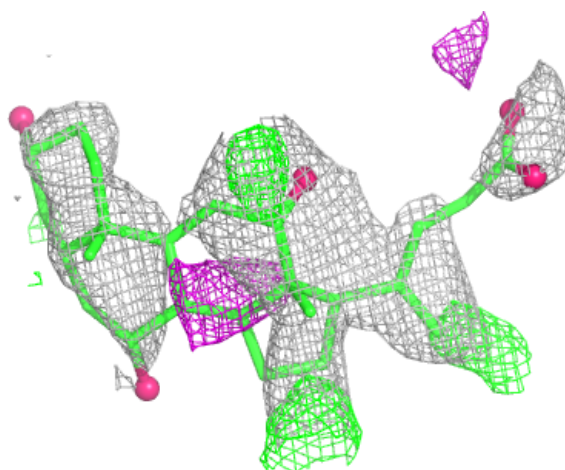
Electron density around PEK T 101:

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



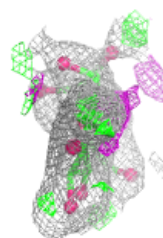
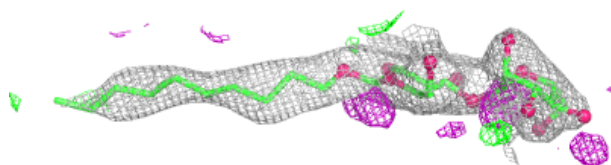
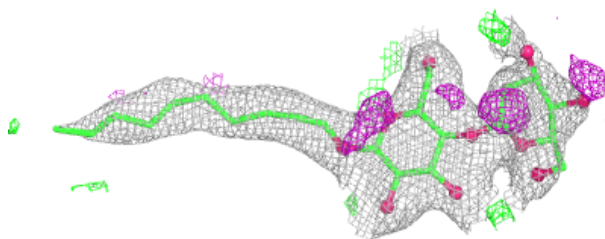
Electron density around CHD W 101:

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

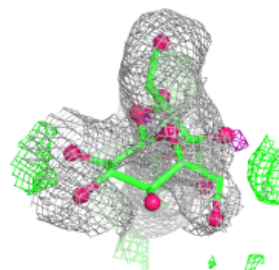
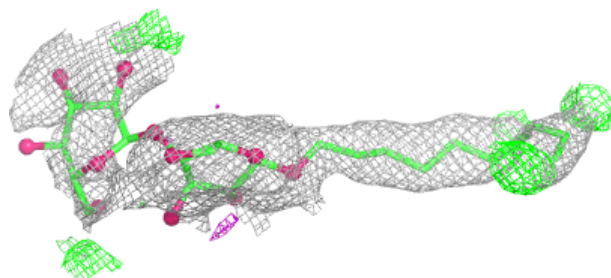
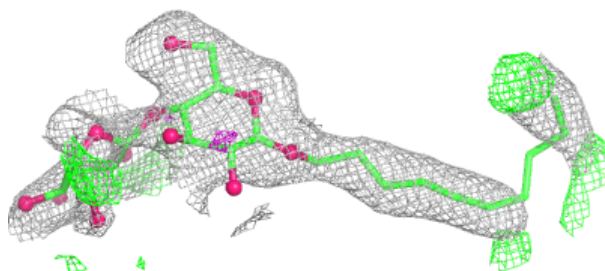


Electron density around DMU C 310:

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

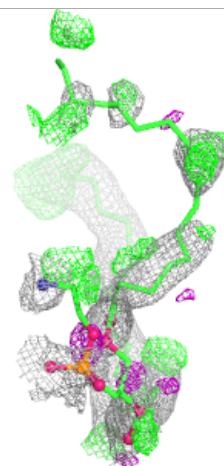
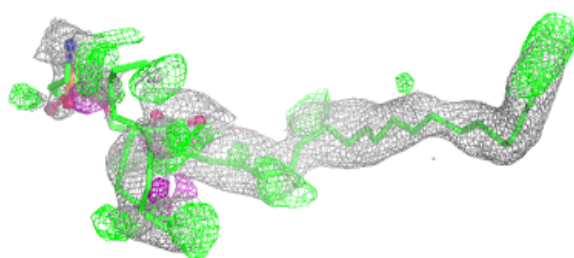
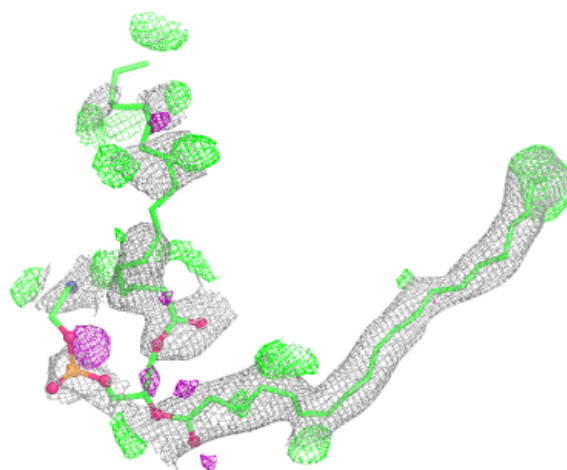
**Electron density around DMU L 102:**

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



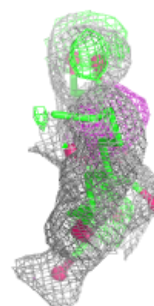
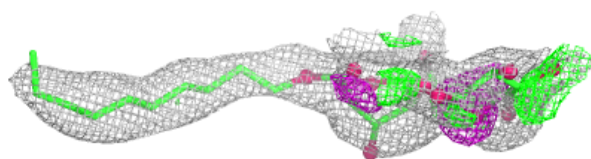
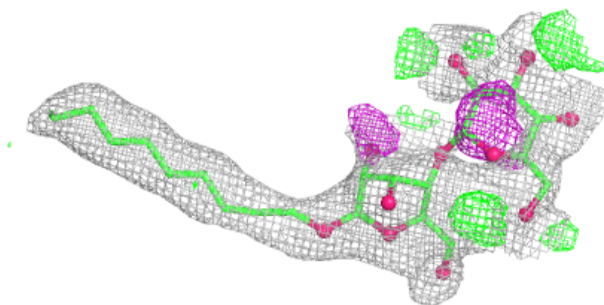
Electron density around PEK G 102:

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

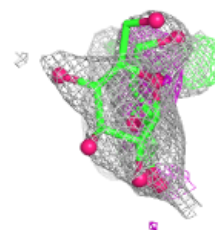
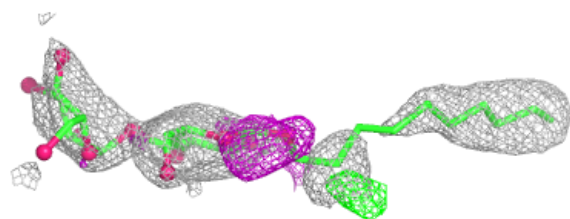
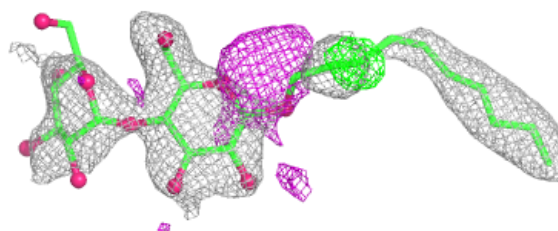


Electron density around DMU C 311:

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

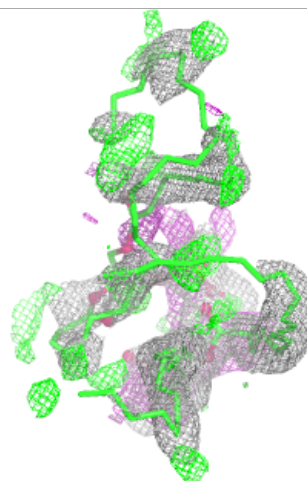
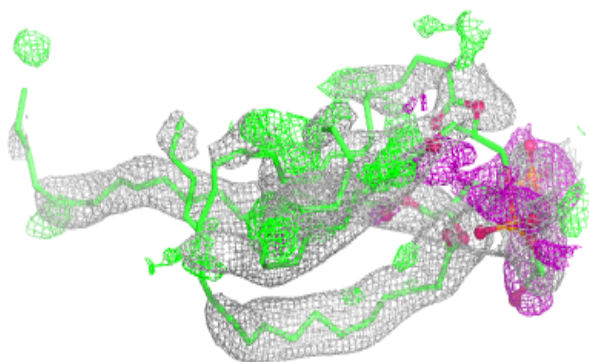
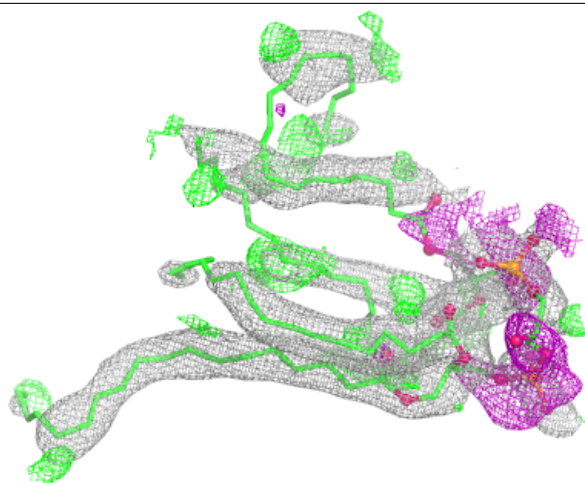
**Electron density around DMU P 306:**

