



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 07:15 AM EDT

PDB ID : 8GCQ / pdb_00008gcq
Title : SFX structure of oxidized cytochrome c oxidase at 2.38 Angstrom resolution
Authors : Ishigami, I.; Yeh, S.-R.; Rousseau, D.L.
Deposited on : 2023-03-02
Resolution : 2.38 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:

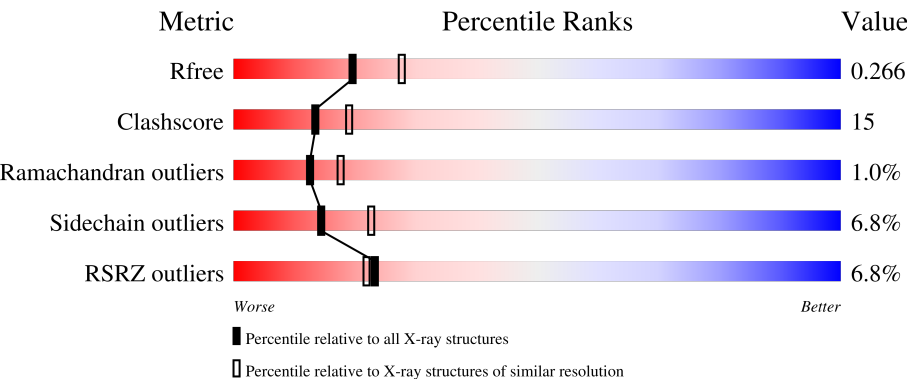
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	59%36%5%
1	N	514	4% 56%41%. .
2	B	227	3% 63%33%. .
2	O	227	11% 67%30%. .
3	C	261	% 67%30%. .

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Mol	Chain	Length	Quality of chain
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	47	
13	Z	47	

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
23	CHD	T	103	X	-	-	-
23	CHD	Y	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	DMU	C	309	X	-	-	-
26	DMU	C	310	X	-	-	-
26	DMU	G	101	X	-	-	-
26	DMU	M	101	X	-	-	-
26	DMU	P	302	X	-	-	-
26	DMU	Q	201	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 31457 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	0	0
			4027	2691	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 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	SER	-	expression tag	UNP P10175
Z	0	SER	-	expression tag	UNP P10175

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

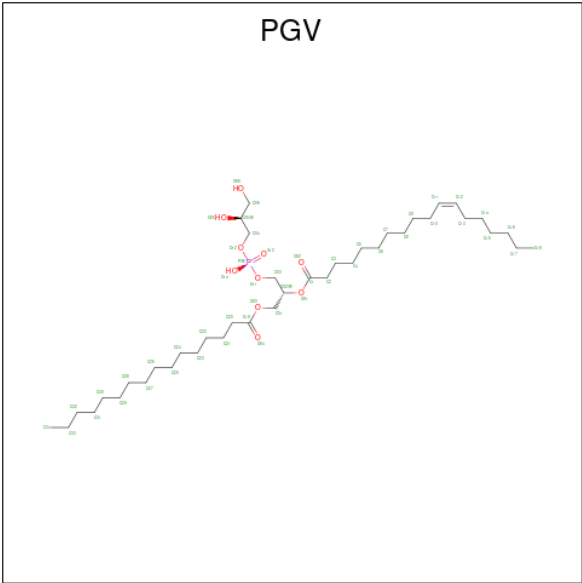
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 17 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P) (labeled as "Ligand of Interest" by depositor).

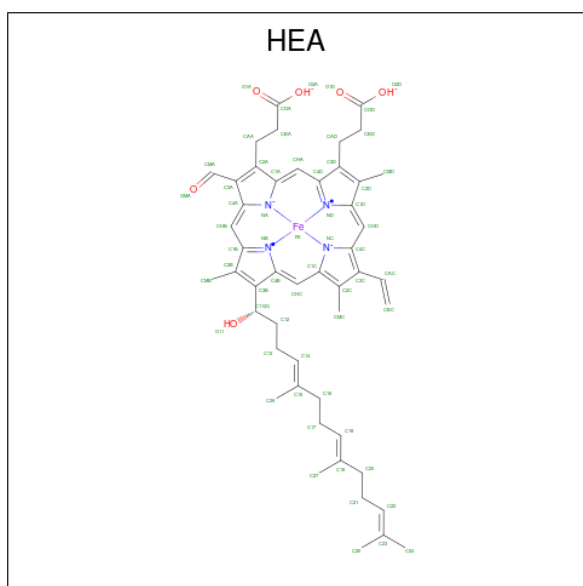


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C O P 51 40 10 1	0	0
17	C	1	Total C O P 51 40 10 1	0	0
17	C	1	Total C O P 51 40 10 1	0	0
17	H	1	Total C O P 51 40 10 1	0	0
17	N	1	Total C O P 51 40 10 1	0	0

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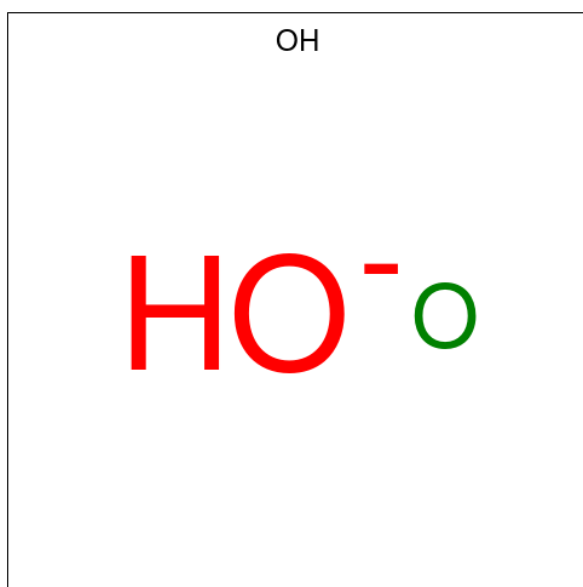
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	N	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



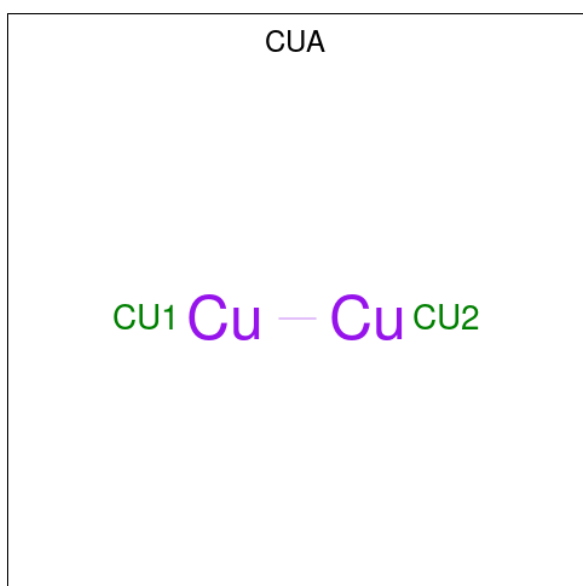
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
18	A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
18	N	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
18	N	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 19 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



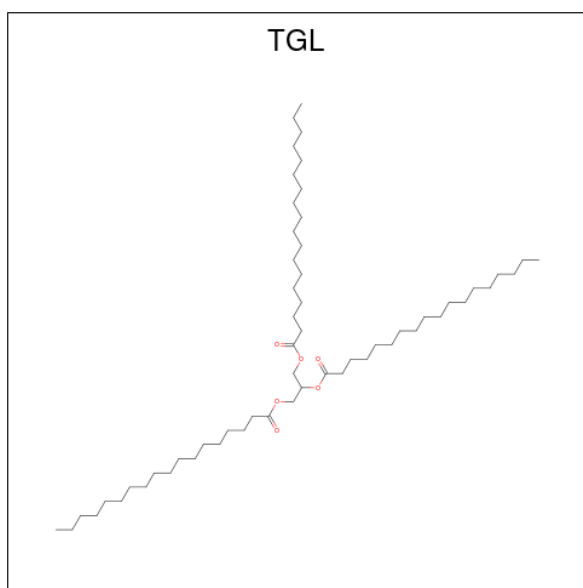
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total O 1 1	0	0
19	N	1	Total O 1 1	0	0

- Molecule 20 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



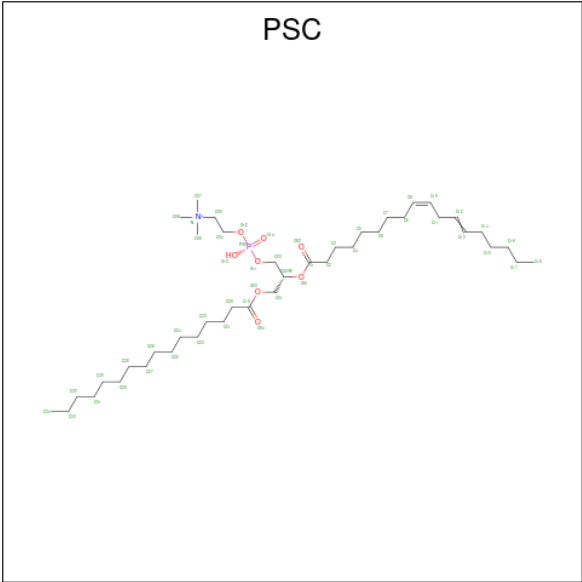
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	B	1	Total Cu 2 2	0	0
20	O	1	Total Cu 2 2	0	0

- Molecule 21 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



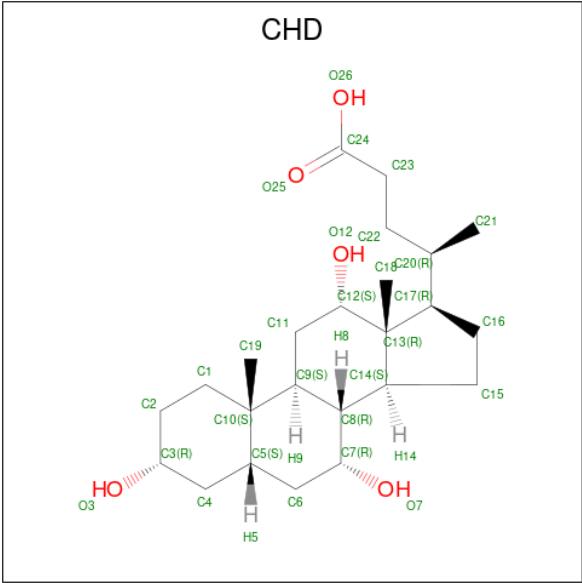
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 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: $C_{42}H_{81}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅) (labeled as "Ligand of Interest" by depositor).



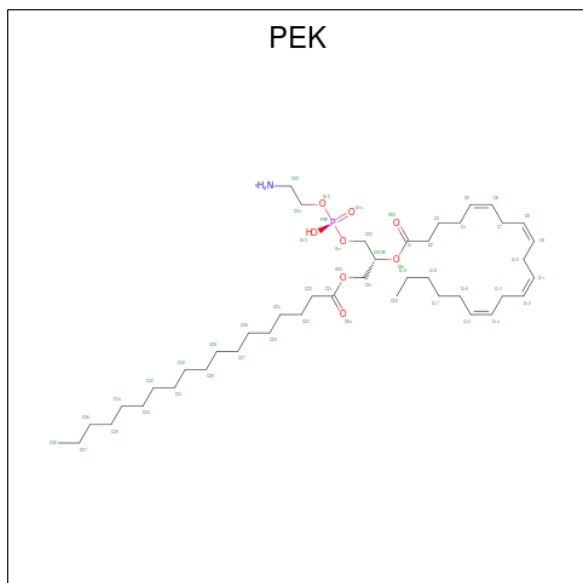
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



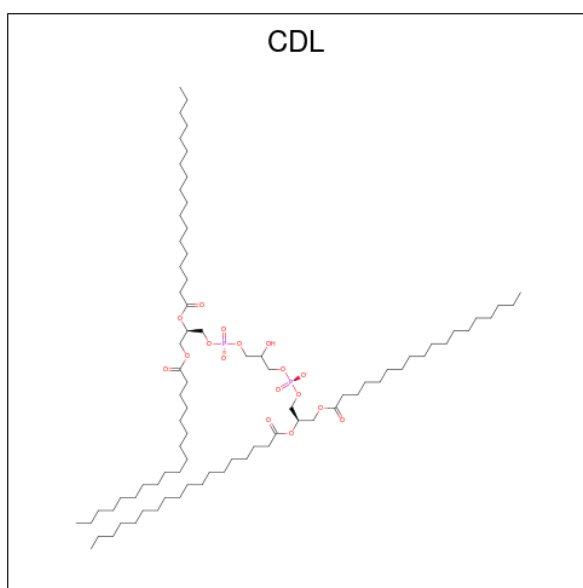
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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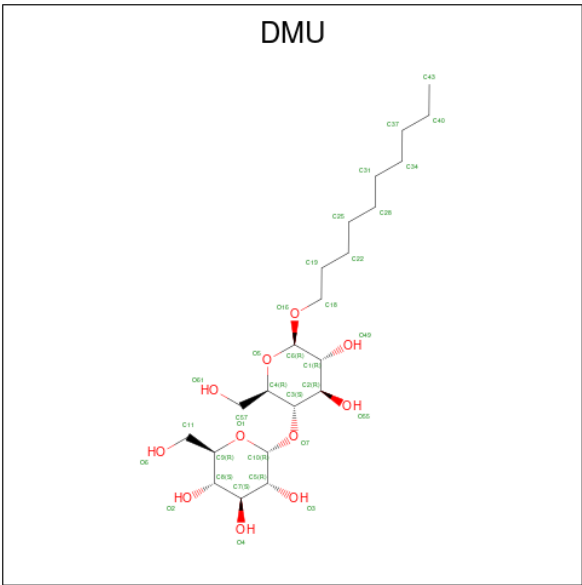
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$) (labeled as "Ligand of Interest" by depositor).

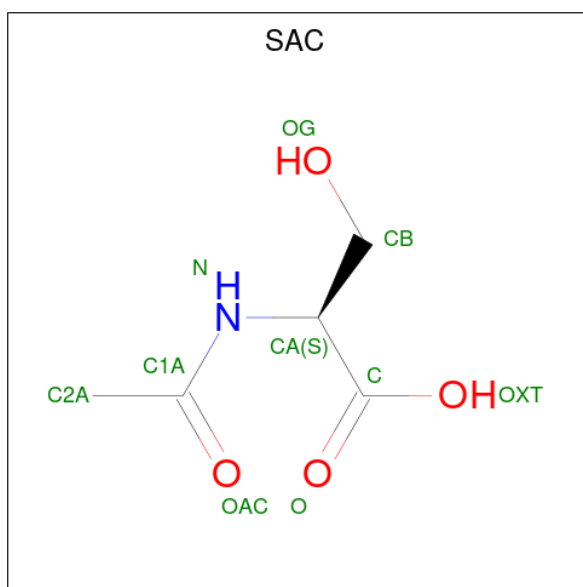


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	C	1	Total	C	O	0	0
			33	22	11		
26	G	1	Total	C	O	0	0
			33	22	11		
26	M	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	Q	1	Total	C	O	0	0
			33	22	11		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 is N-ACETYL-SERINE (CCD ID: SAC) (formula: C₅H₉NO₄) (labeled as "Lig- and of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	I	1	Total	C	N	O	0	0
			9	5	1	3		
28	V	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	104	Total	O	0	0
			104	104		
29	B	46	Total	O	0	0
			46	46		
29	C	44	Total	O	0	0
			44	44		
29	D	23	Total	O	0	0
			23	23		
29	E	23	Total	O	0	0
			23	23		
29	F	20	Total	O	0	0
			20	20		
29	G	13	Total	O	0	0
			13	13		
29	H	26	Total	O	0	0
			26	26		
29	I	8	Total	O	0	0
			8	8		
29	J	11	Total	O	0	0
			11	11		

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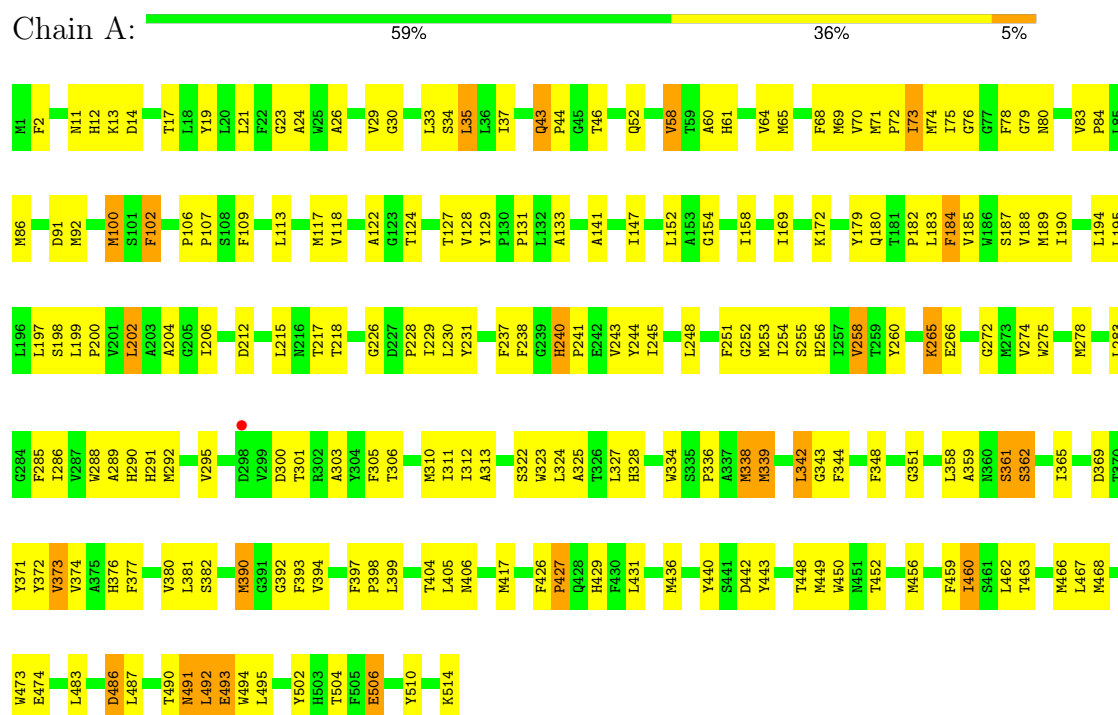
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	K	8	Total 8	O 8	0	0
29	L	13	Total 13	O 13	0	0
29	M	7	Total 7	O 7	0	0
29	N	74	Total 74	O 74	0	0
29	O	39	Total 39	O 39	0	0
29	P	40	Total 40	O 40	0	0
29	Q	28	Total 28	O 28	0	0
29	R	8	Total 8	O 8	0	0
29	S	19	Total 19	O 19	0	0
29	T	17	Total 17	O 17	0	0
29	U	7	Total 7	O 7	0	0
29	V	6	Total 6	O 6	0	0
29	W	5	Total 5	O 5	0	0
29	X	8	Total 8	O 8	0	0
29	Y	1	Total 1	O 1	0	0
29	Z	3	Total 3	O 3	0	0

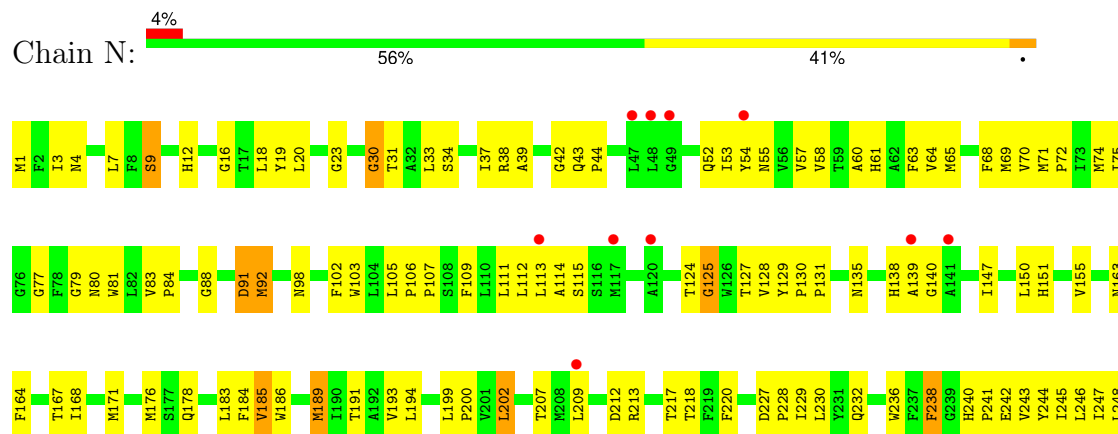
3 Residue-property plots [i](#)

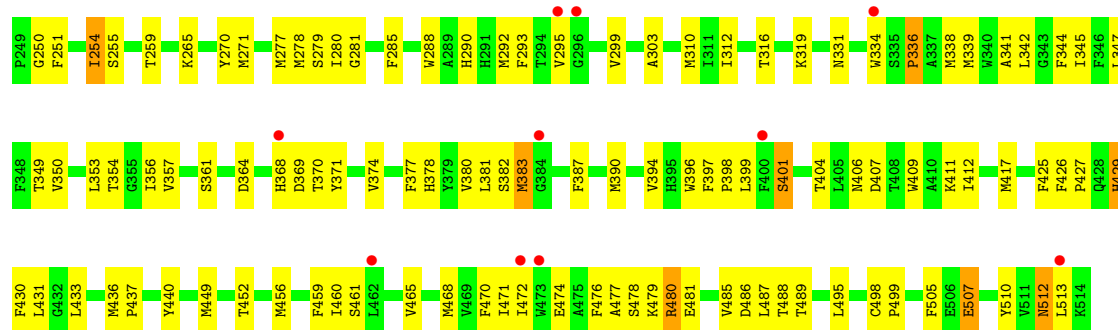
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

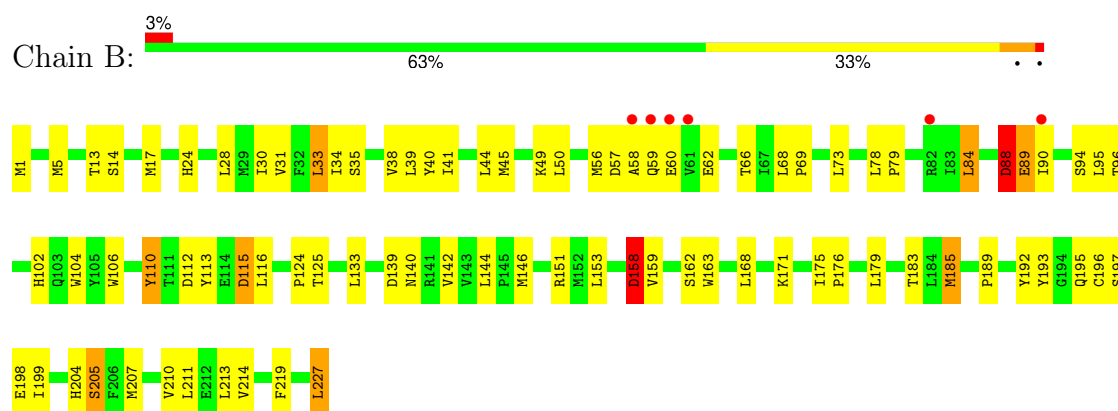


• Molecule 1: Cytochrome c oxidase subunit 1

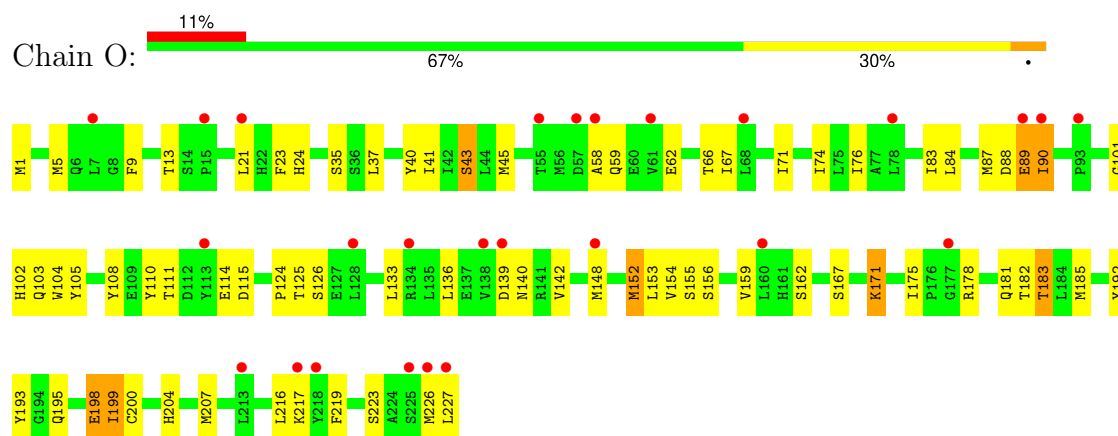




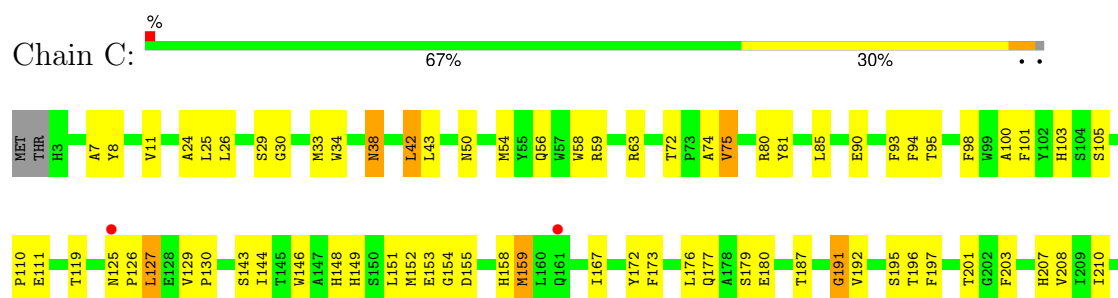
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

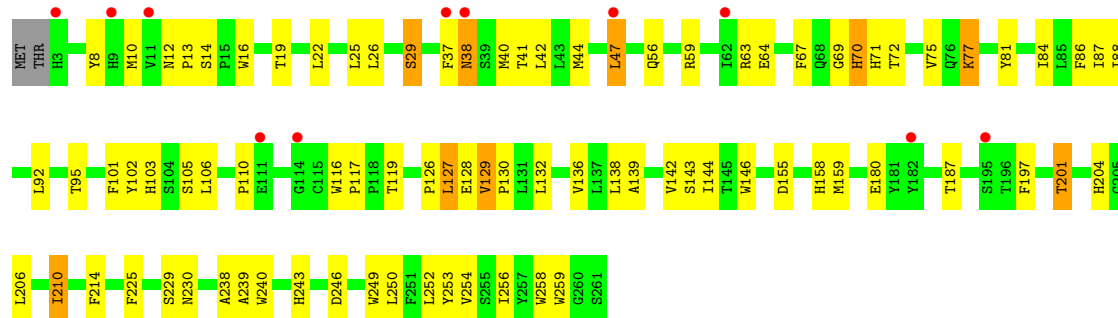


• Molecule 3: Cytochrome c oxidase subunit 3

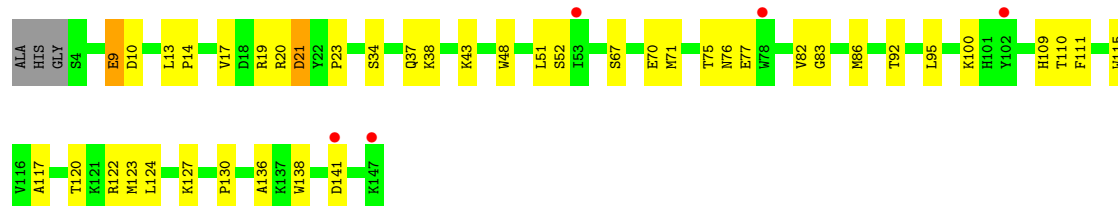




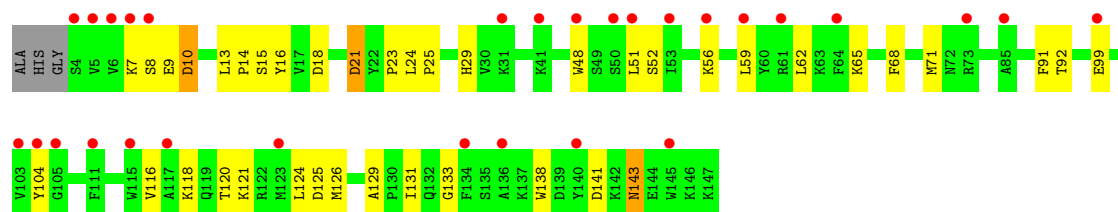
• Molecule 3: Cytochrome c oxidase subunit 3



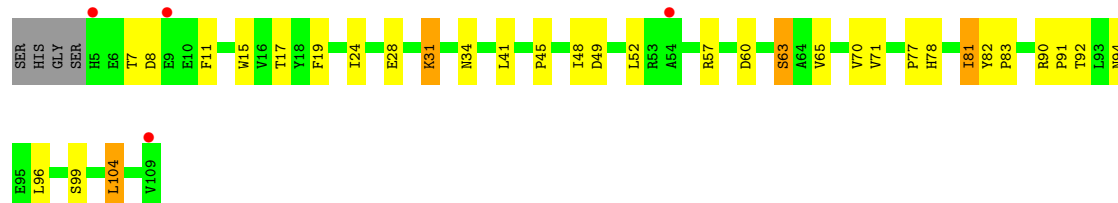
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



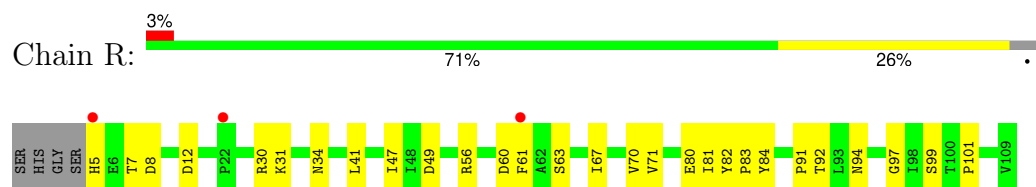
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



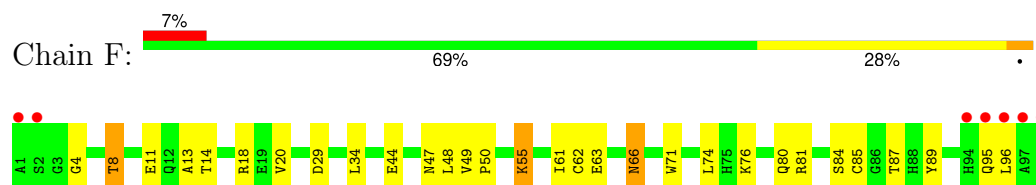
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



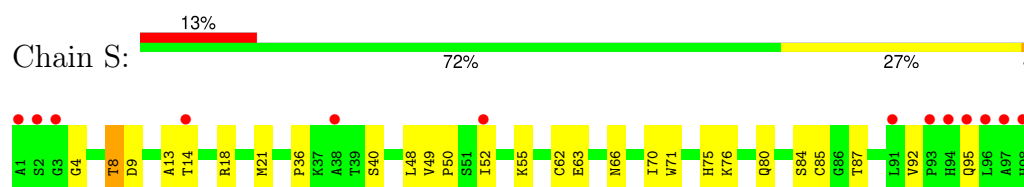
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



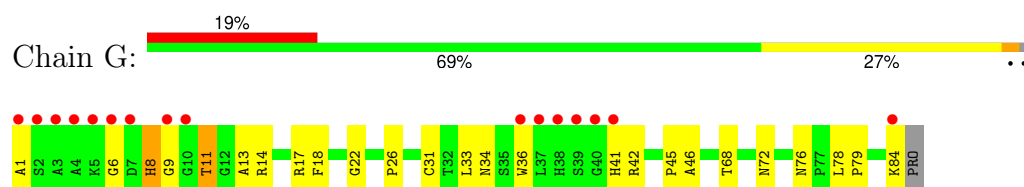
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



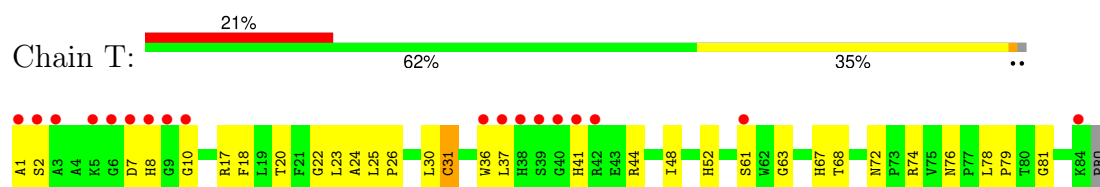
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



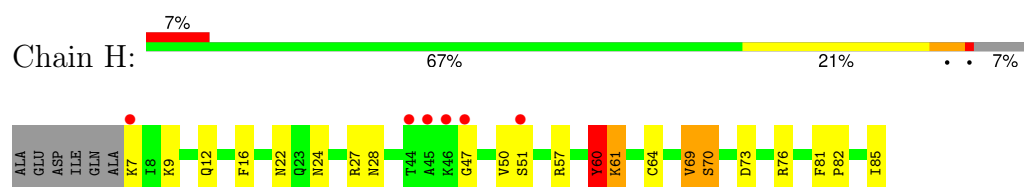
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



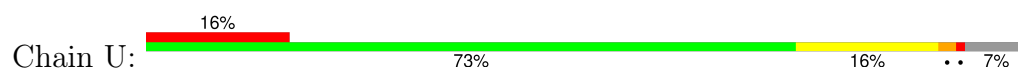
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

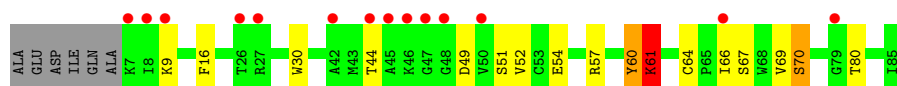


- Molecule 8: Cytochrome c oxidase subunit 6B1

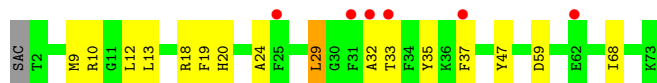
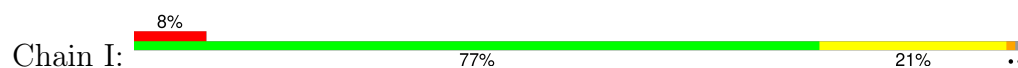


- Molecule 8: Cytochrome c oxidase subunit 6B1

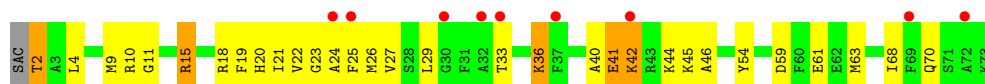




- Molecule 9: Cytochrome c oxidase subunit 6C



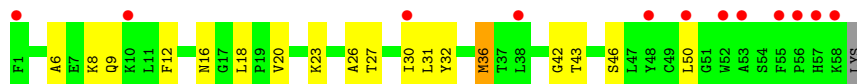
- Molecule 9: Cytochrome c oxidase subunit 6C



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



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



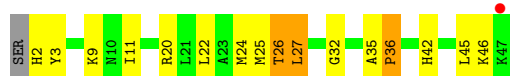
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



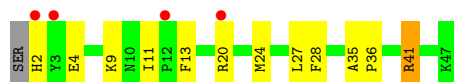
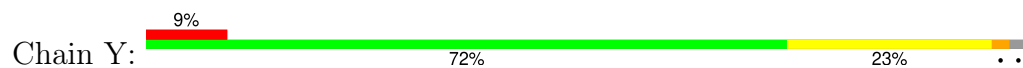
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



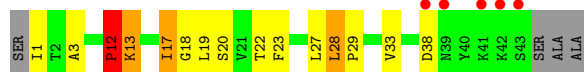
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	178.60Å 189.50Å 211.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.38 33.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.00-2.38) 99.7 (33.00-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.232 , 0.266 0.234 , 0.266	Depositor DCC
R_{free} test set	14182 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	31457	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: CDL, TPO, CHD, CU, PSC, SAC, FME, PEK, OH, ZN, CUA, TGL, HEA, NA, MG, DMU, PGV

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	1.15	5/4156 (0.1%)	1.65	34/5678 (0.6%)
1	N	1.09	0/4156	1.60	30/5678 (0.5%)
2	B	1.14	2/1860 (0.1%)	1.50	3/2534 (0.1%)
2	O	1.07	1/1860 (0.1%)	1.48	1/2534 (0.0%)
3	C	1.05	1/2197 (0.0%)	1.61	15/3005 (0.5%)
3	P	1.06	0/2197	1.60	13/3005 (0.4%)
4	D	1.09	0/1229	1.49	1/1658 (0.1%)
4	Q	1.07	0/1229	1.46	0/1658
5	E	1.03	0/871	1.56	3/1182 (0.3%)
5	R	1.01	0/871	1.56	4/1182 (0.3%)
6	F	1.09	0/765	1.47	1/1038 (0.1%)
6	S	1.11	1/765 (0.1%)	1.48	1/1038 (0.1%)
7	G	1.02	0/690	1.36	0/937
7	T	1.04	0/690	1.40	1/937 (0.1%)
8	H	1.09	1/682 (0.1%)	1.50	5/921 (0.5%)
8	U	0.99	0/682	1.46	2/921 (0.2%)
9	I	1.00	0/605	1.57	0/802
9	V	1.02	0/605	1.62	2/802 (0.2%)
10	J	1.07	0/471	1.70	6/636 (0.9%)
10	W	1.08	0/471	1.60	0/636
11	K	1.13	0/398	1.51	0/546
11	X	1.08	0/398	1.51	2/546 (0.4%)
12	L	1.09	0/393	1.53	2/526 (0.4%)
12	Y	1.03	0/393	1.48	2/526 (0.4%)
13	M	1.15	2/345 (0.6%)	1.61	2/470 (0.4%)
13	Z	1.02	0/345	1.47	2/470 (0.4%)
All	All	1.08	13/29324 (0.0%)	1.56	132/39866 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	12	PRO	C-O	-6.30	1.15	1.24
2	O	198	GLU	C-O	6.03	1.31	1.23
13	M	28	LEU	N-CA	5.97	1.50	1.46
3	C	43	LEU	C-O	5.81	1.30	1.24
1	A	265	LYS	C-O	-5.53	1.17	1.24
2	B	198	GLU	C-O	5.47	1.30	1.23
2	B	205	SER	C-O	5.30	1.30	1.24
8	H	24	ASN	C-O	5.23	1.30	1.24
6	S	49	VAL	N-CA	5.12	1.50	1.46
1	A	348	PHE	C-O	5.12	1.30	1.24
1	A	351	GLY	C-O	5.05	1.30	1.23
1	A	342	LEU	C-O	5.04	1.29	1.24
1	A	228	PRO	C-O	-5.00	1.17	1.24

