



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:06 PM UTC

PDB ID : 5X1F / pdb_00005x1f
Title : CO bound cytochrome c oxidase without pump laser irradiation at 278K
Authors : Shimada, A.; Kubo, M.; Baba, S.; Yamashita, K.; Hirata, K.; Ueno, G.; Nomura, T.; Kimura, T.; Shinzawa-Itoh, K.; Baba, J.; Hatano, K.; Eto, Y.; Miyamoto, A.; Murakami, H.; Kumasaka, T.; Owada, S.; Tono, K.; Yabashi, M.; Yamaguchi, Y.; Yanagisawa, S.; Sakaguchi, M.; Ogura, T.; Komiya, R.; Yan, J.; Yamashita, E.; Yamamoto, M.; Ago, H.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2017-01-25
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

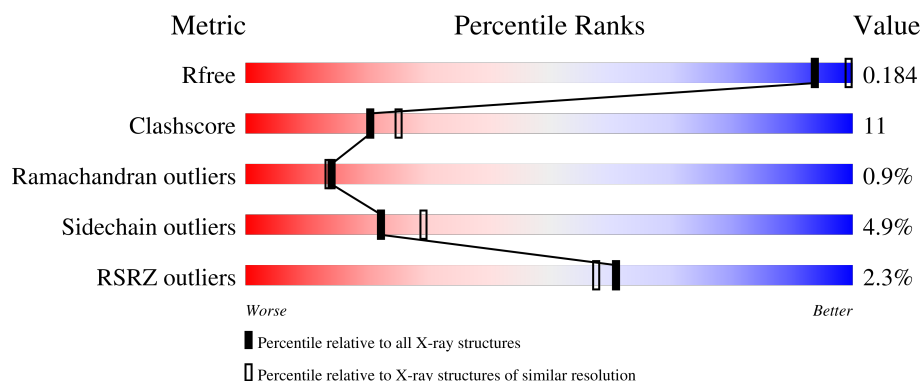
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

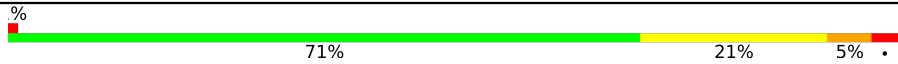
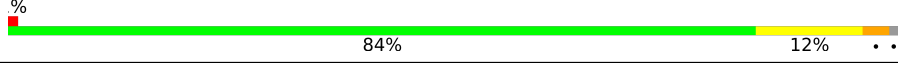
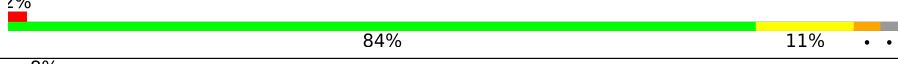
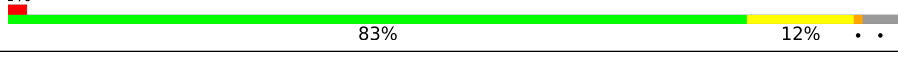
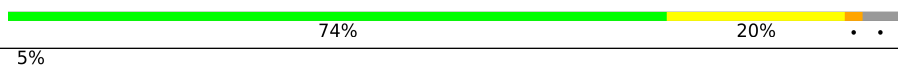
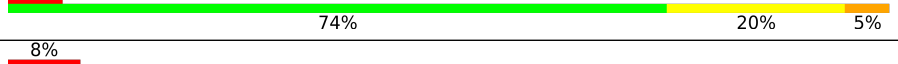
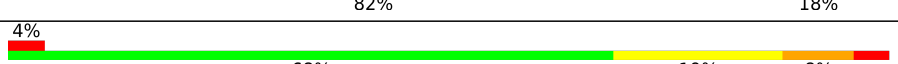
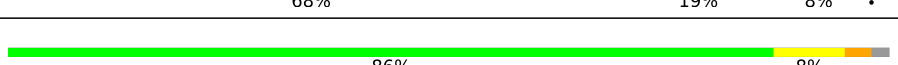
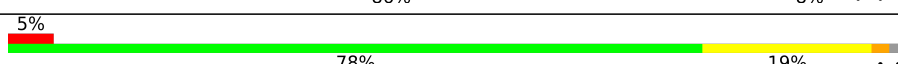
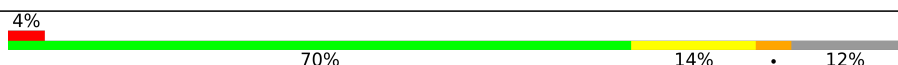
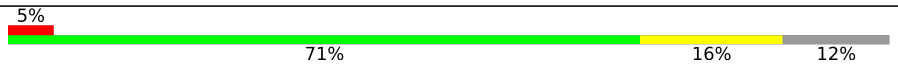
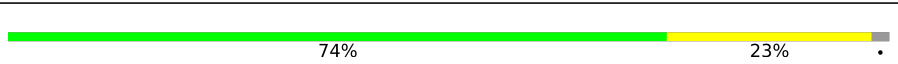
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	82% 17% .
1	N	514	76% 22% .
2	B	227	76% 19% ..

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	O	227	
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CMO	N	606	-	-	X	-
21	EDO	A	613	-	-	X	-
21	EDO	C	312	-	-	X	-
21	EDO	I	101	-	-	X	-
26	UNX	C	301	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32099 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	1	0
			4030	2694	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	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	0	0
			460	297	78	82	3			

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

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

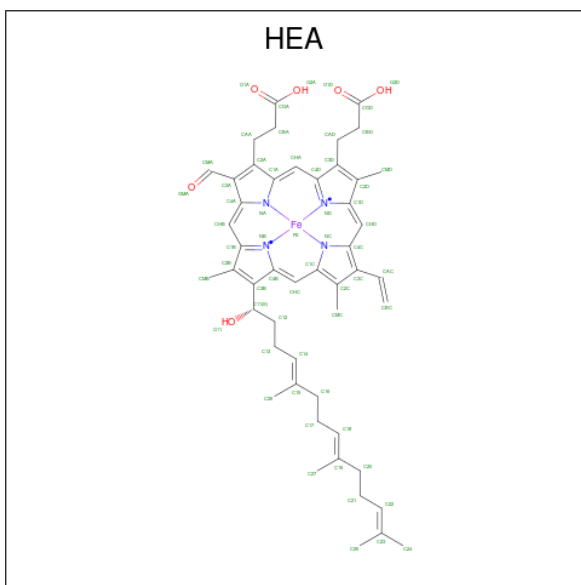
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

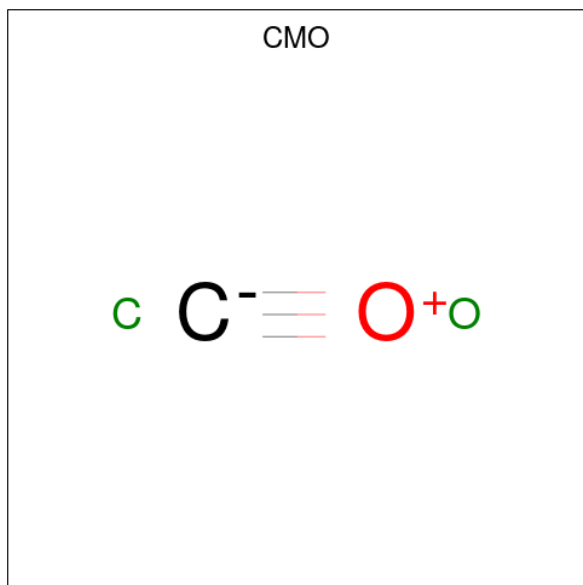
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

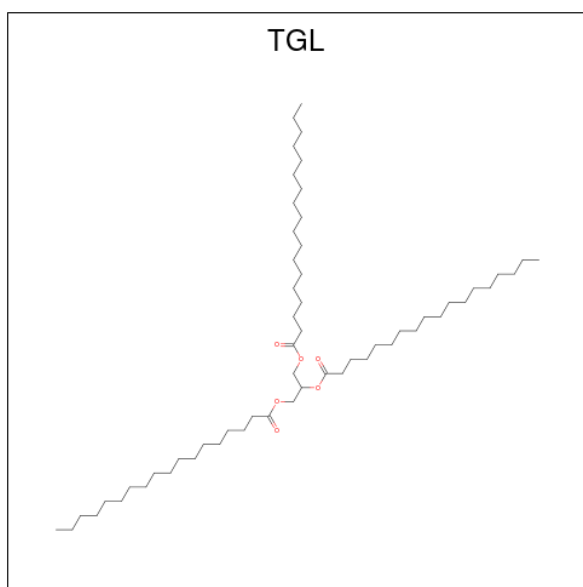
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



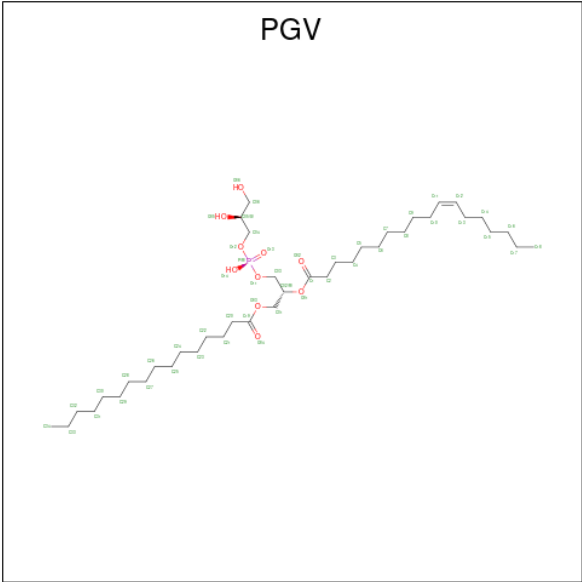
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			2	1	1		
18	N	1	Total	C	O	0	0
			2	1	1		

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



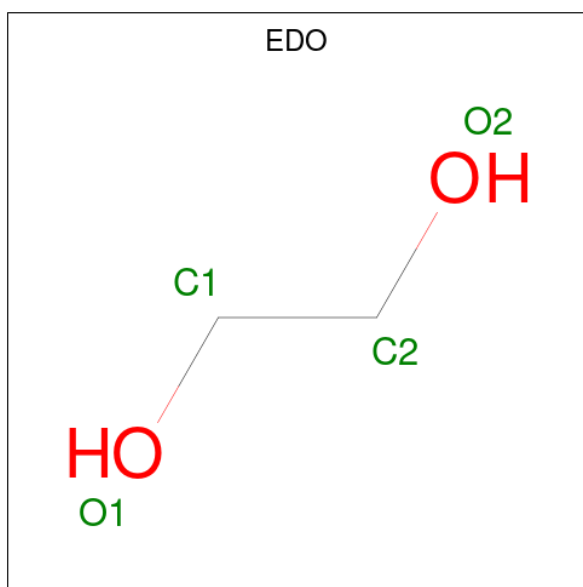
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

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

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



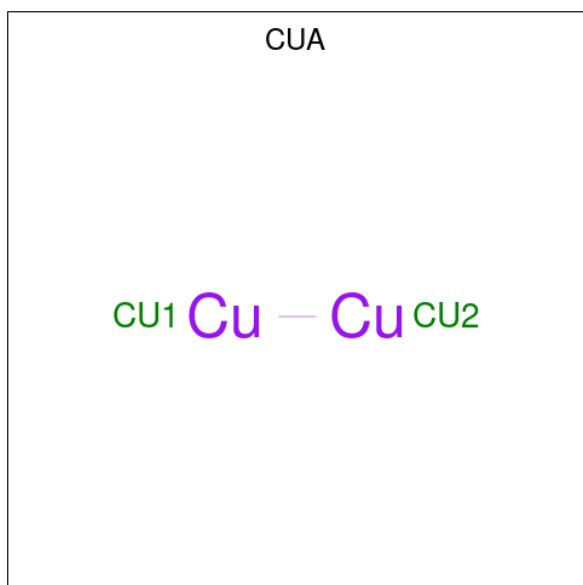
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21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

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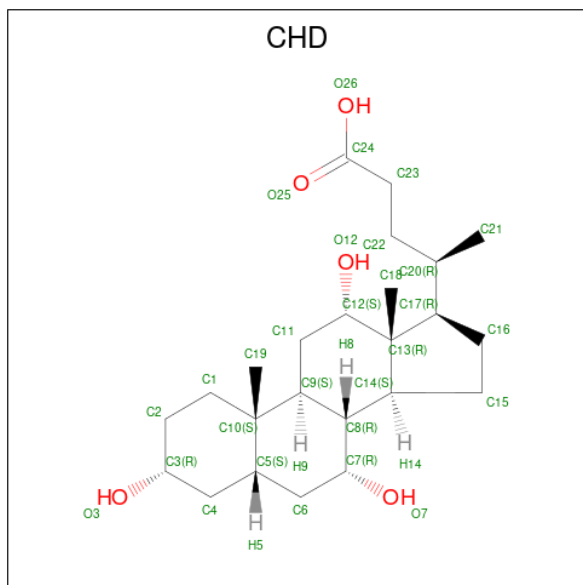
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	K	1	Total 4	C 2	O 2	0	0
21	L	1	Total 4	C 2	O 2	0	0
21	L	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	T	1	Total 4	C 2	O 2	0	0
21	X	1	Total 4	C 2	O 2	0	0

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



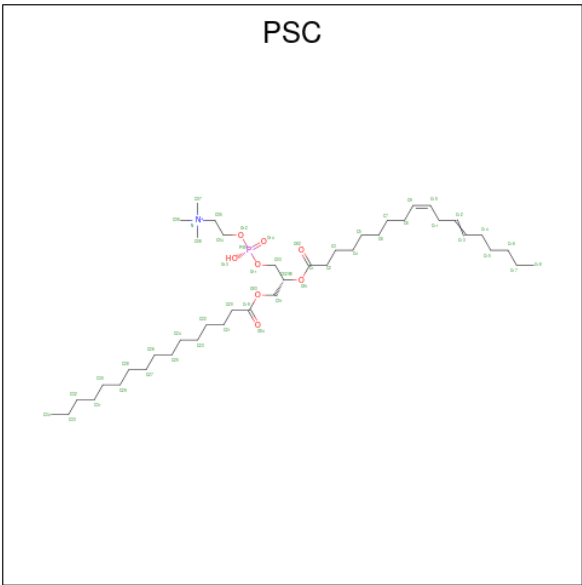
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



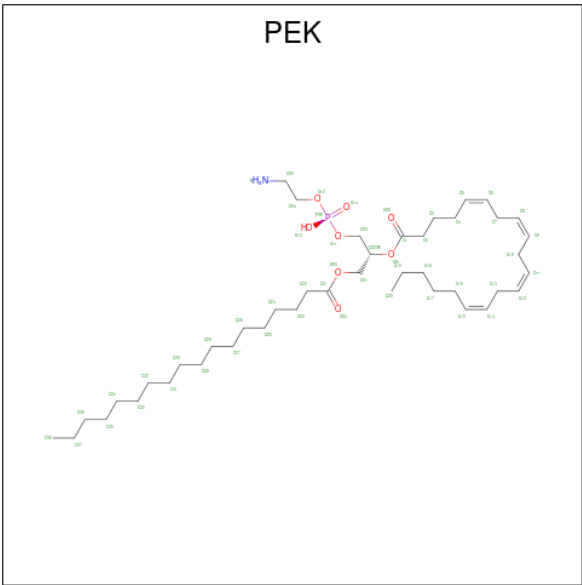
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	G	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0

- Molecule 24 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

- Molecule 25 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
25	B	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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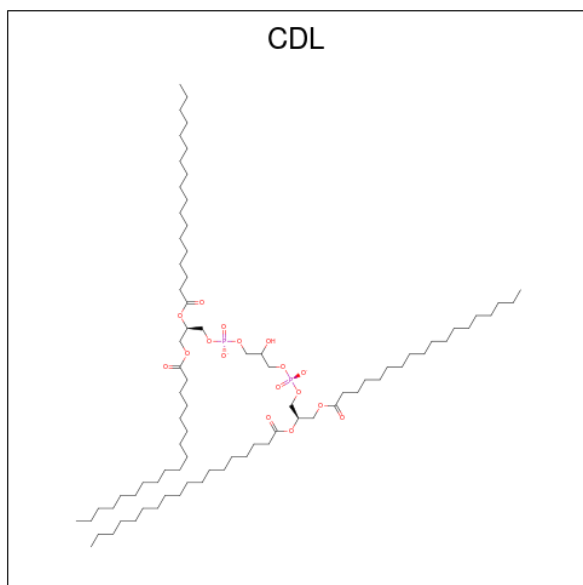
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1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

- Molecule 26 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

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



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

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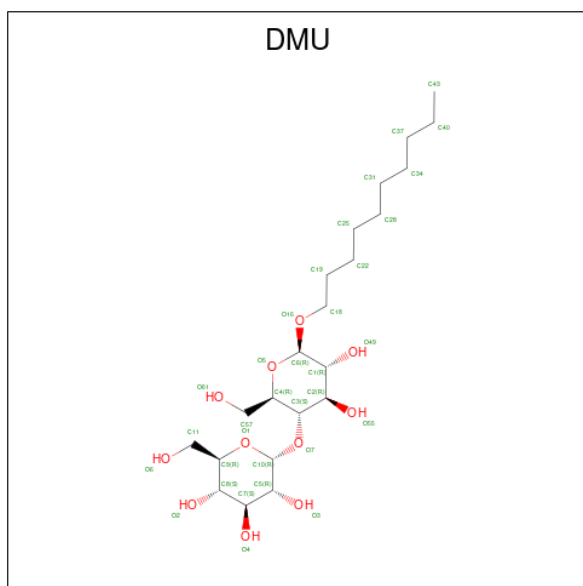
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	P	1	Total	C	O	P	0	0
			100	81	17	2		
27	T	1	Total	C	O	P	0	0
			100	81	17	2		

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

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

- Molecule 29 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	170	Total O 170 170	0	0
30	B	113	Total O 114 114	0	1
30	C	85	Total O 85 85	0	0
30	D	80	Total O 80 80	0	0
30	E	30	Total O 30 30	0	0
30	F	54	Total O 54 54	0	0
30	G	33	Total O 33 33	0	0
30	H	42	Total O 42 42	0	0
30	I	22	Total O 22 22	0	0
30	J	19	Total O 19 19	0	0
30	K	26	Total O 26 26	0	0
30	L	20	Total O 20 20	0	0
30	M	20	Total O 20 20	0	0
30	N	164	Total O 164 164	0	0
30	O	95	Total O 96 96	0	1
30	P	74	Total O 74 74	0	0
30	Q	43	Total O 43 43	0	0
30	R	39	Total O 39 39	0	0
30	S	54	Total O 54 54	0	0
30	T	35	Total O 35 35	0	0
30	U	30	Total O 30 30	0	0
30	V	22	Total O 22 22	0	0

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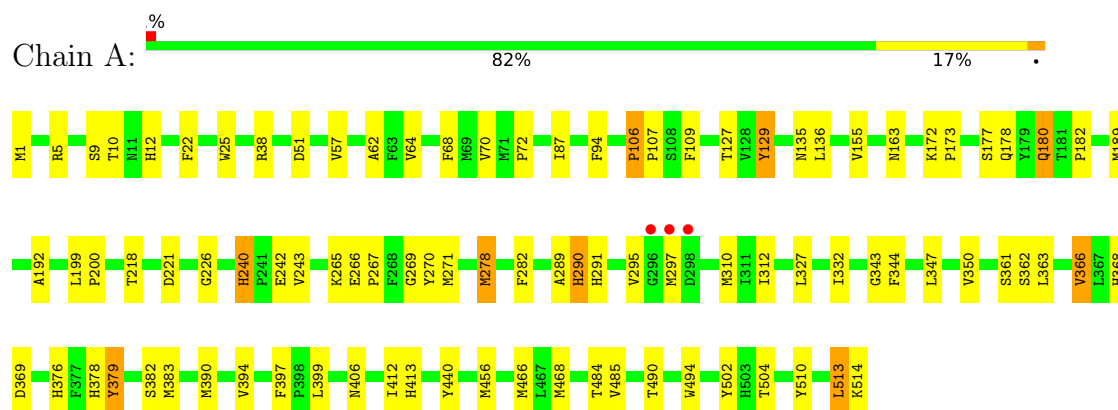
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	W	21	Total 21	O 21	0	0
30	X	12	Total 12	O 12	0	0
30	Y	14	Total 14	O 14	0	0
30	Z	7	Total 7	O 7	0	0

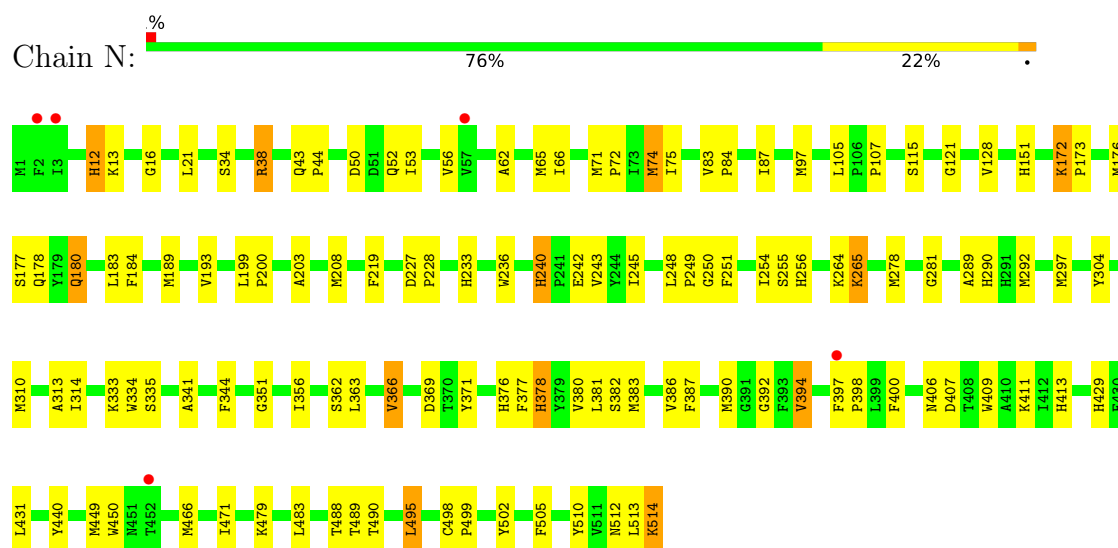
3 Residue-property plots

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

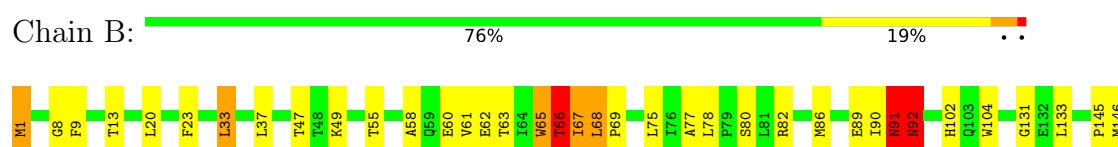
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1

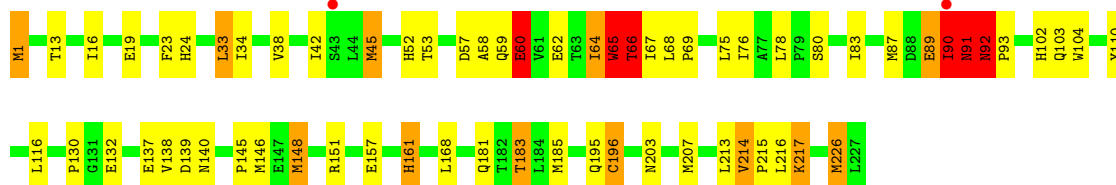


• Molecule 2: Cytochrome c oxidase subunit 2

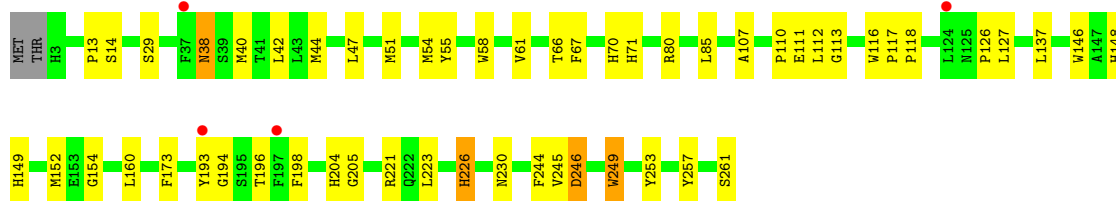
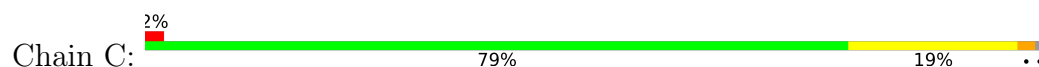




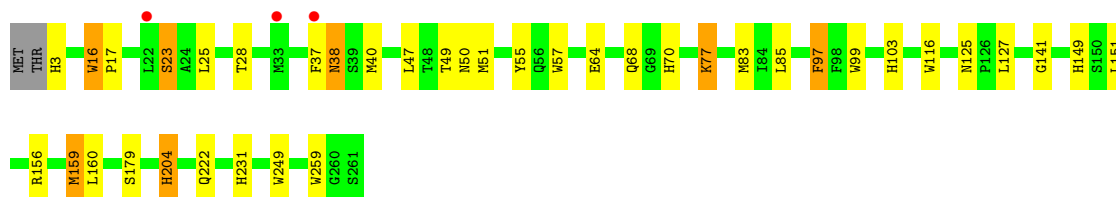
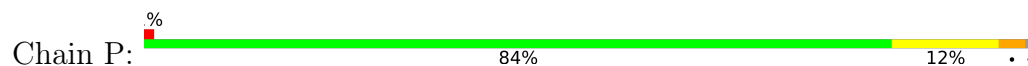
• Molecule 2: Cytochrome c oxidase subunit 2



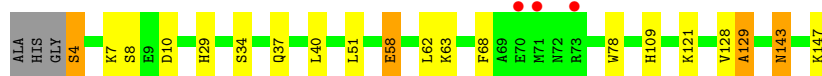
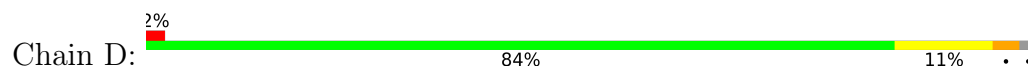
• Molecule 3: Cytochrome c oxidase subunit 3



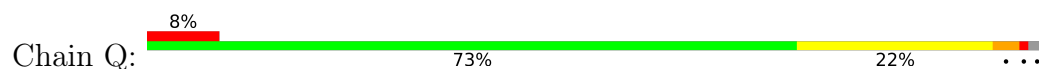
• Molecule 3: Cytochrome c oxidase subunit 3

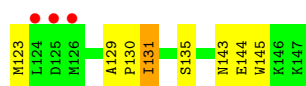


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

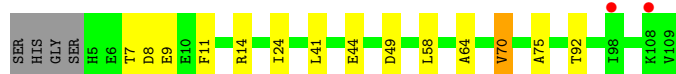
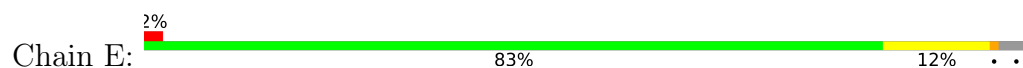


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial





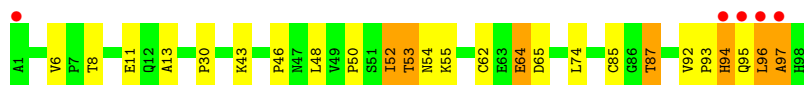
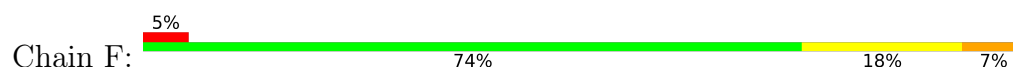
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



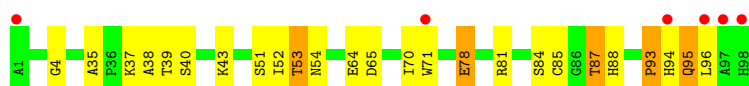
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



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



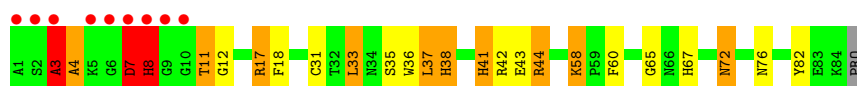
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



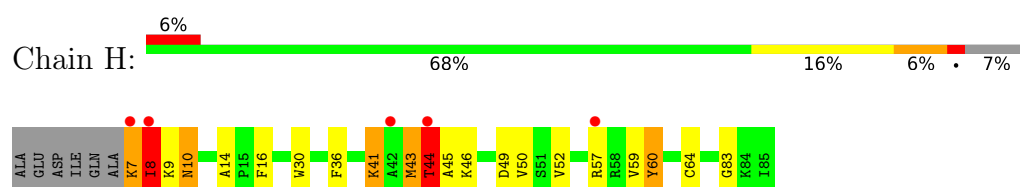
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



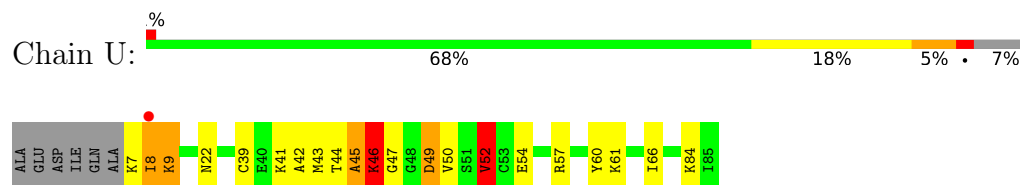
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



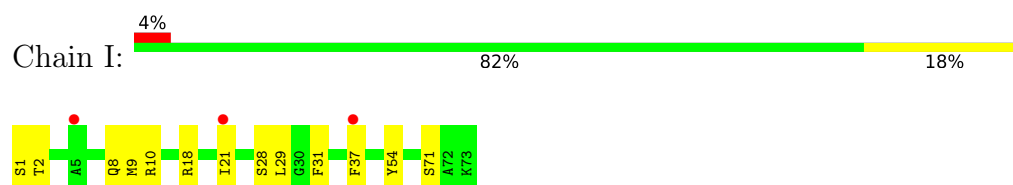
- Molecule 8: Cytochrome c oxidase subunit 6B1



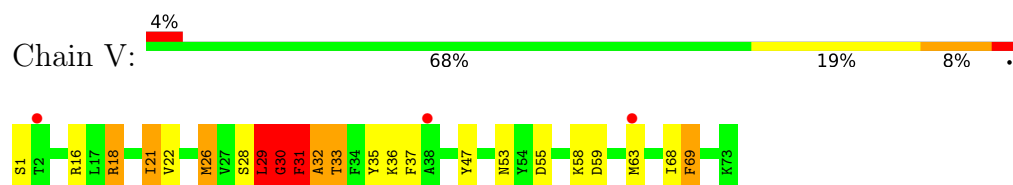
- Molecule 8: Cytochrome c oxidase subunit 6B1



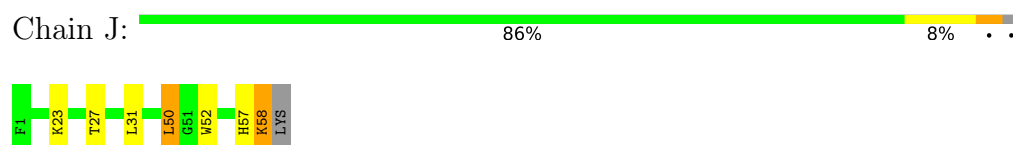
- Molecule 9: Cytochrome c oxidase subunit 6C



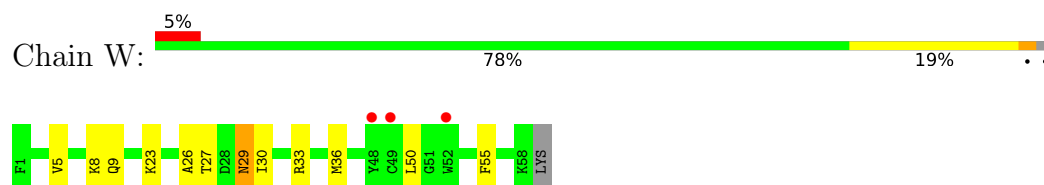
- Molecule 9: Cytochrome c oxidase subunit 6C



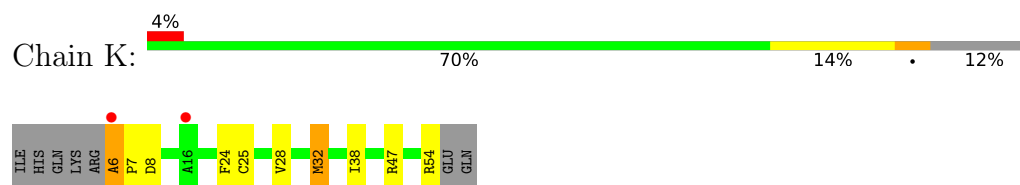
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



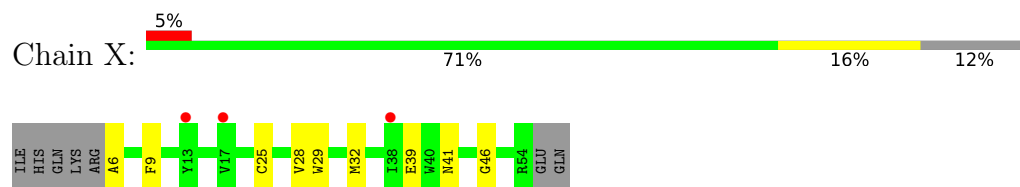
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



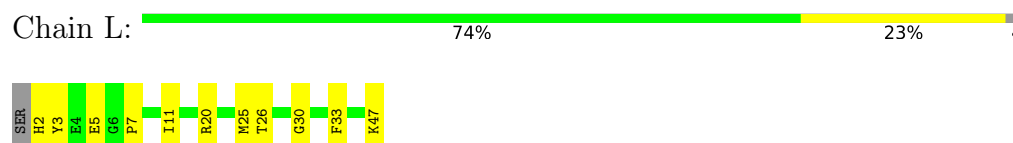
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



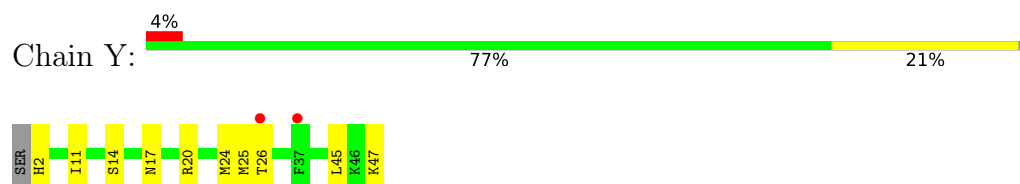
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



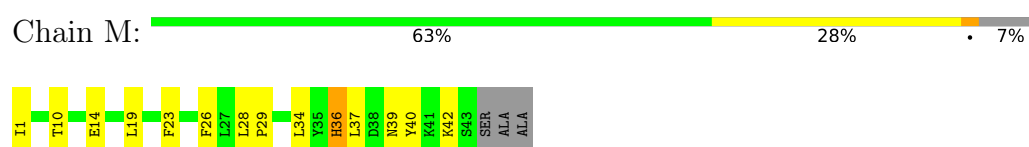
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



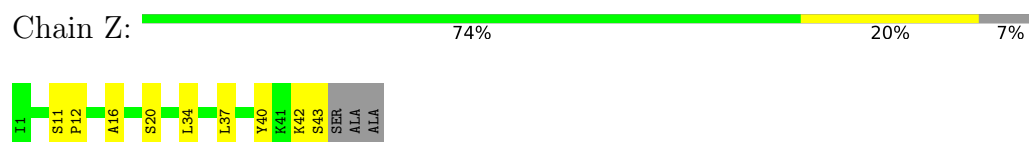
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.81Å 208.49Å 177.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 25.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (25.00-2.20) 96.9 (25.00-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.172 , 0.209 (Not available) , 0.184	Depositor DCC
R_{free} test set	17153 reflections (1.36%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32099	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: DMU, ZN, CMO, CUA, FME, SAC, CDL, CU, NA, TGL, PGV, HEA, EDO, CHD, PSC, PEK, UNX, MG, TPO

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	1.45	20/4164 (0.5%)	1.24	12/5689 (0.2%)
1	N	1.38	15/4156 (0.4%)	1.24	15/5678 (0.3%)
2	B	1.33	7/1860 (0.4%)	1.27	9/2534 (0.4%)
2	O	1.24	10/1860 (0.5%)	1.25	5/2534 (0.2%)
3	C	1.41	8/2197 (0.4%)	1.23	9/3005 (0.3%)
3	P	1.37	9/2197 (0.4%)	1.18	8/3005 (0.3%)
4	D	1.20	3/1229 (0.2%)	1.15	2/1658 (0.1%)
4	Q	1.00	1/1229 (0.1%)	1.09	2/1658 (0.1%)
5	E	1.16	0/871	1.15	2/1182 (0.2%)
5	R	1.05	1/871 (0.1%)	1.12	2/1182 (0.2%)
6	F	1.31	0/765	1.28	3/1038 (0.3%)
6	S	1.22	1/765 (0.1%)	1.28	4/1038 (0.4%)
7	G	1.42	2/690 (0.3%)	1.28	8/937 (0.9%)
7	T	1.33	2/690 (0.3%)	1.21	4/937 (0.4%)
8	H	1.20	0/682	1.25	5/921 (0.5%)
8	U	1.06	0/682	1.22	5/921 (0.5%)
9	I	1.08	0/605	1.21	2/802 (0.2%)
9	V	0.93	0/605	1.31	3/802 (0.4%)
10	J	1.11	0/471	1.13	0/636
10	W	1.01	0/471	1.11	1/636 (0.2%)
11	K	1.20	0/398	1.17	3/546 (0.5%)
11	X	0.99	0/398	1.20	2/546 (0.4%)
12	L	1.26	0/393	1.27	2/526 (0.4%)
12	Y	1.14	0/393	1.16	0/526
13	M	1.20	1/345 (0.3%)	1.17	1/470 (0.2%)
13	Z	1.10	0/345	1.21	1/470 (0.2%)
All	All	1.29	80/29332 (0.3%)	1.22	110/39877 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	O	0	2
6	S	0	1
7	G	0	1
7	T	0	1
9	V	0	2
All	All	0	8

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	204	HIS	ND1-CE1	10.76	1.43	1.32
1	N	290	HIS	CG-CD2	7.79	1.44	1.35
1	N	378	HIS	ND1-CE1	7.50	1.40	1.32
2	B	204	HIS	CG-CD2	7.44	1.44	1.35
1	A	350	VAL	CA-C	7.34	1.61	1.52
2	O	196	CYS	CA-CB	6.98	1.65	1.53
2	B	102	HIS	CE1-NE2	6.72	1.39	1.32
4	D	129	ALA	C-O	-6.64	1.20	1.23
1	A	106	PRO	CA-C	6.60	1.58	1.52
1	A	192	ALA	C-O	6.58	1.31	1.24
7	G	5	LYS	CA-C	6.57	1.59	1.53
1	N	256	HIS	CG-CD2	6.38	1.42	1.35
3	P	204	HIS	CG-CD2	6.36	1.42	1.35
3	C	148	HIS	CG-CD2	6.26	1.42	1.35
1	A	290	HIS	CG-CD2	6.23	1.42	1.35
1	A	376	HIS	CE1-NE2	6.22	1.38	1.32
2	O	66	THR	CA-C	6.20	1.58	1.52
3	P	103	HIS	CG-CD2	6.18	1.42	1.35
3	C	61	VAL	CA-CB	6.07	1.62	1.54
2	O	24	HIS	CE1-NE2	6.07	1.38	1.32
2	B	8	GLY	C-O	6.05	1.29	1.24
1	N	12	HIS	CE1-NE2	6.01	1.38	1.32
1	N	219	PHE	C-O	-6.01	1.17	1.24
1	N	12	HIS	CG-CD2	5.91	1.42	1.35
1	A	242	GLU	C-O	-5.86	1.17	1.24
1	A	135	ASN	N-CA	5.85	1.53	1.46
3	P	149	HIS	ND1-CE1	5.84	1.38	1.32
2	O	24	HIS	CG-CD2	5.83	1.42	1.35
1	N	429	HIS	CG-CD2	5.81	1.42	1.35
1	A	182	PRO	C-O	5.70	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	HIS	ND1-CE1	5.69	1.38	1.32
1	A	378	HIS	CG-ND1	-5.67	1.32	1.38
4	D	29	HIS	CE1-NE2	5.66	1.38	1.32
2	O	52	HIS	CG-CD2	5.63	1.42	1.35
4	Q	129	ALA	N-CA	5.58	1.50	1.46
3	P	70	HIS	CE1-NE2	5.56	1.38	1.32
2	O	196	CYS	N-CA	5.56	1.52	1.46
1	A	379	TYR	N-CA	5.54	1.52	1.46
1	N	290	HIS	CE1-NE2	5.52	1.38	1.32
2	B	161	HIS	CE1-NE2	5.51	1.38	1.32
3	C	14	SER	C-O	-5.46	1.17	1.24
1	N	151	HIS	CG-CD2	5.45	1.41	1.35
1	A	240	HIS	CB-CG	-5.45	1.42	1.50
1	A	163	ASN	CA-C	5.42	1.59	1.52
5	R	78	HIS	CG-CD2	5.42	1.41	1.35
3	C	244	PHE	C-N	-5.39	1.27	1.33
3	P	97	PHE	N-CA	5.39	1.53	1.46
3	P	116	TRP	CD2-CE2	5.38	1.50	1.41
1	N	256	HIS	ND1-CE1	5.36	1.38	1.32
1	A	332	ILE	C-O	-5.36	1.18	1.24
3	P	149	HIS	CG-CD2	5.34	1.41	1.35
6	S	88	HIS	CG-CD2	5.34	1.41	1.35
7	T	58	LYS	CA-C	5.34	1.57	1.52
1	A	368	HIS	CG-CD2	5.31	1.41	1.35
2	B	161	HIS	CG-CD2	5.31	1.41	1.35
1	N	366	VAL	C-O	-5.31	1.19	1.24
3	P	231	HIS	CG-CD2	5.31	1.41	1.35
1	N	97	MET	CA-C	5.30	1.59	1.52
1	A	397	PHE	N-CA	5.30	1.51	1.46
1	N	378	HIS	CG-CD2	5.26	1.41	1.35
13	M	36	HIS	CG-CD2	5.26	1.41	1.35
2	O	161	HIS	CG-CD2	5.24	1.41	1.35
3	C	71	HIS	CG-CD2	5.24	1.41	1.35
2	O	52	HIS	CE1-NE2	5.21	1.37	1.32
3	C	249	TRP	CD2-CE2	5.21	1.50	1.41
2	O	24	HIS	ND1-CE1	5.21	1.37	1.32
1	A	64	VAL	N-CA	-5.20	1.40	1.46
1	A	12	HIS	CB-CG	5.20	1.57	1.50
1	A	57	VAL	CA-CB	5.16	1.60	1.54
2	O	214	VAL	C-O	5.15	1.28	1.24
2	B	165	VAL	CA-C	5.15	1.58	1.52
1	A	295	VAL	C-O	5.13	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	57	TRP	CD2-CE2	5.11	1.50	1.41
4	D	29	HIS	CG-CD2	5.11	1.41	1.35
3	C	226	HIS	CG-CD2	5.09	1.41	1.35
1	N	376	HIS	CE1-NE2	5.08	1.37	1.32
1	N	371	TYR	CA-C	5.05	1.59	1.52
7	T	67	HIS	CG-CD2	5.05	1.41	1.35
3	C	70	HIS	CG-CD2	5.04	1.41	1.35
7	G	20	THR	C-O	-5.01	1.18	1.24

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	31	PHE	N-CA-C	-17.88	91.94	111.07
7	T	3	ALA	N-CA-C	11.40	125.97	108.42
1	N	172	LYS	CA-C-N	-9.01	113.08	119.66
1	N	172	LYS	C-N-CA	-9.01	113.08	119.66
7	G	57	THR	N-CA-C	-8.21	103.41	113.50
3	C	38	ASN	N-CA-C	8.06	122.81	113.38
1	A	94	PHE	CA-C-N	7.95	127.62	119.19
1	A	94	PHE	C-N-CA	7.95	127.62	119.19
3	P	16	TRP	CA-C-N	-7.79	110.87	118.97
3	P	16	TRP	C-N-CA	-7.79	110.87	118.97
7	G	7	ASP	N-CA-C	7.69	127.19	110.80
3	C	113	GLY	N-CA-C	-7.45	104.92	115.43
8	H	9	LYS	N-CA-C	-7.44	104.66	113.21
7	G	72	ASN	CA-C-N	7.25	127.10	119.05
7	G	72	ASN	C-N-CA	7.25	127.10	119.05
1	N	105	LEU	CA-C-N	-7.08	113.09	120.38
1	N	105	LEU	C-N-CA	-7.08	113.09	120.38
12	L	25	MET	CA-C-N	7.02	130.02	120.54
12	L	25	MET	C-N-CA	7.02	130.02	120.54
1	N	16	GLY	N-CA-C	-7.02	104.36	112.50
2	B	67	ILE	CB-CA-C	-6.89	103.00	112.24
1	A	70	VAL	N-CA-C	6.88	117.39	110.23
6	S	53	THR	CB-CA-C	-6.88	97.33	114.11
2	O	89	GLU	N-CA-C	6.86	119.67	110.35
1	A	327	LEU	N-CA-C	-6.81	103.92	111.82
3	C	246	ASP	N-CA-CB	-6.80	100.14	110.01
10	W	55	PHE	CB-CA-C	6.72	118.89	108.61
9	I	37	PHE	CB-CA-C	6.68	120.30	109.07
11	X	41	ASN	CA-C-N	-6.60	113.87	120.21
11	X	41	ASN	C-N-CA	-6.60	113.87	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	CA-CB-CG	-6.59	107.21	113.80
8	U	8	ILE	N-CA-C	6.58	117.92	107.98
1	N	281	GLY	N-CA-C	-6.51	104.94	112.50
11	K	6	ALA	CA-C-N	6.45	126.68	119.90
11	K	6	ALA	C-N-CA	6.45	126.68	119.90
1	A	240	HIS	N-CA-CB	6.27	117.82	110.42
2	B	184	LEU	N-CA-C	-6.17	98.94	109.24
6	F	64	GLU	CA-C-N	-6.12	114.34	125.66
6	F	64	GLU	C-N-CA	-6.12	114.34	125.66
8	U	44	THR	N-CA-C	-6.10	104.91	112.90
1	N	240	HIS	CA-CB-CG	-6.07	107.73	113.80
13	Z	40	TYR	N-CA-C	6.03	118.62	111.33
1	A	278	MET	N-CA-C	5.95	118.25	111.11
1	N	184	PHE	N-CA-C	-5.95	104.87	111.36
5	E	64	ALA	N-CA-C	-5.89	104.94	111.36
7	T	8	HIS	N-CA-C	5.88	123.32	110.80
8	U	49	ASP	N-CA-C	5.88	118.58	110.35
7	G	17	ARG	CB-CG-CD	-5.87	97.79	111.30
2	B	60	GLU	N-CA-C	-5.85	105.39	113.18
7	G	41	HIS	N-CA-C	5.80	118.24	110.35
1	N	392	GLY	N-CA-C	-5.79	105.18	113.86
1	N	240	HIS	N-CA-CB	5.77	117.23	110.42
1	A	412	ILE	N-CA-C	-5.77	104.74	110.62
1	A	310	MET	CA-CB-CG	-5.76	102.57	114.10
3	C	194	GLY	N-CA-C	-5.72	105.86	112.73
9	I	54	TYR	N-CA-C	5.67	118.55	110.10
6	S	40	SER	N-CA-C	-5.66	106.22	113.23
2	O	92	ASN	N-CA-C	5.63	122.26	109.81
4	D	62	LEU	N-CA-C	-5.61	105.55	112.90
1	A	155	VAL	N-CA-C	-5.61	104.90	110.62
3	C	253	TYR	N-CA-C	-5.60	105.09	111.14
1	A	343	GLY	N-CA-C	-5.60	106.01	112.73
1	N	407	ASP	N-CA-C	5.59	117.82	111.11
3	P	159	MET	N-CA-C	-5.59	105.10	111.14
2	O	65	TRP	CB-CA-C	5.59	120.31	110.37
2	B	65	TRP	CB-CA-C	5.53	120.21	110.37
1	N	449	MET	N-CA-C	5.52	117.30	111.28
7	T	72	ASN	CA-C-N	5.49	124.68	118.97
7	T	72	ASN	C-N-CA	5.49	124.68	118.97
8	U	52	VAL	CB-CA-C	-5.49	103.64	112.16
8	H	8	ILE	N-CA-C	5.46	120.71	109.34
9	V	69	PHE	N-CA-C	5.46	118.57	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	28	THR	N-CA-C	-5.46	104.98	111.69
5	R	42	VAL	CA-C-N	-5.45	114.35	119.85
5	R	42	VAL	C-N-CA	-5.45	114.35	119.85
2	O	196	CYS	N-CA-CB	5.43	117.55	109.19
3	P	23	SER	N-CA-C	-5.42	105.53	111.82
3	P	99	TRP	N-CA-C	-5.42	105.45	111.36
2	B	66	THR	CB-CA-C	5.41	117.73	109.34
3	C	85	LEU	N-CA-C	-5.41	105.55	111.82
3	C	245	VAL	N-CA-CB	-5.35	103.26	110.54
6	S	35	ALA	CA-C-N	-5.33	114.22	119.92
6	S	35	ALA	C-N-CA	-5.33	114.22	119.92
3	C	58	TRP	N-CA-C	5.33	117.83	111.71
5	E	75	ALA	N-CA-C	-5.32	106.05	112.54
4	Q	143	ASN	N-CA-C	5.31	118.72	111.39
3	P	83	MET	N-CA-C	-5.31	105.57	111.36
6	F	13	ALA	N-CA-C	-5.29	103.15	110.35
1	A	129	TYR	N-CA-C	5.29	116.35	109.64
2	B	55	THR	N-CA-C	5.25	117.95	110.24
2	O	64	ILE	CB-CA-C	-5.25	105.17	112.04
8	U	60	TYR	N-CA-C	-5.24	105.74	111.82
8	H	83	GLY	N-CA-C	-5.22	104.72	113.02
7	G	25	LEU	CA-C-N	-5.21	113.54	119.28
7	G	25	LEU	C-N-CA	-5.21	113.54	119.28
8	H	64	CYS	CA-C-N	-5.18	114.44	119.78
8	H	64	CYS	C-N-CA	-5.18	114.44	119.78
11	K	47	ARG	N-CA-C	-5.17	106.31	113.18
3	C	196	THR	N-CA-C	-5.13	105.87	111.82
9	V	29	LEU	N-CA-C	-5.10	104.22	110.65
4	D	143	ASN	N-CA-C	5.08	118.45	111.54
1	N	255	SER	N-CA-C	5.06	117.18	111.11
2	B	201	GLY	CA-C-N	5.04	127.03	120.28
2	B	201	GLY	C-N-CA	5.04	127.03	120.28
4	Q	90	GLY	N-CA-C	-5.03	106.66	112.50
13	M	40	TYR	N-CA-C	5.01	116.74	111.28
2	B	77	ALA	N-CA-C	5.01	116.82	111.36
3	P	141	GLY	N-CA-C	-5.01	108.45	114.66
1	N	74	MET	CB-CG-SD	-5.00	97.69	112.70
1	N	479	LYS	N-CA-C	5.00	118.14	111.24