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



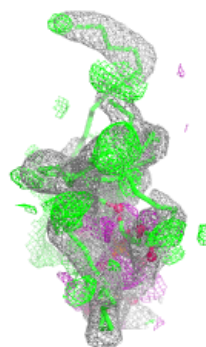
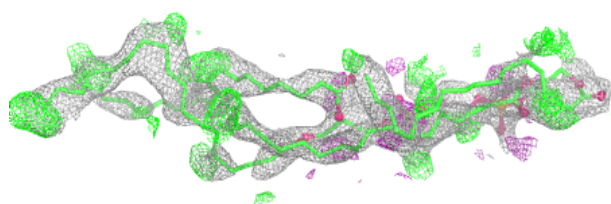
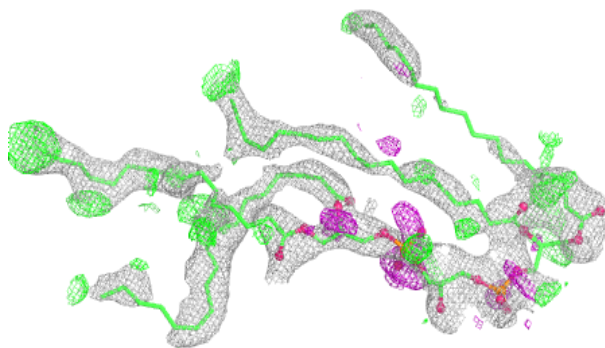
Electron density around CDL P 304:

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

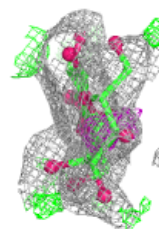
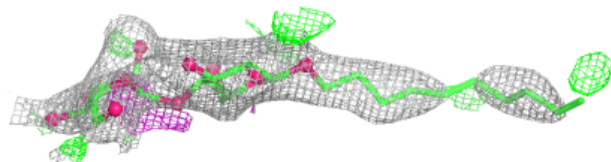
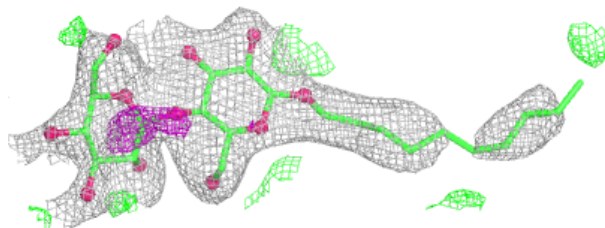


Electron density around CDL T 103:

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

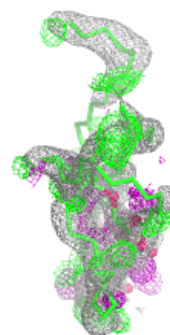
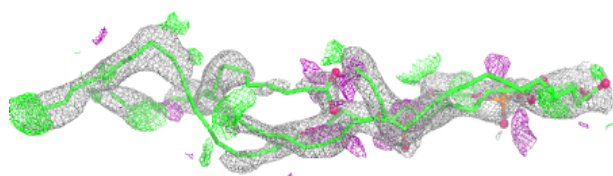
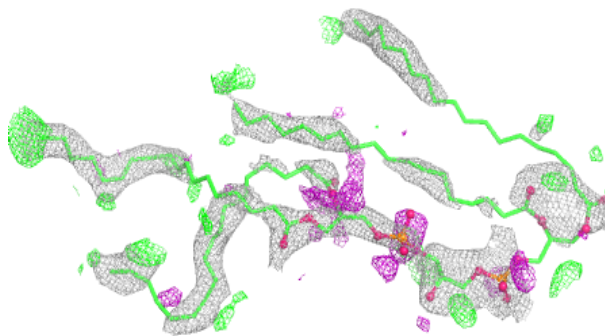
**Electron density around DMU P 308:**

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

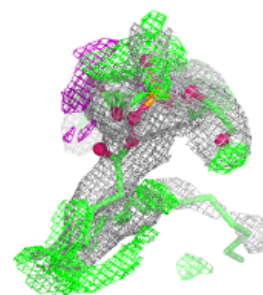
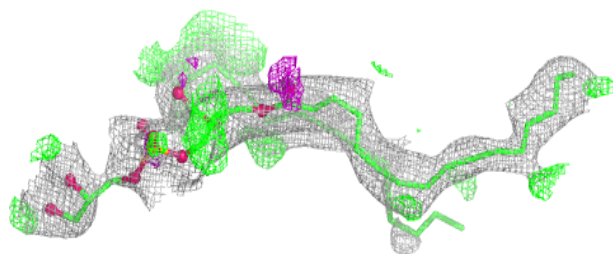
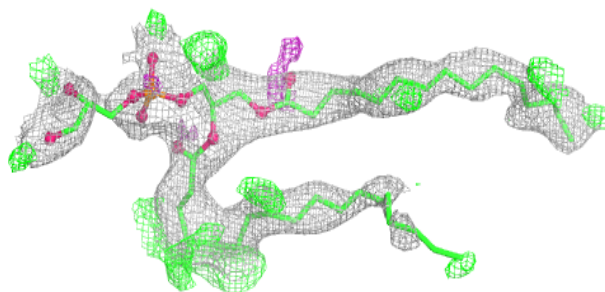


Electron density around CDL N 601:

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

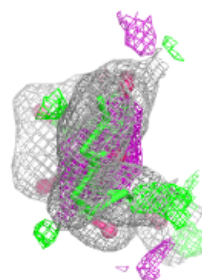
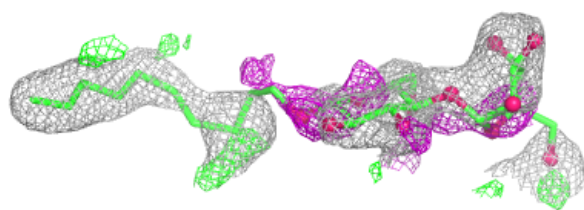
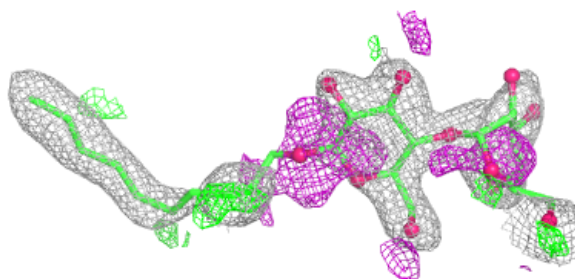
**Electron density around PGV G 103:**

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

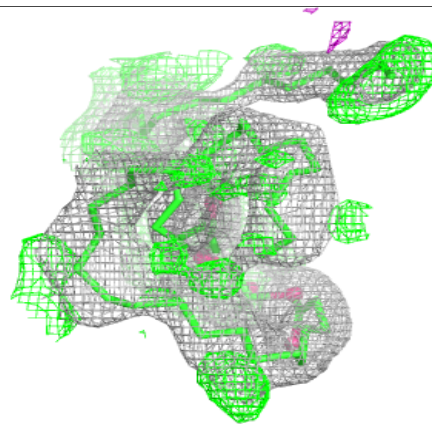
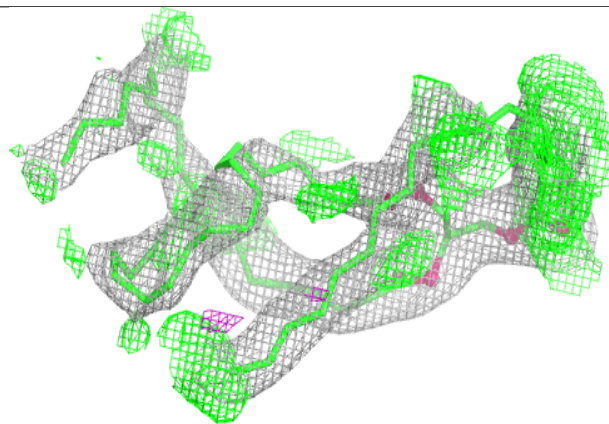
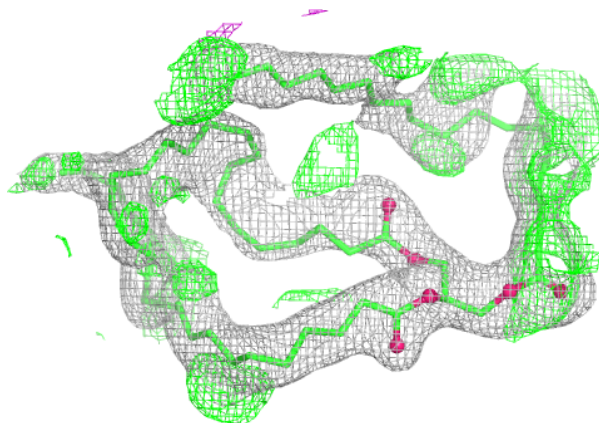