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	VAL	N-CA-C	-7.33	103.19	110.30
1	A	240	HIS	CA-CB-CG	-7.29	106.51	113.80
1	A	184	PHE	N-CA-C	-7.26	103.37	111.28
1	A	58	VAL	O-C-N	7.15	128.92	121.91
1	N	336	PRO	CA-C-N	7.14	130.17	120.38
1	N	336	PRO	C-N-CA	7.14	130.17	120.38
1	N	61	HIS	CA-CB-CG	6.67	120.47	113.80
1	A	102	PHE	CA-CB-CG	-6.59	107.21	113.80
3	P	87	ILE	CA-C-N	6.16	129.22	120.53
3	P	87	ILE	C-N-CA	6.16	129.22	120.53
1	A	427	PRO	CB-CA-C	-6.16	102.69	111.68
1	A	240	HIS	N-CA-CB	6.13	116.21	110.39
6	S	4	GLY	CA-C-O	-6.02	118.30	122.22
1	N	92	MET	CA-C-N	5.91	128.13	120.44
1	N	92	MET	C-N-CA	5.91	128.13	120.44
12	L	3	TYR	CA-C-N	5.83	129.38	121.05
12	L	3	TYR	C-N-CA	5.83	129.38	121.05
1	A	133	ALA	CA-C-N	5.82	129.87	121.54
1	A	133	ALA	C-N-CA	5.82	129.87	121.54
3	C	225	PHE	CA-C-N	5.80	128.06	120.28
3	C	225	PHE	C-N-CA	5.80	128.06	120.28
1	A	506	GLU	N-CA-C	-5.78	104.98	111.28
3	P	42	LEU	CA-C-N	5.75	128.26	120.38
3	P	42	LEU	C-N-CA	5.75	128.26	120.38
10	J	35	THR	CA-C-N	5.72	127.95	120.28
10	J	35	THR	C-N-CA	5.72	127.95	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	22	THR	N-CA-C	-5.67	105.01	111.14
3	C	94	PHE	CA-C-O	-5.67	114.51	120.63
1	N	61	HIS	CB-CA-C	5.66	121.69	110.42
1	A	460	ILE	N-CA-C	-5.66	105.33	110.82
12	Y	41	ARG	CA-C-N	5.63	128.14	120.54
12	Y	41	ARG	C-N-CA	5.63	128.14	120.54
3	C	93	PHE	N-CA-C	-5.58	104.04	111.24
5	R	91	PRO	CA-C-N	5.58	128.02	120.38
5	R	91	PRO	C-N-CA	5.58	128.02	120.38
3	P	201	THR	N-CA-C	-5.57	105.36	111.82
1	A	275	TRP	CA-C-N	5.56	129.16	120.82
1	A	275	TRP	C-N-CA	5.56	129.16	120.82
3	C	93	PHE	CB-CA-C	5.56	120.03	110.86
1	N	114	ALA	CA-C-N	5.54	128.01	120.54
1	N	114	ALA	C-N-CA	5.54	128.01	120.54
1	A	442	ASP	CA-C-O	-5.53	115.15	121.40
1	N	429	HIS	O-C-N	5.49	128.01	122.09
1	A	58	VAL	CA-C-N	5.47	127.88	120.65
1	A	58	VAL	C-N-CA	5.47	127.88	120.65
1	N	512	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	100	MET	N-CA-C	-5.47	105.47	111.82
13	Z	17	ILE	CA-C-N	5.47	126.05	119.98
13	Z	17	ILE	C-N-CA	5.47	126.05	119.98
1	A	463	THR	CB-CA-C	5.44	119.52	110.81
1	N	202	LEU	CA-C-N	5.42	127.48	120.44
1	N	202	LEU	C-N-CA	5.42	127.48	120.44
3	C	94	PHE	CA-C-N	5.41	127.84	120.54
3	C	94	PHE	C-N-CA	5.41	127.84	120.54
2	B	158	ASP	CA-CB-CG	5.37	117.97	112.60
1	N	254	ILE	N-CA-C	-5.36	105.28	110.42
10	J	2	GLU	CA-C-N	5.32	128.89	121.24
10	J	2	GLU	C-N-CA	5.32	128.89	121.24
3	C	210	ILE	CA-C-N	5.31	125.83	119.94
3	C	210	ILE	C-N-CA	5.31	125.83	119.94
1	N	9	SER	CA-C-N	5.30	129.67	121.83
1	N	9	SER	C-N-CA	5.30	129.67	121.83
1	N	281	GLY	CA-C-N	5.28	127.67	120.54
1	N	281	GLY	C-N-CA	5.28	127.67	120.54
3	C	110	PRO	CA-C-N	5.27	128.07	120.38
3	C	110	PRO	C-N-CA	5.27	128.07	120.38
3	P	204	HIS	CA-C-N	5.25	125.81	119.98
3	P	204	HIS	C-N-CA	5.25	125.81	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	173	PHE	CA-C-N	5.25	127.58	120.65
3	C	173	PHE	C-N-CA	5.25	127.58	120.65
1	N	184	PHE	N-CA-C	-5.25	105.56	111.28
8	H	28	ASN	CA-C-N	5.24	127.56	120.38
8	H	28	ASN	C-N-CA	5.24	127.56	120.38
3	P	77	LYS	N-CA-C	-5.24	105.63	112.23
1	A	202	LEU	O-C-N	5.24	127.67	122.12
11	X	24	PHE	CA-C-N	5.24	127.56	120.65
11	X	24	PHE	C-N-CA	5.24	127.56	120.65
1	A	43	GLN	CB-CG-CD	-5.22	103.72	112.60
3	C	75	VAL	O-C-N	5.22	127.14	121.87
1	A	338	MET	CA-C-N	5.21	127.58	120.54
1	A	338	MET	C-N-CA	5.21	127.58	120.54
13	M	33	VAL	N-CA-C	-5.20	105.77	110.82
1	A	204	ALA	CA-C-N	5.19	125.60	119.94
1	A	204	ALA	C-N-CA	5.19	125.60	119.94
1	N	429	HIS	CA-C-N	5.19	127.50	120.65
1	N	429	HIS	C-N-CA	5.19	127.50	120.65
3	P	210	ILE	CA-C-N	5.19	125.70	119.94
3	P	210	ILE	C-N-CA	5.19	125.70	119.94
6	F	50	PRO	CA-C-O	-5.18	115.12	121.03
1	N	30	GLY	O-C-N	5.18	127.15	122.18
2	O	105	TYR	CA-C-O	-5.17	115.92	121.45
8	H	69	VAL	N-CA-C	-5.17	106.04	110.74
3	P	128	GLU	CB-CA-C	5.16	120.69	110.42
10	J	50	LEU	CA-C-N	5.15	125.65	119.94
10	J	50	LEU	C-N-CA	5.15	125.65	119.94
1	A	373	VAL	N-CA-C	-5.13	105.71	110.53
5	E	31	LYS	CA-C-N	5.13	125.67	119.98
5	E	31	LYS	C-N-CA	5.13	125.67	119.98
5	E	65	VAL	N-CA-C	-5.13	105.60	110.42
5	R	31	LYS	CA-C-N	5.12	125.63	119.94
5	R	31	LYS	C-N-CA	5.12	125.63	119.94
1	N	507	GLU	CB-CA-C	5.12	116.04	110.15
2	B	204	HIS	CA-C-N	5.11	127.44	120.54
2	B	204	HIS	C-N-CA	5.11	127.44	120.54
3	P	29	SER	CA-C-N	5.11	125.62	119.94
3	P	29	SER	C-N-CA	5.11	125.62	119.94
8	U	61	LYS	CA-C-N	5.11	127.08	120.44
8	U	61	LYS	C-N-CA	5.11	127.08	120.44
7	T	81	GLY	CA-C-O	-5.10	118.64	122.37
1	N	452	THR	CA-C-N	5.10	127.08	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	452	THR	C-N-CA	5.10	127.08	120.70
1	N	185	VAL	N-CA-C	-5.10	105.36	110.30
1	A	258	VAL	N-CA-C	-5.09	104.73	111.09
1	A	58	VAL	CA-C-O	-5.08	115.79	121.17
1	A	254	ILE	N-CA-C	-5.08	105.59	110.72
8	H	22	ASN	CB-CA-C	5.07	118.16	109.80
4	D	71	MET	N-CA-C	-5.06	106.62	112.89
1	A	194	LEU	CA-C-N	5.05	127.36	120.54
1	A	194	LEU	C-N-CA	5.05	127.36	120.54
1	N	125	GLY	CA-C-O	-5.05	117.85	122.24
3	C	167	ILE	O-C-N	5.05	127.03	121.83
9	V	25	PHE	CA-C-N	5.05	127.31	120.65
9	V	25	PHE	C-N-CA	5.05	127.31	120.65
1	N	30	GLY	CA-C-N	5.04	127.30	120.65
1	N	30	GLY	C-N-CA	5.04	127.30	120.65
1	A	491	ASN	CA-C-N	5.04	131.16	121.54
1	A	491	ASN	C-N-CA	5.04	131.16	121.54
1	A	483	LEU	O-C-N	5.03	127.55	121.76
8	H	60	TYR	CA-C-O	-5.03	114.57	120.20
1	N	270	TYR	CA-C-N	5.02	127.71	120.38
1	N	270	TYR	C-N-CA	5.02	127.71	120.38
1	A	122	ALA	CA-C-O	-5.01	116.47	122.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4002	208	0
1	N	4027	0	4002	189	0
2	B	1824	0	1833	75	0
2	O	1824	0	1833	58	0
3	C	2110	0	2027	57	0
3	P	2110	0	2027	69	0
4	D	1195	0	1183	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	1195	0	1183	37	0
5	E	852	0	845	24	0
5	R	852	0	845	21	0
6	F	748	0	728	17	0
6	S	748	0	728	16	0
7	G	675	0	643	21	0
7	T	675	0	643	27	0
8	H	662	0	623	16	0
8	U	662	0	623	10	0
9	I	592	0	604	14	0
9	V	592	0	604	20	0
10	J	460	0	459	12	0
10	W	460	0	459	13	0
11	K	384	0	366	14	0
11	X	384	0	366	7	0
12	L	380	0	380	13	0
12	Y	380	0	380	9	0
13	M	335	0	352	9	0
13	Z	335	0	352	7	0
14	A	1	0	0	0	0
14	N	1	0	0	0	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	51	0	76	3	0
17	C	102	0	152	3	0
17	H	51	0	76	1	0
17	N	102	0	152	2	0
17	P	102	0	152	2	0
18	A	120	0	108	15	0
18	N	120	0	108	11	0
19	A	1	0	0	0	0
19	N	1	0	0	0	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	63	0	110	2	0
21	D	63	0	110	2	0
21	L	63	0	110	8	0
21	N	126	0	220	7	0
21	O	63	0	110	0	0
22	B	52	0	80	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	52	0	80	2	0
23	C	58	0	78	3	0
23	J	29	0	39	1	0
23	O	29	0	39	0	0
23	P	58	0	78	2	0
23	T	58	0	78	3	0
23	W	29	0	39	0	0
23	Y	29	0	39	2	0
24	C	159	0	231	7	0
24	P	106	0	154	3	0
24	T	53	0	77	1	0
25	C	200	0	312	3	0
25	P	200	0	312	9	0
26	C	66	0	84	6	0
26	G	33	0	42	0	0
26	M	33	0	42	1	0
26	P	33	0	42	0	0
26	Q	33	0	42	0	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	I	9	0	8	0	0
28	V	9	0	8	1	0
29	A	104	0	0	68	0
29	B	46	0	0	16	0
29	C	44	0	0	9	0
29	D	23	0	0	10	0
29	E	23	0	0	4	0
29	F	20	0	0	2	0
29	G	13	0	0	5	0
29	H	26	0	0	10	0
29	I	8	0	0	4	0
29	J	11	0	0	8	0
29	K	8	0	0	5	0
29	L	13	0	0	6	0
29	M	7	0	0	2	0
29	N	74	0	0	47	0
29	O	39	0	0	13	0
29	P	40	0	0	22	0
29	Q	28	0	0	12	0
29	R	8	0	0	0	0
29	S	19	0	0	2	0
29	T	17	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	U	7	0	0	0	0
29	V	6	0	0	0	0
29	W	5	0	0	1	0
29	X	8	0	0	5	0
29	Y	1	0	0	0	0
29	Z	3	0	0	0	0
All	All	31457	0	31478	914	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 15.