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	91	ASN	Peptide
7	G	10	GLY	Peptide
2	O	90	ILE	Peptide
2	O	91	ASN	Peptide
6	S	93	PRO	Peptide
7	T	3	ALA	Peptide
9	V	30	GLY	Peptide
9	V	53	ASN	Peptide

5.2 Too-close contacts [i](#)

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	4030	0	4008	69	0
1	N	4027	0	4001	91	0
2	B	1824	0	1833	38	0
2	O	1824	0	1833	58	0
3	C	2110	0	2027	36	0
3	P	2110	0	2027	26	0
4	D	1195	0	1183	21	0
4	Q	1195	0	1183	33	0
5	E	852	0	845	8	0
5	R	852	0	845	13	0
6	F	748	0	728	27	0
6	S	748	0	728	12	0
7	G	675	0	643	32	0
7	T	675	0	644	25	0
8	H	662	0	623	17	0
8	U	662	0	623	20	0
9	I	601	0	613	8	0
9	V	601	0	613	31	0
10	J	460	0	459	5	0
10	W	460	0	459	9	0
11	K	384	0	366	11	0
11	X	384	0	366	9	0
12	L	380	0	380	14	0
12	Y	380	0	380	16	0
13	M	335	0	352	12	0
13	Z	335	0	352	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	120	0	108	7	0
14	N	120	0	108	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	2	0
19	A	63	0	110	0	0
19	D	63	0	110	10	0
19	L	63	0	110	11	0
19	N	63	0	110	4	0
19	Q	63	0	110	6	0
19	Y	63	0	110	16	0
20	A	102	0	152	7	0
20	C	102	0	152	8	0
20	N	102	0	152	5	0
20	P	51	0	76	1	0
20	Z	51	0	76	5	0
21	A	16	0	24	11	0
21	B	4	0	6	0	0
21	C	16	0	24	5	0
21	F	4	0	6	3	0
21	G	4	0	6	0	0
21	I	4	0	6	5	0
21	K	12	0	18	0	0
21	L	8	0	12	1	0
21	N	12	0	18	0	0
21	P	8	0	12	2	0
21	S	4	0	6	1	0
21	T	4	0	6	1	0
21	X	4	0	6	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	1	0
23	C	58	0	78	1	0
23	G	29	0	39	0	0
23	J	29	0	39	1	0
23	P	58	0	78	5	0
23	W	29	0	39	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	B	52	0	80	2	0
24	O	52	0	80	5	0
25	B	53	0	77	1	0
25	C	106	0	154	4	0
25	G	106	0	154	9	0
25	T	53	0	77	4	0
26	C	1	0	0	0	0
26	P	1	0	0	1	0
27	C	100	0	156	10	0
27	G	100	0	156	16	0
27	P	100	0	156	6	0
27	T	100	0	156	16	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	M	33	0	42	0	0
29	Z	33	0	42	1	0
30	A	170	0	0	27	0
30	B	114	0	0	10	0
30	C	85	0	0	13	0
30	D	80	0	0	5	0
30	E	30	0	0	2	0
30	F	54	0	0	4	0
30	G	33	0	0	6	0
30	H	42	0	0	7	0
30	I	22	0	0	2	0
30	J	19	0	0	1	0
30	K	26	0	0	4	0
30	L	20	0	0	6	0
30	M	20	0	0	4	0
30	N	164	0	0	22	0
30	O	96	0	0	19	0
30	P	74	0	0	4	0
30	Q	43	0	0	7	0
30	R	39	0	0	6	0
30	S	54	0	0	2	0
30	T	35	0	0	8	0
30	U	30	0	0	2	0
30	V	22	0	0	0	0
30	W	21	0	0	1	0
30	X	12	0	0	6	0
30	Y	14	0	0	1	0
30	Z	7	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	32099	0	31390	695	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (695) 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)
13:M:26:PHE:HB2	30:M:201:HOH:O	1.24	1.26
1:N:466:MET:HG2	30:N:795:HOH:O	1.35	1.26
8:H:14:ALA:HB2	30:H:107:HOH:O	1.33	1.25
11:X:28:VAL:HG13	30:X:205:HOH:O	1.35	1.22
1:N:466:MET:HA	30:N:795:HOH:O	1.40	1.21
5:E:44:GLU:OE1	21:I:101:EDO:H21	1.41	1.19
2:O:83:ILE:HG22	30:O:464:HOH:O	1.42	1.17
1:A:62:ALA:HA	30:A:779:HOH:O	1.46	1.15
2:O:65:TRP:CE3	30:O:467:HOH:O	1.98	1.15
3:C:226:HIS:HB3	30:C:402:HOH:O	1.48	1.14
7:G:10:GLY:CA	1:N:177:SER:HB2	1.78	1.13
2:O:69:PRO:HB2	30:O:472:HOH:O	1.44	1.13
2:O:65:TRP:HB3	30:O:467:HOH:O	1.49	1.11
27:G:102:CDL:H242	27:G:102:CDL:H531	1.33	1.09
1:N:178:GLN:HB3	30:N:837:HOH:O	1.51	1.09
12:L:33:PHE:HB3	30:L:210:HOH:O	1.52	1.08
1:N:74:MET:HB3	30:N:808:HOH:O	1.51	1.08
3:C:111:GLU:HG3	30:C:471:HOH:O	1.50	1.07
19:L:101:TGL:OC1	19:L:101:TGL:HC41	1.56	1.05
20:A:609:PGV:H032	20:A:609:PGV:H32	1.32	1.04
1:A:68:PHE:CE1	30:A:702:HOH:O	2.11	1.04
7:G:10:GLY:HA3	1:N:177:SER:HB2	1.36	1.03
6:S:85:CYS:SG	6:S:87:THR:HG23	1.98	1.03
30:A:705:HOH:O	12:L:7:PRO:HG3	1.58	1.03
6:F:85:CYS:SG	6:F:87:THR:HG23	1.98	1.02
3:C:137:LEU:HD12	30:C:472:HOH:O	1.56	1.02
1:A:466:MET:HA	30:A:851:HOH:O	1.60	1.01
1:N:314:ILE:HG12	30:O:472:HOH:O	1.58	1.00
9:V:26:MET:O	9:V:30:GLY:HA3	1.59	1.00
11:X:29:TRP:CD1	30:X:205:HOH:O	2.15	1.00
3:C:149:HIS:NE2	21:C:309:EDO:H22	1.78	0.99
1:N:65:MET:HB2	30:N:744:HOH:O	1.60	0.99
1:A:10:THR:H	21:A:613:EDO:H12	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:72:ASN:H	7:G:76:ASN:HD22	1.11	0.99
2:O:65:TRP:HE3	30:O:467:HOH:O	1.39	0.97
27:C:303:CDL:H361	30:C:479:HOH:O	1.63	0.96
9:V:29:LEU:C	9:V:32:ALA:HB2	1.89	0.96
30:A:780:HOH:O	6:F:96:LEU:HD13	1.66	0.96
27:G:102:CDL:H222	27:G:102:CDL:H511	1.46	0.94
9:I:10:ARG:HH11	21:I:101:EDO:H22	1.32	0.94
4:Q:19:ARG:HH21	4:Q:19:ARG:HG3	1.32	0.94
1:A:22:PHE:CE2	30:A:855:HOH:O	2.21	0.94
7:G:45:PRO:HD2	30:G:208:HOH:O	1.66	0.93
9:I:10:ARG:NH1	21:I:101:EDO:H22	1.83	0.93
1:N:75:ILE:HG13	30:N:808:HOH:O	1.68	0.93
4:Q:78:TRP:HB3	19:Q:201:TGL:HB21	1.51	0.93
1:N:335:SER:HB3	30:N:766:HOH:O	1.69	0.92
30:B:470:HOH:O	7:T:17:ARG:HD2	1.67	0.92
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.51	0.91
4:D:78:TRP:HB3	19:D:201:TGL:CB2	1.99	0.91
20:A:609:PGV:H032	20:A:609:PGV:C3	2.01	0.91
26:P:301:UNX:UNK	30:P:453:HOH:O	1.52	0.91
7:G:76:ASN:HD21	25:G:101:PEK:HN2	1.18	0.90
1:A:109:PHE:HB2	30:A:702:HOH:O	1.71	0.90
19:L:101:TGL:OC1	19:L:101:TGL:CC4	2.19	0.90
4:Q:92:THR:HA	30:Q:301:HOH:O	1.71	0.90
8:H:7:LYS:HB3	8:H:8:ILE:HD12	1.54	0.90
21:A:613:EDO:H21	3:C:13:PRO:HG3	1.53	0.90
1:A:22:PHE:HE2	30:A:855:HOH:O	1.53	0.90
7:G:71:HIS:HA	30:G:204:HOH:O	1.70	0.89
2:B:49:LYS:HG3	30:E:230:HOH:O	1.70	0.89
1:N:400:PHE:HB3	19:Y:101:TGL:H283	1.54	0.89
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.36	0.88
4:Q:9:GLU:HB2	30:Q:336:HOH:O	1.72	0.88
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.38	0.88
27:T:102:CDL:OB4	27:T:102:CDL:H142	1.75	0.86
20:A:609:PGV:H32	20:A:609:PGV:C03	2.05	0.86
1:A:502:TYR:OH	21:A:613:EDO:H11	1.76	0.85
12:L:20:ARG:HH22	19:L:101:TGL:HC62	1.41	0.85
1:A:109:PHE:CB	30:A:702:HOH:O	2.24	0.85
1:A:514:LYS:HE2	30:F:224:HOH:O	1.75	0.85
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.59	0.85
11:K:7:PRO:HB2	30:K:207:HOH:O	1.78	0.84
6:F:64:GLU:O	6:F:65:ASP:HB2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PHE:CA	30:A:702:HOH:O	2.26	0.84
1:N:66:ILE:HG13	30:N:744:HOH:O	1.78	0.83
3:C:67:PHE:HE2	27:C:303:CDL:H1	1.41	0.83
30:A:851:HOH:O	13:M:26:PHE:CE1	2.32	0.83
2:O:217:LYS:NZ	2:O:217:LYS:H	1.76	0.83
2:O:161:HIS:HE1	30:O:460:HOH:O	1.62	0.83
25:C:308:PEK:H342	7:T:3:ALA:HB2	1.59	0.82
4:D:78:TRP:CA	19:D:201:TGL:HB21	2.09	0.82
12:L:2:HIS:CD2	12:L:3:TYR:H	1.98	0.82
30:N:846:HOH:O	4:Q:81:VAL:HG11	1.79	0.82
3:P:77:LYS:HZ2	3:P:77:LYS:HB3	1.44	0.81
9:V:31:PHE:CD1	9:V:32:ALA:N	2.48	0.81
20:Z:101:PGV:H201	30:Z:203:HOH:O	1.78	0.81
3:P:77:LYS:HB3	3:P:77:LYS:NZ	1.96	0.81
30:A:780:HOH:O	6:F:96:LEU:CD1	2.23	0.81
12:L:47:LYS:HA	30:L:216:HOH:O	1.81	0.81
7:T:72:ASN:H	7:T:76:ASN:HD22	1.25	0.81
27:T:102:CDL:H131	27:T:102:CDL:HB22	1.62	0.81
6:F:43:LYS:HB2	30:F:201:HOH:O	1.82	0.80
20:N:608:PGV:H061	8:U:22:ASN:HB2	1.64	0.80
2:O:103:GLN:HA	30:O:460:HOH:O	1.81	0.80
4:Q:92:THR:CA	30:Q:301:HOH:O	2.26	0.80
19:L:101:TGL:HG31	30:L:212:HOH:O	1.81	0.79
25:G:101:PEK:H42	25:G:101:PEK:H8	1.64	0.79
21:C:312:EDO:O2	30:C:401:HOH:O	2.00	0.78
1:A:10:THR:H	21:A:613:EDO:C1	1.95	0.78
21:P:307:EDO:H22	30:P:457:HOH:O	1.82	0.78
2:O:89:GLU:O	30:O:401:HOH:O	2.02	0.78
3:C:173:PHE:CE2	30:C:472:HOH:O	2.37	0.77
4:Q:19:ARG:HH21	4:Q:19:ARG:CG	1.97	0.77
9:V:33:THR:HG23	9:V:37:PHE:CD2	2.20	0.77
20:C:307:PGV:H032	21:C:312:EDO:C1	2.15	0.76
2:O:87:MET:SD	30:O:464:HOH:O	2.42	0.76
12:L:20:ARG:HH22	19:L:101:TGL:HC32	1.49	0.76
27:T:102:CDL:H511	27:T:102:CDL:H222	1.66	0.76
27:G:102:CDL:H761	27:G:102:CDL:H582	1.67	0.75
2:B:89:GLU:O	2:B:91:ASN:OD1	2.05	0.75
3:C:66:THR:OG1	30:C:402:HOH:O	2.04	0.75
3:P:77:LYS:HZ2	3:P:77:LYS:CB	2.01	0.74
5:R:19:PHE:HD2	30:R:208:HOH:O	1.70	0.74
8:H:43:MET:O	8:H:45:ALA:N	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:217:LYS:H	2:O:217:LYS:HZ3	1.34	0.74
2:O:38:VAL:O	2:O:42:ILE:HG13	1.88	0.74
3:P:77:LYS:NZ	3:P:77:LYS:CB	2.51	0.74
5:E:41:LEU:HA	30:I:214:HOH:O	1.87	0.74
20:A:609:PGV:H211	20:A:609:PGV:H031	1.68	0.73
1:N:21:LEU:HD23	19:Y:101:TGL:H221	1.68	0.73
8:H:60:TYR:HA	30:H:123:HOH:O	1.86	0.73
11:X:29:TRP:HD1	30:X:205:HOH:O	1.57	0.73
2:B:207:MET:HE2	30:B:465:HOH:O	1.88	0.73
3:C:221:ARG:NH2	30:C:402:HOH:O	2.20	0.73
6:F:94:HIS:HA	6:F:97:ALA:HB3	1.71	0.72
7:G:10:GLY:HA3	1:N:177:SER:CB	2.16	0.72
9:V:33:THR:HG23	9:V:37:PHE:HD2	1.55	0.72
2:B:47:THR:HB	19:D:201:TGL:H182	1.71	0.72
2:O:45:MET:HA	2:O:45:MET:HE2	1.71	0.72
10:W:29:ASN:HD22	10:W:29:ASN:H	1.36	0.72
9:I:9:MET:HB2	21:I:101:EDO:H11	1.71	0.71
13:M:23:PHE:O	30:M:201:HOH:O	2.08	0.71
1:A:390:MET:HE2	1:A:413:HIS:CE1	2.22	0.71
25:C:308:PEK:H342	7:T:3:ALA:CB	2.20	0.71
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.19	0.71
11:X:39:GLU:HB3	30:X:208:HOH:O	1.89	0.71
6:S:52:ILE:HA	6:S:94:HIS:HB3	1.72	0.70
9:V:28:SER:O	9:V:31:PHE:HD1	1.73	0.70
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.26	0.70
2:O:215:PRO:HB2	2:O:217:LYS:HE2	1.74	0.69
1:N:409:TRP:HB2	30:N:755:HOH:O	1.92	0.69
1:A:10:THR:N	21:A:613:EDO:H12	2.04	0.69
7:T:12:GLY:HA3	30:T:225:HOH:O	1.93	0.69
2:B:92:ASN:HB3	30:B:467:HOH:O	1.92	0.69
8:H:8:ILE:C	8:H:10:ASN:H	1.98	0.69
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.28	0.69
7:T:82:TYR:HB3	30:T:202:HOH:O	1.92	0.69
1:A:510:TYR:OH	21:F:102:EDO:H21	1.93	0.68
2:O:104:TRP:CD1	30:O:460:HOH:O	2.45	0.68
2:O:138:VAL:HG21	30:O:427:HOH:O	1.94	0.68
25:G:101:PEK:H42	25:G:101:PEK:C8	2.22	0.68
12:Y:24:MET:HG2	19:Y:101:TGL:H152	1.76	0.68
9:I:71:SER:O	30:I:201:HOH:O	2.12	0.68
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.57	0.68
9:V:26:MET:O	9:V:30:GLY:CA	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:TYR:OH	21:F:102:EDO:C2	2.42	0.67
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.43	0.67
7:G:10:GLY:HA2	1:N:177:SER:HB2	1.71	0.67
1:N:38:ARG:HD2	14:N:601:HEA:OMA	1.95	0.67
1:N:406:ASN:HD21	20:Z:101:PGV:H32	1.58	0.66
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.75	0.66
7:T:42:ARG:HG3	30:T:229:HOH:O	1.95	0.66
4:Q:98:TRP:CE3	29:Z:102:DMU:H15	2.30	0.66
9:I:9:MET:CB	21:I:101:EDO:H11	2.25	0.66
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.77	0.66
2:B:90:ILE:HA	30:B:476:HOH:O	1.96	0.66
2:O:65:TRP:CD2	30:O:467:HOH:O	2.35	0.66
20:C:302:PGV:O05	30:C:402:HOH:O	2.14	0.66
8:U:45:ALA:O	8:U:47:GLY:N	2.29	0.66
10:W:29:ASN:HD22	10:W:29:ASN:N	1.94	0.66
3:C:137:LEU:CD1	30:C:472:HOH:O	2.27	0.65
27:T:102:CDL:H241	27:T:102:CDL:H531	1.76	0.65
9:V:29:LEU:CA	9:V:32:ALA:HB2	2.26	0.65
1:A:172:LYS:HB2	30:A:728:HOH:O	1.97	0.65
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.78	0.65
10:W:33:ARG:HG2	23:W:101:CHD:H152	1.77	0.65
5:E:9:GLU:H	5:E:9:GLU:CD	2.04	0.65
1:N:74:MET:CB	30:N:808:HOH:O	2.21	0.65
7:T:7:ASP:OD2	30:T:201:HOH:O	2.14	0.65
7:G:72:ASN:H	7:G:76:ASN:ND2	1.89	0.65
2:O:59:GLN:O	2:O:60:GLU:HG3	1.96	0.65
1:A:68:PHE:CZ	30:A:702:HOH:O	2.41	0.65
7:T:76:ASN:HD21	25:T:101:PEK:HN2	1.45	0.64
12:Y:24:MET:HE1	19:Y:101:TGL:HC22	1.79	0.64
1:N:172:LYS:NZ	1:N:178:GLN:HE22	1.95	0.64
9:V:31:PHE:HE2	9:V:35:TYR:H	1.43	0.64
30:N:701:HOH:O	19:Q:201:TGL:HG11	1.97	0.64
27:T:102:CDL:H781	27:T:102:CDL:H561	1.80	0.64
1:N:177:SER:H	1:N:180:GLN:NE2	1.95	0.64
5:R:50:ALA:HB3	30:R:208:HOH:O	1.97	0.64
4:D:78:TRP:CB	19:D:201:TGL:CB2	2.75	0.64
4:D:78:TRP:N	19:D:201:TGL:HB21	2.12	0.64
2:O:33:LEU:HD23	9:V:28:SER:HB3	1.78	0.64
3:P:160:LEU:HD13	23:P:304:CHD:H181	1.79	0.64
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.94	0.64
6:F:93:PRO:O	6:F:94:HIS:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:TRP:CB	19:D:201:TGL:HB21	2.28	0.63
11:K:32:MET:HE3	11:K:38:ILE:CD1	2.27	0.63
1:A:347[A]:LEU:HD13	1:A:383:MET:SD	2.38	0.63
20:C:307:PGV:H032	21:C:312:EDO:H11	1.79	0.63
12:L:20:ARG:NH2	19:L:101:TGL:HC32	2.14	0.63
3:C:67:PHE:CE2	27:C:303:CDL:H1	2.30	0.63
12:Y:17:ASN:H	12:Y:20:ARG:HH12	1.45	0.63
2:O:33:LEU:CD2	9:V:28:SER:HB3	2.29	0.63
1:A:456:MET:HE1	11:K:32:MET:HE1	1.79	0.63
13:M:1:ILE:HG12	30:M:203:HOH:O	1.98	0.62
12:Y:2:HIS:HB2	30:Y:214:HOH:O	1.98	0.62
13:Z:42:LYS:O	13:Z:43:SER:HB2	1.99	0.62
27:C:303:CDL:OA3	27:C:303:CDL:HB22	2.00	0.62
19:Q:201:TGL:H362	9:V:16:ARG:HE	1.65	0.62
25:B:304:PEK:H041	7:T:17:ARG:HH22	1.65	0.62
1:N:488:THR:HB	1:N:495:LEU:HD13	1.82	0.62
4:D:78:TRP:HB3	19:D:201:TGL:HB21	1.78	0.61
6:F:64:GLU:O	6:F:65:ASP:CB	2.47	0.61
1:N:240:HIS:CE1	18:N:606:CMO:C	2.83	0.61
2:B:82:ARG:NH1	2:B:86:MET:HE1	2.15	0.61
10:W:33:ARG:HD2	30:W:211:HOH:O	2.01	0.61
20:A:609:PGV:H311	13:M:19:LEU:HD23	1.83	0.61
1:A:106:PRO:HA	30:A:855:HOH:O	2.01	0.61
1:N:411:LYS:NZ	30:N:701:HOH:O	2.18	0.61
12:Y:24:MET:CE	19:Y:101:TGL:HC22	2.30	0.61
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.83	0.60
6:S:51:SER:O	6:S:94:HIS:HD2	1.83	0.60
3:C:116:TRP:HH2	30:C:420:HOH:O	1.83	0.60
6:F:94:HIS:CA	6:F:97:ALA:HB3	2.30	0.60
24:O:302:PSC:H011	30:R:234:HOH:O	2.01	0.60
3:P:3:HIS:HD2	30:P:462:HOH:O	1.84	0.60
1:A:502:TYR:OH	21:A:613:EDO:C1	2.48	0.60
27:T:102:CDL:H262	27:T:102:CDL:H761	1.82	0.60
4:D:78:TRP:HA	19:D:201:TGL:HB21	1.83	0.60
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.84	0.60
1:A:5:ARG:HA	21:A:613:EDO:O2	2.02	0.60
8:U:43:MET:HE2	8:U:52:VAL:HG21	1.84	0.59
9:V:30:GLY:H	9:V:32:ALA:H	1.48	0.59
30:G:221:HOH:O	1:N:278:MET:HE1	2.02	0.59
20:P:302:PGV:H152	27:P:303:CDL:H622	1.85	0.59
3:C:198:PHE:O	25:G:101:PEK:H31	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:183:THR:HG22	30:O:481:HOH:O	2.01	0.59
1:A:456:MET:CE	11:K:32:MET:HE1	2.33	0.59
8:H:44:THR:HB	30:H:101:HOH:O	2.03	0.59
27:T:102:CDL:OA7	27:T:102:CDL:H331	2.02	0.59
11:K:25:CYS:HB3	30:K:218:HOH:O	2.02	0.59
1:N:513:LEU:O	1:N:514:LYS:HB2	2.03	0.59
6:S:51:SER:O	6:S:94:HIS:CD2	2.56	0.59
11:K:8:ASP:HB3	30:K:219:HOH:O	2.03	0.59
1:A:106:PRO:HG3	30:A:855:HOH:O	2.02	0.58
6:S:78:GLU:HG2	30:S:246:HOH:O	2.01	0.58
6:F:52:ILE:HG23	6:F:96:LEU:HB3	1.85	0.58
11:X:6:ALA:N	30:X:201:HOH:O	2.35	0.58
7:G:17:ARG:HD3	30:G:215:HOH:O	2.03	0.58
7:G:3:ALA:O	7:G:4:ALA:HB2	2.04	0.58
3:P:151:LEU:HB2	3:P:159:MET:HG3	1.84	0.58
24:O:302:PSC:H242	24:O:302:PSC:H012	1.86	0.58
7:T:31:CYS:SG	27:T:102:CDL:H532	2.44	0.58
6:F:46:PRO:O	6:F:48:LEU:HD22	2.04	0.58
2:O:59:GLN:C	2:O:60:GLU:HG3	2.29	0.58
7:G:31:CYS:SG	27:G:102:CDL:H532	2.44	0.57
1:A:289:ALA:HB1	1:A:297:MET:HE1	1.85	0.57
6:F:85:CYS:SG	6:F:87:THR:CG2	2.85	0.57
24:B:303:PSC:H011	24:B:303:PSC:H242	1.87	0.57
3:C:47:LEU:O	3:C:51:MET:HG2	2.05	0.57
1:N:240:HIS:HE1	18:N:606:CMO:C	2.16	0.57
1:N:466:MET:CA	30:N:795:HOH:O	2.16	0.57
20:N:608:PGV:C06	8:U:22:ASN:HD22	2.18	0.56
2:O:45:MET:HE2	2:O:45:MET:CA	2.34	0.56
21:A:613:EDO:H21	3:C:13:PRO:CG	2.32	0.56
9:V:31:PHE:CE1	9:V:32:ALA:HA	2.40	0.56
12:Y:20:ARG:HD2	19:Y:101:TGL:HC62	1.87	0.56
10:W:26:ALA:O	10:W:30:ILE:HD13	2.06	0.56
2:B:221:LYS:NZ	30:B:402:HOH:O	2.37	0.56
1:N:362:SER:HB2	30:O:464:HOH:O	2.05	0.56
27:T:102:CDL:H561	27:T:102:CDL:H762	1.87	0.56
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.87	0.56
10:J:57:HIS:O	10:J:58:LYS:HB2	2.04	0.56
1:A:72:PRO:HA	21:A:612:EDO:O2	2.05	0.56
14:A:601:HEA:HMC3	14:A:601:HEA:HBC1	1.87	0.56
3:C:149:HIS:HA	3:C:152:MET:HE3	1.88	0.56
7:G:8:HIS:O	7:G:8:HIS:CD2	2.58	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:94:HIS:N	6:F:97:ALA:HB3	2.21	0.55
30:A:705:HOH:O	12:L:7:PRO:HD3	2.07	0.55
2:B:161:HIS:HB3	30:B:465:HOH:O	2.05	0.55
8:H:59:VAL:HA	30:H:107:HOH:O	2.06	0.55
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.41	0.55
2:B:90:ILE:HD12	2:B:90:ILE:H	1.72	0.55
27:C:303:CDL:HB32	27:C:303:CDL:HB21	1.87	0.55
4:Q:109:HIS:HD2	30:Q:325:HOH:O	1.89	0.55
1:A:366:VAL:CG1	2:B:9:PHE:CE1	2.90	0.55
7:G:72:ASN:N	7:G:76:ASN:HD22	1.94	0.55
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.89	0.55
7:G:38:HIS:HE1	27:G:102:CDL:H122	1.71	0.55
1:N:115:SER:O	1:N:121:GLY:HA2	2.07	0.55
1:N:249:PRO:HG2	30:N:808:HOH:O	2.07	0.55
3:P:37:PHE:O	3:P:38:ASN:C	2.50	0.54
4:Q:92:THR:OG1	30:Q:301:HOH:O	2.18	0.54
20:C:307:PGV:H032	21:C:312:EDO:O1	2.06	0.54
3:P:125:ASN:H	7:T:42:ARG:HH22	1.56	0.54
1:N:21:LEU:CD2	19:Y:101:TGL:H221	2.37	0.54
9:V:31:PHE:CG	9:V:32:ALA:N	2.76	0.54
8:U:46:LYS:H	8:U:46:LYS:HD3	1.71	0.54
4:Q:8:SER:O	4:Q:10:ASP:N	2.40	0.54
6:S:43:LYS:HD3	30:S:244:HOH:O	2.07	0.54
24:O:302:PSC:H083	30:R:226:HOH:O	2.07	0.54
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.54
2:O:216:LEU:N	2:O:217:LYS:HZ3	2.06	0.54
1:A:390:MET:CE	1:A:413:HIS:HE1	2.13	0.54
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.43	0.54
1:A:347[B]:LEU:HD13	1:A:383:MET:HB3	1.90	0.53
1:A:347[B]:LEU:HD22	1:A:383:MET:SD	2.48	0.53
2:B:131:GLY:N	30:B:403:HOH:O	2.39	0.53
7:G:2:SER:HA	25:G:103:PEK:H361	1.90	0.53
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.90	0.53
27:C:303:CDL:HB21	27:C:303:CDL:CB3	2.38	0.53
1:A:266:GLU:HB2	1:A:267:PRO:HD2	1.90	0.53
2:B:33:LEU:HD13	9:I:28:SER:HB3	1.90	0.53
12:Y:45:LEU:C	12:Y:47:LYS:H	2.15	0.53
25:G:103:PEK:H322	3:P:85:LEU:HD21	1.89	0.53
30:A:705:HOH:O	12:L:7:PRO:CG	2.36	0.53
8:H:49:ASP:HB3	30:H:119:HOH:O	2.08	0.53
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:609:TGL:H283	19:N:609:TGL:H101	1.91	0.53
5:R:36:LEU:HD21	5:R:47:ILE:HG21	1.91	0.53
2:B:37:LEU:HB2	9:I:28:SER:OG	2.09	0.53
1:A:109:PHE:N	30:A:702:HOH:O	2.38	0.52
9:V:33:THR:CG2	9:V:37:PHE:HD2	2.22	0.52
1:A:9:SER:HA	21:A:613:EDO:H12	1.91	0.52
6:F:50:PRO:HB2	6:F:96:LEU:HD12	1.92	0.52
4:Q:33:LEU:HB2	4:Q:38:LYS:HD3	1.91	0.52
3:C:80:ARG:HD3	25:C:308:PEK:O14	2.09	0.52
2:B:33:LEU:C	2:B:33:LEU:HD12	2.35	0.52
4:Q:78:TRP:CB	19:Q:201:TGL:HB21	2.31	0.52
1:A:243:VAL:HG21	18:A:606:CMO:C	2.40	0.52
10:J:52:TRP:O	10:J:57:HIS:HE1	1.93	0.52
8:H:41:LYS:HA	30:H:101:HOH:O	2.09	0.52
1:A:22:PHE:CD2	30:A:855:HOH:O	2.52	0.52
19:L:101:TGL:OC1	19:L:101:TGL:CC5	2.58	0.52
10:J:27:THR:HG22	30:J:202:HOH:O	2.11	0.51
13:M:28:LEU:HB2	13:M:29:PRO:HD3	1.91	0.51
5:R:6:GLU:HB2	5:R:10:GLU:OE1	2.10	0.51
12:Y:14:SER:H	19:Y:101:TGL:HC21	1.74	0.51
2:B:92:ASN:CB	30:B:467:HOH:O	2.53	0.51
4:D:68:PHE:CZ	5:E:70:VAL:HG23	2.45	0.51
6:F:93:PRO:HB3	30:F:232:HOH:O	2.09	0.51
1:N:471:ILE:HG23	30:N:755:HOH:O	2.08	0.51
27:T:102:CDL:H241	27:T:102:CDL:C53	2.40	0.51
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.45	0.51
1:A:106:PRO:CA	30:A:855:HOH:O	2.57	0.51
2:O:1:FME:HE3	4:Q:123:MET:HE3	1.92	0.51
4:Q:131:ILE:HD12	9:V:47:TYR:CE2	2.46	0.51
8:U:39:CYS:O	8:U:43:MET:HG2	2.11	0.51
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.51
3:C:29:SER:HB3	3:C:42:LEU:CD1	2.35	0.50
27:C:303:CDL:H312	27:C:303:CDL:H142	1.93	0.50
7:G:34:ASN:HD22	27:G:102:CDL:H162	1.74	0.50
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.91	0.50
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.46	0.50
27:P:303:CDL:OA4	27:P:303:CDL:H1	2.10	0.50
8:U:54:GLU:OE2	8:U:57:ARG:NH2	2.37	0.50
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.94	0.50
30:O:484:HOH:O	8:U:61:LYS:HE3	2.10	0.50
8:U:50:VAL:HG12	8:U:50:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:5:VAL:O	10:W:9:GLN:HG3	2.11	0.50
8:H:8:ILE:C	8:H:10:ASN:N	2.70	0.50
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.92	0.50
27:P:303:CDL:HB21	10:W:8:LYS:NZ	2.26	0.50
1:A:240:HIS:CD2	1:A:240:HIS:C	2.90	0.50
12:L:47:LYS:HD2	30:L:216:HOH:O	2.10	0.50
19:L:101:TGL:OC1	19:L:101:TGL:HC51	2.12	0.50
5:R:82:TYR:O	5:R:86:ILE:HG12	2.12	0.50
2:O:145:PRO:HA	2:O:214:VAL:O	2.11	0.50
4:Q:40:LEU:HD21	4:Q:58:GLU:HB3	1.93	0.50
4:D:40:LEU:HD21	4:D:58:GLU:HG2	1.92	0.49
11:K:24:PHE:O	11:K:28:VAL:HG12	2.12	0.49
1:N:87:ILE:O	1:N:173:PRO:HD3	2.13	0.49
9:V:21:ILE:O	9:V:22:VAL:C	2.53	0.49
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.93	0.49
25:T:101:PEK:H242	25:T:101:PEK:H12	1.93	0.49
1:N:178:GLN:CB	30:N:837:HOH:O	2.30	0.49
9:V:55:ASP:OD2	9:V:58:LYS:HB2	2.12	0.49
2:B:145:PRO:HA	2:B:214:VAL:O	2.13	0.49
30:A:705:HOH:O	12:L:7:PRO:CD	2.58	0.49
6:F:30:PRO:O	6:F:96:LEU:HD21	2.13	0.49
6:F:52:ILE:CG2	6:F:96:LEU:HB3	2.43	0.49
1:N:334:TRP:CZ3	19:Q:201:TGL:HA62	2.48	0.49
1:N:351:GLY:HA3	1:N:380:VAL:HG13	1.94	0.49
4:Q:92:THR:CB	30:Q:301:HOH:O	2.60	0.49
12:Y:24:MET:CG	19:Y:101:TGL:H152	2.41	0.49
25:G:101:PEK:H161	25:G:101:PEK:H11	1.94	0.49
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.60	0.49
9:V:55:ASP:OD2	9:V:58:LYS:CB	2.61	0.49
7:G:38:HIS:CE1	27:G:102:CDL:H122	2.47	0.49
8:H:60:TYR:CD1	8:H:60:TYR:C	2.91	0.49
19:L:101:TGL:HA92	19:L:101:TGL:H241	1.95	0.49
13:M:10:THR:HA	13:M:14:GLU:OE2	2.12	0.49
1:N:335:SER:CB	30:N:766:HOH:O	2.44	0.49
8:U:42:ALA:O	8:U:46:LYS:HG2	2.13	0.49
2:O:146:MET:HA	2:O:213:LEU:HD12	1.94	0.48
7:T:11:TPO:HA	7:T:11:TPO:O2P	2.12	0.48
20:N:608:PGV:H062	8:U:22:ASN:HD22	1.78	0.48
3:C:55:TYR:CE1	27:C:303:CDL:H512	2.48	0.48
2:B:13:THR:O	2:B:13:THR:HG22	2.12	0.48
6:F:94:HIS:O	6:F:96:LEU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:43:GLN:HB2	1:N:44:PRO:HD2	1.95	0.48
6:S:70:ILE:HG13	6:S:84:SER:HB3	1.95	0.48
4:D:4:SER:HB3	30:D:304:HOH:O	2.14	0.48
4:D:109:HIS:HD2	30:D:319:HOH:O	1.95	0.48
6:F:48:LEU:HD12	6:F:92:VAL:CG1	2.43	0.48
3:P:50:ASN:HD22	3:P:51:MET:HE2	1.79	0.48
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.13	0.48
1:N:50:ASP:HB3	1:N:53:ILE:HD12	1.96	0.48
21:A:612:EDO:H22	30:A:709:HOH:O	2.13	0.48
1:A:513:LEU:O	1:A:514:LYS:HB2	2.12	0.48
8:U:41:LYS:HA	30:U:126:HOH:O	2.14	0.48
1:A:51:ASP:HB2	2:B:202:SER:O	2.14	0.48
13:M:36:HIS:O	13:M:39:ASN:HB2	2.14	0.48
3:P:55:TYR:HE1	27:P:303:CDL:H512	1.79	0.48
1:A:106:PRO:N	1:A:107:PRO:HD2	2.28	0.47
1:A:218:THR:O	1:A:226:GLY:HA3	2.14	0.47
8:H:16:PHE:HE1	30:H:134:HOH:O	1.97	0.47
2:O:161:HIS:CE1	30:O:460:HOH:O	2.50	0.47
10:W:29:ASN:N	10:W:29:ASN:ND2	2.60	0.47
12:Y:24:MET:SD	19:Y:101:TGL:HC22	2.54	0.47
1:A:271:MET:HE3	7:T:18:PHE:CE2	2.49	0.47
1:A:406:ASN:HD21	20:A:609:PGV:H31	1.79	0.47
2:B:58:ALA:O	2:B:62:GLU:HG3	2.13	0.47
1:N:289:ALA:HB1	1:N:297:MET:HE1	1.96	0.47
1:N:390:MET:O	1:N:394:VAL:HG13	2.14	0.47
4:Q:6:VAL:O	4:Q:7:LYS:HB2	2.13	0.47
5:R:19:PHE:HB2	30:R:208:HOH:O	2.15	0.47
3:C:257:TYR:O	3:C:261:SER:HB3	2.13	0.47
30:N:846:HOH:O	4:Q:81:VAL:CG1	2.50	0.47
12:Y:25:MET:HG2	19:Y:101:TGL:HA62	1.95	0.47
2:O:57:ASP:H	24:O:302:PSC:H222	1.79	0.47
2:O:102:HIS:HE1	2:O:157:GLU:OE2	1.97	0.47
4:Q:109:HIS:CD2	30:Q:325:HOH:O	2.67	0.47
3:C:160:LEU:HD13	23:C:304:CHD:H181	1.96	0.47
4:D:4:SER:HA	30:D:304:HOH:O	2.15	0.47
1:N:240:HIS:C	1:N:240:HIS:CD2	2.92	0.47
1:N:264:LYS:HE2	2:O:53:THR:HA	1.95	0.47
2:O:91:ASN:N	2:O:91:ASN:ND2	2.63	0.47
27:C:303:CDL:OA3	27:C:303:CDL:OB7	2.33	0.47
19:N:609:TGL:HC32	19:N:609:TGL:HC61	1.63	0.47
7:T:43:GLU:HB3	30:T:226:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:32:MET:HE3	11:X:32:MET:HB3	1.75	0.47
7:G:9:GLY:HA2	30:N:719:HOH:O	2.15	0.47
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.50	0.47
9:V:29:LEU:C	9:V:32:ALA:CB	2.76	0.47
12:Y:24:MET:HE2	19:Y:101:TGL:HA22	1.96	0.47
4:D:34:SER:H	4:D:37:GLN:HE21	1.63	0.46
1:N:172:LYS:HZ1	1:N:178:GLN:HE22	1.63	0.46
19:N:609:TGL:HA72	19:N:609:TGL:H142	1.96	0.46
27:T:102:CDL:H731	27:T:102:CDL:H541	1.96	0.46
13:Z:11:SER:O	13:Z:12:PRO:C	2.55	0.46
27:G:102:CDL:HB32	1:N:304:TYR:HD1	1.81	0.46
12:L:2:HIS:CD2	12:L:3:TYR:N	2.78	0.46
1:N:333:LYS:HE2	30:Z:202:HOH:O	2.15	0.46
23:P:304:CHD:H212	23:P:304:CHD:H12	1.97	0.46
4:Q:9:GLU:O	4:Q:12:ALA:N	2.42	0.46
10:W:36:MET:HG2	23:W:101:CHD:H183	1.97	0.46
1:A:468:MET:HG3	30:A:865:HOH:O	2.14	0.46
7:G:34:ASN:ND2	27:G:102:CDL:H162	2.30	0.46
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.46	0.46
1:N:199:LEU:N	1:N:200:PRO:CD	2.78	0.46
2:O:151:ARG:HE	2:O:181:GLN:NE2	2.13	0.46
5:R:51:ALA:O	5:R:54:ALA:HB3	2.16	0.46
6:F:53:THR:HB	6:F:54:ASN:H	1.51	0.46
11:K:32:MET:HE3	11:K:38:ILE:HD13	1.97	0.46
9:V:30:GLY:H	9:V:32:ALA:N	2.13	0.46
2:B:63:THR:O	2:B:67:ILE:HG12	2.16	0.46
24:B:303:PSC:H02	24:B:303:PSC:H222	1.98	0.46
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.97	0.46
1:A:106:PRO:CB	30:A:855:HOH:O	2.64	0.46
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.46	0.46
6:S:81:ARG:HA	6:S:87:THR:O	2.16	0.46
21:L:103:EDO:H21	30:L:215:HOH:O	2.16	0.45
14:N:602:HEA:H243	2:O:69:PRO:HB3	1.98	0.45
5:R:19:PHE:CD2	30:R:208:HOH:O	2.56	0.45
1:N:489:THR:HA	6:S:71:TRP:O	2.16	0.45
27:T:102:CDL:H552	27:T:102:CDL:H581	1.49	0.45
3:C:112:LEU:HD22	3:C:118:PRO:HB3	1.97	0.45
7:G:44:ARG:HD2	7:G:74:ARG:O	2.17	0.45
27:G:102:CDL:H781	27:G:102:CDL:H561	1.98	0.45
9:V:30:GLY:N	9:V:32:ALA:N	2.64	0.45
6:S:64:GLU:O	6:S:65:ASP:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:14:ARG:HD2	30:E:221:HOH:O	2.15	0.45
20:N:608:PGV:H061	8:U:22:ASN:CB	2.42	0.45
5:R:80:GLU:C	5:R:83:PRO:HD2	2.41	0.45
1:A:25:TRP:CE3	19:L:101:TGL:HB91	2.51	0.45
4:Q:109:HIS:HE1	4:Q:115:TRP:CZ3	2.35	0.45
19:Y:101:TGL:CA9	19:Y:101:TGL:C23	2.95	0.45
1:A:366:VAL:HG13	2:B:9:PHE:HE1	1.81	0.45
2:O:214:VAL:HB	2:O:215:PRO:HD2	1.97	0.45
4:Q:9:GLU:O	4:Q:10:ASP:C	2.59	0.45
19:Q:201:TGL:HB22	19:Q:201:TGL:OG1	2.17	0.45
8:U:57:ARG:O	8:U:61:LYS:HB2	2.16	0.45
4:D:34:SER:H	4:D:37:GLN:NE2	2.15	0.45
11:K:6:ALA:HA	11:K:7:PRO:HD3	1.76	0.45
1:N:52:GLN:O	1:N:56:VAL:HG23	2.17	0.45
23:P:305:CHD:H212	23:P:305:CHD:H12	1.98	0.45
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.99	0.45
1:A:278:MET:HE3	21:T:103:EDO:O1	2.17	0.45
3:C:193:TYR:CD1	3:C:193:TYR:C	2.94	0.45
25:C:306:PEK:H011	30:C:410:HOH:O	2.17	0.45
6:F:55:LYS:HA	6:F:74:LEU:O	2.16	0.45
11:K:32:MET:HE3	11:K:38:ILE:HD12	1.98	0.45
4:Q:19:ARG:CG	4:Q:19:ARG:NH2	2.67	0.45
5:R:57:ARG:HH11	5:R:57:ARG:HG3	1.82	0.45
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.99	0.44
27:G:102:CDL:H161	27:G:102:CDL:H371	1.99	0.44
3:P:160:LEU:HD21	3:P:222:GLN:HG3	1.99	0.44
25:T:101:PEK:H221	25:T:101:PEK:H251	1.48	0.44
11:K:8:ASP:HA	30:K:201:HOH:O	2.16	0.44
1:N:233:HIS:CE1	1:N:292:MET:HE1	2.53	0.44
20:N:608:PGV:H141	20:N:608:PGV:H301	1.99	0.44
3:P:40:MET:HE3	30:P:429:HOH:O	2.16	0.44
3:P:64:GLU:HA	3:P:68:GLN:HE21	1.82	0.44
6:F:62:CYS:HB3	6:F:85:CYS:HB3	1.99	0.44
1:N:53:ILE:HG13	30:N:852:HOH:O	2.17	0.44
9:V:30:GLY:N	9:V:32:ALA:H	2.15	0.44
2:B:168:LEU:HD23	2:B:184:LEU:HG	1.99	0.44
7:T:44:ARG:NH1	30:T:202:HOH:O	2.48	0.44
8:U:7:LYS:HG2	8:U:8:ILE:N	2.33	0.44
1:A:189:MET:HE2	1:A:189:MET:HB3	1.74	0.44
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.52	0.44
27:T:102:CDL:H222	27:T:102:CDL:C51	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:TYR:CZ	2:B:205:SER:HA	2.52	0.44
25:G:103:PEK:H322	3:P:85:LEU:CD2	2.47	0.44
1:N:498:CYS:HA	1:N:499:PRO:HA	1.80	0.44
5:R:5:HIS:ND1	5:R:6:GLU:HB3	2.33	0.44
1:A:271:MET:HE3	7:T:18:PHE:HE2	1.83	0.44
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.06	0.44
2:B:207:MET:CE	30:B:465:HOH:O	2.56	0.44
4:D:4:SER:N	30:D:303:HOH:O	2.51	0.44
1:N:236:TRP:HH2	14:N:602:HEA:HBD1	1.83	0.44
1:N:383:MET:HA	1:N:387:PHE:CD1	2.53	0.44
19:N:609:TGL:H241	19:N:609:TGL:H272	1.69	0.44
10:J:50:LEU:HD22	10:J:50:LEU:O	2.18	0.43
2:O:92:ASN:HA	2:O:93:PRO:HD3	1.88	0.43
27:T:102:CDL:H152	27:T:102:CDL:H411	1.98	0.43
3:C:116:TRP:HA	3:C:117:PRO:C	2.43	0.43
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.53	0.43
1:N:177:SER:H	1:N:180:GLN:HE21	1.63	0.43
1:N:227:ASP:HA	1:N:228:PRO:HD3	1.85	0.43
1:N:377:PHE:CE1	1:N:378:HIS:CE1	3.06	0.43
2:O:69:PRO:HG2	30:O:403:HOH:O	2.18	0.43
27:T:102:CDL:H1	27:T:102:CDL:OB3	2.18	0.43
14:A:601:HEA:C1D	30:A:779:HOH:O	2.66	0.43
1:N:176:MET:HB2	1:N:176:MET:HE3	1.75	0.43
3:P:156:ARG:HE	23:P:304:CHD:C24	2.32	0.43
7:T:60:PHE:O	7:T:65:GLY:HA2	2.18	0.43
1:A:510:TYR:HH	21:F:102:EDO:H21	1.81	0.43
7:G:30:LEU:HD23	27:G:102:CDL:H472	2.00	0.43
1:N:248:LEU:O	1:N:251:PHE:HB2	2.19	0.43
20:Z:101:PGV:H21	20:Z:101:PGV:H011	1.99	0.43
3:C:154:GLY:HA2	6:F:6:VAL:HB	1.99	0.43
2:O:58:ALA:O	2:O:62:GLU:HG3	2.19	0.43
2:O:62:GLU:O	2:O:66:THR:HB	2.19	0.43
9:V:31:PHE:HE2	9:V:35:TYR:CB	2.31	0.43
5:E:49:ASP:OD2	5:E:92:THR:OG1	2.32	0.43
27:G:102:CDL:H761	27:G:102:CDL:H561	2.00	0.43
10:J:58:LYS:HA	10:J:58:LYS:CE	2.49	0.43
1:N:310:MET:HE1	2:O:76:ILE:HG22	2.00	0.43
2:B:66:THR:HG21	23:B:302:CHD:H3	2.01	0.43
2:B:68:LEU:HB3	2:B:69:PRO:HD3	2.00	0.43
5:E:24:ILE:O	5:E:58:LEU:HD21	2.19	0.43
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:313:ALA:HB2	1:N:356:ILE:HD11	2.01	0.43
1:N:397:PHE:HB3	1:N:398:PRO:HD3	2.00	0.43
30:A:851:HOH:O	13:M:26:PHE:CD1	2.64	0.43
7:T:72:ASN:H	7:T:76:ASN:ND2	2.04	0.43
9:V:31:PHE:CD1	9:V:32:ALA:CA	3.01	0.43
4:D:7:LYS:O	4:D:10:ASP:HB2	2.19	0.43
3:P:77:LYS:HB3	3:P:77:LYS:HZ3	1.82	0.43
4:Q:90:GLY:HA2	30:X:205:HOH:O	2.18	0.43
20:A:609:PGV:H031	20:A:609:PGV:C21	2.45	0.42
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.54	0.42
7:G:5:LYS:O	1:N:193:VAL:HG21	2.19	0.42
14:N:602:HEA:HAD2	14:N:602:HEA:HHA	1.87	0.42
8:U:43:MET:HE3	8:U:43:MET:HB3	1.86	0.42
7:G:36:TRP:HA	7:G:36:TRP:CE3	2.54	0.42
3:P:55:TYR:CE1	27:P:303:CDL:H512	2.54	0.42
4:Q:130:PRO:HA	4:Q:135:SER:HB2	2.00	0.42
5:R:21:LYS:HA	5:R:22:PRO:HD3	1.87	0.42
9:V:29:LEU:O	9:V:29:LEU:HG	2.19	0.42
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.53	0.42
27:G:102:CDL:H781	27:G:102:CDL:C56	2.48	0.42
1:N:83:VAL:HB	1:N:84:PRO:HD3	2.01	0.42
9:V:29:LEU:HA	9:V:32:ALA:HB2	1.98	0.42
2:B:214:VAL:HB	2:B:215:PRO:HD2	2.02	0.42
8:H:36:PHE:CE1	8:H:57:ARG:HB2	2.53	0.42
4:Q:33:LEU:HD22	4:Q:62:LEU:HD13	2.01	0.42
12:Y:11:ILE:CG2	19:Y:101:TGL:H272	2.49	0.42
12:Y:17:ASN:HB3	12:Y:20:ARG:NH1	2.33	0.42
1:A:344:PHE:CD1	1:A:344:PHE:C	2.98	0.42
3:C:249:TRP:CG	30:C:472:HOH:O	2.71	0.42
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.35	0.42
27:G:102:CDL:H222	27:G:102:CDL:C51	2.34	0.42
3:P:259:TRP:HA	21:P:307:EDO:H12	2.00	0.42
30:B:470:HOH:O	7:T:17:ARG:CD	2.41	0.42
3:P:204:HIS:CE1	3:P:249:TRP:HB2	2.54	0.42
7:T:36:TRP:HD1	7:T:37:LEU:HD13	1.85	0.42
14:A:601:HEA:OMA	14:A:601:HEA:HHB	2.19	0.42
12:L:30:GLY:HA2	30:L:210:HOH:O	2.20	0.42
4:Q:63:LYS:HG2	4:Q:64:PHE:CE2	2.55	0.42
2:B:62:GLU:O	2:B:66:THR:HB	2.20	0.42
20:C:302:PGV:H152	20:C:302:PGV:H12	1.66	0.42
6:F:94:HIS:H	6:F:97:ALA:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:5:LYS:HB3	1:N:278:MET:HG2	2.01	0.42
8:H:46:LYS:HG2	8:U:7:LYS:HD2	2.02	0.42
1:N:341:ALA:O	1:N:344:PHE:HB3	2.20	0.42
2:O:66:THR:HG22	2:O:67:ILE:HD13	2.01	0.42
1:A:199:LEU:N	1:A:200:PRO:CD	2.83	0.42
1:A:379:TYR:CZ	1:A:383:MET:HE1	2.55	0.42
2:B:214:VAL:HB	2:B:215:PRO:CD	2.50	0.42
7:G:4:ALA:C	7:G:5:LYS:HG2	2.45	0.42
7:G:56:ARG:NH2	7:G:66:ASN:O	2.45	0.42
14:N:601:HEA:HBC1	14:N:601:HEA:HMC3	2.02	0.42
8:U:9:LYS:HG3	30:U:113:HOH:O	2.20	0.42
12:Y:24:MET:HE3	19:Y:101:TGL:OA1	2.19	0.42
3:C:54:MET:HE1	20:C:302:PGV:H131	2.02	0.42
7:G:45:PRO:CD	30:G:208:HOH:O	2.46	0.42
1:N:495:LEU:HD12	1:N:495:LEU:HA	1.92	0.42
1:N:505:PHE:HB3	30:N:763:HOH:O	2.20	0.42
7:T:8:HIS:HD2	30:T:233:HOH:O	2.02	0.42
8:U:45:ALA:C	8:U:47:GLY:H	2.24	0.42
27:G:102:CDL:H761	27:G:102:CDL:C58	2.44	0.41
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.02	0.41
4:Q:86:MET:O	11:X:25:CYS:HB2	2.20	0.41
14:A:601:HEA:HBC1	14:A:601:HEA:CMC	2.49	0.41
3:C:40:MET:O	3:C:44:MET:HG2	2.20	0.41
3:C:107:ALA:HB2	20:C:307:PGV:H031	2.02	0.41
19:Y:101:TGL:C23	19:Y:101:TGL:HA92	2.50	0.41
1:A:221:ASP:OD1	1:A:221:ASP:C	2.64	0.41
7:G:78:LEU:HB3	7:G:79:PRO:CD	2.50	0.41
13:M:23:PHE:C	30:M:201:HOH:O	2.61	0.41
6:S:39:THR:HG23	21:S:102:EDO:H21	2.02	0.41
4:D:128:VAL:O	4:D:129:ALA:C	2.63	0.41
2:O:13:THR:HB	2:O:168:LEU:HD23	2.03	0.41
24:O:302:PSC:H072	5:R:11:PHE:CD2	2.56	0.41
1:A:87:ILE:O	1:A:173:PRO:HD3	2.21	0.41
1:A:269:GLY:O	1:A:270:TYR:C	2.63	0.41
3:C:223:LEU:HD23	3:C:223:LEU:HA	1.87	0.41
9:I:8:GLN:HE21	9:I:10:ARG:H	1.67	0.41
1:N:12:HIS:CE1	1:N:13:LYS:HG2	2.55	0.41
1:N:381:LEU:O	1:N:386:VAL:HG23	2.21	0.41
7:T:12:GLY:CA	30:T:225:HOH:O	2.61	0.41
14:A:601:HEA:H11	14:A:601:HEA:HHC	1.80	0.41
12:L:20:ARG:HH22	19:L:101:TGL:CC6	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:172:LYS:NZ	1:N:178:GLN:NE2	2.64	0.41
27:P:303:CDL:H151	27:P:303:CDL:H312	2.03	0.41
4:Q:145:TRP:CG	11:X:46:GLY:H	2.39	0.41
9:V:59:ASP:O	9:V:63:MET:HG3	2.20	0.41
1:N:203:ALA:HB1	25:T:101:PEK:H382	2.03	0.41
1:N:250:GLY:O	1:N:254:ILE:HG12	2.21	0.41
2:O:64:ILE:H	2:O:64:ILE:HG13	1.74	0.41
12:Y:20:ARG:CZ	12:Y:20:ARG:HB3	2.50	0.41
1:A:127:THR:HB	1:A:129:TYR:CE1	2.56	0.41
2:B:20:LEU:HA	2:B:20:LEU:HD23	1.87	0.41
6:F:94:HIS:C	6:F:96:LEU:N	2.79	0.41
23:J:101:CHD:H183	23:J:101:CHD:H222	2.02	0.41
1:N:513:LEU:O	1:N:514:LYS:CB	2.69	0.41
2:O:102:HIS:O	2:O:104:TRP:HA	2.20	0.41
9:V:68:ILE:HG13	9:V:69:PHE:N	2.36	0.41
13:Z:16:ALA:HB2	20:Z:101:PGV:H292	2.03	0.41
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.03	0.41
2:O:65:TRP:CB	30:O:467:HOH:O	2.30	0.41
2:O:215:PRO:CB	2:O:217:LYS:HE2	2.49	0.41
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.34	0.40
3:C:205:GLY:HA3	25:G:101:PEK:H181	2.03	0.40
1:N:377:PHE:HA	1:N:380:VAL:HG22	2.02	0.40
1:A:485:VAL:HG22	13:M:1:ILE:HG13	2.04	0.40
3:C:126:PRO:HG2	3:C:127:LEU:HD22	2.02	0.40
4:D:63:LYS:HE3	30:D:361:HOH:O	2.21	0.40
5:E:8:ASP:O	5:E:11:PHE:HB3	2.21	0.40
13:M:36:HIS:HD2	13:M:39:ASN:HD22	1.68	0.40
2:O:130:PRO:HB3	4:Q:118:LYS:HD3	2.04	0.40
2:O:139:ASP:OD1	2:O:140:ASN:N	2.55	0.40
3:P:16:TRP:O	3:P:17:PRO:C	2.61	0.40
3:P:23:SER:HB2	3:P:49:THR:OG1	2.21	0.40
3:P:47:LEU:O	3:P:51:MET:HG2	2.21	0.40
7:T:33:LEU:HD22	7:T:33:LEU:HA	1.82	0.40
1:A:282:PHE:HA	7:T:4:ALA:HB3	2.02	0.40
2:B:146:MET:SD	2:B:189:PRO:HB3	2.61	0.40
27:C:303:CDL:HB22	27:C:303:CDL:PA1	2.61	0.40
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.47	0.40
2:O:90:ILE:H	2:O:90:ILE:HG13	1.77	0.40
23:P:304:CHD:H162	23:P:304:CHD:H232	2.03	0.40
11:X:9:PHE:CE1	20:Z:101:PGV:H232	2.56	0.40
6:F:87:THR:HG21	30:F:224:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:5:LYS:NZ	30:G:202:HOH:O	2.54	0.40
8:H:52:VAL:HB	8:U:46:LYS:HG3	2.03	0.40
1:N:183:LEU:HD23	1:N:183:LEU:HA	1.90	0.40
2:O:45:MET:HE2	2:O:45:MET:N	2.36	0.40
3:C:204:HIS:CE1	3:C:249:TRP:HB2	2.56	0.40
20:C:307:PGV:H152	27:T:102:CDL:H631	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	513/514 (100%)	500 (98%)	13 (2%)	0	100	100
1	N	512/514 (100%)	499 (98%)	12 (2%)	1 (0%)	43	51
2	B	225/227 (99%)	218 (97%)	6 (3%)	1 (0%)	30	34
2	O	225/227 (99%)	216 (96%)	6 (3%)	3 (1%)	9	8
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	248 (96%)	8 (3%)	1 (0%)	30	34
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	132 (93%)	8 (6%)	2 (1%)	9	7
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
6	F	96/98 (98%)	83 (86%)	9 (9%)	4 (4%)	2	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	1
7	G	81/85 (95%)	70 (86%)	8 (10%)	3 (4%)	2	1
7	T	81/85 (95%)	70 (86%)	6 (7%)	5 (6%)	1	0
8	H	77/85 (91%)	68 (88%)	6 (8%)	3 (4%)	2	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	U	77/85 (91%)	69 (90%)	6 (8%)	2 (3%)	4	2
9	I	71/73 (97%)	69 (97%)	1 (1%)	1 (1%)	9	7
9	V	71/73 (97%)	64 (90%)	4 (6%)	3 (4%)	2	1
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	44 (100%)	0	0	100	100
12	Y	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
13	M	41/46 (89%)	40 (98%)	0	1 (2%)	4	3
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3505/3614 (97%)	3351 (96%)	121 (4%)	33 (1%)	14	14