Electron density around DMU C 302:

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

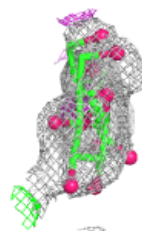
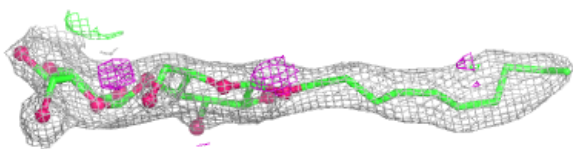
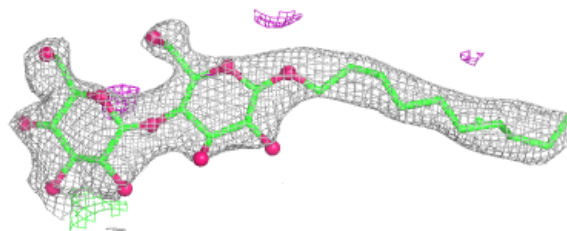
**Electron density around TGL A 608:**

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



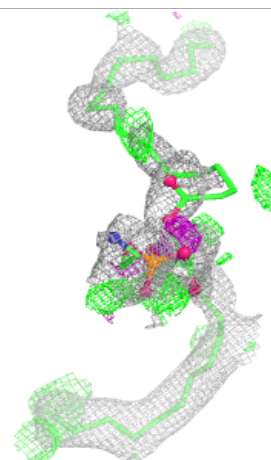
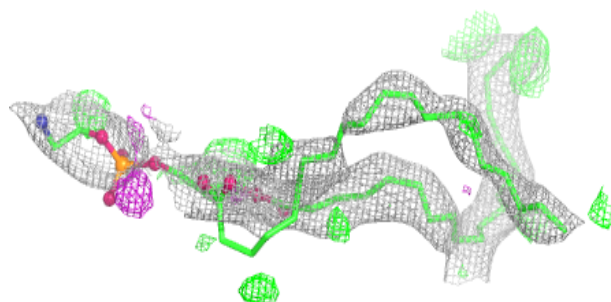
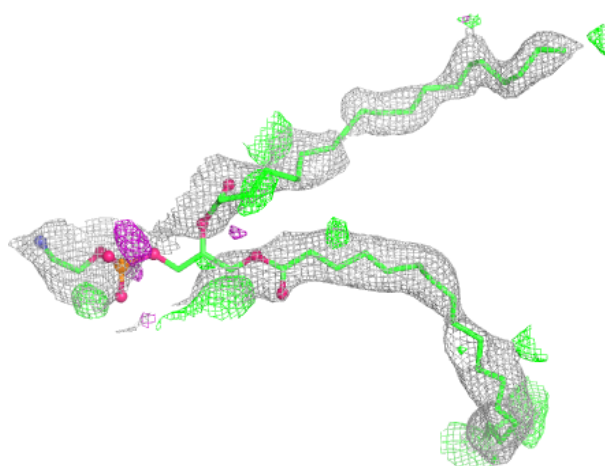
Electron density around DMU P 309:

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



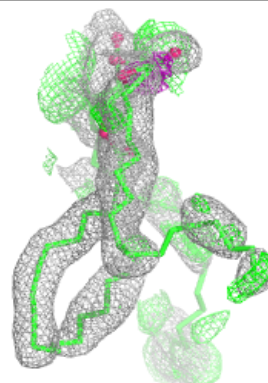
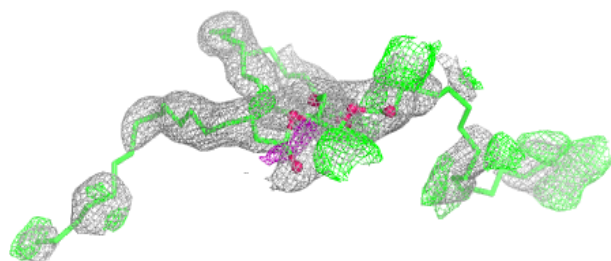
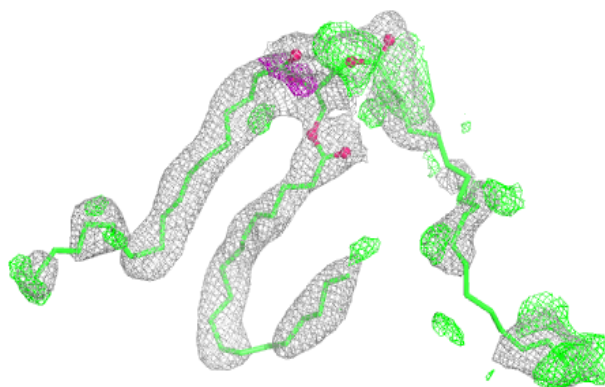
Electron density around PEK C 308:

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



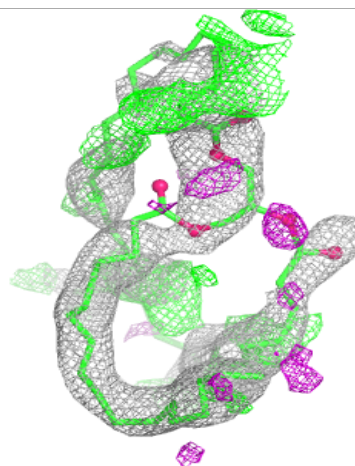
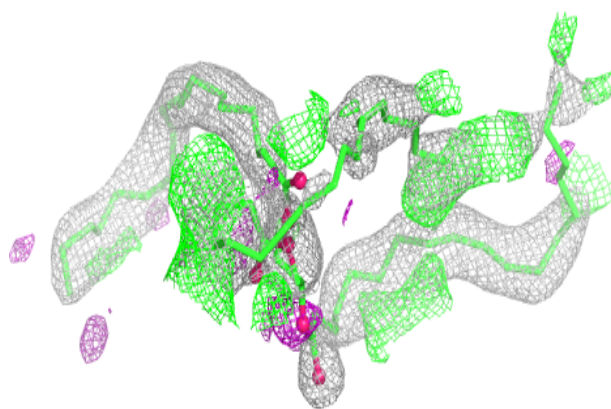
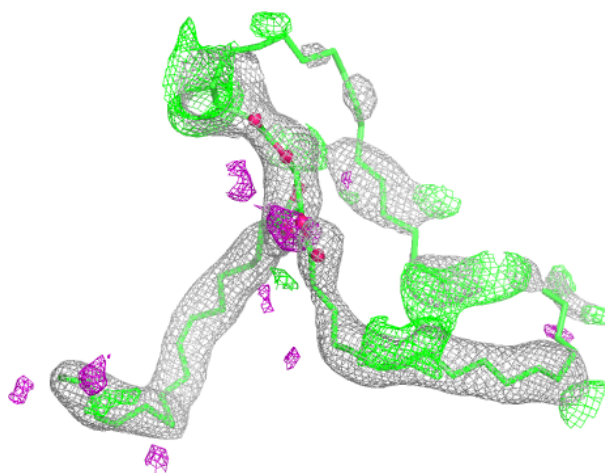
Electron density around TGL Q 201:

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



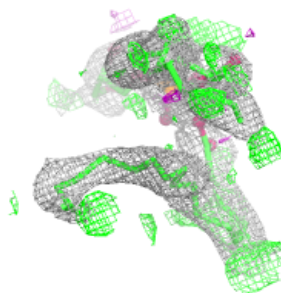
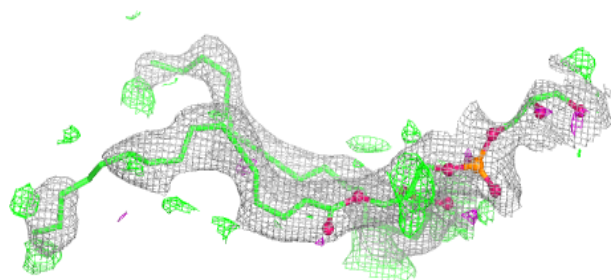
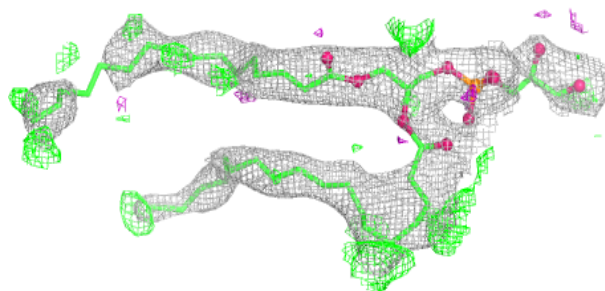
Electron density around TGL Y 101:

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

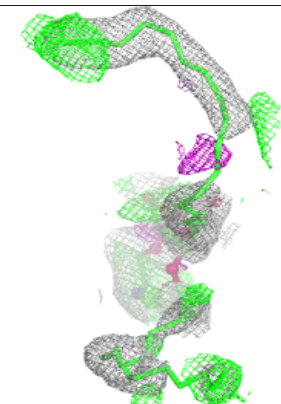
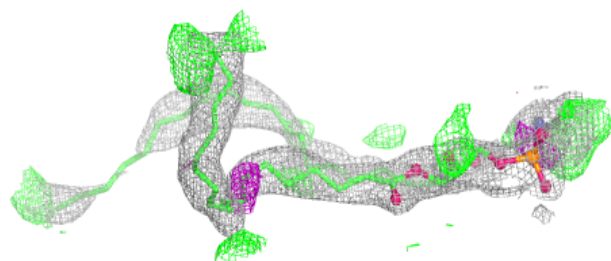
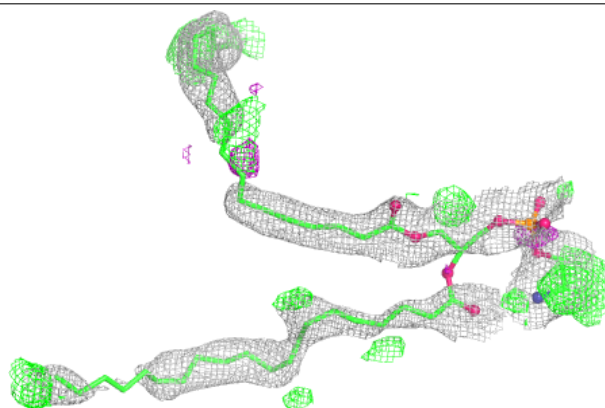


Electron density around PGV C 309:

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

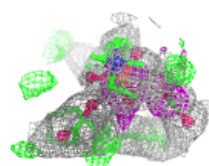
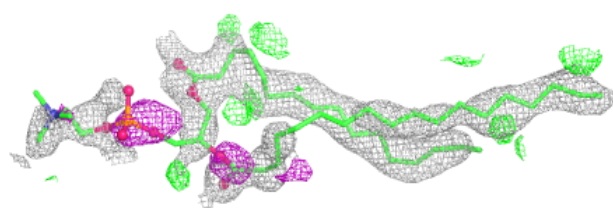
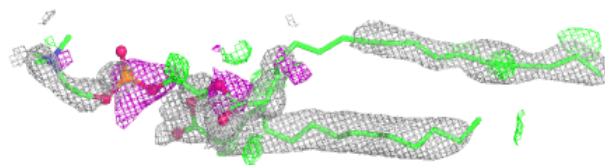
**Electron density around PEK P 307:**

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

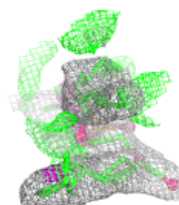
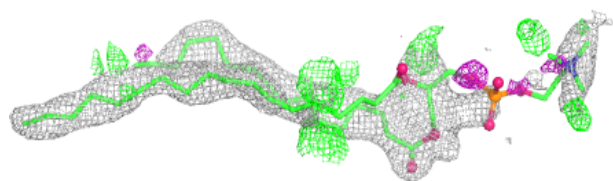
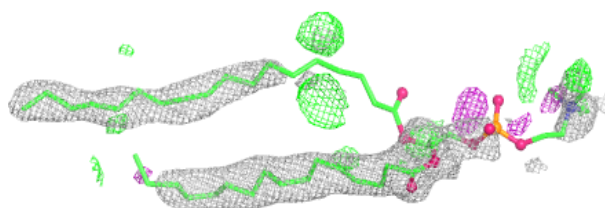


Electron density around PSC B 303:

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

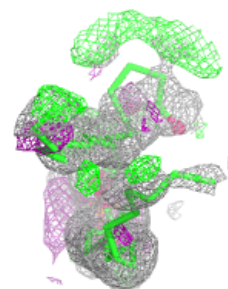
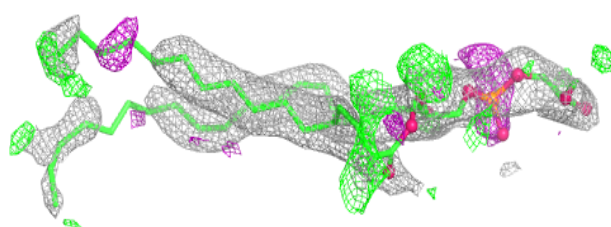
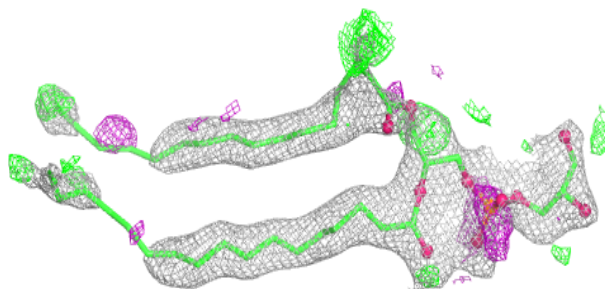
**Electron density around PSC O 302:**

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

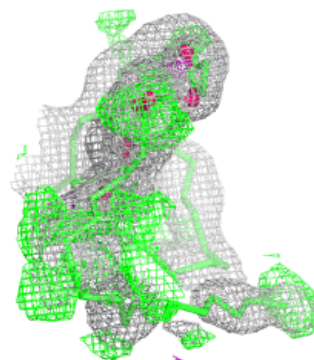
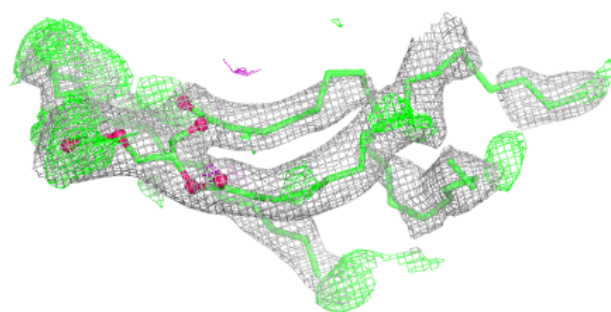
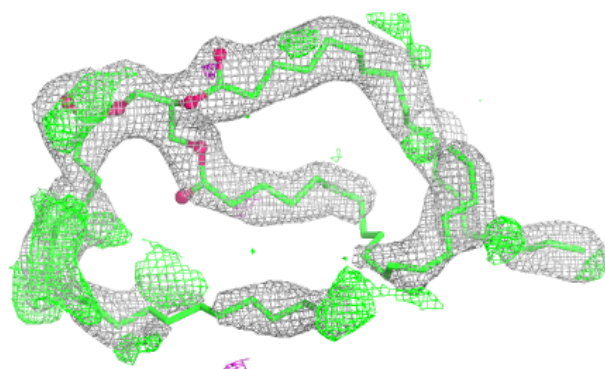


Electron density around PGV A 610:

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

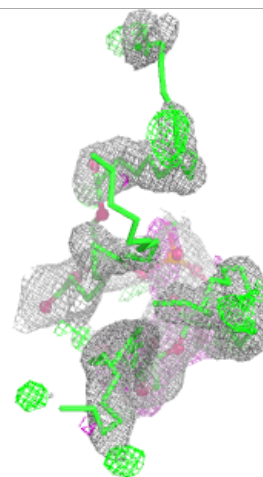
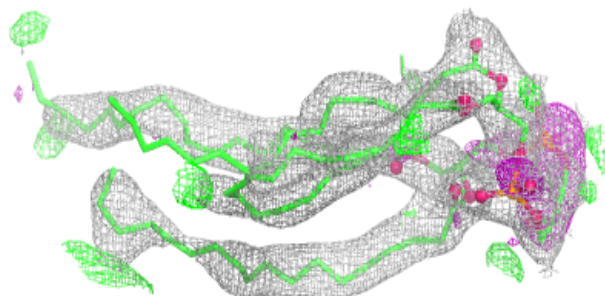
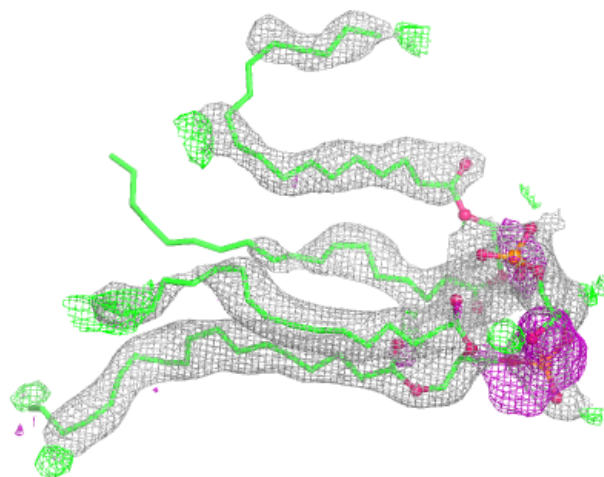
**Electron density around TGL N 610:**

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



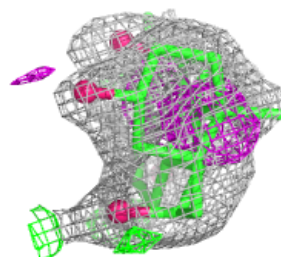
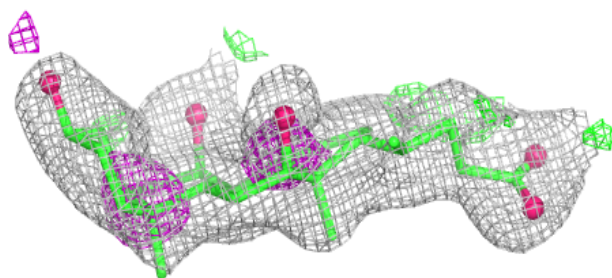
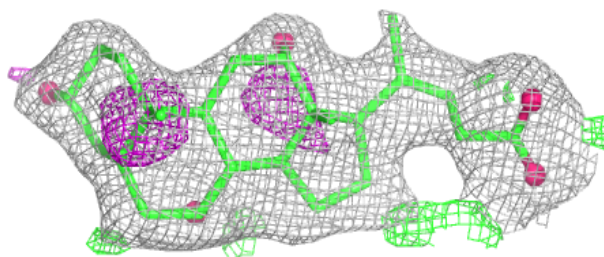
Electron density around CDL C 306:

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

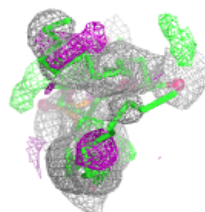
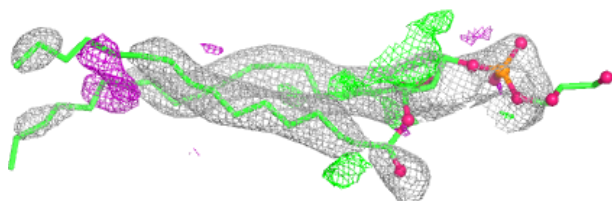
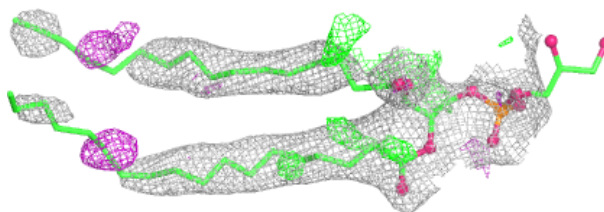


Electron density around CHD P 305:

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

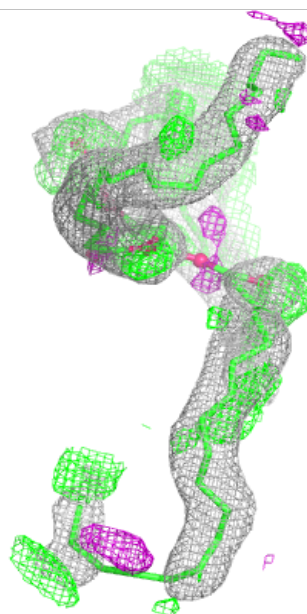
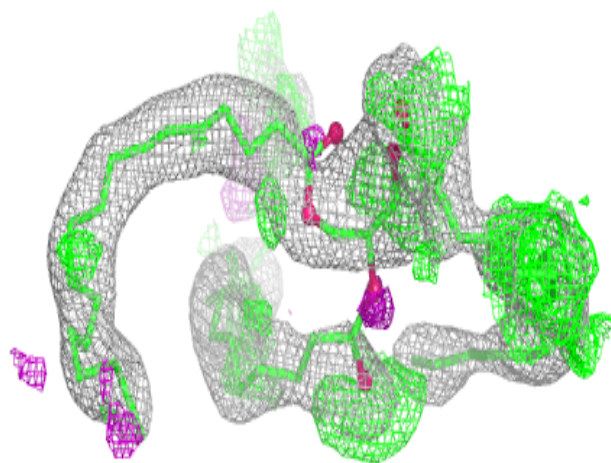
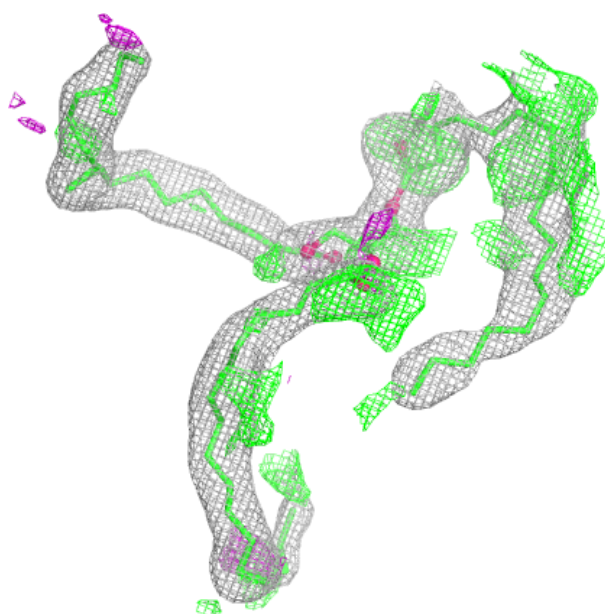
**Electron density around PGV Z 101:**

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



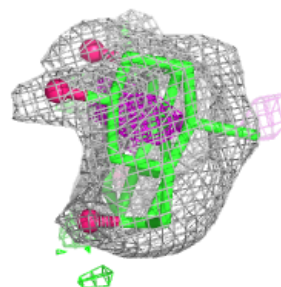
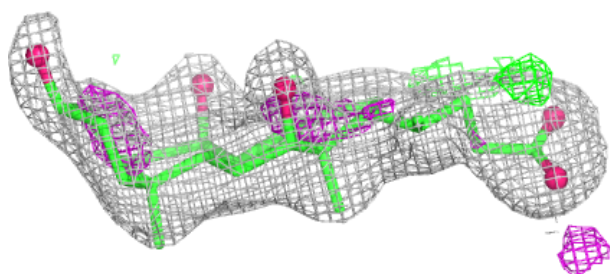
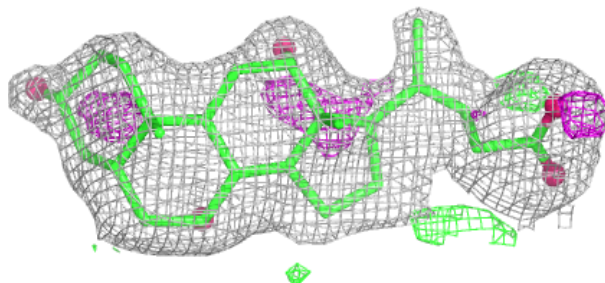
Electron density around TGL L 101:

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

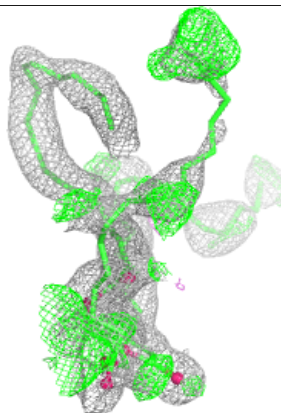
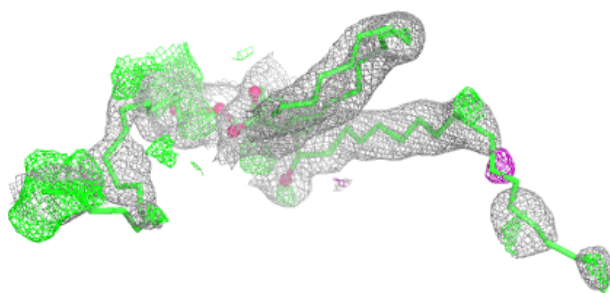
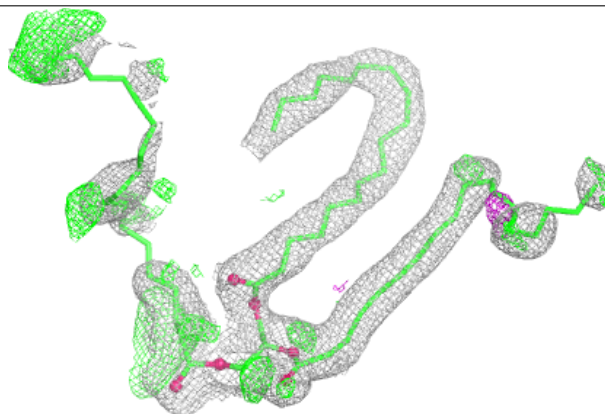


Electron density around CHD C 307:

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

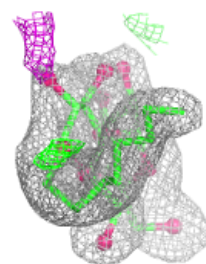
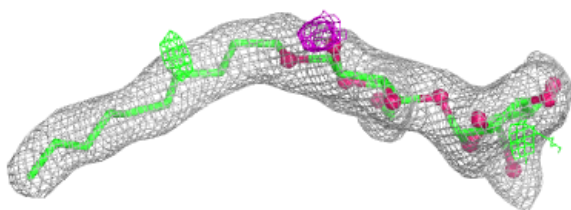
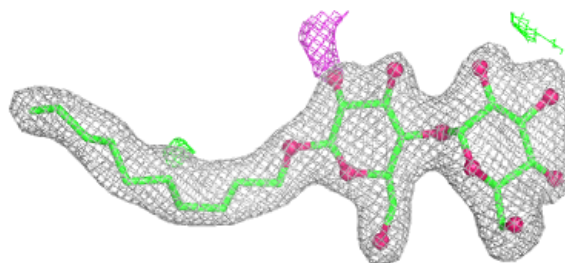
**Electron density around TGL D 201:**

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

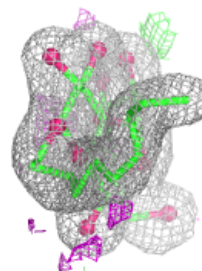
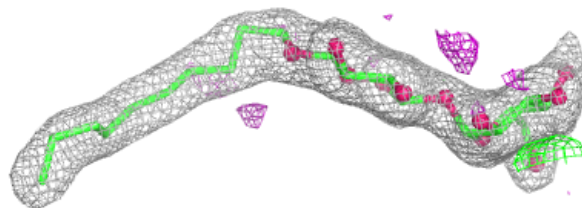


Electron density around DMU Z 102:

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

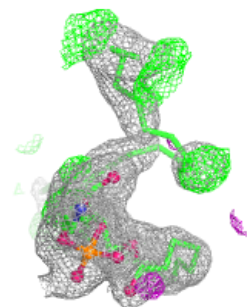
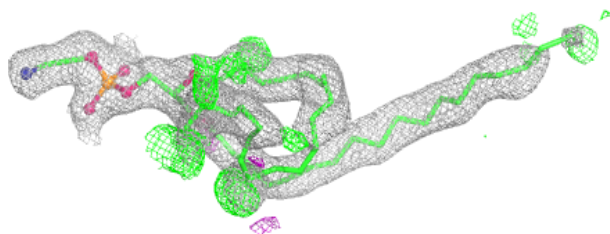
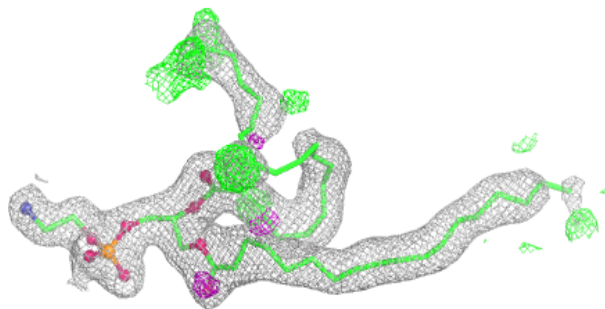
**Electron density around DMU M 101:**

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

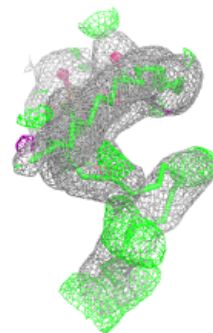
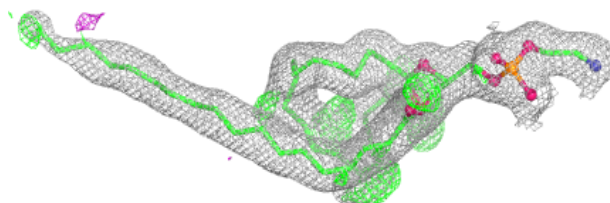
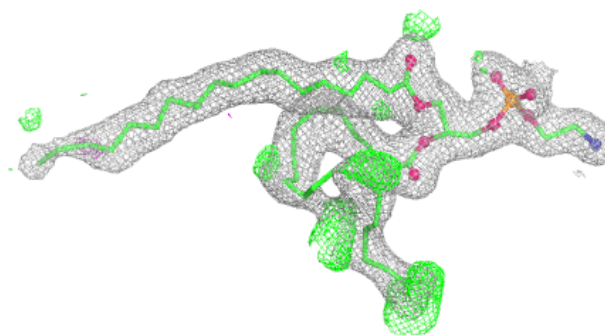


Electron density around PEK T 102:

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

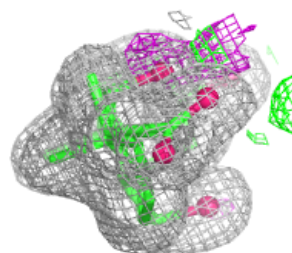
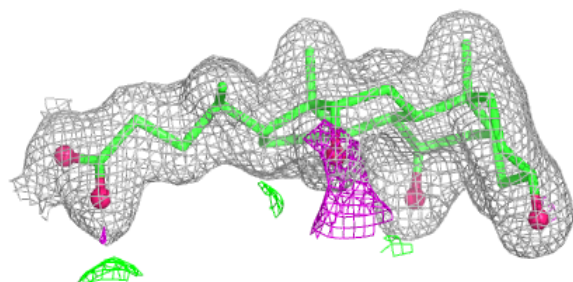
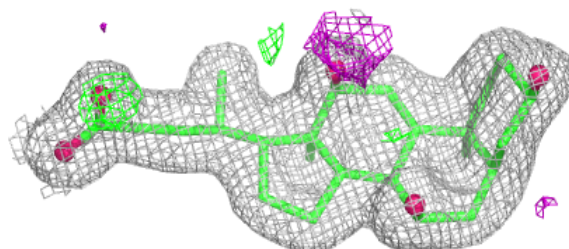
**Electron density around PEK C 304:**

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

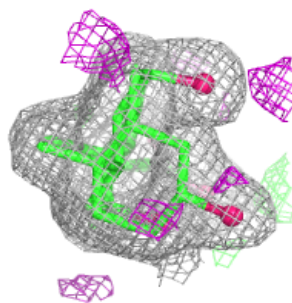
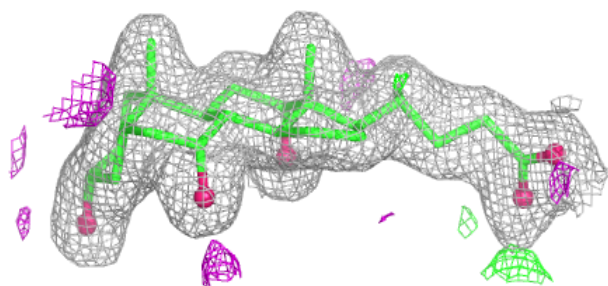
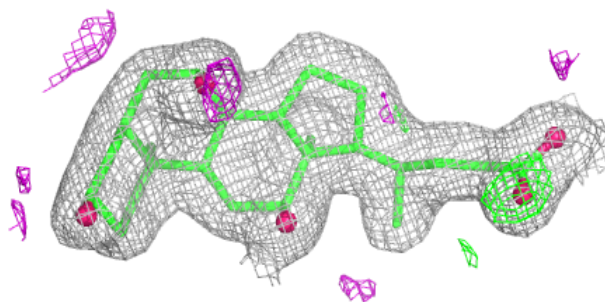


Electron density around CHD C 301:

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

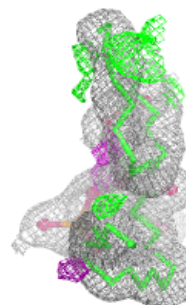
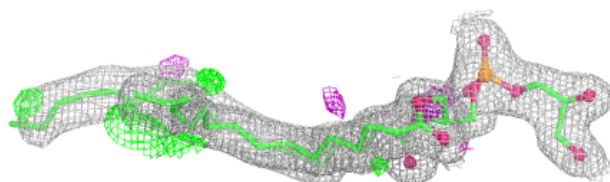
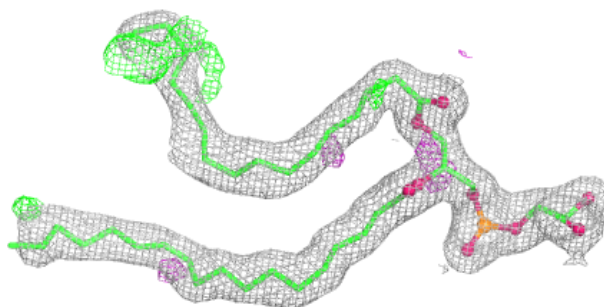
**Electron density around CHD P 301:**

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

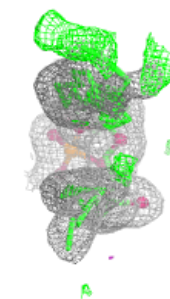
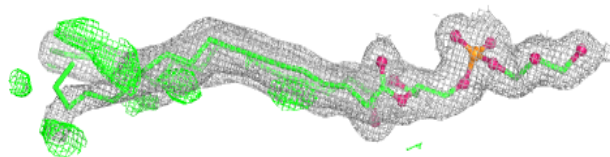
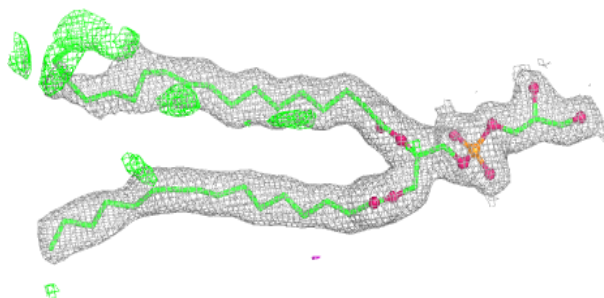


Electron density around PGV N 609:

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

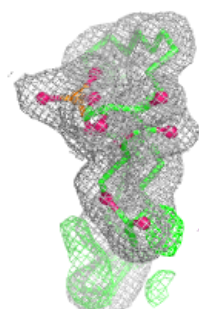
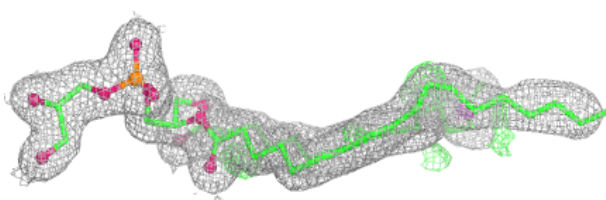
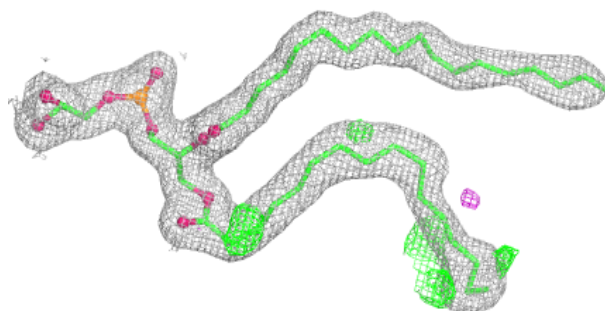
**Electron density around PGV C 305:**

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

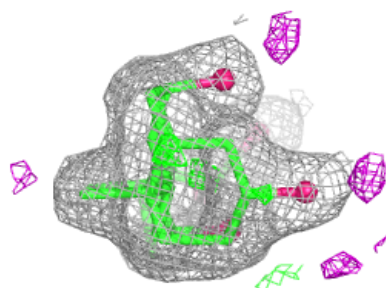
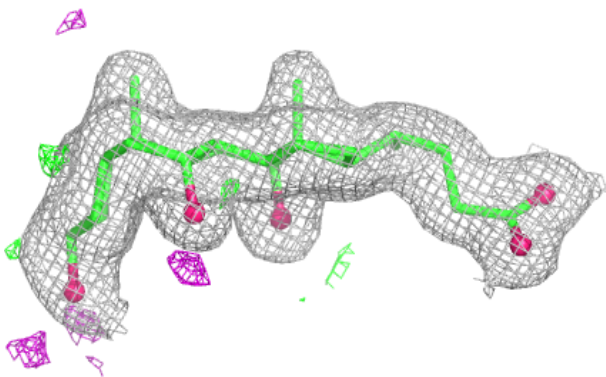
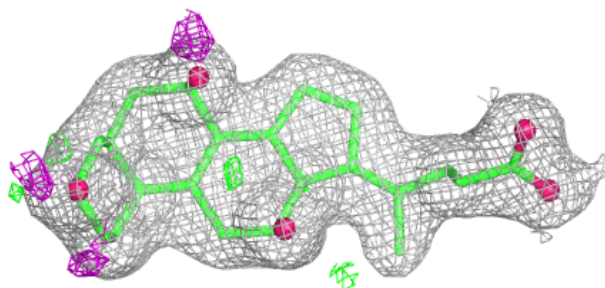


Electron density around PGV A 609:

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

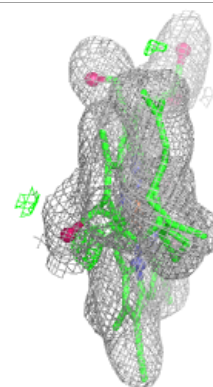
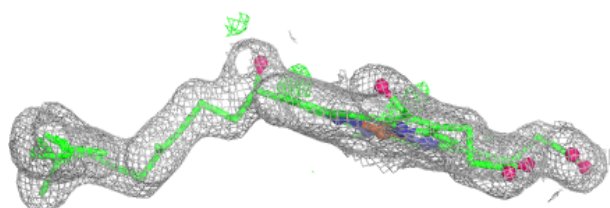
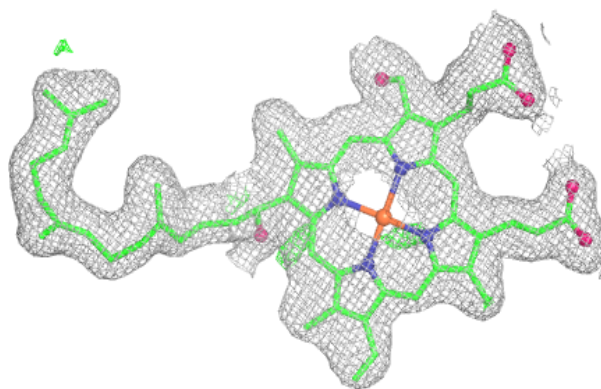
**Electron density around CHD B 301:**

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

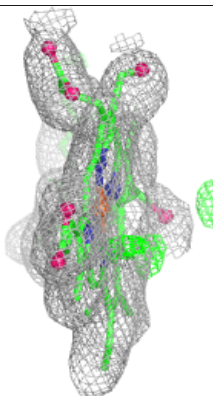
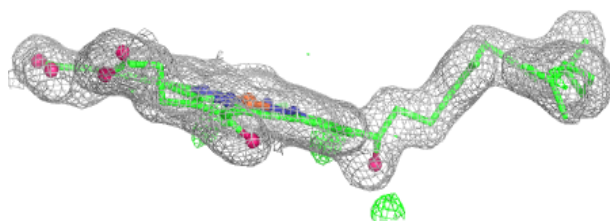
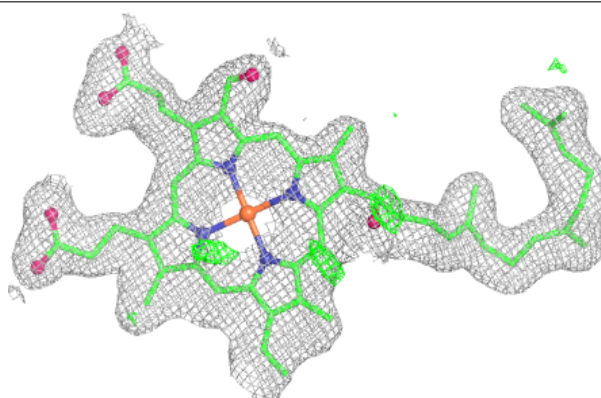


Electron density around HEA N 603 (A):