All (914) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:HIS:NE2	1:A:244:TYR:CE2	1.81	1.47
1:A:240:HIS:NE2	1:A:244:TYR:HE2	0.90	1.37
1:N:240:HIS:NE2	1:N:244:TYR:HE2	1.27	1.30
1:A:394:VAL:HA	29:A:722:HOH:O	1.31	1.28
1:N:240:HIS:NE2	1:N:244:TYR:CE2	2.04	1.26
29:D:311:HOH:O	11:K:25:CYS:SG	2.00	1.18
1:A:338:MET:HE1	29:A:710:HOH:O	1.48	1.13
10:J:55:PHE:HB2	29:J:204:HOH:O	1.49	1.12
1:A:462:LEU:HA	29:A:716:HOH:O	1.49	1.11
11:K:28:VAL:HB	29:K:101:HOH:O	1.52	1.08
3:C:26:LEU:HD23	29:J:205:HOH:O	1.54	1.07
1:A:240:HIS:CD2	1:A:244:TYR:HE2	1.74	1.05
18:N:607:HEA:C3A	29:N:755:HOH:O	2.03	1.03
2:B:34:ILE:HG13	29:B:421:HOH:O	1.58	1.03
3:P:249:TRP:CE2	29:P:406:HOH:O	2.12	1.02
13:M:23:PHE:HA	29:M:203:HOH:O	1.58	1.01
2:B:219:PHE:CD1	29:B:423:HOH:O	2.13	1.00
1:A:73:ILE:HG13	29:A:705:HOH:O	1.63	0.99
1:A:78:PHE:HE1	29:A:726:HOH:O	1.46	0.98
1:N:248:LEU:HD22	29:N:751:HOH:O	1.62	0.98
1:A:374:VAL:HB	29:A:759:HOH:O	1.64	0.96
2:B:24:HIS:HD2	29:B:438:HOH:O	1.49	0.95
2:B:110:TYR:HE2	29:B:434:HOH:O	1.47	0.94
9:I:29:LEU:HB3	29:I:206:HOH:O	1.65	0.94
4:Q:13:LEU:HA	29:Q:301:HOH:O	1.67	0.94
3:P:253:TYR:HB2	29:P:406:HOH:O	1.69	0.91
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:HIS:CD2	1:A:244:TYR:CE2	2.54	0.89
1:N:334:TRP:CD2	29:N:745:HOH:O	2.24	0.89
18:N:607:HEA:CMA	29:N:755:HOH:O	2.19	0.89
1:A:78:PHE:CE1	29:A:726:HOH:O	2.23	0.89
2:O:62:GLU:OE2	29:O:401:HOH:O	1.88	0.89
24:C:303:PEK:HN2	7:G:76:ASN:HD21	1.19	0.88
5:E:94:ASN:HB2	29:E:209:HOH:O	1.73	0.88
1:A:398:PRO:HB2	29:A:723:HOH:O	1.72	0.88
1:N:43:GLN:HB3	4:Q:104:TYR:CE2	2.09	0.87
1:N:396:TRP:HA	29:N:709:HOH:O	1.74	0.87
2:B:39:LEU:HD23	29:B:443:HOH:O	1.73	0.86
29:Q:306:HOH:O	9:V:46:ALA:HB1	1.74	0.86
2:O:74:ILE:HB	29:O:402:HOH:O	1.77	0.84
1:N:39:ALA:O	29:N:702:HOH:O	1.95	0.84
6:S:9:ASP:HB3	6:S:21:MET:HE1	1.57	0.84
11:K:26:VAL:O	11:K:30:VAL:HG23	1.78	0.84
1:N:334:TRP:CG	29:N:745:HOH:O	2.32	0.82
1:N:277:MET:SD	29:N:740:HOH:O	2.36	0.82
1:A:26:ALA:CA	29:A:708:HOH:O	2.30	0.80
4:Q:91:PHE:HA	29:Q:320:HOH:O	1.82	0.80
3:C:119:THR:HA	29:C:426:HOH:O	1.81	0.80
1:A:131:PRO:HG2	2:B:159:VAL:HA	1.65	0.79
1:N:240:HIS:CD2	1:N:244:TYR:CE2	2.70	0.79
1:N:240:HIS:CD2	1:N:244:TYR:HE2	2.01	0.79
1:A:334:TRP:HA	29:A:757:HOH:O	1.83	0.78
1:N:130:PRO:HG2	29:N:729:HOH:O	1.81	0.78
2:B:113:TYR:CE1	29:H:203:HOH:O	2.37	0.78
1:A:288:TRP:CD1	29:A:709:HOH:O	2.37	0.77
1:A:452:THR:HG22	1:A:456:MET:HE3	1.65	0.77
7:G:46:ALA:HB3	29:G:206:HOH:O	1.84	0.77
5:E:49:ASP:OD1	5:E:92:THR:OG1	2.00	0.77
1:A:183:LEU:HD12	1:A:255:SER:HB3	1.67	0.76
4:D:17:VAL:HG11	29:D:320:HOH:O	1.84	0.76
4:D:37:GLN:HG2	29:D:308:HOH:O	1.84	0.76
1:A:306:THR:OG1	1:A:361:SER:OG	2.03	0.76
1:A:23:GLY:HA3	29:A:705:HOH:O	1.87	0.75
1:A:218:THR:OG1	3:C:191:GLY:HA2	1.85	0.75
1:N:228:PRO:HA	29:N:729:HOH:O	1.87	0.75
4:Q:131:ILE:HG22	29:Q:306:HOH:O	1.86	0.75
10:J:50:LEU:HD21	29:J:202:HOH:O	1.87	0.75
1:N:43:GLN:HB3	4:Q:104:TYR:HE2	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ILE:HG13	4:D:92:THR:HG21	1.69	0.74
3:C:80:ARG:NH2	3:C:236:GLU:OE1	2.21	0.74
29:G:201:HOH:O	1:N:278:MET:HE1	1.88	0.74
1:A:26:ALA:HA	29:A:708:HOH:O	1.85	0.74
1:N:74:MET:HE1	1:N:246:LEU:O	1.86	0.74
3:C:149:HIS:CE1	26:C:309:DMU:H2	2.24	0.73
1:A:258:VAL:HG13	29:A:710:HOH:O	1.89	0.73
9:I:32:ALA:HA	29:I:205:HOH:O	1.88	0.73
1:A:17:THR:HG23	21:L:101:TGL:H282	1.70	0.72
1:A:226:GLY:O	29:A:701:HOH:O	2.07	0.72
3:P:92:LEU:HA	29:P:403:HOH:O	1.90	0.72
1:A:398:PRO:C	29:A:723:HOH:O	2.33	0.72
4:D:14:PRO:HB2	29:D:303:HOH:O	1.89	0.72
3:P:12:ASN:HD22	10:W:20:VAL:H	1.37	0.72
7:G:18:PHE:CZ	29:N:703:HOH:O	2.44	0.71
18:N:607:HEA:C2A	29:N:755:HOH:O	2.31	0.71
5:E:60:ASP:OD2	5:E:63:SER:OG	2.09	0.71
10:J:29:ASN:OD1	29:J:201:HOH:O	2.09	0.71
3:C:25:LEU:O	3:C:29:SER:OG	2.06	0.70
1:N:390:MET:HA	1:N:390:MET:HE3	1.71	0.70
5:E:41:LEU:O	5:E:41:LEU:HD12	1.90	0.70
1:A:12:HIS:HD2	1:A:80:ASN:O	1.74	0.70
17:N:605:PGV:H183	29:N:774:HOH:O	1.90	0.70
4:D:17:VAL:CG1	29:D:320:HOH:O	2.39	0.70
3:P:71:HIS:CD2	29:P:421:HOH:O	2.43	0.70
2:B:49:LYS:HE3	29:D:312:HOH:O	1.92	0.70
7:G:72:ASN:H	7:G:76:ASN:HD22	1.40	0.69
18:A:605:HEA:HBC1	18:A:605:HEA:HMC3	1.75	0.69
1:A:188:VAL:HG23	29:A:706:HOH:O	1.91	0.69
9:V:40:ALA:C	9:V:42:LYS:H	2.01	0.69
1:N:83:VAL:HB	1:N:84:PRO:HD3	1.75	0.69
1:A:324:LEU:HA	1:A:327:LEU:HD12	1.74	0.69
2:O:24:HIS:HE1	29:O:434:HOH:O	1.76	0.69
1:N:232:GLN:OE1	29:N:704:HOH:O	2.11	0.68
1:A:117:MET:HB2	29:J:202:HOH:O	1.93	0.68
2:O:207:MET:C	29:O:407:HOH:O	2.36	0.68
1:A:374:VAL:CG1	29:A:759:HOH:O	2.42	0.68
1:N:271:MET:O	29:N:703:HOH:O	2.09	0.68
12:L:24:MET:SD	29:L:201:HOH:O	2.52	0.68
5:R:41:LEU:HD12	5:R:41:LEU:O	1.93	0.68
29:B:420:HOH:O	4:D:21:ASP:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:77:GLU:HB3	21:D:201:TGL:HB32	1.74	0.67
1:A:260:TYR:CE2	29:A:785:HOH:O	2.46	0.67
5:E:99:SER:HB2	5:E:104:LEU:HD11	1.75	0.67
1:N:371:TYR:CE2	29:N:731:HOH:O	2.46	0.67
1:A:371:TYR:CD2	29:A:759:HOH:O	2.46	0.67
5:E:78:HIS:CD2	9:I:12:LEU:HD22	2.29	0.67
18:A:606:HEA:H121	29:A:762:HOH:O	1.93	0.67
2:B:66:THR:HB	29:B:442:HOH:O	1.94	0.67
1:N:33:LEU:O	1:N:37:ILE:HG13	1.95	0.67
1:N:513:LEU:HA	29:N:741:HOH:O	1.93	0.67
1:N:19:TYR:O	29:N:705:HOH:O	2.12	0.67
4:D:23:PRO:HD2	5:E:34:ASN:OD1	1.95	0.67
12:Y:11:ILE:HD12	12:Y:13:PHE:CE2	2.30	0.66
1:A:392:GLY:C	29:A:726:HOH:O	2.37	0.66
1:A:466:MET:SD	29:M:203:HOH:O	2.52	0.66
1:N:189:MET:O	1:N:193:VAL:HG23	1.95	0.66
1:N:369:ASP:OD1	29:N:706:HOH:O	2.13	0.66
4:Q:118:LYS:HG2	29:X:102:HOH:O	1.95	0.66
2:B:34:ILE:O	2:B:38:VAL:HG23	1.95	0.66
2:B:195:GLN:HG2	29:B:415:HOH:O	1.94	0.66
1:N:183:LEU:HD22	29:N:747:HOH:O	1.94	0.66
7:G:45:PRO:HA	29:G:204:HOH:O	1.96	0.65
1:A:19:TYR:O	29:A:702:HOH:O	2.13	0.65
1:A:288:TRP:CG	29:A:709:HOH:O	2.48	0.65
2:B:68:LEU:HB2	2:B:69:PRO:HD3	1.77	0.65
1:A:494:TRP:HZ3	29:A:723:HOH:O	1.80	0.65
7:G:1:ALA:HB2	24:P:301:PEK:H382	1.78	0.65
21:L:101:TGL:OC1	29:L:201:HOH:O	2.15	0.65
2:O:71:ILE:O	29:O:402:HOH:O	2.15	0.65
11:K:24:PHE:O	29:K:101:HOH:O	2.14	0.65
3:P:249:TRP:CZ2	29:P:406:HOH:O	2.40	0.65
9:V:54:TYR:OH	9:V:59:ASP:OD2	2.14	0.65
1:N:151:HIS:O	1:N:155:VAL:HG23	1.98	0.64
3:P:71:HIS:HD2	29:P:421:HOH:O	1.77	0.64
1:A:266:GLU:OE1	29:A:703:HOH:O	2.15	0.64
2:O:108:TYR:CE2	2:O:142:VAL:HG21	2.33	0.64
2:O:88:ASP:O	2:O:89:GLU:O	2.15	0.64
25:P:309:CDL:H271	24:T:102:PEK:H383	1.79	0.64
2:O:102:HIS:HD2	29:O:438:HOH:O	1.80	0.63
29:Q:306:HOH:O	9:V:46:ALA:CB	2.41	0.63
1:A:256:HIS:CD2	29:A:747:HOH:O	2.49	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:ASP:OD2	3:C:158:HIS:HD2	1.80	0.63
2:O:71:ILE:HA	29:O:402:HOH:O	1.98	0.63
4:Q:56:LYS:NZ	5:R:99:SER:OG	2.32	0.63
1:A:73:ILE:N	29:A:705:HOH:O	2.30	0.63
6:F:95:GLN:HB2	29:F:213:HOH:O	1.98	0.63
2:O:207:MET:HG3	2:O:207:MET:O	1.99	0.63
11:X:52:GLU:C	29:X:102:HOH:O	2.41	0.63
1:A:240:HIS:CE1	1:A:244:TYR:CE2	2.81	0.62
18:N:607:HEA:CHB	29:N:722:HOH:O	2.46	0.62
3:P:22:LEU:HD22	29:W:203:HOH:O	1.99	0.62
3:P:40:MET:HE2	3:P:44:MET:CE	2.28	0.62
4:Q:9:GLU:OE2	6:S:55:LYS:NZ	2.26	0.62
1:A:313:ALA:HB3	2:B:73:LEU:HD11	1.80	0.62
7:G:22:GLY:O	7:G:26:PRO:HG2	1.99	0.62
1:N:130:PRO:HB2	29:N:716:HOH:O	1.99	0.62
1:A:390:MET:HE3	1:A:390:MET:HA	1.81	0.62
1:N:344:PHE:HB2	29:N:730:HOH:O	2.00	0.62
1:N:411:LYS:HE3	29:N:762:HOH:O	1.99	0.62
10:W:26:ALA:O	10:W:30:ILE:HD12	2.00	0.62
1:A:405:LEU:HD11	29:A:722:HOH:O	1.99	0.62
2:B:110:TYR:CE2	29:B:434:HOH:O	2.31	0.62
1:A:26:ALA:N	29:A:708:HOH:O	2.31	0.61
4:D:82:VAL:O	4:D:86:MET:HG3	2.00	0.61
3:C:149:HIS:NE2	26:C:309:DMU:H2	2.15	0.61
3:C:187:THR:HB	7:G:68:THR:HG21	1.82	0.61
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.83	0.61
1:N:240:HIS:CE1	1:N:244:TYR:HE2	2.11	0.61
1:N:336:PRO:HB2	1:N:394:VAL:HG11	1.81	0.61
1:A:215:LEU:HD13	29:C:412:HOH:O	2.00	0.61
12:Y:35:ALA:HB3	12:Y:36:PRO:CD	2.27	0.61
1:N:364:ASP:OD1	18:N:606:HEA:O2A	2.17	0.61
8:H:81:PHE:CE2	8:H:85:ILE:HD11	2.36	0.61
1:A:406:ASN:OD1	1:A:406:ASN:C	2.43	0.61
13:M:17:ILE:O	13:M:20:SER:N	2.34	0.60
1:N:477:ALA:O	13:Z:8:THR:OG1	2.19	0.60
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.83	0.60
21:B:302:TGL:HC31	29:I:201:HOH:O	2.01	0.60
1:N:236:TRP:O	1:N:288:TRP:HB2	2.01	0.60
1:N:396:TRP:CA	29:N:709:HOH:O	2.42	0.60
3:P:75:VAL:HG12	29:P:420:HOH:O	2.00	0.60
4:Q:118:LYS:HA	29:X:102:HOH:O	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:255:SER:O	1:N:259:THR:OG1	2.11	0.60
13:Z:34:LEU:HA	13:Z:37:LEU:HD23	1.82	0.60
6:F:20:VAL:HG13	29:F:208:HOH:O	2.02	0.60
1:N:409:TRP:HA	1:N:412:ILE:HD12	1.84	0.60
12:L:2:HIS:HB2	29:L:205:HOH:O	2.02	0.60
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.84	0.60
8:U:60:TYR:CD1	8:U:60:TYR:C	2.80	0.60
1:A:92:MET:SD	29:A:714:HOH:O	2.57	0.59
3:P:40:MET:HE2	3:P:44:MET:HE3	1.84	0.59
1:N:163:ASN:O	1:N:167:THR:OG1	2.15	0.59
24:P:304:PEK:HN2	7:T:76:ASN:HD21	1.51	0.59
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.83	0.59
11:X:6:ALA:HA	29:X:107:HOH:O	2.02	0.59
3:C:192:VAL:O	3:C:196:THR:HG23	2.02	0.59
2:B:207:MET:HE1	29:B:439:HOH:O	2.01	0.59
5:E:15:TRP:HB3	29:E:222:HOH:O	2.01	0.59
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.90	0.59
3:P:88:ILE:O	3:P:92:LEU:HD23	2.03	0.59
2:B:139:ASP:OD1	2:B:140:ASN:N	2.35	0.59
3:P:132:LEU:O	3:P:136:VAL:HG23	2.03	0.59
8:H:60:TYR:O	8:H:64:CYS:HB2	2.03	0.59
2:O:40:TYR:O	2:O:43:SER:OG	2.18	0.59
1:N:397:PHE:O	1:N:401:SER:OG	2.21	0.58
3:P:214:PHE:CE2	3:P:238:ALA:HA	2.39	0.58
12:Y:41:ARG:NH1	23:Y:101:CHD:H182	2.18	0.58
4:D:34:SER:O	4:D:38:LYS:HG3	2.04	0.58
9:V:2:THR:N	28:V:102:SAC:HG	2.01	0.58
2:B:146:MET:SD	2:B:189:PRO:HB3	2.44	0.58
26:C:310:DMU:H34	29:C:438:HOH:O	2.03	0.58
1:N:31:THR:HG23	18:N:607:HEA:H14	1.86	0.58
7:T:10:GLY:O	23:T:103:CHD:H41	2.03	0.58
1:A:198:SER:OG	29:A:704:HOH:O	2.17	0.58
1:A:338:MET:HG2	29:A:757:HOH:O	2.03	0.58
3:C:111:GLU:HG3	29:C:440:HOH:O	2.04	0.58
1:N:349:THR:O	1:N:353:LEU:HG	2.04	0.58
1:A:117:MET:HE3	29:J:202:HOH:O	2.03	0.58
29:P:417:HOH:O	10:W:12:PHE:HE2	1.85	0.58
2:B:153:LEU:HD13	2:B:179:LEU:HD21	1.86	0.58
2:O:1:FME:HE1	2:O:133:LEU:HD11	1.86	0.57
7:T:17:ARG:HD2	29:T:203:HOH:O	2.04	0.57
1:A:169:ILE:HD12	7:T:7:ASP:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:171:MET:HE3	3:P:8:TYR:CD1	2.39	0.57
1:A:372:TYR:HD1	29:A:713:HOH:O	1.87	0.57
8:H:60:TYR:CD1	8:H:60:TYR:C	2.82	0.57
1:N:112:LEU:O	1:N:115:SER:HB3	2.03	0.57
1:N:399:LEU:CB	29:N:709:HOH:O	2.52	0.57
2:O:1:FME:SD	2:O:133:LEU:HD11	2.44	0.57
10:W:8:LYS:O	10:W:12:PHE:HD2	1.86	0.57
1:N:72:PRO:HB2	29:N:705:HOH:O	2.05	0.57
10:W:32:TYR:HE1	10:W:36:MET:HE2	1.68	0.57
1:N:399:LEU:HB2	29:N:709:HOH:O	2.04	0.57
1:A:195:LEU:CD2	1:A:245:ILE:HD13	2.35	0.56
2:O:226:MET:HE2	2:O:226:MET:HA	1.87	0.56
25:P:309:CDL:H761	29:P:412:HOH:O	2.04	0.56
1:A:69:MET:O	29:A:705:HOH:O	2.17	0.56
1:N:33:LEU:HD23	1:N:57:VAL:HG23	1.87	0.56
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.06	0.56
1:A:23:GLY:HA3	29:A:702:HOH:O	2.05	0.56
1:A:179:TYR:C	1:A:180:GLN:HG3	2.31	0.56
1:A:358:LEU:HD13	18:A:605:HEA:CBA	2.36	0.56
1:A:377:PHE:HA	1:A:380:VAL:HG22	1.87	0.56
3:C:111:GLU:CG	29:C:440:HOH:O	2.53	0.56
4:D:67:SER:OG	4:D:70:GLU:HG3	2.04	0.56
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.40	0.56
6:F:85:CYS:SG	6:F:87:THR:OG1	2.58	0.56
1:A:83:VAL:HB	1:A:84:PRO:HD3	1.88	0.56
10:J:8:LYS:O	10:J:12:PHE:HD2	1.89	0.56
1:A:80:ASN:HA	29:A:714:HOH:O	2.04	0.56
2:B:90:ILE:O	2:B:90:ILE:HG23	2.05	0.56
1:N:486:ASP:HB3	1:N:487:LEU:HG	1.86	0.56
3:P:126:PRO:HB2	29:P:412:HOH:O	2.05	0.56
2:B:50:LEU:HD21	5:E:77:PRO:HD2	1.88	0.56
25:P:309:CDL:HA32	25:P:309:CDL:HA22	1.86	0.56
6:F:63:GLU:O	6:F:66:ASN:HB2	2.06	0.56
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.86	0.56
1:N:417:MET:HE3	29:N:764:HOH:O	2.06	0.56
4:Q:56:LYS:NZ	5:R:97:GLY:O	2.36	0.56
1:N:92:MET:HE1	1:N:164:PHE:CD1	2.41	0.56
3:P:252:LEU:CD2	3:P:256:ILE:HD12	2.36	0.56
1:A:70:VAL:O	1:A:74:MET:HB2	2.05	0.55
3:P:70:HIS:HB2	29:P:421:HOH:O	2.05	0.55
1:A:373:VAL:HA	29:A:713:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:81:ARG:HA	6:F:87:THR:O	2.06	0.55
1:N:331:ASN:ND2	4:Q:21:ASP:OD1	2.37	0.55
2:B:40:TYR:CE1	9:I:24:ALA:HB2	2.41	0.55
1:N:474:GLU:OE1	1:N:480:ARG:NH2	2.28	0.55
1:A:283:LEU:HD23	1:A:286:ILE:HD11	1.88	0.55
4:D:14:PRO:CB	29:D:303:HOH:O	2.50	0.55
1:A:23:GLY:CA	29:A:702:HOH:O	2.54	0.55
1:N:250:GLY:O	1:N:254:ILE:HG12	2.07	0.55
1:A:34:SER:CB	29:A:762:HOH:O	2.54	0.55
6:F:55:LYS:HA	6:F:74:LEU:O	2.06	0.55
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.72	0.55
1:N:303:ALA:HB2	2:O:84:LEU:HD21	1.87	0.55
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.88	0.55
23:T:103:CHD:H182	23:T:103:CHD:H9	1.87	0.55
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.89	0.55
2:O:40:TYR:CE1	9:V:24:ALA:HB2	2.42	0.55
23:C:307:CHD:H212	23:C:307:CHD:H183	1.87	0.55
26:C:309:DMU:H7	24:C:311:PEK:HN1	1.70	0.55
1:N:480:ARG:NE	29:N:714:HOH:O	2.40	0.55
6:S:50:PRO:HA	6:S:92:VAL:HG23	1.89	0.55
7:T:67:HIS:CE1	7:T:78:LEU:HD11	2.42	0.55
8:U:69:VAL:O	8:U:70:SER:C	2.50	0.55
21:L:101:TGL:HG2	29:L:209:HOH:O	2.06	0.54
12:L:20:ARG:O	12:L:24:MET:HG2	2.07	0.54
1:N:489:THR:HA	6:S:71:TRP:O	2.07	0.54
1:A:184:PHE:CD1	29:A:706:HOH:O	2.54	0.54
1:A:322:SER:O	1:A:323:TRP:C	2.49	0.54
3:P:258:TRP:CD1	25:P:309:CDL:H781	2.43	0.54
4:Q:14:PRO:HD3	29:Q:301:HOH:O	2.07	0.54
2:B:44:LEU:HD11	9:I:20:HIS:CG	2.42	0.54
3:C:11:VAL:HG13	29:C:414:HOH:O	2.07	0.54
5:E:99:SER:CB	5:E:104:LEU:HD11	2.38	0.54
1:N:310:MET:HE1	2:O:76:ILE:CG2	2.38	0.54
1:A:372:TYR:C	29:A:713:HOH:O	2.50	0.54
12:Y:20:ARG:NH1	12:Y:24:MET:SD	2.80	0.54
18:N:607:HEA:OMA	18:N:607:HEA:HHB	2.06	0.54
1:A:73:ILE:CG1	29:A:705:HOH:O	2.37	0.54
1:A:169:ILE:CD1	7:T:7:ASP:HB3	2.38	0.54
2:O:111:THR:HA	2:O:114:GLU:O	2.07	0.54
1:N:481:GLU:HB2	13:Z:4:LYS:HE3	1.89	0.54
1:A:486:ASP:OD1	1:A:486:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:113:LEU:CA	21:N:604:TGL:H323	2.38	0.53
1:A:118:VAL:HG11	1:A:141:ALA:HB3	1.90	0.53
1:A:303:ALA:HB2	2:B:84:LEU:CD2	2.38	0.53
7:G:8:HIS:ND1	7:G:8:HIS:N	2.56	0.53
1:N:34:SER:HA	29:N:722:HOH:O	2.08	0.53
1:A:462:LEU:O	1:A:466:MET:HG3	2.08	0.53
2:B:95:LEU:HD12	2:B:96:THR:H	1.73	0.53
1:N:113:LEU:HD22	21:N:604:TGL:H291	1.90	0.53
3:P:26:LEU:HD21	10:W:42:GLY:C	2.34	0.53
1:A:190:ILE:HG22	1:A:248:LEU:HD13	1.89	0.53
5:E:45:PRO:HD3	9:I:9:MET:HE1	1.91	0.53
2:O:152:MET:HB2	2:O:182:THR:HG23	1.90	0.53
1:A:377:PHE:O	1:A:381:LEU:HB2	2.08	0.53
29:A:771:HOH:O	21:D:201:TGL:HG11	2.08	0.53
1:N:240:HIS:ND1	1:N:290:HIS:CE1	2.76	0.53
1:N:383:MET:HA	1:N:387:PHE:CE1	2.43	0.53
1:A:292:MET:O	1:A:295:VAL:HG22	2.08	0.53
8:H:61:LYS:HD2	29:H:207:HOH:O	2.09	0.53
3:P:103:HIS:ND1	23:P:303:CHD:O26	2.34	0.53
3:C:246:ASP:OD1	3:C:246:ASP:C	2.52	0.53
3:P:47:LEU:HD23	29:P:439:HOH:O	2.09	0.53
6:S:8:THR:HG22	29:S:213:HOH:O	2.09	0.53
1:A:100:MET:HE1	17:C:301:PGV:H81	1.90	0.53
3:C:30:GLY:HA2	3:C:42:LEU:HB3	1.91	0.53
12:L:25:MET:HE3	21:L:101:TGL:HA91	1.91	0.53
3:P:92:LEU:HD13	29:P:403:HOH:O	2.08	0.53
3:P:159:MET:SD	3:P:159:MET:O	2.67	0.53
4:Q:29:HIS:HB3	29:Q:316:HOH:O	2.09	0.53
1:A:117:MET:CB	29:J:202:HOH:O	2.56	0.52
1:A:127:THR:HB	1:A:129:TYR:CE1	2.45	0.52
6:F:62:CYS:SG	6:F:84:SER:HB3	2.49	0.52
1:N:183:LEU:HD12	1:N:255:SER:HB3	1.91	0.52
2:O:139:ASP:OD1	2:O:140:ASN:N	2.40	0.52
1:A:373:VAL:N	29:A:713:HOH:O	2.42	0.52
2:B:113:TYR:CD1	29:H:203:HOH:O	2.59	0.52
3:C:8:TYR:CE1	3:C:74:ALA:HB1	2.43	0.52
7:T:23:LEU:C	7:T:26:PRO:HD2	2.34	0.52
24:C:303:PEK:C12	24:C:303:PEK:H162	2.40	0.52
8:H:47:GLY:HA2	29:H:225:HOH:O	2.09	0.52
8:H:12:GLN:HG3	29:H:210:HOH:O	2.09	0.52
29:N:750:HOH:O	2:O:199:ILE:HG12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:25:LEU:O	3:P:29:SER:OG	2.14	0.52
5:R:41:LEU:HD12	5:R:41:LEU:C	2.35	0.52
1:N:30:GLY:O	1:N:33:LEU:HB2	2.10	0.52
2:B:13:THR:C	29:B:417:HOH:O	2.51	0.52
3:P:229:SER:OG	29:P:401:HOH:O	2.19	0.52
3:C:125:ASN:OD1	3:C:126:PRO:HD2	2.10	0.52
5:E:11:PHE:CE2	5:E:41:LEU:HD21	2.44	0.52
1:N:460:ILE:HG13	4:Q:92:THR:HG21	1.91	0.52
7:T:22:GLY:C	7:T:26:PRO:HG2	2.35	0.52
1:A:30:GLY:HA3	1:A:65:MET:SD	2.50	0.52
1:A:373:VAL:CA	29:A:713:HOH:O	2.57	0.52
1:N:478:SER:O	13:Z:6:ALA:HB1	2.09	0.52
1:A:436:MET:HE3	1:A:443:TYR:HB3	1.92	0.52
1:A:106:PRO:O	1:A:107:PRO:C	2.53	0.52
1:N:65:MET:O	1:N:70:VAL:HG23	2.10	0.52
12:Y:35:ALA:CB	12:Y:36:PRO:HD3	2.33	0.51
1:N:43:GLN:OE1	4:Q:104:TYR:CD2	2.64	0.51
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.93	0.51
1:N:310:MET:HE1	2:O:76:ILE:HG21	1.91	0.51
4:D:10:ASP:HB3	4:D:13:LEU:HD12	1.92	0.51
2:O:136:LEU:HB3	2:O:193:TYR:CD2	2.45	0.51
2:B:33:LEU:HB3	29:B:421:HOH:O	2.10	0.51
5:E:48:ILE:O	5:E:52:LEU:HG	2.10	0.51
6:F:8:THR:HG23	6:F:11:GLU:OE2	2.11	0.51
2:B:90:ILE:HD11	8:H:16:PHE:CD2	2.45	0.51
3:C:148:HIS:O	3:C:152:MET:HG3	2.11	0.51
1:A:289:ALA:HB3	1:A:305:PHE:CD1	2.46	0.51
7:G:6:GLY:O	7:G:8:HIS:ND1	2.44	0.51
2:O:108:TYR:CE2	2:O:142:VAL:CG2	2.93	0.51
3:P:142:VAL:HG11	7:T:24:ALA:HB2	1.92	0.51
4:Q:126:MET:HB3	9:V:68:ILE:HD12	1.92	0.51
29:O:415:HOH:O	9:V:70:GLN:HG3	2.11	0.51
4:Q:25:PRO:O	5:R:30:ARG:HD2	2.11	0.51
29:Q:320:HOH:O	11:X:24:PHE:HZ	1.92	0.51
1:A:443:TYR:HE2	1:A:448:THR:HA	1.76	0.51
4:D:95:LEU:HD22	26:M:101:DMU:H17	1.92	0.51
1:N:178:GLN:HG3	1:N:186:TRP:CZ2	2.46	0.51
1:N:227:ASP:OD2	3:P:103:HIS:NE2	2.44	0.51
23:P:308:CHD:H183	23:P:308:CHD:H212	1.92	0.51
1:N:290:HIS:HA	1:N:293:PHE:CZ	2.46	0.51
2:B:142:VAL:HG12	2:B:144:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:60:ALA:O	1:N:64:VAL:HG23	2.11	0.51
1:A:184:PHE:CE1	29:A:706:HOH:O	2.64	0.50
3:C:127:LEU:HD23	25:C:308:CDL:HA21	1.92	0.50
3:P:129:VAL:N	3:P:130:PRO:CD	2.75	0.50
3:P:143:SER:O	3:P:146:TRP:HB3	2.11	0.50
1:A:258:VAL:HA	29:A:710:HOH:O	2.11	0.50
1:N:102:PHE:O	1:N:105:LEU:HB2	2.11	0.50
1:N:299:VAL:HB	2:O:88:ASP:OD2	2.10	0.50
1:A:274:VAL:O	1:A:278:MET:HG3	2.12	0.50
1:A:358:LEU:HD13	18:A:605:HEA:HBA2	1.93	0.50
18:A:606:HEA:C3B	29:A:762:HOH:O	2.59	0.50
5:E:19:PHE:O	5:E:57:ARG:NH2	2.44	0.50
8:H:69:VAL:O	8:H:70:SER:C	2.55	0.50
1:N:127:THR:HB	1:N:129:TYR:CD1	2.46	0.50
2:O:1:FME:SD	2:O:133:LEU:CD1	2.99	0.50
10:W:43:THR:O	10:W:46:SER:OG	2.24	0.50
10:W:32:TYR:CE1	10:W:36:MET:HE2	2.46	0.50
1:A:152:LEU:HD22	3:C:24:ALA:HB1	1.94	0.50
3:C:24:ALA:HB2	29:C:427:HOH:O	2.12	0.50
4:Q:29:HIS:CE1	4:Q:65:LYS:HD2	2.47	0.50
1:A:510:TYR:CD2	6:F:49:VAL:HG13	2.47	0.50
3:C:75:VAL:HG21	29:C:402:HOH:O	2.11	0.50
1:N:65:MET:HE2	29:N:713:HOH:O	2.11	0.50
2:O:83:ILE:O	2:O:87:MET:HG3	2.12	0.50
4:Q:121:LYS:O	4:Q:125:ASP:N	2.45	0.50
1:A:306:THR:HA	1:A:359:ALA:O	2.12	0.50
2:B:41:ILE:O	2:B:45:MET:HG2	2.11	0.50
3:C:58:TRP:CG	17:C:305:PGV:H41	2.46	0.50
21:L:101:TGL:HA22	29:L:208:HOH:O	2.11	0.50
1:N:449:MET:SD	2:O:5:MET:HG2	2.52	0.50
1:A:61:HIS:O	1:A:65:MET:HG2	2.12	0.49
1:A:86:MET:HB3	1:A:182:PRO:HG2	1.94	0.49
1:A:336:PRO:HB2	1:A:394:VAL:HG11	1.93	0.49
6:F:13:ALA:O	6:F:18:ARG:HD2	2.12	0.49
1:A:21:LEU:CD2	21:L:101:TGL:H212	2.42	0.49
1:A:426:PHE:N	1:A:427:PRO:CD	2.75	0.49
7:G:45:PRO:CA	29:G:204:HOH:O	2.56	0.49
1:N:168:ILE:HD13	1:N:185:VAL:HG13	1.93	0.49
1:N:292:MET:O	1:N:295:VAL:HG22	2.12	0.49
1:N:374:VAL:HG11	29:N:755:HOH:O	2.12	0.49
2:O:115:ASP:OD2	8:U:61:LYS:NZ	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:HIS:O	2:B:104:TRP:HA	2.12	0.49
1:N:43:GLN:CB	4:Q:104:TYR:CE2	2.89	0.49
1:N:80:ASN:ND2	1:N:98:ASN:HD21	2.10	0.49
1:N:128:VAL:HG12	1:N:128:VAL:O	2.12	0.49
6:S:55:LYS:NZ	29:S:202:HOH:O	2.39	0.49
1:A:490:THR:C	1:A:491:ASN:HD22	2.21	0.49
3:P:225:PHE:HZ	29:P:416:HOH:O	1.95	0.49
1:A:21:LEU:HD21	21:L:101:TGL:H212	1.94	0.49
1:N:113:LEU:HB2	21:N:604:TGL:H323	1.93	0.49
1:N:398:PRO:HG2	29:N:726:HOH:O	2.13	0.49
6:S:70:ILE:HG13	6:S:84:SER:HB2	1.94	0.49
1:A:212:ASP:OD1	1:A:217:THR:OG1	2.28	0.49
1:A:338:MET:O	1:A:342:LEU:HG	2.12	0.49
17:C:305:PGV:H142	25:C:306:CDL:H652	1.94	0.49
3:P:259:TRP:CG	29:P:434:HOH:O	2.66	0.49
1:A:303:ALA:HB2	2:B:84:LEU:HD21	1.94	0.49
24:P:304:PEK:C1	29:P:408:HOH:O	2.60	0.49
1:A:199:LEU:N	1:A:200:PRO:CD	2.75	0.49
2:B:14:SER:OG	2:B:168:LEU:O	2.31	0.49
2:B:116:LEU:HB2	2:B:227:LEU:HD23	1.95	0.49
1:N:9:SER:HA	29:N:738:HOH:O	2.12	0.49
3:P:12:ASN:O	3:P:13:PRO:C	2.54	0.49
8:U:49:ASP:O	8:U:52:VAL:HG22	2.13	0.49
3:P:252:LEU:HD22	3:P:256:ILE:HD12	1.94	0.48
1:A:202:LEU:HD13	1:A:238:PHE:CD2	2.48	0.48
1:A:440:TYR:CE2	2:B:205:SER:HA	2.48	0.48
7:T:72:ASN:H	7:T:76:ASN:HD22	1.60	0.48
9:V:23:GLY:O	9:V:27:VAL:HG23	2.13	0.48
1:A:248:LEU:O	1:A:251:PHE:HB2	2.13	0.48
2:B:106:TRP:CD2	29:B:439:HOH:O	2.66	0.48
2:B:124:PRO:O	2:B:125:THR:C	2.56	0.48
1:N:75:ILE:O	1:N:79:GLY:HA3	2.13	0.48
1:N:341:ALA:O	1:N:344:PHE:HB3	2.12	0.48
1:N:397:PHE:N	1:N:398:PRO:CD	2.77	0.48
23:T:101:CHD:H151	29:T:201:HOH:O	2.14	0.48
1:A:12:HIS:CD2	1:A:84:PRO:HG2	2.48	0.48
1:A:306:THR:O	1:A:310:MET:HG3	2.14	0.48
5:E:41:LEU:HD12	5:E:41:LEU:C	2.39	0.48
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.96	0.48
29:Q:301:HOH:O	6:S:75:HIS:CE1	2.66	0.48
3:C:143:SER:O	3:C:146:TRP:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:76:ASN:O	11:K:10:HIS:HB3	2.13	0.48
1:N:251:PHE:HB3	1:N:319:LYS:HE2	1.94	0.48
1:N:312:ILE:HG22	1:N:312:ILE:O	2.12	0.48
7:T:25:LEU:N	7:T:26:PRO:CD	2.76	0.48
2:B:78:LEU:HB3	2:B:79:PRO:HD3	1.96	0.48
3:C:203:PHE:O	3:C:207:HIS:HD2	1.96	0.48
17:H:101:PGV:H181	7:T:1:ALA:HB2	1.96	0.48
13:M:28:LEU:HB2	13:M:29:PRO:HD3	1.96	0.48
1:N:229:ILE:O	1:N:230:LEU:C	2.57	0.48
4:Q:129:ALA:HB1	4:Q:133:GLY:HA3	1.95	0.48
1:A:492:LEU:HD13	6:F:71:TRP:CD2	2.49	0.47
2:B:1:FME:SD	2:B:133:LEU:HD11	2.54	0.47
3:C:7:ALA:O	3:C:72:THR:OG1	2.22	0.47
8:H:9:LYS:HG2	29:H:208:HOH:O	2.14	0.47
1:N:472:ILE:HG21	21:N:604:TGL:H201	1.97	0.47
1:A:183:LEU:CD1	1:A:255:SER:HB3	2.42	0.47
1:A:358:LEU:HD13	18:A:605:HEA:HBA1	1.95	0.47
26:C:309:DMU:O1	26:C:309:DMU:O55	2.18	0.47
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.95	0.47
2:B:88:ASP:O	2:B:89:GLU:O	2.32	0.47
1:A:343:GLY:O	1:A:344:PHE:C	2.58	0.47
2:B:142:VAL:HG12	2:B:142:VAL:O	2.13	0.47
12:L:45:LEU:HD23	12:L:45:LEU:HA	1.71	0.47
1:A:417:MET:CE	18:A:606:HEA:H263	2.45	0.47
9:V:40:ALA:O	9:V:42:LYS:N	2.45	0.47
1:A:231:TYR:CD1	1:A:231:TYR:C	2.92	0.47
3:C:63:ARG:HD3	10:J:12:PHE:CE1	2.49	0.47
7:G:11:TPO:HG23	7:G:14:ARG:HB3	1.96	0.47
1:N:383:MET:HA	1:N:387:PHE:CD1	2.49	0.47
1:A:73:ILE:HG13	29:A:702:HOH:O	2.14	0.47
1:A:440:TYR:CZ	2:B:205:SER:HA	2.49	0.47
18:A:605:HEA:HBC1	18:A:605:HEA:CMC	2.42	0.47
4:D:48:TRP:HB2	5:E:96:LEU:O	2.15	0.47
1:N:232:GLN:O	1:N:236:TRP:HB2	2.15	0.47
1:N:488:THR:HB	1:N:495:LEU:HD13	1.95	0.47
2:O:90:ILE:CD1	8:U:16:PHE:CD2	2.97	0.47
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.50	0.47
1:N:55:ASN:HA	1:N:58:VAL:HB	1.96	0.47
1:N:339:MET:HE1	1:N:411:LYS:CD	2.44	0.47
5:R:60:ASP:OD2	5:R:63:SER:OG	2.25	0.47
5:E:94:ASN:CB	29:E:209:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:57:ARG:HG2	29:H:207:HOH:O	2.14	0.47
1:N:3:ILE:HD13	1:N:7:LEU:HD22	1.97	0.47
5:R:8:ASP:HA	22:V:101:PSC:H081	1.96	0.47
17:A:604:PGV:O02	17:A:604:PGV:H72	2.15	0.47
1:N:380:VAL:HG21	18:N:606:HEA:C3C	2.45	0.47
3:P:197:PHE:O	3:P:201:THR:OG1	2.32	0.47
1:A:109:PHE:CE1	1:A:113:LEU:HD11	2.50	0.46
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.96	0.46
2:O:200:CYS:SG	2:O:204:HIS:HA	2.54	0.46
6:S:85:CYS:SG	6:S:87:THR:HG23	2.55	0.46
1:A:328:HIS:HD2	2:B:56:MET:HE1	1.80	0.46
1:A:358:LEU:HD11	29:A:713:HOH:O	2.15	0.46
18:A:606:HEA:H212	29:A:733:HOH:O	2.14	0.46
2:B:31:VAL:O	2:B:35:SER:OG	2.26	0.46
1:N:42:GLY:C	4:Q:104:TYR:OH	2.58	0.46
1:N:124:THR:OG1	1:N:125:GLY:O	2.33	0.46
3:P:70:HIS:CB	29:P:421:HOH:O	2.60	0.46
5:R:81:ILE:HD13	9:V:9:MET:HG2	1.98	0.46
6:S:62:CYS:SG	6:S:84:SER:HB3	2.55	0.46
3:C:243:HIS:HD2	29:C:406:HOH:O	1.98	0.46
1:N:135:ASN:O	1:N:139:ALA:HB2	2.16	0.46
1:N:429:HIS:O	1:N:433:LEU:HG	2.15	0.46
2:O:155:SER:CB	29:O:412:HOH:O	2.63	0.46
4:Q:10:ASP:CB	29:Q:322:HOH:O	2.64	0.46
1:N:23:GLY:N	29:N:705:HOH:O	2.47	0.46
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.96	0.46
1:A:75:ILE:O	1:A:79:GLY:HA3	2.16	0.46
8:H:27:ARG:HD3	29:H:222:HOH:O	2.15	0.46
9:I:29:LEU:O	9:I:32:ALA:HB3	2.16	0.46
1:N:140:GLY:O	1:N:213:ARG:NH2	2.48	0.46
1:N:371:TYR:O	1:N:374:VAL:HB	2.16	0.46
3:P:116:TRP:HA	3:P:117:PRO:C	2.41	0.46
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.16	0.46
1:N:303:ALA:HB2	2:O:84:LEU:CD2	2.45	0.46
2:O:124:PRO:O	2:O:125:THR:C	2.58	0.46
1:N:361:SER:OG	2:O:84:LEU:HD13	2.15	0.46
10:W:16:ASN:CG	10:W:18:LEU:HD12	2.41	0.46
5:E:24:ILE:HA	5:E:28:GLU:OE1	2.16	0.46
1:N:127:THR:HB	1:N:129:TYR:CE1	2.51	0.46
1:N:344:PHE:O	1:N:345:ILE:C	2.58	0.46
4:D:14:PRO:HD2	29:D:303:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:MET:O	11:K:25:CYS:HB2	2.16	0.46
1:N:251:PHE:HB2	29:N:740:HOH:O	2.15	0.46
2:O:199:ILE:HG23	2:O:199:ILE:O	2.16	0.46
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.98	0.46
1:N:377:PHE:O	1:N:381:LEU:HB2	2.16	0.46
1:N:498:CYS:HA	1:N:499:PRO:HA	1.85	0.46
2:O:216:LEU:HB2	29:O:426:HOH:O	2.16	0.46
25:P:309:CDL:H231	7:T:30:LEU:HD13	1.98	0.46
1:A:12:HIS:CD2	1:A:80:ASN:O	2.61	0.45
2:B:14:SER:CB	2:B:185:MET:O	2.64	0.45
2:B:96:THR:HA	2:B:151:ARG:O	2.15	0.45
1:N:356:ILE:HD13	1:N:356:ILE:HA	1.86	0.45
2:B:14:SER:HB2	2:B:185:MET:O	2.16	0.45
4:D:83:GLY:HA3	11:K:18:LEU:HA	1.98	0.45
1:N:378:HIS:CE1	18:N:607:HEA:NA	2.84	0.45
1:A:11:ASN:HB3	1:A:14:ASP:HB2	1.99	0.45
3:C:56:GLN:O	3:C:59:ARG:HB3	2.16	0.45
12:L:22:LEU:HD21	13:M:18:GLY:HA2	1.97	0.45
2:O:102:HIS:O	2:O:104:TRP:HA	2.16	0.45
3:P:127:LEU:HD13	25:P:309:CDL:H782	1.97	0.45
3:C:81:TYR:O	3:C:85:LEU:HG	2.17	0.45
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.99	0.45
1:A:44:PRO:HD3	1:A:448:THR:HG23	1.98	0.45
2:B:90:ILE:CD1	8:H:16:PHE:CD2	2.98	0.45
3:C:129:VAL:N	3:C:130:PRO:CD	2.79	0.45
4:D:100:LYS:HD2	4:D:100:LYS:O	2.17	0.45
4:Q:10:ASP:HB3	29:Q:322:HOH:O	2.16	0.45
1:N:248:LEU:HB3	29:N:751:HOH:O	2.16	0.45
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.99	0.45
3:P:95:THR:CB	29:P:403:HOH:O	2.64	0.45
29:Q:326:HOH:O	11:X:28:VAL:HG21	2.17	0.45
7:T:72:ASN:C	7:T:72:ASN:OD1	2.60	0.45
1:A:289:ALA:HB3	1:A:305:PHE:CG	2.52	0.45
1:N:43:GLN:HB2	1:N:44:PRO:HD2	1.97	0.45
1:N:151:HIS:CE1	1:N:207:THR:OG1	2.69	0.45
1:N:199:LEU:N	1:N:200:PRO:CD	2.80	0.45
5:R:67:ILE:O	5:R:70:VAL:HG12	2.16	0.45
8:U:60:TYR:O	8:U:64:CYS:HB2	2.16	0.45
1:A:43:GLN:HB2	1:A:44:PRO:HD2	1.99	0.45
2:B:1:FME:HE3	4:D:123:MET:HE3	1.99	0.45
5:E:81:ILE:HD13	9:I:9:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:65:MET:HE3	18:N:607:HEA:HMC3	1.99	0.45
3:P:206:LEU:HB2	29:P:414:HOH:O	2.16	0.45
6:S:13:ALA:O	6:S:18:ARG:HD2	2.17	0.45
1:A:301:THR:HG23	23:C:302:CHD:H112	1.98	0.45
12:L:22:LEU:O	12:L:26:THR:HB	2.17	0.45
1:N:202:LEU:HD13	1:N:238:PHE:CD2	2.52	0.45
12:Y:4:GLU:HB3	12:Y:9:LYS:HB3	1.98	0.45
3:C:192:VAL:HA	3:C:195:SER:HB2	1.99	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.99	0.45
1:N:111:LEU:HD21	3:P:25:LEU:HD12	1.99	0.45
1:N:200:PRO:HB2	3:P:92:LEU:HB3	1.99	0.45
2:O:23:PHE:HB2	2:O:83:ILE:CD1	2.47	0.45
3:P:138:LEU:O	3:P:139:ALA:C	2.59	0.45
1:A:37:ILE:HD11	1:A:58:VAL:HA	1.98	0.44
1:A:230:LEU:HD21	3:C:100:ALA:HA	1.99	0.44
1:A:60:ALA:O	1:A:64:VAL:HG23	2.17	0.44
11:K:9:PHE:HA	29:K:107:HOH:O	2.17	0.44
1:A:405:LEU:CD1	29:A:722:HOH:O	2.63	0.44
1:A:514:LYS:CE	6:F:61:ILE:O	2.65	0.44
3:C:98:PHE:O	3:C:101:PHE:HB3	2.18	0.44
1:N:280:ILE:HD11	1:N:316:THR:HA	1.99	0.44
2:O:1:FME:CE	2:O:133:LEU:HD11	2.46	0.44
1:A:154:GLY:O	1:A:158:ILE:HG13	2.17	0.44
3:C:50:ASN:OD1	3:C:54:MET:HE2	2.17	0.44
3:C:103:HIS:ND1	23:C:302:CHD:O26	2.46	0.44
1:N:378:HIS:CG	1:N:425:PHE:CE1	3.05	0.44
1:N:470:PHE:CD1	1:N:470:PHE:C	2.95	0.44
4:Q:21:ASP:OD1	4:Q:21:ASP:N	2.50	0.44
1:A:68:PHE:HA	1:A:72:PRO:HG2	1.99	0.44
2:B:58:ALA:O	2:B:60:GLU:N	2.50	0.44
1:N:347:LEU:HD13	1:N:383:MET:HB3	1.99	0.44
1:N:396:TRP:C	29:N:709:HOH:O	2.58	0.44
3:P:86:PHE:CE2	17:P:305:PGV:H261	2.52	0.44
1:A:278:MET:HE1	7:T:8:HIS:NE2	2.33	0.44
1:A:459:PHE:O	4:D:92:THR:HG23	2.18	0.44
11:K:6:ALA:HB1	11:K:7:PRO:HD2	1.99	0.44
7:T:72:ASN:N	7:T:76:ASN:HD22	2.16	0.44
1:A:393:PHE:HA	29:A:726:HOH:O	2.18	0.44
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.17	0.44
2:B:95:LEU:HD12	2:B:112:ASP:OD2	2.18	0.44
2:B:162:SER:HB3	2:B:197:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.17	0.44
13:M:12:PRO:O	13:M:13:LYS:C	2.61	0.44
2:O:216:LEU:O	2:O:219:PHE:HB3	2.18	0.44
3:P:159:MET:SD	3:P:159:MET:C	3.01	0.44
3:P:206:LEU:O	3:P:210:ILE:HG13	2.18	0.44
7:T:48:ILE:HG22	8:U:80:THR:HG22	2.00	0.44
12:Y:41:ARG:HH11	23:Y:101:CHD:H182	1.81	0.44
29:A:804:HOH:O	21:L:101:TGL:H291	2.16	0.44
2:B:110:TYR:CD1	2:B:110:TYR:N	2.86	0.44
3:C:247:VAL:O	3:C:250:LEU:HB2	2.17	0.44
4:D:117:ALA:HB1	11:K:51:LYS:HB2	1.99	0.44
5:E:19:PHE:HE2	29:E:222:HOH:O	2.01	0.44
1:N:54:TYR:O	1:N:57:VAL:HG12	2.17	0.44
1:N:88:GLY:HA2	1:N:505:PHE:CZ	2.52	0.44
1:N:468:MET:HE2	1:N:468:MET:HB3	1.93	0.44
1:A:285:PHE:C	29:A:724:HOH:O	2.60	0.44
1:A:399:LEU:N	29:A:723:HOH:O	2.48	0.44
1:A:443:TYR:CE2	1:A:448:THR:HA	2.53	0.44
1:N:220:PHE:HB3	29:N:729:HOH:O	2.18	0.44
1:N:407:ASP:HB3	29:N:762:HOH:O	2.17	0.44
3:P:102:TYR:O	3:P:106:LEU:HG	2.18	0.44
1:A:11:ASN:HB2	1:A:502:TYR:CZ	2.53	0.43
1:A:24:ALA:HA	29:A:733:HOH:O	2.19	0.43
1:A:362:SER:O	1:A:365:ILE:HB	2.18	0.43
2:B:58:ALA:HB1	2:B:62:GLU:HG3	2.00	0.43
3:C:90:GLU:OE1	3:C:207:HIS:HE1	2.00	0.43
10:J:8:LYS:O	10:J:12:PHE:CD2	2.71	0.43
13:M:13:LYS:HE3	13:M:17:ILE:HD11	2.00	0.43
1:N:106:PRO:O	1:N:107:PRO:C	2.61	0.43
1:N:147:ILE:HD11	1:N:209:LEU:HD23	1.99	0.43
29:P:417:HOH:O	10:W:12:PHE:CE2	2.56	0.43
2:B:163:TRP:O	2:B:171:LYS:HA	2.18	0.43
8:H:57:ARG:CG	29:H:207:HOH:O	2.66	0.43
1:N:111:LEU:HD21	3:P:25:LEU:CD1	2.48	0.43
1:A:258:VAL:CG1	29:A:710:HOH:O	2.54	0.43
1:A:260:TYR:CE2	1:A:487:LEU:HB2	2.53	0.43
1:A:417:MET:HE1	18:A:606:HEA:H263	2.00	0.43
1:A:493:GLU:HG2	1:A:494:TRP:N	2.33	0.43
2:B:40:TYR:CD1	9:I:24:ALA:HB2	2.52	0.43
4:D:109:HIS:C	4:D:111:PHE:H	2.24	0.43
1:N:77:GLY:O	1:N:81:TRP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:113:LEU:HB2	21:N:604:TGL:C31	2.48	0.43
2:O:101:GLY:H	2:O:156:SER:HA	1.82	0.43
1:A:179:TYR:OH	7:T:8:HIS:HB3	2.18	0.43
2:B:28:LEU:HD23	9:I:35:TYR:OH	2.18	0.43
2:B:57:ASP:HB2	22:B:303:PSC:H212	2.00	0.43
10:J:33:ARG:HD2	29:J:201:HOH:O	2.17	0.43
1:N:18:LEU:HA	29:N:753:HOH:O	2.18	0.43
1:N:409:TRP:O	1:N:412:ILE:HB	2.17	0.43
5:R:84:TYR:CD1	5:R:84:TYR:C	2.96	0.43
1:A:377:PHE:CD1	1:A:377:PHE:C	2.97	0.43
2:B:96:THR:HG23	2:B:151:ARG:HD2	2.00	0.43
10:J:30:ILE:O	10:J:34:VAL:HG23	2.18	0.43
1:N:68:PHE:HA	1:N:72:PRO:HG2	1.99	0.43
1:N:339:MET:HE1	1:N:411:LYS:HD3	2.00	0.43
2:O:103:GLN:HB3	2:O:104:TRP:CE2	2.54	0.43
6:S:63:GLU:O	6:S:66:ASN:HB2	2.18	0.43
1:A:328:HIS:CD2	2:B:56:MET:HE1	2.54	0.43
1:A:449:MET:SD	2:B:5:MET:HG2	2.59	0.43
2:B:1:FME:SD	2:B:133:LEU:CD1	3.06	0.43
3:C:197:PHE:O	3:C:201:THR:OG1	2.17	0.43
4:D:23:PRO:CB	5:E:70:VAL:HG21	2.49	0.43
1:N:103:TRP:O	1:N:107:PRO:HD2	2.18	0.43
1:N:476:PHE:O	1:N:479:LYS:HG2	2.17	0.43
1:A:197:LEU:HD21	24:C:311:PEK:H311	2.01	0.43
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.90	0.43
1:A:218:THR:OG1	3:C:191:GLY:CA	2.63	0.43
2:B:144:LEU:HD23	29:B:434:HOH:O	2.18	0.43
2:O:126:SER:HA	29:O:439:HOH:O	2.18	0.43
7:T:78:LEU:HB3	7:T:79:PRO:CD	2.49	0.43
1:A:187:SER:OG	29:A:706:HOH:O	2.22	0.43
2:B:158:ASP:O	2:B:176:PRO:HG3	2.19	0.43
3:C:149:HIS:CE1	26:C:309:DMU:C2	2.98	0.43
4:D:110:THR:HG22	4:D:115:TRP:CE2	2.54	0.43
5:E:31:LYS:HE2	6:F:84:SER:O	2.18	0.43
21:N:609:TGL:HG11	29:N:770:HOH:O	2.18	0.43
4:Q:24:LEU:HD12	5:R:30:ARG:HA	2.01	0.43
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.00	0.43
10:W:6:ALA:O	10:W:9:GLN:HB2	2.18	0.43
21:B:302:TGL:HC41	21:B:302:TGL:H151	2.00	0.43
2:O:199:ILE:HG13	29:O:435:HOH:O	2.18	0.43
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:PHE:CD1	1:A:2:PHE:C	2.97	0.43
1:A:29:VAL:HG22	12:L:32:GLY:O	2.18	0.43
4:D:19:ARG:HD2	29:D:320:HOH:O	2.19	0.43
10:J:25:GLY:O	10:J:27:THR:N	2.52	0.43
23:J:101:CHD:O7	23:J:101:CHD:H41	2.19	0.43
12:L:9:LYS:HA	12:L:9:LYS:HD3	1.79	0.43
1:A:468:MET:HE1	18:A:606:HEA:H211	2.01	0.42
25:P:309:CDL:H542	7:T:31:CYS:SG	2.59	0.42
1:A:240:HIS:O	1:A:243:VAL:HG22	2.18	0.42
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.01	0.42
4:D:21:ASP:OD1	4:D:21:ASP:N	2.52	0.42
9:I:19:PHE:HD1	9:I:20:HIS:CD2	2.37	0.42
1:N:212:ASP:OD1	1:N:217:THR:OG1	2.32	0.42
1:N:507:GLU:HB2	6:S:52:ILE:CD1	2.49	0.42
1:A:468:MET:HE1	18:A:606:HEA:C21	2.49	0.42
2:B:13:THR:HG21	2:B:192:TYR:CE2	2.54	0.42
3:C:119:THR:HG21	8:H:82:PRO:HA	2.01	0.42
3:C:258:TRP:CD1	25:C:308:CDL:H562	2.55	0.42
4:Q:16:TYR:OH	4:Q:18:ASP:OD1	2.30	0.42
4:Q:68:PHE:CZ	5:R:70:VAL:HG23	2.55	0.42
5:R:49:ASP:OD1	5:R:92:THR:OG1	2.30	0.42
9:V:40:ALA:C	9:V:42:LYS:N	2.70	0.42
1:A:245:ILE:HD13	1:A:245:ILE:HG21	1.81	0.42
1:A:289:ALA:HB3	1:A:305:PHE:CE1	2.55	0.42
1:A:361:SER:HB2	2:B:84:LEU:HD13	2.00	0.42
3:C:155:ASP:OD2	3:C:158:HIS:CD2	2.67	0.42
10:J:50:LEU:HD22	10:J:50:LEU:O	2.19	0.42
11:K:21:GLY:N	29:K:102:HOH:O	2.52	0.42
1:N:43:GLN:CG	4:Q:104:TYR:CE2	3.02	0.42
1:N:354:THR:O	1:N:357:VAL:HB	2.19	0.42
2:O:41:ILE:HD13	22:V:101:PSC:C34	2.49	0.42
7:T:17:ARG:NE	29:T:204:HOH:O	2.52	0.42
9:V:11:GLY:O	9:V:15:ARG:NH1	2.51	0.42
9:V:22:VAL:O	9:V:26:MET:HG2	2.20	0.42
1:A:147:ILE:HG23	1:A:206:ILE:HD12	2.01	0.42
1:A:467:LEU:HD12	1:A:467:LEU:HA	1.87	0.42
1:A:494:TRP:CD1	29:A:785:HOH:O	2.71	0.42
3:C:34:TRP:O	3:C:38:ASN:HA	2.19	0.42
11:K:28:VAL:CB	29:K:101:HOH:O	2.32	0.42
1:N:368:HIS:O	2:O:171:LYS:HE2	2.19	0.42
1:N:459:PHE:CE2	4:Q:99:GLU:OE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:14:GLU:O	13:Z:17:ILE:HB	2.20	0.42
3:C:153:GLU:OE1	7:G:13:ALA:HB3	2.19	0.42
4:D:14:PRO:CD	29:D:303:HOH:O	2.66	0.42
1:N:12:HIS:HD2	1:N:80:ASN:O	2.02	0.42
1:N:70:VAL:CG1	1:N:246:LEU:HD22	2.49	0.42
3:P:16:TRP:HA	3:P:19:THR:OG1	2.20	0.42
3:P:72:THR:O	3:P:75:VAL:N	2.52	0.42
3:P:77:LYS:O	3:P:81:TYR:CD2	2.73	0.42
3:P:139:ALA:O	3:P:142:VAL:N	2.53	0.42
4:Q:48:TRP:HA	4:Q:51:LEU:HD13	2.02	0.42
6:S:9:ASP:HB3	6:S:21:MET:CE	2.38	0.42
1:A:12:HIS:CE1	1:A:13:LYS:HG3	2.54	0.42
1:A:102:PHE:CD2	1:A:102:PHE:C	2.98	0.42
5:E:8:ASP:HB3	9:I:10:ARG:CZ	2.50	0.42
5:R:82:TYR:OH	5:R:101:PRO:HD2	2.19	0.42
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.85	0.42
1:A:322:SER:O	1:A:325:ALA:N	2.52	0.42
1:A:397:PHE:N	1:A:398:PRO:CD	2.83	0.42
6:F:29:ASP:OD2	6:F:34:LEU:N	2.36	0.42
1:N:131:PRO:HG2	2:O:159:VAL:HA	2.02	0.42
1:N:338:MET:O	1:N:342:LEU:HG	2.19	0.42
2:O:13:THR:HG21	2:O:192:TYR:CE2	2.55	0.42
11:X:34:THR:OG1	11:X:35:GLN:HG2	2.20	0.42
1:A:374:VAL:HA	1:A:377:PHE:CE2	2.53	0.42
17:A:604:PGV:H062	13:M:3:ALA:HB3	2.01	0.42
2:B:193:TYR:CD2	2:B:210:VAL:HG22	2.55	0.42
3:C:172:TYR:O	3:C:176:LEU:HD12	2.19	0.42
6:F:47:ASN:HB2	6:F:89:TYR:CD1	2.55	0.42
12:L:26:THR:HG22	12:L:27:LEU:HD23	2.01	0.42
1:N:33:LEU:HD22	1:N:60:ALA:HB3	2.01	0.42
3:P:59:ARG:HD2	3:P:63:ARG:NH2	2.34	0.42
5:R:94:ASN:N	5:R:94:ASN:HD22	2.17	0.42
1:A:24:ALA:HB1	29:A:733:HOH:O	2.20	0.42
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.68	0.42
2:B:5:MET:HE2	2:B:5:MET:HB3	1.90	0.42
1:N:430:PHE:O	1:N:431:LEU:C	2.63	0.42
3:P:25:LEU:O	3:P:29:SER:CB	2.68	0.42
3:P:44:MET:SD	25:P:307:CDL:H473	2.59	0.42
3:P:64:GLU:OE2	10:W:20:VAL:HG11	2.19	0.42
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.55	0.42
9:V:42:LYS:HA	9:V:45:LYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:LEU:HD21	10:J:42:GLY:C	2.45	0.41
9:I:47:TYR:HB3	29:I:203:HOH:O	2.20	0.41
2:O:162:SER:HB2	2:O:198:GLU:HB2	2.02	0.41
9:V:36:LYS:HD3	9:V:41:GLU:HG2	2.01	0.41
7:G:11:TPO:HG23	7:G:14:ARG:CB	2.50	0.41
12:L:2:HIS:CD2	29:L:210:HOH:O	2.73	0.41
1:N:354:THR:HG21	1:N:429:HIS:HE1	1.85	0.41
1:N:377:PHE:CD1	1:N:377:PHE:C	2.99	0.41
18:N:607:HEA:C1C	29:N:763:HOH:O	2.68	0.41
3:P:37:PHE:O	3:P:38:ASN:C	2.63	0.41
1:A:473:TRP:O	1:A:474:GLU:C	2.63	0.41
7:G:1:ALA:HA	17:P:306:PGV:H301	2.01	0.41
3:P:67:PHE:HA	10:W:9:GLN:HG2	2.02	0.41
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.56	0.41
1:A:33:LEU:HB3	1:A:61:HIS:HB2	2.02	0.41
4:Q:48:TRP:CE2	5:R:56:ARG:NH1	2.87	0.41
4:Q:116:VAL:O	4:Q:120:THR:OG1	2.30	0.41
1:A:76:GLY:O	1:A:80:ASN:HB2	2.21	0.41
1:A:393:PHE:N	29:A:726:HOH:O	2.50	0.41
3:C:159:MET:O	3:C:159:MET:SD	2.79	0.41
1:N:54:TYR:O	1:N:57:VAL:CG1	2.68	0.41
1:N:176:MET:HE3	1:N:176:MET:HB2	1.99	0.41
1:N:240:HIS:O	1:N:241:PRO:C	2.60	0.41
2:O:24:HIS:CE1	29:O:434:HOH:O	2.61	0.41
2:O:153:LEU:HD23	2:O:181:GLN:HA	2.01	0.41
3:P:69:GLY:HA3	6:S:14:THR:O	2.21	0.41
3:P:119:THR:O	7:T:52:HIS:HE1	2.04	0.41
3:P:155:ASP:OD2	3:P:158:HIS:HB2	2.21	0.41
24:C:303:PEK:C12	24:C:303:PEK:C16	2.98	0.41
10:J:50:LEU:HD22	10:J:50:LEU:C	2.45	0.41
12:L:35:ALA:O	12:L:36:PRO:C	2.62	0.41
1:N:65:MET:SD	1:N:69:MET:HE2	2.60	0.41
1:N:91:ASP:HB2	3:P:10:MET:HE1	2.03	0.41
1:N:510:TYR:CE2	6:S:36:PRO:HG3	2.56	0.41
3:P:56:GLN:O	3:P:59:ARG:HB3	2.20	0.41
4:Q:59:LEU:HD13	5:R:61:PHE:HB3	2.03	0.41
4:Q:121:LYS:HA	4:Q:124:LEU:HD12	2.03	0.41
1:A:35:LEU:HD11	1:A:462:LEU:HD22	2.03	0.41
1:A:240:HIS:CD2	1:A:244:TYR:CD2	3.07	0.41
1:A:272:GLY:HA2	29:T:201:HOH:O	2.19	0.41
1:A:380:VAL:HG21	18:A:605:HEA:C3C	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:CD1	2:B:211:LEU:HD12	2.50	0.41
3:C:187:THR:HA	24:C:303:PEK:O12	2.20	0.41
7:G:9:GLY:HA3	29:G:211:HOH:O	2.21	0.41
8:H:73:ASP:OD1	8:H:76:ARG:NH2	2.45	0.41
11:K:43:SER:OG	11:K:45:VAL:HG23	2.21	0.41
1:N:16:GLY:O	1:N:20:LEU:HG	2.21	0.41
1:N:72:PRO:CB	29:N:705:HOH:O	2.66	0.41
12:Y:35:ALA:CB	12:Y:36:PRO:CD	2.95	0.41
1:A:285:PHE:CG	7:T:2:SER:OG	2.74	0.41
1:A:311:ILE:CD1	25:P:309:CDL:H181	2.51	0.41
18:A:606:HEA:C4B	29:A:762:HOH:O	2.68	0.41
2:B:78:LEU:N	2:B:79:PRO:HD2	2.36	0.41
2:B:115:ASP:HB2	29:B:424:HOH:O	2.20	0.41
3:C:33:MET:HG3	3:C:42:LEU:HD12	2.02	0.41
24:C:303:PEK:C05	7:G:76:ASN:HD21	2.33	0.41
1:N:404:THR:HG21	13:Z:3:ALA:HB2	2.02	0.41
1:N:426:PHE:N	1:N:427:PRO:CD	2.84	0.41
2:O:175:ILE:HD12	2:O:178:ARG:HD3	2.03	0.41
7:T:17:ARG:O	7:T:18:PHE:C	2.63	0.41
1:A:24:ALA:CA	29:A:733:HOH:O	2.68	0.41
1:N:406:ASN:HD21	17:N:610:PGV:H61	1.86	0.41
1:N:461:SER:O	1:N:465:VAL:HG23	2.21	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.21	0.41
1:A:404:THR:HG21	13:M:3:ALA:HB2	2.03	0.40
2:B:17:MET:HE2	29:B:440:HOH:O	2.21	0.40
3:C:151:LEU:HD21	3:C:232:HIS:CG	2.56	0.40
4:D:120:THR:O	4:D:124:LEU:HG	2.21	0.40
4:D:130:PRO:O	4:D:136:ALA:HB2	2.21	0.40
1:N:377:PHE:HA	1:N:380:VAL:HG22	2.03	0.40
1:N:387:PHE:HB3	29:N:730:HOH:O	2.21	0.40
3:P:243:HIS:O	3:P:246:ASP:HB3	2.21	0.40
7:T:44:ARG:HD2	7:T:74:ARG:O	2.20	0.40
11:X:54:ARG:HD3	29:X:108:HOH:O	2.21	0.40
1:A:24:ALA:CB	18:A:606:HEA:H243	2.51	0.40
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.87	0.40
1:A:429:HIS:CD2	29:A:793:HOH:O	2.74	0.40
3:C:127:LEU:HD12	3:C:127:LEU:HA	1.95	0.40
4:D:127:LYS:HD2	9:I:59:ASP:OD1	2.22	0.40
3:P:239:ALA:O	3:P:240:TRP:C	2.64	0.40
8:U:54:GLU:OE1	8:U:54:GLU:HA	2.20	0.40
1:A:183:LEU:HD12	1:A:255:SER:CB	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PHE:CG	29:A:706:HOH:O	2.72	0.40
1:A:237:PHE:CA	29:A:709:HOH:O	2.68	0.40
1:A:336:PRO:HA	1:A:339:MET:HG3	2.03	0.40
3:C:154:GLY:O	6:F:4:GLY:HA2	2.22	0.40
8:H:7:LYS:N	29:H:204:HOH:O	2.54	0.40
3:P:187:THR:HB	7:T:68:THR:HG21	2.03	0.40
5:R:12:ASP:CG	9:V:10:ARG:HH22	2.29	0.40
7:T:20:THR:O	7:T:24:ALA:HB3	2.22	0.40
9:V:29:LEU:HD23	9:V:29:LEU:HA	1.90	0.40
1:A:198:SER:HB2	1:A:238:PHE:HA	2.02	0.40
1:A:492:LEU:HD13	6:F:71:TRP:CG	2.55	0.40
7:G:34:ASN:O	7:G:34:ASN:CG	2.63	0.40
1:N:113:LEU:HD22	21:N:604:TGL:C29	2.50	0.40
1:N:191:THR:HG23	1:N:245:ILE:HA	2.02	0.40
1:N:240:HIS:ND1	1:N:290:HIS:HE1	2.16	0.40
1:N:370:THR:HA	1:N:437:PRO:HA	2.03	0.40
9:V:19:PHE:HD1	9:V:20:HIS:CD2	2.39	0.40
1:A:172:LYS:HE2	1:A:172:LYS:HB2	1.87	0.40
1:A:406:ASN:HD21	17:A:604:PGV:H71	1.86	0.40
3:C:187:THR:CB	7:G:68:THR:HG21	2.51	0.40
13:M:23:PHE:O	13:M:27:LEU:HG	2.21	0.40
1:N:63:PHE:CE1	1:N:150:LEU:HD21	2.56	0.40
1:N:247:ILE:O	1:N:250:GLY:N	2.54	0.40
2:O:182:THR:OG1	2:O:183:THR:N	2.54	0.40
3:P:101:PHE:O	3:P:105:SER:OG	2.33	0.40
3:P:249:TRP:HD1	29:P:430:HOH:O	2.05	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	512/514 (100%)	455 (89%)	52 (10%)	5 (1%)	12	17
1	N	512/514 (100%)	451 (88%)	60 (12%)	1 (0%)	43	56
2	B	225/227 (99%)	199 (88%)	22 (10%)	4 (2%)	6	8
2	O	225/227 (99%)	194 (86%)	27 (12%)	4 (2%)	6	8
3	C	257/261 (98%)	240 (93%)	15 (6%)	2 (1%)	16	23
3	P	257/261 (98%)	226 (88%)	30 (12%)	1 (0%)	30	40
4	D	142/147 (97%)	124 (87%)	17 (12%)	1 (1%)	18	26
4	Q	142/147 (97%)	130 (92%)	10 (7%)	2 (1%)	9	11
5	E	103/109 (94%)	93 (90%)	9 (9%)	1 (1%)	12	17
5	R	103/109 (94%)	99 (96%)	4 (4%)	0	100	100
6	F	96/98 (98%)	86 (90%)	9 (9%)	1 (1%)	12	17
6	S	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
7	G	81/85 (95%)	68 (84%)	12 (15%)	1 (1%)	10	14
7	T	81/85 (95%)	66 (82%)	13 (16%)	2 (2%)	4	4
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	4	4
8	U	77/85 (91%)	65 (84%)	10 (13%)	2 (3%)	4	4
9	I	70/73 (96%)	64 (91%)	5 (7%)	1 (1%)	9	11
9	V	70/73 (96%)	62 (89%)	7 (10%)	1 (1%)	9	11
10	J	56/59 (95%)	50 (89%)	5 (9%)	1 (2%)	6	8
10	W	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	43 (92%)	4 (8%)	0	100	100
12	L	44/47 (94%)	39 (89%)	4 (9%)	1 (2%)	5	5
12	Y	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	5	5
13	M	41/47 (87%)	35 (85%)	4 (10%)	2 (5%)	1	1
13	Z	41/47 (87%)	37 (90%)	4 (10%)	0	100	100
All	All	3502/3616 (97%)	3123 (89%)	343 (10%)	36 (1%)	12	17

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	GLN
2	B	89	GLU
7	G	41	HIS

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Mol	Chain	Res	Type
10	J	26	ALA
12	L	46	LYS
2	O	59	GLN
2	O	89	GLU
1	A	52	GLN
3	C	229	SER
6	F	66	ASN
8	H	70	SER
1	N	52	GLN
2	O	90	ILE
7	T	41	HIS
8	U	70	SER
1	A	252	GLY
1	A	362	SER
2	B	88	ASP
2	B	158	ASP
8	H	51	SER
2	O	58	ALA
8	U	51	SER
9	V	41	GLU
13	M	17	ILE
3	P	38	ASN
4	Q	141	ASP
4	Q	143	ASN
1	A	492	LEU
4	D	9	GLU
9	I	37	PHE
13	M	12	PRO
7	T	63	GLY
12	Y	28	PHE
1	A	73	ILE
3	C	191	GLY
5	E	91	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	406 (95%)	20 (5%)	23	37
1	N	426/426 (100%)	404 (95%)	22 (5%)	21	33
2	B	210/210 (100%)	197 (94%)	13 (6%)	16	26
2	O	210/210 (100%)	193 (92%)	17 (8%)	11	16
3	C	224/226 (99%)	210 (94%)	14 (6%)	16	26
3	P	224/226 (99%)	212 (95%)	12 (5%)	20	32
4	D	128/129 (99%)	119 (93%)	9 (7%)	14	21
4	Q	128/129 (99%)	119 (93%)	9 (7%)	14	21
5	E	92/95 (97%)	85 (92%)	7 (8%)	12	19
5	R	92/95 (97%)	88 (96%)	4 (4%)	26	41
6	F	81/81 (100%)	73 (90%)	8 (10%)	7	10
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	19
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	13
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	28
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	42
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	15
9	I	57/57 (100%)	52 (91%)	5 (9%)	9	14
9	V	57/57 (100%)	47 (82%)	10 (18%)	2	2
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	43
10	W	49/50 (98%)	44 (90%)	5 (10%)	7	9
11	K	39/46 (85%)	34 (87%)	5 (13%)	4	5
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	34
12	L	39/40 (98%)	34 (87%)	5 (13%)	4	5
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	34
13	M	37/39 (95%)	33 (89%)	4 (11%)	6	8
13	Z	37/39 (95%)	30 (81%)	7 (19%)	1	2
All	All	3040/3084 (99%)	2833 (93%)	207 (7%)	14	23

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	46	THR
1	A	91	ASP

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Mol	Chain	Res	Type
1	A	124	THR
1	A	128	VAL
1	A	189	MET
1	A	253	MET
1	A	265	LYS
1	A	300	ASP
1	A	312	ILE
1	A	339	MET
1	A	361	SER
1	A	369	ASP
1	A	376	HIS
1	A	382	SER
1	A	390	MET
1	A	486	ASP
1	A	493	GLU
1	A	504	THR
1	A	506	GLU
2	B	30	ILE
2	B	33	LEU
2	B	84	LEU
2	B	88	ASP
2	B	94	SER
2	B	110	TYR
2	B	115	ASP
2	B	183	THR
2	B	185	MET
2	B	199	ILE
2	B	213	LEU
2	B	214	VAL
2	B	227	LEU
3	C	38	ASN
3	C	42	LEU
3	C	95	THR
3	C	105	SER
3	C	127	LEU
3	C	144	ILE
3	C	159	MET
3	C	179	SER
3	C	180	GLU
3	C	208	VAL
3	C	230	ASN
3	C	246	ASP

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Mol	Chain	Res	Type
3	C	254	VAL
3	C	261	SER
4	D	9	GLU
4	D	20	ARG
4	D	21	ASP
4	D	43	LYS
4	D	51	LEU
4	D	52	SER
4	D	75	THR
4	D	122	ARG
4	D	141	ASP
5	E	7	THR
5	E	17	THR
5	E	63	SER
5	E	71	VAL
5	E	81	ILE
5	E	90	ARG
5	E	104	LEU
6	F	8	THR
6	F	14	THR
6	F	44	GLU
6	F	48	LEU
6	F	55	LYS
6	F	76	LYS
6	F	80	GLN
6	F	96	LEU
7	G	8	HIS
7	G	31	CYS
7	G	33	LEU
7	G	36	TRP
7	G	42	ARG
7	G	84	LYS
8	H	50	VAL
8	H	60	TYR
8	H	61	LYS
9	I	13	LEU
9	I	18	ARG
9	I	29	LEU
9	I	33	THR
9	I	68	ILE
10	J	31	LEU
10	J	50	LEU

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Mol	Chain	Res	Type
11	K	23	THR
11	K	38	ILE
11	K	49	THR
11	K	51	LYS
11	K	54	ARG
12	L	11	ILE
12	L	26	THR
12	L	27	LEU
12	L	36	PRO
12	L	42	HIS
13	M	1	ILE
13	M	13	LYS
13	M	19	LEU
13	M	38	ASP
1	N	4	ASN
1	N	38	ARG
1	N	53	ILE
1	N	91	ASP
1	N	109	PHE
1	N	138	HIS
1	N	189	MET
1	N	218	THR
1	N	238	PHE
1	N	243	VAL
1	N	265	LYS
1	N	279	SER
1	N	350	VAL
1	N	382	SER
1	N	383	MET
1	N	401	SER
1	N	436	MET
1	N	456	MET
1	N	471	ILE
1	N	480	ARG
1	N	485	VAL
1	N	512	ASN
2	O	35	SER
2	O	37	LEU
2	O	43	SER
2	O	66	THR
2	O	67	ILE
2	O	110	TYR

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Mol	Chain	Res	Type
2	O	148	MET
2	O	152	MET
2	O	154	VAL
2	O	167	SER
2	O	171	LYS
2	O	183	THR
2	O	185	MET
2	O	199	ILE
2	O	217	LYS
2	O	223	SER
2	O	227	LEU
3	P	14	SER
3	P	41	THR
3	P	47	LEU
3	P	70	HIS
3	P	84	ILE
3	P	127	LEU
3	P	129	VAL
3	P	144	ILE
3	P	180	GLU
3	P	230	ASN
3	P	250	LEU
3	P	254	VAL
4	Q	7	LYS
4	Q	8	SER
4	Q	10	ASP
4	Q	15	SER
4	Q	21	ASP
4	Q	52	SER
4	Q	62	LEU
4	Q	71	MET
4	Q	143	ASN
5	R	5	HIS
5	R	7	THR
5	R	71	VAL
5	R	80	GLU
6	S	8	THR
6	S	40	SER
6	S	48	LEU
6	S	76	LYS
6	S	80	GLN
6	S	95	GLN