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	96	LEU
6	F	97	ALA
7	G	4	ALA
8	H	8	ILE
8	H	43	MET
8	H	44	THR
4	Q	9	GLU
7	T	8	HIS
8	U	45	ALA
8	U	46	LYS
9	V	32	ALA
9	I	2	THR
2	O	60	GLU
3	P	38	ASN
6	S	4	GLY
7	T	7	ASP
7	T	38	HIS
7	T	41	HIS
9	V	33	THR
6	F	95	GLN
6	S	95	GLN

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Mol	Chain	Res	Type
7	T	4	ALA
9	V	30	GLY
7	G	8	HIS
13	M	42	LYS
1	N	502	TYR
4	Q	65	LYS
2	O	91	ASN
6	S	93	PRO
2	B	92	ASN
2	O	92	ASN
7	G	6	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/426 (100%)	412 (96%)	15 (4%)	32	43
1	N	426/426 (100%)	412 (97%)	14 (3%)	33	45
2	B	210/210 (100%)	201 (96%)	9 (4%)	26	35
2	O	210/210 (100%)	191 (91%)	19 (9%)	9	9
3	C	224/226 (99%)	221 (99%)	3 (1%)	61	76
3	P	224/226 (99%)	221 (99%)	3 (1%)	61	76
4	D	128/129 (99%)	121 (94%)	7 (6%)	19	24
4	Q	128/129 (99%)	120 (94%)	8 (6%)	16	19
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	61
5	R	92/95 (97%)	85 (92%)	7 (8%)	12	14
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	41
6	S	81/81 (100%)	74 (91%)	7 (9%)	10	10
7	G	67/68 (98%)	65 (97%)	2 (3%)	36	49
7	T	67/68 (98%)	58 (87%)	9 (13%)	4	3
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	11
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	16
9	V	57/57 (100%)	51 (90%)	6 (10%)	6	6
10	J	49/50 (98%)	45 (92%)	4 (8%)	10	12
10	W	49/50 (98%)	45 (92%)	4 (8%)	10	12
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	27
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	36 (92%)	3 (8%)	12	13
12	Y	39/40 (98%)	38 (97%)	1 (3%)	40	55
13	M	37/38 (97%)	35 (95%)	2 (5%)	20	25
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	12
All	All	3041/3082 (99%)	2892 (95%)	149 (5%)	22	29

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	136	LEU
1	A	178	GLN
1	A	180	GLN
1	A	312	ILE
1	A	361	SER
1	A	362	SER
1	A	363	LEU
1	A	366	VAL
1	A	369	ASP
1	A	382	SER
1	A	394	VAL
1	A	484	THR
1	A	504	THR
1	A	513	LEU
2	B	33	LEU
2	B	61	VAL
2	B	65	TRP
2	B	66	THR
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU

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Mol	Chain	Res	Type
2	B	91	ASN
2	B	92	ASN
3	C	38	ASN
3	C	230	ASN
3	C	246	ASP
4	D	4	SER
4	D	8	SER
4	D	51	LEU
4	D	58	GLU
4	D	121	LYS
4	D	143	ASN
4	D	147	LYS
5	E	7	THR
5	E	70	VAL
6	F	52	ILE
6	F	53	THR
6	F	87	THR
7	G	5	LYS
7	G	36	TRP
8	H	7	LYS
8	H	10	ASN
8	H	41	LYS
8	H	44	THR
8	H	50	VAL
8	H	60	TYR
9	I	18	ARG
9	I	21	ILE
9	I	29	LEU
9	I	31	PHE
10	J	23	LYS
10	J	31	LEU
10	J	50	LEU
10	J	58	LYS
11	K	32	MET
11	K	54	ARG
12	L	5	GLU
12	L	11	ILE
12	L	26	THR
13	M	34	LEU
13	M	37	LEU
1	N	38	ARG
1	N	128	VAL

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Mol	Chain	Res	Type
1	N	180	GLN
1	N	189	MET
1	N	243	VAL
1	N	265	LYS
1	N	363	LEU
1	N	366	VAL
1	N	369	ASP
1	N	382	SER
1	N	394	VAL
1	N	483	LEU
1	N	495	LEU
1	N	514	LYS
2	O	16	ILE
2	O	19	GLU
2	O	33	LEU
2	O	34	ILE
2	O	45	MET
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	90	ILE
2	O	91	ASN
2	O	110	TYR
2	O	148	MET
2	O	183	THR
2	O	185	MET
2	O	217	LYS
2	O	226	MET
3	P	77	LYS
3	P	127	LEU
3	P	179	SER
4	Q	4	SER
4	Q	9	GLU
4	Q	19	ARG
4	Q	51	LEU
4	Q	62	LEU
4	Q	112	GLU
4	Q	131	ILE
4	Q	144	GLU

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Mol	Chain	Res	Type
5	R	6	GLU
5	R	7	THR
5	R	14	ARG
5	R	70	VAL
5	R	79	LYS
5	R	80	GLU
5	R	108	LYS
6	S	37	LYS
6	S	53	THR
6	S	54	ASN
6	S	78	GLU
6	S	87	THR
6	S	95	GLN
6	S	96	LEU
7	T	7	ASP
7	T	17	ARG
7	T	33	LEU
7	T	35	SER
7	T	37	LEU
7	T	38	HIS
7	T	41	HIS
7	T	44	ARG
7	T	58	LYS
8	U	9	LYS
8	U	46	LYS
8	U	49	ASP
8	U	52	VAL
8	U	66	ILE
8	U	84	LYS
9	V	18	ARG
9	V	21	ILE
9	V	26	MET
9	V	29	LEU
9	V	31	PHE
9	V	36	LYS
10	W	23	LYS
10	W	27	THR
10	W	29	ASN
10	W	50	LEU
12	Y	26	THR
13	Z	20	SER
13	Z	34	LEU

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Mol	Chain	Res	Type
13	Z	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	413	HIS
1	A	422	ASN
1	A	512	ASN
2	B	52	HIS
2	B	181	GLN
3	C	50	ASN
4	D	29	HIS
4	D	37	GLN
4	D	119	GLN
5	E	78	HIS
5	E	94	ASN
6	F	98	HIS
7	G	8	HIS
7	G	34	ASN
7	G	41	HIS
7	G	76	ASN
8	H	23	GLN
8	H	31	GLN
8	H	32	ASN
9	I	8	GLN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
12	L	2	HIS
13	M	39	ASN
1	N	178	GLN
1	N	180	GLN
1	N	413	HIS
1	N	503	HIS
1	N	512	ASN
2	O	10	GLN
2	O	24	HIS
2	O	59	GLN
2	O	181	GLN
2	O	195	GLN

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Mol	Chain	Res	Type
3	P	38	ASN
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
3	P	149	HIS
3	P	161	GLN
4	Q	29	HIS
4	Q	32	ASN
4	Q	37	GLN
4	Q	109	HIS
4	Q	119	GLN
4	Q	143	ASN
5	R	94	ASN
6	S	54	ASN
6	S	94	HIS
6	S	95	GLN
7	T	8	HIS
7	T	76	ASN
8	U	22	ASN
10	W	29	ASN
11	X	35	GLN
13	Z	36	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	N	1	1	8,9,10	0.62	0	8,9,11	1.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TPO	T	11	7	8,10,11	1.65	2 (25%)	10,14,16	1.28	2 (20%)
9	SAC	V	1	9	7,8,9	1.36	1 (14%)	7,9,11	1.84	1 (14%)
7	TPO	G	11	7	8,10,11	2.18	2 (25%)	10,14,16	0.97	0
1	FME	A	1	1	8,9,10	0.59	0	8,9,11	1.33	2 (25%)
9	SAC	I	1	9	7,8,9	1.14	1 (14%)	7,9,11	1.57	2 (28%)
2	FME	B	1	2	8,9,10	1.07	1 (12%)	8,9,11	1.05	0
2	FME	O	1	2	8,9,10	1.12	1 (12%)	8,9,11	1.30	1 (12%)

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.80	1.66	1.59
7	G	11	TPO	P-O1P	3.57	1.61	1.50
9	V	1	SAC	CA-N	3.40	1.51	1.46
7	T	11	TPO	P-O1P	2.82	1.59	1.50
9	I	1	SAC	CA-N	2.72	1.50	1.46
2	O	1	FME	CA-N	2.26	1.49	1.46
7	T	11	TPO	P-OG1	2.19	1.63	1.59
2	B	1	FME	CA-N	2.09	1.49	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	C-CA-N	4.08	117.36	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	SAC	C-CA-N	3.24	115.75	109.50
1	A	1	FME	C-CA-N	2.66	114.63	109.50
7	T	11	TPO	CG2-CB-CA	2.50	118.14	113.26
7	T	11	TPO	O2P-P-OG1	2.25	114.64	105.85
2	O	1	FME	O-C-CA	-2.23	119.02	124.77
9	I	1	SAC	O-C-CA	-2.22	119.06	124.77
1	A	1	FME	O-C-CA	-2.02	119.56	124.77

There are no chirality outliers.

All (25) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
2	B	1	FME	1	0
2	O	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 79 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 69 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	$\# Z > 2$
21	EDO	C	311	-	3,3,3	0.40	0	2,2,2	0.53	0
21	EDO	A	610	-	3,3,3	0.61	0	2,2,2	0.38	0
23	CHD	C	305	-	32,32,32	1.07	3 (9%)	51,51,51	1.68	10 (19%)
29	DMU	Z	102	-	34,34,34	0.45	0	45,45,45	1.61	9 (20%)
29	DMU	M	101	-	34,34,34	0.60	1 (2%)	45,45,45	1.14	4 (8%)
20	PGV	N	608	-	50,50,50	1.11	2 (4%)	53,56,56	1.34	5 (9%)
21	EDO	N	610	-	3,3,3	0.70	0	2,2,2	0.05	0
21	EDO	F	102	-	3,3,3	0.59	0	2,2,2	0.27	0
27	CDL	C	303	-	99,99,99	1.50	13 (13%)	105,111,111	1.20	7 (6%)
19	TGL	L	101	-	62,62,62	1.22	3 (4%)	65,65,65	1.60	9 (13%)
14	HEA	A	602	1	67,67,67	2.13	21 (31%)	81,103,103	1.95	22 (27%)
14	HEA	N	602	18,1	67,67,67	2.12	22 (32%)	81,103,103	1.91	23 (28%)
19	TGL	Y	101	-	62,62,62	1.27	3 (4%)	65,65,65	1.28	7 (10%)
21	EDO	B	305	-	3,3,3	0.55	0	2,2,2	0.16	0
21	EDO	P	306	-	3,3,3	0.70	0	2,2,2	0.49	0
19	TGL	D	201	-	62,62,62	1.25	4 (6%)	65,65,65	1.26	6 (9%)
23	CHD	P	304	-	32,32,32	0.79	1 (3%)	51,51,51	1.64	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHD	G	104	-	32,32,32	0.97	1 (3%)	51,51,51	1.63	14 (27%)
14	HEA	N	601	1	67,67,67	2.15	26 (38%)	81,103,103	1.42	9 (11%)
27	CDL	P	303	-	99,99,99	1.48	12 (12%)	105,111,111	1.29	11 (10%)
18	CMO	A	606	15	0,1,1	-	-	-	-	-
21	EDO	K	102	-	3,3,3	0.41	0	2,2,2	0.56	0
20	PGV	A	609	-	50,50,50	1.15	2 (4%)	53,56,56	1.11	6 (11%)
21	EDO	A	612	-	3,3,3	0.58	0	2,2,2	0.55	0
23	CHD	J	101	-	32,32,32	1.05	1 (3%)	51,51,51	2.18	20 (39%)
18	CMO	N	606	14	0,1,1	-	-	-	-	-
21	EDO	C	309	-	3,3,3	0.69	0	2,2,2	0.28	0
21	EDO	I	101	-	3,3,3	0.70	0	2,2,2	0.28	0
21	EDO	K	103	-	3,3,3	0.48	0	2,2,2	0.46	0
21	EDO	N	612	-	3,3,3	0.68	0	2,2,2	0.56	0
25	PEK	C	308	-	52,52,52	1.04	2 (3%)	55,57,57	1.00	3 (5%)
23	CHD	P	305	-	32,32,32	0.99	0	51,51,51	1.92	10 (19%)
20	PGV	C	307	-	50,50,50	1.07	2 (4%)	53,56,56	1.00	3 (5%)
21	EDO	P	307	-	3,3,3	0.56	0	2,2,2	0.14	0
22	CUA	O	301	2,30	0,1,1	-	-	-	-	-
20	PGV	N	607	-	50,50,50	0.97	2 (4%)	53,56,56	1.30	5 (9%)
24	PSC	O	302	-	51,51,51	1.25	3 (5%)	57,59,59	1.13	4 (7%)
20	PGV	A	608	-	50,50,50	0.89	3 (6%)	53,56,56	1.43	7 (13%)
25	PEK	C	306	-	52,52,52	1.14	2 (3%)	55,57,57	1.12	5 (9%)
20	PGV	P	302	-	50,50,50	0.89	3 (6%)	53,56,56	1.29	9 (16%)
14	HEA	A	601	1	67,67,67	1.95	21 (31%)	81,103,103	1.94	22 (27%)
20	PGV	Z	101	-	50,50,50	1.13	2 (4%)	53,56,56	1.13	4 (7%)
25	PEK	B	304	-	52,52,52	1.19	2 (3%)	55,57,57	1.07	3 (5%)
21	EDO	C	312	-	3,3,3	0.48	0	2,2,2	0.17	0
27	CDL	T	102	-	99,99,99	1.43	12 (12%)	105,111,111	1.24	10 (9%)
23	CHD	C	304	-	32,32,32	0.73	0	51,51,51	2.40	18 (35%)
21	EDO	N	611	-	3,3,3	0.53	0	2,2,2	0.12	0
25	PEK	G	101	-	52,52,52	0.87	3 (5%)	55,57,57	1.41	5 (9%)
19	TGL	A	607	-	62,62,62	1.23	4 (6%)	65,65,65	1.53	7 (10%)
21	EDO	G	105	-	3,3,3	0.56	0	2,2,2	0.31	0
21	EDO	K	101	-	3,3,3	0.49	0	2,2,2	0.38	0
23	CHD	B	302	-	32,32,32	1.00	2 (6%)	51,51,51	1.67	15 (29%)
24	PSC	B	303	-	51,51,51	1.20	3 (5%)	57,59,59	1.07	2 (3%)
27	CDL	G	102	-	99,99,99	1.45	12 (12%)	105,111,111	1.28	12 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEK	G	103	-	52,52,52	1.15	2 (3%)	55,57,57	1.10	4 (7%)
19	TGL	N	609	-	62,62,62	1.19	3 (4%)	65,65,65	1.38	9 (13%)
21	EDO	A	611	-	3,3,3	0.46	0	2,2,2	0.35	0
21	EDO	C	310	-	3,3,3	0.47	0	2,2,2	0.33	0
21	EDO	L	103	-	3,3,3	0.55	0	2,2,2	0.03	0
21	EDO	X	101	-	3,3,3	0.54	0	2,2,2	0.17	0
21	EDO	A	613	-	3,3,3	0.52	0	2,2,2	0.43	0
21	EDO	S	102	-	3,3,3	0.78	0	2,2,2	0.27	0
22	CUA	B	301	2,30	0,1,1	-	-	-	-	-
25	PEK	T	101	-	52,52,52	0.99	3 (5%)	55,57,57	1.19	5 (9%)
20	PGV	C	302	-	50,50,50	0.89	2 (4%)	53,56,56	1.17	6 (11%)
21	EDO	L	102	-	3,3,3	0.43	0	2,2,2	0.46	0
23	CHD	W	101	-	32,32,32	0.84	0	51,51,51	2.20	21 (41%)
19	TGL	Q	201	-	62,62,62	1.22	3 (4%)	65,65,65	1.02	6 (9%)
21	EDO	T	103	-	3,3,3	0.64	0	2,2,2	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	C	311	-	-	1/1/1/1	-
21	EDO	A	610	-	-	0/1/1/1	-
23	CHD	C	305	-	-	0/9/74/74	0/4/4/4
29	DMU	Z	102	-	-	7/19/59/59	0/2/2/2
29	DMU	M	101	-	-	7/19/59/59	0/2/2/2
20	PGV	N	608	-	-	23/55/55/55	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
27	CDL	C	303	-	-	65/110/110/110	-
19	TGL	L	101	-	-	34/65/65/65	-
14	HEA	A	602	1	-	6/36/76/76	-
14	HEA	N	602	18,1	-	9/36/76/76	-
19	TGL	Y	101	-	-	37/65/65/65	-
21	EDO	B	305	-	-	0/1/1/1	-
21	EDO	P	306	-	-	0/1/1/1	-
19	TGL	D	201	-	-	29/65/65/65	-
23	CHD	P	304	-	-	4/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	G	104	-	-	3/9/74/74	0/4/4/4
14	HEA	N	601	1	-	4/36/76/76	-
27	CDL	P	303	-	-	71/110/110/110	-
21	EDO	K	102	-	-	1/1/1/1	-
20	PGV	A	609	-	-	28/55/55/55	-
21	EDO	A	612	-	-	1/1/1/1	-
23	CHD	J	101	-	-	7/9/74/74	0/4/4/4
21	EDO	I	101	-	-	1/1/1/1	-
21	EDO	C	309	-	-	0/1/1/1	-
21	EDO	K	103	-	-	1/1/1/1	-
21	EDO	N	612	-	-	0/1/1/1	-
25	PEK	C	308	-	-	31/56/56/56	-
23	CHD	P	305	-	-	3/9/74/74	0/4/4/4
20	PGV	C	307	-	-	32/55/55/55	-
21	EDO	P	307	-	-	1/1/1/1	-
20	PGV	N	607	-	-	11/55/55/55	-
24	PSC	O	302	-	-	23/55/55/55	-
20	PGV	A	608	-	-	20/55/55/55	-
25	PEK	C	306	-	-	25/56/56/56	-
20	PGV	P	302	-	-	12/55/55/55	-
14	HEA	A	601	1	-	4/36/76/76	-
20	PGV	Z	101	-	-	32/55/55/55	-
25	PEK	B	304	-	-	36/56/56/56	-
21	EDO	C	312	-	-	1/1/1/1	-
27	CDL	T	102	-	-	54/110/110/110	-
23	CHD	C	304	-	-	8/9/74/74	0/4/4/4
21	EDO	N	611	-	-	1/1/1/1	-
25	PEK	G	101	-	-	21/56/56/56	-
19	TGL	A	607	-	-	35/65/65/65	-
21	EDO	G	105	-	-	0/1/1/1	-
21	EDO	K	101	-	-	0/1/1/1	-
23	CHD	B	302	-	-	3/9/74/74	0/4/4/4
24	PSC	B	303	-	-	30/55/55/55	-
27	CDL	G	102	-	-	59/110/110/110	-
25	PEK	G	103	-	-	36/56/56/56	-
19	TGL	N	609	-	-	41/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	A	611	-	-	1/1/1/1	-
21	EDO	C	310	-	-	0/1/1/1	-
21	EDO	L	103	-	-	1/1/1/1	-
21	EDO	X	101	-	-	0/1/1/1	-
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
25	PEK	T	101	-	-	22/56/56/56	-
20	PGV	C	302	-	-	20/55/55/55	-
21	EDO	L	102	-	-	1/1/1/1	-
23	CHD	W	101	-	-	8/9/74/74	0/4/4/4
19	TGL	Q	201	-	-	34/65/65/65	-
21	EDO	T	103	-	-	1/1/1/1	-

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	FE-ND	6.67	2.15	1.94
19	L	101	TGL	OG2-CB1	5.99	1.51	1.34
19	Y	101	TGL	OG3-CC1	5.84	1.50	1.33
19	N	609	TGL	OG2-CB1	5.82	1.50	1.34
19	Y	101	TGL	OG2-CB1	5.48	1.49	1.34
25	G	103	PEK	O01-C1	5.46	1.49	1.34
19	A	607	TGL	OG2-CB1	5.45	1.49	1.34
25	B	304	PEK	O01-C1	5.39	1.49	1.34
20	N	608	PGV	O01-C1	5.26	1.49	1.34
19	D	201	TGL	OG1-CA1	5.25	1.48	1.33
20	A	609	PGV	O01-C1	5.20	1.49	1.34
20	C	307	PGV	O01-C1	5.18	1.48	1.34
27	P	303	CDL	OB8-CB7	5.12	1.48	1.33
25	B	304	PEK	O03-C21	5.08	1.48	1.33
24	O	302	PSC	O03-C19	5.04	1.48	1.33
25	G	103	PEK	O03-C21	5.02	1.48	1.33
19	Q	201	TGL	OG1-CA1	4.99	1.47	1.33
19	L	101	TGL	OG3-CC1	4.98	1.47	1.33
27	G	102	CDL	OA8-CA7	4.95	1.47	1.33
19	A	607	TGL	OG1-CA1	4.95	1.47	1.33
19	Q	201	TGL	OG2-CB1	4.94	1.48	1.34
20	Z	101	PGV	O01-C1	4.92	1.48	1.34
25	C	306	PEK	O03-C21	4.92	1.47	1.33
27	C	303	CDL	OA8-CA7	4.92	1.47	1.33
20	Z	101	PGV	O03-C19	4.91	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	306	PEK	O01-C1	4.87	1.48	1.34
27	C	303	CDL	OB8-CB7	4.85	1.47	1.33
19	N	609	TGL	OG1-CA1	4.84	1.47	1.33
24	B	303	PSC	O01-C1	4.81	1.47	1.34
24	B	303	PSC	O03-C19	4.79	1.47	1.33
14	N	601	HEA	FE-NB	4.79	2.09	1.94
14	N	602	HEA	C1D-ND	-4.76	1.32	1.40
20	A	609	PGV	O03-C19	4.75	1.47	1.33
14	N	602	HEA	FE-ND	4.71	2.09	1.94
27	T	102	CDL	OB8-CB7	4.71	1.47	1.33
27	T	102	CDL	OA8-CA7	4.71	1.47	1.33
24	O	302	PSC	O01-C1	4.71	1.47	1.34
25	C	308	PEK	O01-C1	4.69	1.47	1.34
27	G	102	CDL	OA6-CA5	4.68	1.47	1.34
27	C	303	CDL	OA6-CA5	4.67	1.47	1.34
27	P	303	CDL	OB6-CB5	4.65	1.47	1.34
27	P	303	CDL	OA8-CA7	4.60	1.46	1.33
27	P	303	CDL	OA6-CA5	4.56	1.47	1.34
27	G	102	CDL	OB8-CB7	4.55	1.46	1.33
27	C	303	CDL	OB6-CB5	4.53	1.47	1.34
14	N	601	HEA	CHA-C1A	4.53	1.47	1.38
25	C	308	PEK	O03-C21	4.53	1.46	1.33
27	T	102	CDL	OA6-CA5	4.49	1.47	1.34
14	N	602	HEA	C4B-NB	-4.46	1.32	1.40
19	Y	101	TGL	OG1-CA1	4.43	1.46	1.33
14	N	601	HEA	C1D-ND	-4.41	1.32	1.40
27	T	102	CDL	OB6-CB5	4.41	1.46	1.34
19	Q	201	TGL	OG3-CC1	4.41	1.46	1.33
19	D	201	TGL	OG3-CC1	4.36	1.46	1.33
27	G	102	CDL	OB6-CB5	4.36	1.46	1.34
20	N	608	PGV	O03-C19	4.35	1.46	1.33
19	D	201	TGL	OG2-CB1	4.35	1.46	1.34
14	A	601	HEA	CHB-C4A	4.32	1.46	1.38
19	L	101	TGL	OG1-CA1	4.27	1.45	1.33
14	N	602	HEA	FE-NB	4.25	2.08	1.94
14	A	601	HEA	FE-NA	4.24	2.09	1.95
20	C	302	PGV	O03-C19	4.22	1.45	1.33
14	N	601	HEA	FE-ND	4.22	2.07	1.94
20	N	607	PGV	O03-C19	4.19	1.45	1.33
14	N	601	HEA	C4B-NB	-4.15	1.33	1.40
19	N	609	TGL	OG3-CC1	4.13	1.45	1.33
25	T	101	PEK	O03-C21	4.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	FE-ND	4.02	2.07	1.94
24	O	302	PSC	C13-C12	4.01	1.54	1.31
14	N	602	HEA	C1A-C2A	-4.00	1.38	1.45
14	N	601	HEA	FE-NC	3.99	2.08	1.95
14	N	602	HEA	C4C-NC	-3.96	1.32	1.39
14	A	602	HEA	C4B-NB	-3.90	1.33	1.40
14	A	602	HEA	FE-NB	3.87	2.06	1.94
24	B	303	PSC	C13-C12	3.80	1.53	1.31
14	N	602	HEA	C1B-C2B	-3.79	1.36	1.44
14	N	601	HEA	C1C-NC	-3.74	1.32	1.39
20	C	307	PGV	O03-C19	3.73	1.44	1.33
27	C	303	CDL	C59-C58	-3.69	1.33	1.51
14	A	602	HEA	C4D-ND	-3.69	1.31	1.38
19	A	607	TGL	OG3-CC1	3.67	1.44	1.33
14	A	602	HEA	FE-NA	3.65	2.07	1.95
14	N	602	HEA	C4A-NA	-3.63	1.32	1.39
27	T	102	CDL	C79-C78	-3.63	1.33	1.51
25	G	101	PEK	O01-C1	3.63	1.44	1.34
27	T	102	CDL	C19-C18	-3.62	1.33	1.51
14	A	602	HEA	CHA-C1A	3.62	1.45	1.38
27	G	102	CDL	C19-C18	-3.61	1.33	1.51
14	A	602	HEA	C1D-ND	-3.61	1.34	1.40
20	P	302	PGV	O01-C1	3.60	1.44	1.34
27	C	303	CDL	C62-C61	-3.59	1.33	1.51
27	C	303	CDL	C22-C21	-3.59	1.33	1.51
27	C	303	CDL	C79-C78	-3.58	1.34	1.51
14	N	601	HEA	C4B-C3B	-3.58	1.38	1.44
20	A	608	PGV	O03-C19	3.58	1.43	1.33
27	G	102	CDL	C59-C58	-3.57	1.34	1.51
27	P	303	CDL	C59-C58	-3.57	1.34	1.51
27	T	102	CDL	C22-C21	-3.56	1.34	1.51
14	A	602	HEA	O11-C11	3.56	1.50	1.42
27	P	303	CDL	C19-C18	-3.54	1.34	1.51
25	T	101	PEK	O01-C1	3.53	1.44	1.34
27	P	303	CDL	C79-C78	-3.52	1.34	1.51
14	N	602	HEA	C4B-C3B	-3.51	1.38	1.44
27	C	303	CDL	C39-C38	-3.50	1.34	1.51
14	A	601	HEA	O11-C11	3.50	1.50	1.42
27	C	303	CDL	C19-C18	-3.49	1.34	1.51
27	P	303	CDL	C42-C41	-3.49	1.34	1.51
27	T	102	CDL	C39-C38	-3.48	1.34	1.51
27	P	303	CDL	C22-C21	-3.47	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	P	303	CDL	C62-C61	-3.46	1.34	1.51
14	A	602	HEA	C1B-NB	-3.45	1.32	1.38
27	P	303	CDL	C39-C38	-3.44	1.34	1.51
27	G	102	CDL	C79-C78	-3.43	1.34	1.51
27	C	303	CDL	C82-C81	-3.42	1.34	1.51
27	P	303	CDL	C82-C81	-3.42	1.34	1.51
27	G	102	CDL	C62-C61	-3.40	1.34	1.51
27	G	102	CDL	C22-C21	-3.39	1.34	1.51
14	A	601	HEA	C4B-NB	-3.37	1.34	1.40
14	N	601	HEA	FE-NA	3.36	2.06	1.95
27	C	303	CDL	C42-C41	-3.35	1.35	1.51
14	A	602	HEA	C3A-C4A	-3.34	1.40	1.46
14	A	601	HEA	C1D-ND	-3.32	1.34	1.40
25	G	101	PEK	O03-C21	3.32	1.43	1.33
14	N	602	HEA	O11-C11	3.31	1.50	1.42
14	A	602	HEA	C1A-C2A	-3.28	1.39	1.45
27	T	102	CDL	C42-C41	-3.26	1.35	1.51
27	T	102	CDL	C82-C81	-3.26	1.35	1.51
27	T	102	CDL	C62-C61	-3.25	1.35	1.51
27	T	102	CDL	C59-C58	-3.18	1.35	1.51
27	G	102	CDL	C82-C81	-3.18	1.36	1.51
14	N	602	HEA	C1C-NC	-3.17	1.33	1.39
14	A	601	HEA	C3B-C2B	3.17	1.41	1.34
20	N	607	PGV	O01-C1	3.16	1.43	1.34
14	N	601	HEA	C3A-C4A	-3.14	1.40	1.46
14	N	602	HEA	C3A-C4A	-3.14	1.40	1.46
14	A	601	HEA	FE-NB	3.13	2.04	1.94
27	G	102	CDL	C42-C41	-3.11	1.36	1.51
27	G	102	CDL	C39-C38	-3.11	1.36	1.51
20	A	608	PGV	O01-C1	3.07	1.43	1.34
14	A	601	HEA	CHA-C1A	3.06	1.44	1.38
14	A	602	HEA	CHB-C1B	3.03	1.46	1.39
14	N	601	HEA	CHB-C4A	2.96	1.44	1.38
14	A	602	HEA	CHD-C1D	2.95	1.44	1.38
14	A	602	HEA	C4D-C3D	-2.94	1.40	1.45
14	N	601	HEA	CHA-C4D	2.94	1.45	1.39
14	A	602	HEA	C4C-NC	-2.93	1.34	1.39
14	A	601	HEA	C4C-NC	-2.92	1.34	1.39
19	A	607	TGL	OC1-CC1	-2.89	1.13	1.22
14	A	601	HEA	C4D-ND	-2.88	1.33	1.38
14	A	601	HEA	C3A-C4A	-2.82	1.41	1.46
14	N	602	HEA	C1B-NB	-2.81	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	CHC-C4B	2.81	1.44	1.38
25	T	101	PEK	O01-C02	-2.78	1.40	1.46
14	N	601	HEA	C4C-NC	-2.78	1.34	1.39
14	N	601	HEA	CHC-C1C	2.72	1.45	1.39
14	A	602	HEA	C4B-C3B	-2.71	1.40	1.44
14	N	601	HEA	C1D-C2D	-2.70	1.39	1.44
14	N	602	HEA	CMA-C3A	2.69	1.51	1.45
14	A	601	HEA	C11-C3B	2.69	1.54	1.51
14	N	601	HEA	CHD-C1D	2.68	1.43	1.38
14	A	601	HEA	C4B-C3B	-2.65	1.40	1.44
14	N	602	HEA	CHB-C4A	2.64	1.43	1.38
14	A	601	HEA	C1D-C2D	-2.62	1.39	1.44
14	N	602	HEA	CHA-C1A	2.60	1.43	1.38
14	A	602	HEA	CHD-C4C	2.60	1.45	1.39
14	A	601	HEA	CHB-C1B	2.58	1.45	1.39
14	N	602	HEA	C4D-ND	-2.56	1.33	1.38
23	C	305	CHD	O12-C12	2.54	1.47	1.43
14	N	601	HEA	C4D-ND	-2.54	1.33	1.38
14	N	601	HEA	C4D-C3D	-2.53	1.40	1.45
14	A	602	HEA	C4A-NA	-2.53	1.34	1.39
14	N	601	HEA	C1B-C2B	-2.53	1.39	1.44
14	N	601	HEA	CMA-C3A	2.52	1.51	1.45
14	N	602	HEA	CHD-C4C	2.49	1.45	1.39
23	P	304	CHD	C20-C17	2.48	1.58	1.54
20	C	302	PGV	O01-C1	2.42	1.41	1.34
14	A	602	HEA	CHC-C1C	2.40	1.44	1.39
14	A	601	HEA	C1A-NA	-2.40	1.35	1.39
23	J	101	CHD	C23-C24	2.40	1.56	1.50
20	P	302	PGV	O03-C19	2.38	1.40	1.33
23	G	104	CHD	O7-C7	2.35	1.48	1.43
14	A	601	HEA	C4D-C3D	-2.29	1.41	1.45
14	N	602	HEA	CHD-C1D	2.29	1.43	1.38
23	C	305	CHD	C4-C3	2.27	1.56	1.52
14	A	602	HEA	C1C-C2C	-2.26	1.37	1.43
19	D	201	TGL	OB1-CB1	2.26	1.29	1.22
20	A	608	PGV	O01-C02	-2.26	1.41	1.46
14	N	602	HEA	O1D-CGD	2.23	1.29	1.22
23	B	302	CHD	C4-C3	2.23	1.55	1.52
14	N	601	HEA	CHB-C1B	2.22	1.44	1.39
14	N	601	HEA	CMC-C2C	2.21	1.55	1.50
23	B	302	CHD	C13-C17	-2.20	1.51	1.55
14	A	601	HEA	CHD-C1D	2.20	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	305	CHD	O26-C24	-2.18	1.23	1.30
14	N	602	HEA	CHA-C4D	2.16	1.44	1.39
14	N	602	HEA	C3B-C2B	2.16	1.39	1.34
14	A	601	HEA	C1A-C2A	-2.15	1.41	1.45
29	M	101	DMU	O16-C6	2.12	1.43	1.40
20	P	302	PGV	O01-C02	-2.11	1.41	1.46
14	N	601	HEA	O1D-CGD	2.10	1.28	1.22
25	G	101	PEK	O01-C02	-2.06	1.41	1.46
14	N	601	HEA	C1B-NB	-2.03	1.34	1.38
27	C	303	CDL	CB2-C1	2.02	1.57	1.51
14	N	601	HEA	CBD-CGD	2.01	1.55	1.50
14	N	601	HEA	C3A-C2A	2.01	1.41	1.37
14	A	602	HEA	CHC-C4B	2.01	1.42	1.38