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

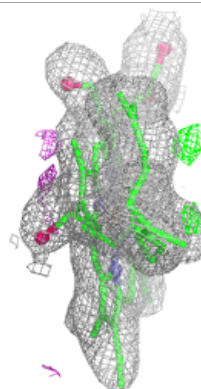
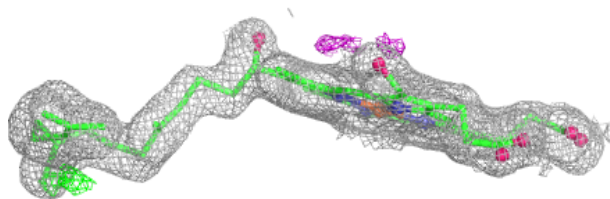
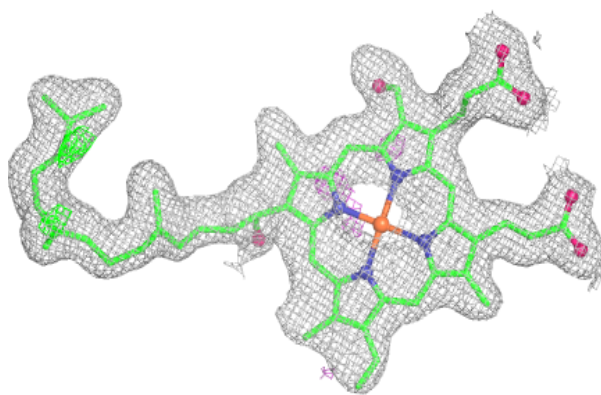
**Electron density around HEA N 603 (B):**

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

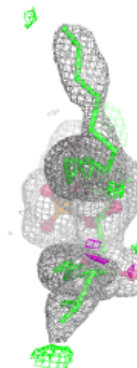
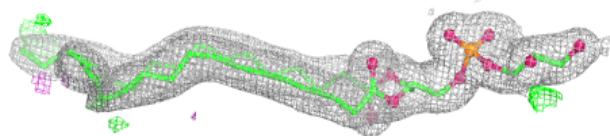
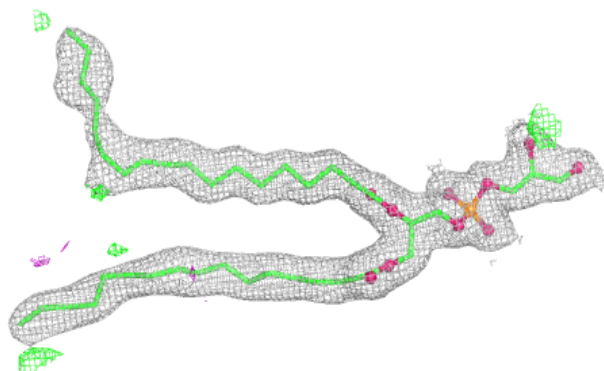


Electron density around HEA A 602 (A):

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

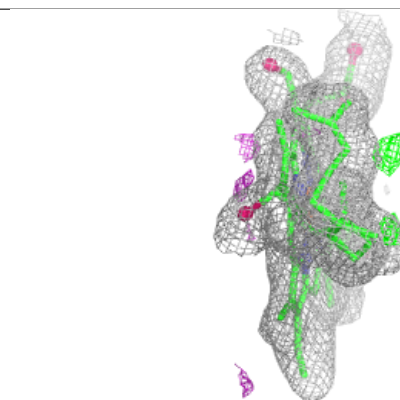
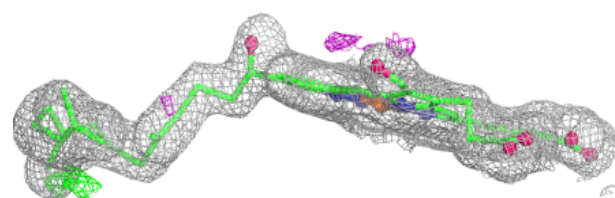
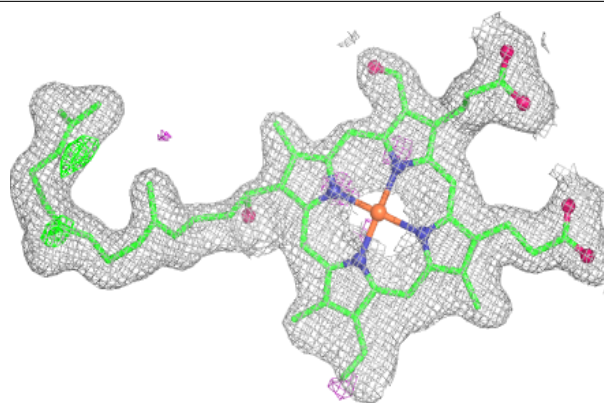
**Electron density around PGV P 303:**

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

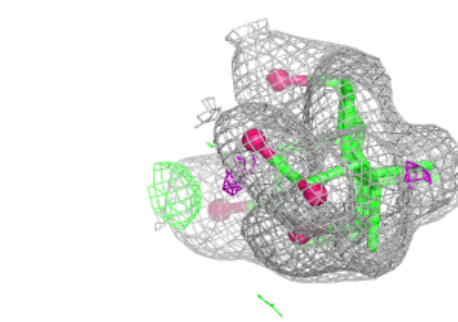
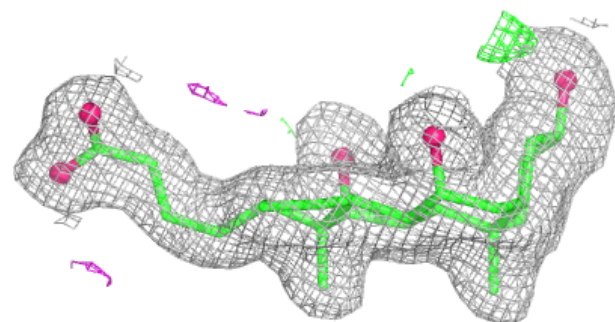
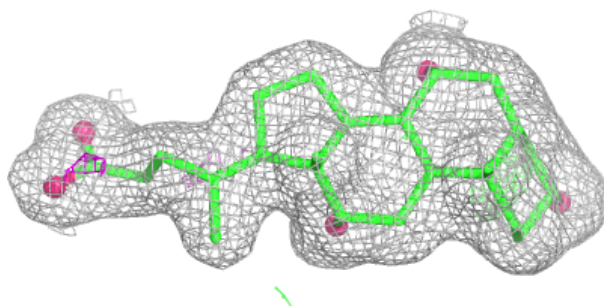


Electron density around HEA A 602 (B):

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

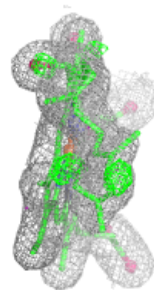
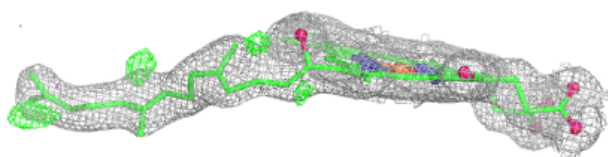
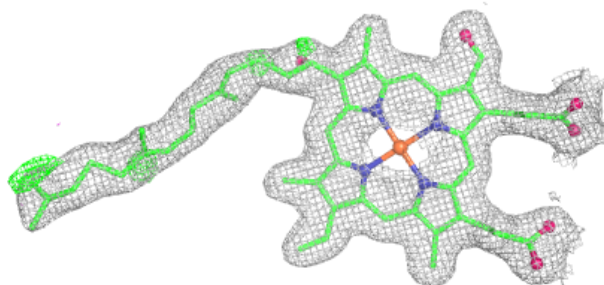
**Electron density around CHD G 101:**

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

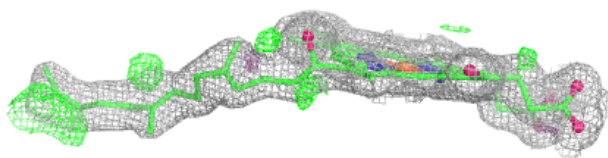
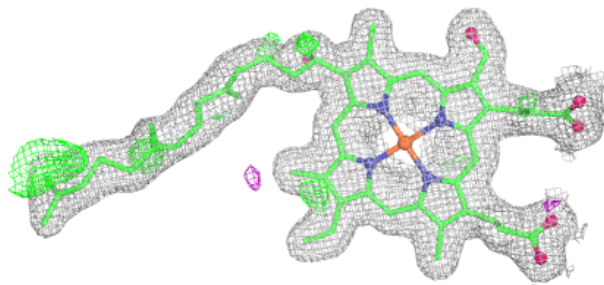


Electron density around HEA N 602:

$2mF_o-DF_c$ (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:**

$2mF_o-DF_c$ (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.