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Mol	Chain	Res	Type
7	T	31	CYS
7	T	36	TRP
7	T	37	LEU
7	T	61	SER
8	U	9	LYS
8	U	44	THR
8	U	60	TYR
8	U	61	LYS
8	U	66	ILE
8	U	67	SER
9	V	2	THR
9	V	4	LEU
9	V	15	ARG
9	V	18	ARG
9	V	21	ILE
9	V	33	THR
9	V	36	LYS
9	V	42	LYS
9	V	44	LYS
9	V	61	GLU
10	W	23	LYS
10	W	27	THR
10	W	31	LEU
10	W	36	MET
10	W	50	LEU
11	X	20	SER
11	X	49	THR
12	Y	2	HIS
12	Y	27	LEU
13	Z	1	ILE
13	Z	10	THR
13	Z	22	THR
13	Z	34	LEU
13	Z	37	LEU
13	Z	41	LYS
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	12	HIS

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Mol	Chain	Res	Type
1	A	491	ASN
2	B	24	HIS
2	B	59	GLN
3	C	12	ASN
3	C	38	ASN
3	C	158	HIS
3	C	207	HIS
3	C	222	GLN
4	D	101	HIS
5	E	20	ASN
7	G	76	ASN
8	H	32	ASN
8	H	37	HIS
9	I	20	HIS
10	J	13	GLN
11	K	15	ASN
1	N	4	ASN
1	N	12	HIS
1	N	80	ASN
1	N	98	ASN
1	N	138	HIS
1	N	151	HIS
1	N	214	ASN
1	N	422	ASN
1	N	429	HIS
2	O	24	HIS
2	O	26	HIS
2	O	91	ASN
2	O	102	HIS
3	P	12	ASN
3	P	68	GLN
3	P	232	HIS
4	Q	101	HIS
5	R	78	HIS
5	R	94	ASN
6	S	47	ASN
6	S	75	HIS
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
6	S	98	HIS
7	T	38	HIS

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Mol	Chain	Res	Type
7	T	52	HIS
7	T	67	HIS
7	T	76	ASN
8	U	22	ASN
8	U	28	ASN
8	U	31	GLN
9	V	20	HIS
10	W	21	HIS
11	X	10	HIS
12	Y	2	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	O	1	2	8,9,10	0.68	0	8,9,11	0.99	0
1	FME	A	1	1	8,9,10	0.64	0	8,9,11	0.96	0
2	FME	B	1	2	8,9,10	0.39	0	8,9,11	1.02	0
7	TPO	G	11	7	8,10,11	0.94	1 (12%)	10,14,16	0.98	1 (10%)
1	FME	N	1	1	8,9,10	0.50	0	8,9,11	0.91	1 (12%)
7	TPO	T	11	7	8,10,11	0.84	0	10,14,16	0.78	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
2	FME	O	1	2	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	7/9/11/13	-
1	FME	N	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	2.18	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	11	TPO	O-C-CA	-2.03	119.54	124.77
1	N	1	FME	O-C-CA	-2.01	119.59	124.77

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
2	B	1	FME	CB-CA-N-CN
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	CA-CB-OG1-P
1	N	1	FME	C-CA-CB-CG
2	O	1	FME	CB-CA-N-CN
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	O-C-CA-CB
1	A	1	FME	CA-CB-CG-SD
1	N	1	FME	CB-CG-SD-CE
2	O	1	FME	CB-CG-SD-CE
1	N	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
7	G	11	TPO	CG2-CB-OG1-P
7	T	11	TPO	CA-CB-OG1-P

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Mol	Chain	Res	Type	Atoms
7	G	11	TPO	CB-OG1-P-O1P
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	4	0
2	B	1	FME	3	0
7	G	11	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 50 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	$\# Z > 2$
26	DMU	C	310	-	34,34,34	0.83	1 (2%)	45,45,45	1.28	5 (11%)
17	PGV	A	604	-	50,50,50	0.32	0	53,56,56	0.51	0
23	CHD	T	101	-	32,32,32	0.65	0	51,51,51	1.43	11 (21%)
24	PEK	C	311	-	52,52,52	0.38	0	55,57,57	0.45	0
21	TGL	D	201	-	62,62,62	0.23	0	65,65,65	0.28	0
17	PGV	N	605	-	50,50,50	0.31	0	53,56,56	0.74	2 (3%)
24	PEK	P	304	-	52,52,52	0.29	0	55,57,57	0.51	0
20	CUA	O	302	2	0,1,1	-	-	-	-	-
22	PSC	V	101	-	51,51,51	0.31	0	57,59,59	0.45	0
17	PGV	C	305	-	50,50,50	0.37	0	53,56,56	0.55	0
21	TGL	O	301	-	62,62,62	0.27	0	65,65,65	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHD	O	303	-	32,32,32	0.56	0	51,51,51	1.04	3 (5%)
17	PGV	N	610	-	50,50,50	0.32	0	53,56,56	0.39	0
21	TGL	N	604	-	62,62,62	0.22	0	65,65,65	0.34	0
22	PSC	B	303	-	51,51,51	0.29	0	57,59,59	0.38	0
23	CHD	T	103	-	32,32,32	0.63	0	51,51,51	0.92	2 (3%)
17	PGV	C	301	-	50,50,50	0.35	0	53,56,56	0.68	2 (3%)
23	CHD	Y	101	-	32,32,32	0.63	0	51,51,51	0.95	1 (1%)
23	CHD	P	308	-	32,32,32	0.58	0	51,51,51	0.90	0
26	DMU	M	101	-	34,34,34	0.67	0	45,45,45	1.55	8 (17%)
28	SAC	V	102	-	7,8,9	0.55	0	7,9,11	1.50	1 (14%)
23	CHD	P	303	-	32,32,32	0.66	1 (3%)	51,51,51	1.13	3 (5%)
23	CHD	W	101	-	32,32,32	0.60	0	51,51,51	0.71	0
25	CDL	C	306	-	99,99,99	0.30	0	105,111,111	0.38	0
24	PEK	C	304	-	52,52,52	0.29	0	55,57,57	0.38	0
18	HEA	A	606	1	67,67,67	2.37	25 (37%)	81,103,103	2.67	34 (41%)
21	TGL	B	302	-	62,62,62	0.35	0	65,65,65	0.40	0
28	SAC	I	101	-	7,8,9	0.57	0	7,9,11	1.11	1 (14%)
17	PGV	H	101	-	50,50,50	0.31	0	53,56,56	0.42	0
23	CHD	C	302	-	32,32,32	0.67	0	51,51,51	0.94	1 (1%)
26	DMU	P	302	-	34,34,34	0.64	1 (2%)	45,45,45	1.29	7 (15%)
26	DMU	C	309	-	34,34,34	0.92	1 (2%)	45,45,45	1.39	7 (15%)
24	PEK	P	301	-	52,52,52	0.31	0	55,57,57	0.36	0
25	CDL	P	307	-	99,99,99	0.31	0	105,111,111	0.47	1 (0%)
23	CHD	C	307	-	32,32,32	0.64	0	51,51,51	1.07	2 (3%)
26	DMU	Q	201	-	34,34,34	0.65	1 (2%)	45,45,45	1.15	5 (11%)
18	HEA	N	607	1	67,67,67	2.46	23 (34%)	81,103,103	2.76	32 (39%)
24	PEK	C	303	-	52,52,52	0.29	0	55,57,57	0.66	1 (1%)
21	TGL	L	101	-	62,62,62	0.27	0	65,65,65	0.34	0
26	DMU	G	101	-	34,34,34	0.84	1 (2%)	45,45,45	1.10	3 (6%)
17	PGV	P	306	-	50,50,50	0.32	0	53,56,56	0.39	0
18	HEA	A	605	1,19	67,67,67	2.46	23 (34%)	81,103,103	2.81	30 (37%)
20	CUA	B	301	2	0,1,1	-	-	-	-	-
24	PEK	T	102	-	52,52,52	0.33	0	55,57,57	0.72	1 (1%)
25	CDL	P	309	-	99,99,99	0.31	0	105,111,111	0.38	0
17	PGV	P	305	-	50,50,50	0.33	0	53,56,56	0.53	0
21	TGL	N	609	-	62,62,62	0.27	0	65,65,65	0.24	0
18	HEA	N	606	1,19	67,67,67	2.51	25 (37%)	81,103,103	2.57	28 (34%)
23	CHD	J	101	-	32,32,32	0.63	0	51,51,51	1.06	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CDL	C	308	-	99,99,99	0.32	0	105,111,111	0.39	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
26	DMU	C	310	-	2/2/10/10	9/19/59/59	0/2/2/2
17	PGV	A	604	-	-	31/55/55/55	-
23	CHD	T	101	-	-	7/9/74/74	0/4/4/4
24	PEK	C	311	-	-	24/56/56/56	-
21	TGL	D	201	-	-	39/65/65/65	-
17	PGV	N	605	-	-	21/55/55/55	-
24	PEK	P	304	-	-	20/56/56/56	-
22	PSC	V	101	-	-	30/55/55/55	-
17	PGV	C	305	-	-	17/55/55/55	-
21	TGL	O	301	-	-	34/65/65/65	-
23	CHD	O	303	-	-	2/9/74/74	0/4/4/4
17	PGV	N	610	-	-	34/55/55/55	-
21	TGL	N	604	-	-	38/65/65/65	-
22	PSC	B	303	-	-	28/55/55/55	-
23	CHD	T	103	-	1/1/12/12	3/9/74/74	0/4/4/4
23	CHD	Y	101	-	1/1/12/12	5/9/74/74	0/4/4/4
26	DMU	M	101	-	2/2/10/10	7/19/59/59	0/2/2/2
17	PGV	C	301	-	-	16/55/55/55	-
23	CHD	P	308	-	-	3/9/74/74	0/4/4/4
28	SAC	V	102	-	-	2/7/8/10	-
23	CHD	P	303	-	-	7/9/74/74	0/4/4/4
23	CHD	W	101	-	-	1/9/74/74	0/4/4/4
25	CDL	C	306	-	-	56/110/110/110	-
24	PEK	C	304	-	-	25/56/56/56	-
18	HEA	A	606	1	-	7/36/76/76	-
21	TGL	B	302	-	-	34/65/65/65	-
28	SAC	I	101	-	-	2/7/8/10	-
17	PGV	H	101	-	-	30/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	C	302	-	-	3/9/74/74	0/4/4/4
26	DMU	P	302	-	2/2/10/10	9/19/59/59	0/2/2/2
26	DMU	C	309	-	2/2/10/10	9/19/59/59	0/2/2/2
24	PEK	P	301	-	-	32/56/56/56	-
25	CDL	P	307	-	-	61/110/110/110	-
23	CHD	C	307	-	-	6/9/74/74	0/4/4/4
26	DMU	Q	201	-	2/2/10/10	9/19/59/59	0/2/2/2
18	HEA	N	607	1	-	5/36/76/76	-
24	PEK	C	303	-	-	17/56/56/56	-
21	TGL	L	101	-	-	34/65/65/65	-
26	DMU	G	101	-	2/2/10/10	13/19/59/59	0/2/2/2
17	PGV	P	306	-	-	33/55/55/55	-
18	HEA	A	605	1,19	-	9/36/76/76	-
24	PEK	T	102	-	-	33/56/56/56	-
25	CDL	P	309	-	-	49/110/110/110	-
17	PGV	P	305	-	-	24/55/55/55	-
21	TGL	N	609	-	-	34/65/65/65	-
18	HEA	N	606	1,19	-	9/36/76/76	-
23	CHD	J	101	-	-	3/9/74/74	0/4/4/4
25	CDL	C	308	-	-	56/110/110/110	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	607	HEA	C3B-C2B	6.35	1.49	1.34
18	A	606	HEA	CHB-C4A	5.69	1.49	1.38
18	N	607	HEA	FE-ND	5.49	2.11	1.94
18	N	607	HEA	C3D-C2D	5.41	1.48	1.36
18	N	606	HEA	C4B-NB	-5.38	1.30	1.40
18	N	606	HEA	C3D-C2D	5.38	1.48	1.36
18	A	606	HEA	CHA-C1A	5.38	1.48	1.38
18	A	605	HEA	FE-NB	5.31	2.11	1.94
18	N	606	HEA	CHC-C4B	5.29	1.49	1.38
18	N	606	HEA	C3B-C2B	5.21	1.46	1.34
18	A	606	HEA	FE-NB	5.20	2.10	1.94
18	A	605	HEA	C3D-C2D	5.17	1.47	1.36
18	A	605	HEA	CHC-C4B	5.14	1.48	1.38
18	A	605	HEA	C3B-C2B	5.05	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	606	HEA	FE-NB	4.93	2.10	1.94
18	A	605	HEA	CHB-C4A	4.88	1.47	1.38
18	N	606	HEA	FE-ND	4.86	2.09	1.94
18	N	606	HEA	CHA-C1A	4.86	1.47	1.38
18	N	607	HEA	CHA-C1A	4.82	1.47	1.38
18	A	605	HEA	FE-NC	4.75	2.10	1.95
18	A	605	HEA	C3A-C2A	4.71	1.48	1.37
18	N	607	HEA	CHC-C4B	4.62	1.47	1.38
18	A	605	HEA	CHB-C1B	4.56	1.49	1.39
18	N	607	HEA	CHC-C1C	4.51	1.49	1.39
18	N	607	HEA	C4A-NA	-4.50	1.31	1.39
18	A	606	HEA	CHB-C1B	4.32	1.49	1.39
18	A	605	HEA	CHA-C4D	4.32	1.49	1.39
18	N	606	HEA	C4B-C3B	4.27	1.52	1.44
18	N	607	HEA	FE-NB	4.22	2.07	1.94
18	A	605	HEA	FE-NA	4.18	2.08	1.95
18	A	606	HEA	C3B-C2B	4.13	1.44	1.34
18	N	606	HEA	FE-NA	4.13	2.08	1.95
18	A	605	HEA	FE-ND	4.11	2.07	1.94
18	A	606	HEA	C3D-C2D	4.07	1.45	1.36
18	N	607	HEA	FE-NA	4.05	2.08	1.95
18	A	605	HEA	CHA-C1A	4.01	1.46	1.38
18	N	606	HEA	C1C-C2C	3.97	1.52	1.43
18	A	606	HEA	CHA-C4D	3.95	1.48	1.39
18	A	606	HEA	CHC-C4B	3.89	1.46	1.38
18	N	606	HEA	CHC-C1C	3.86	1.48	1.39
18	N	607	HEA	FE-NC	3.86	2.07	1.95
18	N	606	HEA	CHB-C4A	3.83	1.45	1.38
18	N	607	HEA	C3A-C2A	3.80	1.45	1.37
18	N	606	HEA	FE-NC	3.78	2.07	1.95
18	A	606	HEA	FE-ND	3.78	2.06	1.94
18	A	605	HEA	C1A-NA	-3.76	1.32	1.39
18	A	606	HEA	CHC-C1C	3.75	1.47	1.39
18	A	606	HEA	FE-NA	3.74	2.07	1.95
18	A	606	HEA	FE-NC	3.69	2.07	1.95
18	A	606	HEA	C1D-ND	-3.62	1.34	1.40
18	A	606	HEA	CHD-C4C	3.59	1.47	1.39
18	A	606	HEA	C3A-C2A	3.57	1.45	1.37
18	N	607	HEA	C4B-C3B	3.55	1.51	1.44
18	N	606	HEA	CHD-C4C	3.54	1.47	1.39
18	A	606	HEA	CHD-C1D	3.53	1.45	1.38
18	A	605	HEA	C4D-ND	-3.49	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	607	HEA	CHB-C4A	3.43	1.45	1.38
18	N	606	HEA	C1D-ND	-3.41	1.34	1.40
18	A	606	HEA	C11-C3B	-3.41	1.47	1.51
18	A	605	HEA	CHD-C1D	3.40	1.45	1.38
18	N	607	HEA	CHD-C1D	3.40	1.45	1.38
18	N	606	HEA	CHA-C4D	3.37	1.46	1.39
18	A	605	HEA	CHD-C4C	3.33	1.46	1.39
18	N	607	HEA	C1C-NC	-3.27	1.33	1.39
18	N	607	HEA	CHD-C4C	3.26	1.46	1.39
26	G	101	DMU	O16-C6	3.23	1.45	1.40
18	N	607	HEA	C1C-C2C	3.23	1.50	1.43
18	A	606	HEA	C1B-C2B	3.23	1.51	1.44
18	A	606	HEA	C4A-NA	-3.16	1.33	1.39
26	C	309	DMU	O16-C6	3.16	1.45	1.40
18	A	606	HEA	C4D-ND	-3.11	1.32	1.38
18	N	606	HEA	CHD-C1D	3.11	1.44	1.38
18	N	606	HEA	C1A-NA	-3.10	1.33	1.39
18	N	606	HEA	CHB-C1B	3.09	1.46	1.39
18	N	607	HEA	CHB-C1B	3.08	1.46	1.39
18	N	607	HEA	C1B-NB	-3.05	1.32	1.38
18	N	606	HEA	C4A-NA	-3.03	1.33	1.39
18	N	607	HEA	CHA-C4D	2.98	1.46	1.39
18	N	607	HEA	C4D-C3D	2.97	1.50	1.45
18	A	605	HEA	C4B-NB	-2.93	1.35	1.40
18	A	605	HEA	CHC-C1C	2.93	1.46	1.39
18	N	606	HEA	C3A-C2A	2.91	1.43	1.37
18	A	605	HEA	C1C-C2C	2.87	1.49	1.43
18	A	605	HEA	C4D-C3D	2.73	1.49	1.45
18	N	606	HEA	C1B-NB	-2.68	1.33	1.38
18	N	607	HEA	C1D-ND	-2.67	1.35	1.40
18	A	606	HEA	C1C-C2C	2.56	1.49	1.43
26	C	310	DMU	O16-C6	2.51	1.44	1.40
18	N	606	HEA	C1C-NC	-2.49	1.34	1.39
26	Q	201	DMU	O16-C6	2.46	1.44	1.40
18	A	606	HEA	C3C-C4C	2.45	1.49	1.42
18	A	606	HEA	C4B-C3B	2.42	1.49	1.44
18	A	605	HEA	C1A-C2A	2.41	1.49	1.45
18	A	605	HEA	C1D-C2D	2.39	1.49	1.44
18	N	606	HEA	C1D-C2D	2.38	1.49	1.44
26	P	302	DMU	O16-C6	2.37	1.44	1.40
18	N	606	HEA	C3C-C4C	2.36	1.49	1.42
18	A	606	HEA	C1B-NB	-2.20	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	303	CHD	O26-C24	-2.20	1.23	1.30
18	N	607	HEA	C4B-NB	-2.16	1.36	1.40
18	A	606	HEA	C4C-NC	-2.12	1.35	1.39
18	A	605	HEA	C1B-C2B	2.07	1.48	1.44

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	607	HEA	C3A-C2A-C1A	-8.87	98.66	107.05
18	N	607	HEA	C3C-C4C-NC	7.83	116.39	109.80
18	A	605	HEA	C3A-C2A-C1A	-7.70	99.76	107.05
18	A	605	HEA	C1D-C2D-C3D	-7.57	99.02	106.98
18	N	607	HEA	C2D-C1D-ND	7.54	118.50	109.84
18	A	605	HEA	C2A-C1A-NA	7.18	117.25	110.32
18	A	605	HEA	CMD-C2D-C1D	7.11	136.15	125.03
18	N	606	HEA	C2A-C1A-NA	6.97	117.05	110.32
18	N	607	HEA	C2A-C1A-NA	6.81	116.89	110.32
18	N	606	HEA	C3D-C4D-ND	6.76	116.88	110.35
18	A	606	HEA	C3A-C2A-C1A	-6.68	100.72	107.05
18	N	606	HEA	C2B-C1B-NB	6.61	117.54	109.90
18	A	605	HEA	C2D-C1D-ND	6.56	117.38	109.84
18	N	606	HEA	C3C-C4C-NC	6.54	115.31	109.80
18	N	607	HEA	C3D-C4D-ND	6.49	116.62	110.35
18	N	606	HEA	C3A-C2A-C1A	-6.22	101.16	107.05
18	A	606	HEA	C2D-C1D-ND	6.08	116.83	109.84
18	A	606	HEA	C3B-C4B-NB	5.98	116.71	109.84
18	A	605	HEA	C3C-C4C-NC	5.89	114.76	109.80
18	N	607	HEA	C1D-C2D-C3D	-5.63	101.06	106.98
18	A	606	HEA	C2A-C1A-NA	5.58	115.71	110.32
18	A	606	HEA	CMB-C2B-C1B	5.44	133.54	125.03
18	A	605	HEA	CAD-CBD-CGD	-5.40	99.34	113.67
18	A	605	HEA	C3B-C4B-NB	5.20	115.82	109.84
18	A	606	HEA	C3D-C4D-ND	5.05	115.24	110.35
18	A	605	HEA	C3C-C2C-C1C	-5.04	101.23	107.17
18	N	607	HEA	C4C-C3C-C2C	-4.98	101.11	107.30
18	A	606	HEA	O11-C11-C3B	-4.89	102.29	111.26
18	A	606	HEA	C3C-C2C-C1C	-4.87	101.43	107.17
18	N	606	HEA	C12-C11-C3B	4.71	119.49	112.12
18	N	606	HEA	C2D-C1D-ND	4.66	115.19	109.84
18	A	605	HEA	CMB-C2B-C1B	4.61	132.24	125.03
18	N	606	HEA	CHB-C1B-C2B	-4.60	117.76	125.03
18	A	606	HEA	C2B-C1B-NB	4.59	115.21	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	606	HEA	C1B-C2B-C3B	-4.55	101.52	106.80
18	A	606	HEA	CAA-CBA-CGA	-4.49	101.76	113.67
18	N	607	HEA	C2B-C1B-NB	4.46	115.06	109.90
18	A	605	HEA	C3D-C4D-ND	4.46	114.66	110.35
18	A	606	HEA	C1D-C2D-C3D	-4.44	102.31	106.98
18	N	607	HEA	OMA-CMA-C3A	-4.34	115.83	125.62
18	A	606	HEA	CMB-C2B-C3B	-4.26	122.03	130.28
18	A	606	HEA	CHA-C1A-C2A	-4.14	118.33	124.86
18	A	605	HEA	C13-C12-C11	-4.13	107.79	114.39
18	N	606	HEA	CHA-C4D-C3D	-4.11	118.79	124.77
18	A	606	HEA	C3C-C4C-NC	4.04	113.20	109.80
24	T	102	PEK	O01-C1-C2	3.97	120.06	111.48
26	M	101	DMU	O5-C4-C57	3.96	116.25	106.44
18	A	606	HEA	CBD-CAD-C3D	-3.95	101.62	112.53
18	A	605	HEA	C2B-C1B-NB	3.94	114.46	109.90
18	N	607	HEA	C4B-C3B-C2B	-3.85	100.97	107.44
18	N	607	HEA	C3B-C4B-NB	3.85	114.27	109.84
18	N	606	HEA	C1D-C2D-C3D	-3.85	102.93	106.98
18	A	605	HEA	C2C-C1C-NC	3.85	116.31	110.14
23	J	101	CHD	C4-C3-C2	3.83	115.29	110.62
26	C	309	DMU	C1-C2-C3	3.76	118.21	109.68
18	N	606	HEA	C4C-C3C-C2C	-3.70	102.70	107.30
18	N	607	HEA	CHA-C1A-C2A	-3.65	119.09	124.86
23	P	303	CHD	C16-C17-C13	-3.60	100.05	103.54
17	N	605	PGV	O11-P-O13	-3.60	94.69	108.94
28	V	102	SAC	O-C-CA	-3.57	115.59	124.77
18	N	606	HEA	C4D-C3D-C2D	-3.55	101.72	106.89
18	A	606	HEA	C17-C18-C19	-3.54	119.52	127.62
23	T	101	CHD	C19-C10-C1	-3.54	102.67	108.31
18	N	607	HEA	CHB-C1B-C2B	-3.53	119.46	125.03
18	N	606	HEA	C3B-C4B-NB	3.53	113.89	109.84
18	N	607	HEA	CAA-CBA-CGA	-3.45	104.51	113.67
18	A	606	HEA	C4B-C3B-C2B	-3.41	101.71	107.44
26	C	310	DMU	C10-O1-C9	3.40	120.36	113.72
18	N	606	HEA	C3C-C2C-C1C	-3.34	103.23	107.17
23	J	101	CHD	C5-C4-C3	3.33	117.73	112.71
18	N	606	HEA	CHA-C1A-C2A	-3.33	119.61	124.86
18	N	607	HEA	C1D-ND-C4D	-3.28	101.32	105.21
26	P	302	DMU	C10-C5-C7	3.27	116.89	110.01
26	Q	201	DMU	O16-C6-C1	3.25	113.21	108.27
18	A	606	HEA	C2C-C1C-NC	3.25	115.35	110.14
18	A	605	HEA	C1B-C2B-C3B	-3.25	103.03	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	606	HEA	CHD-C1D-C2D	-3.25	117.72	126.95
26	M	101	DMU	O7-C3-C4	-3.25	100.96	109.48
26	C	310	DMU	O16-C6-C1	3.24	113.20	108.27
18	N	607	HEA	CHD-C1D-C2D	-3.21	117.83	126.95
18	A	605	HEA	CHA-C1A-NA	-3.17	121.00	124.45
26	M	101	DMU	O5-C6-C1	3.15	116.84	110.37
18	A	605	HEA	OMA-CMA-C3A	-3.15	118.52	125.62
23	P	303	CHD	C13-C17-C20	3.11	123.25	119.48
18	N	607	HEA	CAA-C2A-C1A	3.08	131.12	124.85
26	G	101	DMU	C10-C5-C7	3.07	116.47	110.01
18	A	605	HEA	CMC-C2C-C1C	3.05	130.06	125.42
18	N	606	HEA	CAA-CBA-CGA	-3.04	105.59	113.67
26	P	302	DMU	O5-C4-C57	3.03	113.96	106.44
18	N	607	HEA	C4D-C3D-C2D	-3.02	102.49	106.89
18	A	606	HEA	C4D-C3D-C2D	-2.97	102.56	106.89
26	G	101	DMU	C6-O5-C4	2.97	119.53	113.72
18	N	607	HEA	CHC-C4B-NB	-2.97	120.69	124.37
18	A	606	HEA	C12-C11-C3B	2.92	116.69	112.12
23	O	303	CHD	C17-C13-C14	2.90	103.02	100.11
18	A	606	HEA	CAD-C3D-C4D	2.88	129.72	124.70
18	A	605	HEA	CMB-C2B-C3B	-2.87	124.72	130.28
18	N	606	HEA	C4B-C3B-C2B	-2.87	102.61	107.44
26	C	310	DMU	C18-O16-C6	2.87	118.58	113.68
23	Y	101	CHD	C5-C6-C7	-2.83	111.04	114.40
18	A	606	HEA	C4B-NB-C1B	-2.83	101.86	105.21
23	C	307	CHD	C4-C5-C10	2.82	115.67	112.66
25	P	307	CDL	OB6-CB5-C51	2.80	117.55	111.48
18	A	605	HEA	O1D-CGD-CBD	-2.79	114.24	123.09
28	I	101	SAC	O-C-CA	-2.79	117.60	124.77
18	N	606	HEA	CHC-C4B-NB	-2.77	120.94	124.37
18	A	606	HEA	CHC-C1C-C2C	-2.77	119.38	127.43
18	N	607	HEA	C13-C12-C11	-2.75	110.00	114.39
26	Q	201	DMU	C8-C7-C5	2.75	115.65	110.83
18	N	606	HEA	CAD-CBD-CGD	-2.74	106.39	113.67
18	N	606	HEA	CAA-C2A-C1A	2.74	130.42	124.85
18	A	606	HEA	CHC-C4B-C3B	-2.74	118.89	125.80
18	N	606	HEA	C4A-C3A-C2A	-2.74	104.44	106.81
18	A	605	HEA	C27-C19-C20	2.67	119.86	115.23
17	C	301	PGV	O12-P-O13	-2.65	98.42	108.94
26	M	101	DMU	C1-C2-C3	-2.60	103.77	109.68
23	C	307	CHD	C15-C14-C13	2.56	106.02	103.54
23	T	101	CHD	C10-C9-C8	2.56	114.69	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	605	HEA	O2D-CGD-CBD	2.55	122.07	114.00
26	G	101	DMU	C18-O16-C6	2.54	118.01	113.68
26	M	101	DMU	O55-C2-C1	2.53	116.33	110.38
18	N	607	HEA	CMD-C2D-C3D	2.51	132.95	126.15
26	P	302	DMU	C7-C8-C9	-2.50	105.70	110.23
18	N	607	HEA	CHA-C4D-ND	-2.49	121.74	124.42
18	A	606	HEA	CMC-C2C-C3C	2.49	132.41	126.55
18	A	606	HEA	OMA-CMA-C3A	-2.49	120.00	125.62
18	N	606	HEA	OMA-CMA-C3A	-2.47	120.05	125.62
18	A	606	HEA	C27-C19-C20	2.47	119.51	115.23
18	A	606	HEA	CHA-C4D-C3D	-2.46	121.19	124.77
26	M	101	DMU	O4-C7-C8	2.45	116.14	110.38
18	A	605	HEA	CHC-C1C-C2C	-2.43	120.36	127.43
26	C	309	DMU	O1-C9-C11	2.43	112.47	106.44
17	C	301	PGV	O14-P-O13	2.42	123.72	112.44
23	P	303	CHD	C15-C14-C13	2.42	105.89	103.54
18	A	605	HEA	C4B-C3B-C2B	-2.42	103.37	107.44
18	N	607	HEA	C12-C11-C3B	-2.39	108.39	112.12
18	N	606	HEA	C2C-C1C-NC	2.37	113.94	110.14
23	T	101	CHD	O12-C12-C11	-2.36	104.31	109.12
23	T	101	CHD	C17-C13-C14	2.36	102.48	100.11
26	C	310	DMU	C6-O5-C4	2.35	118.31	113.72
18	N	606	HEA	CMB-C2B-C1B	2.35	128.70	125.03
26	P	302	DMU	O1-C10-C5	2.34	115.18	110.37
26	Q	201	DMU	O5-C4-C57	2.32	112.19	106.44
18	A	606	HEA	C26-C15-C16	2.28	119.19	115.23
26	C	309	DMU	C7-C8-C9	2.28	114.36	110.23
17	N	605	PGV	O14-P-O13	2.28	123.04	112.44
26	M	101	DMU	C28-C25-C22	-2.27	102.87	114.37
26	M	101	DMU	C8-C7-C5	-2.27	106.84	110.83
18	N	607	HEA	C3C-C2C-C1C	-2.27	104.50	107.17
23	T	101	CHD	C9-C8-C7	2.25	114.69	111.86
26	P	302	DMU	O1-C9-C8	-2.24	105.66	109.70
18	A	606	HEA	CHB-C1B-C2B	-2.24	121.49	125.03
18	A	606	HEA	O2D-CGD-CBD	2.23	121.05	114.00
18	N	607	HEA	C17-C18-C19	-2.22	122.54	127.62
26	P	302	DMU	O1-C9-C11	2.21	111.92	106.44
26	C	309	DMU	O55-C2-C3	-2.20	104.29	109.94
23	O	303	CHD	C13-C17-C20	-2.20	116.82	119.48
18	A	605	HEA	CHC-C4B-C3B	-2.20	120.26	125.80
23	T	101	CHD	C14-C8-C7	-2.19	108.94	111.85
18	A	605	HEA	CHA-C4D-C3D	-2.19	121.58	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	T	101	CHD	C19-C10-C5	2.19	114.10	110.44
26	Q	201	DMU	O1-C9-C11	2.18	111.85	106.44
18	N	607	HEA	C1B-C2B-C3B	-2.18	104.27	106.80
18	N	607	HEA	O2D-CGD-O1D	-2.18	117.72	123.33
23	T	103	CHD	C5-C6-C7	-2.16	111.83	114.40
18	N	607	HEA	CHA-C4D-C3D	-2.15	121.63	124.77
18	A	605	HEA	CHD-C1D-ND	-2.15	121.70	124.37
23	T	101	CHD	O12-C12-C13	2.15	114.65	111.02
18	N	607	HEA	CHD-C4C-C3C	-2.13	118.12	127.37
18	N	606	HEA	CAD-C3D-C2D	2.13	131.86	127.87
18	A	605	HEA	CHD-C1D-C2D	-2.13	120.90	126.95
23	T	101	CHD	C9-C10-C5	-2.12	105.57	108.51
23	C	302	CHD	C13-C17-C20	2.11	122.05	119.48
18	A	605	HEA	C26-C15-C16	2.11	118.90	115.23
26	C	309	DMU	O1-C10-C5	2.09	114.67	110.37
23	O	303	CHD	C13-C14-C8	-2.09	112.07	114.72
18	N	607	HEA	C2C-C1C-NC	2.09	113.49	110.14
18	N	606	HEA	CMD-C2D-C1D	2.09	128.30	125.03
23	J	101	CHD	C1-C2-C3	2.09	113.25	110.48
18	A	605	HEA	C16-C15-C14	-2.08	116.49	121.17
18	N	607	HEA	CAD-C3D-C4D	2.08	128.33	124.70
23	T	103	CHD	C11-C9-C10	2.08	115.81	113.70
26	C	309	DMU	C10-C5-C7	2.08	114.38	110.01
18	N	606	HEA	CHB-C4A-NA	-2.07	122.20	124.45
24	C	303	PEK	O13-P-O14	2.06	122.05	112.44
26	Q	201	DMU	C7-C8-C9	2.04	113.94	110.23
18	A	606	HEA	C1B-C2B-C3B	-2.04	104.43	106.80
23	T	101	CHD	C18-C13-C17	-2.04	108.01	111.20
18	A	606	HEA	C13-C12-C11	-2.04	111.14	114.39
23	T	101	CHD	C5-C6-C7	2.04	116.82	114.40
26	P	302	DMU	O16-C6-C1	2.03	111.35	108.27
18	N	607	HEA	C16-C15-C14	-2.02	116.62	121.17
26	C	309	DMU	C10-O1-C9	2.01	117.64	113.72
26	C	310	DMU	C7-C8-C9	2.00	113.86	110.23

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	T	103	CHD	C9
23	Y	101	CHD	C3
26	C	309	DMU	C6
26	C	309	DMU	C5

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Mol	Chain	Res	Type	Atom
26	C	310	DMU	C6
26	C	310	DMU	C5
26	G	101	DMU	C6
26	G	101	DMU	C5
26	M	101	DMU	C6
26	M	101	DMU	C5
26	P	302	DMU	C6
26	P	302	DMU	C5
26	Q	201	DMU	C6
26	Q	201	DMU	C5

All (980) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C03-O11-P-O12
17	A	604	PGV	C04-O12-P-O11
17	A	604	PGV	C04-O12-P-O13
17	A	604	PGV	C04-O12-P-O14
17	A	604	PGV	C04-C05-C06-O06
17	A	604	PGV	O02-C1-O01-C02
17	A	604	PGV	C2-C1-O01-C02
17	C	305	PGV	C04-O12-P-O11
17	C	305	PGV	C04-O12-P-O13
17	C	305	PGV	C04-O12-P-O14
17	C	305	PGV	O12-C04-C05-O05
17	H	101	PGV	C03-O11-P-O12
17	H	101	PGV	C03-O11-P-O14
17	H	101	PGV	C04-O12-P-O11
17	H	101	PGV	C04-O12-P-O14
17	H	101	PGV	C04-C05-C06-O06
17	H	101	PGV	O02-C1-O01-C02
17	N	605	PGV	C04-C05-C06-O06
17	N	610	PGV	C03-O11-P-O14
17	N	610	PGV	C04-O12-P-O13
17	N	610	PGV	C2-C1-O01-C02
17	P	305	PGV	C03-O11-P-O12
17	P	305	PGV	C03-O11-P-O13
17	P	305	PGV	C04-O12-P-O14
17	P	306	PGV	C03-O11-P-O12
17	P	306	PGV	C03-O11-P-O13
17	P	306	PGV	C04-O12-P-O11
17	P	306	PGV	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
17	P	306	PGV	O12-C04-C05-C06
17	P	306	PGV	C2-C1-O01-C02
18	N	606	HEA	C2A-C3A-CMA-OMA
21	D	201	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	CB2-CB1-OG2-CG2
21	N	604	TGL	CB2-CB1-OG2-CG2
21	N	604	TGL	OB1-CB1-OG2-CG2
22	B	303	PSC	O12-C04-C05-N
22	V	101	PSC	C03-O11-P-O12
22	V	101	PSC	C03-O11-P-O13
22	V	101	PSC	C03-O11-P-O14
22	V	101	PSC	O12-C04-C05-N
22	V	101	PSC	C2-C1-O01-C02
24	C	303	PEK	C03-O11-P-O13
24	C	303	PEK	C12-C13-C14-C15
24	C	304	PEK	C03-O11-P-O12
24	C	304	PEK	C03-O11-P-O13
24	C	304	PEK	C04-O12-P-O11
24	C	304	PEK	C04-O12-P-O13
24	C	304	PEK	C04-O12-P-O14
24	C	304	PEK	O12-C04-C05-N
24	C	311	PEK	C03-O11-P-O12
24	C	311	PEK	C03-O11-P-O13
24	P	301	PEK	C03-O11-P-O12
24	P	301	PEK	C03-O11-P-O13
24	P	301	PEK	C03-O11-P-O14
24	P	301	PEK	O12-C04-C05-N
24	P	304	PEK	C03-O11-P-O12
24	P	304	PEK	C03-O11-P-O13
24	P	304	PEK	O12-C04-C05-N
24	T	102	PEK	C03-O11-P-O12
24	T	102	PEK	C03-O11-P-O14
24	T	102	PEK	C04-O12-P-O14
24	T	102	PEK	C02-C03-O11-P
24	T	102	PEK	O12-C04-C05-N
24	T	102	PEK	O02-C1-O01-C02
24	T	102	PEK	C2-C1-O01-C02
25	C	306	CDL	CB2-C1-CA2-OA2
25	C	306	CDL	C1-CA2-OA2-PA1
25	C	306	CDL	CA3-OA5-PA1-OA3
25	C	306	CDL	OA7-CA5-OA6-CA4
25	C	306	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
25	C	306	CDL	C51-CB5-OB6-CB4
25	C	308	CDL	CB2-C1-CA2-OA2
25	C	308	CDL	CA2-C1-CB2-OB2
25	C	308	CDL	CA3-OA5-PA1-OA2
25	C	308	CDL	CA3-OA5-PA1-OA3
25	C	308	CDL	CA3-OA5-PA1-OA4
25	C	308	CDL	C11-CA5-OA6-CA4
25	C	308	CDL	CB2-OB2-PB2-OB3
25	C	308	CDL	CB3-OB5-PB2-OB3
25	P	307	CDL	CA2-OA2-PA1-OA3
25	P	307	CDL	CA2-OA2-PA1-OA4
25	P	307	CDL	CA2-OA2-PA1-OA5
25	P	307	CDL	CA3-OA5-PA1-OA2
25	P	307	CDL	CA3-OA5-PA1-OA3
25	P	307	CDL	CB2-OB2-PB2-OB4
25	P	309	CDL	O1-C1-CA2-OA2
25	P	309	CDL	CB3-OB5-PB2-OB2
26	M	101	DMU	O5-C6-O16-C18
28	I	101	SAC	C-CA-CB-OG
28	V	102	SAC	C2A-C1A-N-CA
28	V	102	SAC	OAC-C1A-N-CA
17	A	604	PGV	O04-C19-O03-C01
22	V	101	PSC	O04-C19-O03-C01
25	P	309	CDL	OB9-CB7-OB8-CB6
17	A	604	PGV	C20-C19-O03-C01
17	N	610	PGV	O04-C19-O03-C01
21	B	302	TGL	OC1-CC1-OG3-CG3
21	N	609	TGL	OC1-CC1-OG3-CG3
24	C	304	PEK	O04-C21-O03-C01
25	P	307	CDL	OA9-CA7-OA8-CA6
25	P	309	CDL	OA9-CA7-OA8-CA6
26	C	309	DMU	O1-C10-O7-C3
17	N	610	PGV	O02-C1-O01-C02
17	P	306	PGV	O02-C1-O01-C02
21	D	201	TGL	OB1-CB1-OG2-CG2
21	L	101	TGL	OB1-CB1-OG2-CG2
25	C	306	CDL	OB7-CB5-OB6-CB4
21	N	609	TGL	CC2-CC1-OG3-CG3
22	V	101	PSC	C20-C19-O03-C01
25	C	306	CDL	C31-CA7-OA8-CA6
25	P	307	CDL	C31-CA7-OA8-CA6
25	P	309	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
25	P	309	CDL	C71-CB7-OB8-CB6
17	H	101	PGV	C2-C1-O01-C02
25	C	306	CDL	C11-CA5-OA6-CA4
26	C	309	DMU	O6-C11-C9-O1
17	N	610	PGV	C20-C19-O03-C01
17	P	306	PGV	C20-C19-O03-C01
21	B	302	TGL	CC2-CC1-OG3-CG3
21	D	201	TGL	CC2-CC1-OG3-CG3
22	B	303	PSC	C20-C19-O03-C01
24	C	304	PEK	C22-C21-O03-C01
24	P	301	PEK	C22-C21-O03-C01
26	Q	201	DMU	O5-C4-C57-O61
22	B	303	PSC	O04-C19-O03-C01
25	C	306	CDL	OA9-CA7-OA8-CA6
22	V	101	PSC	O02-C1-O01-C02
25	C	308	CDL	OA7-CA5-OA6-CA4
17	P	306	PGV	O12-C04-C05-O05
25	C	306	CDL	O1-C1-CA2-OA2
25	C	306	CDL	O1-C1-CB2-OB2
25	C	308	CDL	O1-C1-CA2-OA2
25	C	308	CDL	O1-C1-CB2-OB2
25	P	307	CDL	O1-C1-CB2-OB2
21	N	604	TGL	CA2-CA1-OG1-CG1
24	C	311	PEK	C22-C21-O03-C01
26	M	101	DMU	O6-C11-C9-O1
26	G	101	DMU	O6-C11-C9-C8
26	Q	201	DMU	C3-C4-C57-O61
26	G	101	DMU	O6-C11-C9-O1
26	C	309	DMU	O6-C11-C9-C8
17	A	604	PGV	C3-C4-C5-C6
23	C	307	CHD	C13-C17-C20-C21
23	P	303	CHD	C13-C17-C20-C21
17	A	604	PGV	C1-C2-C3-C4
22	V	101	PSC	C19-C20-C21-C22
23	P	303	CHD	C16-C17-C20-C22
25	C	308	CDL	C71-CB7-OB8-CB6
18	A	606	HEA	C26-C15-C16-C17
18	A	606	HEA	C14-C15-C16-C17
17	P	306	PGV	O04-C19-O03-C01
24	C	311	PEK	O04-C21-O03-C01
24	P	301	PEK	O04-C21-O03-C01
18	A	606	HEA	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
26	M	101	DMU	O6-C11-C9-C8
17	H	101	PGV	C02-C03-O11-P
17	P	306	PGV	C05-C04-O12-P
21	D	201	TGL	OC1-CC1-OG3-CG3
26	C	310	DMU	O5-C6-O16-C18
26	G	101	DMU	O5-C6-O16-C18
21	O	301	TGL	CC2-CC1-OG3-CG3
26	C	310	DMU	O5-C4-C57-O61
23	Y	101	CHD	C17-C20-C22-C23
25	C	308	CDL	OB9-CB7-OB8-CB6
21	B	302	TGL	CA1-CA2-CA3-CA4
21	N	604	TGL	C23-C24-C25-C26
23	Y	101	CHD	C21-C20-C22-C23
21	N	604	TGL	OA1-CA1-OG1-CG1
17	C	305	PGV	O12-C04-C05-C06
25	C	306	CDL	CA2-C1-CB2-OB2
25	P	307	CDL	CA2-C1-CB2-OB2
21	N	604	TGL	CC2-CC1-OG3-CG3
21	O	301	TGL	CA2-CA1-OG1-CG1
26	C	310	DMU	C1-C6-O16-C18
26	G	101	DMU	C1-C6-O16-C18
21	D	201	TGL	CB1-CB2-CB3-CB4
24	C	311	PEK	C1-C2-C3-C4
21	O	301	TGL	OA1-CA1-OG1-CG1
21	O	301	TGL	OC1-CC1-OG3-CG3
21	N	604	TGL	OC1-CC1-OG3-CG3
17	H	101	PGV	C20-C19-O03-C01
24	T	102	PEK	C22-C21-O03-C01
17	P	305	PGV	C1-C2-C3-C4
25	C	308	CDL	CA7-C31-C32-C33
26	C	310	DMU	O16-C18-C19-C22
17	P	306	PGV	C26-C27-C28-C29
17	N	610	PGV	C19-C20-C21-C22
21	D	201	TGL	CC1-CC2-CC3-CC4
24	T	102	PEK	C1-C2-C3-C4
24	T	102	PEK	C21-C22-C23-C24
25	C	306	CDL	CA7-C31-C32-C33
25	C	306	CDL	CB7-C71-C72-C73
25	C	308	CDL	CA5-C11-C12-C13
23	T	101	CHD	C20-C22-C23-C24
21	N	609	TGL	CB1-CB2-CB3-CB4
26	C	309	DMU	C5-C10-O7-C3