All (369) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	101	CHD	C13-C17-C20	7.23	128.24	119.48
23	J	101	CHD	C13-C17-C20	7.03	128.00	119.48
19	L	101	TGL	OG2-CB1-CB2	6.97	126.57	111.48
23	P	305	CHD	C18-C13-C12	-6.89	102.16	109.06
19	N	609	TGL	OG2-CB1-CB2	6.39	125.31	111.48
20	N	608	PGV	O01-C1-C2	6.24	124.99	111.48
19	A	607	TGL	CG3-CG2-CG1	-6.12	97.52	111.78
14	A	601	HEA	C12-C11-C3B	6.05	121.58	112.12
23	C	304	CHD	C10-C9-C8	5.85	118.36	111.84
14	N	602	HEA	C13-C12-C11	-5.83	105.08	114.39
25	G	101	PEK	C2-C3-C4	-5.75	100.79	113.35
23	C	304	CHD	C16-C17-C20	5.63	120.70	112.18
14	A	601	HEA	C26-C15-C14	-5.32	109.97	123.63
19	L	101	TGL	CG2-OG2-CB1	5.31	130.51	117.80
19	Y	101	TGL	OG2-CB1-CB2	5.29	122.93	111.48
14	A	602	HEA	CAD-CBD-CGD	-5.28	99.65	113.67
19	A	607	TGL	OG2-CB1-CB2	5.25	122.84	111.48
23	W	101	CHD	C10-C9-C8	5.21	117.65	111.84
27	T	102	CDL	OB6-CB5-C51	5.16	122.64	111.48
27	P	303	CDL	OB6-CB5-C51	5.11	122.53	111.48
23	C	304	CHD	C17-C13-C14	-5.10	95.00	100.11
27	G	102	CDL	OB6-CB5-C51	5.09	122.50	111.48
23	C	304	CHD	C1-C2-C3	5.05	117.17	110.48
20	A	608	PGV	O03-C19-C20	4.99	127.05	111.83
14	N	601	HEA	C13-C12-C11	-4.85	106.65	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	201	TGL	CG2-OG2-CB1	-4.82	106.25	117.80
20	Z	101	PGV	O01-C1-C2	4.79	121.84	111.48
25	C	306	PEK	O01-C1-C2	4.74	121.74	111.48
23	C	304	CHD	C14-C13-C12	4.70	111.71	107.42
23	J	101	CHD	C22-C20-C17	4.69	120.06	110.33
19	A	607	TGL	OG3-CC1-CC2	4.68	126.09	111.83
27	C	303	CDL	OB6-CB5-C51	4.65	121.53	111.48
27	P	303	CDL	OA6-CA5-C11	4.64	121.53	111.48
23	P	305	CHD	C19-C10-C1	-4.63	100.94	108.31
27	C	303	CDL	OA6-CA5-C11	4.53	121.28	111.48
14	A	602	HEA	C13-C14-C15	-4.52	117.29	127.62
25	T	101	PEK	O01-C1-C2	4.46	121.14	111.48
23	C	305	CHD	C19-C10-C1	-4.46	101.21	108.31
27	G	102	CDL	OA6-CA5-C11	4.45	121.12	111.48
20	N	607	PGV	O03-C19-C20	4.42	125.31	111.83
23	P	304	CHD	C16-C17-C20	4.37	118.78	112.18
14	A	602	HEA	C3A-C2A-C1A	-4.35	102.93	107.05
14	N	601	HEA	C3C-C4C-NC	4.33	113.44	109.80
25	G	101	PEK	O03-C01-C02	-4.31	95.97	108.40
25	B	304	PEK	O01-C1-C2	4.25	120.67	111.48
23	C	304	CHD	C2-C1-C10	4.22	119.86	112.74
24	B	303	PSC	O01-C1-C2	4.20	120.57	111.48
23	P	305	CHD	C21-C20-C22	-4.19	103.85	110.34
23	J	101	CHD	C6-C7-C8	4.19	116.07	111.50
14	A	601	HEA	C16-C15-C14	4.17	130.53	121.17
19	D	201	TGL	OG3-CC1-CC2	4.13	124.42	111.83
19	A	607	TGL	OG3-CC1-OC1	-4.12	113.31	123.63
29	Z	102	DMU	C7-C8-C9	4.12	117.70	110.23
23	P	305	CHD	C14-C13-C12	4.09	111.15	107.42
19	D	201	TGL	OG3-CC1-OC1	-4.05	113.50	123.63
20	A	609	PGV	O01-C1-C2	4.03	120.19	111.48
20	A	608	PGV	O03-C19-O04	-4.01	113.59	123.63
23	J	101	CHD	C10-C9-C8	4.00	116.29	111.84
23	J	101	CHD	C11-C12-C13	3.99	115.32	111.26
14	N	602	HEA	CAD-CBD-CGD	-3.98	103.10	113.67
23	G	104	CHD	C13-C17-C20	-3.92	114.74	119.48
23	C	304	CHD	C23-C22-C20	-3.87	107.22	114.46
14	A	602	HEA	C1D-C2D-C3D	-3.86	102.92	106.98
27	T	102	CDL	OA6-CA5-C11	3.86	119.83	111.48
24	O	302	PSC	O01-C1-C2	3.86	119.83	111.48
14	A	601	HEA	C27-C19-C20	3.83	121.88	115.23
14	A	601	HEA	C2D-C1D-ND	3.81	114.22	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	C12-C11-C3B	3.79	118.05	112.12
20	N	607	PGV	O01-C1-O02	-3.78	114.87	123.70
19	Q	201	TGL	OG1-CA1-CA2	3.77	123.32	111.83
14	A	602	HEA	C21-C20-C19	3.76	125.64	113.19
23	C	305	CHD	C6-C5-C10	3.76	116.66	112.66
23	B	302	CHD	C18-C13-C12	-3.74	105.31	109.06
14	N	602	HEA	C3A-C2A-C1A	-3.73	103.52	107.05
23	P	304	CHD	C6-C5-C4	-3.72	106.98	111.23
14	N	602	HEA	O11-C11-C12	3.71	118.97	109.14
19	N	609	TGL	OG1-CA1-CA2	3.68	123.05	111.83
19	L	101	TGL	OG3-CC1-CC2	3.67	123.04	111.83
23	W	101	CHD	C9-C8-C7	3.67	116.48	111.86
25	C	308	PEK	O01-C1-C2	3.67	119.41	111.48
25	G	103	PEK	O01-C1-C2	3.65	119.38	111.48
20	N	608	PGV	O03-C19-C20	3.64	122.93	111.83
14	A	602	HEA	CAA-CBA-CGA	-3.64	104.02	113.67
23	C	304	CHD	C15-C14-C13	3.63	107.06	103.54
14	N	602	HEA	C25-C23-C24	3.60	122.87	114.59
14	N	602	HEA	C2D-C1D-ND	3.58	113.95	109.84
19	Y	101	TGL	OG3-CC1-CC2	3.57	122.72	111.83
20	C	302	PGV	O03-C19-C20	3.56	122.68	111.83
23	P	305	CHD	C17-C13-C12	3.56	120.87	117.67
14	A	601	HEA	OMA-CMA-C3A	-3.56	117.59	125.62
29	Z	102	DMU	C6-O5-C4	-3.52	106.84	113.72
20	C	307	PGV	C01-O03-C19	3.52	129.98	117.12
25	T	101	PEK	O03-C21-C22	3.52	122.56	111.83
23	C	305	CHD	C4-C3-C2	3.51	114.91	110.62
23	P	305	CHD	C1-C10-C5	3.49	112.75	107.75
19	Y	101	TGL	OG3-CG3-CG2	3.46	118.37	108.40
20	P	302	PGV	C03-C02-C01	-3.46	103.73	111.78
14	A	602	HEA	C27-C19-C20	3.44	121.21	115.23
19	N	609	TGL	OG3-CC1-CC2	3.40	122.22	111.83
14	N	602	HEA	C3C-C4C-NC	3.38	112.64	109.80
20	C	307	PGV	O01-C1-C2	3.38	118.78	111.48
23	P	304	CHD	C15-C14-C13	3.37	106.81	103.54
25	G	103	PEK	O03-C21-C22	3.37	122.12	111.83
20	N	608	PGV	O01-C1-O02	-3.37	115.83	123.70
23	W	101	CHD	C6-C7-C8	3.36	115.17	111.50
14	N	602	HEA	C1D-C2D-C3D	-3.36	103.45	106.98
27	C	303	CDL	OA8-CA7-C31	3.35	122.04	111.83
23	B	302	CHD	C16-C17-C13	3.34	106.78	103.54
25	G	101	PEK	C01-O03-C21	3.34	129.32	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	303	CDL	OB8-CB7-C71	3.33	121.97	111.83
19	A	607	TGL	OG1-CA1-CA2	3.32	121.96	111.83
23	G	104	CHD	C1-C2-C3	-3.32	106.09	110.48
23	W	101	CHD	C14-C8-C7	3.31	116.24	111.85
24	O	302	PSC	O03-C19-C20	3.30	121.89	111.83
23	W	101	CHD	C14-C8-C9	-3.29	105.16	109.75
23	C	305	CHD	C6-C5-C4	-3.26	107.50	111.23
23	W	101	CHD	C6-C5-C10	3.26	116.12	112.66
19	Q	201	TGL	OG2-CB1-CB2	3.25	118.52	111.48
14	A	601	HEA	CHC-C4B-NB	3.25	128.38	124.37
29	Z	102	DMU	C18-O16-C6	-3.24	108.15	113.68
14	N	601	HEA	C4A-C3A-C2A	-3.22	104.02	106.81
20	P	302	PGV	O03-C01-C02	-3.22	99.11	108.40
25	T	101	PEK	O01-C1-O02	-3.22	116.18	123.70
14	A	602	HEA	CHD-C4C-NC	3.22	129.69	123.86
23	B	302	CHD	C15-C14-C13	3.21	106.65	103.54
19	D	201	TGL	OG1-CA1-CA2	3.20	121.59	111.83
20	Z	101	PGV	O03-C19-C20	3.20	121.58	111.83
23	C	304	CHD	C15-C14-C8	3.20	122.74	118.36
14	A	601	HEA	C3C-C2C-C1C	-3.20	103.40	107.17
20	P	302	PGV	O03-C19-O04	-3.19	115.66	123.63
25	B	304	PEK	O03-C21-C22	3.18	121.53	111.83
14	A	602	HEA	O1A-CGA-CBA	-3.17	113.05	123.09
14	A	601	HEA	C17-C16-C15	-3.16	102.72	113.19
19	N	609	TGL	OG3-CC1-OC1	-3.16	115.73	123.63
23	G	104	CHD	C5-C6-C7	-3.13	110.68	114.40
14	A	602	HEA	CHB-C4A-NA	-3.12	121.06	124.45
23	P	304	CHD	C19-C10-C1	-3.12	103.35	108.31
19	Q	201	TGL	OG3-CC1-CC2	3.11	121.33	111.83
14	A	602	HEA	C13-C12-C11	-3.11	109.43	114.39
14	N	602	HEA	C4B-NB-C1B	3.09	108.86	105.21
14	A	602	HEA	O11-C11-C12	3.09	117.32	109.14
25	C	306	PEK	O03-C21-C22	3.08	121.22	111.83
23	G	104	CHD	C15-C14-C13	3.08	106.52	103.54
27	G	102	CDL	OA8-CA7-C31	3.07	121.19	111.83
14	N	602	HEA	C3D-C4D-ND	3.06	113.31	110.35
27	T	102	CDL	OA8-CA7-C31	3.06	121.18	111.83
14	N	602	HEA	CAD-C3D-C2D	3.06	133.60	127.87
24	O	302	PSC	O03-C01-C02	3.06	117.23	108.40
14	A	601	HEA	CAA-C2A-C1A	3.06	131.07	124.85
29	Z	102	DMU	O1-C9-C8	3.05	115.19	109.70
20	C	307	PGV	O03-C19-C20	3.04	121.11	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C2A-C1A-NA	3.04	113.25	110.32
20	C	302	PGV	O03-C19-O04	-3.03	116.05	123.63
24	B	303	PSC	O03-C19-C20	3.03	121.06	111.83
27	P	303	CDL	OB8-CB6-CB4	3.03	117.12	108.40
14	N	602	HEA	O11-C11-C3B	-3.01	105.73	111.26
14	A	601	HEA	CAA-CBA-CGA	-3.01	105.69	113.67
23	G	104	CHD	O7-C7-C6	2.99	117.28	109.86
23	W	101	CHD	C22-C20-C17	2.97	116.50	110.33
20	N	607	PGV	O03-C19-O04	-2.97	116.21	123.63
23	W	101	CHD	C1-C2-C3	2.94	114.38	110.48
20	P	302	PGV	O01-C1-C2	2.94	117.84	111.48
25	G	101	PEK	O01-C1-C2	2.94	117.84	111.48
27	P	303	CDL	OB8-CB7-C71	2.94	120.79	111.83
20	A	609	PGV	O03-C01-C02	2.93	116.84	108.40
20	C	302	PGV	O01-C1-C2	2.92	117.80	111.48
27	G	102	CDL	OB8-CB7-OB9	-2.91	116.34	123.63
23	J	101	CHD	C14-C8-C7	2.91	115.72	111.85
20	A	609	PGV	O03-C19-C20	2.91	120.72	111.83
14	N	602	HEA	CHB-C1B-NB	2.90	127.55	124.42
23	B	302	CHD	O12-C12-C13	-2.90	106.13	111.02
27	G	102	CDL	OB8-CB7-C71	2.89	120.63	111.83
29	M	101	DMU	O49-C1-C6	-2.89	103.20	110.08
19	D	201	TGL	CG3-CG2-CG1	2.88	118.50	111.78
23	W	101	CHD	C9-C10-C5	2.87	112.50	108.51
23	P	304	CHD	C15-C14-C8	2.87	122.29	118.36
23	C	304	CHD	O12-C12-C13	2.86	115.86	111.02
25	C	308	PEK	O03-C21-O04	-2.84	116.51	123.63
23	B	302	CHD	C17-C13-C12	2.84	120.22	117.67
23	P	304	CHD	C22-C20-C17	2.84	116.21	110.33
25	G	103	PEK	C02-O01-C1	2.83	124.58	117.80
23	G	104	CHD	C11-C9-C8	2.80	115.04	110.89
29	M	101	DMU	C6-O5-C4	2.79	119.18	113.72
25	C	308	PEK	O03-C21-C22	2.79	120.34	111.83
14	N	602	HEA	C2A-C1A-NA	2.78	113.01	110.32
27	P	303	CDL	CB6-OB8-CB7	2.78	127.29	117.12
23	C	304	CHD	C19-C10-C1	-2.78	103.88	108.31
25	C	306	PEK	O03-C01-C02	2.77	116.39	108.40
14	A	601	HEA	C1D-C2D-C3D	-2.77	104.07	106.98
20	N	608	PGV	C03-C02-C01	-2.75	105.38	111.78
27	P	303	CDL	OB6-CB5-OB7	-2.74	117.29	123.70
23	P	304	CHD	C14-C13-C12	2.74	109.92	107.42
23	C	305	CHD	C11-C9-C10	-2.74	110.92	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	303	CDL	OA8-CA7-C31	2.73	120.15	111.83
19	N	609	TGL	OB1-CB1-CB2	-2.72	113.15	123.78
19	Q	201	TGL	OG3-CC1-OC1	-2.72	116.83	123.63
23	B	302	CHD	C11-C9-C8	2.71	114.91	110.89
29	Z	102	DMU	O49-C1-C6	-2.69	103.67	110.08
14	A	602	HEA	C3C-C2C-C1C	-2.68	104.01	107.17
23	J	101	CHD	C21-C20-C17	-2.68	108.86	112.88
23	J	101	CHD	C22-C23-C24	2.68	119.64	112.49
23	C	304	CHD	C6-C5-C10	2.66	115.49	112.66
20	C	302	PGV	O03-C01-C02	2.65	116.05	108.40
23	C	304	CHD	O25-C24-C23	-2.65	114.70	123.09
19	L	101	TGL	CB4-CB3-CB2	-2.64	103.43	113.13
14	A	602	HEA	O2A-CGA-CBA	2.64	122.34	114.00
23	C	305	CHD	C23-C22-C20	-2.63	109.54	114.46
19	L	101	TGL	OG2-CG2-CG1	2.63	117.78	108.34
20	A	608	PGV	C26-C25-C24	-2.61	101.17	114.37
23	C	304	CHD	C9-C11-C12	-2.60	110.89	114.29
27	G	102	CDL	CA6-OA8-CA7	2.59	126.58	117.12
14	A	601	HEA	C27-C19-C18	-2.59	116.98	123.63
25	G	101	PEK	C3-C2-C1	-2.59	104.22	113.69
23	C	305	CHD	O7-C7-C6	-2.58	103.44	109.86
23	B	302	CHD	C4-C3-C2	-2.58	107.47	110.62
23	J	101	CHD	C1-C2-C3	2.57	113.89	110.48
27	T	102	CDL	OB8-CB7-OB9	-2.56	117.21	123.63
14	A	602	HEA	CHC-C1C-C2C	-2.55	120.01	127.43
14	N	602	HEA	C27-C19-C20	2.55	119.66	115.23
19	Y	101	TGL	CG2-OG2-CB1	2.55	123.89	117.80
27	P	303	CDL	OA6-CA5-OA7	-2.55	117.75	123.70
23	C	304	CHD	C5-C4-C3	-2.54	108.87	112.71
20	A	608	PGV	O01-C1-C2	2.54	116.98	111.48
19	Y	101	TGL	OG1-CA1-CA2	2.54	119.57	111.83
24	O	302	PSC	C01-O03-C19	2.53	126.35	117.12
19	Q	201	TGL	OG1-CG1-CG2	2.51	115.64	108.40
23	J	101	CHD	C23-C22-C20	2.51	119.16	114.46
25	C	306	PEK	O03-C21-O04	-2.51	117.36	123.63
23	J	101	CHD	C5-C4-C3	2.50	116.48	112.71
23	G	104	CHD	C16-C15-C14	-2.50	100.26	105.14
20	P	302	PGV	O01-C1-O02	-2.48	117.92	123.70
23	G	104	CHD	C9-C8-C7	2.47	114.96	111.86
20	P	302	PGV	C02-O01-C1	2.47	123.70	117.80
14	A	601	HEA	C13-C12-C11	-2.46	110.46	114.39
23	G	104	CHD	C16-C17-C20	2.46	115.89	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	104	CHD	O26-C24-C23	2.46	121.76	114.00
19	A	607	TGL	CG3-OG3-CC1	2.45	126.09	117.12
23	W	101	CHD	C5-C4-C3	2.45	116.41	112.71
14	A	601	HEA	C3A-C2A-C1A	-2.45	104.73	107.05
14	N	601	HEA	C1B-C2B-C3B	-2.45	103.96	106.80
27	C	303	CDL	OA6-CA5-OA7	-2.45	117.98	123.70
27	G	102	CDL	OB6-CB5-OB7	-2.45	117.99	123.70
23	W	101	CHD	C11-C9-C8	-2.44	107.28	110.89
23	P	305	CHD	C22-C23-C24	-2.43	106.00	112.49
23	B	302	CHD	C18-C13-C14	2.42	115.00	111.20
19	N	609	TGL	OG2-CG2-CG3	2.42	117.02	108.34
27	T	102	CDL	C72-C71-CB7	2.41	122.53	113.69
23	C	305	CHD	C14-C8-C9	-2.41	106.39	109.75
23	B	302	CHD	C13-C17-C20	-2.41	116.57	119.48
27	G	102	CDL	C40-C39-C38	2.40	126.50	114.37
23	C	305	CHD	C1-C10-C5	2.40	111.19	107.75
23	J	101	CHD	C17-C13-C14	-2.40	97.71	100.11
20	Z	101	PGV	C01-O03-C19	2.38	125.83	117.12
14	A	601	HEA	C3D-C4D-ND	2.38	112.66	110.35
23	P	305	CHD	O26-C24-C23	2.38	121.51	114.00
27	T	102	CDL	OB6-CB5-OB7	-2.38	118.15	123.70
14	A	601	HEA	C26-C15-C16	2.37	119.34	115.23
19	N	609	TGL	OG1-CA1-OA1	-2.37	117.71	123.63
14	A	602	HEA	CMD-C2D-C1D	2.36	128.72	125.03
23	J	101	CHD	C18-C13-C17	2.36	114.90	111.20
19	L	101	TGL	CG3-CG2-CG1	-2.35	106.30	111.78
14	A	601	HEA	C2A-C1A-NA	2.35	112.59	110.32
23	B	302	CHD	O12-C12-C11	2.35	113.90	109.12
23	P	305	CHD	C15-C14-C13	2.35	105.82	103.54
29	M	101	DMU	O1-C9-C11	2.34	112.25	106.44
20	A	608	PGV	O01-C02-C01	-2.34	99.93	108.34
19	Y	101	TGL	OC1-CC1-CC2	-2.34	114.62	123.78
14	N	602	HEA	C3C-C2C-C1C	-2.34	104.41	107.17
23	J	101	CHD	C4-C3-C2	2.34	113.47	110.62
14	N	602	HEA	CHA-C1A-C2A	-2.34	121.17	124.86
27	G	102	CDL	OA6-CA5-OA7	-2.33	118.25	123.70
14	N	602	HEA	C2C-C1C-NC	2.33	113.88	110.14
25	B	304	PEK	O03-C21-O04	-2.32	117.82	123.63
20	Z	101	PGV	C02-O01-C1	2.32	123.35	117.80
29	Z	102	DMU	C8-C7-C5	2.32	114.91	110.83
14	N	601	HEA	O11-C11-C3B	-2.32	107.00	111.26
25	G	103	PEK	O03-C01-C02	2.32	115.09	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	101	CHD	C17-C13-C12	2.32	119.75	117.67
14	N	601	HEA	C26-C15-C16	2.31	119.24	115.23
20	A	608	PGV	O03-C01-C02	2.30	115.04	108.40
29	Z	102	DMU	O2-C8-C7	-2.30	104.95	110.38
19	L	101	TGL	OG2-CB1-OB1	-2.30	118.32	123.70
27	T	102	CDL	C42-C41-C40	2.30	125.98	114.37
23	B	302	CHD	O3-C3-C2	-2.29	104.18	110.17
14	N	602	HEA	CHC-C1C-C2C	-2.28	120.80	127.43
20	P	302	PGV	O14-P-O13	2.28	123.06	112.44
23	B	302	CHD	O26-C24-C23	2.28	121.20	114.00
19	Y	101	TGL	OG2-CB1-OB1	-2.28	118.39	123.70
20	N	607	PGV	O03-C01-C02	2.27	114.94	108.40
20	C	302	PGV	O01-C1-O02	-2.26	118.42	123.70
14	A	602	HEA	C16-C15-C14	2.26	126.23	121.17
25	T	101	PEK	O03-C21-O04	-2.26	117.98	123.63
20	P	302	PGV	O03-C19-C20	2.24	118.66	111.83
20	N	607	PGV	O01-C1-C2	2.24	116.32	111.48
23	G	104	CHD	C15-C16-C17	2.23	109.51	105.14
25	T	101	PEK	C23-C22-C21	-2.23	105.52	113.69
23	C	304	CHD	C22-C23-C24	-2.23	106.55	112.49
27	G	102	CDL	C42-C41-C40	2.23	125.62	114.37
23	J	101	CHD	C14-C8-C9	-2.22	106.64	109.75
23	B	302	CHD	C1-C2-C3	2.22	113.43	110.48
14	A	602	HEA	C4C-CHD-C1D	-2.22	121.03	126.25
23	W	101	CHD	C6-C5-C4	-2.22	108.69	111.23
19	L	101	TGL	OB1-CB1-CB2	-2.22	115.10	123.78
14	N	602	HEA	CMD-C2D-C3D	2.22	132.14	126.15
23	P	304	CHD	C6-C7-C8	2.21	113.92	111.50
19	N	609	TGL	CG3-OG3-CC1	2.21	125.21	117.12
23	J	101	CHD	C9-C10-C5	2.21	111.58	108.51
27	P	303	CDL	OA8-CA7-OA9	-2.21	118.11	123.63
19	N	609	TGL	CG3-CG2-CG1	-2.20	106.65	111.78
29	M	101	DMU	O49-C1-C2	-2.20	105.20	110.38
19	D	201	TGL	CG1-OG1-CA1	2.19	125.12	117.12
14	N	602	HEA	CAD-C3D-C4D	-2.18	120.91	124.70
27	T	102	CDL	OB8-CB7-C71	2.17	118.46	111.83
23	P	304	CHD	C23-C22-C20	-2.16	110.42	114.46
14	A	601	HEA	O1A-CGA-CBA	-2.16	116.23	123.09
14	N	601	HEA	C4C-C3C-C2C	-2.16	104.61	107.30
25	C	306	PEK	O01-C1-O02	-2.15	118.67	123.70
14	A	601	HEA	C13-C14-C15	-2.15	122.70	127.62
20	A	609	PGV	O03-C19-O04	-2.15	118.25	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	104	CHD	O3-C3-C4	-2.15	105.57	109.84
27	T	102	CDL	C83-C82-C81	2.14	125.21	114.37
23	W	101	CHD	C4-C3-C2	2.14	113.23	110.62
20	P	302	PGV	C01-O03-C19	2.14	124.92	117.12
20	A	609	PGV	C02-O01-C1	2.13	122.90	117.80
23	P	304	CHD	C1-C2-C3	2.13	113.31	110.48
29	Z	102	DMU	O5-C4-C57	2.13	111.72	106.44
19	A	607	TGL	OG1-CA1-OA1	-2.13	118.30	123.63
27	P	303	CDL	O1-C1-CB2	2.12	117.03	109.70
23	G	104	CHD	O12-C12-C13	-2.12	107.44	111.02
19	Q	201	TGL	OG1-CA1-OA1	-2.12	118.33	123.63
27	C	303	CDL	OB6-CB5-OB7	-2.11	118.76	123.70
14	N	602	HEA	C20-C19-C18	-2.11	116.43	121.17
20	A	608	PGV	C21-C20-C19	-2.11	105.98	113.69
19	L	101	TGL	CB6-CB5-CB4	-2.10	103.75	114.37
23	W	101	CHD	C15-C14-C8	2.10	121.24	118.36
27	C	303	CDL	OA8-CA7-OA9	-2.09	118.39	123.63
23	C	305	CHD	C5-C4-C3	2.09	115.86	112.71
20	A	609	PGV	C01-O03-C19	2.08	124.72	117.12
23	W	101	CHD	C1-C10-C5	2.08	110.73	107.75
29	Z	102	DMU	O7-C3-C2	2.08	112.52	107.23
23	P	304	CHD	C9-C10-C5	2.08	111.40	108.51
14	A	602	HEA	CHA-C1A-C2A	-2.08	121.58	124.86
14	A	601	HEA	CHC-C4B-C3B	-2.08	120.56	125.80
23	J	101	CHD	C16-C17-C13	2.07	105.55	103.54
14	A	602	HEA	O2D-CGD-O1D	-2.06	118.03	123.33
23	C	304	CHD	C6-C5-C4	-2.05	108.88	111.23
20	N	608	PGV	C02-O01-C1	2.05	122.70	117.80
23	C	304	CHD	C1-C10-C5	2.04	110.68	107.75
23	P	304	CHD	C1-C10-C5	2.04	110.67	107.75
23	J	101	CHD	C15-C14-C8	2.03	121.14	118.36
14	N	602	HEA	CHB-C1B-C2B	-2.03	121.83	125.03
23	W	101	CHD	C21-C20-C22	2.03	113.47	110.34
23	G	104	CHD	C21-C20-C17	2.03	115.92	112.88
27	G	102	CDL	OA8-CA7-OA9	-2.03	118.56	123.63
23	B	302	CHD	C13-C14-C8	-2.02	112.15	114.72
23	B	302	CHD	C22-C20-C17	2.02	114.52	110.33
20	C	302	PGV	O14-P-O13	2.02	121.85	112.44
23	P	305	CHD	C9-C10-C5	2.02	111.32	108.51
27	P	303	CDL	CB6-CB4-CB3	-2.02	107.08	111.78
14	A	602	HEA	C2D-C1D-ND	2.02	112.16	109.84
23	W	101	CHD	O26-C24-C23	2.02	120.38	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	101	CHD	C9-C8-C7	2.02	114.40	111.86
27	G	102	CDL	C23-C22-C21	2.02	124.56	114.37
23	J	101	CHD	O26-C24-O25	-2.01	118.16	123.33
14	A	601	HEA	C21-C20-C19	-2.01	106.53	113.19
14	N	601	HEA	CHC-C4B-NB	2.01	126.85	124.37
23	W	101	CHD	C11-C12-C13	2.00	113.30	111.26
27	T	102	CDL	C60-C59-C58	2.00	124.50	114.37
23	W	101	CHD	C14-C13-C12	2.00	109.25	107.42

There are no chirality outliers.

All (946) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602	HEA	C2A-C3A-CMA-OMA
14	N	601	HEA	C2A-C3A-CMA-OMA
14	N	602	HEA	C2A-C3A-CMA-OMA
14	N	602	HEA	C4A-C3A-CMA-OMA
19	D	201	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	OB1-CB1-OG2-CG2
19	Q	201	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	OB1-CB1-OG2-CG2
20	A	609	PGV	C02-C03-O11-P
20	A	609	PGV	C05-C04-O12-P
20	A	609	PGV	C2-C1-O01-C02
20	C	302	PGV	C12-C13-C14-C15
20	C	307	PGV	C03-O11-P-O13
20	C	307	PGV	O01-C02-C03-O11
20	C	307	PGV	O12-C04-C05-C06
20	C	307	PGV	C04-C05-C06-O06
20	N	608	PGV	C04-O12-P-O11
20	N	608	PGV	O01-C02-C03-O11
20	N	608	PGV	O02-C1-O01-C02
20	N	608	PGV	C2-C1-O01-C02
20	Z	101	PGV	O02-C1-O01-C02
20	Z	101	PGV	C2-C1-O01-C02
23	C	304	CHD	C13-C17-C20-C21
23	C	304	CHD	C16-C17-C20-C21
23	J	101	CHD	C13-C17-C20-C22
23	W	101	CHD	C13-C17-C20-C22
23	W	101	CHD	C16-C17-C20-C21
23	W	101	CHD	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
24	B	303	PSC	C03-O11-P-O12
24	O	302	PSC	O12-C04-C05-N
25	B	304	PEK	C03-O11-P-O12
25	B	304	PEK	C03-O11-P-O13
25	B	304	PEK	C04-O12-P-O11
25	C	306	PEK	C03-O11-P-O12
25	C	306	PEK	C03-O11-P-O13
25	C	306	PEK	O01-C02-C03-O11
25	C	306	PEK	O12-C04-C05-N
25	C	306	PEK	O02-C1-O01-C02
25	C	306	PEK	C2-C1-O01-C02
25	C	308	PEK	C03-O11-P-O13
25	C	308	PEK	O12-C04-C05-N
25	G	103	PEK	C03-O11-P-O12
25	G	103	PEK	C03-O11-P-O13
25	G	103	PEK	C03-O11-P-O14
25	G	103	PEK	C04-O12-P-O13
25	G	103	PEK	O01-C02-C03-O11
25	G	103	PEK	O02-C1-O01-C02
25	G	103	PEK	C2-C1-O01-C02
25	G	103	PEK	O04-C21-O03-C01
25	G	103	PEK	C22-C21-O03-C01
25	T	101	PEK	C9-C10-C11-C12
25	T	101	PEK	C12-C13-C14-C15
27	C	303	CDL	CA2-OA2-PA1-OA4
27	C	303	CDL	CA3-OA5-PA1-OA2
27	C	303	CDL	CA3-OA5-PA1-OA3
27	C	303	CDL	CA3-OA5-PA1-OA4
27	C	303	CDL	OA7-CA5-OA6-CA4
27	C	303	CDL	CB2-OB2-PB2-OB3
27	C	303	CDL	CB2-OB2-PB2-OB4
27	G	102	CDL	CA3-OA5-PA1-OA2
27	G	102	CDL	C1-CB2-OB2-PB2
27	G	102	CDL	CB2-OB2-PB2-OB4
27	G	102	CDL	CB2-OB2-PB2-OB5
27	G	102	CDL	CB3-OB5-PB2-OB2
27	G	102	CDL	CB3-OB5-PB2-OB3
27	P	303	CDL	C1-CA2-OA2-PA1
27	P	303	CDL	CA3-OA5-PA1-OA2
27	P	303	CDL	CA3-OA5-PA1-OA3
27	P	303	CDL	CA3-OA5-PA1-OA4
27	P	303	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
27	P	303	CDL	CB2-OB2-PB2-OB3
27	P	303	CDL	CB2-OB2-PB2-OB5
27	P	303	CDL	C51-CB5-OB6-CB4
27	P	303	CDL	CB4-CB6-OB8-CB7
27	T	102	CDL	CA2-OA2-PA1-OA4
27	T	102	CDL	C11-CA5-OA6-CA4
27	T	102	CDL	C1-CB2-OB2-PB2
25	C	308	PEK	C22-C21-O03-C01
20	Z	101	PGV	O04-C19-O03-C01
25	C	308	PEK	O04-C21-O03-C01
23	C	304	CHD	C16-C17-C20-C22
23	J	101	CHD	C16-C17-C20-C22
23	C	304	CHD	C13-C17-C20-C22
29	Z	102	DMU	O6-C11-C9-O1
19	D	201	TGL	OB1-CB1-OG2-CG2
19	Q	201	TGL	OB1-CB1-OG2-CG2
24	B	303	PSC	O02-C1-O01-C02
27	P	303	CDL	OA7-CA5-OA6-CA4
27	P	303	CDL	OB7-CB5-OB6-CB4
27	T	102	CDL	OA7-CA5-OA6-CA4
20	Z	101	PGV	C20-C19-O03-C01
27	G	102	CDL	C31-CA7-OA8-CA6
27	T	102	CDL	C71-CB7-OB8-CB6
19	Y	101	TGL	CB2-CB1-OG2-CG2
27	C	303	CDL	C11-CA5-OA6-CA4
27	P	303	CDL	C71-CB7-OB8-CB6
20	A	609	PGV	C10-C11-C12-C13
25	B	304	PEK	C4-C5-C6-C7
19	N	609	TGL	OC1-CC1-OG3-CG3
19	Q	201	TGL	OC1-CC1-OG3-CG3
24	O	302	PSC	O04-C19-O03-C01
27	G	102	CDL	OA9-CA7-OA8-CA6
20	A	609	PGV	O02-C1-O01-C02
19	Q	201	TGL	CC2-CC1-OG3-CG3
27	P	303	CDL	C31-CA7-OA8-CA6
24	B	303	PSC	C2-C1-O01-C02
27	G	102	CDL	C11-CA5-OA6-CA4
27	T	102	CDL	C51-CB5-OB6-CB4
23	C	304	CHD	C21-C20-C22-C23
27	T	102	CDL	OB9-CB7-OB8-CB6
19	L	101	TGL	CC1-CC2-CC3-CC4
19	N	609	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
24	O	302	PSC	C20-C19-O03-C01
27	P	303	CDL	OB9-CB7-OB8-CB6
29	Z	102	DMU	O6-C11-C9-C8
23	P	304	CHD	C21-C20-C22-C23
27	P	303	CDL	OA9-CA7-OA8-CA6
25	T	101	PEK	C22-C23-C24-C25
29	M	101	DMU	O6-C11-C9-O1
23	W	101	CHD	C17-C20-C22-C23
20	C	307	PGV	C10-C11-C12-C13
20	Z	101	PGV	C10-C11-C12-C13
24	O	302	PSC	C11-C10-C9-C8
25	C	306	PEK	C10-C11-C12-C13
25	T	101	PEK	C13-C14-C15-C16
27	T	102	CDL	C60-C61-C62-C63
27	T	102	CDL	CB7-C71-C72-C73
27	G	102	CDL	OA7-CA5-OA6-CA4
27	T	102	CDL	OB7-CB5-OB6-CB4
27	C	303	CDL	CB2-C1-CA2-OA2
19	D	201	TGL	CC2-CC1-OG3-CG3
19	N	609	TGL	CA2-CA1-OG1-CG1
19	Y	101	TGL	CA2-CA1-OG1-CG1
24	B	303	PSC	C20-C19-O03-C01
27	C	303	CDL	C71-CB7-OB8-CB6
19	L	101	TGL	CC3-CC4-CC5-CC6
23	C	304	CHD	C17-C20-C22-C23
29	M	101	DMU	O6-C11-C9-C8
19	N	609	TGL	CC3-CC4-CC5-CC6
19	L	101	TGL	CA1-CA2-CA3-CA4
27	C	303	CDL	O1-C1-CA2-OA2
24	B	303	PSC	C20-C21-C22-C23
14	N	602	HEA	C2D-C3D-CAD-CBD
27	C	303	CDL	OB9-CB7-OB8-CB6
23	P	304	CHD	C17-C20-C22-C23
27	G	102	CDL	OB6-CB4-CB6-OB8
19	A	607	TGL	CC2-CC1-OG3-CG3
27	G	102	CDL	C71-CB7-OB8-CB6
24	B	303	PSC	C11-C10-C9-C8
25	B	304	PEK	C13-C14-C15-C16
25	G	101	PEK	C7-C8-C9-C10
25	G	103	PEK	C7-C8-C9-C10
25	T	101	PEK	C10-C11-C12-C13
20	C	307	PGV	O05-C05-C06-O06

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Mol	Chain	Res	Type	Atoms
23	J	101	CHD	C16-C17-C20-C21
20	N	608	PGV	C1-C2-C3-C4
19	Y	101	TGL	OA1-CA1-OG1-CG1
27	T	102	CDL	C55-C56-C57-C58
19	A	607	TGL	CB1-CB2-CB3-CB4
19	Y	101	TGL	CC1-CC2-CC3-CC4
27	G	102	CDL	CB7-C71-C72-C73
19	D	201	TGL	OC1-CC1-OG3-CG3
19	N	609	TGL	OA1-CA1-OG1-CG1
20	Z	101	PGV	C19-C20-C21-C22
25	G	103	PEK	C1-C2-C3-C4
19	Y	101	TGL	CA9-C20-C21-C22
29	Z	102	DMU	O16-C18-C19-C22
20	C	302	PGV	O12-C04-C05-O05
27	C	303	CDL	O1-C1-CB2-OB2
27	P	303	CDL	O1-C1-CA2-OA2
27	T	102	CDL	O1-C1-CB2-OB2
19	A	607	TGL	CA2-CA1-OG1-CG1
19	A	607	TGL	OC1-CC1-OG3-CG3
24	B	303	PSC	O04-C19-O03-C01
25	C	308	PEK	C13-C14-C15-C16
20	A	608	PGV	C19-C20-C21-C22
20	P	302	PGV	C27-C28-C29-C30
27	G	102	CDL	C40-C41-C42-C43
19	N	609	TGL	OB1-CB1-OG2-CG2
27	P	303	CDL	CB2-C1-CA2-OA2
27	T	102	CDL	CA2-C1-CB2-OB2
19	A	607	TGL	CC9-C15-C16-C17
27	G	102	CDL	OB9-CB7-OB8-CB6
19	N	609	TGL	CB2-CB1-OG2-CG2
25	C	308	PEK	C2-C1-O01-C02
27	C	303	CDL	C51-CB5-OB6-CB4
24	O	302	PSC	O02-C1-O01-C02
25	C	308	PEK	O02-C1-O01-C02
27	C	303	CDL	OB7-CB5-OB6-CB4
23	W	101	CHD	C13-C17-C20-C21
25	B	304	PEK	C10-C11-C12-C13
25	G	101	PEK	C4-C5-C6-C7
25	G	101	PEK	C13-C14-C15-C16
25	G	103	PEK	C21-C22-C23-C24
20	N	608	PGV	C04-C05-C06-O06
27	T	102	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
24	O	302	PSC	C2-C1-O01-C02
20	C	307	PGV	C20-C19-O03-C01
20	C	302	PGV	C1-C2-C3-C4
19	A	607	TGL	OA1-CA1-OG1-CG1
19	D	201	TGL	CA6-CA7-CA8-CA9
19	D	201	TGL	C13-C14-C29-C30
19	N	609	TGL	C11-C12-C13-C14
25	G	101	PEK	C28-C29-C30-C31
19	A	607	TGL	CC4-CC5-CC6-CC7
19	A	607	TGL	C20-C21-C22-C23
19	Q	201	TGL	CC4-CC5-CC6-CC7
19	Y	101	TGL	C16-C15-CC9-CC8
20	C	307	PGV	C24-C25-C26-C27
20	C	307	PGV	C25-C26-C27-C28
24	B	303	PSC	C3-C4-C5-C6
25	G	103	PEK	C4-C5-C6-C7
25	G	103	PEK	C13-C14-C15-C16
25	T	101	PEK	C7-C8-C9-C10
25	G	103	PEK	C28-C29-C30-C31
19	A	607	TGL	CA7-CA8-CA9-C20
19	D	201	TGL	CA3-CA4-CA5-CA6
19	L	101	TGL	CA3-CA4-CA5-CA6
19	L	101	TGL	CA5-CA6-CA7-CA8
19	L	101	TGL	C16-C15-CC9-CC8
19	N	609	TGL	CA5-CA6-CA7-CA8
19	Q	201	TGL	C21-C20-CA9-CA8
20	C	307	PGV	C4-C5-C6-C7
27	C	303	CDL	C58-C59-C60-C61
27	P	303	CDL	C78-C79-C80-C81
19	A	607	TGL	C12-C13-C14-C29
19	N	609	TGL	CC2-CC3-CC4-CC5
19	Q	201	TGL	CA9-C20-C21-C22
19	Q	201	TGL	C21-C22-C23-C24
20	Z	101	PGV	C20-C21-C22-C23
20	Z	101	PGV	C21-C22-C23-C24
25	C	308	PEK	C30-C31-C32-C33
27	G	102	CDL	C35-C36-C37-C38
27	T	102	CDL	C32-C33-C34-C35
27	T	102	CDL	C78-C79-C80-C81
19	N	609	TGL	CA1-CA2-CA3-CA4
25	C	308	PEK	C29-C30-C31-C32
27	G	102	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
20	C	302	PGV	C24-C25-C26-C27
20	C	307	PGV	C6-C7-C8-C9
27	G	102	CDL	C51-CB5-OB6-CB4
19	N	609	TGL	CA2-CA3-CA4-CA5
19	Q	201	TGL	CA6-CA7-CA8-CA9
19	A	607	TGL	CC2-CC3-CC4-CC5
20	A	609	PGV	C4-C5-C6-C7
27	G	102	CDL	O1-C1-CB2-OB2
19	A	607	TGL	CC1-CC2-CC3-CC4
19	N	609	TGL	CC1-CC2-CC3-CC4
20	C	307	PGV	C1-C2-C3-C4
19	D	201	TGL	C11-C10-CB9-CB8
19	N	609	TGL	CA4-CA5-CA6-CA7
19	N	609	TGL	CB4-CB5-CB6-CB7
19	N	609	TGL	C18-C19-C33-C34
20	C	302	PGV	C14-C15-C16-C17
20	N	607	PGV	C23-C24-C25-C26
20	P	302	PGV	C13-C14-C15-C16
25	G	101	PEK	C31-C32-C33-C34
27	C	303	CDL	C17-C18-C19-C20
27	G	102	CDL	C11-C12-C13-C14
27	G	102	CDL	C13-C14-C15-C16
27	T	102	CDL	C73-C74-C75-C76
20	C	307	PGV	O04-C19-O03-C01
19	L	101	TGL	C21-C20-CA9-CA8
19	N	609	TGL	CC6-CC7-CC8-CC9
19	N	609	TGL	C17-C18-C19-C33
27	C	303	CDL	C37-C38-C39-C40
27	C	303	CDL	C38-C39-C40-C41
19	Y	101	TGL	CB4-CB5-CB6-CB7
25	G	101	PEK	C26-C27-C28-C29
19	Y	101	TGL	C21-C22-C23-C24
25	B	304	PEK	C24-C25-C26-C27
27	P	303	CDL	C82-C83-C84-C85
24	B	303	PSC	C21-C22-C23-C24
19	A	607	TGL	CA1-CA2-CA3-CA4
24	O	302	PSC	C1-C2-C3-C4
27	P	303	CDL	CA5-C11-C12-C13
19	A	607	TGL	CA9-C20-C21-C22
20	A	608	PGV	C30-C31-C32-C33
20	A	609	PGV	C7-C8-C9-C10
20	N	608	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	O	302	PSC	C30-C31-C32-C33
25	C	306	PEK	C29-C30-C31-C32
27	G	102	CDL	C80-C81-C82-C83
27	P	303	CDL	C22-C23-C24-C25
27	P	303	CDL	C43-C44-C45-C46
19	D	201	TGL	CC6-CC7-CC8-CC9
19	Y	101	TGL	C10-C11-C12-C13
20	C	307	PGV	C2-C3-C4-C5
20	N	608	PGV	C2-C3-C4-C5
27	P	303	CDL	C54-C55-C56-C57
27	P	303	CDL	C60-C61-C62-C63
27	P	303	CDL	C81-C82-C83-C84
21	A	611	EDO	O1-C1-C2-O2
21	N	611	EDO	O1-C1-C2-O2
21	P	307	EDO	O1-C1-C2-O2
21	T	103	EDO	O1-C1-C2-O2
19	L	101	TGL	C20-C21-C22-C23
19	N	609	TGL	C19-C33-C34-C35
25	G	103	PEK	C24-C25-C26-C27
24	B	303	PSC	C04-C05-N-C06
24	B	303	PSC	C04-C05-N-C08
19	N	609	TGL	C21-C22-C23-C24
25	C	308	PEK	C31-C32-C33-C34
25	T	101	PEK	C33-C34-C35-C36
27	C	303	CDL	C54-C55-C56-C57
27	G	102	CDL	C75-C76-C77-C78
19	A	607	TGL	C23-C24-C25-C26
19	N	609	TGL	C16-C15-CC9-CC8
27	T	102	CDL	C13-C14-C15-C16
19	D	201	TGL	C21-C22-C23-C24
19	Q	201	TGL	CA1-CA2-CA3-CA4
19	Y	101	TGL	C11-C12-C13-C14
19	L	101	TGL	CC4-CC5-CC6-CC7
20	N	608	PGV	C13-C14-C15-C16
25	B	304	PEK	C26-C27-C28-C29
25	C	306	PEK	C26-C27-C28-C29
27	G	102	CDL	OB7-CB5-OB6-CB4
19	L	101	TGL	C19-C33-C34-C35
19	Q	201	TGL	C20-C21-C22-C23
20	C	307	PGV	C3-C4-C5-C6
20	N	608	PGV	C30-C31-C32-C33
27	G	102	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	P	303	CDL	C80-C81-C82-C83
19	L	101	TGL	C24-C25-C26-C27
19	N	609	TGL	CA9-C20-C21-C22
24	O	302	PSC	C3-C4-C5-C6
25	B	304	PEK	C25-C26-C27-C28
27	P	303	CDL	C74-C75-C76-C77
27	T	102	CDL	C40-C41-C42-C43
27	T	102	CDL	C76-C77-C78-C79
19	D	201	TGL	CA9-C20-C21-C22
19	Y	101	TGL	CC5-CC6-CC7-CC8
19	Y	101	TGL	C22-C23-C24-C25
20	Z	101	PGV	C14-C15-C16-C17
20	N	607	PGV	C14-C15-C16-C17
24	O	302	PSC	C29-C30-C31-C32
27	P	303	CDL	C58-C59-C60-C61
19	D	201	TGL	C16-C15-CC9-CC8
19	N	609	TGL	CC4-CC5-CC6-CC7
20	C	307	PGV	C22-C23-C24-C25
19	N	609	TGL	CB6-CB7-CB8-CB9
19	Y	101	TGL	CB6-CB7-CB8-CB9
25	T	101	PEK	C28-C29-C30-C31
27	C	303	CDL	C60-C61-C62-C63
19	D	201	TGL	C12-C13-C14-C29
19	Y	101	TGL	CC7-CC8-CC9-C15
20	C	302	PGV	C26-C27-C28-C29
27	C	303	CDL	C51-C52-C53-C54
27	C	303	CDL	C62-C63-C64-C65
29	Z	102	DMU	C28-C31-C34-C37
19	A	607	TGL	CA5-CA6-CA7-CA8
19	A	607	TGL	C11-C10-CB9-CB8
20	C	307	PGV	C14-C15-C16-C17
20	N	607	PGV	C29-C30-C31-C32
20	Z	101	PGV	C29-C30-C31-C32
25	C	306	PEK	C33-C34-C35-C36
27	T	102	CDL	C19-C20-C21-C22
27	T	102	CDL	C43-C44-C45-C46
27	P	303	CDL	C36-C37-C38-C39
23	J	101	CHD	C13-C17-C20-C21
20	C	307	PGV	C2-C1-O01-C02
27	P	303	CDL	C18-C19-C20-C21
19	A	607	TGL	CB6-CB7-CB8-CB9
19	N	609	TGL	CA7-CA8-CA9-C20

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Mol	Chain	Res	Type	Atoms
25	B	304	PEK	C22-C23-C24-C25
20	A	608	PGV	C12-C13-C14-C15
20	C	302	PGV	C11-C10-C9-C8
20	N	607	PGV	C12-C13-C14-C15
24	O	302	PSC	C6-C7-C8-C9
25	G	103	PEK	C2-C3-C4-C5
25	G	103	PEK	C15-C16-C17-C18
25	T	101	PEK	C15-C16-C17-C18
24	O	302	PSC	C20-C21-C22-C23
25	C	308	PEK	C27-C28-C29-C30
25	G	103	PEK	C23-C24-C25-C26
27	T	102	CDL	C12-C13-C14-C15
25	C	306	PEK	C4-C5-C6-C7
25	C	306	PEK	C13-C14-C15-C16
19	L	101	TGL	C13-C14-C29-C30
27	P	303	CDL	C42-C43-C44-C45
24	B	303	PSC	C04-C05-N-C07
19	D	201	TGL	C20-C21-C22-C23
19	Q	201	TGL	CB6-CB7-CB8-CB9
20	A	608	PGV	C29-C30-C31-C32
27	G	102	CDL	C17-C18-C19-C20
20	A	608	PGV	C23-C24-C25-C26
27	P	303	CDL	C37-C38-C39-C40
19	L	101	TGL	C22-C23-C24-C25
27	P	303	CDL	C61-C62-C63-C64
20	A	609	PGV	C20-C19-O03-C01
27	P	303	CDL	CB5-C51-C52-C53
20	N	608	PGV	C4-C5-C6-C7
20	Z	101	PGV	C27-C28-C29-C30
25	G	101	PEK	C23-C24-C25-C26
27	P	303	CDL	C79-C80-C81-C82
20	C	307	PGV	O02-C1-O01-C02
25	C	308	PEK	O01-C02-C03-O11
19	L	101	TGL	CA9-C20-C21-C22
20	A	609	PGV	C2-C3-C4-C5
27	P	303	CDL	C11-C12-C13-C14
19	L	101	TGL	CC5-CC6-CC7-CC8
19	Y	101	TGL	CC4-CC5-CC6-CC7
27	G	102	CDL	C57-C58-C59-C60
29	M	101	DMU	C25-C28-C31-C34
25	B	304	PEK	O03-C01-C02-O01
25	C	308	PEK	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
25	G	101	PEK	C15-C16-C17-C18
19	D	201	TGL	C17-C18-C19-C33
19	L	101	TGL	C11-C12-C13-C14
27	C	303	CDL	C63-C64-C65-C66
27	P	303	CDL	C56-C57-C58-C59
19	L	101	TGL	C23-C24-C25-C26
20	A	608	PGV	C14-C15-C16-C17
20	P	302	PGV	C26-C27-C28-C29
27	G	102	CDL	C52-C53-C54-C55
19	D	201	TGL	C10-C11-C12-C13
20	P	302	PGV	C7-C8-C9-C10
27	C	303	CDL	C11-C12-C13-C14
27	T	102	CDL	C22-C23-C24-C25
19	Y	101	TGL	CB2-CB3-CB4-CB5
19	Y	101	TGL	C13-C14-C29-C30
20	C	307	PGV	C27-C28-C29-C30
27	C	303	CDL	C16-C17-C18-C19
27	P	303	CDL	C14-C15-C16-C17
19	L	101	TGL	CB5-CB6-CB7-CB8
14	N	602	HEA	C4D-C3D-CAD-CBD
20	C	302	PGV	O12-C04-C05-C06
20	C	302	PGV	C27-C28-C29-C30
20	C	307	PGV	C30-C31-C32-C33
24	O	302	PSC	C21-C22-C23-C24
25	B	304	PEK	C34-C35-C36-C37
25	G	101	PEK	C16-C17-C18-C19
27	C	303	CDL	C33-C34-C35-C36
23	P	304	CHD	C20-C22-C23-C24
29	Z	102	DMU	C19-C22-C25-C28
27	C	303	CDL	CA4-CA6-OA8-CA7
27	C	303	CDL	C80-C81-C82-C83
19	D	201	TGL	C21-C20-CA9-CA8
25	T	101	PEK	C27-C28-C29-C30
27	P	303	CDL	C19-C20-C21-C22
20	N	608	PGV	O05-C05-C06-O06
19	A	607	TGL	CC5-CC6-CC7-CC8
19	D	201	TGL	C19-C33-C34-C35
27	T	102	CDL	C75-C76-C77-C78
24	O	302	PSC	C13-C14-C15-C16
27	T	102	CDL	C42-C43-C44-C45
20	C	307	PGV	C01-C02-C03-O11
25	C	306	PEK	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
25	C	308	PEK	C01-C02-C03-O11
27	C	303	CDL	OB5-CB3-CB4-CB6
27	P	303	CDL	OB5-CB3-CB4-CB6
19	L	101	TGL	C12-C13-C14-C29
27	G	102	CDL	C16-C17-C18-C19
20	Z	101	PGV	C4-C5-C6-C7
24	B	303	PSC	C30-C31-C32-C33
19	Y	101	TGL	C25-C26-C27-C28
27	T	102	CDL	C34-C35-C36-C37
20	A	609	PGV	O04-C19-O03-C01
20	A	608	PGV	C26-C27-C28-C29
27	C	303	CDL	C74-C75-C76-C77
29	M	101	DMU	C22-C25-C28-C31
27	P	303	CDL	C34-C35-C36-C37
20	A	608	PGV	C10-C11-C12-C13
19	A	607	TGL	C21-C22-C23-C24
19	A	607	TGL	OG1-CG1-CG2-CG3
19	L	101	TGL	OG1-CG1-CG2-CG3
19	Y	101	TGL	OG1-CG1-CG2-CG3
27	C	303	CDL	CB3-CB4-CB6-OB8
27	G	102	CDL	CB3-CB4-CB6-OB8
19	Q	201	TGL	C11-C10-CB9-CB8
27	T	102	CDL	C54-C55-C56-C57
20	Z	101	PGV	C11-C10-C9-C8
25	C	308	PEK	C15-C16-C17-C18
27	C	303	CDL	C73-C74-C75-C76
25	C	308	PEK	C21-C22-C23-C24
19	N	609	TGL	C20-C21-C22-C23
19	Y	101	TGL	C17-C18-C19-C33
20	C	307	PGV	C23-C24-C25-C26
25	C	308	PEK	C25-C26-C27-C28
27	C	303	CDL	C18-C19-C20-C21
27	C	303	CDL	C23-C24-C25-C26
21	A	612	EDO	O1-C1-C2-O2
21	C	311	EDO	O1-C1-C2-O2
21	K	103	EDO	O1-C1-C2-O2
20	A	609	PGV	C21-C22-C23-C24
24	B	303	PSC	C5-C6-C7-C8
20	N	607	PGV	C13-C14-C15-C16
19	L	101	TGL	C18-C19-C33-C34
19	A	607	TGL	C11-C12-C13-C14
27	G	102	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	CG1-CG2-OG2-CB1
20	A	609	PGV	C03-C02-O01-C1
25	G	103	PEK	C31-C32-C33-C34
27	G	102	CDL	C55-C56-C57-C58
27	G	102	CDL	C63-C64-C65-C66
27	P	303	CDL	C33-C34-C35-C36
20	A	609	PGV	C25-C26-C27-C28
20	C	302	PGV	C25-C26-C27-C28
20	N	608	PGV	C20-C21-C22-C23
20	Z	101	PGV	C13-C14-C15-C16
25	B	304	PEK	C33-C34-C35-C36
27	G	102	CDL	C61-C62-C63-C64
27	G	102	CDL	C72-C73-C74-C75
19	Q	201	TGL	CA2-CA3-CA4-CA5
19	Q	201	TGL	C10-C11-C12-C13
27	T	102	CDL	C36-C37-C38-C39
20	A	608	PGV	C4-C5-C6-C7
27	T	102	CDL	C31-C32-C33-C34
19	N	609	TGL	C29-C30-C31-C32
27	P	303	CDL	OB5-CB3-CB4-OB6
20	A	608	PGV	C31-C32-C33-C34
25	C	306	PEK	C31-C32-C33-C34
19	D	201	TGL	CA2-CA3-CA4-CA5
19	Y	101	TGL	CA5-CA6-CA7-CA8
19	N	609	TGL	C15-C16-C17-C18
27	C	303	CDL	C34-C35-C36-C37
27	P	303	CDL	C71-C72-C73-C74
20	P	302	PGV	C29-C30-C31-C32
24	O	302	PSC	C31-C32-C33-C34
27	P	303	CDL	C84-C85-C86-C87
20	P	302	PGV	C25-C26-C27-C28
27	C	303	CDL	C71-C72-C73-C74
23	G	104	CHD	C17-C20-C22-C23
20	C	307	PGV	C13-C14-C15-C16
25	T	101	PEK	C34-C35-C36-C37
27	P	303	CDL	C52-C51-CB5-OB6
25	G	101	PEK	C35-C36-C37-C38
20	C	307	PGV	C12-C13-C14-C15
19	Q	201	TGL	C13-C14-C29-C30
20	Z	101	PGV	C31-C32-C33-C34
20	C	302	PGV	C23-C24-C25-C26
27	G	102	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
27	T	102	CDL	C53-C54-C55-C56
25	T	101	PEK	C17-C18-C19-C20
19	A	607	TGL	C33-C34-C35-C36
19	D	201	TGL	C29-C30-C31-C32
29	M	101	DMU	C34-C37-C40-C43
25	C	306	PEK	C30-C31-C32-C33
25	G	101	PEK	C32-C33-C34-C35
25	T	101	PEK	C30-C31-C32-C33
27	G	102	CDL	C59-C60-C61-C62
20	C	302	PGV	C31-C32-C33-C34
25	B	304	PEK	C17-C18-C19-C20
27	P	303	CDL	C44-C45-C46-C47
19	D	201	TGL	CB1-CB2-CB3-CB4
25	T	101	PEK	C4-C5-C6-C7
19	Y	101	TGL	C12-C13-C14-C29
19	L	101	TGL	CA4-CA5-CA6-CA7
19	N	609	TGL	C10-C11-C12-C13
20	Z	101	PGV	C24-C25-C26-C27
25	B	304	PEK	C29-C30-C31-C32
20	C	302	PGV	C02-C03-O11-P
27	C	303	CDL	C1-CA2-OA2-PA1
27	G	102	CDL	CB4-CB3-OB5-PB2
20	Z	101	PGV	C3-C4-C5-C6
20	Z	101	PGV	C2-C3-C4-C5
25	G	101	PEK	C30-C31-C32-C33
24	O	302	PSC	C2-C3-C4-C5
27	P	303	CDL	C40-C41-C42-C43
19	N	609	TGL	C25-C26-C27-C28
20	C	307	PGV	C31-C32-C33-C34
25	C	308	PEK	C17-C18-C19-C20
20	A	609	PGV	C01-C02-C03-O11
24	B	303	PSC	C01-C02-C03-O11
25	B	304	PEK	C01-C02-C03-O11
25	G	103	PEK	C01-C02-C03-O11
27	P	303	CDL	OA5-CA3-CA4-CA6
25	B	304	PEK	C28-C29-C30-C31
27	C	303	CDL	C75-C76-C77-C78
27	T	102	CDL	C72-C73-C74-C75
25	G	103	PEK	C35-C36-C37-C38
20	C	302	PGV	C15-C16-C17-C18
27	T	102	CDL	C59-C60-C61-C62
19	N	609	TGL	CB2-CB3-CB4-CB5