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Mol	Chain	Res	Type	Atoms
21	B	302	TGL	C11-C10-CB9-CB8
25	P	309	CDL	O1-C1-CB2-OB2
21	D	201	TGL	CA2-CA1-OG1-CG1
24	C	304	PEK	C1-C2-C3-C4
26	Q	201	DMU	O16-C18-C19-C22
24	T	102	PEK	O04-C21-O03-C01
17	P	305	PGV	C19-C20-C21-C22
17	H	101	PGV	O04-C19-O03-C01
23	C	307	CHD	C16-C17-C20-C22
21	N	604	TGL	CC6-CC7-CC8-CC9
25	P	309	CDL	CB2-C1-CA2-OA2
25	P	309	CDL	CA2-C1-CB2-OB2
21	O	301	TGL	CA1-CA2-CA3-CA4
21	D	201	TGL	OA1-CA1-OG1-CG1
23	J	101	CHD	C20-C22-C23-C24
17	N	610	PGV	C1-C2-C3-C4
25	C	306	CDL	C39-C40-C41-C42
17	C	305	PGV	C12-C13-C14-C15
21	B	302	TGL	C21-C20-CA9-CA8
24	T	102	PEK	O01-C02-C03-O11
26	G	101	DMU	O16-C18-C19-C22
21	L	101	TGL	C24-C25-C26-C27
24	C	311	PEK	C27-C28-C29-C30
25	C	308	CDL	C73-C74-C75-C76
26	C	309	DMU	C19-C22-C25-C28
21	L	101	TGL	CB2-CB3-CB4-CB5
24	C	303	PEK	C23-C24-C25-C26
24	C	311	PEK	C25-C26-C27-C28
25	C	306	CDL	C15-C16-C17-C18
25	C	306	CDL	C61-C62-C63-C64
25	P	307	CDL	C55-C56-C57-C58
25	P	307	CDL	C78-C79-C80-C81
25	P	309	CDL	C43-C44-C45-C46
21	L	101	TGL	CB6-CB7-CB8-CB9
21	N	604	TGL	CC3-CC4-CC5-CC6
21	N	609	TGL	CB5-CB6-CB7-CB8
21	N	609	TGL	C16-C15-CC9-CC8
25	C	308	CDL	C15-C16-C17-C18
17	C	305	PGV	C25-C26-C27-C28
17	N	605	PGV	C23-C24-C25-C26
17	N	610	PGV	C27-C28-C29-C30
21	B	302	TGL	C14-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
21	L	101	TGL	C18-C19-C33-C34
21	O	301	TGL	C10-C11-C12-C13
22	B	303	PSC	C27-C28-C29-C30
24	C	303	PEK	C22-C23-C24-C25
25	C	306	CDL	C32-C33-C34-C35
25	C	308	CDL	C12-C13-C14-C15
25	C	308	CDL	C79-C80-C81-C82
25	P	307	CDL	C36-C37-C38-C39
25	P	307	CDL	C41-C42-C43-C44
26	Q	201	DMU	C25-C28-C31-C34
17	A	604	PGV	O05-C05-C06-O06
17	H	101	PGV	O05-C05-C06-O06
17	N	605	PGV	O05-C05-C06-O06
26	P	302	DMU	C19-C18-O16-C6
24	C	303	PEK	C25-C26-C27-C28
25	C	308	CDL	C60-C61-C62-C63
21	L	101	TGL	CC6-CC7-CC8-CC9
21	O	301	TGL	C15-C16-C17-C18
21	B	302	TGL	CB5-CB6-CB7-CB8
21	D	201	TGL	CA6-CA7-CA8-CA9
21	N	604	TGL	C13-C14-C29-C30
25	P	307	CDL	C19-C20-C21-C22
22	B	303	PSC	C2-C1-O01-C02
21	O	301	TGL	CB7-CB8-CB9-C10
21	N	604	TGL	C10-C11-C12-C13
17	N	610	PGV	O12-C04-C05-O05
21	B	302	TGL	CB1-CB2-CB3-CB4
21	B	302	TGL	CA5-CA6-CA7-CA8
21	L	101	TGL	CC7-CC8-CC9-C15
21	N	609	TGL	C13-C14-C29-C30
21	O	301	TGL	CC7-CC8-CC9-C15
24	P	301	PEK	C34-C35-C36-C37
25	C	306	CDL	C83-C84-C85-C86
17	C	301	PGV	C5-C6-C7-C8
28	I	101	SAC	N-CA-CB-OG
26	G	101	DMU	C18-C19-C22-C25
17	P	305	PGV	C6-C7-C8-C9
25	P	309	CDL	C31-C32-C33-C34
21	O	301	TGL	CB9-C10-C11-C12
25	C	306	CDL	C76-C77-C78-C79
25	P	307	CDL	C72-C73-C74-C75
25	C	306	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	C	308	CDL	C31-CA7-OA8-CA6
17	N	610	PGV	C7-C8-C9-C10
21	N	604	TGL	C21-C20-CA9-CA8
21	N	604	TGL	CB9-C10-C11-C12
21	N	609	TGL	CC3-CC4-CC5-CC6
25	P	309	CDL	C34-C35-C36-C37
17	N	605	PGV	C19-C20-C21-C22
21	O	301	TGL	CB1-CB2-CB3-CB4
17	H	101	PGV	C23-C24-C25-C26
17	N	605	PGV	C13-C14-C15-C16
21	B	302	TGL	C11-C12-C13-C14
21	B	302	TGL	CC9-C15-C16-C17
21	D	201	TGL	C12-C13-C14-C29
21	N	604	TGL	CB2-CB3-CB4-CB5
21	N	609	TGL	C10-C11-C12-C13
21	O	301	TGL	C11-C12-C13-C14
24	C	311	PEK	C16-C17-C18-C19
24	P	301	PEK	C29-C30-C31-C32
25	C	308	CDL	C33-C34-C35-C36
25	P	309	CDL	C16-C17-C18-C19
25	P	309	CDL	C20-C21-C22-C23
17	C	305	PGV	C30-C31-C32-C33
17	N	605	PGV	C30-C31-C32-C33
25	C	308	CDL	C53-C54-C55-C56
25	P	307	CDL	C58-C59-C60-C61
25	P	307	CDL	C83-C84-C85-C86
25	C	306	CDL	C43-C44-C45-C46
25	C	308	CDL	C41-C42-C43-C44
17	C	301	PGV	C7-C8-C9-C10
21	L	101	TGL	C11-C12-C13-C14
25	P	309	CDL	C82-C83-C84-C85
26	P	302	DMU	C31-C34-C37-C40
24	P	304	PEK	C1-C2-C3-C4
17	N	610	PGV	C24-C25-C26-C27
21	N	609	TGL	C24-C25-C26-C27
25	C	306	CDL	C14-C15-C16-C17
24	P	301	PEK	C2-C1-O01-C02
24	P	301	PEK	C15-C16-C17-C18
17	N	610	PGV	C02-C03-O11-P
24	P	301	PEK	C7-C8-C9-C10
17	A	604	PGV	C4-C5-C6-C7
21	N	609	TGL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	B	302	TGL	C33-C34-C35-C36
21	B	302	TGL	CC7-CC8-CC9-C15
21	D	201	TGL	CA3-CA4-CA5-CA6
26	M	101	DMU	C19-C22-C25-C28
21	O	301	TGL	CC3-CC4-CC5-CC6
21	D	201	TGL	C16-C15-CC9-CC8
21	D	201	TGL	C23-C24-C25-C26
21	N	604	TGL	C16-C15-CC9-CC8
25	C	308	CDL	C23-C24-C25-C26
25	P	309	CDL	C12-C13-C14-C15
21	B	302	TGL	C12-C13-C14-C29
21	B	302	TGL	CA9-C20-C21-C22
21	N	609	TGL	CA9-C20-C21-C22
21	O	301	TGL	CC5-CC6-CC7-CC8
25	C	306	CDL	C60-C61-C62-C63
25	C	306	CDL	C62-C63-C64-C65
17	C	301	PGV	C29-C30-C31-C32
25	P	307	CDL	C77-C78-C79-C80
21	L	101	TGL	CA4-CA5-CA6-CA7
24	P	304	PEK	C16-C17-C18-C19
24	T	102	PEK	C31-C32-C33-C34
21	D	201	TGL	CA9-C20-C21-C22
17	N	610	PGV	C29-C30-C31-C32
21	B	302	TGL	C23-C24-C25-C26
21	L	101	TGL	C20-C21-C22-C23
21	N	604	TGL	CC5-CC6-CC7-CC8
25	P	309	CDL	C61-C62-C63-C64
21	N	609	TGL	C15-C16-C17-C18
21	O	301	TGL	C17-C18-C19-C33
23	P	303	CHD	C16-C17-C20-C21
17	P	305	PGV	C2-C1-O01-C02
21	N	609	TGL	CB2-CB1-OG2-CG2
24	C	304	PEK	C2-C1-O01-C02
25	P	307	CDL	C11-CA5-OA6-CA4
25	C	308	CDL	OA9-CA7-OA8-CA6
21	D	201	TGL	CA1-CA2-CA3-CA4
22	B	303	PSC	O02-C1-O01-C02
25	P	307	CDL	OA7-CA5-OA6-CA4
21	L	101	TGL	C12-C13-C14-C29
21	L	101	TGL	CC9-C15-C16-C17
24	C	311	PEK	C29-C30-C31-C32
25	C	306	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
17	H	101	PGV	C12-C13-C14-C15
22	B	303	PSC	C6-C7-C8-C9
26	M	101	DMU	C34-C37-C40-C43
25	P	309	CDL	C83-C84-C85-C86
17	H	101	PGV	C19-C20-C21-C22
25	C	306	CDL	C77-C78-C79-C80
21	N	609	TGL	CB4-CB5-CB6-CB7
17	A	604	PGV	C10-C11-C12-C13
17	C	305	PGV	C22-C23-C24-C25
21	D	201	TGL	CB6-CB7-CB8-CB9
21	O	301	TGL	CB4-CB5-CB6-CB7
24	C	304	PEK	C28-C29-C30-C31
25	P	309	CDL	C58-C59-C60-C61
25	P	307	CDL	C11-C12-C13-C14
17	P	305	PGV	O02-C1-O01-C02
24	C	304	PEK	O02-C1-O01-C02
24	C	311	PEK	C24-C25-C26-C27
24	C	311	PEK	C28-C29-C30-C31
24	P	301	PEK	C26-C27-C28-C29
24	P	301	PEK	C30-C31-C32-C33
25	C	308	CDL	C76-C77-C78-C79
25	C	306	CDL	C56-C57-C58-C59
21	N	609	TGL	C20-C21-C22-C23
22	B	303	PSC	C4-C5-C6-C7
25	P	309	CDL	C77-C78-C79-C80
17	P	305	PGV	C13-C14-C15-C16
21	N	609	TGL	CA7-CA8-CA9-C20
17	H	101	PGV	C11-C10-C9-C8
24	P	301	PEK	C23-C24-C25-C26
25	P	309	CDL	C59-C60-C61-C62
25	P	309	CDL	C74-C75-C76-C77
17	N	605	PGV	C24-C25-C26-C27
24	C	303	PEK	C24-C25-C26-C27
25	P	307	CDL	C17-C18-C19-C20
25	P	307	CDL	C74-C75-C76-C77
24	C	304	PEK	C02-C03-O11-P
17	N	610	PGV	C14-C15-C16-C17
17	N	610	PGV	C23-C24-C25-C26
21	B	302	TGL	CB2-CB3-CB4-CB5
21	B	302	TGL	C18-C19-C33-C34
21	L	101	TGL	CC4-CC5-CC6-CC7
24	C	304	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	C	310	DMU	C25-C28-C31-C34
17	C	305	PGV	C7-C8-C9-C10
21	O	301	TGL	C21-C22-C23-C24
25	P	307	CDL	C22-C23-C24-C25
25	P	309	CDL	C41-C42-C43-C44
26	P	302	DMU	C22-C25-C28-C31
21	B	302	TGL	CC4-CC5-CC6-CC7
21	D	201	TGL	C15-C16-C17-C18
26	Q	201	DMU	C28-C31-C34-C37
17	H	101	PGV	C13-C14-C15-C16
25	C	308	CDL	C52-C53-C54-C55
17	H	101	PGV	C6-C7-C8-C9
21	N	609	TGL	C19-C33-C34-C35
25	P	307	CDL	C52-C53-C54-C55
17	A	604	PGV	C5-C6-C7-C8
17	H	101	PGV	C29-C30-C31-C32
24	T	102	PEK	C27-C28-C29-C30
17	C	301	PGV	C11-C10-C9-C8
22	B	303	PSC	C13-C14-C15-C16
24	P	301	PEK	C2-C3-C4-C5
24	T	102	PEK	C15-C16-C17-C18
22	B	303	PSC	C20-C21-C22-C23
25	P	309	CDL	C35-C36-C37-C38
24	T	102	PEK	C01-C02-C03-O11
25	P	307	CDL	OA5-CA3-CA4-CA6
21	N	609	TGL	OB1-CB1-OG2-CG2
24	P	301	PEK	O02-C1-O01-C02
23	P	303	CHD	C17-C20-C22-C23
25	P	309	CDL	C53-C54-C55-C56
21	O	301	TGL	CB3-CB4-CB5-CB6
21	L	101	TGL	CA6-CA7-CA8-CA9
21	N	604	TGL	CA4-CA5-CA6-CA7
25	C	306	CDL	C18-C19-C20-C21
21	O	301	TGL	C22-C23-C24-C25
18	A	605	HEA	C4D-C3D-CAD-CBD
26	P	302	DMU	C1-C6-O16-C18
24	P	304	PEK	C7-C8-C9-C10
21	L	101	TGL	CC1-CC2-CC3-CC4
17	P	305	PGV	O03-C01-C02-C03
21	L	101	TGL	CG1-CG2-CG3-OG3
25	C	306	CDL	CA3-CA4-CA6-OA8
25	P	309	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
24	C	311	PEK	C15-C16-C17-C18
24	P	304	PEK	C15-C16-C17-C18
17	A	604	PGV	C20-C21-C22-C23
21	N	604	TGL	CB7-CB8-CB9-C10
25	P	307	CDL	C43-C44-C45-C46
17	N	610	PGV	C3-C4-C5-C6
24	P	301	PEK	C14-C15-C16-C17
21	B	302	TGL	CA3-CA4-CA5-CA6
25	P	309	CDL	C56-C57-C58-C59
17	P	306	PGV	C30-C31-C32-C33
17	N	605	PGV	C7-C8-C9-C10
25	P	309	CDL	C13-C14-C15-C16
21	B	302	TGL	C21-C22-C23-C24
24	C	311	PEK	C32-C33-C34-C35
24	T	102	PEK	C23-C24-C25-C26
17	P	306	PGV	C2-C3-C4-C5
25	P	309	CDL	C57-C58-C59-C60
24	P	304	PEK	C2-C3-C4-C5
21	D	201	TGL	CC6-CC7-CC8-CC9
22	V	101	PSC	C23-C24-C25-C26
25	P	309	CDL	C11-C12-C13-C14
18	A	605	HEA	C2A-C3A-CMA-OMA
24	P	304	PEK	C33-C34-C35-C36
23	C	307	CHD	C16-C17-C20-C21
17	A	604	PGV	C15-C16-C17-C18
21	L	101	TGL	CA5-CA6-CA7-CA8
26	Q	201	DMU	C22-C25-C28-C31
24	C	304	PEK	C24-C25-C26-C27
25	P	307	CDL	C21-C22-C23-C24
21	N	604	TGL	C33-C34-C35-C36
17	N	605	PGV	C22-C23-C24-C25
21	N	609	TGL	CA3-CA4-CA5-CA6
22	B	303	PSC	C24-C25-C26-C27
25	P	309	CDL	C18-C19-C20-C21
24	C	304	PEK	C35-C36-C37-C38
24	C	311	PEK	C35-C36-C37-C38
25	P	309	CDL	C84-C85-C86-C87
17	A	604	PGV	C13-C14-C15-C16
17	N	610	PGV	C20-C21-C22-C23
17	P	306	PGV	C21-C22-C23-C24
25	P	307	CDL	OA6-CA4-CA6-OA8
25	P	307	CDL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
25	P	307	CDL	C71-CB7-OB8-CB6
25	C	308	CDL	C44-C45-C46-C47
24	T	102	PEK	C25-C26-C27-C28
21	N	604	TGL	C25-C26-C27-C28
24	C	303	PEK	C16-C17-C18-C19
17	N	610	PGV	C6-C7-C8-C9
21	O	301	TGL	C29-C30-C31-C32
18	A	605	HEA	C3B-C11-C12-C13
24	T	102	PEK	C17-C18-C19-C20
25	P	307	CDL	C54-C55-C56-C57
26	C	309	DMU	C34-C37-C40-C43
17	C	305	PGV	C27-C28-C29-C30
17	N	610	PGV	C21-C22-C23-C24
17	N	610	PGV	C5-C6-C7-C8
24	T	102	PEK	C28-C29-C30-C31
25	C	306	CDL	C78-C79-C80-C81
26	C	309	DMU	C19-C18-O16-C6
26	G	101	DMU	C19-C18-O16-C6
26	Q	201	DMU	C19-C18-O16-C6
25	C	308	CDL	C19-C20-C21-C22
25	C	308	CDL	C62-C63-C64-C65
17	A	604	PGV	C02-C03-O11-P
25	P	307	CDL	C1-CA2-OA2-PA1
21	N	609	TGL	CC5-CC6-CC7-CC8
25	C	308	CDL	C21-C22-C23-C24
17	P	306	PGV	C24-C25-C26-C27
26	Q	201	DMU	C34-C37-C40-C43
17	A	604	PGV	C24-C25-C26-C27
21	O	301	TGL	C20-C21-C22-C23
25	C	306	CDL	C20-C21-C22-C23
25	C	306	CDL	C57-C58-C59-C60
25	C	308	CDL	C74-C75-C76-C77
21	D	201	TGL	C21-C20-CA9-CA8
21	L	101	TGL	CA1-CA2-CA3-CA4
17	C	305	PGV	C31-C32-C33-C34
25	P	307	CDL	C20-C21-C22-C23
25	C	306	CDL	C80-C81-C82-C83
25	P	307	CDL	C37-C38-C39-C40
25	C	306	CDL	C37-C38-C39-C40
25	C	308	CDL	C64-C65-C66-C67
21	L	101	TGL	C21-C20-CA9-CA8
24	P	301	PEK	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	V	101	PSC	C30-C31-C32-C33
17	C	301	PGV	C4-C5-C6-C7
17	N	610	PGV	C31-C32-C33-C34
25	P	307	CDL	C24-C25-C26-C27
17	P	306	PGV	C4-C5-C6-C7
21	L	101	TGL	CB7-CB8-CB9-C10
25	C	306	CDL	C52-C53-C54-C55
21	D	201	TGL	C18-C19-C33-C34
17	H	101	PGV	C31-C32-C33-C34
21	D	201	TGL	C29-C30-C31-C32
21	D	201	TGL	C21-C22-C23-C24
21	N	609	TGL	CC2-CC3-CC4-CC5
25	C	306	CDL	CB3-CB4-CB6-OB8
25	P	307	CDL	CB3-CB4-CB6-OB8
22	B	303	PSC	C26-C27-C28-C29
25	C	308	CDL	C83-C84-C85-C86
25	P	309	CDL	C54-C55-C56-C57
21	B	302	TGL	CC1-CC2-CC3-CC4
25	C	308	CDL	CB5-C51-C52-C53
24	T	102	PEK	C16-C17-C18-C19
25	C	306	CDL	C13-C14-C15-C16
21	B	302	TGL	C25-C26-C27-C28
25	P	307	CDL	OA5-CA3-CA4-OA6
17	C	301	PGV	C6-C7-C8-C9
17	H	101	PGV	C2-C3-C4-C5
17	C	305	PGV	C02-C03-O11-P
17	P	305	PGV	C05-C04-O12-P
24	P	301	PEK	C02-C03-O11-P
22	V	101	PSC	C21-C22-C23-C24
24	P	301	PEK	C16-C17-C18-C19
17	P	305	PGV	C30-C31-C32-C33
21	N	609	TGL	C21-C20-CA9-CA8
26	G	101	DMU	C5-C10-O7-C3
21	B	302	TGL	OG1-CG1-CG2-OG2
25	C	306	CDL	OA6-CA4-CA6-OA8
25	C	308	CDL	OA6-CA4-CA6-OA8
17	H	101	PGV	C30-C31-C32-C33
22	V	101	PSC	C10-C11-C12-C13
24	C	304	PEK	C6-C7-C8-C9
24	C	304	PEK	C12-C13-C14-C15
24	C	311	PEK	C9-C10-C11-C12
24	C	311	PEK	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	P	301	PEK	C5-C6-C7-C8
24	P	301	PEK	C11-C12-C13-C14
24	P	301	PEK	C12-C13-C14-C15
24	P	304	PEK	C9-C10-C11-C12
24	T	102	PEK	C11-C10-C9-C8
24	T	102	PEK	C11-C12-C13-C14
17	H	101	PGV	C26-C27-C28-C29
17	C	305	PGV	C1-C2-C3-C4
25	C	306	CDL	C21-C22-C23-C24
21	D	201	TGL	CA2-CA3-CA4-CA5
25	P	309	CDL	CB7-C71-C72-C73
24	C	304	PEK	C27-C28-C29-C30
25	P	309	CDL	C21-C22-C23-C24
24	P	304	PEK	C28-C29-C30-C31
24	T	102	PEK	C29-C30-C31-C32
25	C	306	CDL	C73-C74-C75-C76
21	O	301	TGL	C12-C13-C14-C29
22	V	101	PSC	C3-C4-C5-C6
24	C	304	PEK	C14-C15-C16-C17
24	C	304	PEK	C34-C35-C36-C37
21	N	604	TGL	CC9-C15-C16-C17
22	V	101	PSC	C20-C21-C22-C23
25	C	308	CDL	C16-C17-C18-C19
17	N	610	PGV	C26-C27-C28-C29
21	B	302	TGL	CA4-CA5-CA6-CA7
21	N	604	TGL	CB4-CB5-CB6-CB7
17	N	605	PGV	C12-C13-C14-C15
24	C	303	PEK	C30-C31-C32-C33
26	Q	201	DMU	C19-C22-C25-C28
21	B	302	TGL	CB4-CB5-CB6-CB7
21	N	609	TGL	CA6-CA7-CA8-CA9
25	C	306	CDL	C71-C72-C73-C74
26	M	101	DMU	C18-C19-C22-C25
17	P	305	PGV	C10-C11-C12-C13
18	N	607	HEA	C26-C15-C16-C17
25	P	307	CDL	C84-C85-C86-C87
17	C	305	PGV	C26-C27-C28-C29
21	O	301	TGL	CB5-CB6-CB7-CB8
17	N	610	PGV	C03-C02-O01-C1
22	V	101	PSC	C03-C02-O01-C1
25	C	308	CDL	CA6-CA4-OA6-CA5
21	D	201	TGL	CC2-CC3-CC4-CC5

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Mol	Chain	Res	Type	Atoms
17	C	301	PGV	C21-C22-C23-C24
24	T	102	PEK	C24-C25-C26-C27
21	N	604	TGL	C29-C30-C31-C32
25	P	307	CDL	OB9-CB7-OB8-CB6
25	P	307	CDL	O1-C1-CA2-OA2
21	O	301	TGL	CA9-C20-C21-C22
17	N	610	PGV	C28-C29-C30-C31
22	V	101	PSC	O01-C02-C03-O11
17	H	101	PGV	C27-C28-C29-C30
22	B	303	PSC	C3-C4-C5-C6
23	P	303	CHD	C13-C17-C20-C22
17	A	604	PGV	O03-C01-C02-C03
17	P	306	PGV	O03-C01-C02-C03
25	P	309	CDL	CA3-CA4-CA6-OA8
17	N	610	PGV	C25-C26-C27-C28
21	N	609	TGL	CB2-CB3-CB4-CB5
24	P	301	PEK	C35-C36-C37-C38
17	N	610	PGV	C2-C3-C4-C5
17	P	306	PGV	C13-C14-C15-C16
22	B	303	PSC	C11-C12-C13-C14
21	N	604	TGL	C18-C19-C33-C34
21	O	301	TGL	CA5-CA6-CA7-CA8
22	B	303	PSC	C30-C31-C32-C33
17	A	604	PGV	O03-C01-C02-O01
17	P	305	PGV	O03-C01-C02-O01
22	V	101	PSC	O03-C01-C02-O01
25	P	307	CDL	OB6-CB4-CB6-OB8
17	N	605	PGV	C5-C6-C7-C8
25	P	309	CDL	C81-C82-C83-C84
26	C	310	DMU	C28-C31-C34-C37
26	G	101	DMU	O1-C10-O7-C3
24	P	304	PEK	C26-C27-C28-C29
25	C	306	CDL	C17-C18-C19-C20
21	D	201	TGL	CC4-CC5-CC6-CC7
23	C	307	CHD	C13-C17-C20-C22
25	P	309	CDL	C36-C37-C38-C39
17	N	605	PGV	C26-C27-C28-C29
21	D	201	TGL	C33-C34-C35-C36
26	C	310	DMU	C19-C18-O16-C6
21	N	604	TGL	CB5-CB6-CB7-CB8
21	L	101	TGL	CA2-CA3-CA4-CA5
24	C	311	PEK	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	P	307	CDL	C62-C63-C64-C65
17	P	305	PGV	C23-C24-C25-C26
25	C	306	CDL	C81-C82-C83-C84
17	N	605	PGV	C31-C32-C33-C34
17	N	605	PGV	C11-C12-C13-C14
21	N	609	TGL	C22-C23-C24-C25
24	P	301	PEK	C22-C23-C24-C25
25	P	307	CDL	C40-C41-C42-C43
25	P	307	CDL	OB5-CB3-CB4-CB6
17	C	301	PGV	C22-C23-C24-C25
17	P	306	PGV	C22-C23-C24-C25
22	V	101	PSC	C24-C25-C26-C27
17	H	101	PGV	O12-C04-C05-O05
22	B	303	PSC	C14-C15-C16-C17
22	V	101	PSC	C02-C03-O11-P
25	P	307	CDL	OB5-CB3-CB4-OB6
17	P	306	PGV	C31-C32-C33-C34
21	N	604	TGL	CA9-C20-C21-C22
25	C	306	CDL	C54-C55-C56-C57
25	P	309	CDL	C33-C34-C35-C36
18	N	606	HEA	C4A-C3A-CMA-OMA
25	P	307	CDL	C15-C16-C17-C18
17	P	306	PGV	C19-C20-C21-C22
23	C	302	CHD	C13-C17-C20-C21
21	N	604	TGL	OG2-CG2-CG3-OG3
25	P	309	CDL	OA6-CA4-CA6-OA8
17	H	101	PGV	O12-C04-C05-C06
26	P	302	DMU	C5-C10-O7-C3
21	B	302	TGL	OG1-CG1-CG2-CG3
21	D	201	TGL	OG1-CG1-CG2-CG3
21	N	604	TGL	CG1-CG2-CG3-OG3
24	P	301	PEK	O03-C01-C02-C03
25	P	307	CDL	CA3-CA4-CA6-OA8
21	N	604	TGL	CC7-CC8-CC9-C15
24	C	304	PEK	C16-C17-C18-C19
26	P	302	DMU	O5-C6-O16-C18
21	N	609	TGL	CA2-CA3-CA4-CA5
21	B	302	TGL	C16-C17-C18-C19
21	D	201	TGL	C10-C11-C12-C13
17	A	604	PGV	C03-O11-P-O13
17	C	301	PGV	C04-O12-P-O13
17	N	605	PGV	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
17	N	610	PGV	C04-O12-P-O11
17	N	610	PGV	C04-O12-P-O14
17	P	305	PGV	C03-O11-P-O14
17	P	305	PGV	C04-O12-P-O11
22	B	303	PSC	C04-O12-P-O14
24	C	311	PEK	O12-C04-C05-N
24	P	301	PEK	C04-O12-P-O14
24	P	304	PEK	C03-O11-P-O14
24	T	102	PEK	C04-O12-P-O11
24	T	102	PEK	C04-O12-P-O13
25	C	308	CDL	CA2-OA2-PA1-OA3
25	P	307	CDL	CA3-OA5-PA1-OA4
25	P	307	CDL	CB2-OB2-PB2-OB3
25	P	307	CDL	CB2-OB2-PB2-OB5
25	P	309	CDL	CB3-OB5-PB2-OB3
17	P	305	PGV	C28-C29-C30-C31
23	P	303	CHD	C21-C20-C22-C23
24	C	303	PEK	C02-C03-O11-P
24	P	304	PEK	C02-C03-O11-P
25	P	309	CDL	C1-CA2-OA2-PA1
17	C	301	PGV	C13-C14-C15-C16
25	C	308	CDL	OB7-CB5-OB6-CB4
25	C	306	CDL	C44-C45-C46-C47
17	P	306	PGV	C1-C2-C3-C4
17	A	604	PGV	C14-C15-C16-C17
21	N	604	TGL	CC2-CC3-CC4-CC5
24	P	301	PEK	C25-C26-C27-C28
23	C	302	CHD	C16-C17-C20-C21
25	P	309	CDL	CB6-CB4-OB6-CB5
21	L	101	TGL	C29-C30-C31-C32
25	C	306	CDL	C40-C41-C42-C43
17	H	101	PGV	C15-C16-C17-C18
23	T	101	CHD	C13-C17-C20-C21
22	B	303	PSC	C01-C02-C03-O11
25	C	306	CDL	OA5-CA3-CA4-CA6
17	C	301	PGV	C14-C15-C16-C17
18	N	606	HEA	C4D-C3D-CAD-CBD
17	P	305	PGV	O12-C04-C05-C06
17	P	306	PGV	C3-C4-C5-C6
17	P	306	PGV	C7-C8-C9-C10
25	C	306	CDL	OB9-CB7-OB8-CB6
25	C	308	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
21	B	302	TGL	OB1-CB1-OG2-CG2
25	P	309	CDL	CA4-CA3-OA5-PA1
25	P	307	CDL	C63-C64-C65-C66
21	L	101	TGL	OG2-CG2-CG3-OG3
25	C	306	CDL	OB6-CB4-CB6-OB8
17	P	305	PGV	C15-C16-C17-C18
26	G	101	DMU	C22-C25-C28-C31
26	G	101	DMU	C34-C37-C40-C43
22	V	101	PSC	O03-C01-C02-C03
18	N	606	HEA	C2D-C3D-CAD-CBD
17	C	301	PGV	C20-C19-O03-C01
23	Y	101	CHD	C20-C22-C23-C24
17	A	604	PGV	C25-C26-C27-C28
24	P	304	PEK	C32-C33-C34-C35
26	C	310	DMU	C22-C25-C28-C31
23	C	302	CHD	C16-C17-C20-C22
21	N	609	TGL	CA5-CA6-CA7-CA8
25	C	306	CDL	C71-CB7-OB8-CB6
17	C	301	PGV	C9-C10-C11-C12
17	A	604	PGV	C29-C30-C31-C32
21	D	201	TGL	C16-C17-C18-C19
25	P	309	CDL	C19-C20-C21-C22
21	N	604	TGL	CB3-CB4-CB5-CB6
26	C	309	DMU	C4-C3-O7-C10
17	P	306	PGV	C14-C15-C16-C17
17	P	306	PGV	C20-C21-C22-C23
25	C	308	CDL	C61-C62-C63-C64
22	B	303	PSC	C12-C13-C14-C15
24	P	304	PEK	C3-C4-C5-C6
21	N	609	TGL	CC9-C15-C16-C17
25	P	307	CDL	C82-C83-C84-C85
25	P	309	CDL	C72-C73-C74-C75
23	T	101	CHD	C16-C17-C20-C22
21	L	101	TGL	CA9-C20-C21-C22
18	A	605	HEA	CAD-CBD-CGD-O1D
18	N	606	HEA	C26-C15-C16-C17
24	C	303	PEK	C27-C28-C29-C30
25	P	307	CDL	CB2-C1-CA2-OA2
18	N	607	HEA	CAA-CBA-CGA-O2A
23	Y	101	CHD	C22-C23-C24-O25
24	P	304	PEK	C14-C15-C16-C17
17	P	305	PGV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
17	P	305	PGV	C04-C05-C06-O06
24	P	301	PEK	C17-C18-C19-C20
21	D	201	TGL	CB2-CB3-CB4-CB5
21	O	301	TGL	C11-C10-CB9-CB8
18	N	606	HEA	CAD-CBD-CGD-O1D
23	Y	101	CHD	C22-C23-C24-O26
21	O	301	TGL	C18-C19-C33-C34
18	N	606	HEA	CAD-CBD-CGD-O2D
18	A	605	HEA	C26-C15-C16-C17
25	C	306	CDL	C79-C80-C81-C82
17	N	605	PGV	O03-C19-C20-C21
22	B	303	PSC	C15-C16-C17-C18
17	P	306	PGV	O01-C02-C03-O11
23	C	307	CHD	C22-C23-C24-O25
23	P	308	CHD	C22-C23-C24-O26
26	C	310	DMU	C3-C4-C57-O61
17	P	306	PGV	C02-C03-O11-P
25	P	307	CDL	CA4-CA3-OA5-PA1
25	P	307	CDL	CB4-CB3-OB5-PB2
21	L	101	TGL	C19-C33-C34-C35
18	A	605	HEA	CAD-CBD-CGD-O2D
23	P	308	CHD	C22-C23-C24-O25
17	P	306	PGV	O03-C01-C02-O01
17	C	301	PGV	O04-C19-O03-C01
24	C	304	PEK	C11-C10-C9-C8
24	C	304	PEK	C11-C12-C13-C14
24	C	311	PEK	C5-C6-C7-C8
24	C	311	PEK	C12-C13-C14-C15
24	P	301	PEK	C9-C10-C11-C12
24	T	102	PEK	C6-C7-C8-C9
24	T	102	PEK	C9-C10-C11-C12
24	T	102	PEK	C12-C13-C14-C15
24	C	303	PEK	C34-C35-C36-C37
17	N	605	PGV	C11-C10-C9-C8
24	P	304	PEK	C25-C26-C27-C28
23	O	303	CHD	C22-C23-C24-O25
23	T	101	CHD	C22-C23-C24-O25
17	A	604	PGV	C22-C23-C24-C25
22	V	101	PSC	C5-C6-C7-C8
23	P	308	CHD	C20-C22-C23-C24
21	D	201	TGL	C13-C14-C29-C30
25	C	306	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
18	N	606	HEA	C14-C15-C16-C17
18	N	607	HEA	C14-C15-C16-C17
22	V	101	PSC	C14-C15-C16-C17
23	T	101	CHD	C13-C17-C20-C22
23	C	307	CHD	C22-C23-C24-O26
21	L	101	TGL	C10-C11-C12-C13
18	A	605	HEA	C2D-C3D-CAD-CBD
21	O	301	TGL	CB2-CB3-CB4-CB5
25	P	307	CDL	C53-C54-C55-C56
25	C	308	CDL	CA3-CA4-CA6-OA8
23	T	101	CHD	C16-C17-C20-C21
18	N	607	HEA	CAA-CBA-CGA-O1A
23	O	303	CHD	C22-C23-C24-O26
17	P	305	PGV	O05-C05-C06-O06
26	C	309	DMU	C2-C3-O7-C10
22	B	303	PSC	O01-C02-C03-O11
18	A	606	HEA	CAA-CBA-CGA-O2A
21	L	101	TGL	CA3-CA4-CA5-CA6
17	C	301	PGV	C24-C25-C26-C27
23	J	101	CHD	C22-C23-C24-O26
17	N	605	PGV	O12-C04-C05-C06
24	C	304	PEK	C2-C3-C4-C5
18	N	607	HEA	C11-C12-C13-C14
24	T	102	PEK	C32-C33-C34-C35
25	P	307	CDL	C16-C17-C18-C19
22	V	101	PSC	C01-C02-C03-O11
25	C	308	CDL	OB5-CB3-CB4-CB6
22	B	303	PSC	C1-C2-C3-C4
17	P	306	PGV	C9-C10-C11-C12
17	A	604	PGV	C7-C8-C9-C10
26	M	101	DMU	C28-C31-C34-C37
21	N	604	TGL	CA1-CA2-CA3-CA4
21	N	604	TGL	C14-C29-C30-C31
21	D	201	TGL	CC3-CC4-CC5-CC6
24	C	303	PEK	C1-C2-C3-C4
25	C	308	CDL	CB7-C71-C72-C73
17	C	305	PGV	C11-C12-C13-C14
24	C	303	PEK	C14-C15-C16-C17
24	C	311	PEK	C3-C4-C5-C6
24	C	303	PEK	C10-C11-C12-C13
21	O	301	TGL	CA7-CA8-CA9-C20
22	V	101	PSC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	T	102	PEK	C14-C15-C16-C17
17	N	605	PGV	C6-C7-C8-C9
21	N	609	TGL	CA4-CA5-CA6-CA7
17	A	604	PGV	C11-C12-C13-C14
17	N	610	PGV	C9-C10-C11-C12
18	A	606	HEA	CAA-CBA-CGA-O1A
23	J	101	CHD	C22-C23-C24-O25
22	V	101	PSC	C15-C16-C17-C18
25	P	309	CDL	C24-C25-C26-C27
17	A	604	PGV	C26-C27-C28-C29
22	B	303	PSC	C29-C30-C31-C32
17	C	301	PGV	C11-C12-C13-C14
21	N	609	TGL	CB7-CB8-CB9-C10
21	O	301	TGL	C16-C15-CC9-CC8
23	W	101	CHD	C20-C22-C23-C24
21	D	201	TGL	C11-C10-CB9-CB8
25	P	309	CDL	C37-C38-C39-C40
21	D	201	TGL	C25-C26-C27-C28
23	T	103	CHD	C22-C23-C24-O26
21	D	201	TGL	OG2-CB1-CB2-CB3
21	N	609	TGL	CB9-C10-C11-C12
25	C	308	CDL	C22-C23-C24-C25
23	T	103	CHD	C22-C23-C24-O25
17	H	101	PGV	C9-C10-C11-C12
17	N	610	PGV	O03-C19-C20-C21
24	C	311	PEK	O03-C21-C22-C23
21	D	201	TGL	CB4-CB5-CB6-CB7
22	B	303	PSC	C31-C32-C33-C34
21	B	302	TGL	CB2-CB1-OG2-CG2
21	O	301	TGL	C14-C29-C30-C31
17	P	306	PGV	C5-C6-C7-C8
17	N	605	PGV	C25-C26-C27-C28
21	O	301	TGL	CA4-CA5-CA6-CA7
17	H	101	PGV	C11-C12-C13-C14
23	P	303	CHD	C20-C22-C23-C24
25	C	308	CDL	C51-CB5-OB6-CB4
18	A	606	HEA	CAD-CBD-CGD-O2D
22	B	303	PSC	O03-C19-C20-C21
25	C	308	CDL	C63-C64-C65-C66
26	P	302	DMU	O1-C10-O7-C3
21	L	101	TGL	OG3-CC1-CC2-CC3
22	V	101	PSC	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	V	101	PSC	O03-C19-C20-C21
22	B	303	PSC	C23-C24-C25-C26
21	B	302	TGL	C15-C16-C17-C18
21	N	604	TGL	CC4-CC5-CC6-CC7
21	L	101	TGL	OG1-CA1-CA2-CA3
21	N	604	TGL	OG2-CB1-CB2-CB3
24	C	303	PEK	O01-C1-C2-C3
24	T	102	PEK	O01-C1-C2-C3
25	C	308	CDL	C12-C11-CA5-OA6
17	N	605	PGV	O12-C04-C05-O05
18	A	605	HEA	CAA-CBA-CGA-O2A
24	P	304	PEK	C27-C28-C29-C30
21	N	609	TGL	OG2-CB1-CB2-CB3
18	A	605	HEA	CAA-CBA-CGA-O1A
21	D	201	TGL	OG1-CA1-CA2-CA3
21	B	302	TGL	C13-C14-C29-C30
25	C	308	CDL	C81-C82-C83-C84
21	O	301	TGL	C24-C25-C26-C27
17	N	610	PGV	C01-C02-C03-O11
21	B	302	TGL	OG1-CA1-CA2-CA3
21	O	301	TGL	OG3-CC1-CC2-CC3
25	C	308	CDL	C24-C25-C26-C27
17	H	101	PGV	C21-C22-C23-C24
24	C	311	PEK	C30-C31-C32-C33
26	G	101	DMU	C31-C34-C37-C40
17	A	604	PGV	C23-C24-C25-C26
25	C	306	CDL	C16-C17-C18-C19
17	P	305	PGV	C24-C25-C26-C27
21	B	302	TGL	C10-C11-C12-C13
25	C	308	CDL	C32-C31-CA7-OA8
24	C	303	PEK	C29-C30-C31-C32
26	P	302	DMU	C28-C31-C34-C37
21	L	101	TGL	OC1-CC1-CC2-CC3
21	N	604	TGL	CA6-CA7-CA8-CA9
25	P	307	CDL	C56-C57-C58-C59
18	A	606	HEA	CAD-CBD-CGD-O1D
22	V	101	PSC	O04-C19-C20-C21
24	C	311	PEK	O04-C21-C22-C23
23	T	101	CHD	C22-C23-C24-O26
25	C	306	CDL	C59-C60-C61-C62
25	C	308	CDL	C55-C56-C57-C58
25	P	307	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
17	H	101	PGV	C22-C23-C24-C25
17	P	306	PGV	C23-C24-C25-C26
24	P	304	PEK	C31-C32-C33-C34
22	B	303	PSC	O04-C19-C20-C21
18	N	606	HEA	CAA-CBA-CGA-O2A
21	L	101	TGL	CC5-CC6-CC7-CC8
21	L	101	TGL	OA1-CA1-CA2-CA3
21	N	609	TGL	OB1-CB1-CB2-CB3
26	G	101	DMU	C19-C22-C25-C28
24	P	301	PEK	O03-C01-C02-O01
26	P	302	DMU	O5-C4-C57-O61
17	N	610	PGV	O04-C19-C20-C21
21	D	201	TGL	OA1-CA1-CA2-CA3
21	D	201	TGL	OG3-CC1-CC2-CC3
23	T	103	CHD	C21-C20-C22-C23
17	N	610	PGV	C11-C12-C13-C14
21	N	609	TGL	C16-C17-C18-C19
25	P	309	CDL	C71-C72-C73-C74
24	C	303	PEK	O02-C1-C2-C3
25	C	308	CDL	C12-C11-CA5-OA7
24	P	301	PEK	C33-C34-C35-C36
17	C	305	PGV	O03-C19-C20-C21
21	N	604	TGL	OB1-CB1-CB2-CB3
22	V	101	PSC	O02-C1-C2-C3
25	C	308	CDL	C31-C32-C33-C34
22	B	303	PSC	C2-C3-C4-C5
21	L	101	TGL	C17-C18-C19-C33
21	N	604	TGL	C21-C22-C23-C24

There are no ring outliers.