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	C17-C18-C19-C33
25	B	304	PEK	C27-C28-C29-C30
25	B	304	PEK	O03-C01-C02-C03
27	C	303	CDL	CA3-CA4-CA6-OA8
27	G	102	CDL	CA3-CA4-CA6-OA8
27	G	102	CDL	C64-C65-C66-C67
27	P	303	CDL	C24-C25-C26-C27
25	B	304	PEK	C1-C2-C3-C4
20	A	609	PGV	C31-C32-C33-C34
25	C	306	PEK	C25-C26-C27-C28
21	I	101	EDO	O1-C1-C2-O2
21	L	103	EDO	O1-C1-C2-O2
19	Q	201	TGL	C17-C18-C19-C33
25	B	304	PEK	C16-C17-C18-C19
19	Y	101	TGL	CB5-CB6-CB7-CB8
27	C	303	CDL	C77-C78-C79-C80
19	N	609	TGL	CB1-CB2-CB3-CB4
25	B	304	PEK	O01-C02-C03-O11
27	C	303	CDL	OB5-CB3-CB4-OB6
25	G	101	PEK	C17-C18-C19-C20
25	B	304	PEK	C15-C16-C17-C18
27	P	303	CDL	CA4-CA3-OA5-PA1
19	D	201	TGL	CC3-CC4-CC5-CC6
27	T	102	CDL	C77-C78-C79-C80
20	N	608	PGV	C21-C22-C23-C24
25	G	103	PEK	C25-C26-C27-C28
20	A	608	PGV	C25-C26-C27-C28
19	Q	201	TGL	C16-C15-CC9-CC8
27	C	303	CDL	C15-C16-C17-C18
27	G	102	CDL	C42-C43-C44-C45
25	C	306	PEK	C1-C2-C3-C4
19	A	607	TGL	OG1-CG1-CG2-OG2
19	D	201	TGL	OG2-CG2-CG3-OG3
19	Y	101	TGL	OG1-CG1-CG2-OG2
19	Y	101	TGL	OG2-CG2-CG3-OG3
20	A	609	PGV	O03-C01-C02-O01
27	C	303	CDL	OB6-CB4-CB6-OB8
27	G	102	CDL	OA6-CA4-CA6-OA8
27	P	303	CDL	OA6-CA4-CA6-OA8
27	P	303	CDL	OB6-CB4-CB6-OB8
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
25	B	304	PEK	C9-C10-C11-C12
25	B	304	PEK	C11-C12-C13-C14
25	C	306	PEK	C5-C6-C7-C8
25	C	306	PEK	C11-C10-C9-C8
25	C	306	PEK	C9-C10-C11-C12
25	C	306	PEK	C11-C12-C13-C14
25	C	308	PEK	C11-C10-C9-C8
25	C	308	PEK	C9-C10-C11-C12
25	C	308	PEK	C12-C13-C14-C15
25	G	101	PEK	C6-C7-C8-C9
25	G	103	PEK	C11-C10-C9-C8
25	G	103	PEK	C11-C12-C13-C14
25	G	103	PEK	C12-C13-C14-C15
25	T	101	PEK	C6-C7-C8-C9
25	T	101	PEK	C11-C10-C9-C8
19	N	609	TGL	C24-C25-C26-C27
24	B	303	PSC	C14-C15-C16-C17
27	T	102	CDL	C35-C36-C37-C38
25	G	101	PEK	C24-C25-C26-C27
19	Y	101	TGL	C14-C29-C30-C31
19	Q	201	TGL	CB1-CB2-CB3-CB4
20	P	302	PGV	C12-C13-C14-C15
19	Q	201	TGL	C16-C17-C18-C19
19	Y	101	TGL	CB9-C10-C11-C12
20	C	307	PGV	C29-C30-C31-C32
27	G	102	CDL	C76-C77-C78-C79
20	Z	101	PGV	C7-C8-C9-C10
29	M	101	DMU	C28-C31-C34-C37
20	N	607	PGV	C15-C16-C17-C18
20	Z	101	PGV	O05-C05-C06-O06
25	G	103	PEK	C29-C30-C31-C32
24	B	303	PSC	C25-C26-C27-C28
25	T	101	PEK	C26-C27-C28-C29
19	Q	201	TGL	C12-C13-C14-C29
20	N	608	PGV	C25-C26-C27-C28
25	T	101	PEK	C2-C3-C4-C5
27	P	303	CDL	C12-C13-C14-C15
20	N	608	PGV	C01-C02-C03-O11
27	C	303	CDL	C61-C62-C63-C64
19	L	101	TGL	C10-C11-C12-C13
23	W	101	CHD	C21-C20-C22-C23
19	Y	101	TGL	CC2-CC3-CC4-CC5

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Mol	Chain	Res	Type	Atoms
24	B	303	PSC	C26-C27-C28-C29
19	D	201	TGL	C33-C34-C35-C36
19	Y	101	TGL	C23-C24-C25-C26
20	Z	101	PGV	C25-C26-C27-C28
20	A	608	PGV	C21-C22-C23-C24
19	L	101	TGL	C21-C22-C23-C24
19	A	607	TGL	CA2-CA3-CA4-CA5
27	T	102	CDL	C79-C80-C81-C82
19	D	201	TGL	CG1-CG2-CG3-OG3
25	G	103	PEK	O03-C01-C02-C03
27	P	303	CDL	CA3-CA4-CA6-OA8
27	P	303	CDL	CB3-CB4-CB6-OB8
19	Q	201	TGL	C33-C34-C35-C36
24	B	303	PSC	C31-C32-C33-C34
25	G	101	PEK	C05-C04-O12-P
21	L	102	EDO	O1-C1-C2-O2
19	N	609	TGL	OG2-CG2-CG3-OG3
24	B	303	PSC	O03-C01-C02-O01
25	G	103	PEK	O03-C01-C02-O01
27	C	303	CDL	C84-C85-C86-C87
25	T	101	PEK	C23-C24-C25-C26
27	G	102	CDL	C62-C63-C64-C65
27	T	102	CDL	C15-C16-C17-C18
27	T	102	CDL	C71-C72-C73-C74
20	P	302	PGV	C30-C31-C32-C33
27	C	303	CDL	C31-C32-C33-C34
24	B	303	PSC	C02-C03-O11-P
25	C	308	PEK	C32-C33-C34-C35
19	Q	201	TGL	CA3-CA4-CA5-CA6
20	A	609	PGV	C24-C25-C26-C27
27	P	303	CDL	C38-C39-C40-C41
20	A	608	PGV	C15-C16-C17-C18
19	Q	201	TGL	C18-C19-C33-C34
19	N	609	TGL	C33-C34-C35-C36
27	C	303	CDL	C83-C84-C85-C86
19	N	609	TGL	C16-C17-C18-C19
27	P	303	CDL	C31-C32-C33-C34
19	D	201	TGL	CC2-CC3-CC4-CC5
20	N	608	PGV	C6-C7-C8-C9
27	C	303	CDL	C19-C20-C21-C22
27	C	303	CDL	C40-C41-C42-C43
25	B	304	PEK	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	B	303	PSC	C4-C5-C6-C7
19	L	101	TGL	CA7-CA8-CA9-C20
27	G	102	CDL	C1-CA2-OA2-PA1
27	T	102	CDL	C38-C39-C40-C41
27	C	303	CDL	C78-C79-C80-C81
24	B	303	PSC	O01-C02-C03-O11
25	G	101	PEK	C1-C2-C3-C4
14	A	602	HEA	C4A-C3A-CMA-OMA
14	N	601	HEA	C4A-C3A-CMA-OMA
20	Z	101	PGV	C1-C2-C3-C4
19	Y	101	TGL	C11-C10-CB9-CB8
19	L	101	TGL	OG1-CG1-CG2-OG2
24	O	302	PSC	O03-C01-C02-O01
27	C	303	CDL	OA6-CA4-CA6-OA8
19	A	607	TGL	CC3-CC4-CC5-CC6
19	Y	101	TGL	CG1-CG2-CG3-OG3
24	O	302	PSC	O03-C01-C02-C03
25	C	308	PEK	O03-C01-C02-C03
20	N	607	PGV	C11-C10-C9-C8
19	Q	201	TGL	C15-C16-C17-C18
20	A	608	PGV	C20-C21-C22-C23
19	L	101	TGL	CB7-CB8-CB9-C10
19	N	609	TGL	CA3-CA4-CA5-CA6
20	C	302	PGV	C13-C14-C15-C16
20	N	608	PGV	C15-C16-C17-C18
27	T	102	CDL	C16-C17-C18-C19
20	C	307	PGV	C03-O11-P-O12
20	N	608	PGV	C04-O12-P-O13
20	Z	101	PGV	C03-O11-P-O12
20	Z	101	PGV	C03-O11-P-O13
20	Z	101	PGV	C03-O11-P-O14
24	B	303	PSC	C03-O11-P-O14
24	O	302	PSC	C03-O11-P-O14
25	B	304	PEK	C03-O11-P-O14
25	B	304	PEK	C04-O12-P-O14
25	B	304	PEK	O12-C04-C05-N
25	C	308	PEK	C03-O11-P-O12
25	G	103	PEK	C04-O12-P-O11
25	G	103	PEK	C04-O12-P-O14
27	C	303	CDL	CB2-OB2-PB2-OB5
27	G	102	CDL	CA3-OA5-PA1-OA3
27	G	102	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
27	T	102	CDL	CA2-OA2-PA1-OA3
27	T	102	CDL	CA2-OA2-PA1-OA5
27	T	102	CDL	CA3-OA5-PA1-OA3
27	T	102	CDL	CB2-OB2-PB2-OB3
27	T	102	CDL	CB3-OB5-PB2-OB3
27	G	102	CDL	C41-C42-C43-C44
19	Q	201	TGL	CA4-CA5-CA6-CA7
20	C	302	PGV	C05-C04-O12-P
20	P	302	PGV	C02-C03-O11-P
25	G	101	PEK	C21-C22-C23-C24
19	N	609	TGL	C21-C20-CA9-CA8
27	G	102	CDL	C20-C21-C22-C23
25	C	308	PEK	C35-C36-C37-C38
27	G	102	CDL	C54-C55-C56-C57
27	P	303	CDL	C16-C17-C18-C19
27	C	303	CDL	C22-C23-C24-C25
25	G	101	PEK	C10-C11-C12-C13
20	A	609	PGV	O01-C02-C03-O11
27	P	303	CDL	OA5-CA3-CA4-OA6
20	C	302	PGV	C22-C23-C24-C25
27	T	102	CDL	C41-C42-C43-C44
19	A	607	TGL	C14-C29-C30-C31
24	O	302	PSC	C22-C23-C24-C25
29	Z	102	DMU	C31-C34-C37-C40
25	T	101	PEK	C31-C32-C33-C34
20	C	302	PGV	C10-C11-C12-C13
25	T	101	PEK	O03-C21-C22-C23
19	Y	101	TGL	CA1-CA2-CA3-CA4
25	C	308	PEK	C1-C2-C3-C4
20	A	608	PGV	C6-C7-C8-C9
27	C	303	CDL	C43-C44-C45-C46
20	A	609	PGV	O03-C01-C02-C03
27	P	303	CDL	C76-C77-C78-C79
27	P	303	CDL	C75-C76-C77-C78
27	G	102	CDL	C31-C32-C33-C34
20	N	607	PGV	C31-C32-C33-C34
27	P	303	CDL	C52-C53-C54-C55
29	M	101	DMU	O16-C18-C19-C22
27	T	102	CDL	C57-C58-C59-C60
19	A	607	TGL	C16-C15-CC9-CC8
19	A	607	TGL	OB1-CB1-OG2-CG2
20	A	609	PGV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	C	308	PEK	C28-C29-C30-C31
27	C	303	CDL	C59-C60-C61-C62
19	Y	101	TGL	CA4-CA5-CA6-CA7
23	P	305	CHD	C16-C17-C20-C22
23	J	101	CHD	C22-C23-C24-O26
19	A	607	TGL	C24-C25-C26-C27
19	Q	201	TGL	CC6-CC7-CC8-CC9
20	A	609	PGV	C1-C2-C3-C4
25	G	103	PEK	C32-C33-C34-C35
19	A	607	TGL	CC6-CC7-CC8-CC9
14	A	602	HEA	C26-C15-C16-C17
19	D	201	TGL	OG2-CB1-CB2-CB3
27	C	303	CDL	CA2-C1-CB2-OB2
23	B	302	CHD	C22-C23-C24-O26
23	W	101	CHD	C22-C23-C24-O25
19	N	609	TGL	OG1-CG1-CG2-CG3
23	B	302	CHD	C22-C23-C24-O25
23	C	304	CHD	C22-C23-C24-O25
23	J	101	CHD	C22-C23-C24-O25
23	G	104	CHD	C22-C23-C24-O26
20	N	607	PGV	O03-C19-C20-C21
14	A	602	HEA	CAD-CBD-CGD-O1D
20	P	302	PGV	O05-C05-C06-O06
20	A	609	PGV	C15-C16-C17-C18
14	N	602	HEA	CAD-CBD-CGD-O2D
20	C	307	PGV	O12-C04-C05-O05
14	A	601	HEA	CAD-CBD-CGD-O1D
27	G	102	CDL	C74-C75-C76-C77
27	C	303	CDL	CA4-CA3-OA5-PA1
23	G	104	CHD	C22-C23-C24-O25
19	Q	201	TGL	C11-C12-C13-C14
27	P	303	CDL	C52-C51-CB5-OB7
19	A	607	TGL	CB7-CB8-CB9-C10
27	P	303	CDL	C62-C63-C64-C65
20	P	302	PGV	C9-C10-C11-C12
25	B	304	PEK	C5-C6-C7-C8
25	B	304	PEK	C6-C7-C8-C9
25	B	304	PEK	C11-C10-C9-C8
25	B	304	PEK	C12-C13-C14-C15
19	Q	201	TGL	CC7-CC8-CC9-C15
27	G	102	CDL	C32-C33-C34-C35
23	W	101	CHD	C22-C23-C24-O26

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	C22-C23-C24-C25
24	O	302	PSC	C23-C24-C25-C26
27	C	303	CDL	C35-C36-C37-C38
14	N	602	HEA	C26-C15-C16-C17
19	Y	101	TGL	OG1-CA1-CA2-CA3
20	A	608	PGV	O03-C19-C20-C21
14	N	601	HEA	CAD-CBD-CGD-O1D
20	C	302	PGV	C29-C30-C31-C32
19	N	609	TGL	CC5-CC6-CC7-CC8
20	A	608	PGV	C7-C8-C9-C10
25	G	103	PEK	C26-C27-C28-C29
27	G	102	CDL	C60-C61-C62-C63
27	G	102	CDL	C24-C25-C26-C27
27	T	102	CDL	C44-C45-C46-C47
24	O	302	PSC	C24-C25-C26-C27
27	T	102	CDL	C37-C38-C39-C40
14	N	601	HEA	CAD-CBD-CGD-O2D
27	T	102	CDL	C52-C53-C54-C55
14	A	602	HEA	C14-C15-C16-C17
19	Q	201	TGL	CB3-CB4-CB5-CB6
20	A	609	PGV	C22-C23-C24-C25
27	T	102	CDL	C39-C40-C41-C42
23	C	304	CHD	C22-C23-C24-O26
20	N	608	PGV	C5-C6-C7-C8
21	K	102	EDO	O1-C1-C2-O2
14	A	601	HEA	CAD-CBD-CGD-O2D
20	P	302	PGV	C10-C11-C12-C13
27	C	303	CDL	C36-C37-C38-C39
14	N	602	HEA	CAD-CBD-CGD-O1D
19	Y	101	TGL	CA7-CA8-CA9-C20
27	C	303	CDL	C82-C83-C84-C85
19	L	101	TGL	CB4-CB5-CB6-CB7
23	B	302	CHD	C17-C20-C22-C23
20	A	609	PGV	O03-C19-C20-C21
20	A	609	PGV	C20-C21-C22-C23
27	P	303	CDL	C51-C52-C53-C54
14	A	602	HEA	CAD-CBD-CGD-O2D
20	C	302	PGV	C30-C31-C32-C33
20	N	607	PGV	C21-C22-C23-C24
20	Z	101	PGV	C9-C10-C11-C12
27	G	102	CDL	C77-C78-C79-C80
20	N	608	PGV	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
20	A	609	PGV	C04-C05-C06-O06
23	P	305	CHD	C22-C23-C24-O26
24	O	302	PSC	C25-C26-C27-C28
19	L	101	TGL	CC2-CC3-CC4-CC5
20	N	608	PGV	C11-C12-C13-C14
24	B	303	PSC	C12-C13-C14-C15
25	C	306	PEK	C3-C4-C5-C6
23	J	101	CHD	C17-C20-C22-C23
27	P	303	CDL	C63-C64-C65-C66
20	C	307	PGV	C20-C21-C22-C23
19	D	201	TGL	CB2-CB3-CB4-CB5
19	L	101	TGL	CC9-C15-C16-C17
27	G	102	CDL	CA2-C1-CB2-OB2
25	G	101	PEK	C34-C35-C36-C37
24	B	303	PSC	O03-C01-C02-C03
20	C	307	PGV	C5-C6-C7-C8
25	G	103	PEK	C27-C28-C29-C30
20	Z	101	PGV	O01-C1-C2-C3
25	T	101	PEK	C24-C25-C26-C27
19	L	101	TGL	CB3-CB4-CB5-CB6
21	C	312	EDO	O1-C1-C2-O2
20	Z	101	PGV	O03-C01-C02-O01
25	C	306	PEK	C16-C17-C18-C19
20	N	607	PGV	C11-C12-C13-C14
20	Z	101	PGV	O03-C19-C20-C21
24	B	303	PSC	O01-C1-C2-C3
27	T	102	CDL	C33-C34-C35-C36
19	A	607	TGL	CB2-CB1-OG2-CG2
20	A	608	PGV	C11-C12-C13-C14
25	B	304	PEK	C3-C4-C5-C6
25	B	304	PEK	O01-C1-C2-C3
19	Q	201	TGL	OG1-CA1-CA2-CA3
20	A	608	PGV	C27-C28-C29-C30
25	G	103	PEK	O03-C21-C22-C23
19	Q	201	TGL	OG3-CC1-CC2-CC3
14	N	602	HEA	CAA-CBA-CGA-O1A
25	C	308	PEK	C33-C34-C35-C36
25	G	101	PEK	C25-C26-C27-C28
25	C	306	PEK	O01-C1-C2-C3
20	N	608	PGV	C26-C27-C28-C29
27	C	303	CDL	C41-C42-C43-C44
27	C	303	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
20	Z	101	PGV	O03-C01-C02-C03
27	P	303	CDL	C72-C71-CB7-OB8
20	A	609	PGV	C3-C4-C5-C6
25	C	308	PEK	C23-C24-C25-C26
20	A	608	PGV	C28-C29-C30-C31
14	N	602	HEA	CAA-CBA-CGA-O2A
23	P	305	CHD	C22-C23-C24-O25
25	C	308	PEK	C22-C23-C24-C25
27	C	303	CDL	C31-CA7-OA8-CA6
23	P	304	CHD	C22-C23-C24-O26
20	A	609	PGV	C9-C10-C11-C12
25	B	304	PEK	O02-C1-C2-C3
19	Q	201	TGL	OA1-CA1-CA2-CA3
27	P	303	CDL	C72-C71-CB7-OB9
19	Y	101	TGL	C20-C21-C22-C23
19	D	201	TGL	OG1-CA1-CA2-CA3
27	P	303	CDL	C12-C11-CA5-OA6
25	C	308	PEK	C3-C4-C5-C6
20	Z	101	PGV	O02-C1-C2-C3
24	B	303	PSC	O02-C1-C2-C3
29	Z	102	DMU	C18-C19-C22-C25
14	A	601	HEA	C4A-C3A-CMA-OMA
27	G	102	CDL	C32-C31-CA7-OA8
14	A	601	HEA	CAA-CBA-CGA-O2A
25	G	103	PEK	O04-C21-C22-C23
20	Z	101	PGV	O04-C19-C20-C21
25	C	306	PEK	O02-C1-C2-C3
20	C	307	PGV	C05-C04-O12-P
19	Q	201	TGL	OC1-CC1-CC2-CC3
27	C	303	CDL	C52-C51-CB5-OB6
27	G	102	CDL	C23-C24-C25-C26
27	T	102	CDL	C52-C51-CB5-OB6
27	T	102	CDL	C72-C71-CB7-OB8
19	N	609	TGL	OG1-CA1-CA2-CA3
27	P	303	CDL	C15-C16-C17-C18

There are no ring outliers.

46 monomers are involved in 199 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	Z	102	DMU	1	0
20	N	608	PGV	5	0

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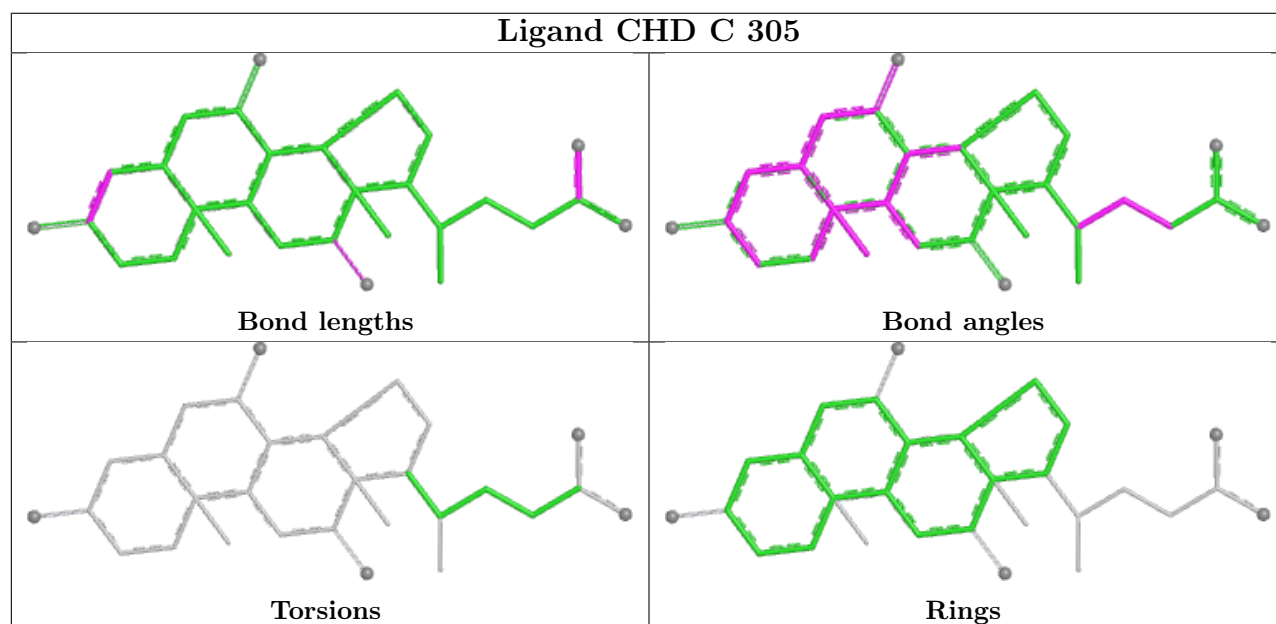
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	F	102	EDO	3	0
27	C	303	CDL	10	0
19	L	101	TGL	11	0
14	A	602	HEA	1	0
14	N	602	HEA	4	0
19	Y	101	TGL	16	0
19	D	201	TGL	10	0
23	P	304	CHD	4	0
14	N	601	HEA	4	0
27	P	303	CDL	6	0
18	A	606	CMO	1	0
20	A	609	PGV	7	0
21	A	612	EDO	2	0
23	J	101	CHD	1	0
18	N	606	CMO	2	0
21	C	309	EDO	1	0
21	I	101	EDO	5	0
25	C	308	PEK	3	0
23	P	305	CHD	1	0
20	C	307	PGV	5	0
21	P	307	EDO	2	0
24	O	302	PSC	5	0
25	C	306	PEK	1	0
20	P	302	PGV	1	0
14	A	601	HEA	6	0
20	Z	101	PGV	5	0
25	B	304	PEK	1	0
21	C	312	EDO	4	0
27	T	102	CDL	16	0
23	C	304	CHD	1	0
25	G	101	PEK	6	0
23	B	302	CHD	1	0
24	B	303	PSC	2	0
27	G	102	CDL	16	0
25	G	103	PEK	3	0
19	N	609	TGL	4	0
21	L	103	EDO	1	0
21	A	613	EDO	9	0
21	S	102	EDO	1	0
25	T	101	PEK	4	0
20	C	302	PGV	3	0
23	W	101	CHD	2	0

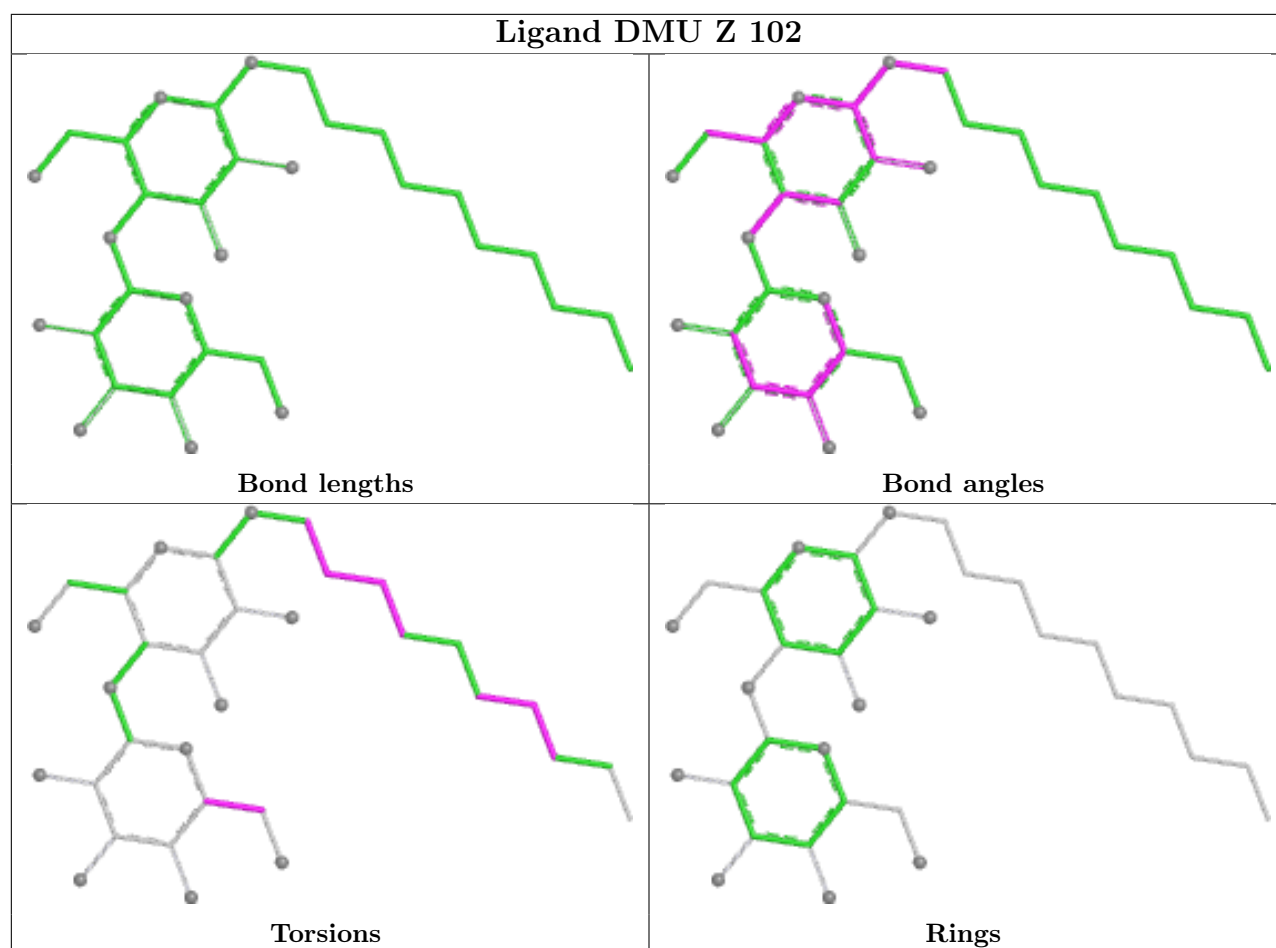
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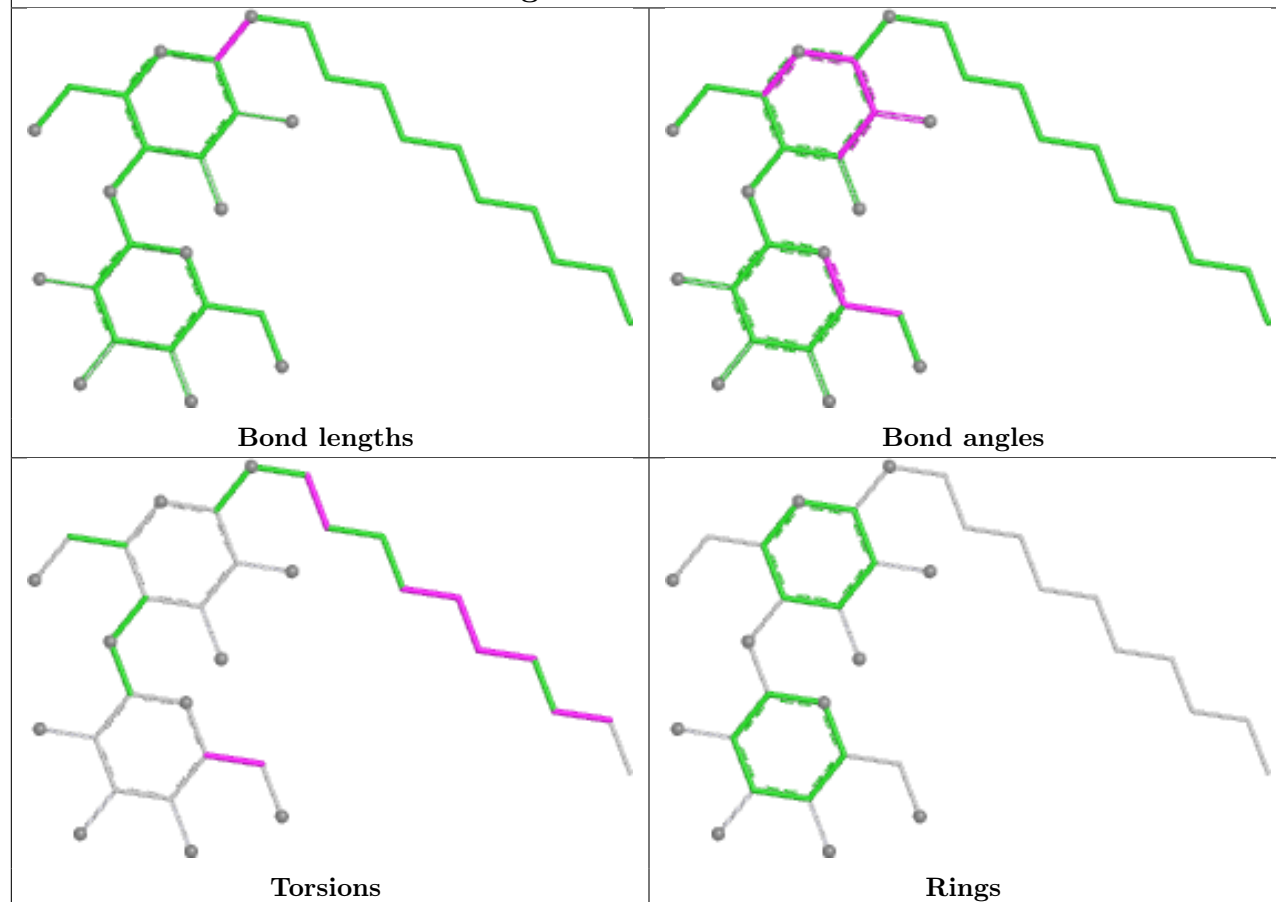
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Q	201	TGL	6	0
21	T	103	EDO	1	0

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

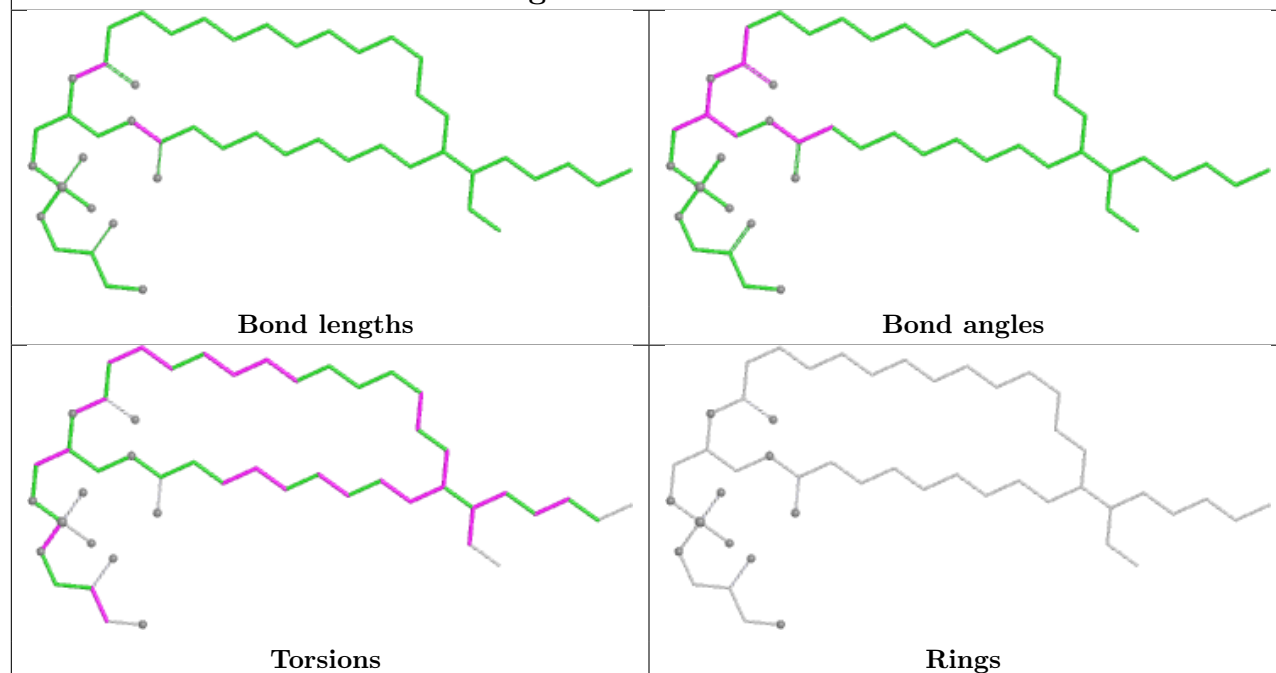


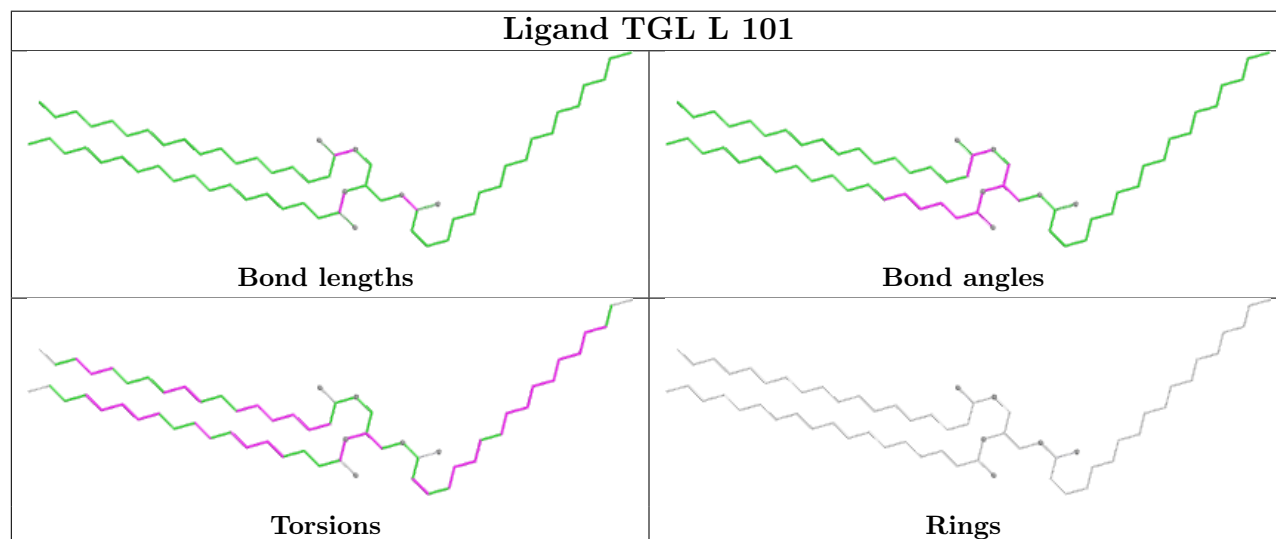
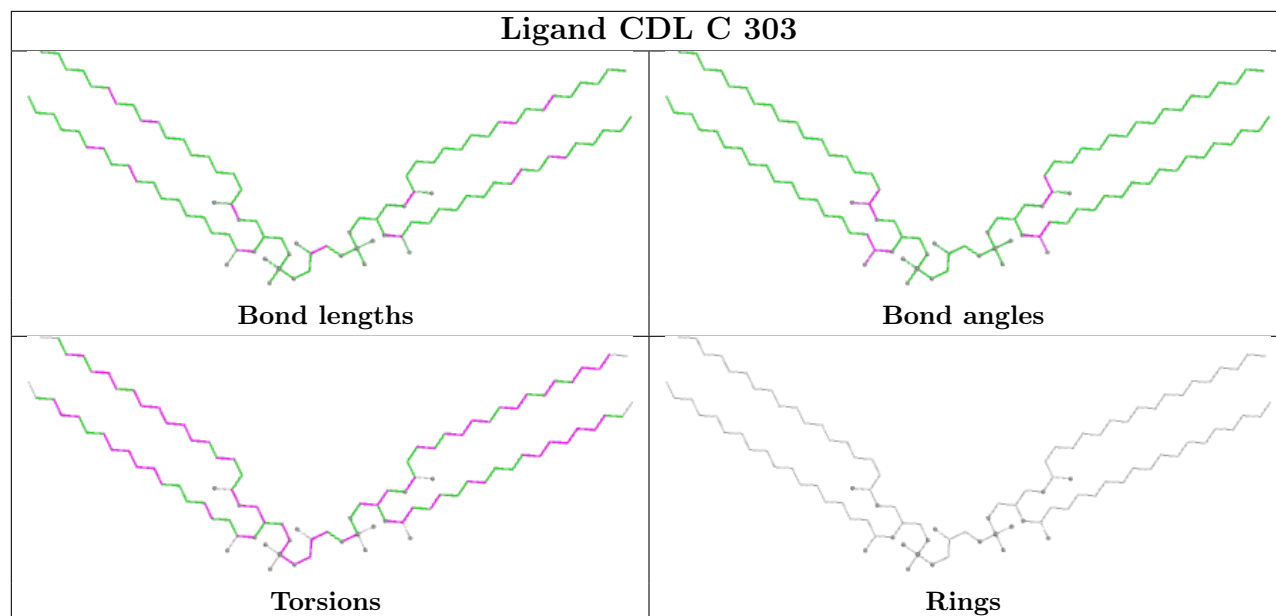


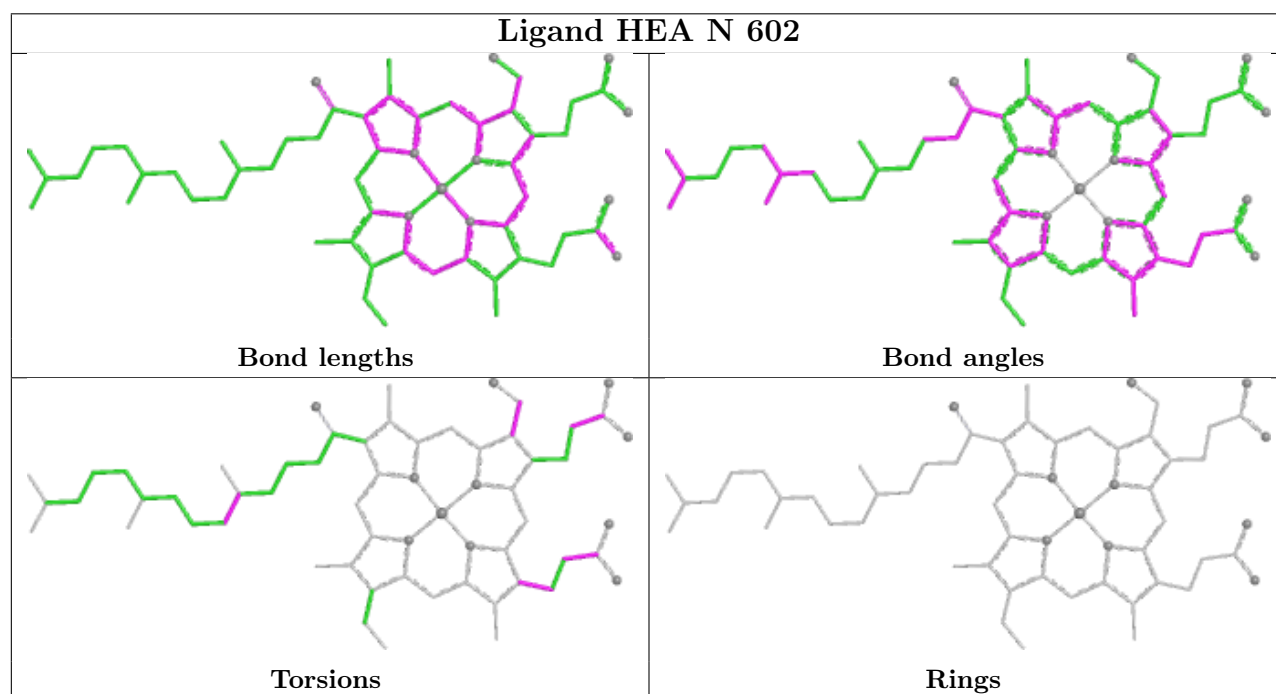
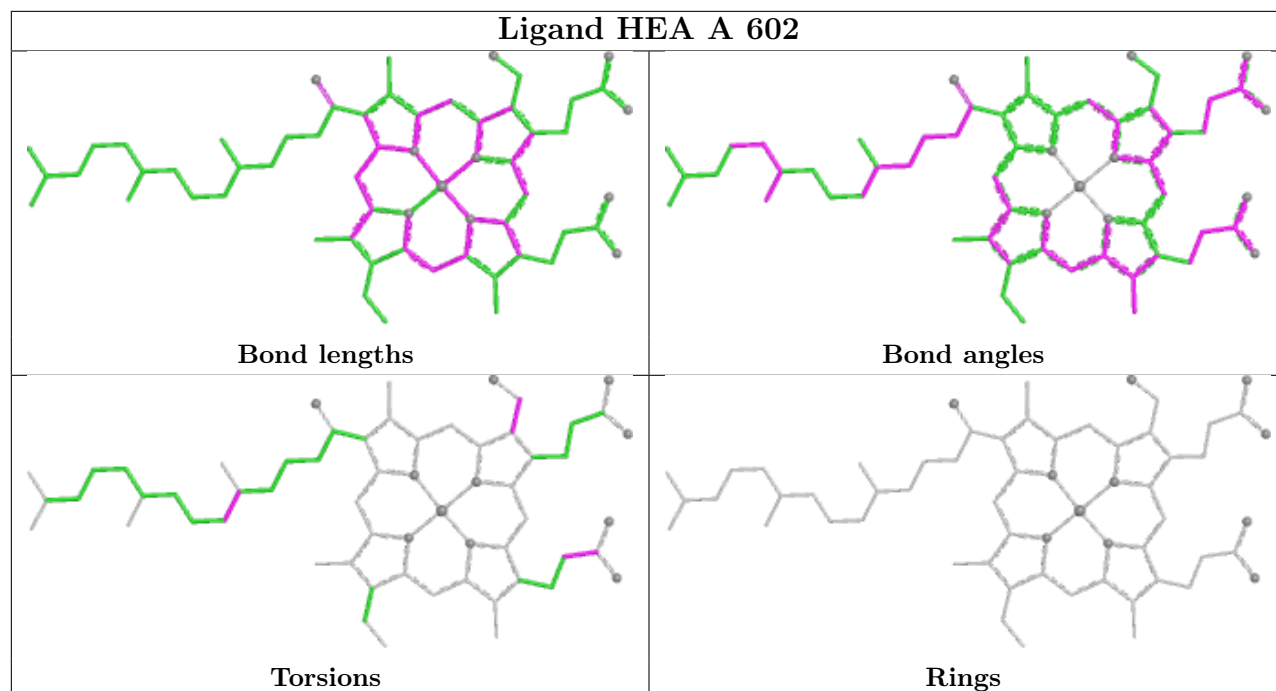
Ligand DMU M 101

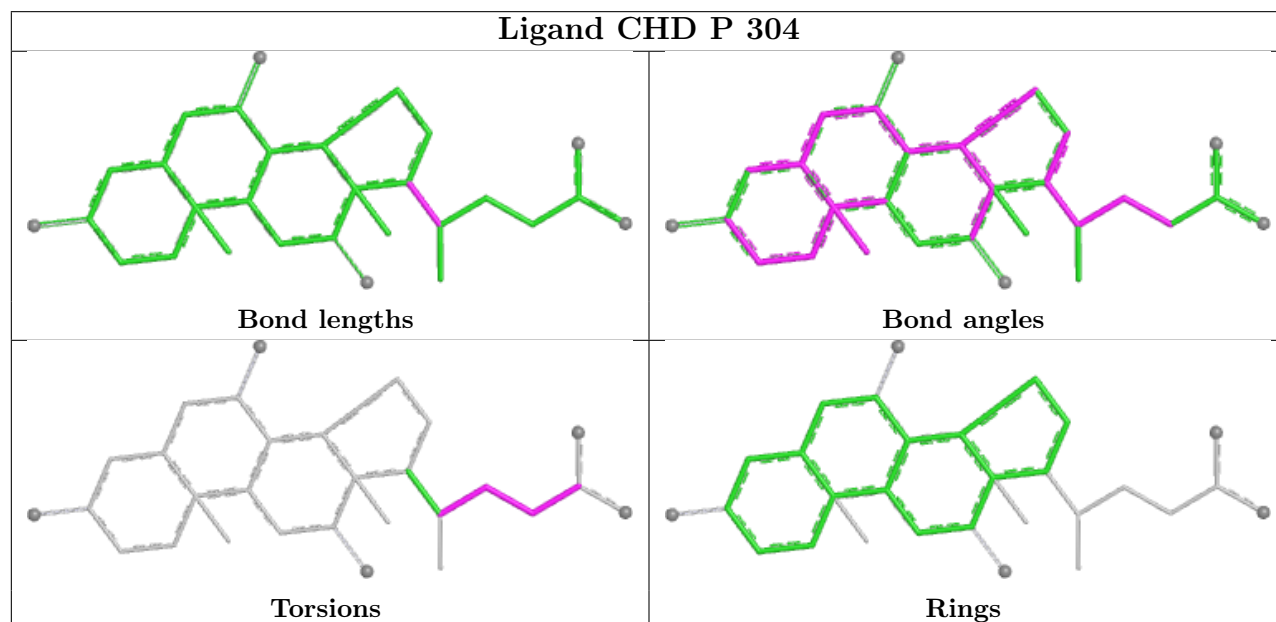
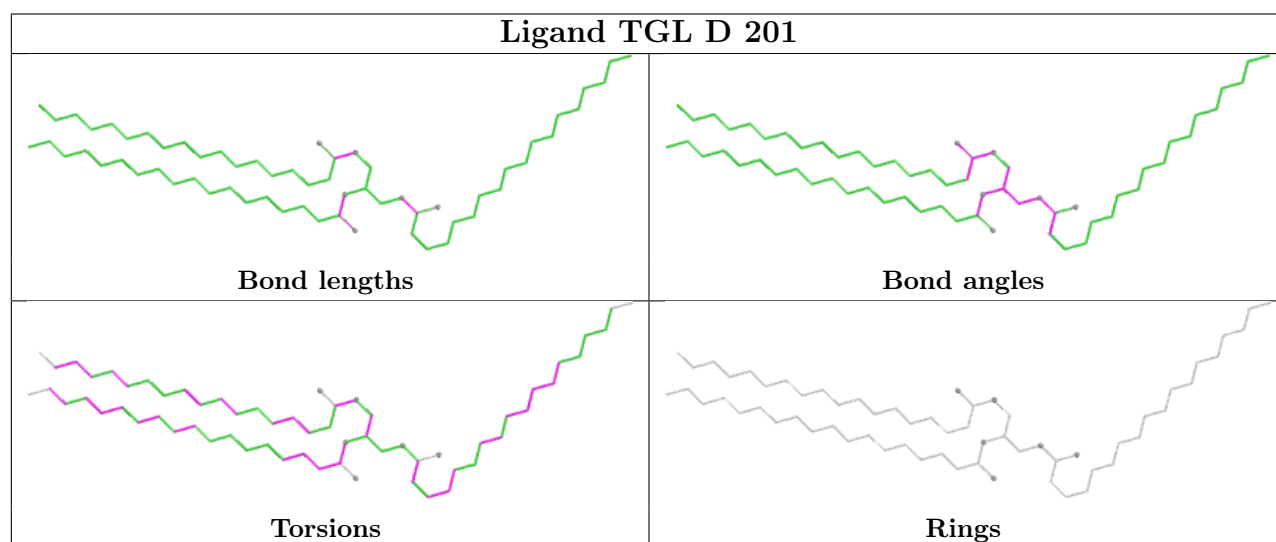
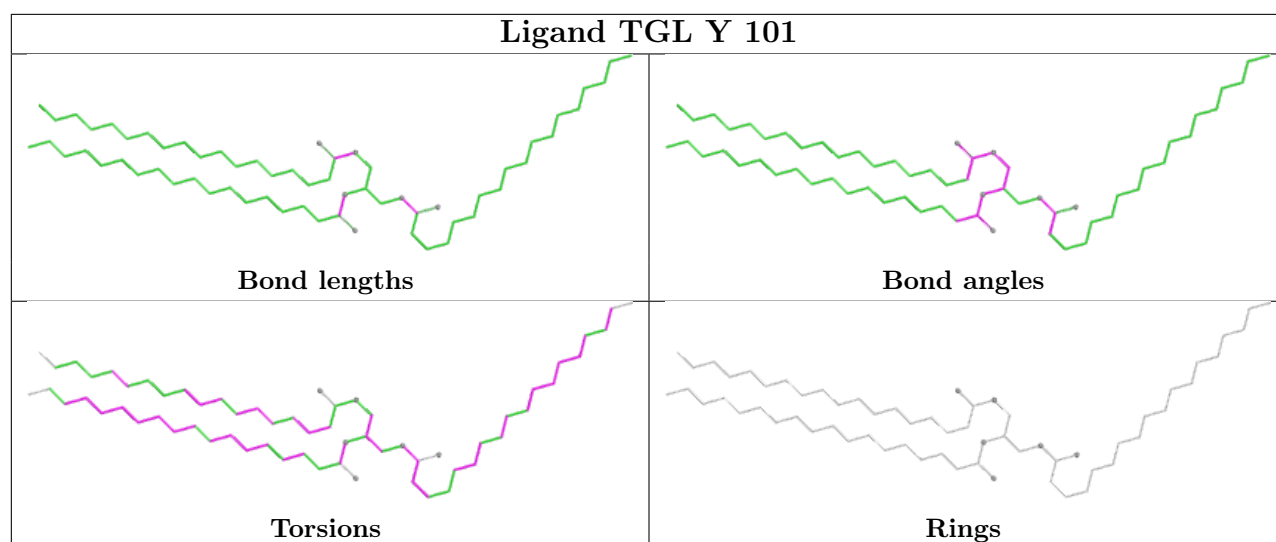


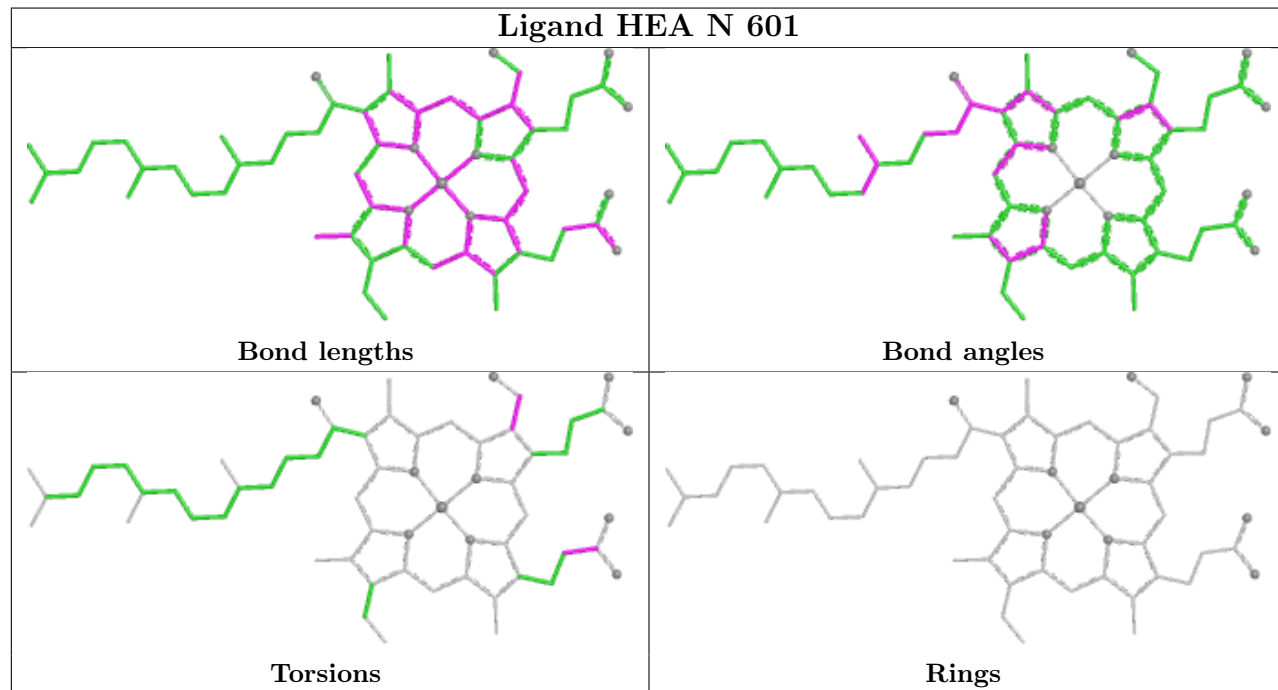
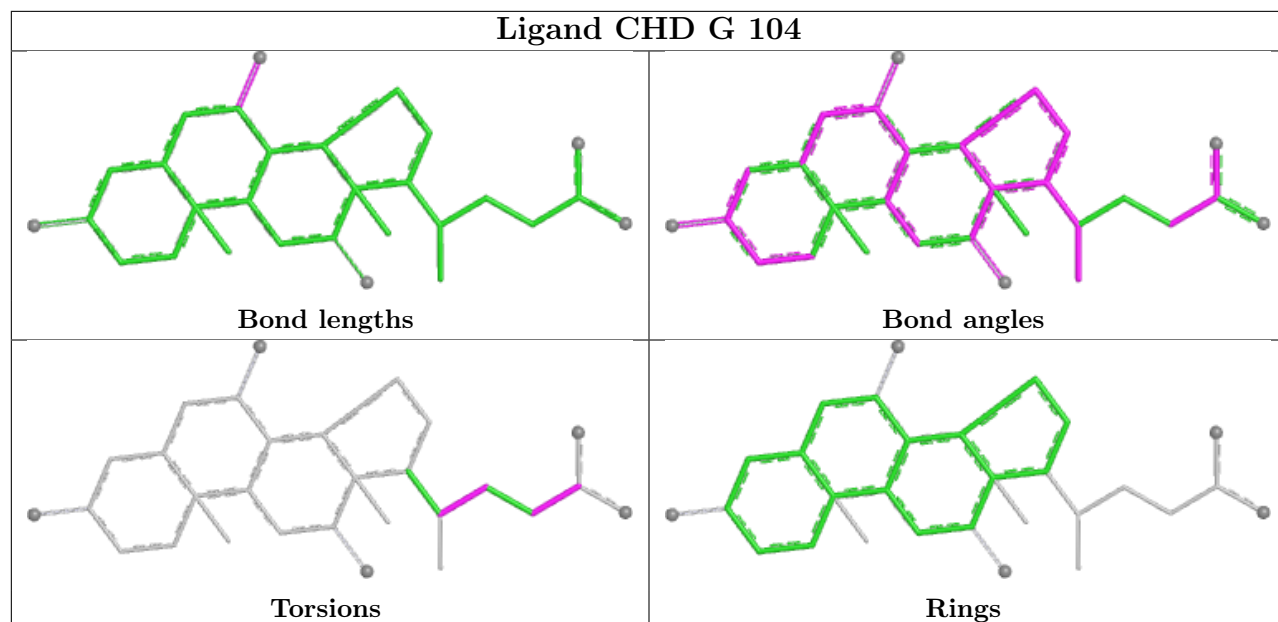
Ligand PGV N 608

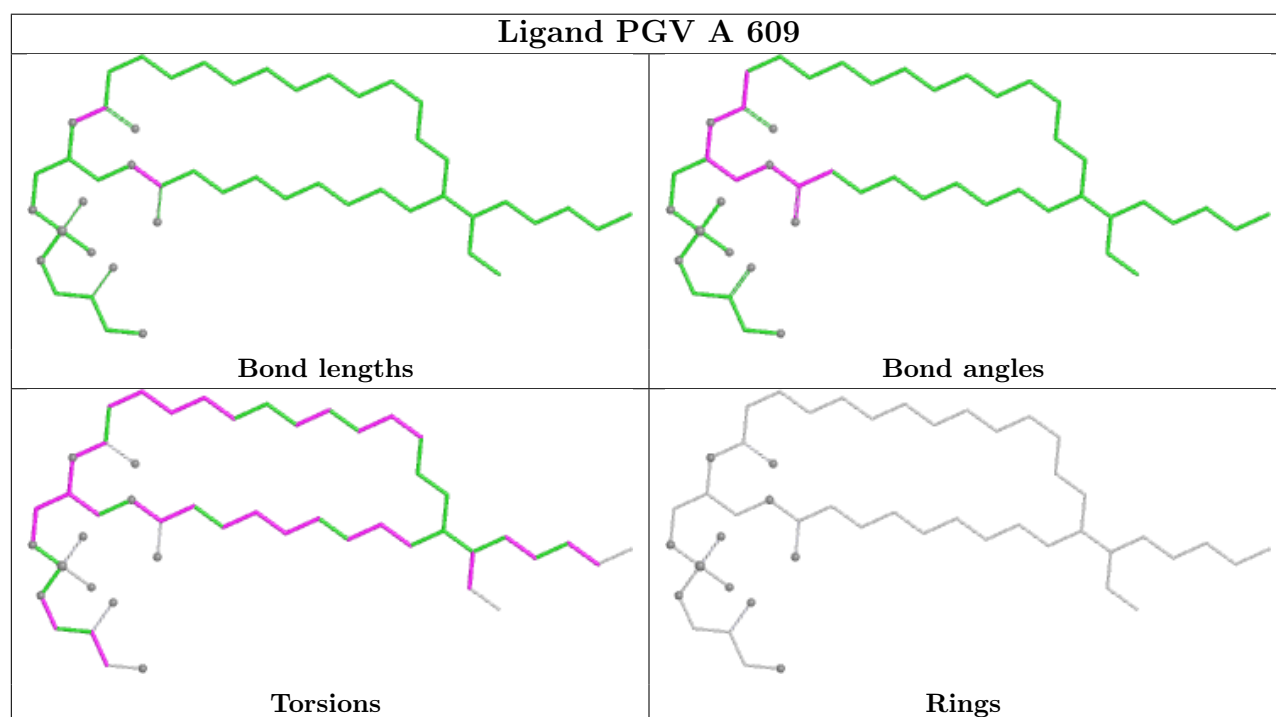
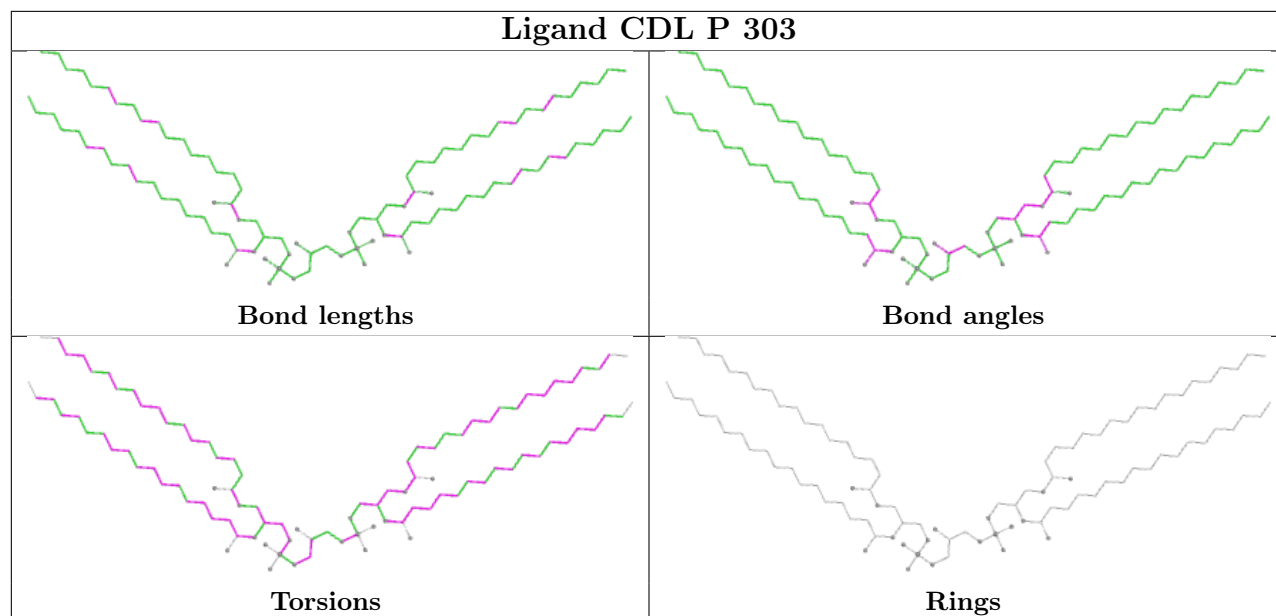




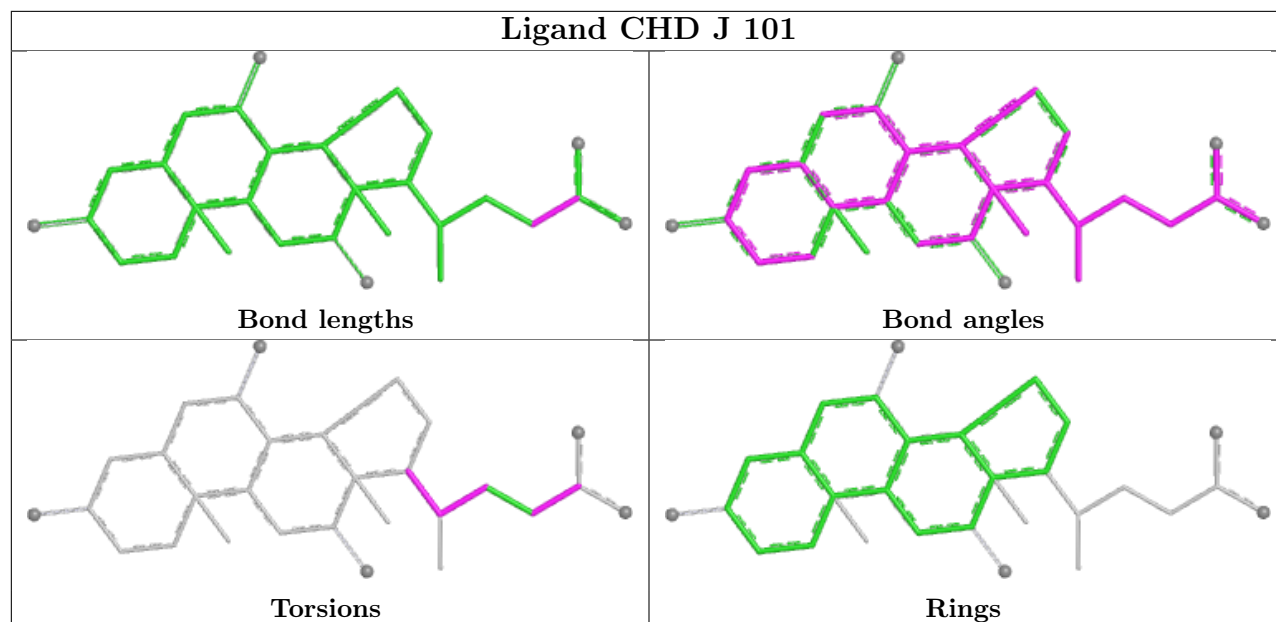




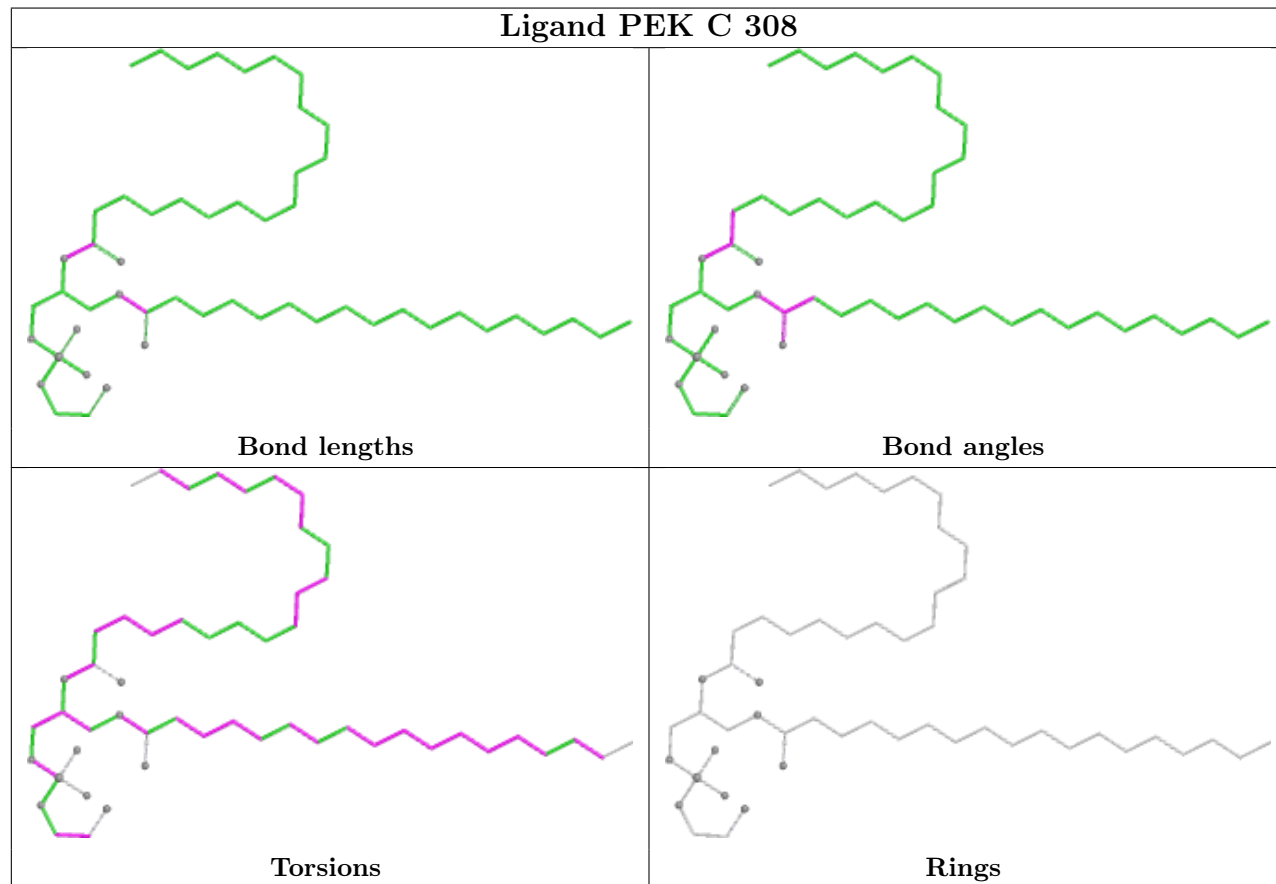


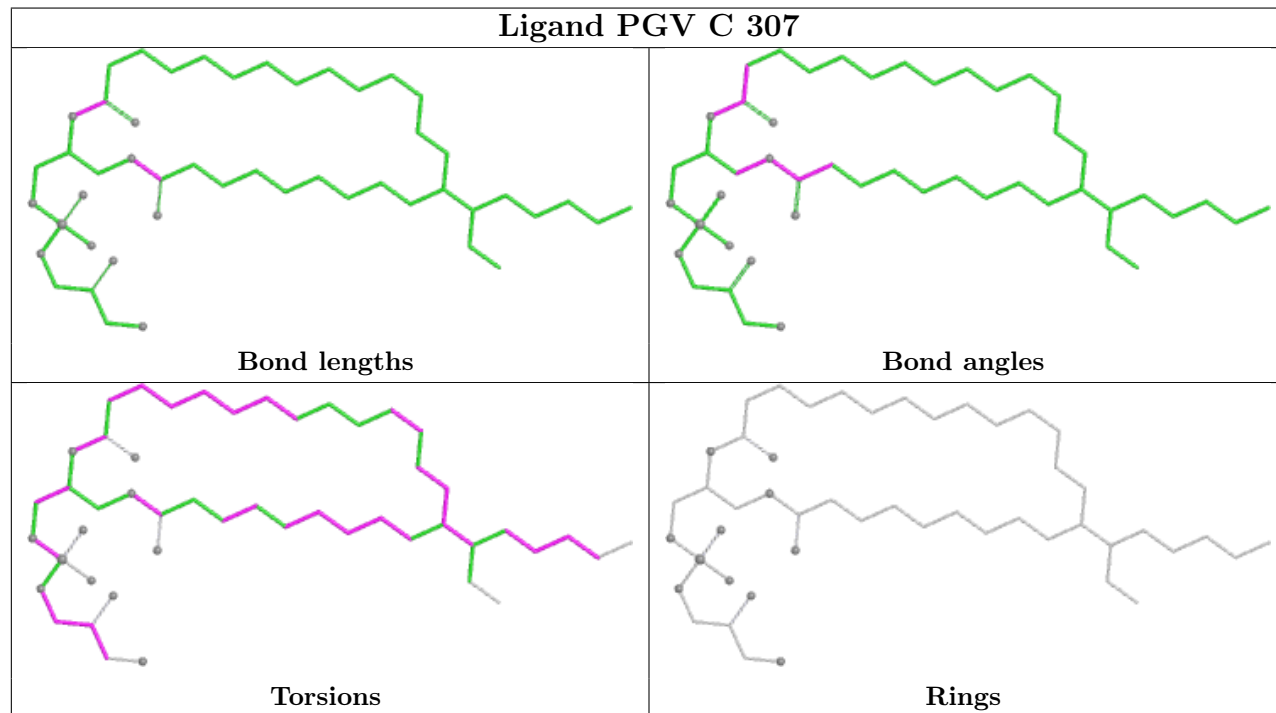
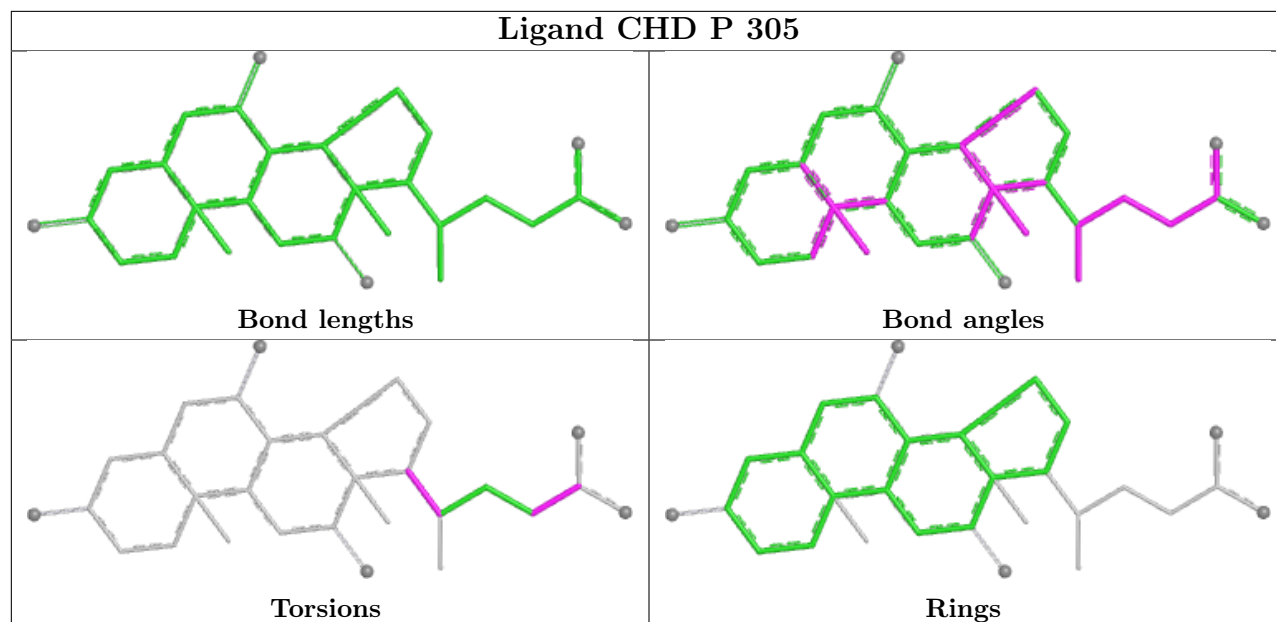


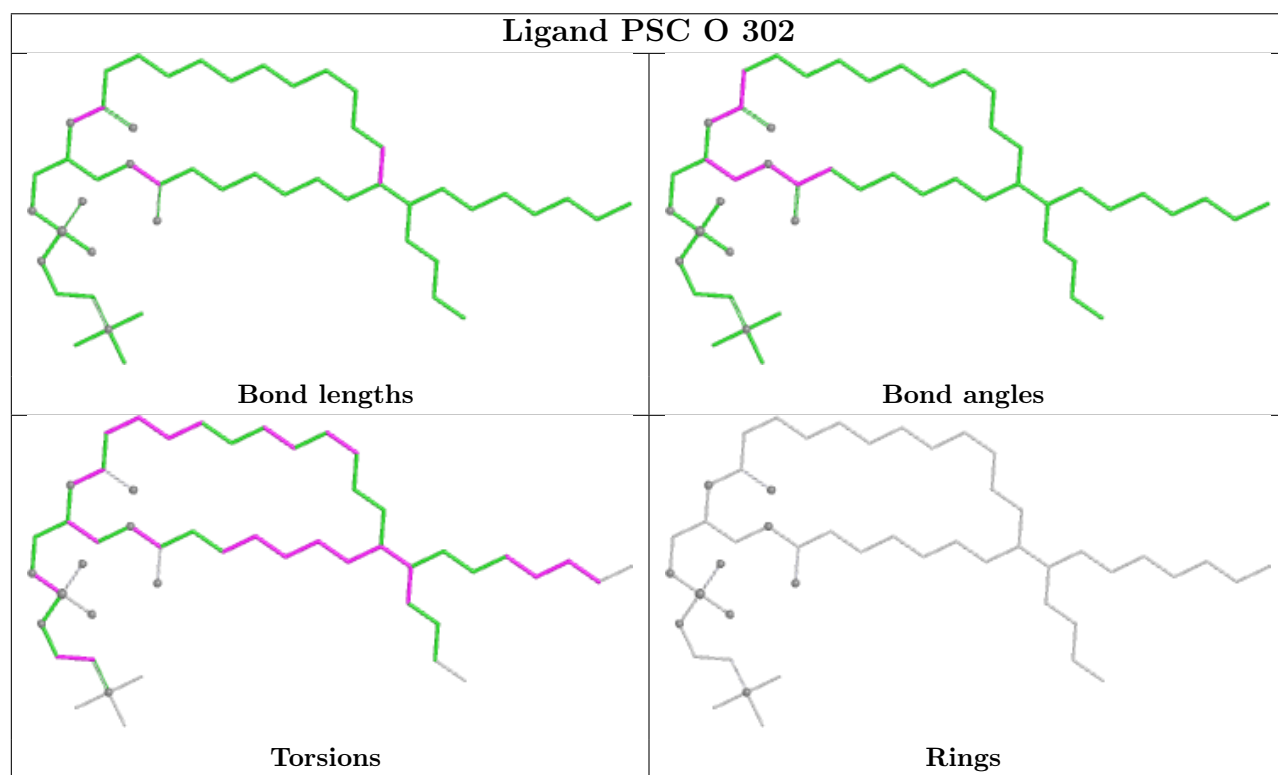
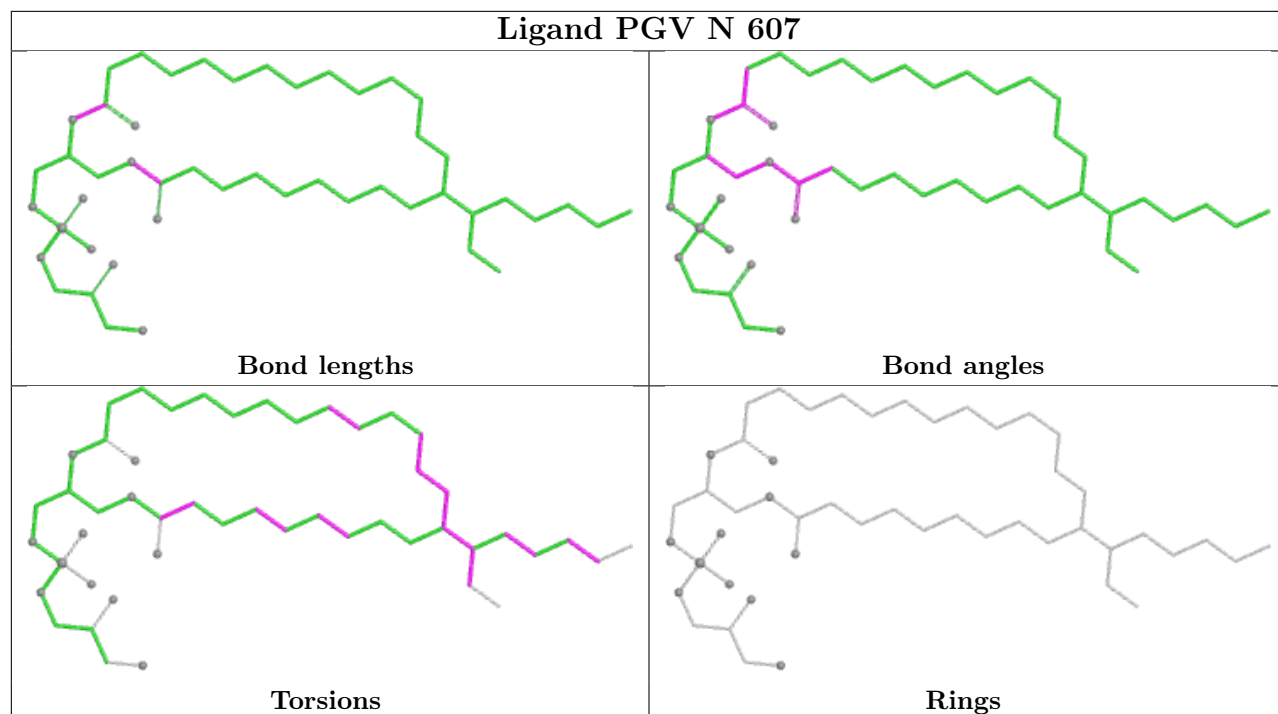
Ligand CHD J 101

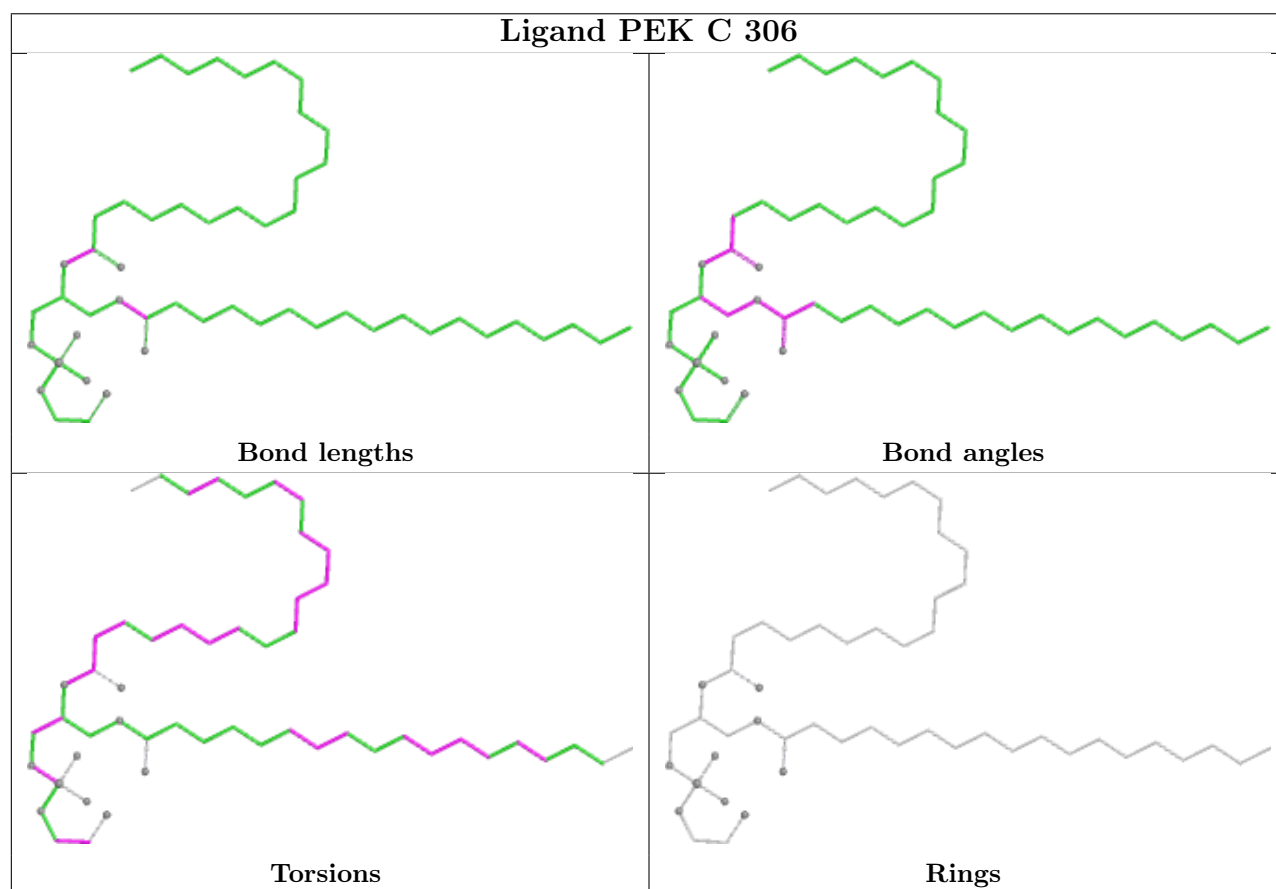
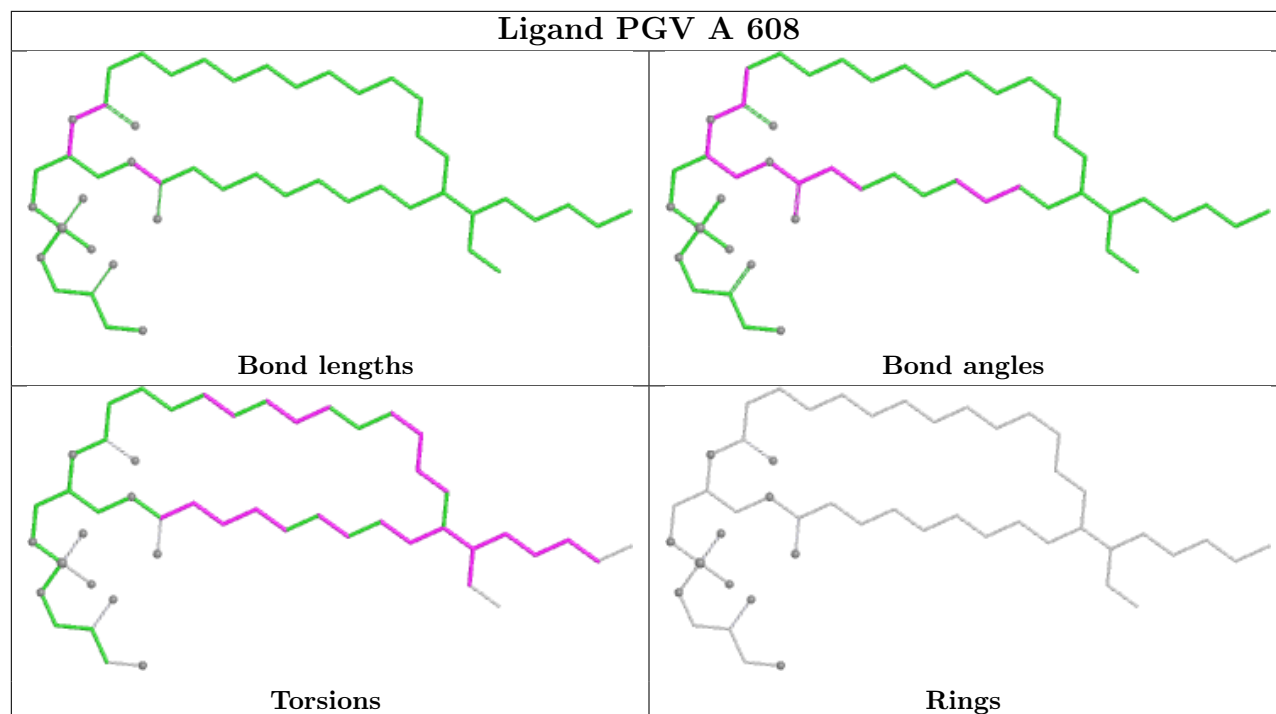


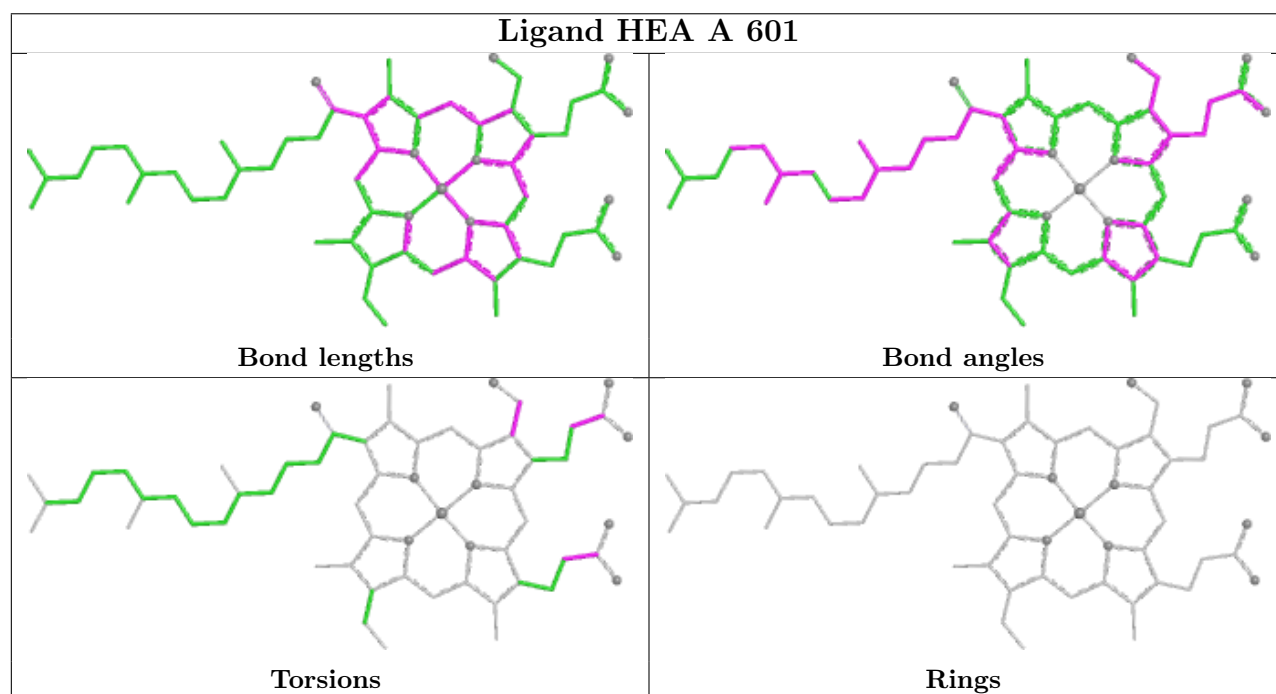
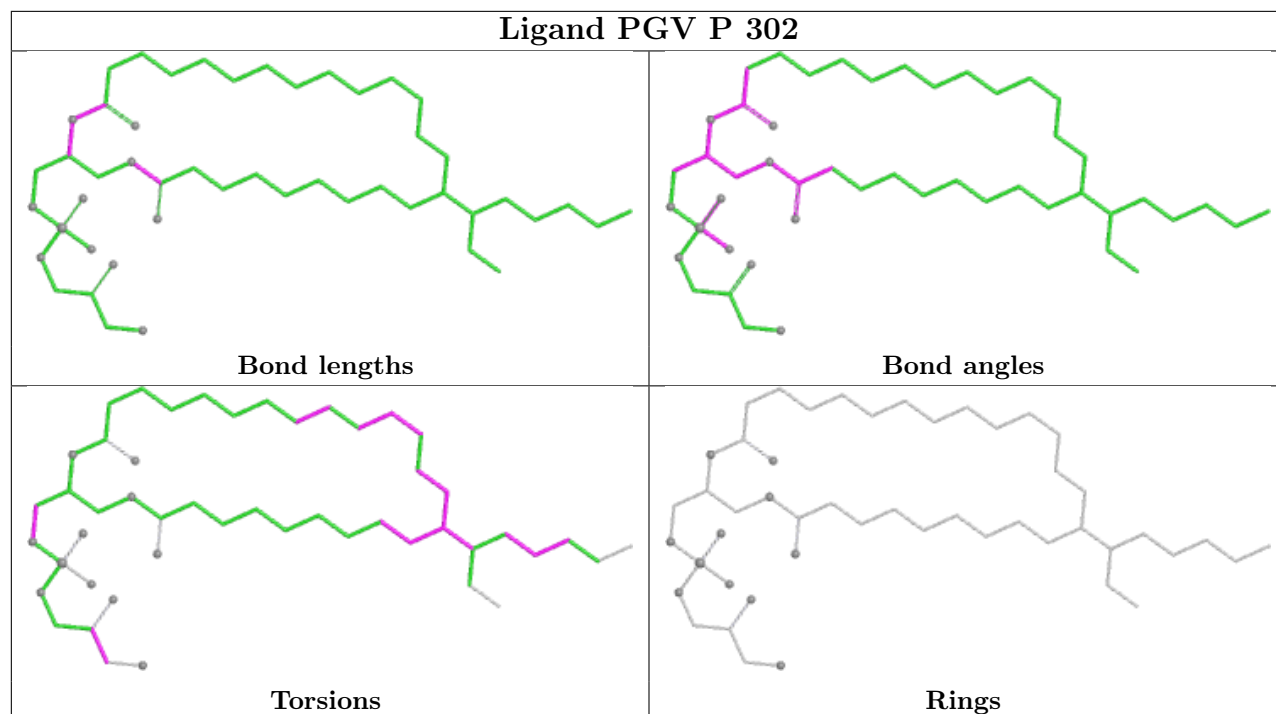
Ligand PEK C 308

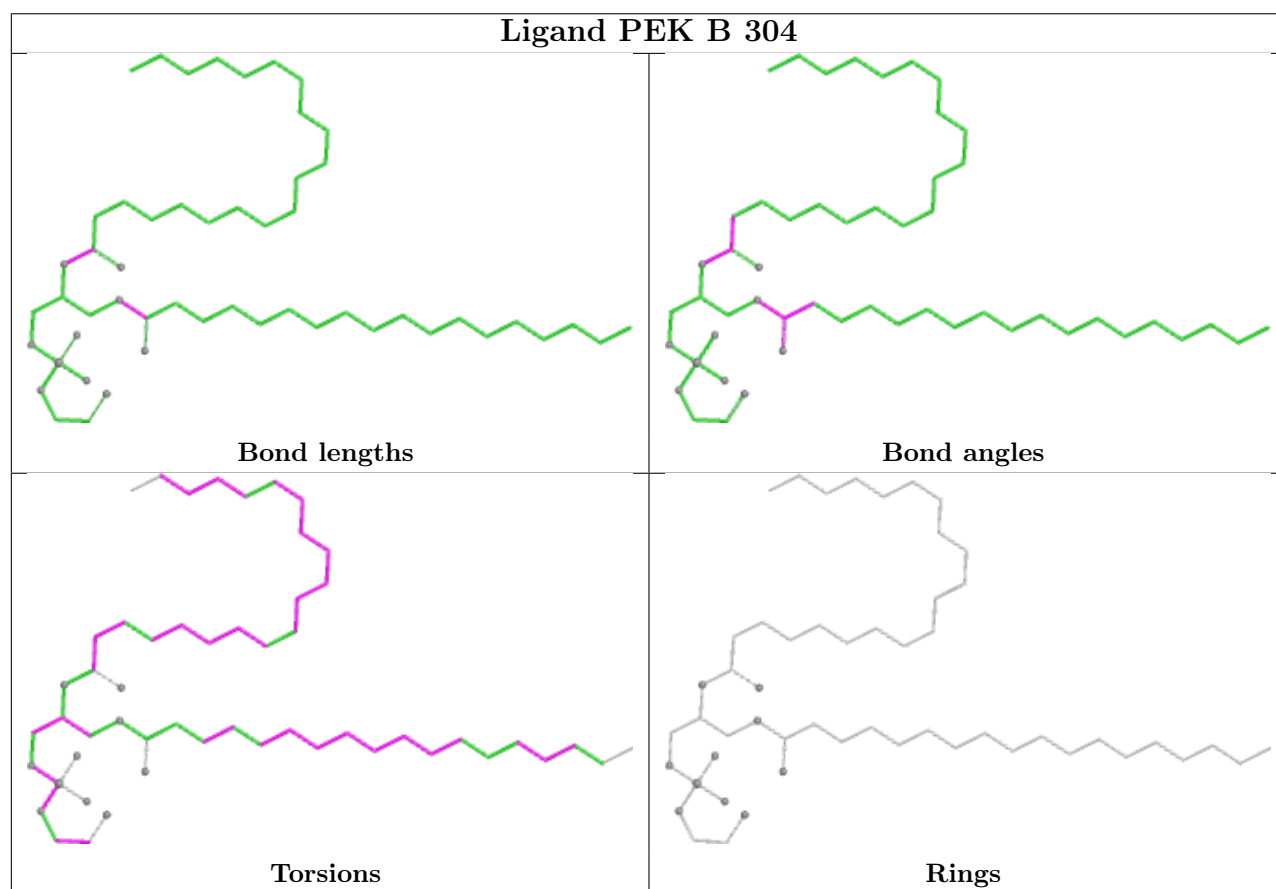
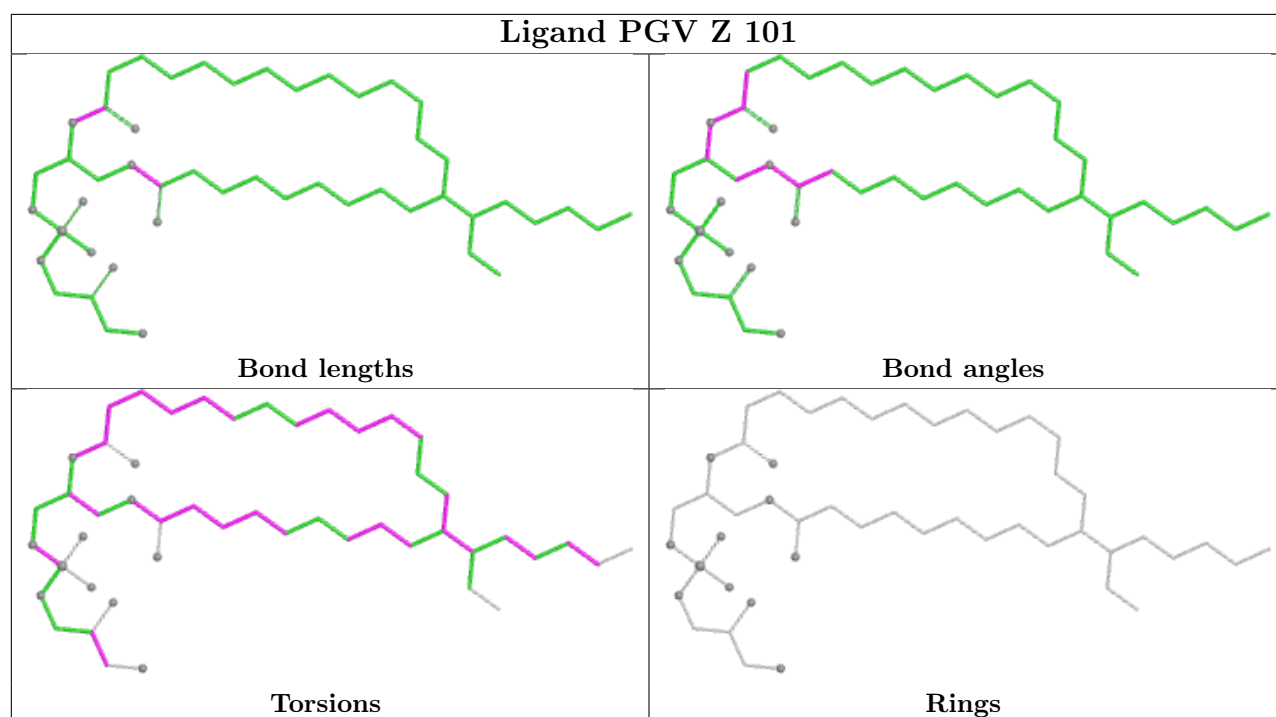