40 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	310	DMU	1	0
17	A	604	PGV	3	0
23	T	101	CHD	1	0
24	C	311	PEK	2	0
21	D	201	TGL	2	0
17	N	605	PGV	1	0
24	P	304	PEK	2	0
22	V	101	PSC	2	0
17	C	305	PGV	2	0

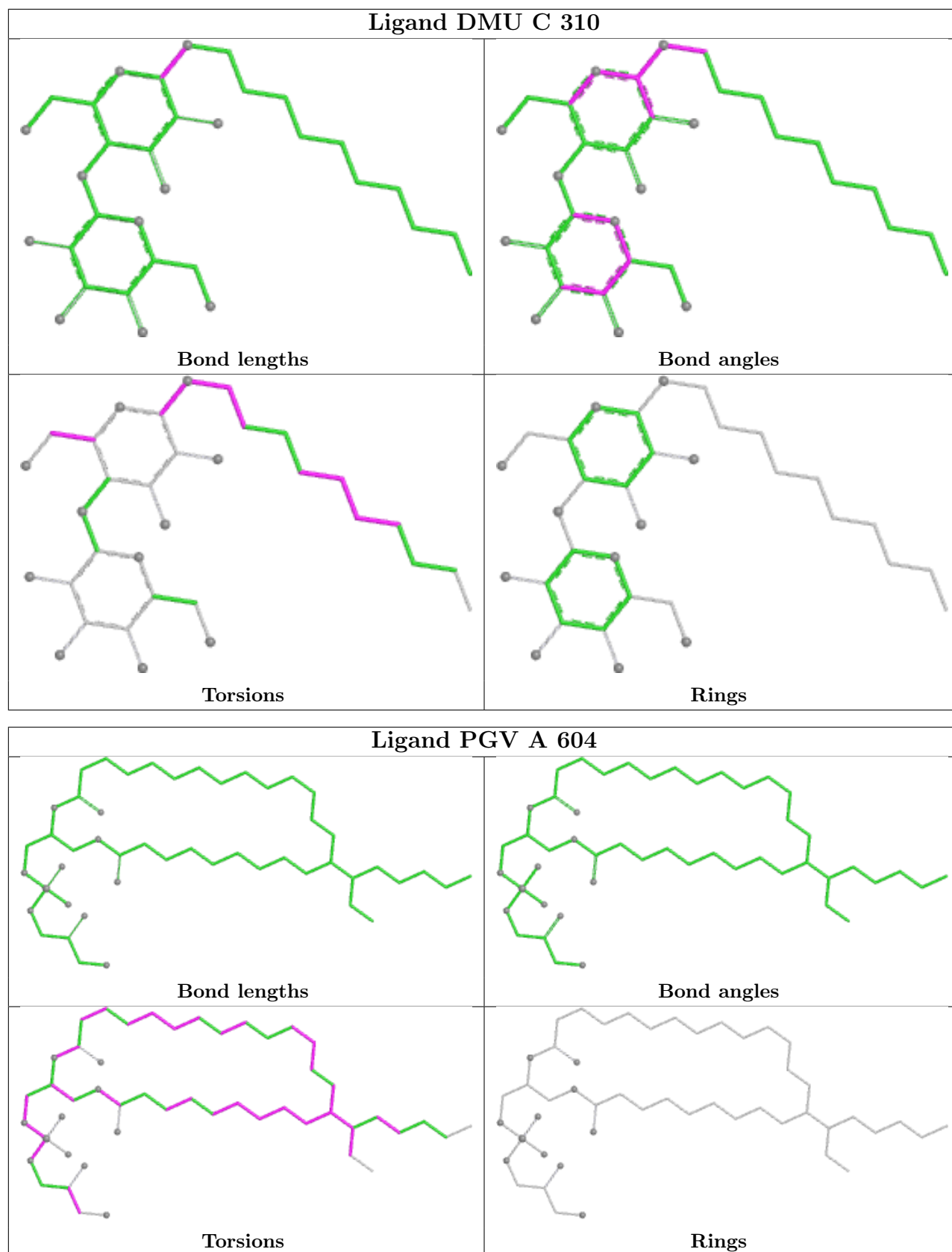
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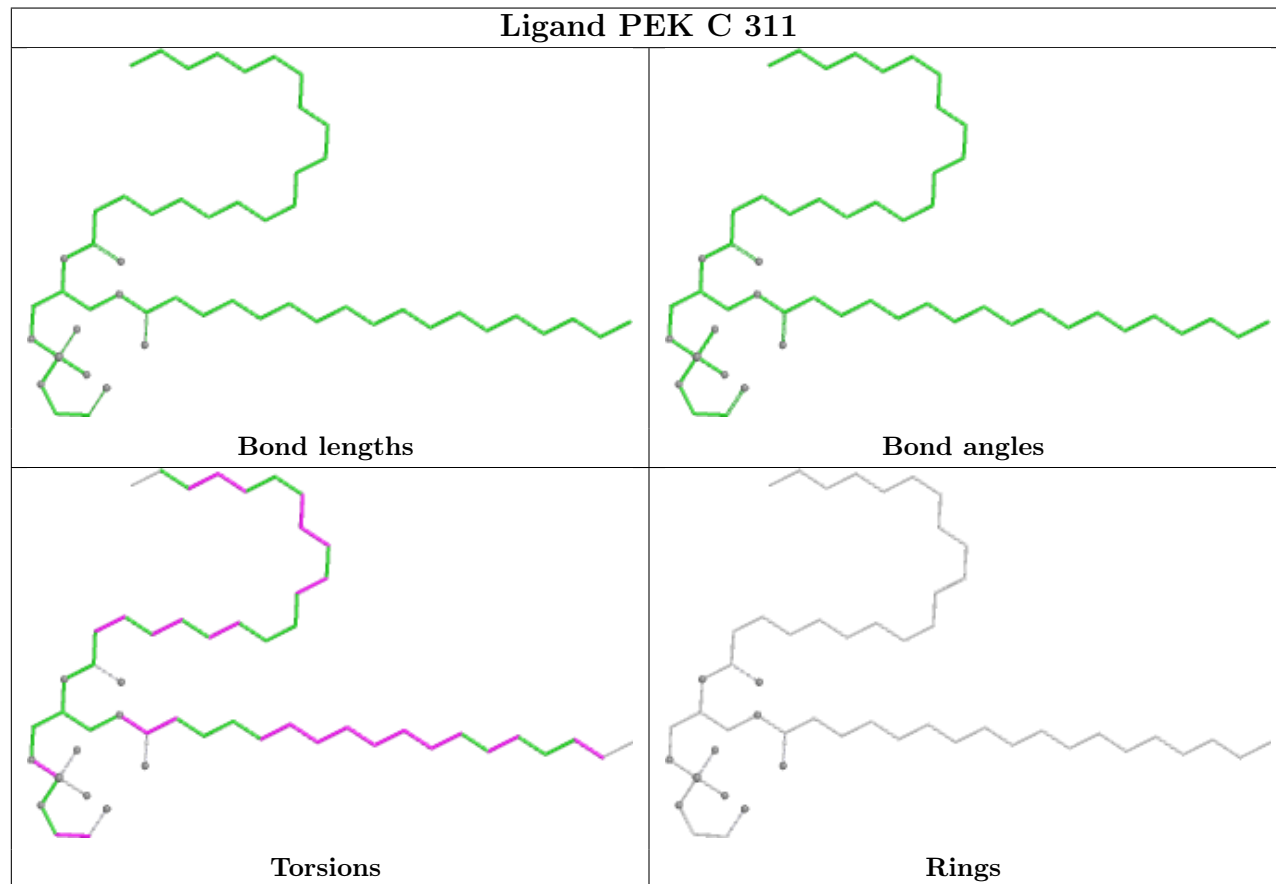
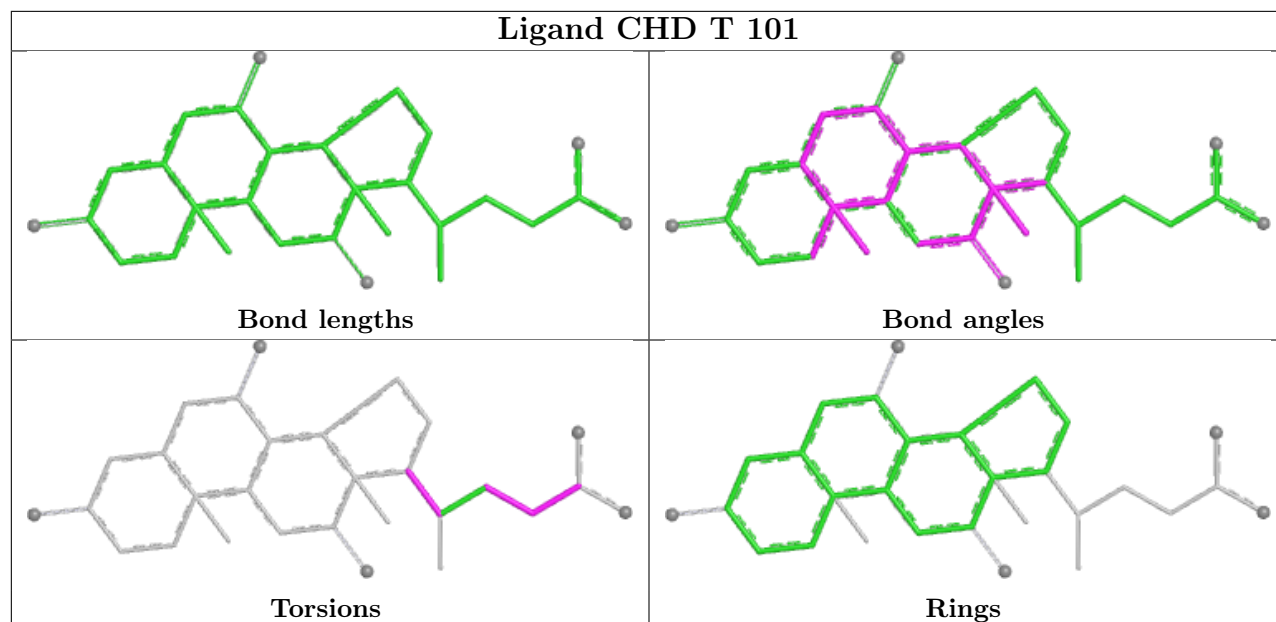
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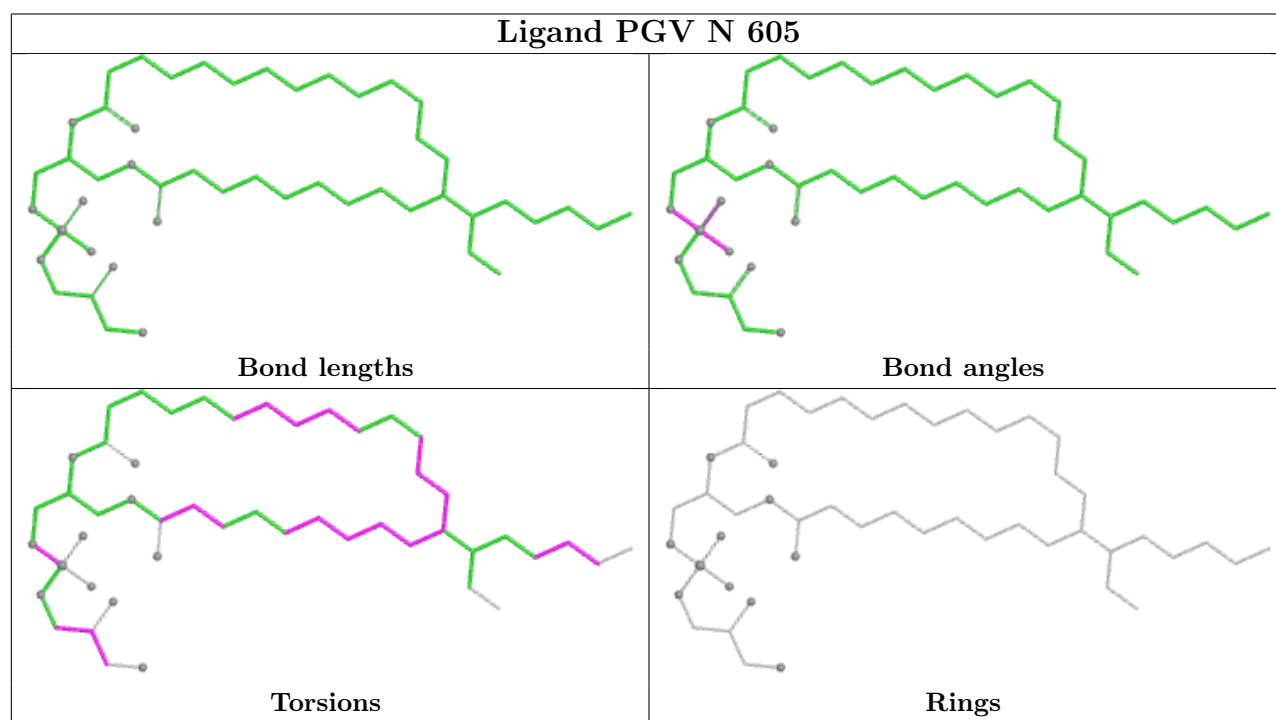
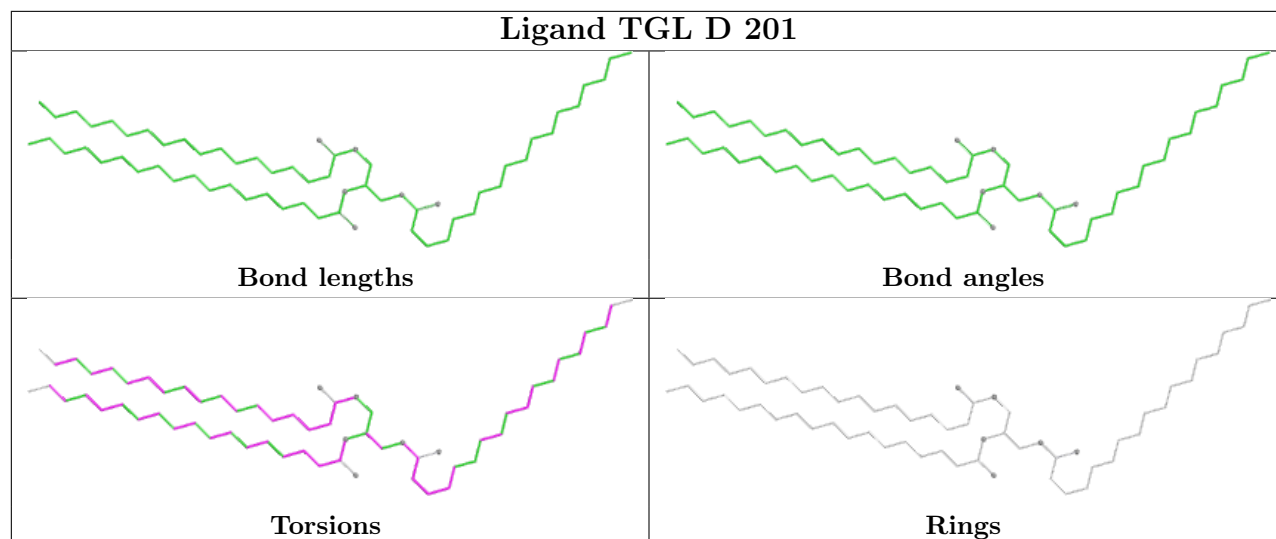
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	610	PGV	1	0
21	N	604	TGL	6	0
22	B	303	PSC	1	0
23	T	103	CHD	2	0
17	C	301	PGV	1	0
23	Y	101	CHD	2	0
23	P	308	CHD	1	0
26	M	101	DMU	1	0
28	V	102	SAC	1	0
23	P	303	CHD	1	0
25	C	306	CDL	1	0
18	A	606	HEA	9	0
21	B	302	TGL	2	0
17	H	101	PGV	1	0
23	C	302	CHD	2	0
26	C	309	DMU	5	0
24	P	301	PEK	1	0
25	P	307	CDL	1	0
23	C	307	CHD	1	0
18	N	607	HEA	9	0
24	C	303	PEK	5	0
21	L	101	TGL	8	0
17	P	306	PGV	1	0
18	A	605	HEA	6	0
24	T	102	PEK	1	0
25	P	309	CDL	8	0
17	P	305	PGV	1	0
21	N	609	TGL	1	0
18	N	606	HEA	2	0
23	J	101	CHD	1	0
25	C	308	CDL	2	0

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

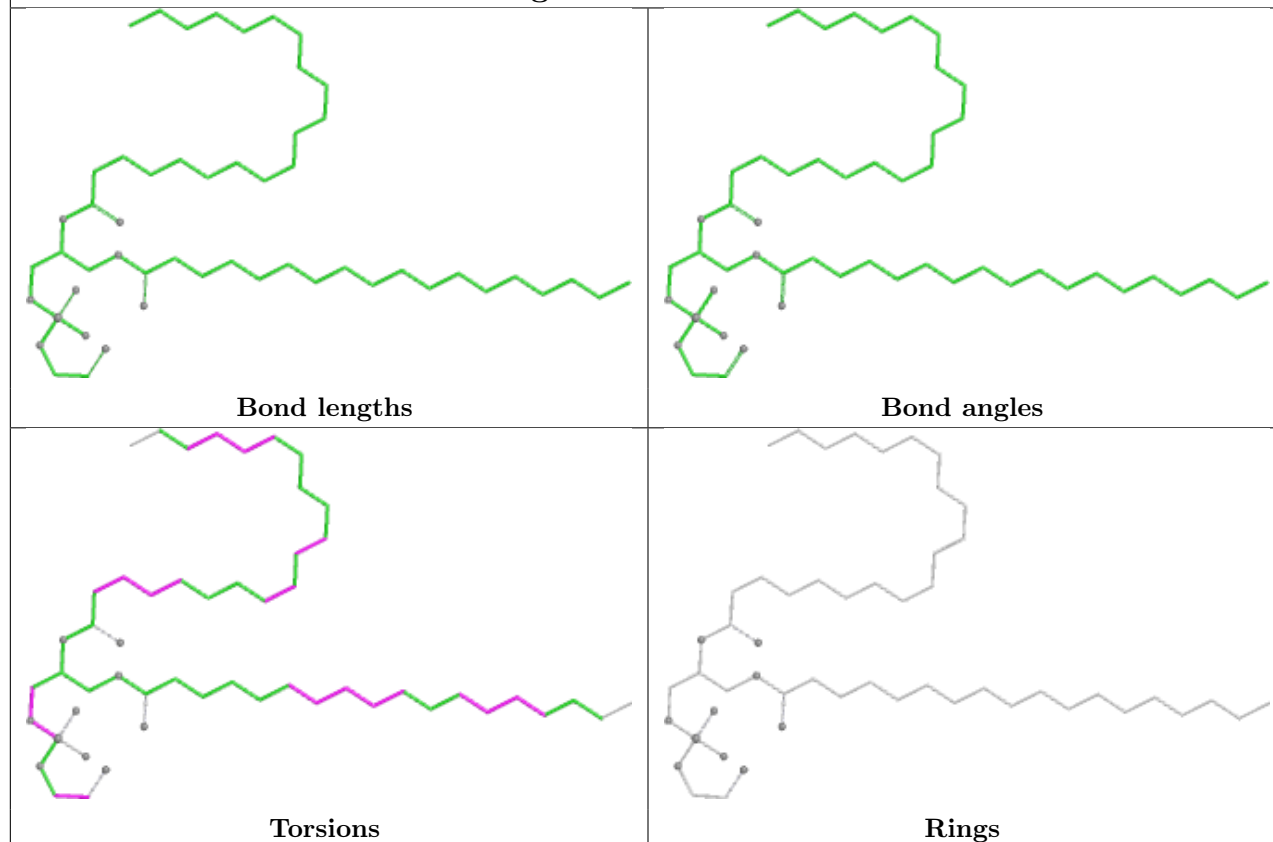
equivalents in the CSD to analyse the geometry.



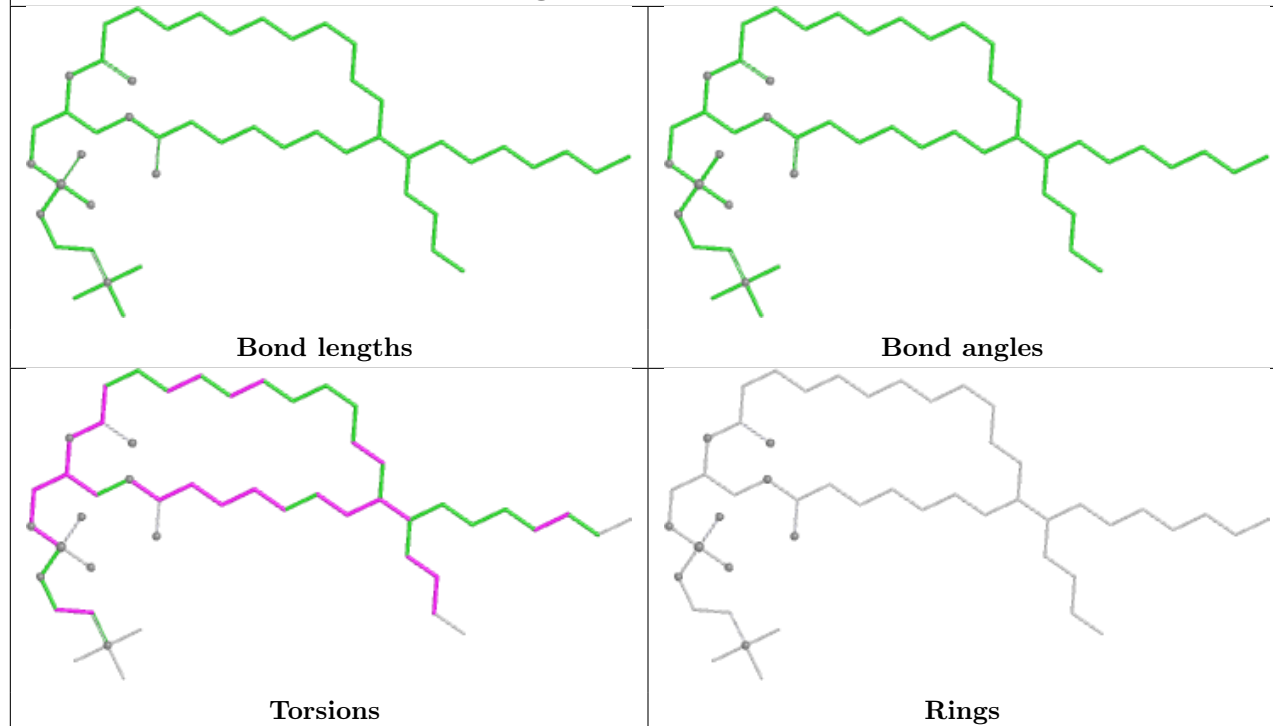


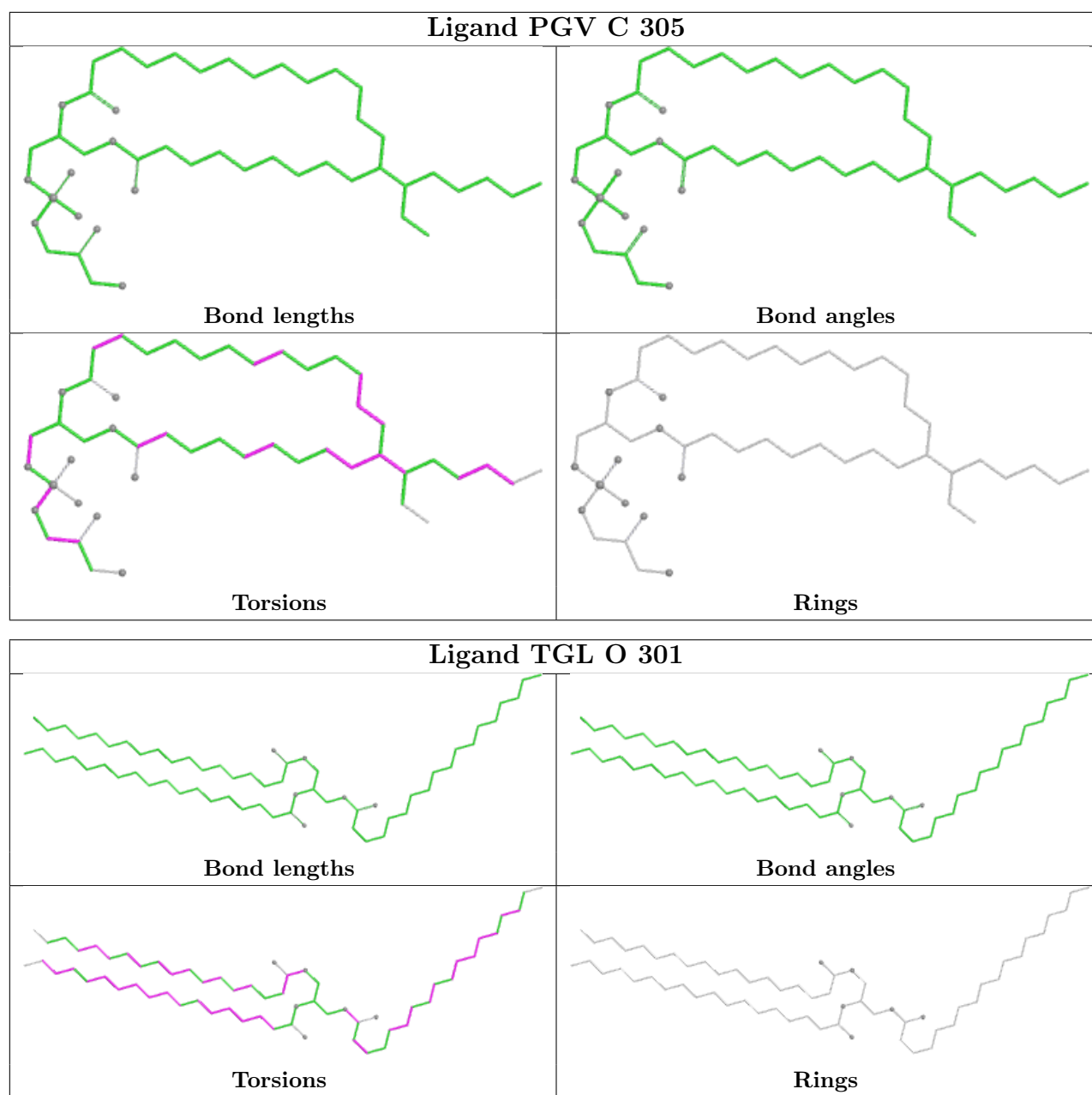


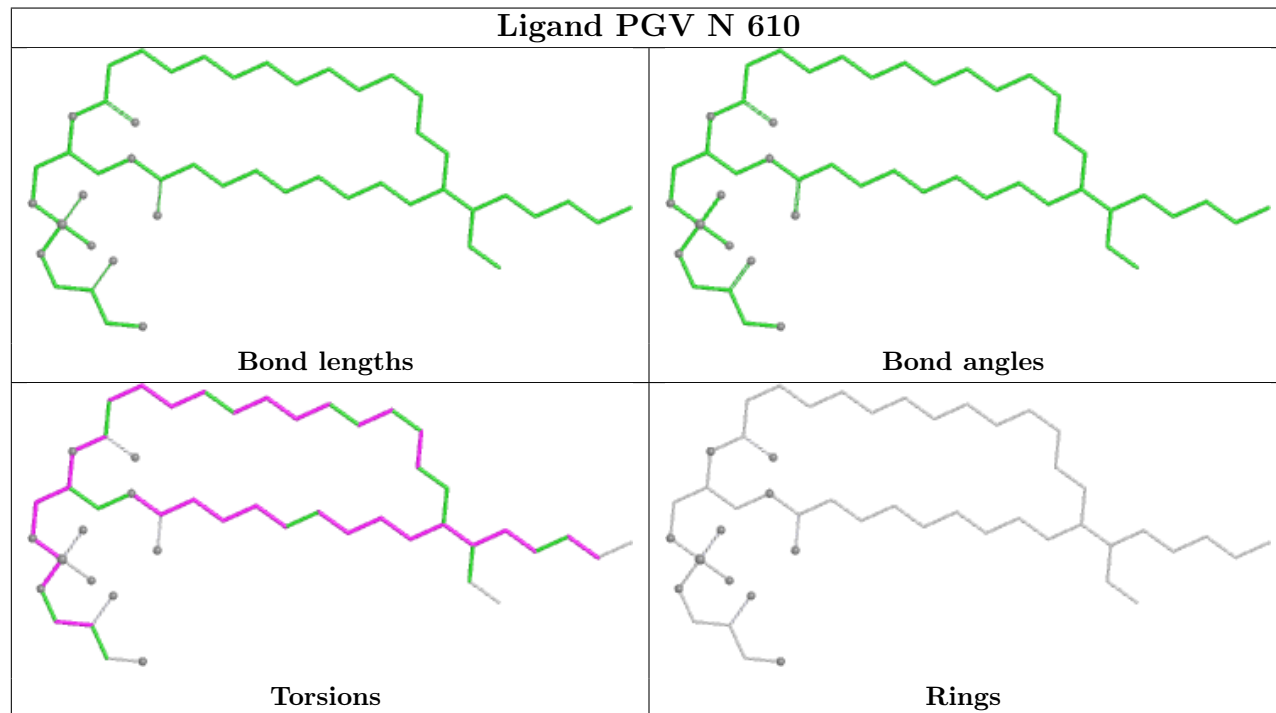
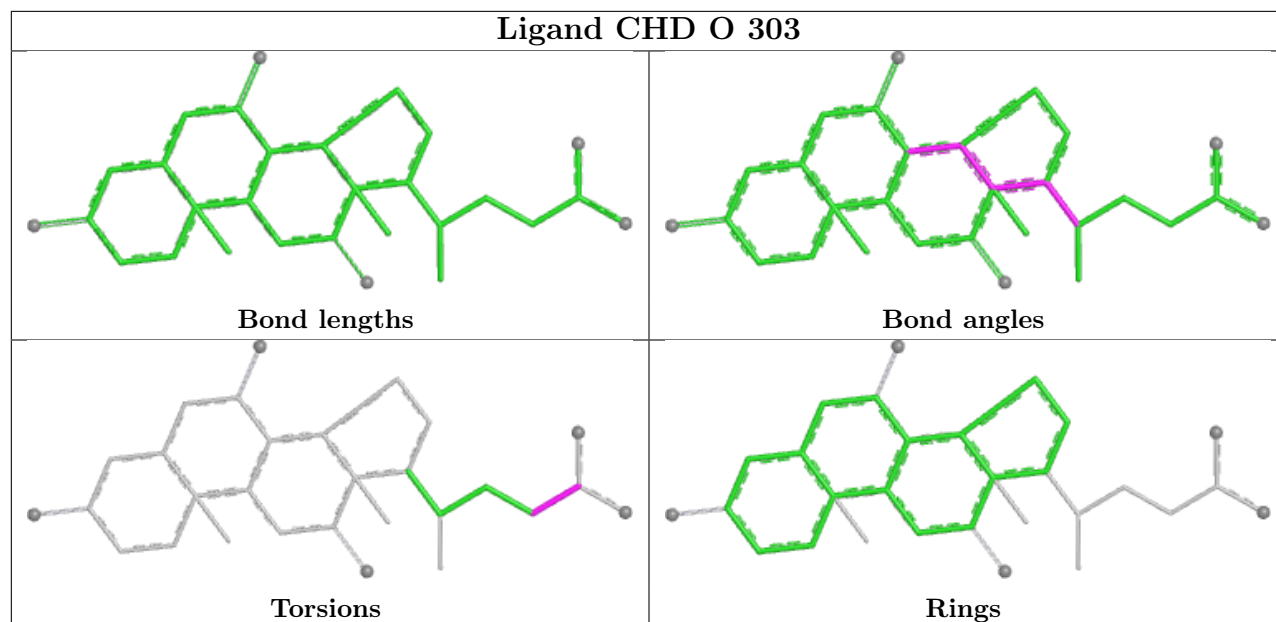
Ligand PEK P 304

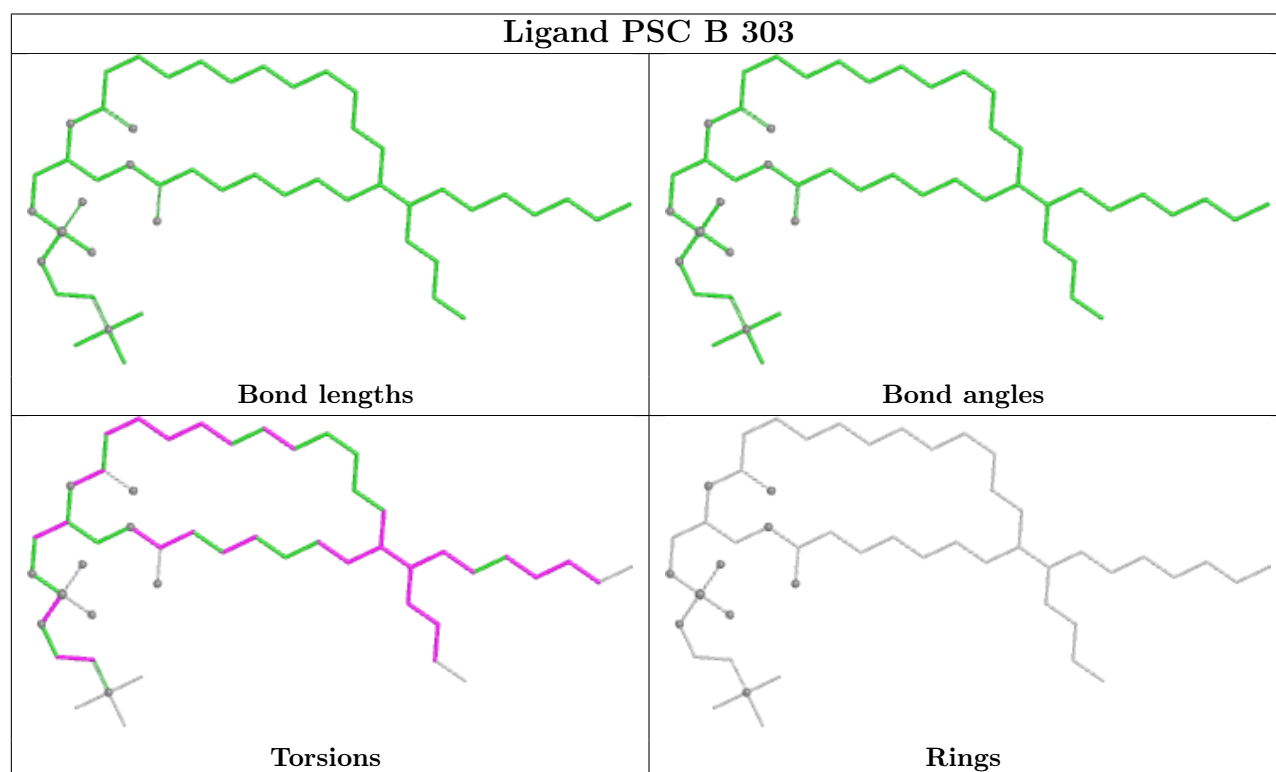
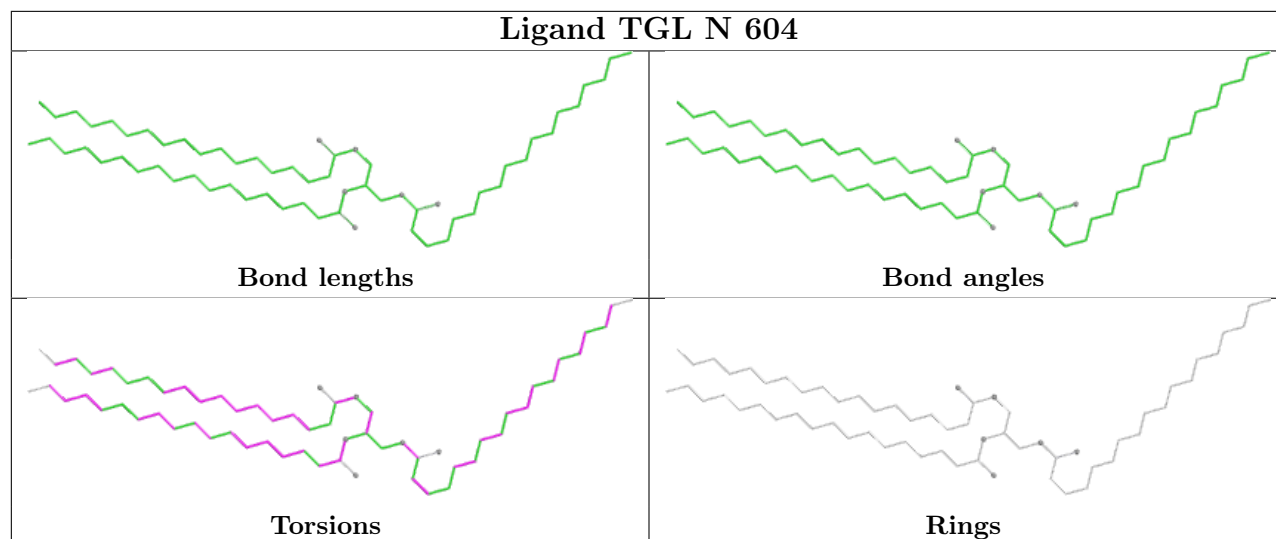


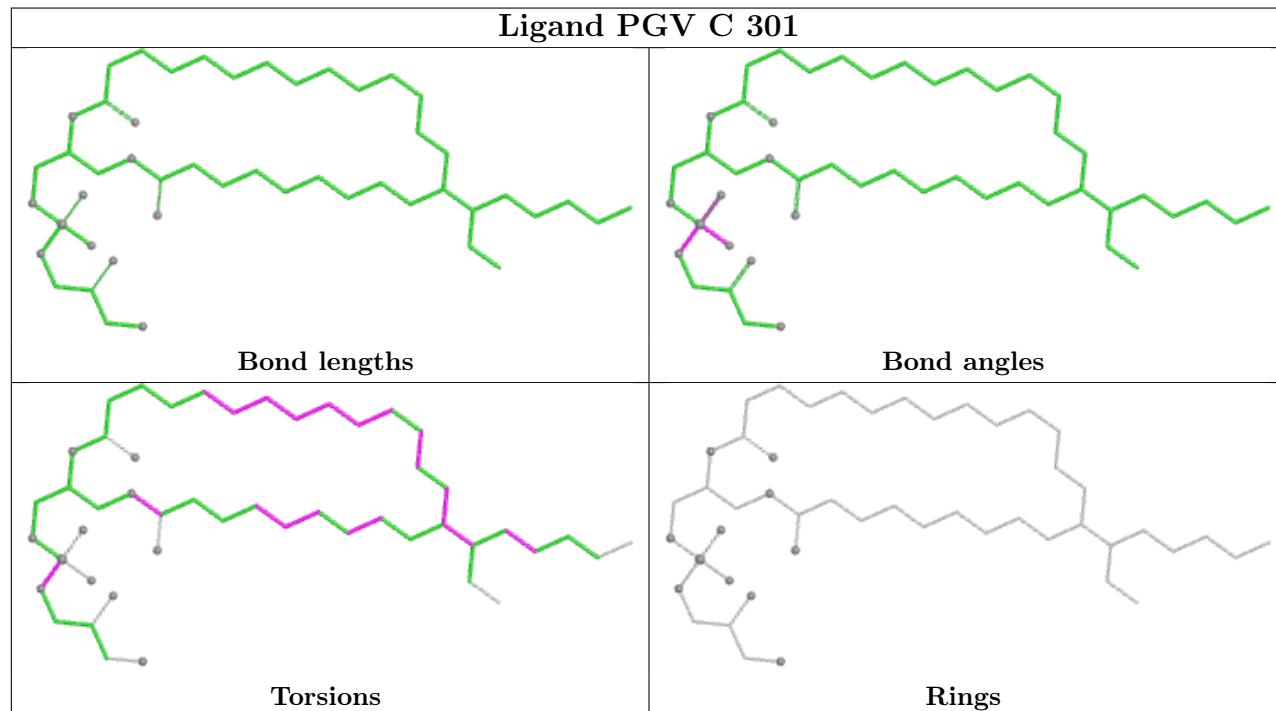
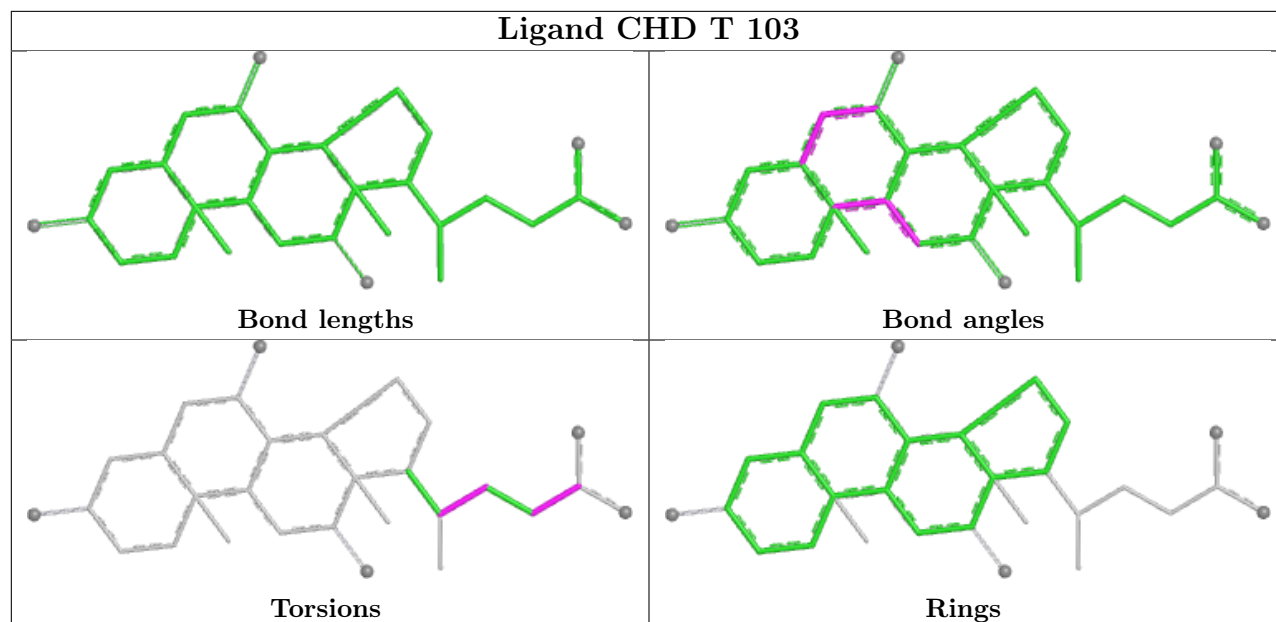
Ligand PSC V 101