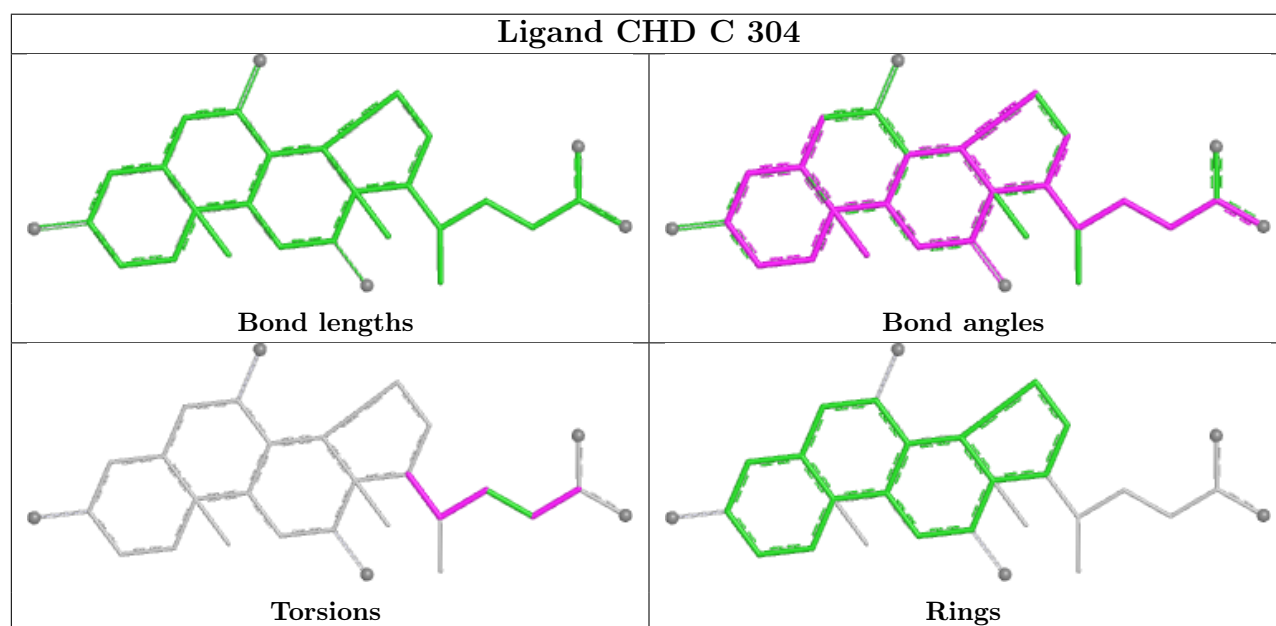
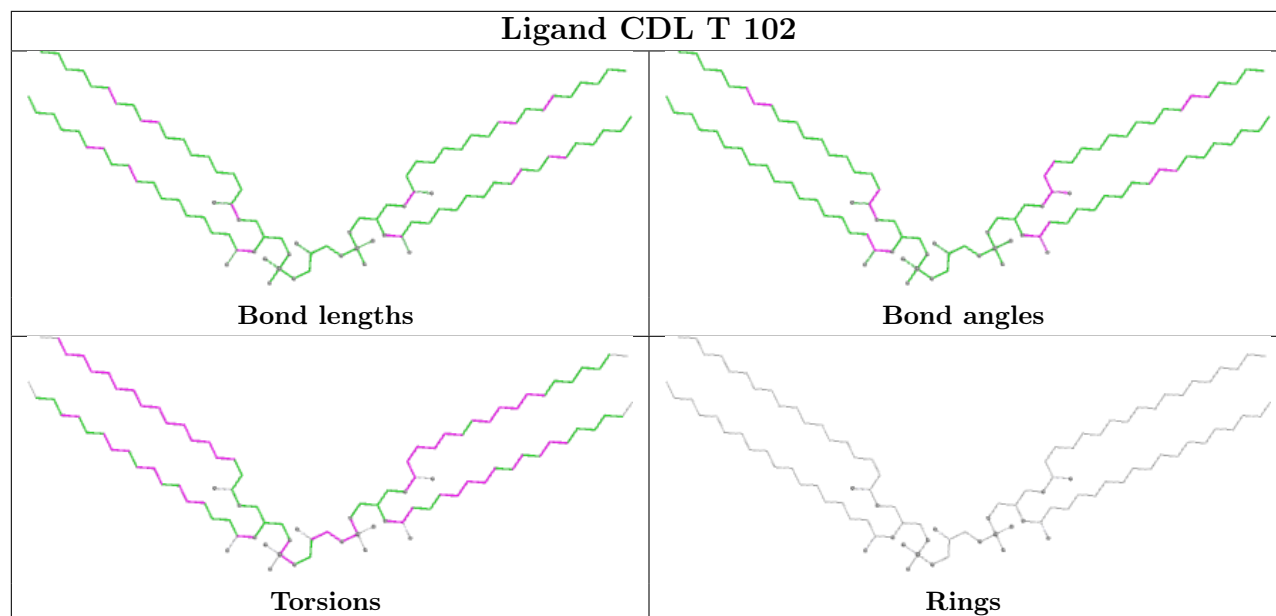


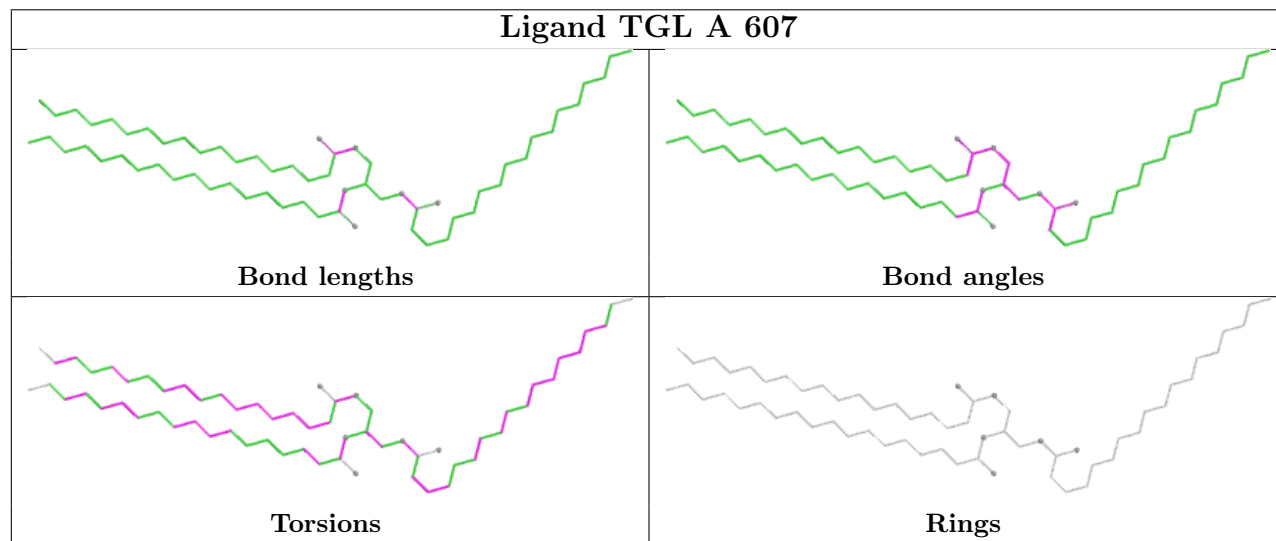
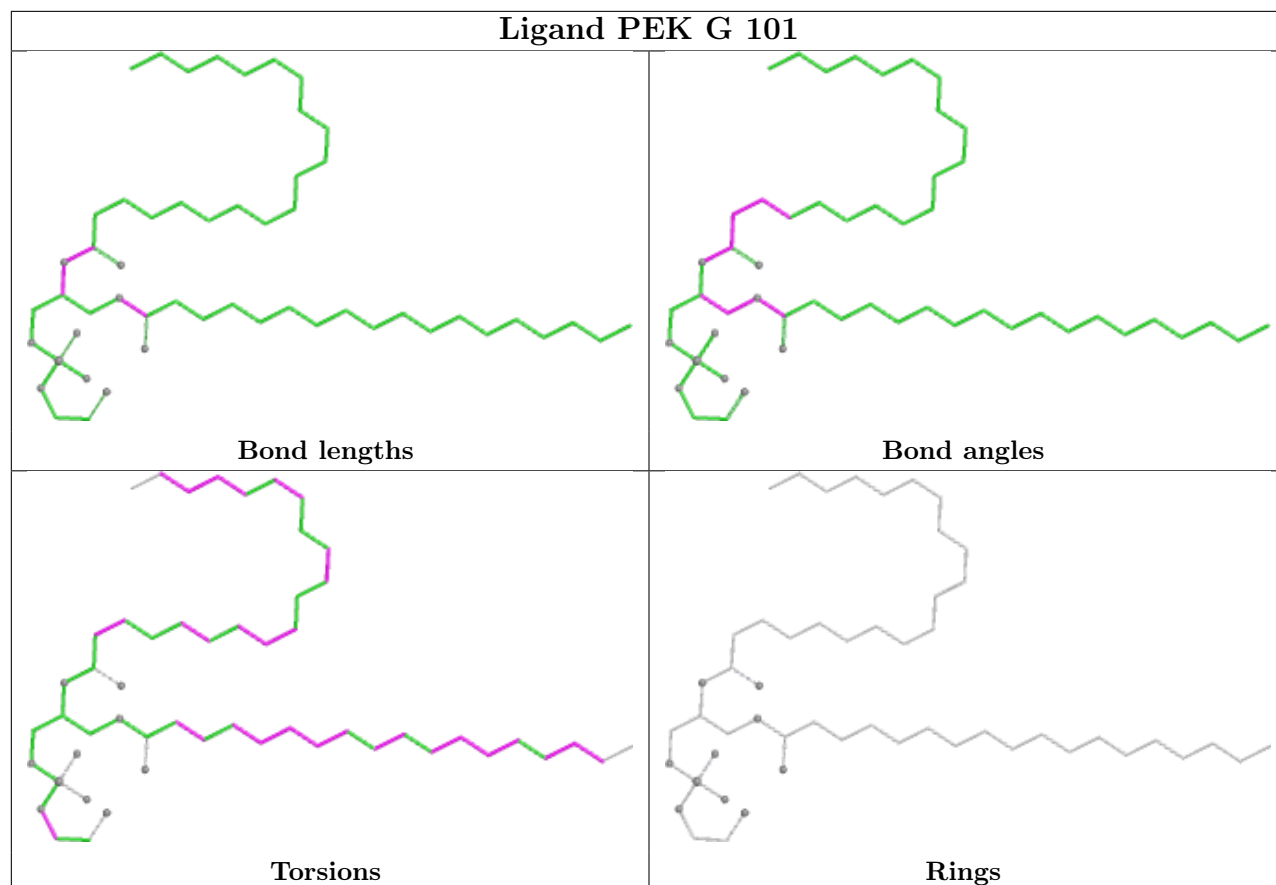


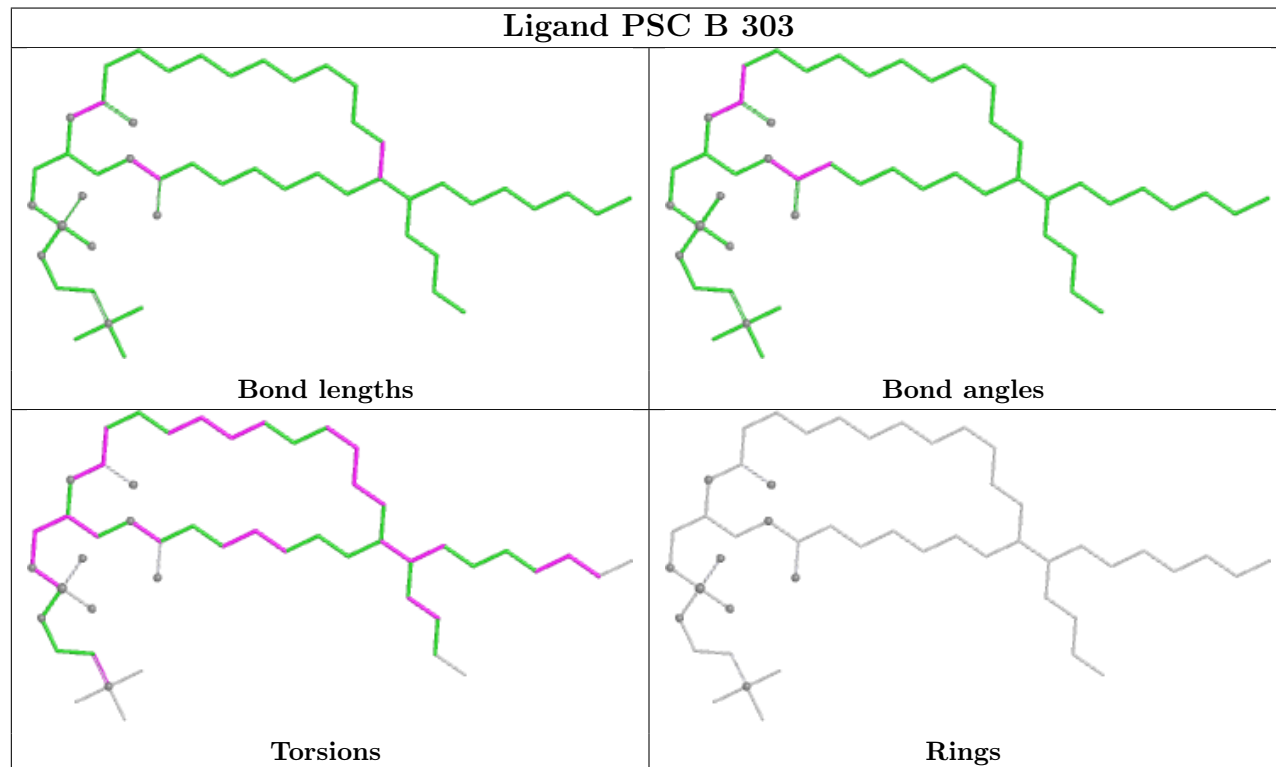
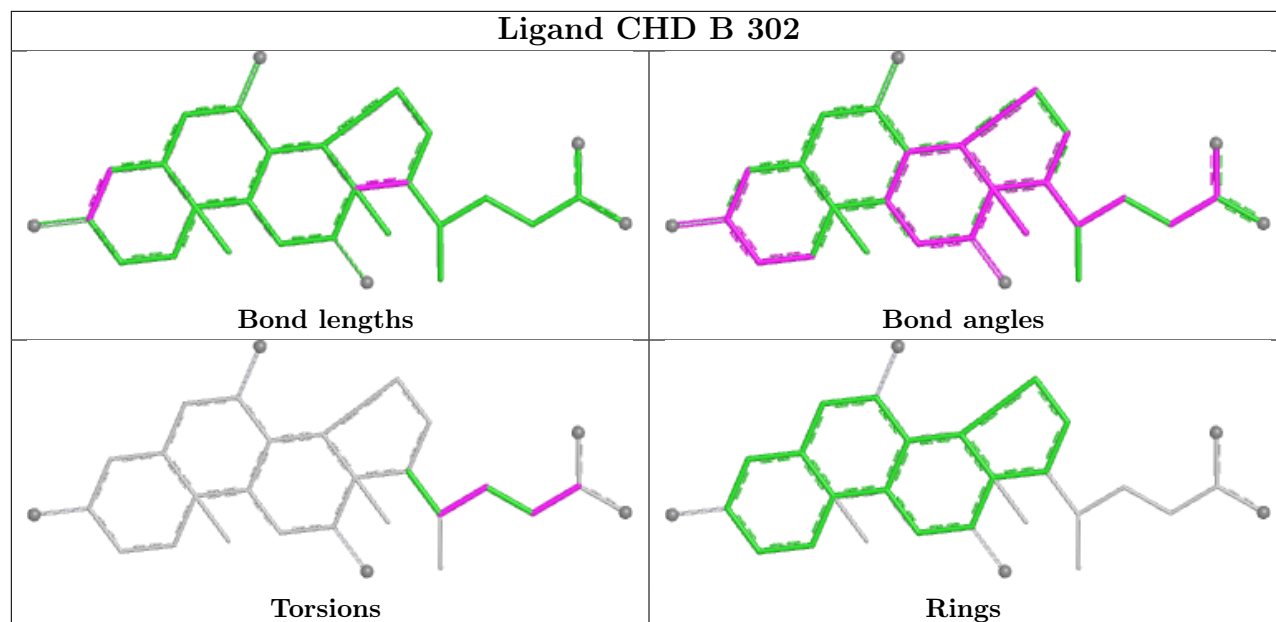


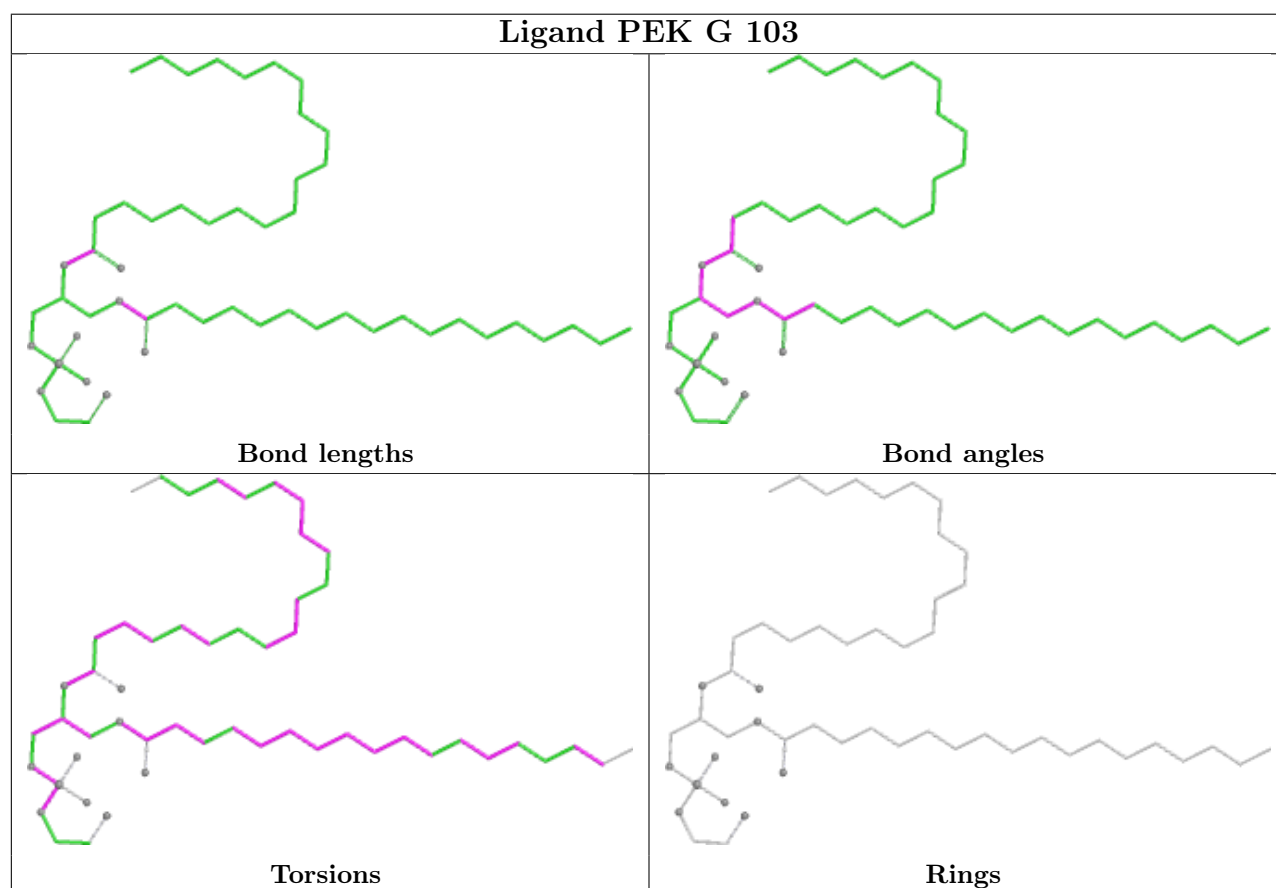
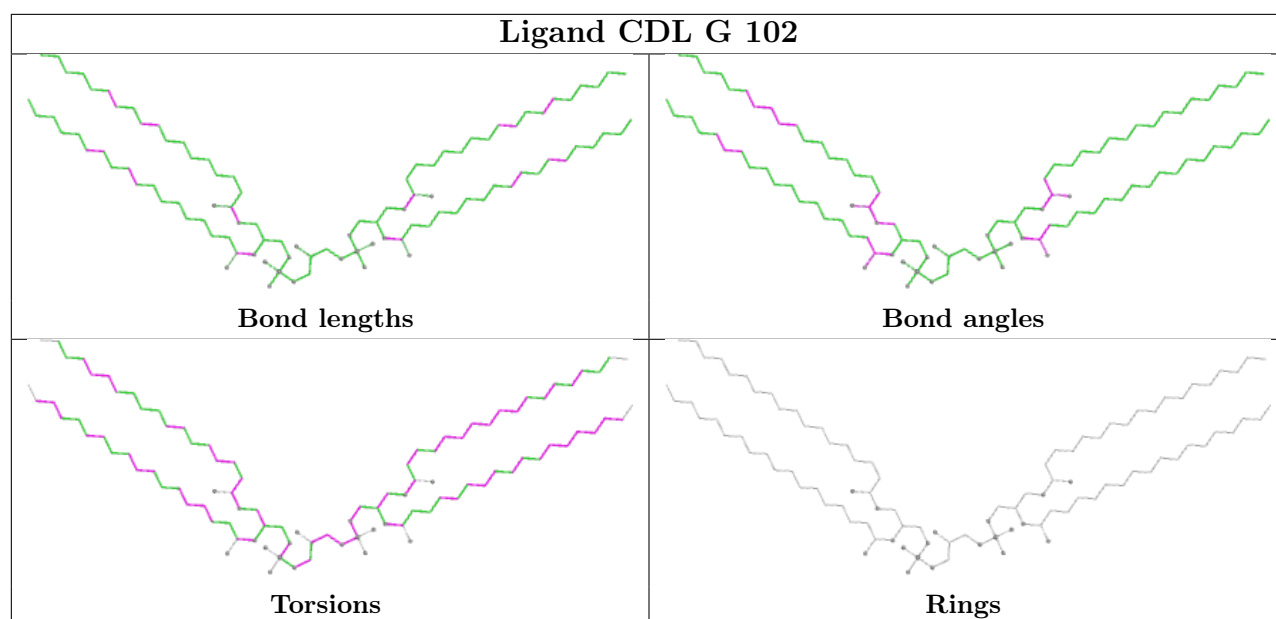


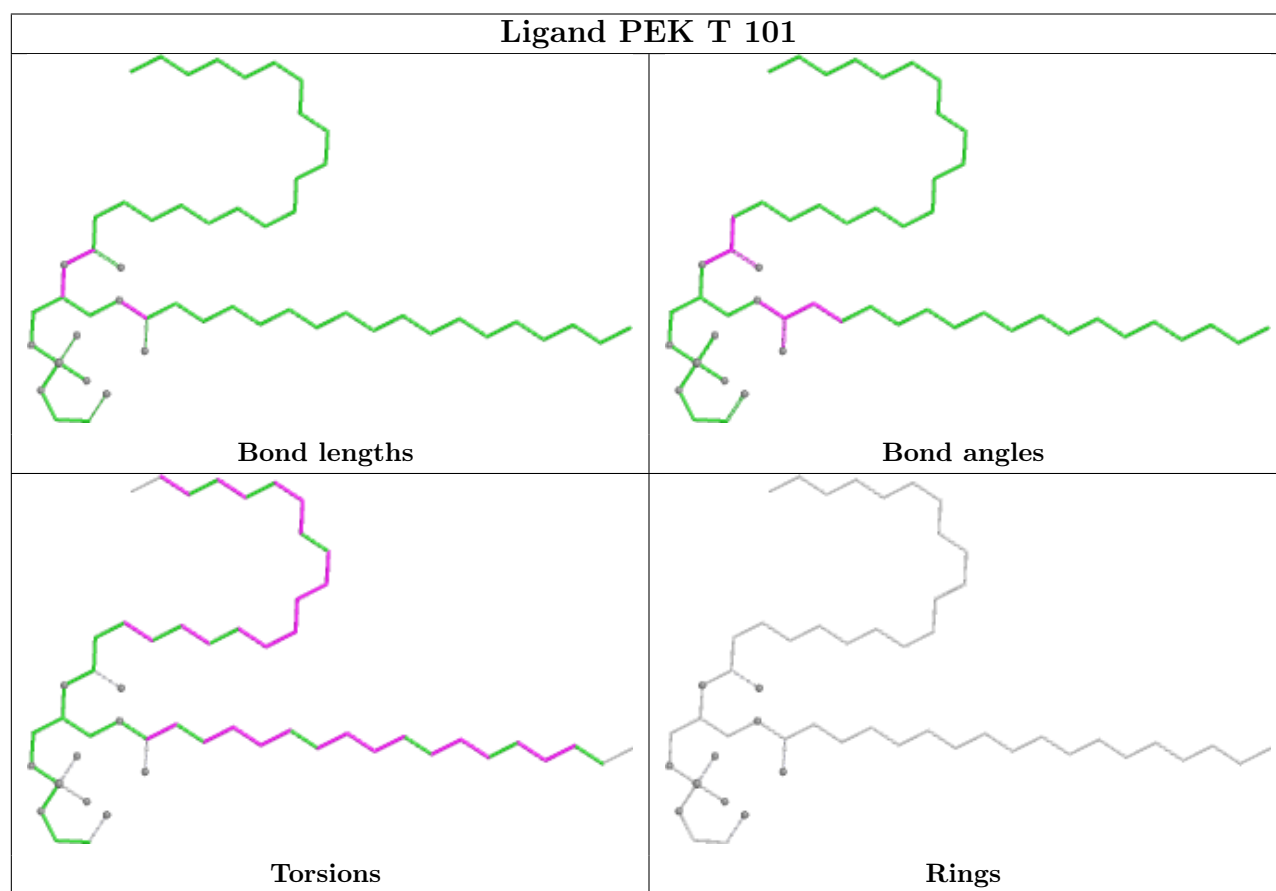
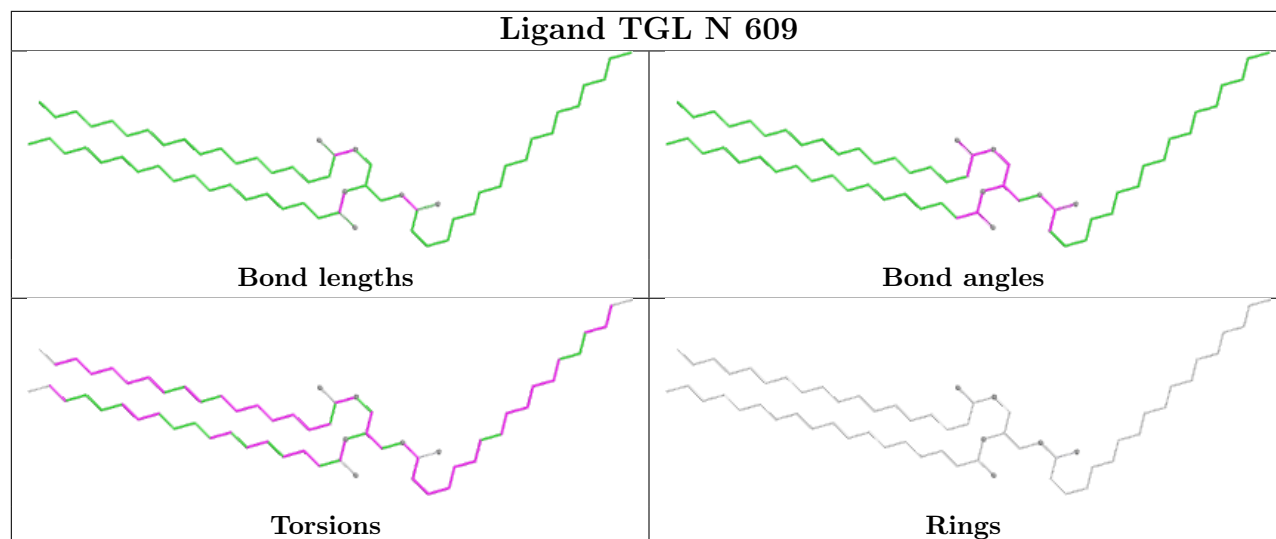


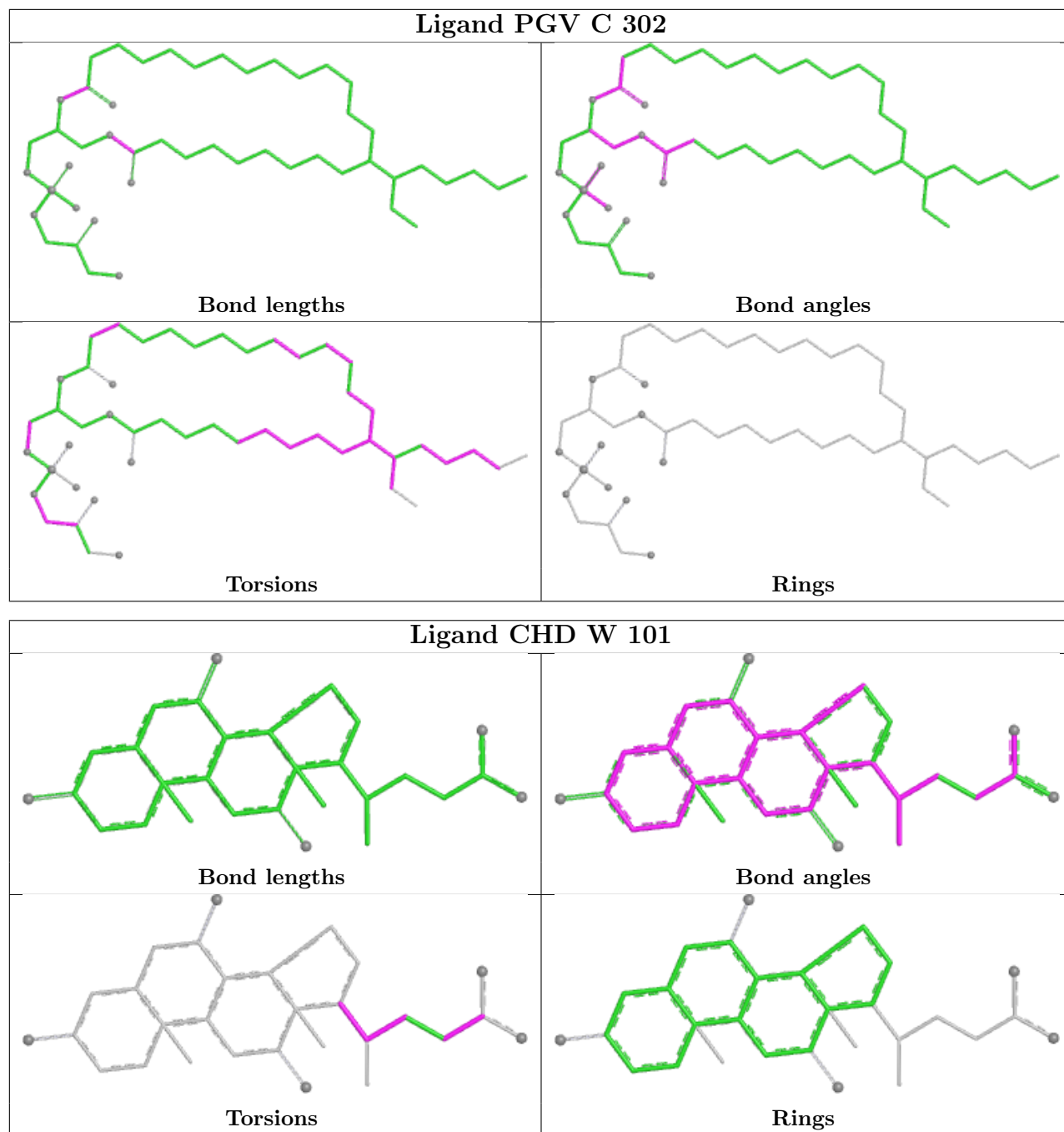


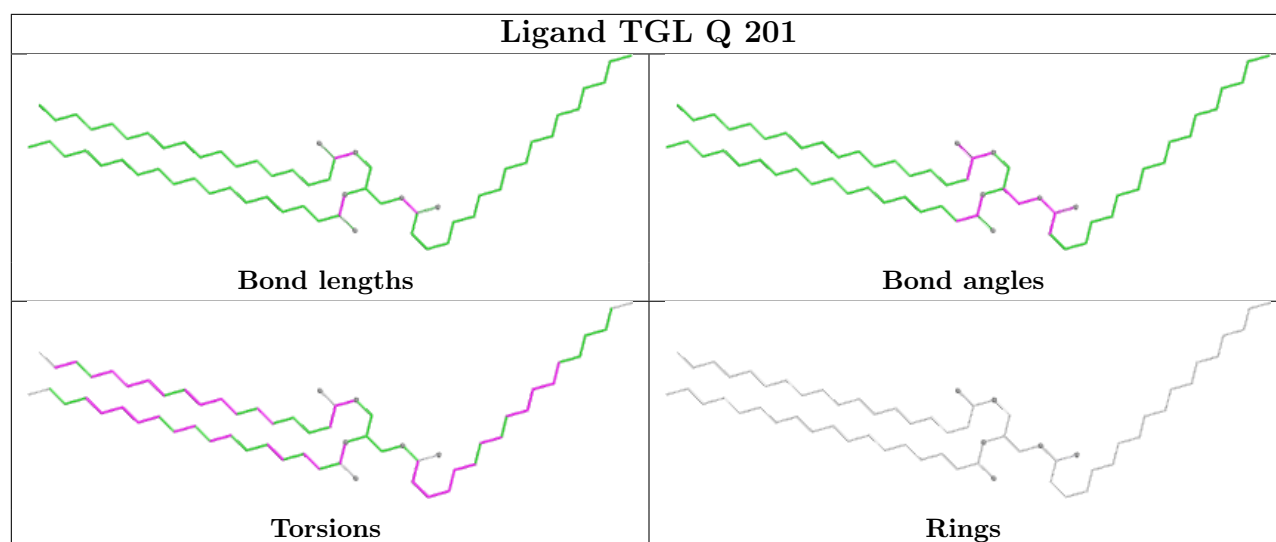












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.50	3 (0%) 85 83	33, 42, 53, 87	1 (0%)
1	N	513/514 (99%)	-0.26	5 (0%) 79 77	40, 48, 63, 83	0
2	B	226/227 (99%)	-0.39	0 100 100	38, 49, 73, 112	0
2	O	226/227 (99%)	-0.22	2 (0%) 81 79	45, 56, 89, 138	0
3	C	259/261 (99%)	-0.33	4 (1%) 72 69	38, 46, 65, 117	0
3	P	259/261 (99%)	-0.16	3 (1%) 76 74	41, 51, 69, 107	0
4	D	144/147 (97%)	-0.26	3 (2%) 63 60	43, 54, 77, 115	0
4	Q	144/147 (97%)	0.33	12 (8%) 17 15	54, 71, 118, 159	0
5	E	105/109 (96%)	-0.14	2 (1%) 66 63	44, 54, 88, 136	0
5	R	105/109 (96%)	-0.34	0 100 100	49, 65, 91, 133	0
6	F	98/98 (100%)	-0.12	5 (5%) 33 30	41, 55, 135, 155	0
6	S	98/98 (100%)	0.08	6 (6%) 27 24	47, 62, 126, 160	0
7	G	83/85 (97%)	0.33	7 (8%) 17 14	44, 56, 142, 157	0
7	T	83/85 (97%)	0.27	9 (10%) 11 8	45, 61, 144, 158	0
8	H	79/85 (92%)	0.07	5 (6%) 26 23	44, 57, 123, 140	0
8	U	79/85 (92%)	-0.03	1 (1%) 75 73	51, 65, 132, 156	0
9	I	72/73 (98%)	-0.15	3 (4%) 40 37	48, 62, 88, 114	0
9	V	72/73 (98%)	0.19	3 (4%) 40 37	50, 73, 105, 147	0
10	J	58/59 (98%)	-0.07	0 100 100	45, 59, 101, 140	0
10	W	58/59 (98%)	0.33	3 (5%) 33 29	51, 70, 110, 156	0
11	K	49/56 (87%)	0.16	2 (4%) 41 38	50, 60, 82, 106	0
11	X	49/56 (87%)	0.31	3 (6%) 27 24	59, 71, 95, 119	0
12	L	46/47 (97%)	-0.41	0 100 100	43, 49, 68, 107	0
12	Y	46/47 (97%)	0.06	2 (4%) 40 36	51, 62, 90, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.11	0 100 100	43, 51, 80, 150	0
13	Z	43/46 (93%)	-0.05	0 100 100	57, 66, 100, 154	0
All	All	3550/3614 (98%)	-0.18	83 (2%) 61 58	33, 53, 94, 160	1 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	3	ALA	7.5
7	G	5	LYS	7.1
4	Q	6	VAL	6.3
4	Q	5	VAL	6.1
10	W	48	TYR	5.8
7	G	2	SER	5.7
6	S	97	ALA	5.4
3	P	33	MET	5.4
1	N	452	THR	5.3
3	P	37	PHE	5.2
7	G	4	ALA	5.1
6	S	1	ALA	5.1
9	V	38	ALA	4.7
7	G	6	GLY	4.7
10	W	49	CYS	4.6
6	S	94	HIS	4.4
1	A	298	ASP	4.4
6	S	96	LEU	4.3
4	Q	124	LEU	4.3
8	H	8	ILE	4.3
7	T	9	GLY	4.2
6	F	97	ALA	4.2
6	F	96	LEU	4.2
1	A	296	GLY	4.1
6	S	71	TRP	4.1
6	F	95	GLN	4.0
7	T	3	ALA	4.0
4	Q	125	ASP	4.0
8	H	7	LYS	3.9
6	F	94	HIS	3.9
7	T	5	LYS	3.8
7	T	2	SER	3.8
6	F	1	ALA	3.7
1	N	57	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
7	G	37	LEU	3.5
2	O	90	ILE	3.4
7	G	36	TRP	3.3
8	H	42	ALA	3.2
3	C	37	PHE	3.1
7	T	6	GLY	3.0
10	W	52	TRP	3.0
9	I	21	ILE	2.9
1	A	297	MET	2.9
1	N	2	PHE	2.9
5	E	108	LYS	2.9
9	I	37	PHE	2.9
11	K	16	ALA	2.9
1	N	397	PHE	2.8
8	U	8	ILE	2.8
7	T	1	ALA	2.8
11	X	17	VAL	2.8
12	Y	37	PHE	2.7
7	T	8	HIS	2.7
9	V	63	MET	2.7
11	K	6	ALA	2.6
11	X	13	TYR	2.6
4	Q	95	LEU	2.5
4	Q	126	MET	2.5
7	T	7	ASP	2.5
8	H	44	THR	2.5
11	X	38	ILE	2.5
4	Q	103	VAL	2.5
1	N	3	ILE	2.4
9	V	2	THR	2.4
2	O	43	SER	2.4
6	S	98	HIS	2.4
4	Q	66	GLU	2.3
4	Q	4	SER	2.2
4	Q	89	ILE	2.2
4	D	71	MET	2.2
8	H	57	ARG	2.2
3	P	22	LEU	2.2
5	E	98	ILE	2.2
7	T	10	GLY	2.1
4	Q	7	LYS	2.1
9	I	5	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	124	LEU	2.1
3	C	197	PHE	2.1
4	D	73	ARG	2.1
4	D	70	GLU	2.0
3	C	193	TYR	2.0
4	Q	31	LYS	2.0
12	Y	26	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.43	0.15	100,128,158,158	0
7	TPO	T	11	11/12	0.60	0.15	110,133,150,157	0
9	SAC	I	1	9/10	0.70	0.11	105,118,134,139	0
9	SAC	V	1	9/10	0.74	0.13	139,151,162,164	0
1	FME	N	1	10/11	0.81	0.17	75,79,131,135	0
1	FME	A	1	10/11	0.91	0.14	53,68,109,123	0
2	FME	O	1	10/11	0.97	0.09	50,55,65,65	0
2	FME	B	1	10/11	0.98	0.07	46,51,52,55	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	UNX	C	301	1/1	0.64	0.52	19,19,19,19	1
27	CDL	G	102	100/100	0.78	0.24	78,118,150,150	0
19	TGL	D	201	63/63	0.80	0.25	60,99,130,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	TGL	Q	201	63/63	0.80	0.29	72,107,141,149	0
27	CDL	T	102	100/100	0.80	0.26	64,118,150,150	0
21	EDO	C	309	4/4	0.81	0.13	74,80,83,84	0
25	PEK	B	304	53/53	0.82	0.21	58,127,150,150	0
20	PGV	N	608	51/51	0.83	0.19	70,109,144,150	0
25	PEK	C	308	53/53	0.83	0.21	68,122,150,150	0
19	TGL	A	607	63/63	0.83	0.22	53,93,127,141	0
21	EDO	N	611	4/4	0.83	0.23	79,84,87,95	0
23	CHD	W	101	29/29	0.83	0.17	85,138,150,150	0
27	CDL	P	303	100/100	0.84	0.16	55,127,150,150	0
23	CHD	J	101	29/29	0.84	0.14	79,102,129,130	0
25	PEK	C	306	53/53	0.85	0.20	63,117,150,150	0
19	TGL	N	609	63/63	0.85	0.20	57,100,138,150	0
25	PEK	G	103	53/53	0.85	0.16	68,116,150,150	0
20	PGV	Z	101	51/51	0.85	0.26	63,121,150,150	0
27	CDL	C	303	100/100	0.85	0.17	57,114,156,159	0
20	PGV	A	609	51/51	0.85	0.22	64,103,157,158	0
24	PSC	O	302	52/52	0.85	0.23	67,130,150,150	0
21	EDO	C	312	4/4	0.85	0.15	92,93,108,109	0
20	PGV	C	307	51/51	0.86	0.17	57,105,146,150	0
21	EDO	I	101	4/4	0.86	0.16	72,74,89,95	0
19	TGL	Y	101	63/63	0.86	0.21	70,105,147,150	0
21	EDO	S	102	4/4	0.86	0.15	71,73,74,87	0
23	CHD	P	304	29/29	0.87	0.11	73,92,104,114	0
21	EDO	K	103	4/4	0.87	0.18	91,97,99,99	0
21	EDO	T	103	4/4	0.88	0.15	87,92,97,100	0
24	PSC	B	303	52/52	0.88	0.20	71,129,150,150	0
19	TGL	L	101	63/63	0.88	0.21	53,87,129,144	0
21	EDO	L	103	4/4	0.88	0.16	76,83,84,90	0
21	EDO	C	311	4/4	0.89	0.09	74,76,81,97	0
21	EDO	A	613	4/4	0.89	0.16	56,63,74,80	0
21	EDO	P	306	4/4	0.90	0.17	69,70,80,84	0
23	CHD	C	304	29/29	0.90	0.09	74,98,117,117	0
21	EDO	P	307	4/4	0.90	0.08	88,89,91,94	0
21	EDO	K	101	4/4	0.90	0.14	84,86,93,96	0
29	DMU	Z	102	33/33	0.90	0.10	64,81,111,121	0
21	EDO	N	610	4/4	0.92	0.12	63,71,74,75	0
21	EDO	A	611	4/4	0.93	0.16	81,81,82,88	0
21	EDO	N	612	4/4	0.93	0.10	52,61,67,68	0
21	EDO	A	612	4/4	0.94	0.25	58,59,71,78	0
21	EDO	F	102	4/4	0.94	0.11	63,64,72,80	0
21	EDO	K	102	4/4	0.94	0.10	82,82,86,89	0

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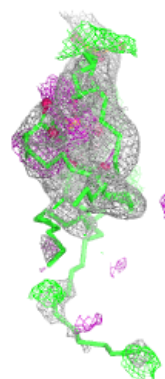
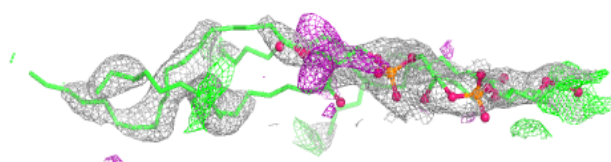
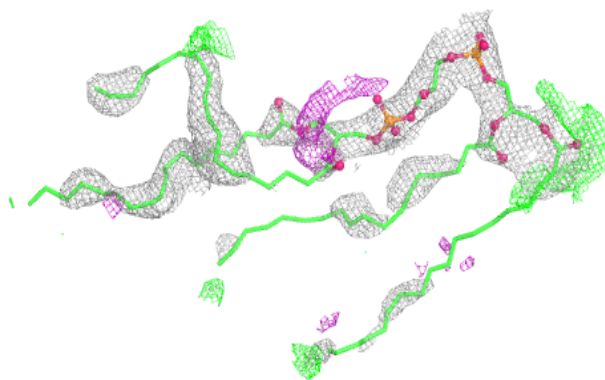
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	X	101	4/4	0.94	0.13	88,102,104,111	0
26	UNX	P	301	1/1	0.95	0.21	23,23,23,23	1
21	EDO	L	102	4/4	0.95	0.10	78,80,81,83	0
29	DMU	M	101	33/33	0.95	0.09	56,69,89,103	0
23	CHD	P	305	29/29	0.95	0.07	42,47,53,53	0
23	CHD	C	305	29/29	0.96	0.06	41,46,54,59	0
23	CHD	G	104	29/29	0.96	0.07	39,46,50,64	0
21	EDO	G	105	4/4	0.96	0.15	59,70,73,73	0
21	EDO	C	310	4/4	0.96	0.12	63,69,77,80	0
21	EDO	B	305	4/4	0.97	0.23	52,56,62,66	0
21	EDO	A	610	4/4	0.97	0.09	44,47,55,57	0
20	PGV	C	302	51/51	0.97	0.09	41,54,96,101	0
25	PEK	G	101	53/53	0.97	0.12	44,65,105,130	0
20	PGV	P	302	51/51	0.97	0.10	40,58,132,137	0
25	PEK	T	101	53/53	0.97	0.10	48,72,118,128	0
20	PGV	N	607	51/51	0.97	0.10	41,60,86,93	0
23	CHD	B	302	29/29	0.98	0.06	40,47,52,65	0
18	CMO	A	606	2/2	0.98	0.10	34,34,34,48	0
18	CMO	N	606	2/2	0.98	0.10	43,43,43,49	0
20	PGV	A	608	51/51	0.98	0.07	38,57,76,78	0
14	HEA	A	601	60/60	0.98	0.06	31,41,59,66	0
14	HEA	N	601	60/60	0.98	0.07	41,50,67,74	0
14	HEA	N	602	60/60	0.98	0.06	38,44,52,56	0
16	MG	N	604	1/1	0.98	0.03	46,46,46,46	0
17	NA	N	605	1/1	0.99	0.03	52,52,52,52	0
14	HEA	A	602	60/60	0.99	0.06	34,38,45,54	0
17	NA	A	605	1/1	0.99	0.03	43,43,43,43	0
22	CUA	O	301	2/2	0.99	0.06	55,55,55,57	0
15	CU	A	603	1/1	1.00	0.01	39,39,39,39	0
15	CU	N	603	1/1	1.00	0.02	45,45,45,45	0
28	ZN	F	101	1/1	1.00	0.03	52,52,52,52	0
28	ZN	S	101	1/1	1.00	0.02	56,56,56,56	0
22	CUA	B	301	2/2	1.00	0.02	43,43,43,44	0
16	MG	A	604	1/1	1.00	0.01	39,39,39,39	0

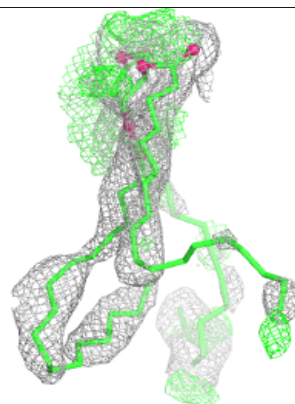
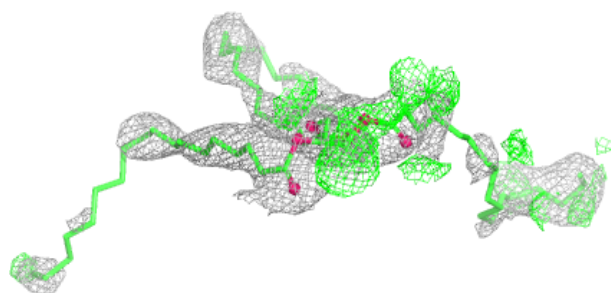
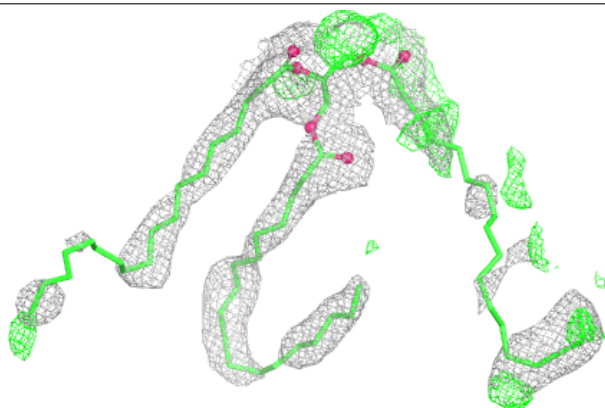
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CDL G 102:

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

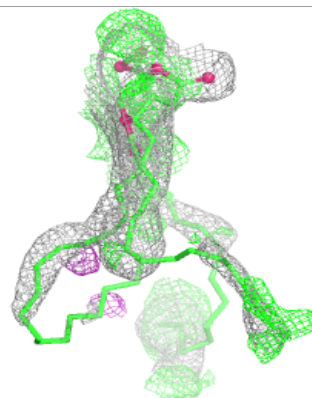
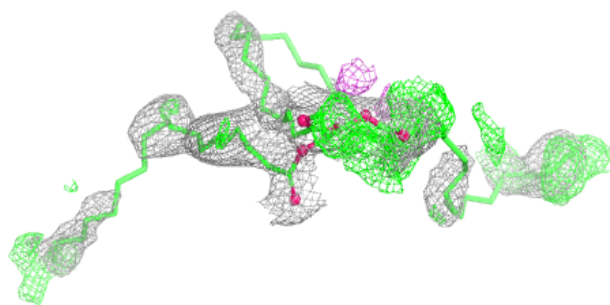
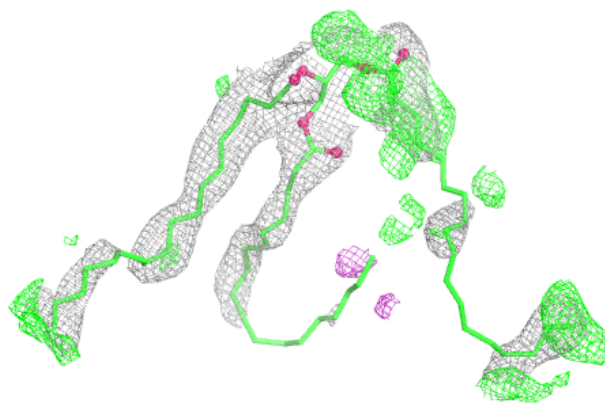
**Electron density around TGL D 201:**

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

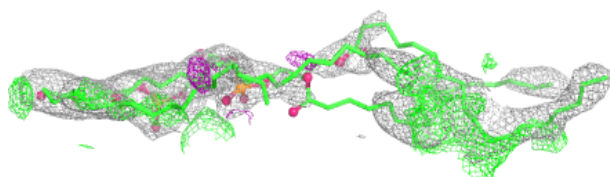
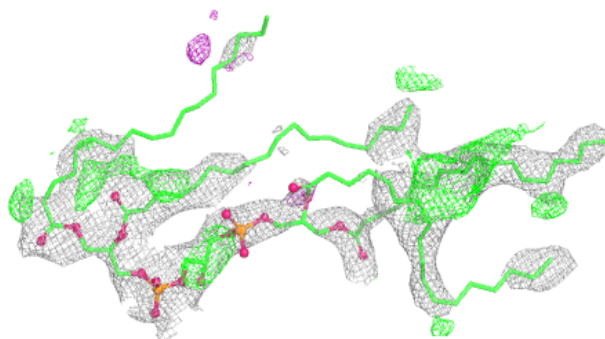


Electron density around TGL Q 201:

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

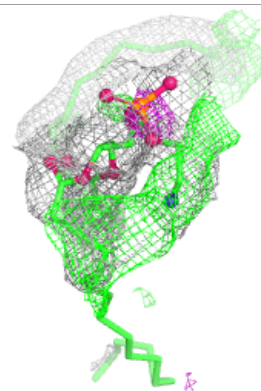
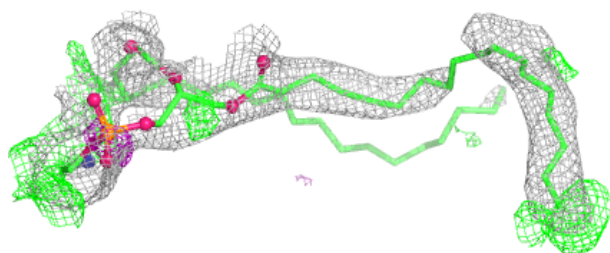
**Electron density around CDL T 102:**

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

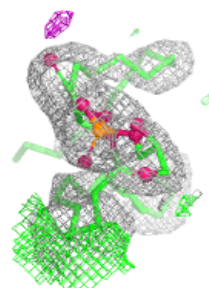
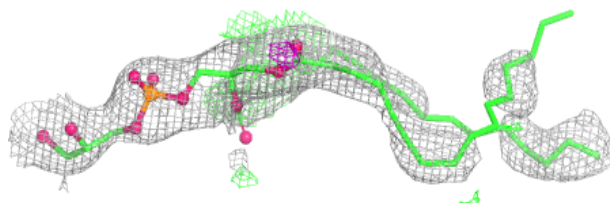
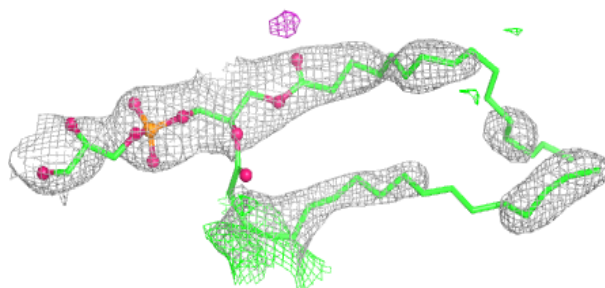


Electron density around PEK B 304:

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

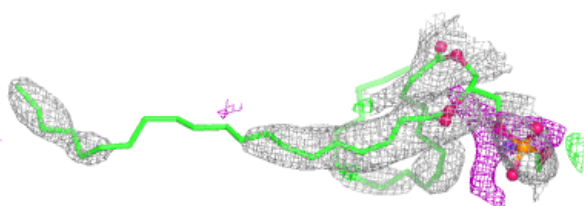
**Electron density around PGV N 608:**

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

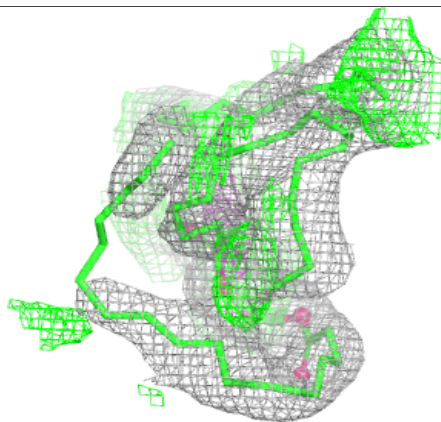
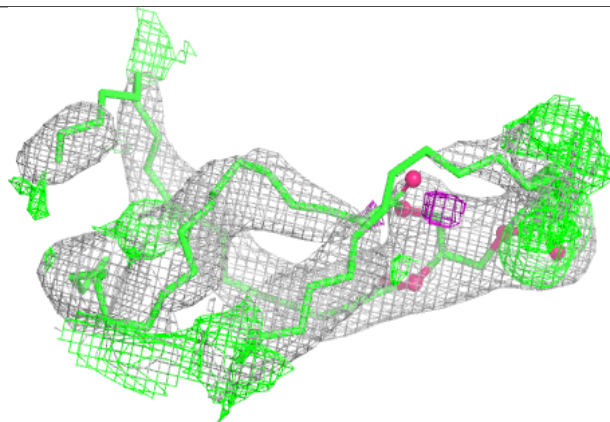
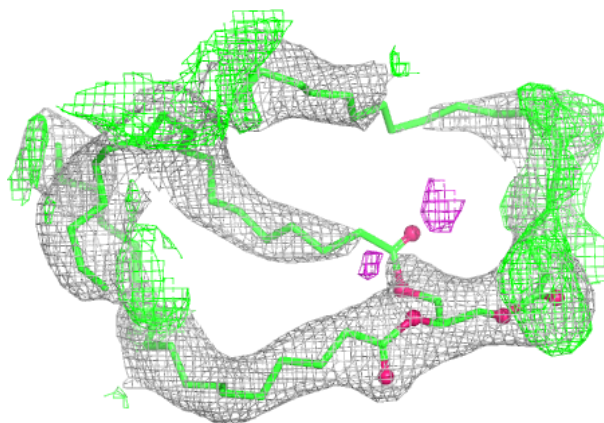


Electron density around PEK C 308:

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

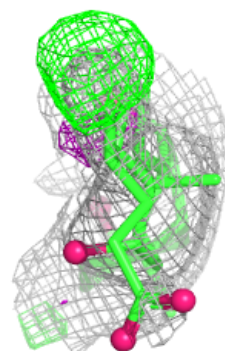
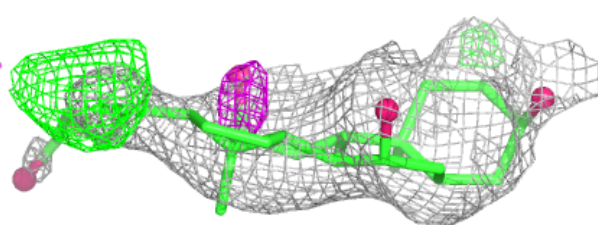
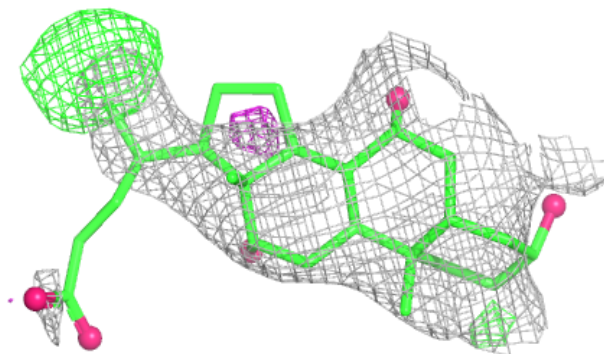
**Electron density around TGL A 607:**

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

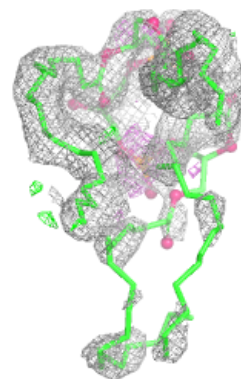
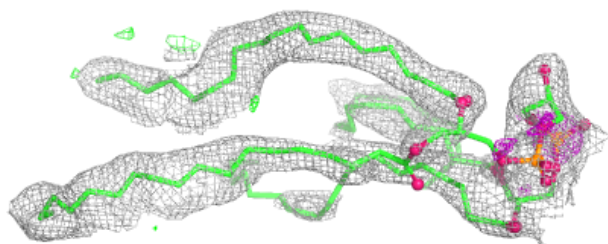
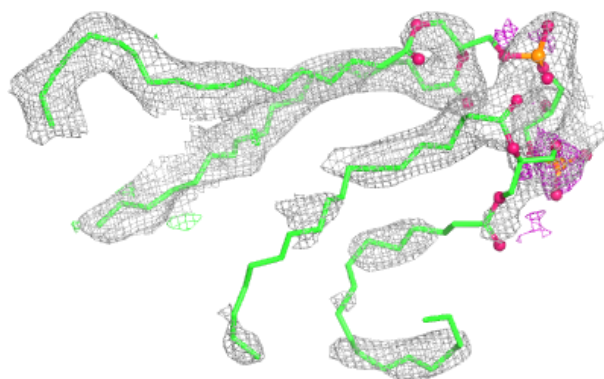


Electron density around CHD W 101:

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

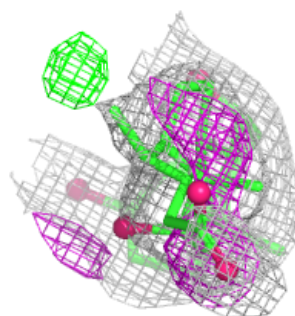
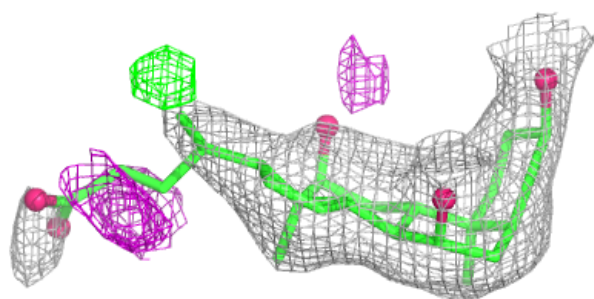
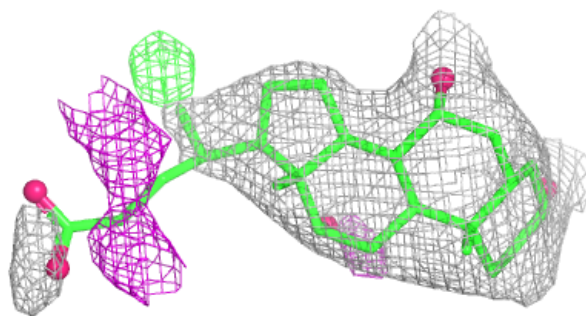
**Electron density around CDL P 303:**

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

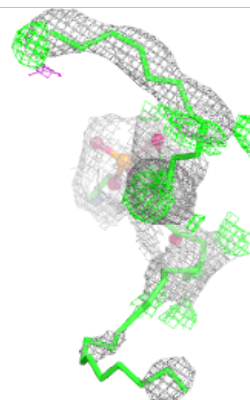
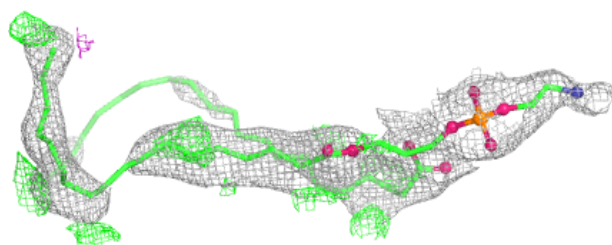
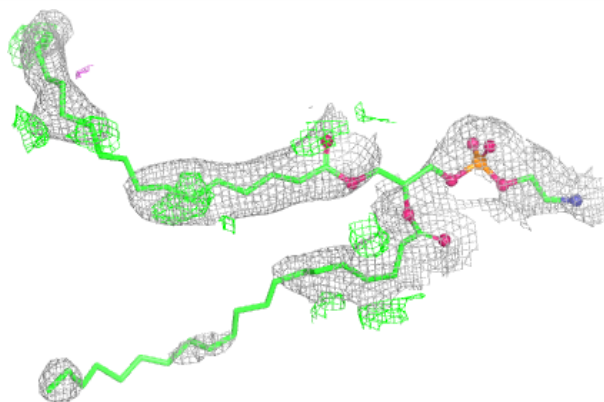


Electron density around CHD J 101:

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

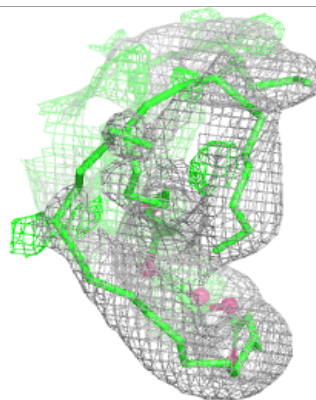
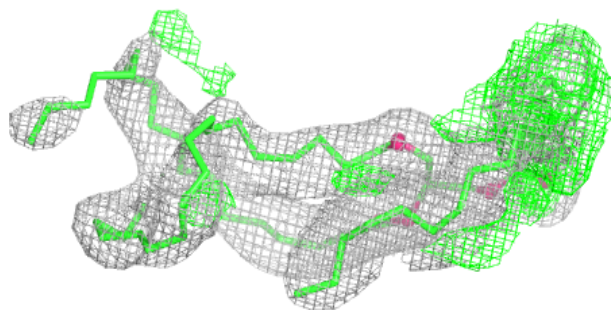
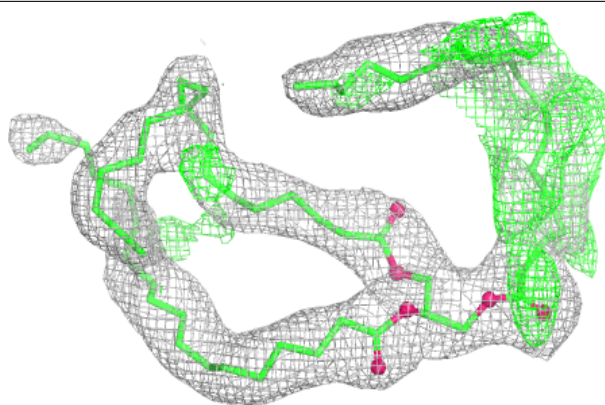
**Electron density around PEK C 306:**

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



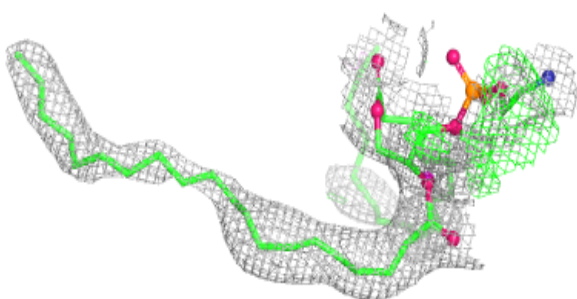
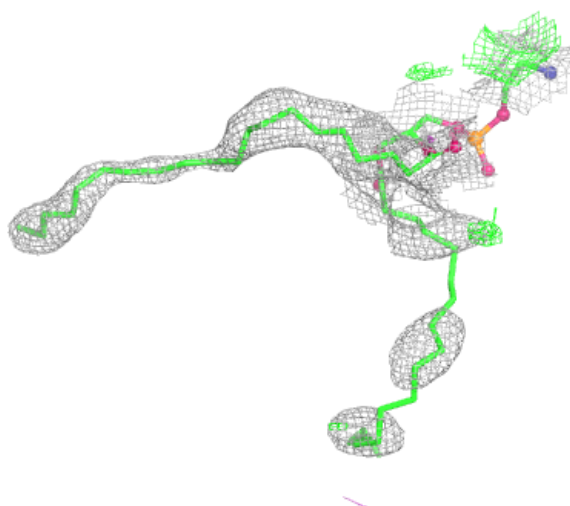
Electron density around TGL N 609:

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



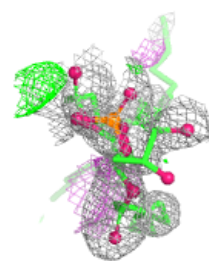
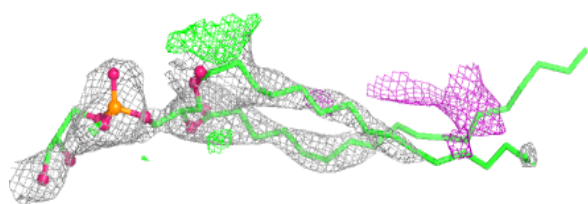
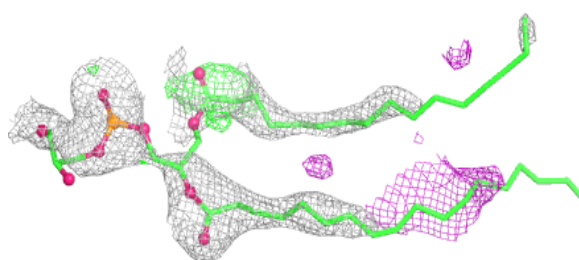
Electron density around PEK G 103:

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

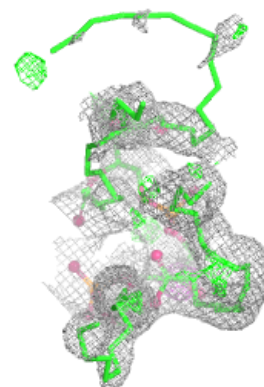
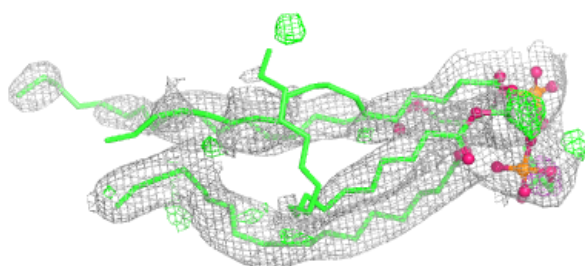
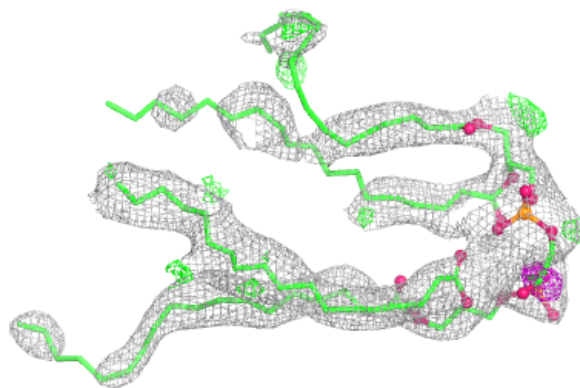


Electron density around PGV Z 101:

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

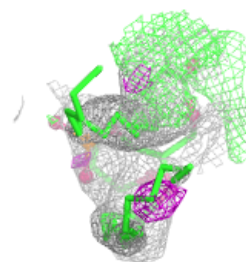
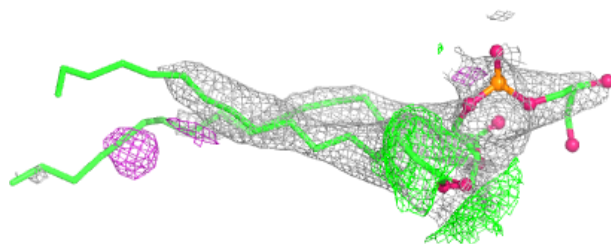
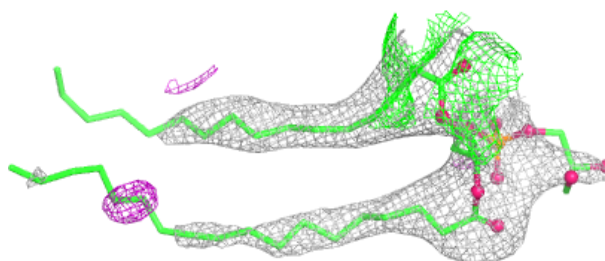
**Electron density around CDL C 303:**

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

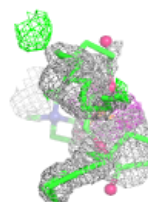
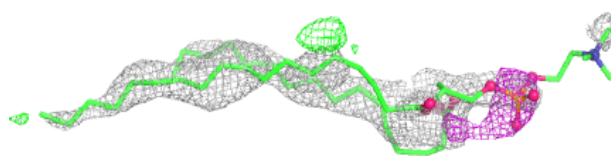
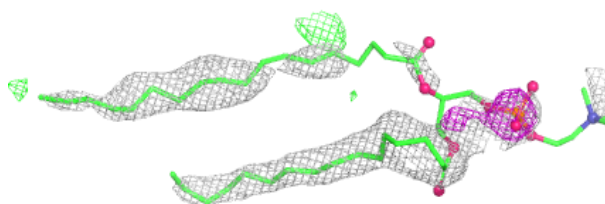


Electron density around PGV A 609:

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

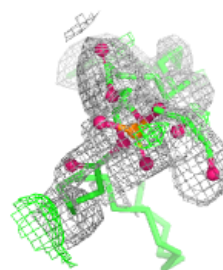
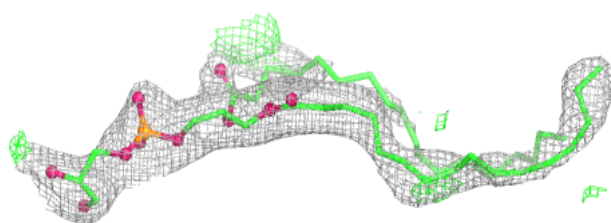
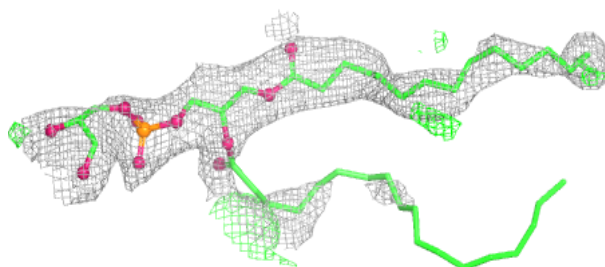
**Electron density around PSC O 302:**

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



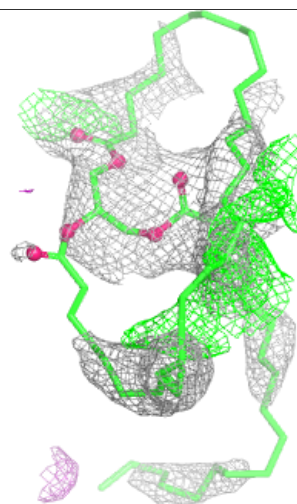
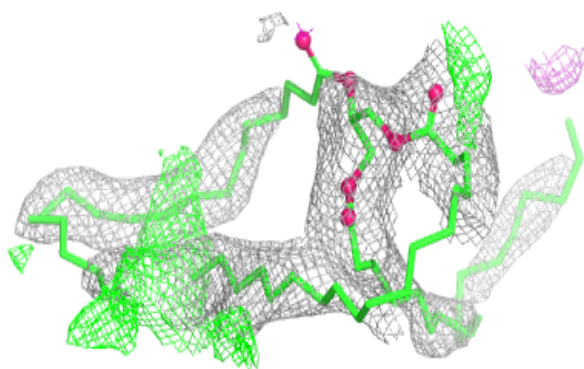
Electron density around PGV C 307:

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



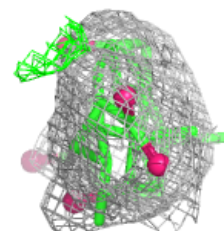
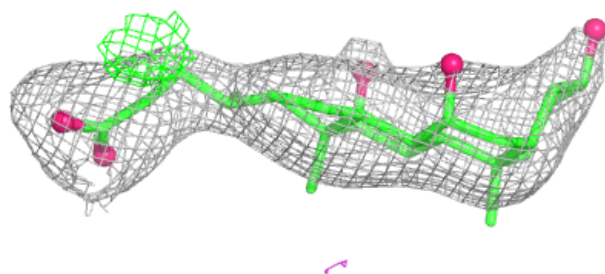
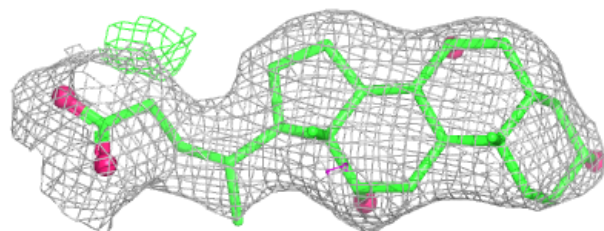
Electron density around TGL Y 101:

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

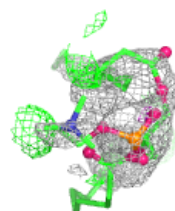
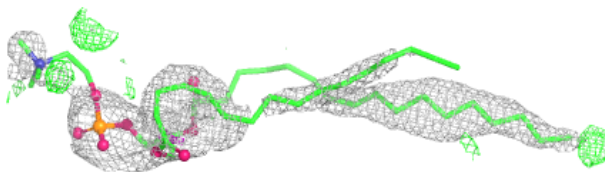
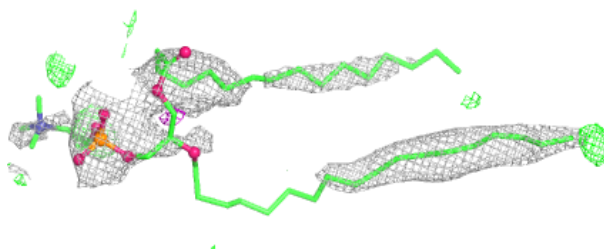


Electron density around CHD P 304:

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

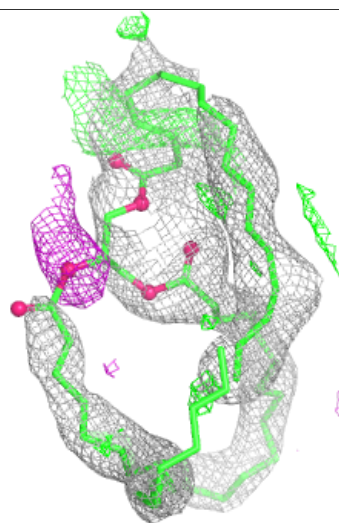
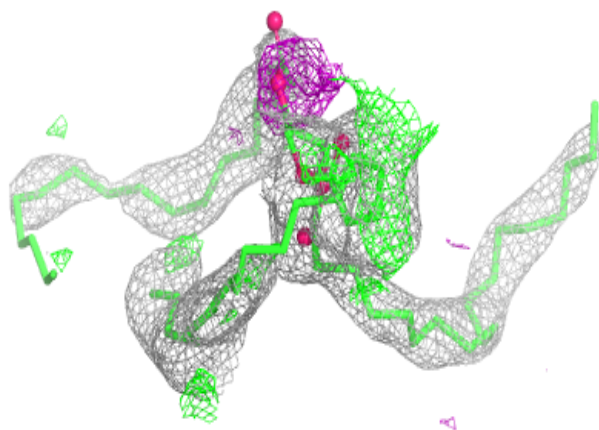
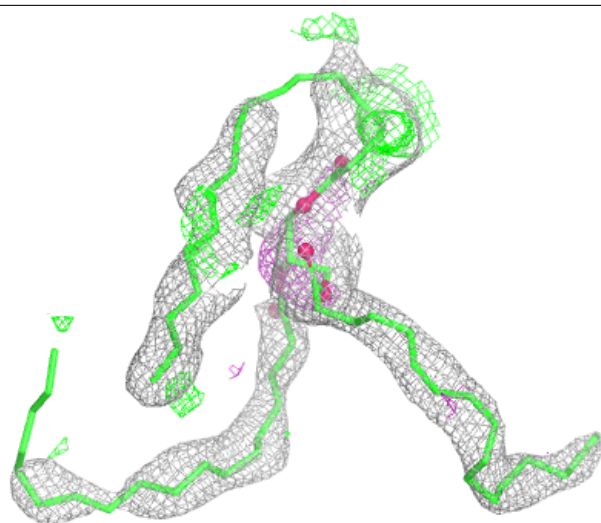
**Electron density around PSC B 303:**

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



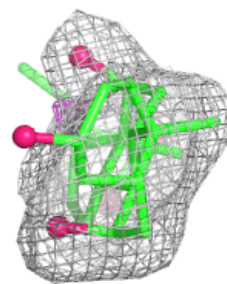
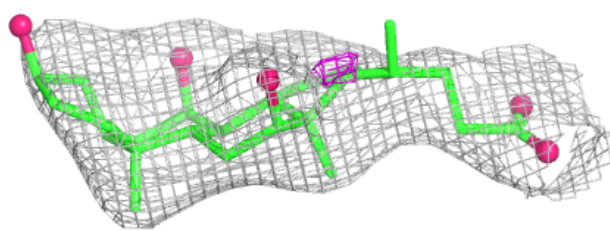
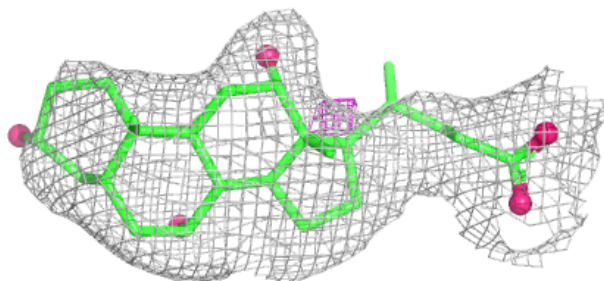
Electron density around TGL L 101:

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

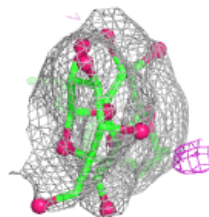
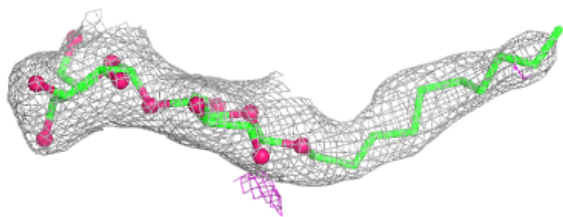
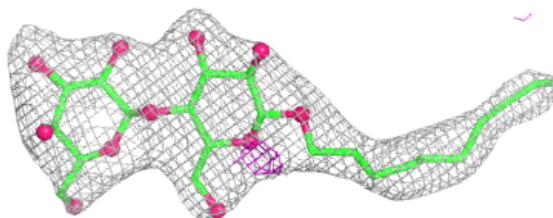


Electron density around CHD C 304:

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

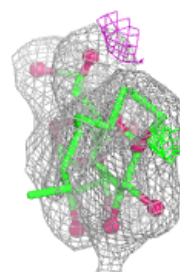
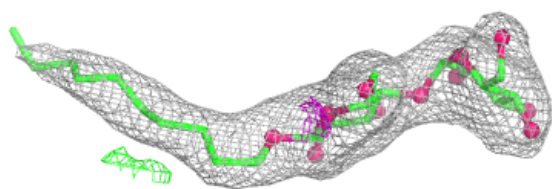
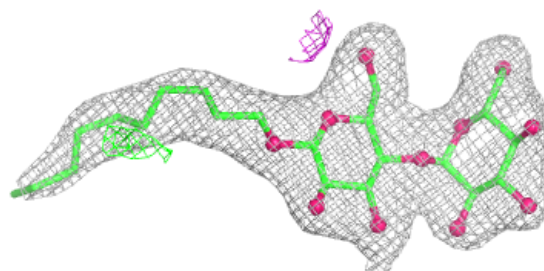
**Electron density around DMU Z 102:**

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

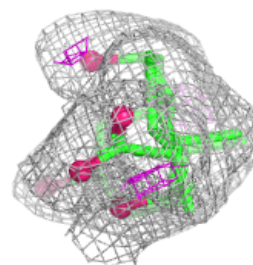
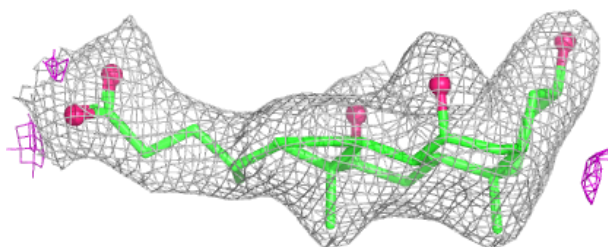
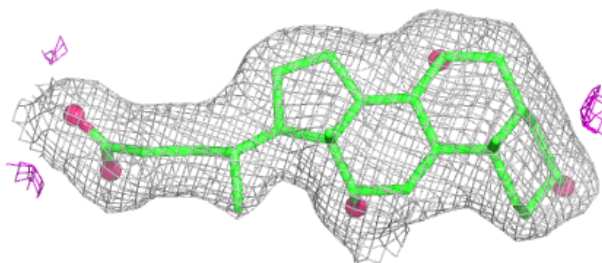


Electron density around DMU M 101:

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

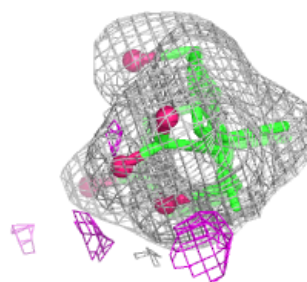
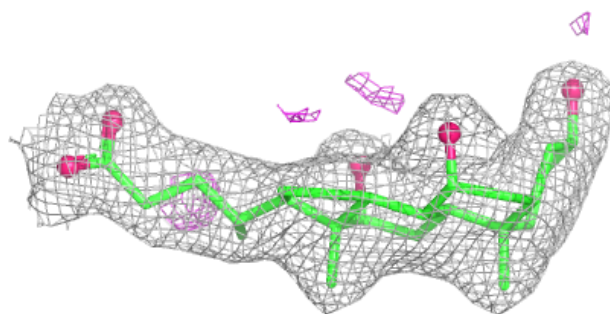
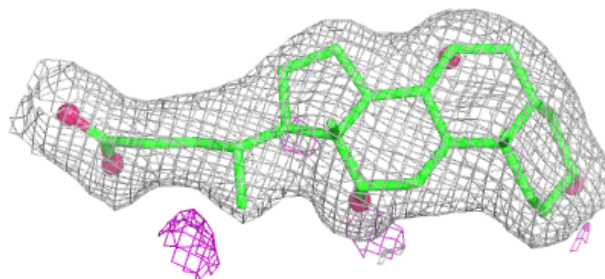
**Electron density around CHD P 305:**

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

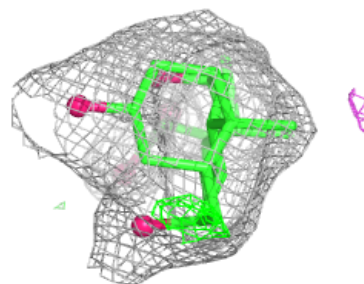
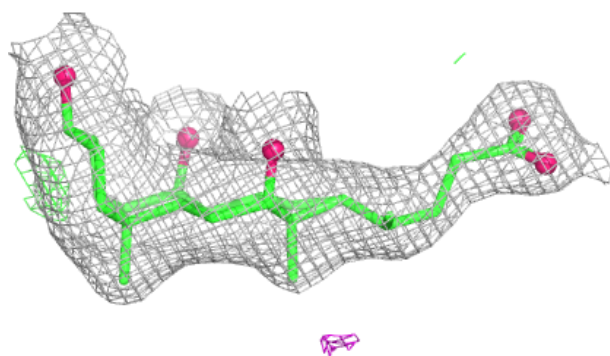
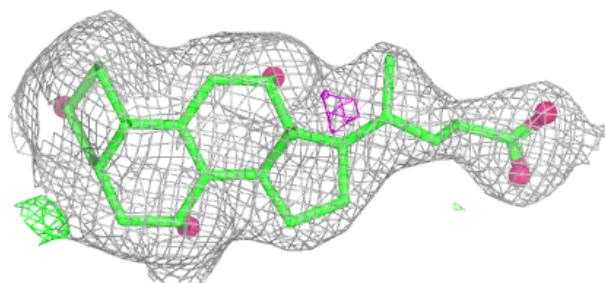


Electron density around CHD C 305:

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

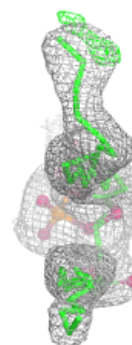
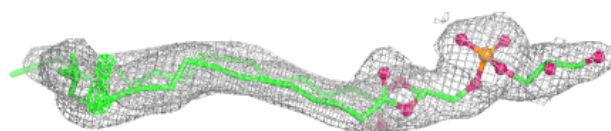
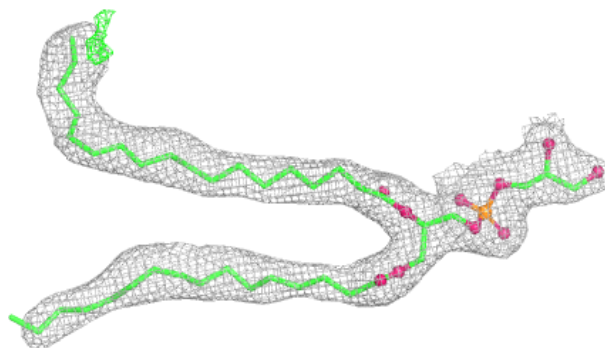
**Electron density around CHD G 104:**

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

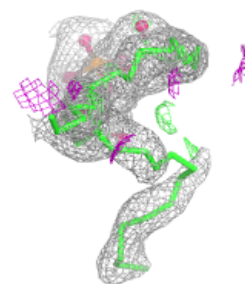
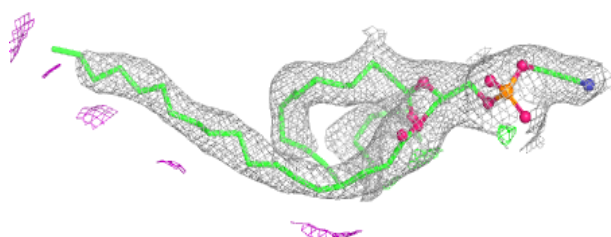
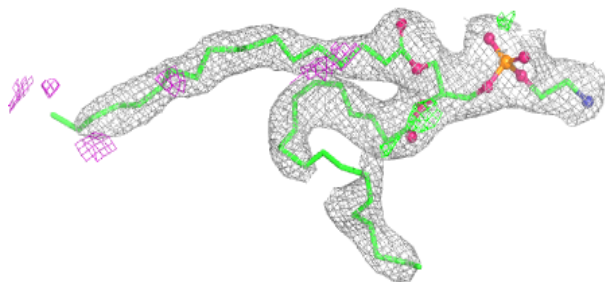


Electron density around PGV C 302:

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

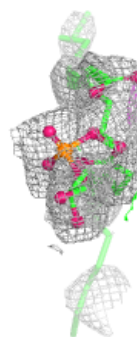
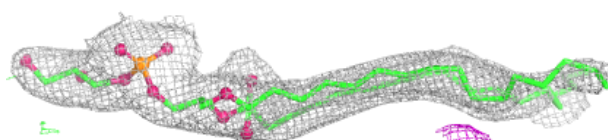
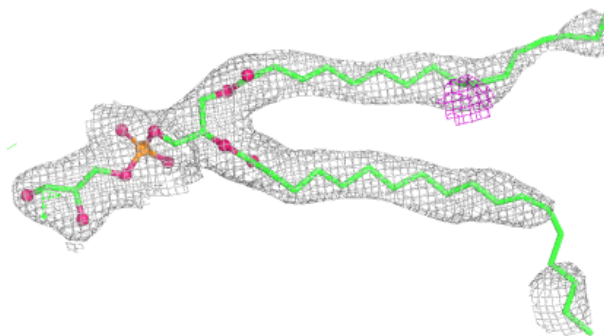
**Electron density around PEK G 101:**

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

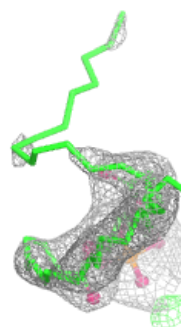
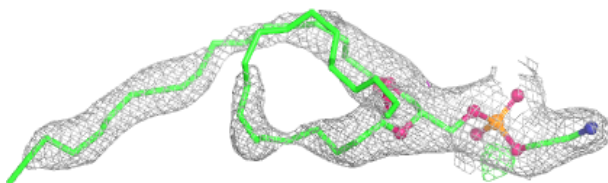
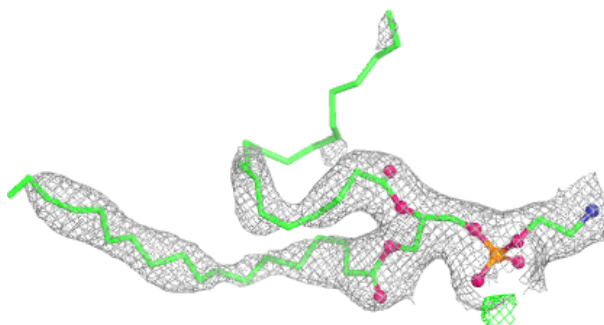


Electron density around PGV P 302:

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

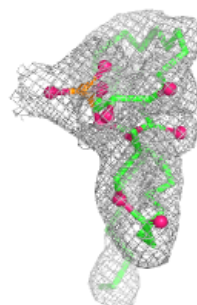
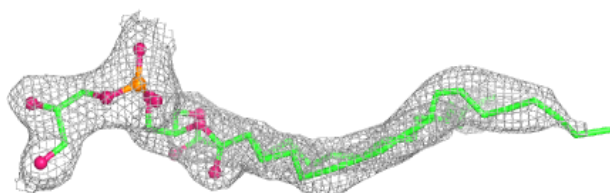
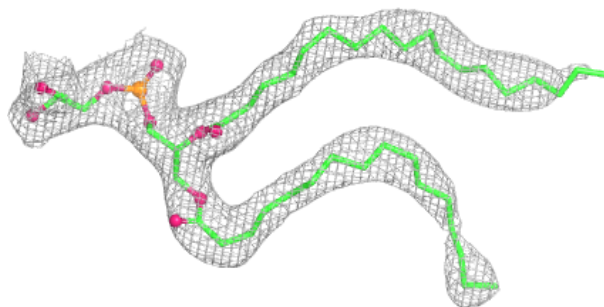
**Electron density around PEK T 101:**

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

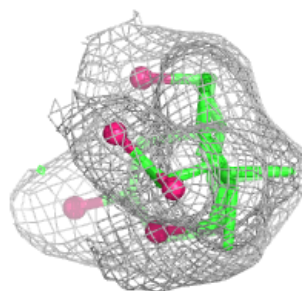
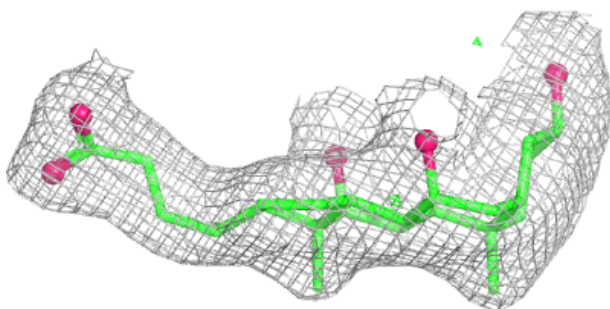
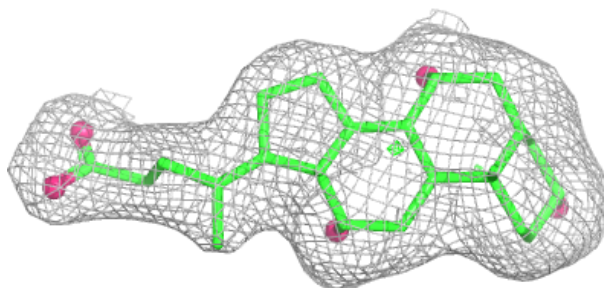


Electron density around PGV N 607:

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

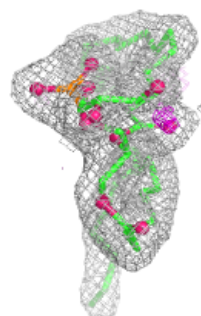
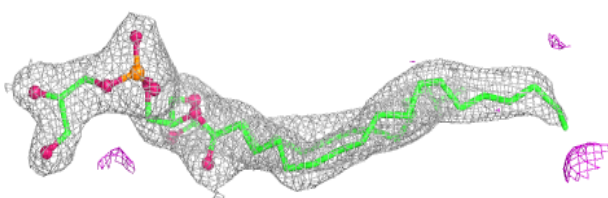
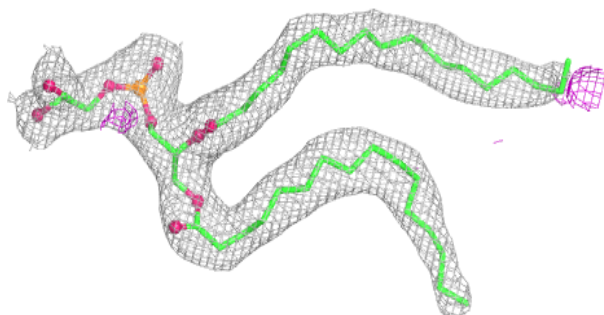
**Electron density around CHD B 302:**

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

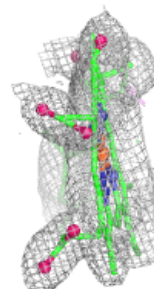
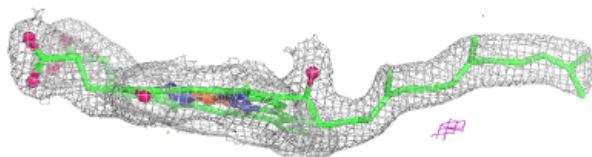
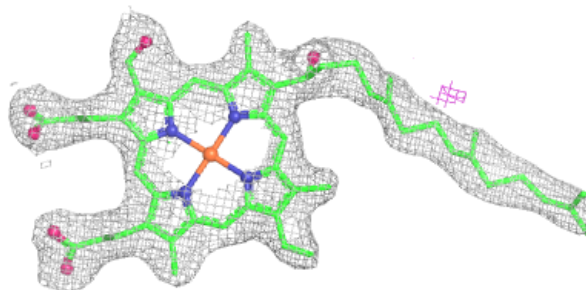


Electron density around PGV A 608:

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

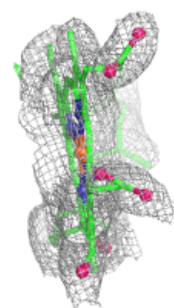
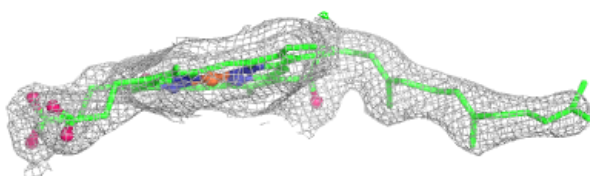
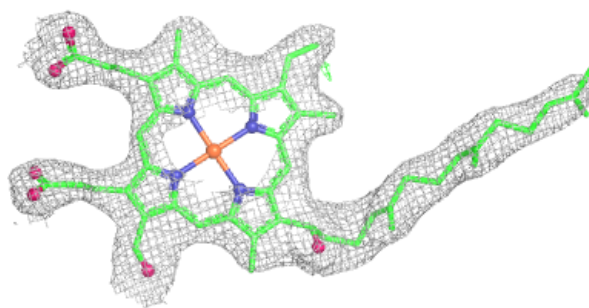
**Electron density around HEA A 601:**

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

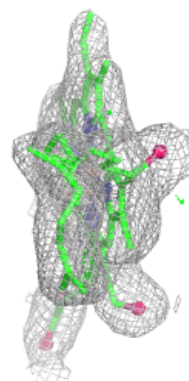
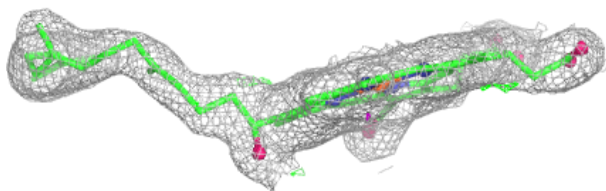
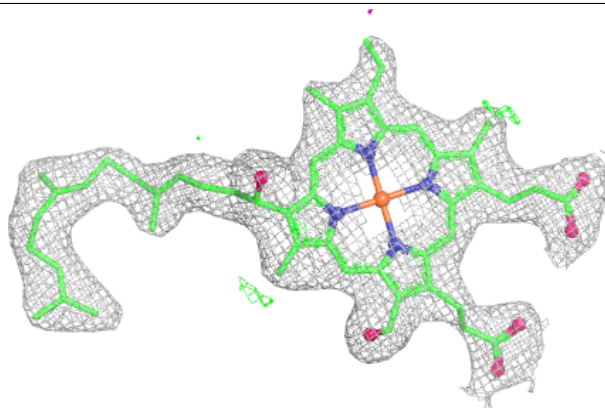


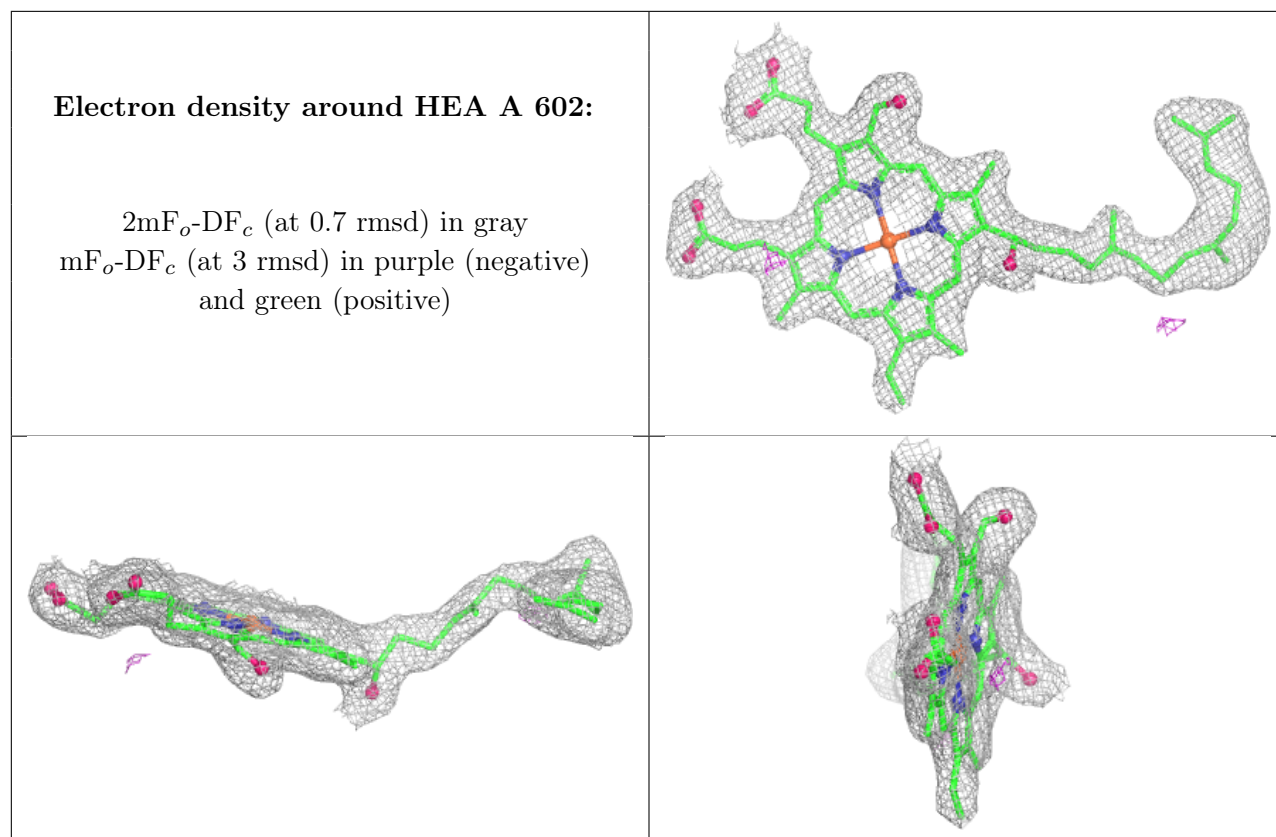
Electron density around HEA N 601:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.