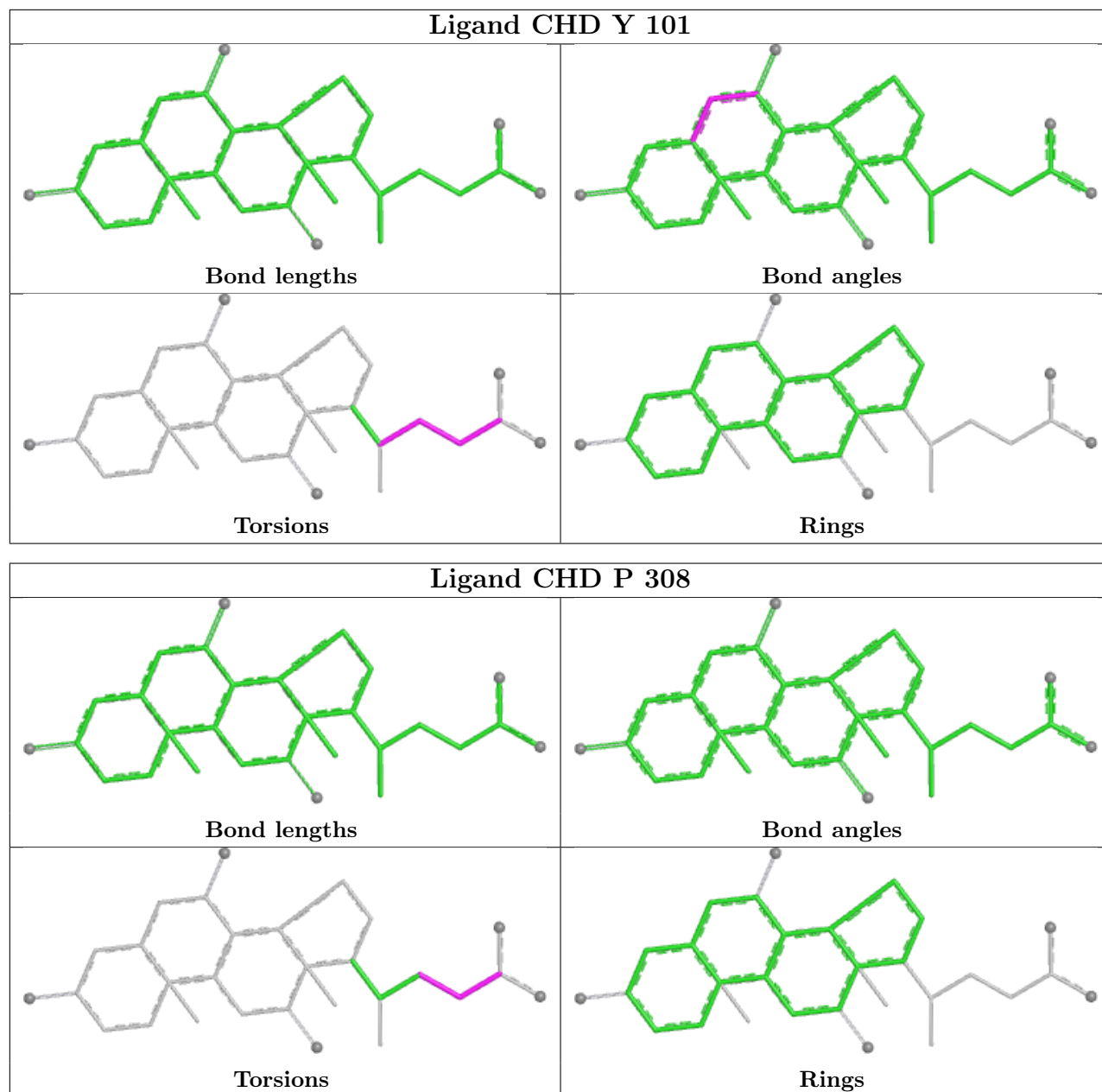


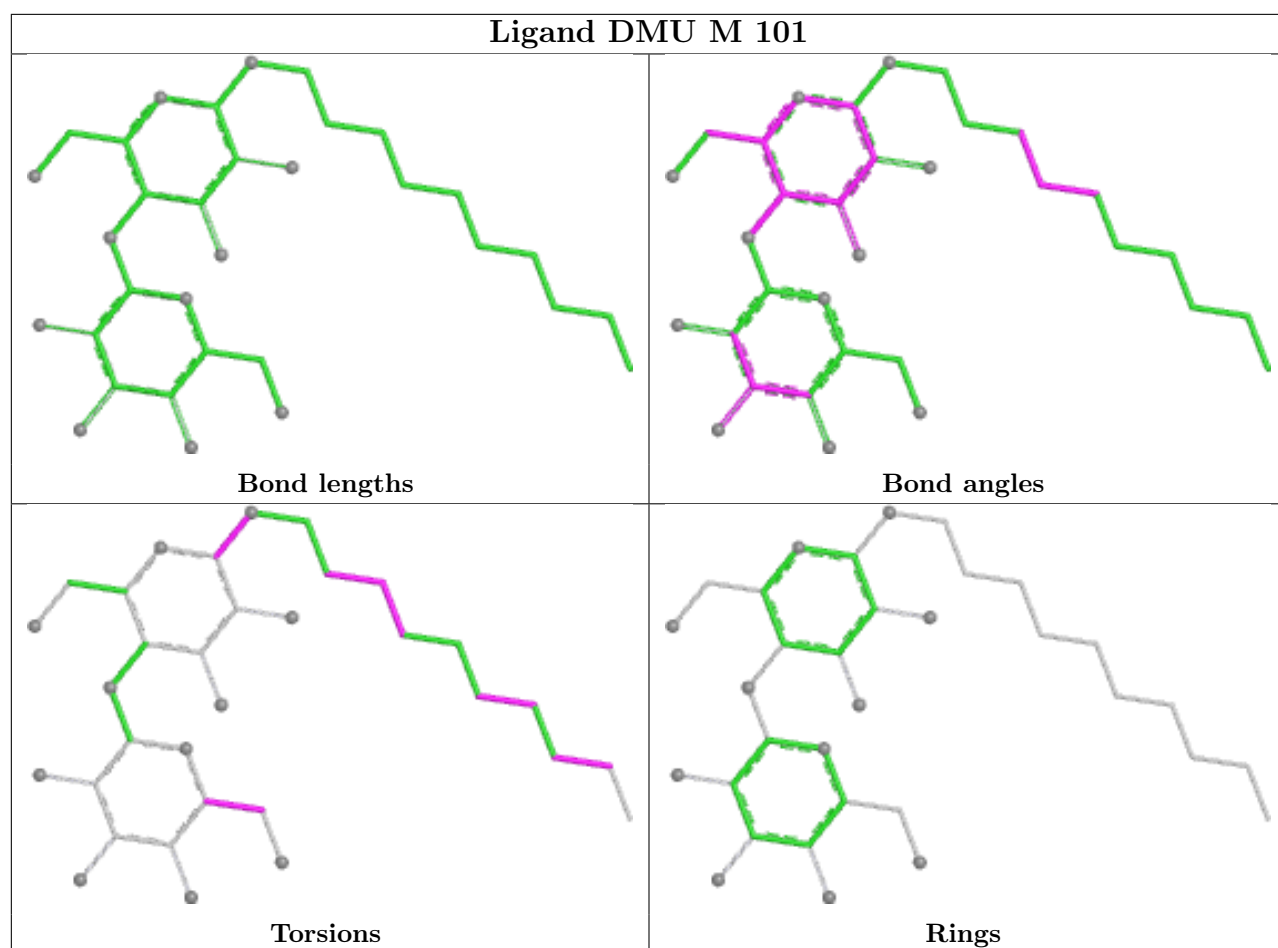


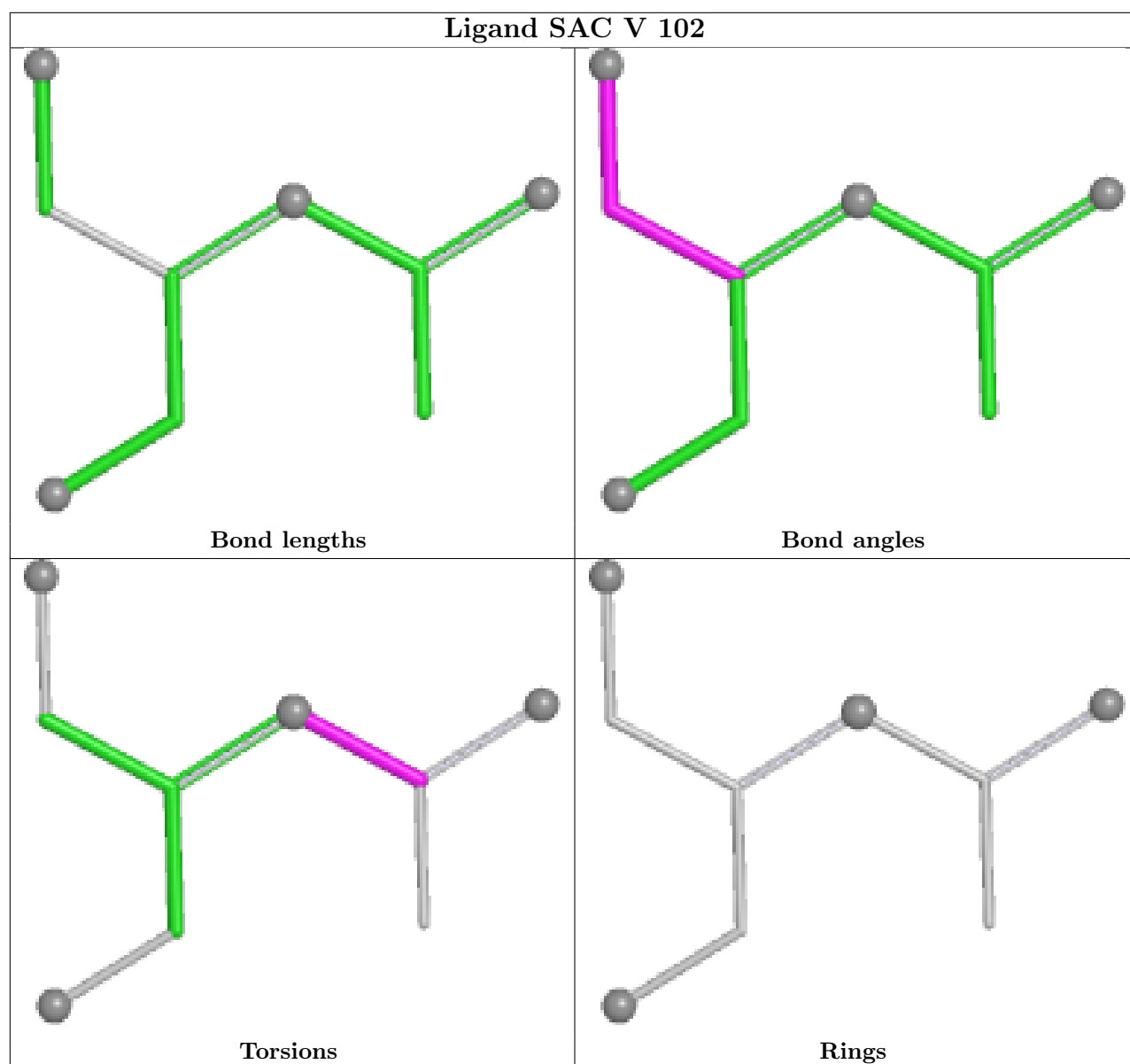




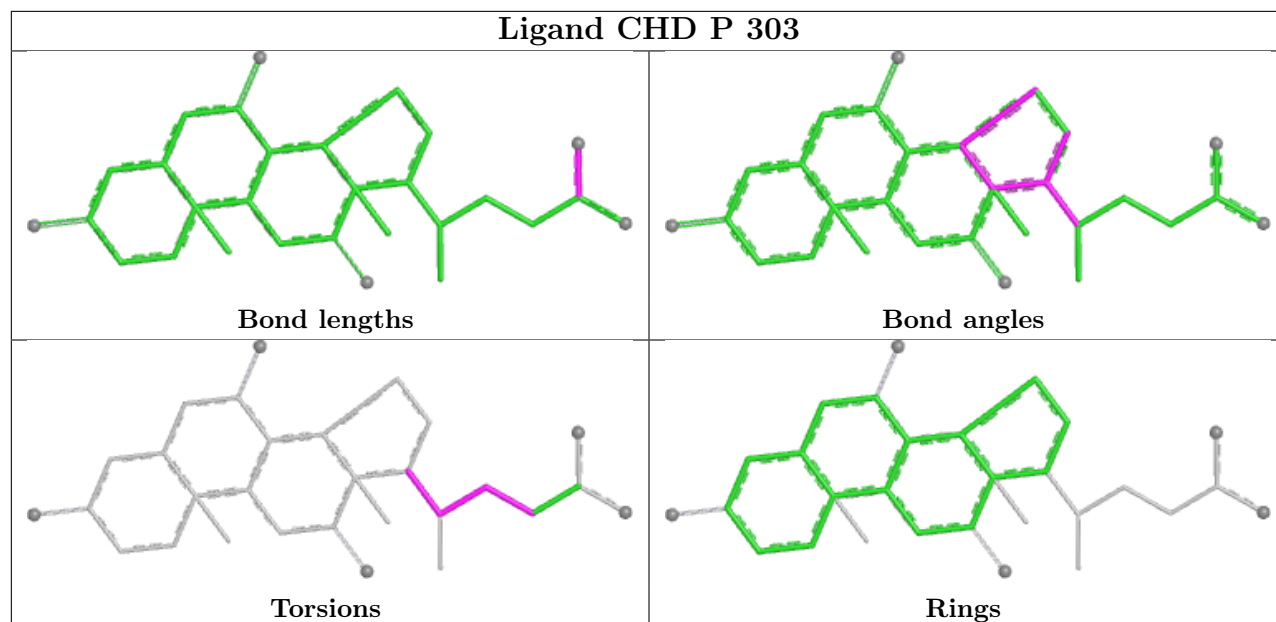




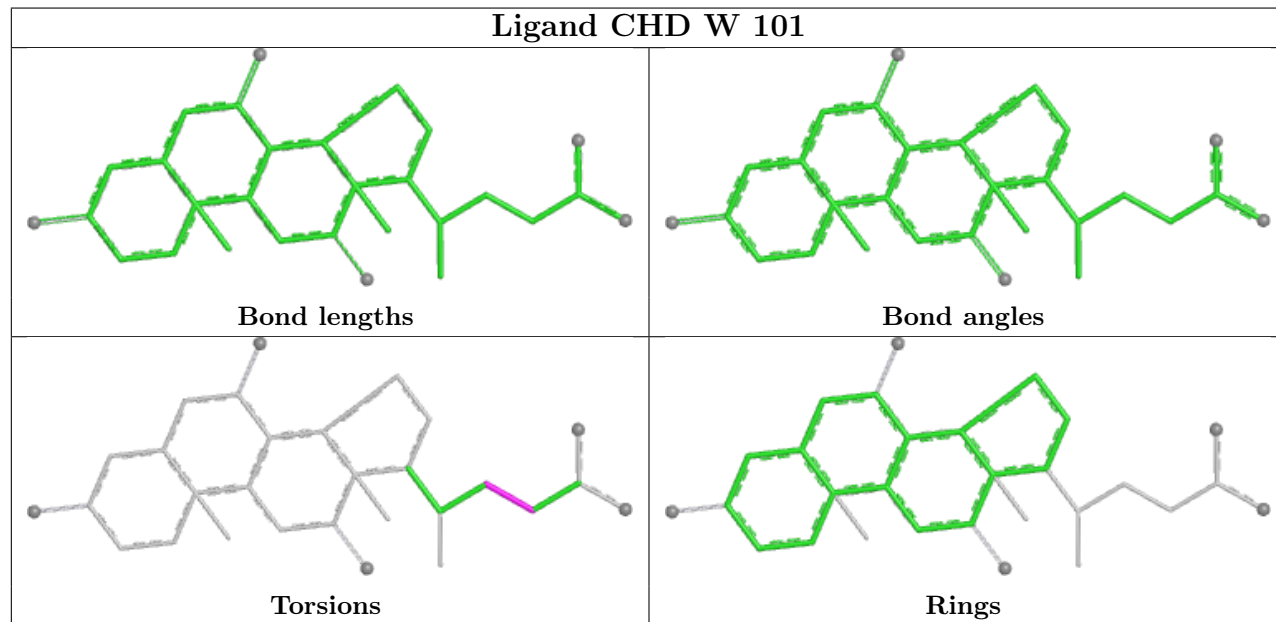


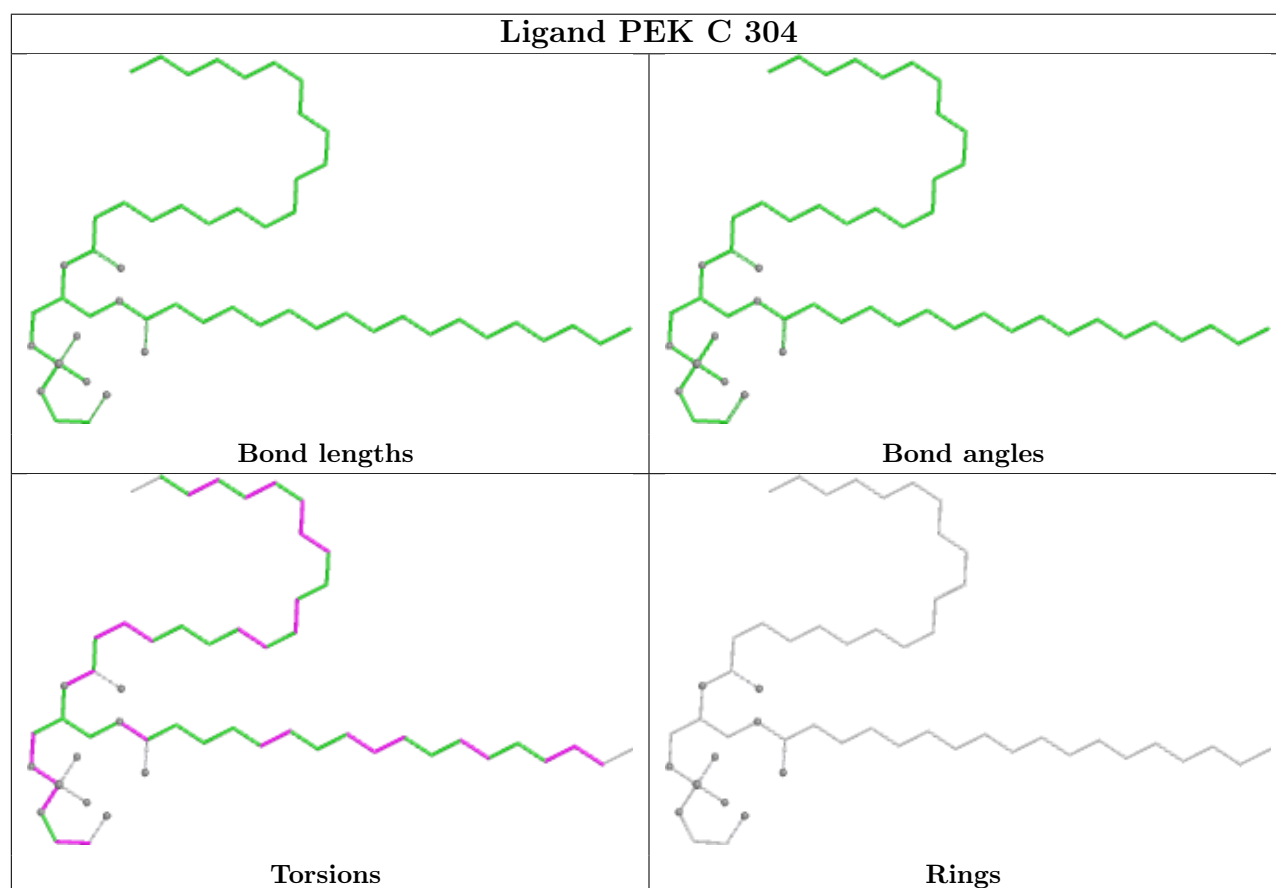
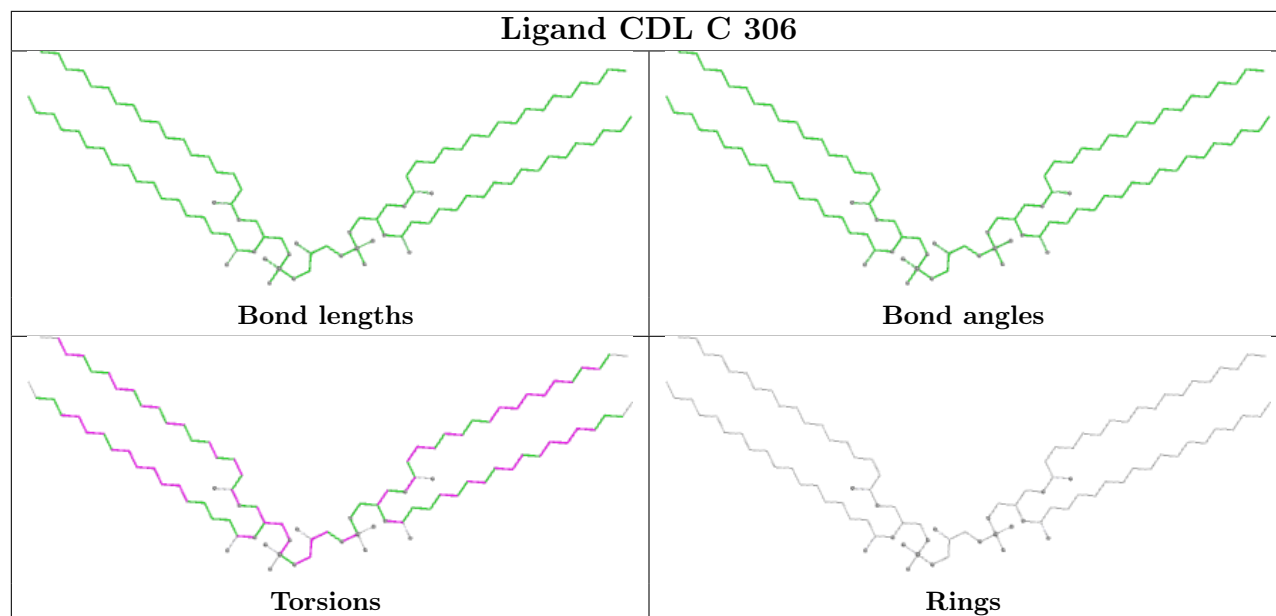


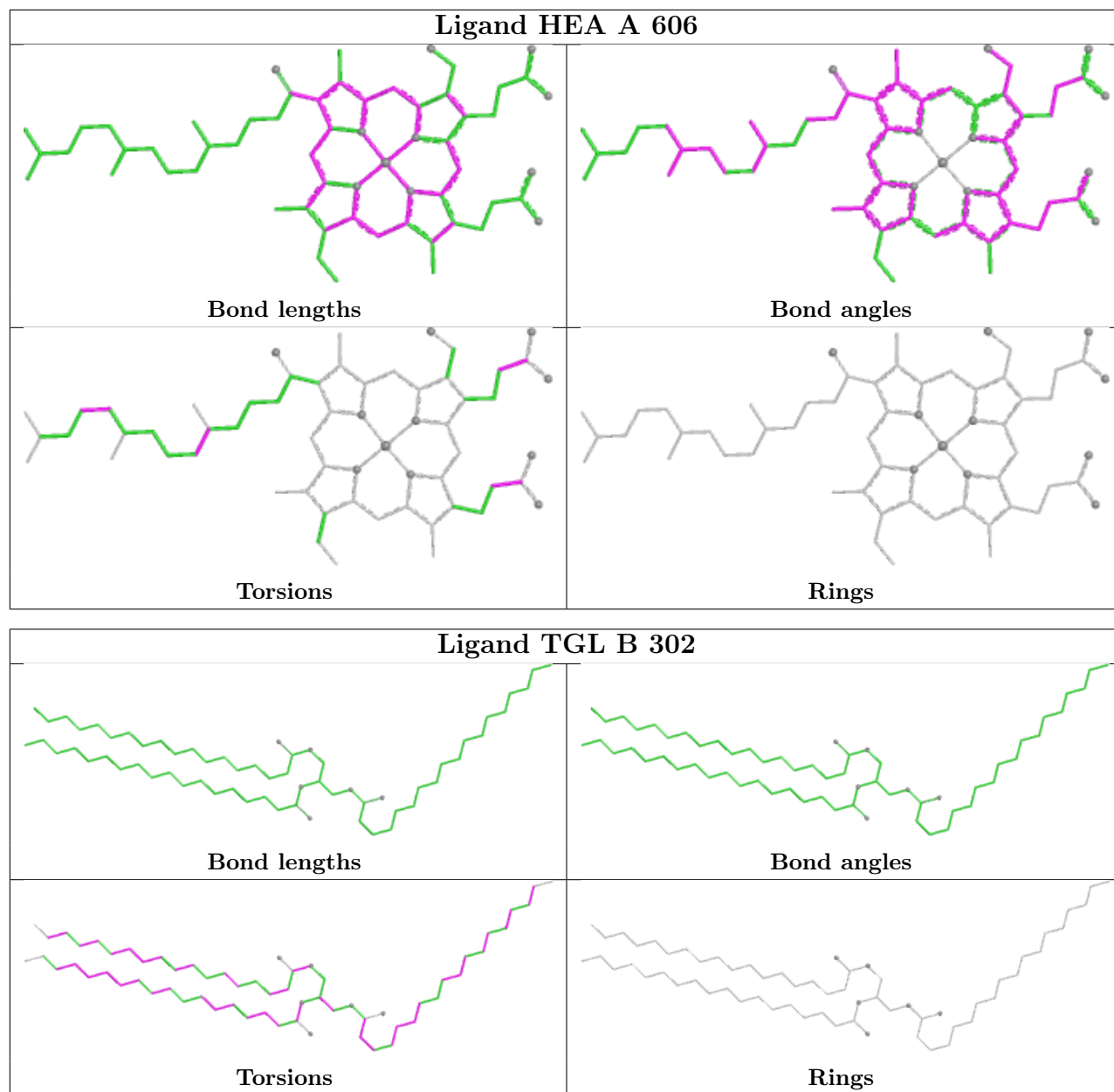
Ligand CHD P 303

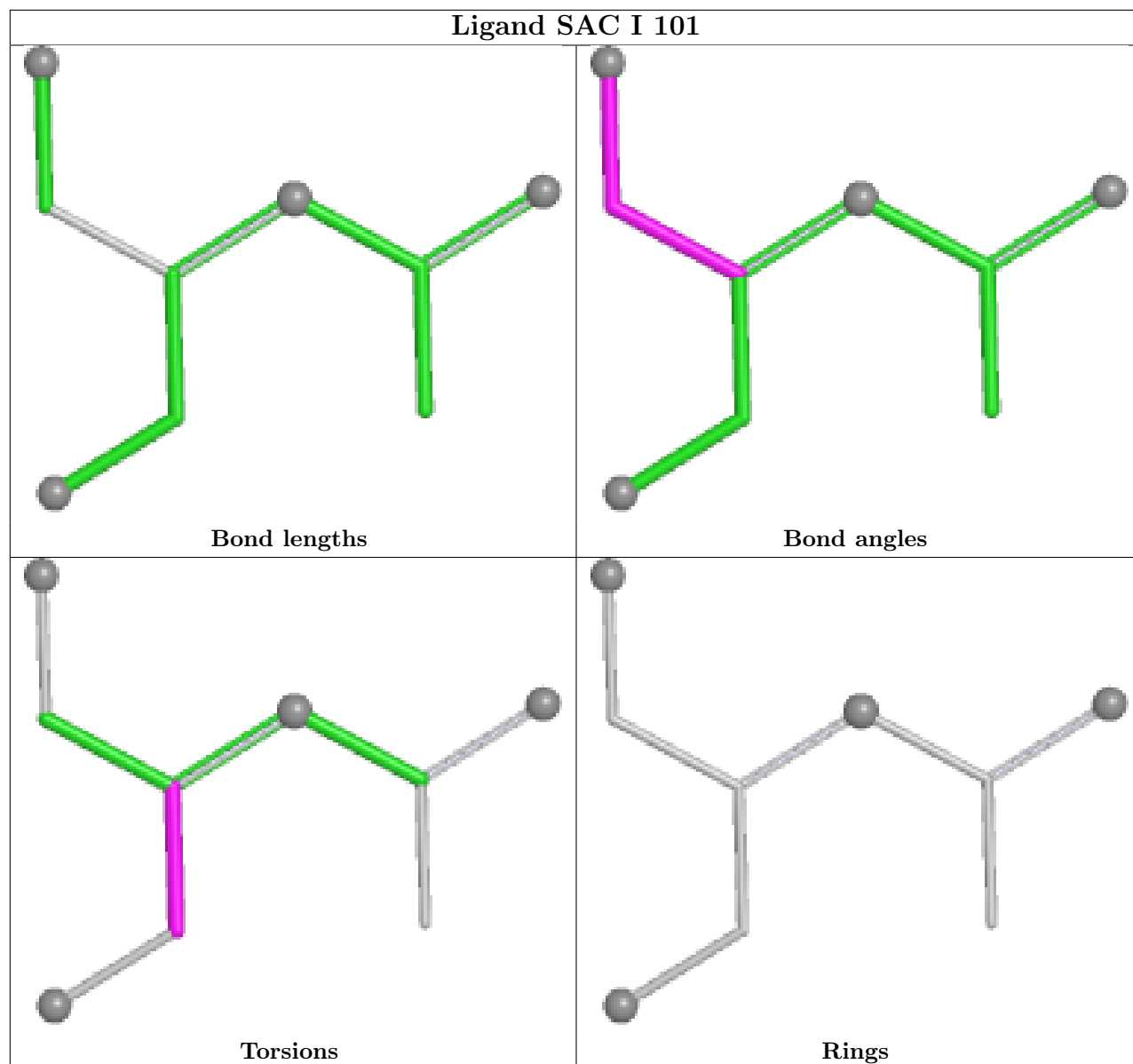


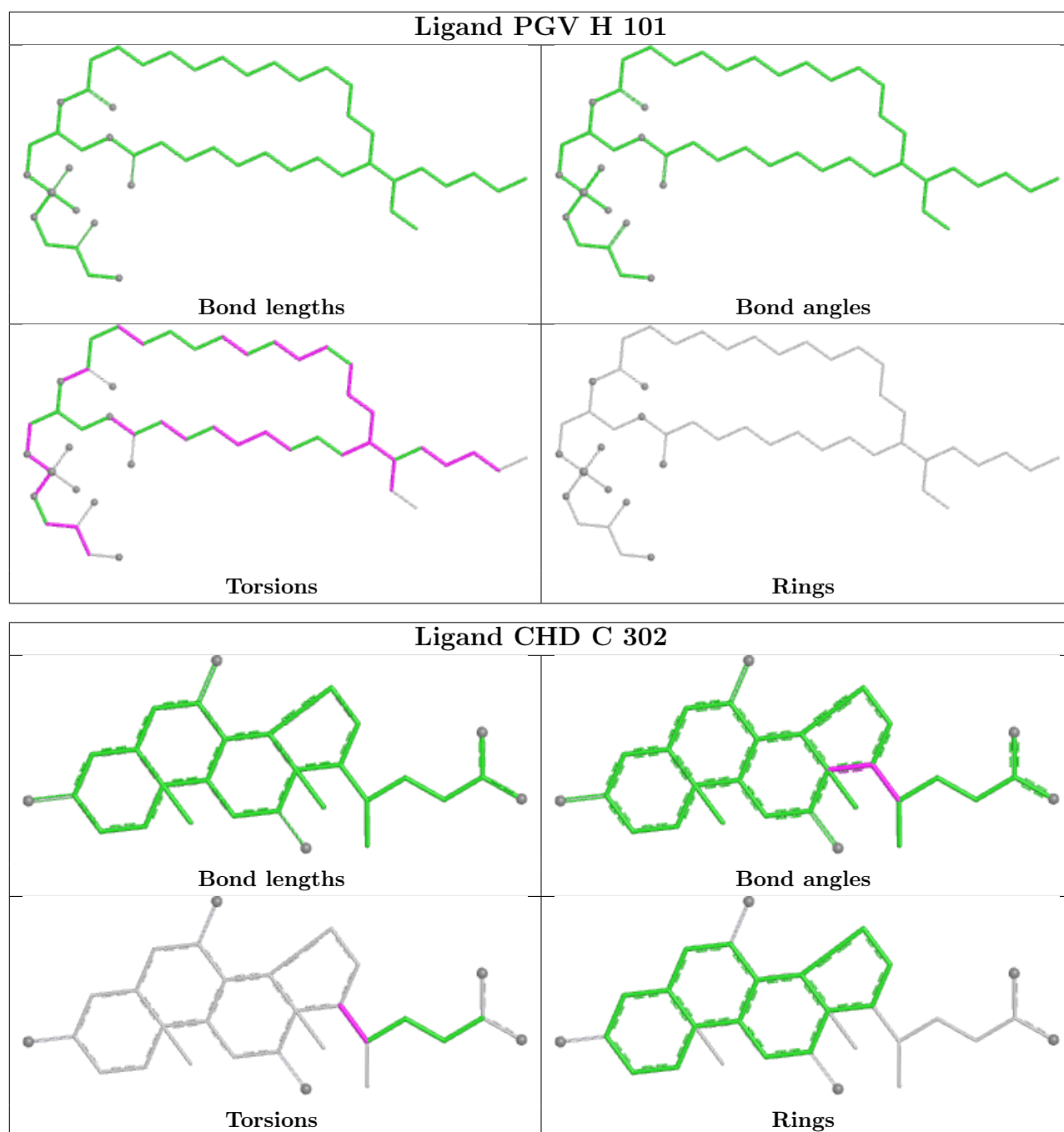
Ligand CHD W 101

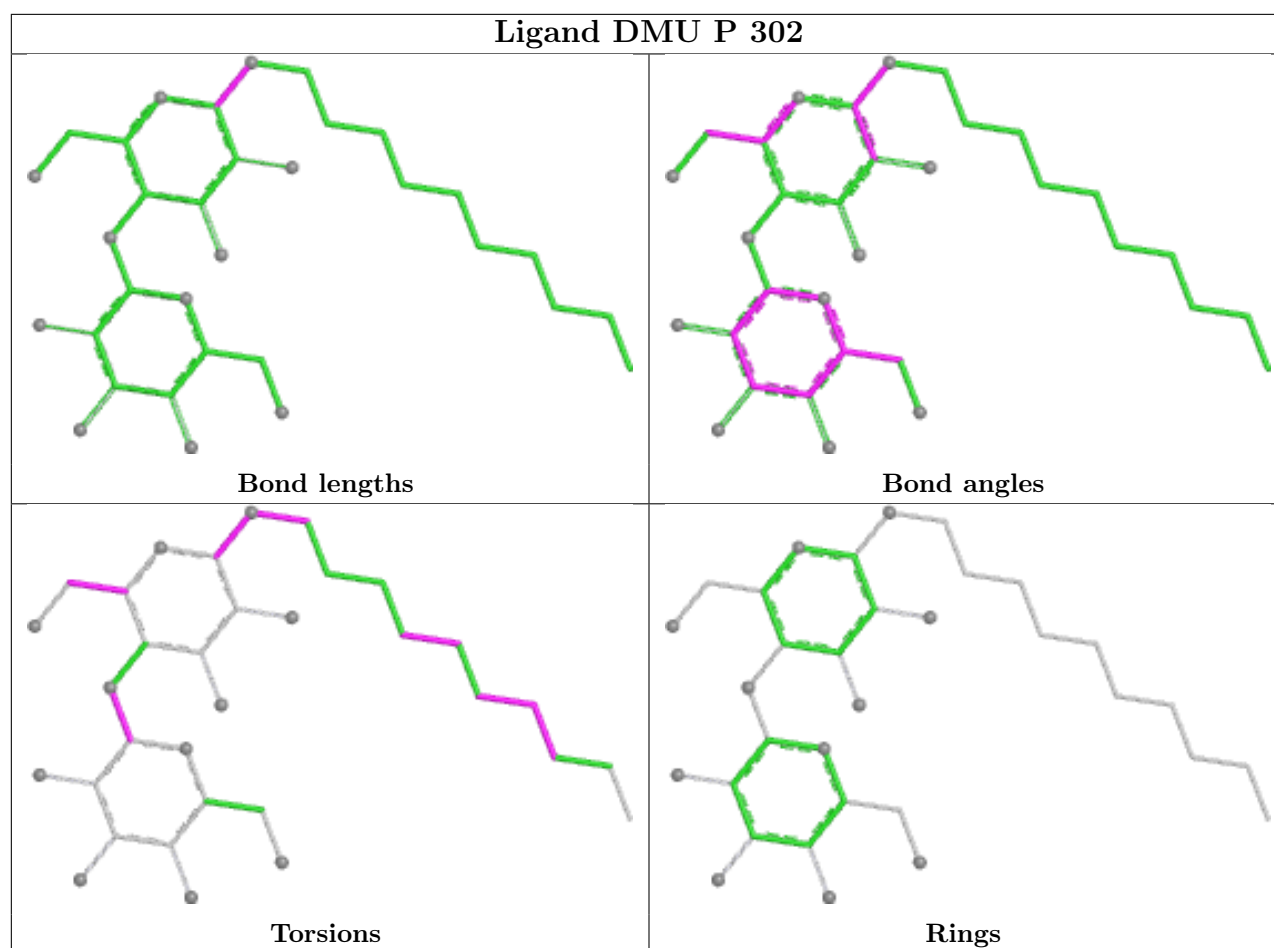


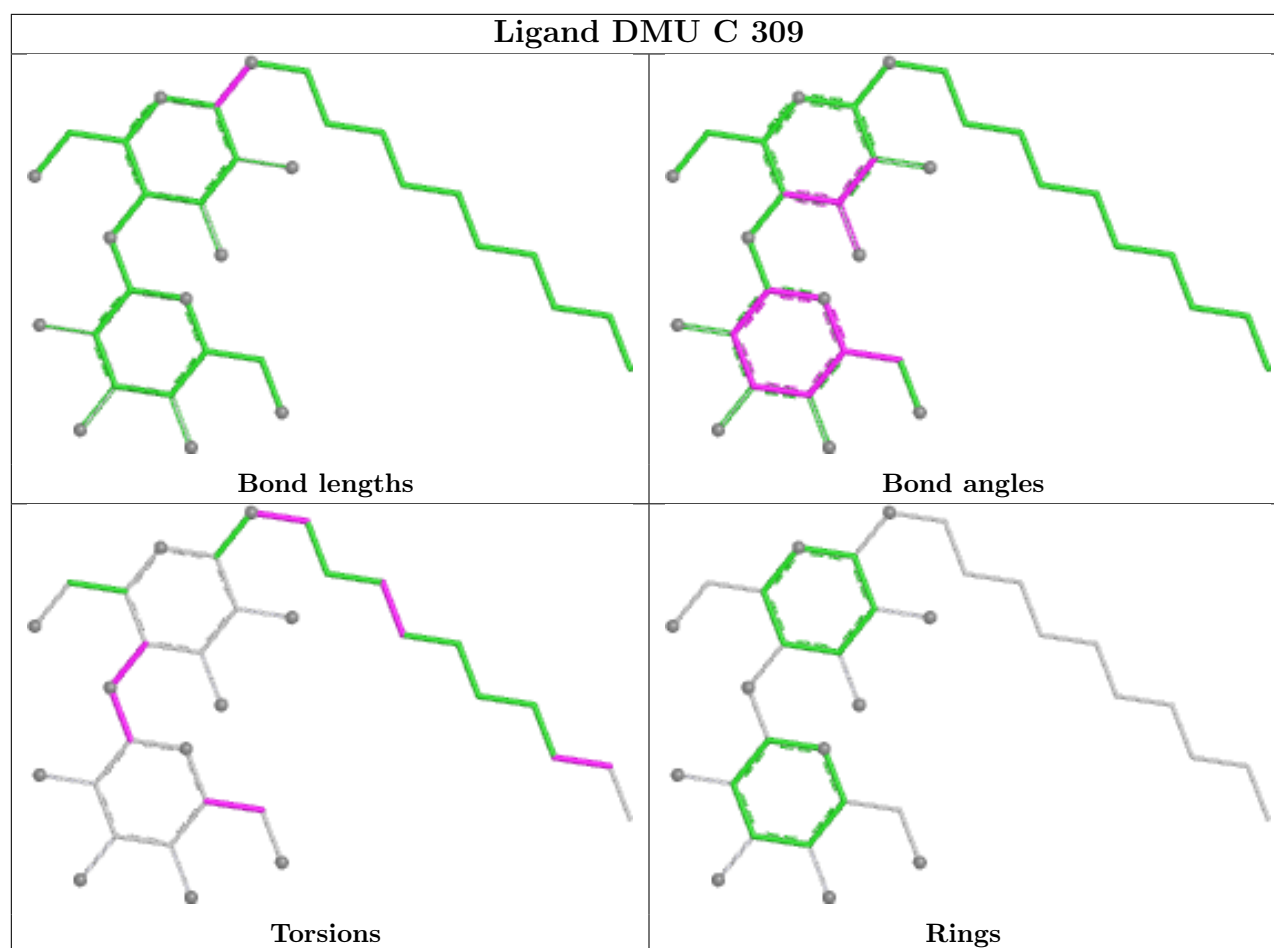




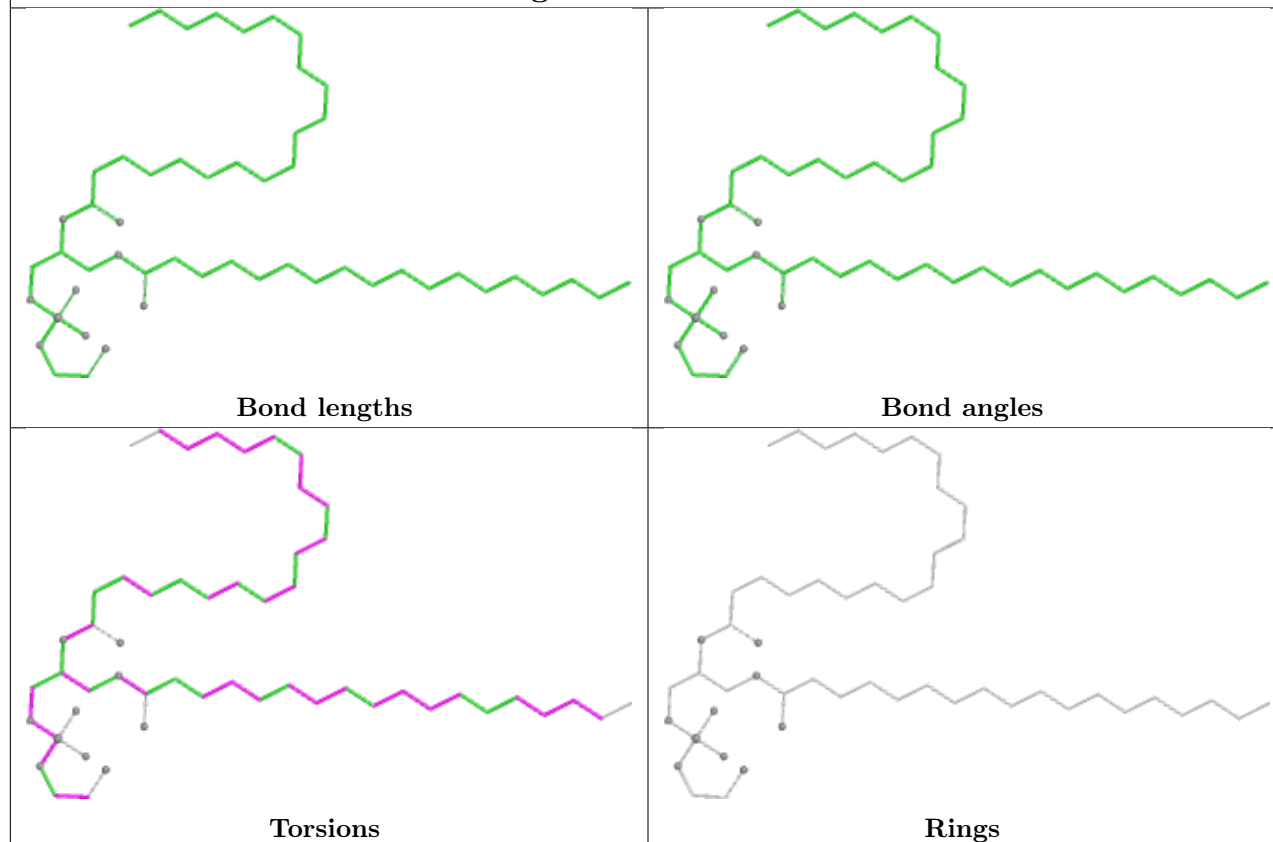




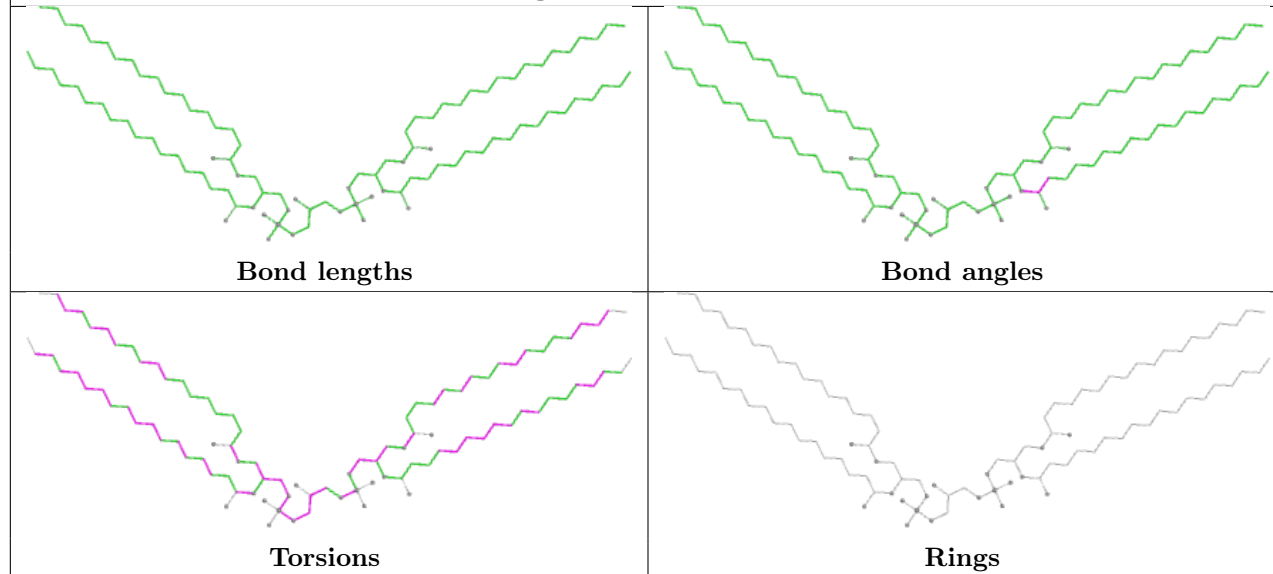


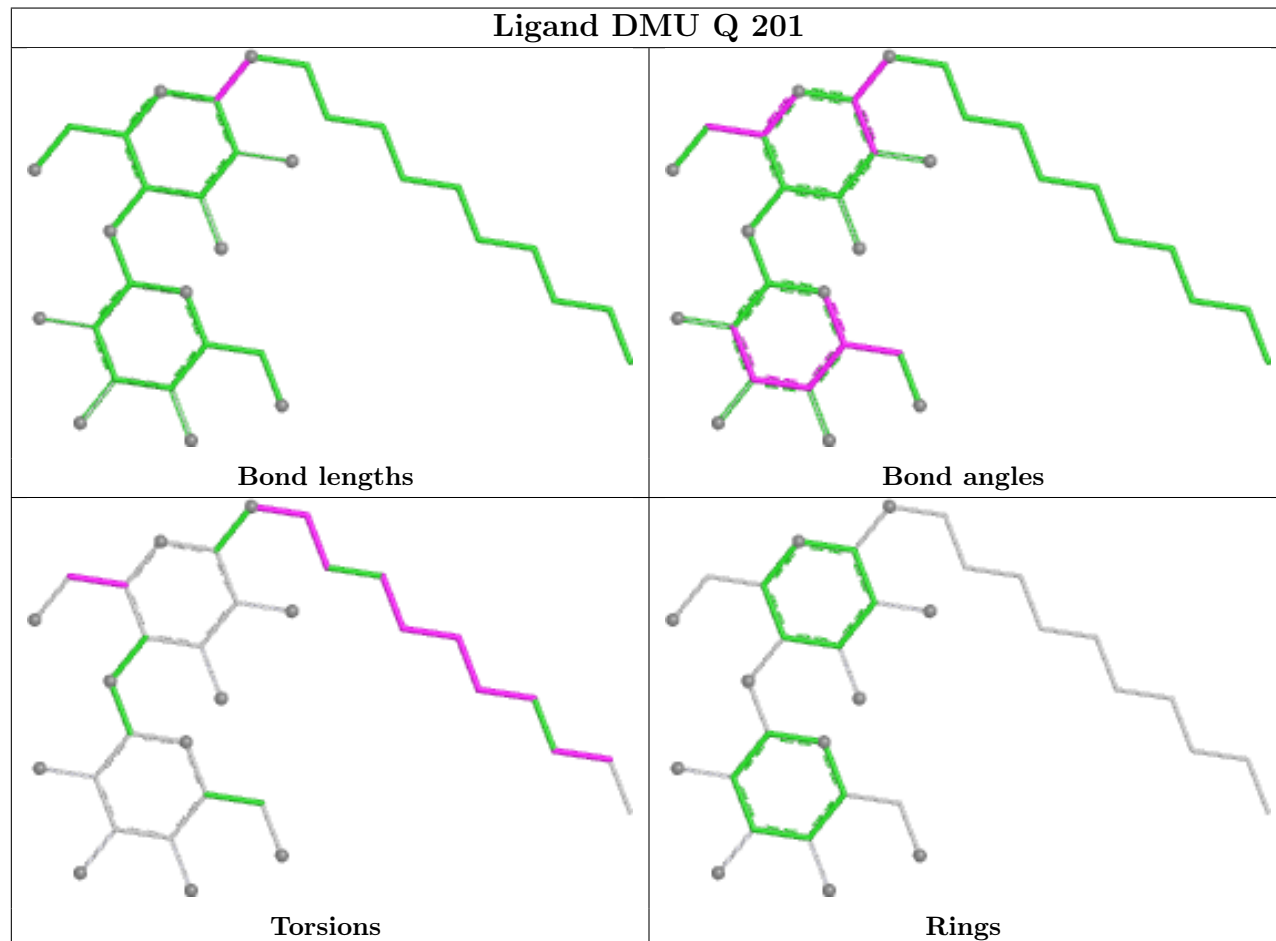
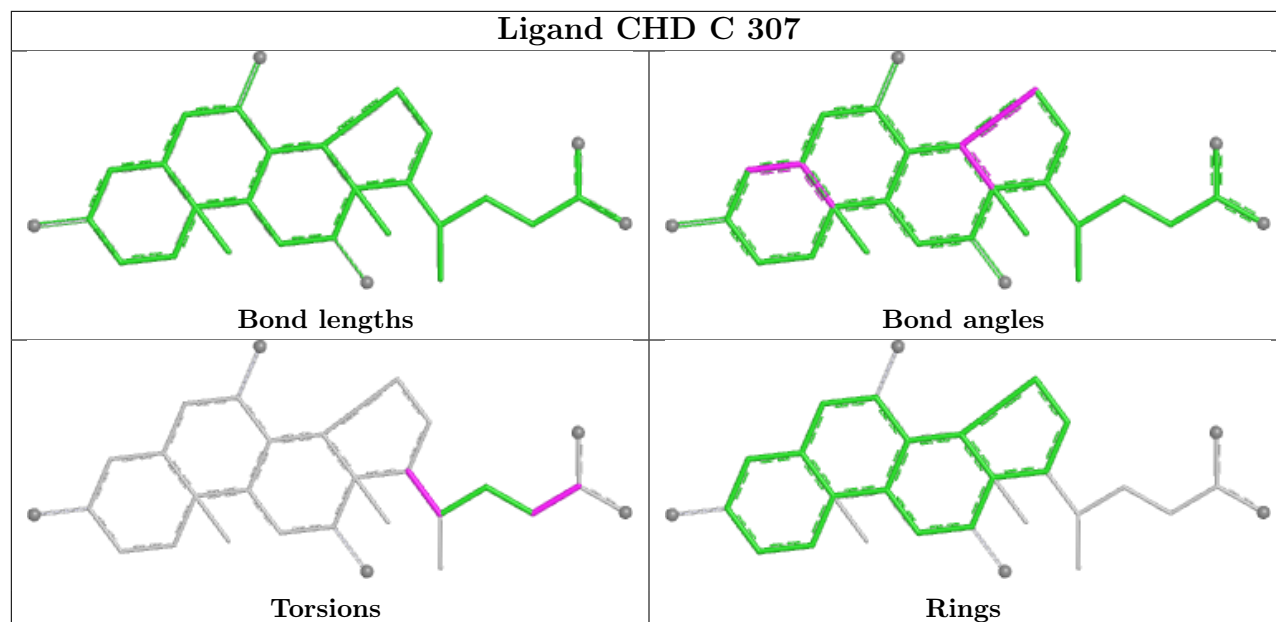


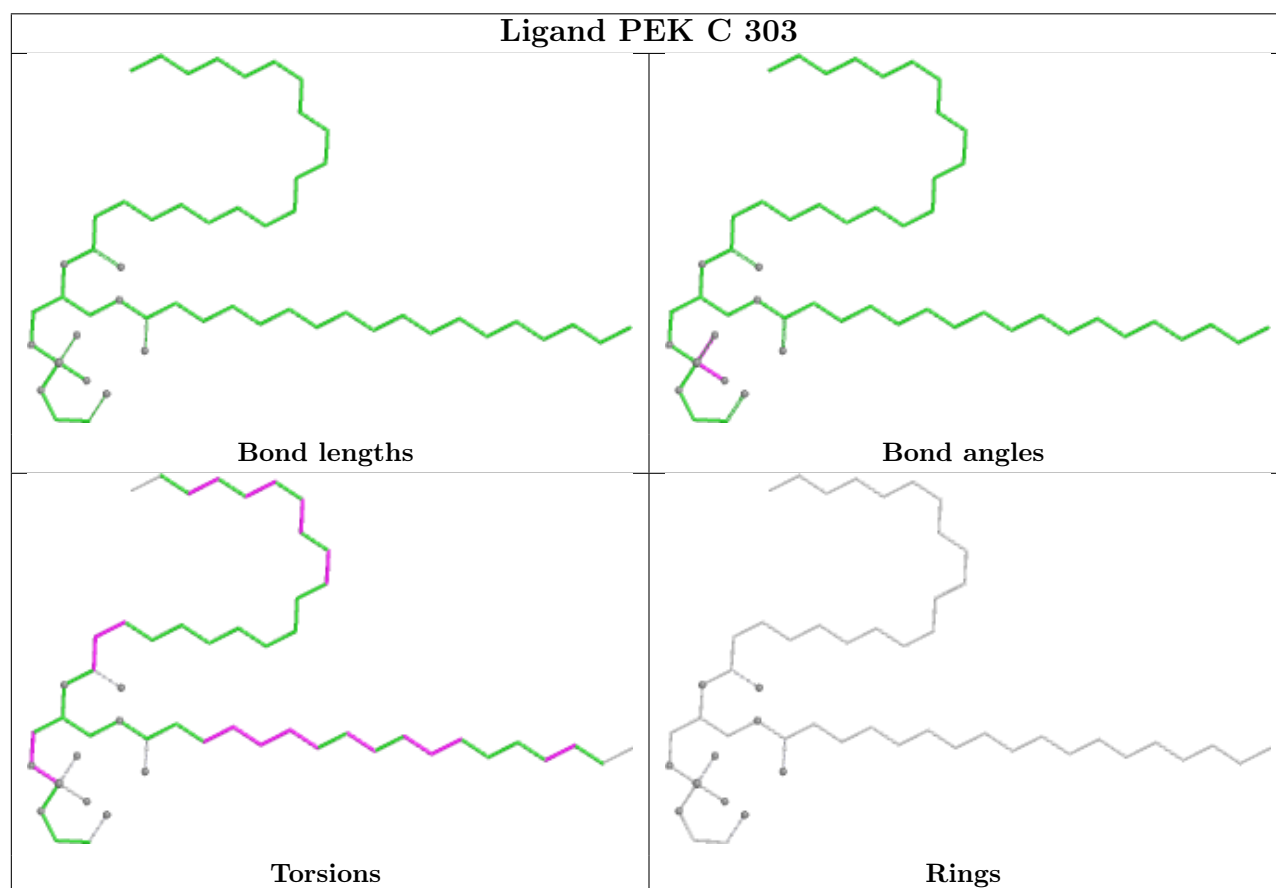
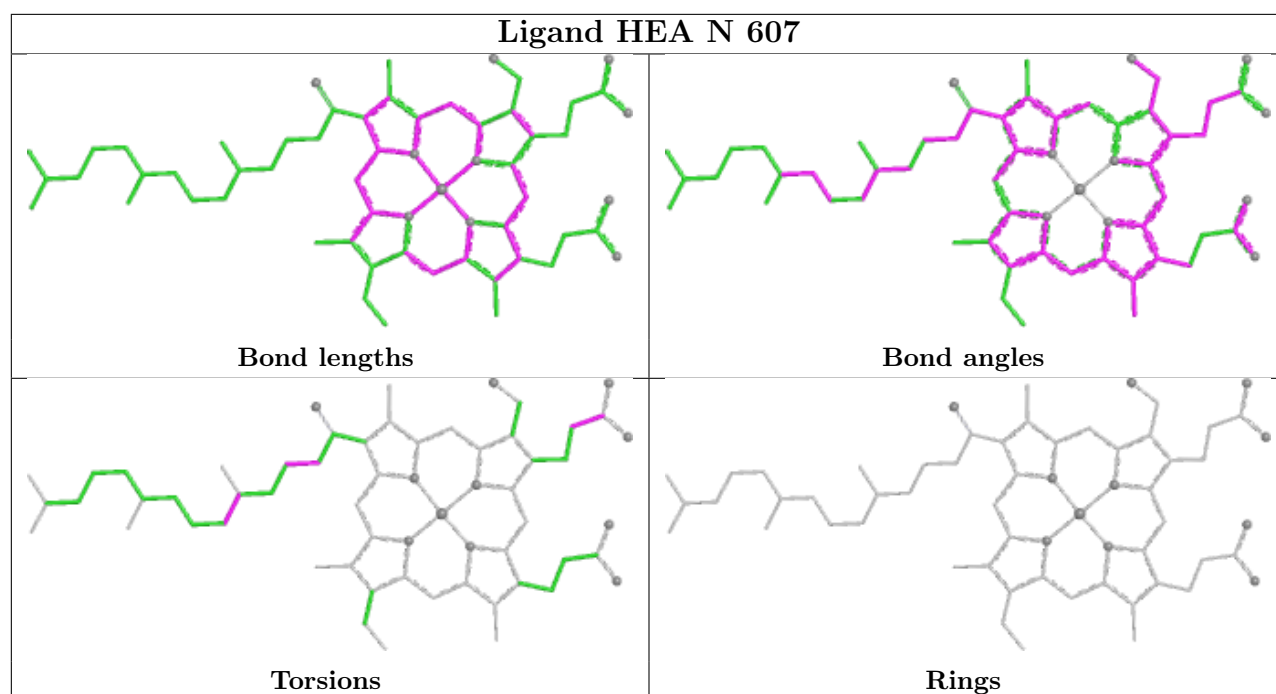
Ligand PEK P 301

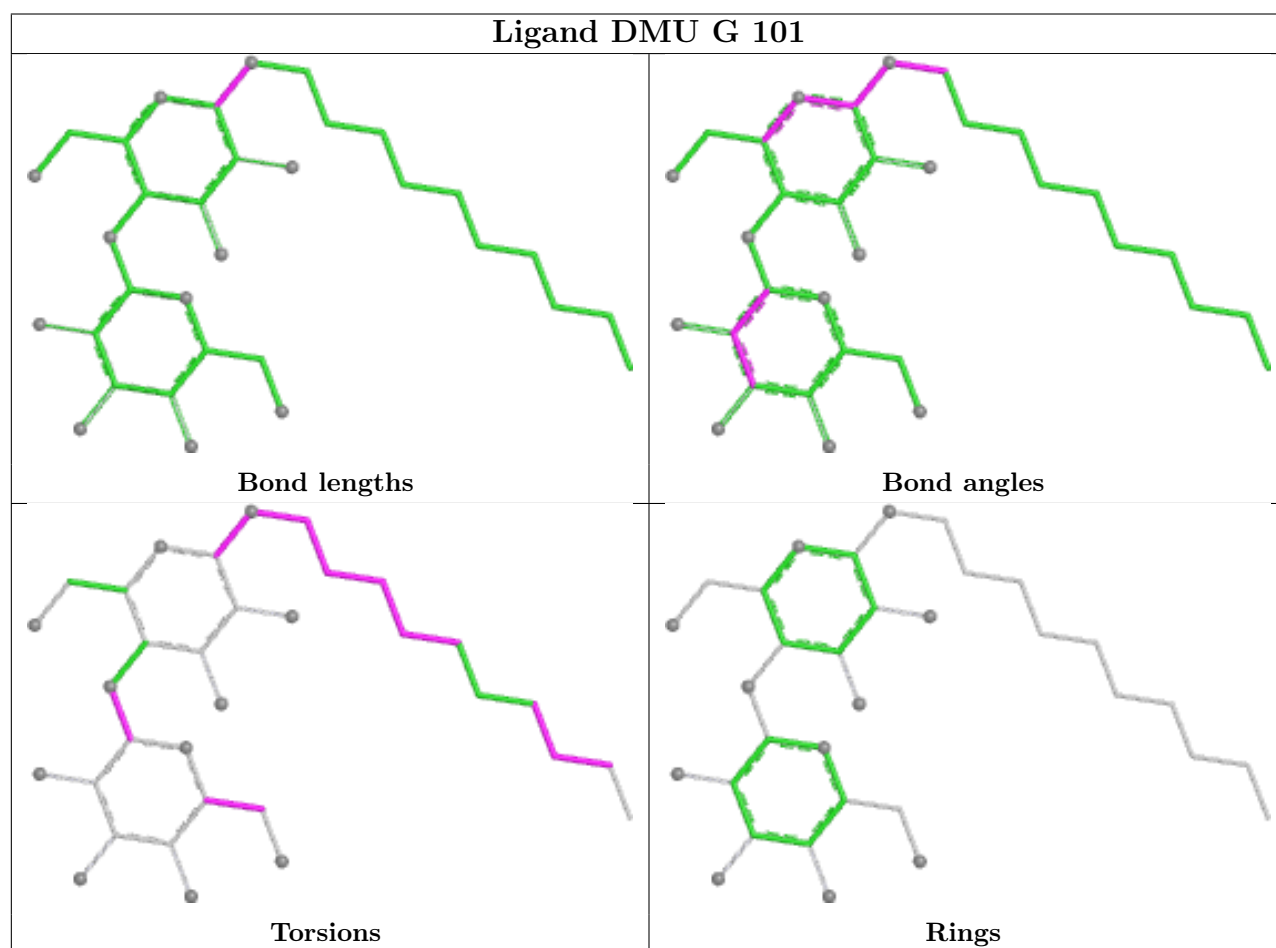
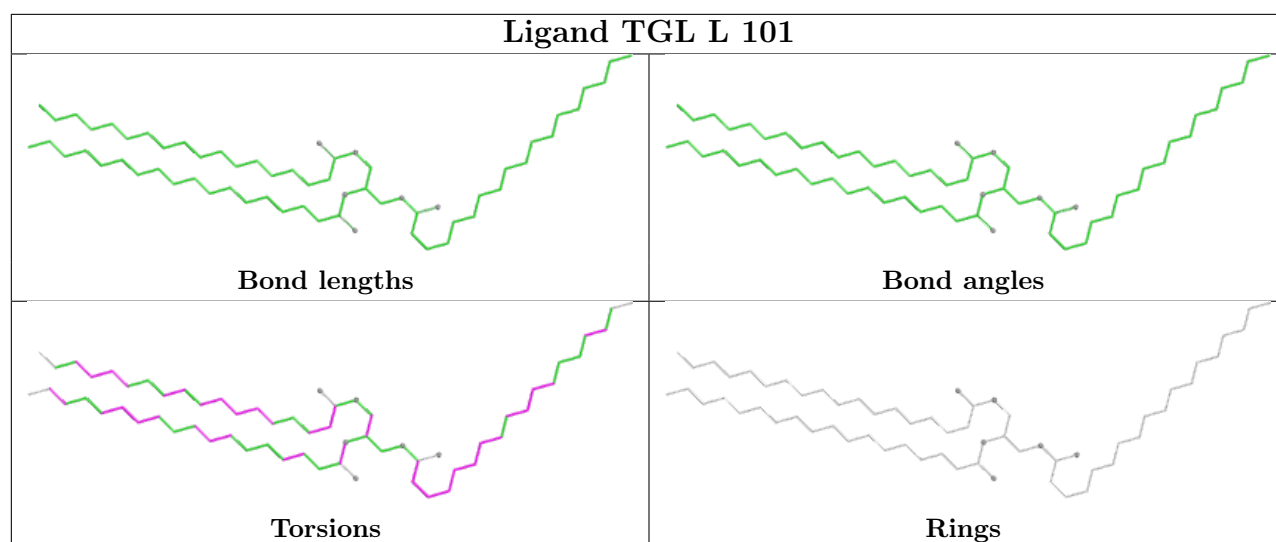


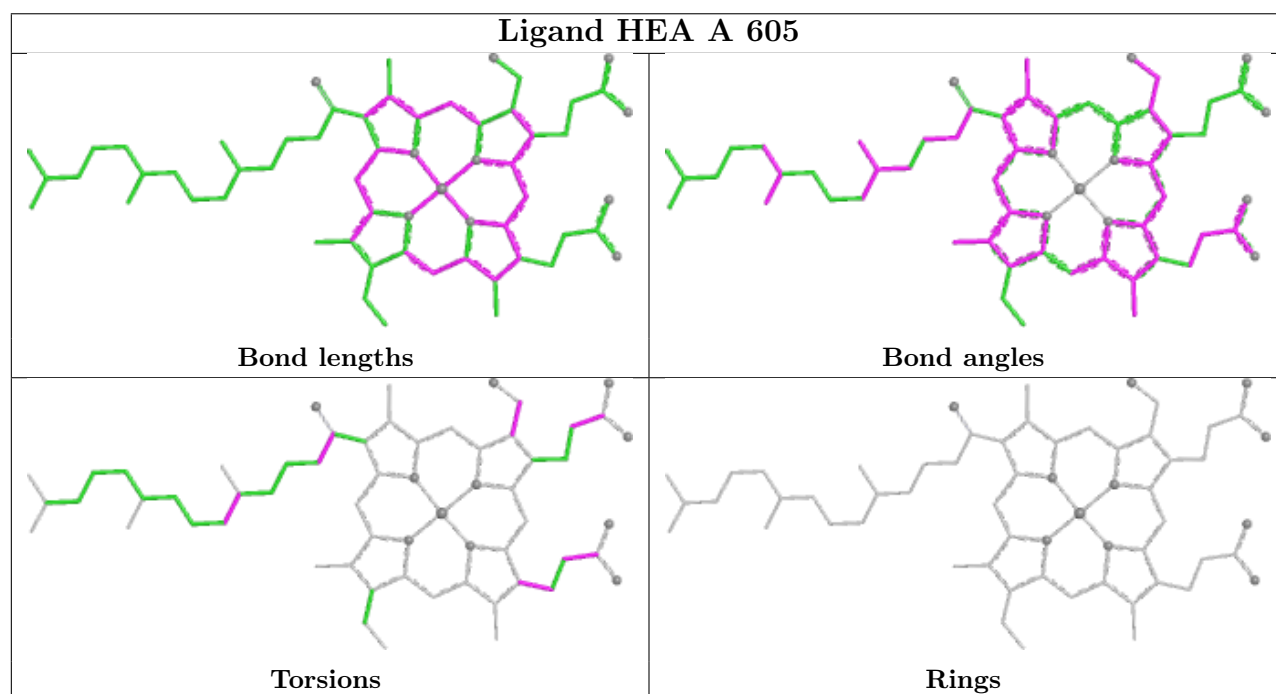
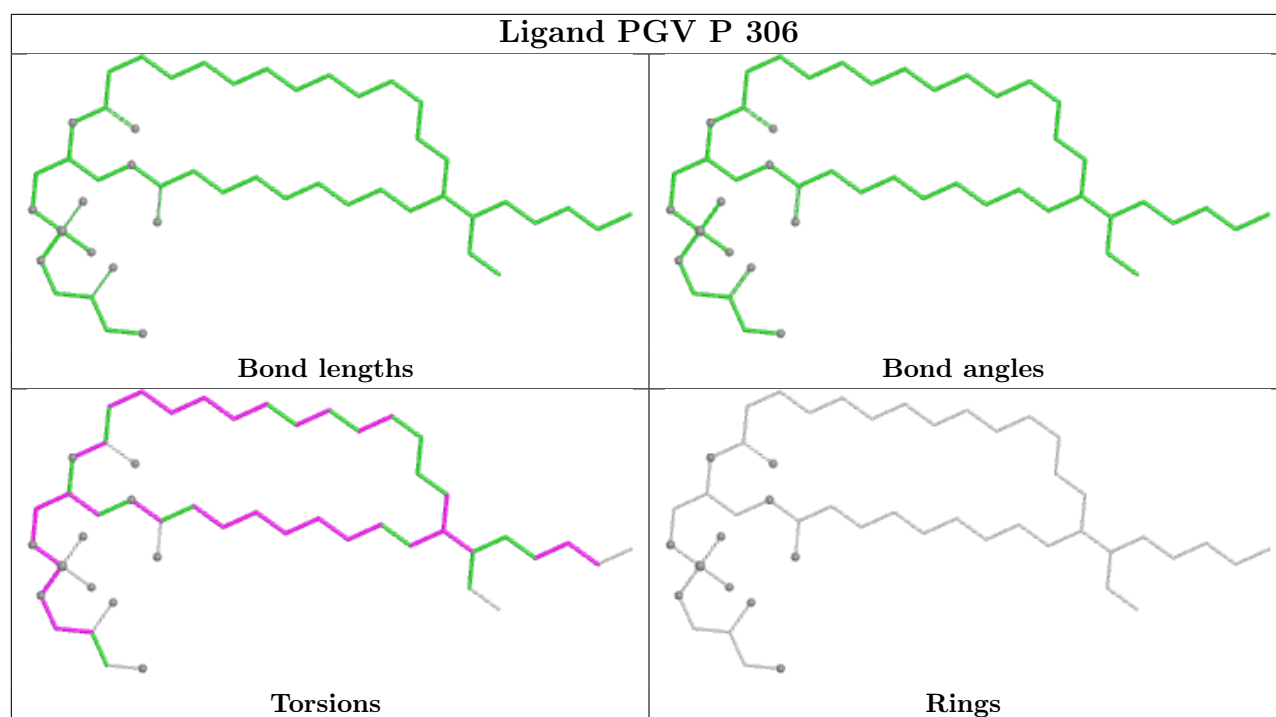
Ligand CDL P 307



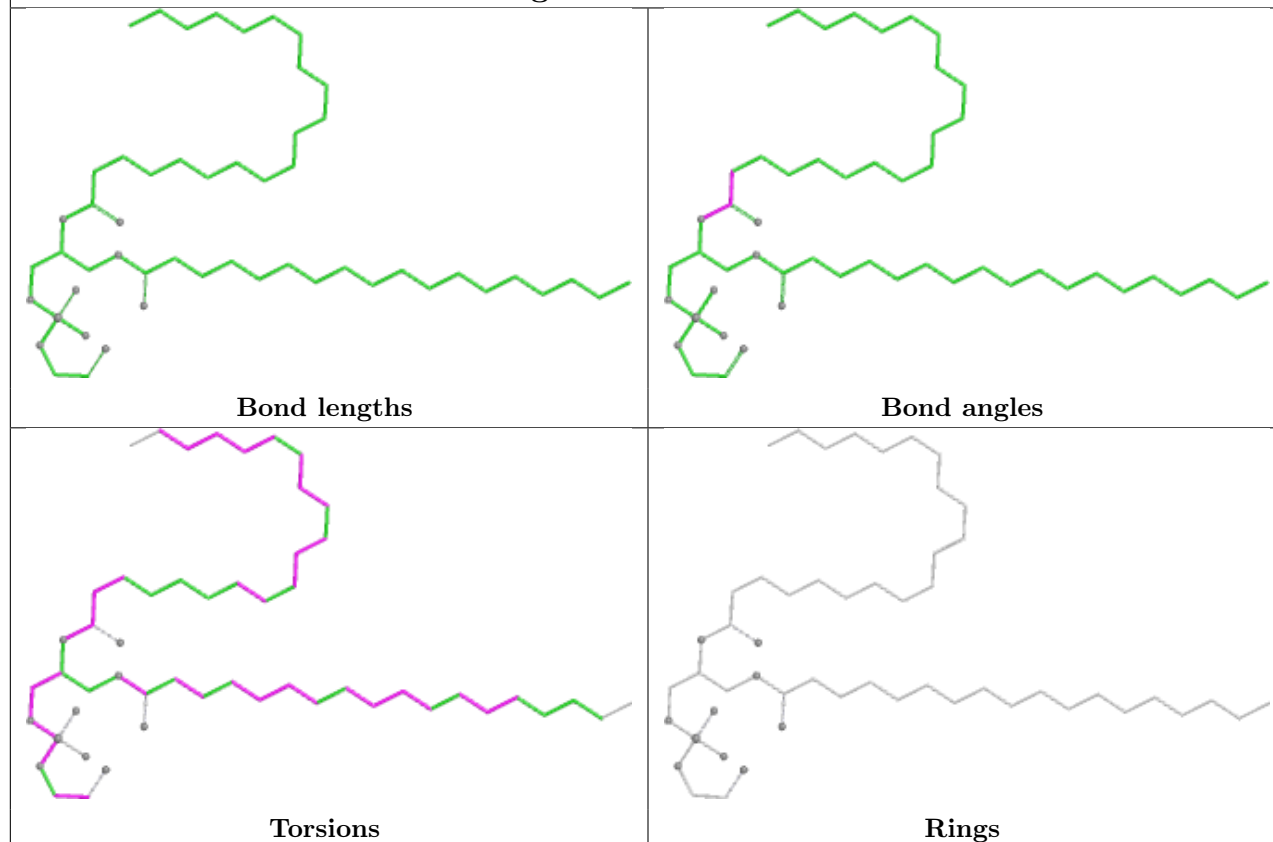




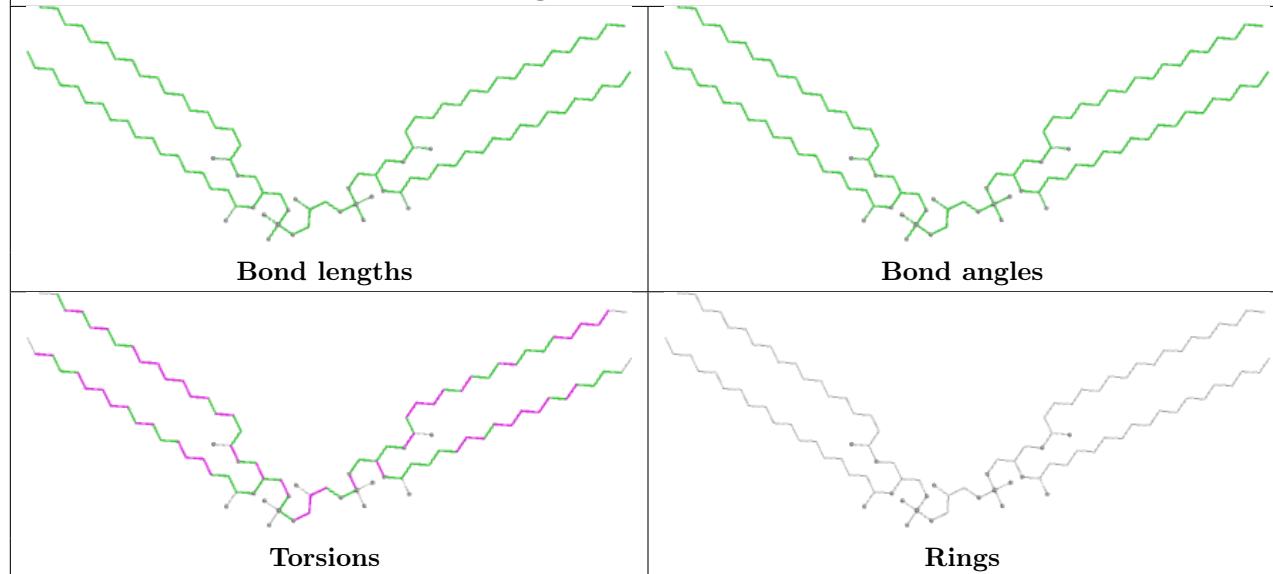


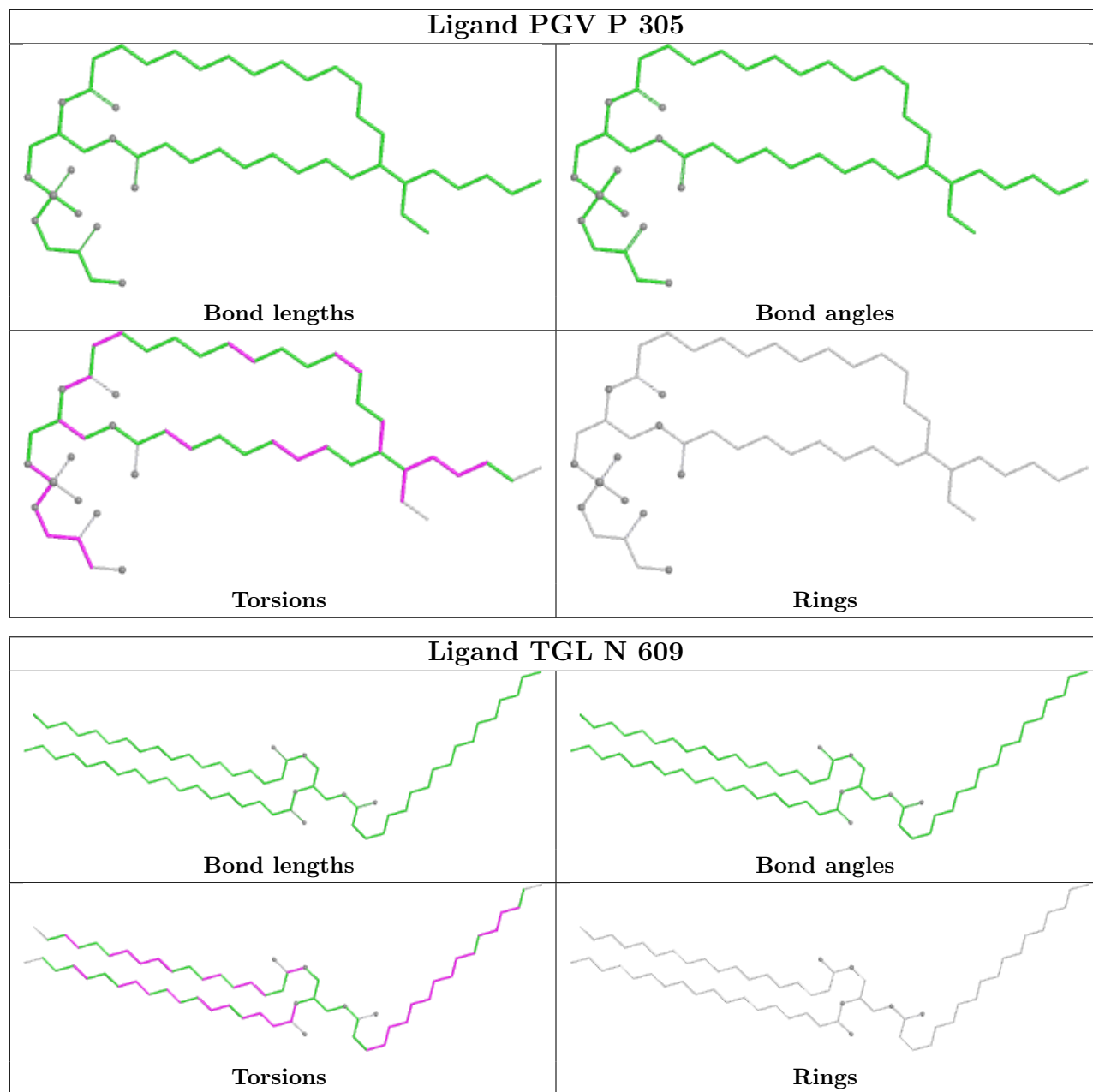


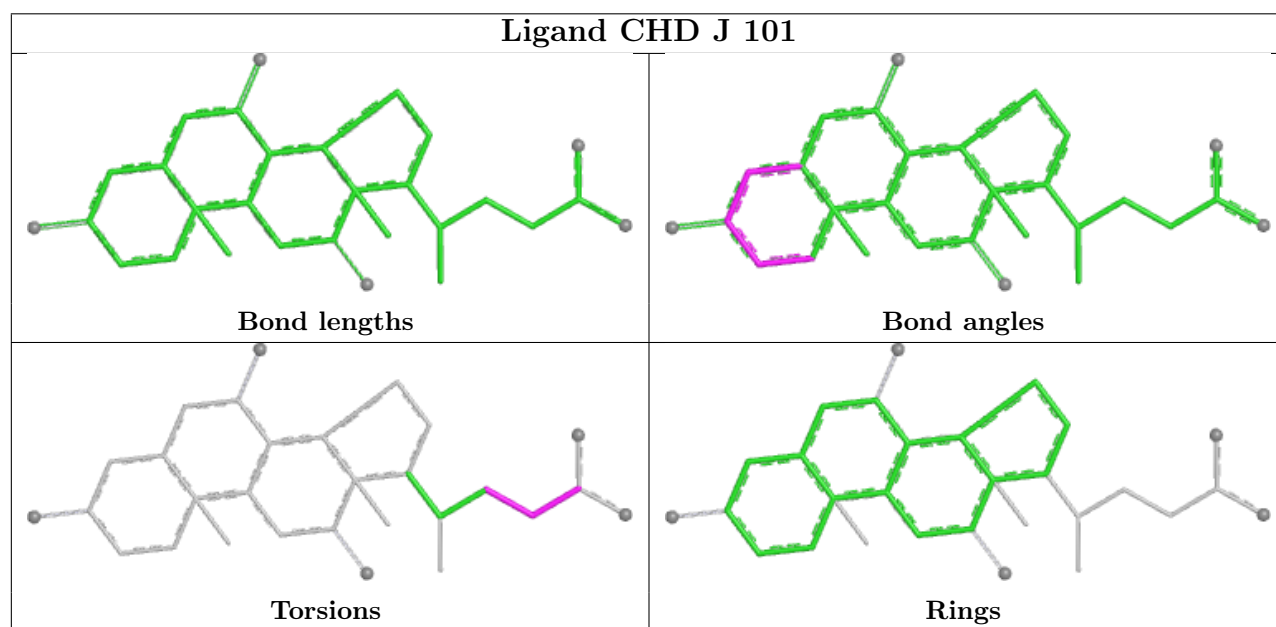
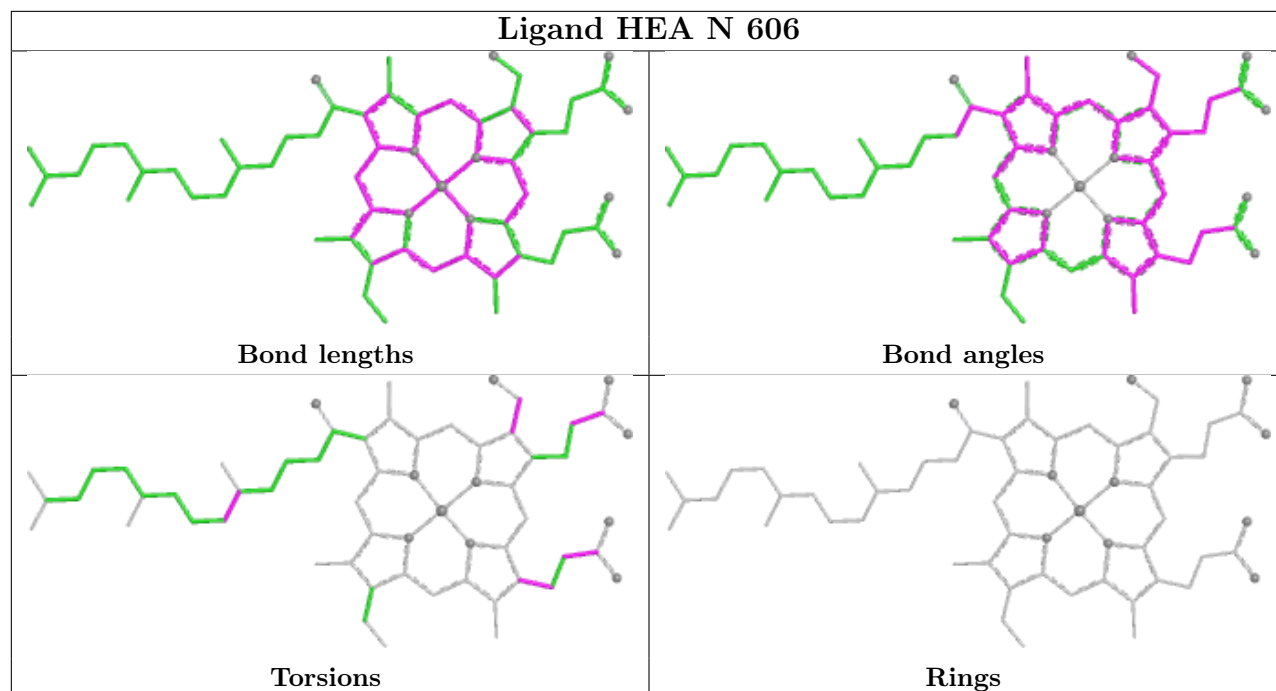
Ligand PEK T 102

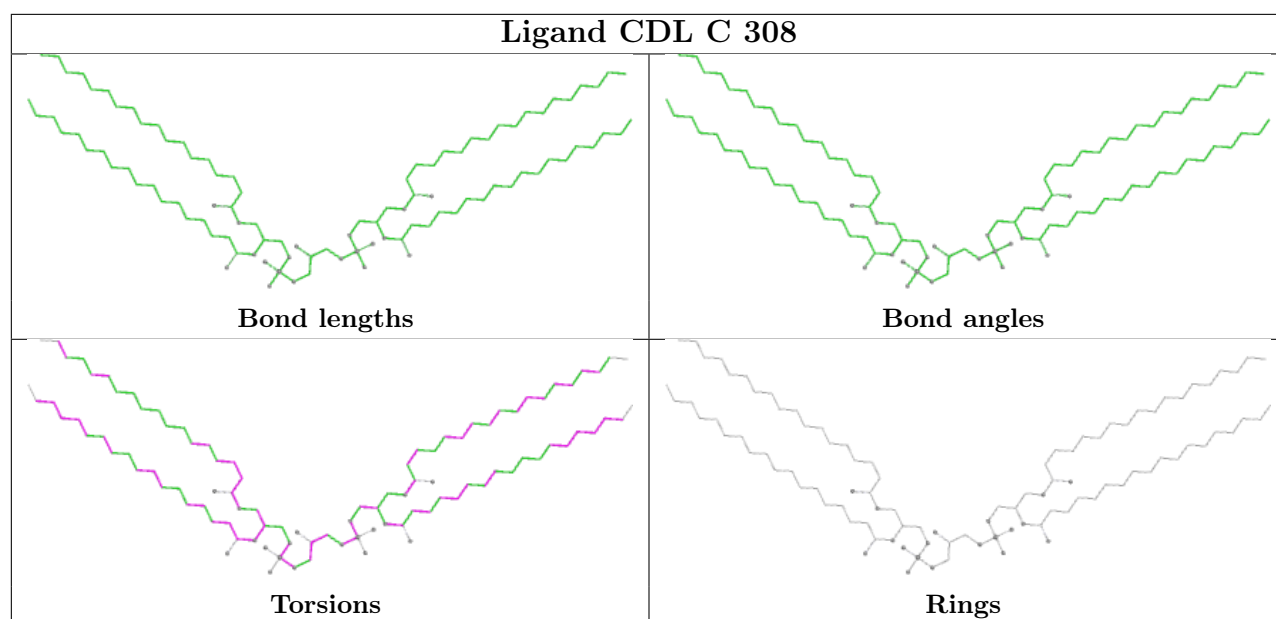


Ligand CDL P 309









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%)	-0.25	1 (0%) 91 90	5, 15, 24, 48	0
1	N	513/514 (99%)	0.33	20 (3%) 43 43	12, 27, 44, 62	0
2	B	226/227 (99%)	0.05	6 (2%) 56 56	8, 20, 45, 91	0
2	O	226/227 (99%)	0.90	26 (11%) 9 8	19, 39, 65, 116	0
3	C	259/261 (99%)	-0.00	2 (0%) 82 82	10, 20, 33, 50	0
3	P	259/261 (99%)	0.40	11 (4%) 40 40	13, 28, 49, 78	0
4	D	144/147 (97%)	0.11	5 (3%) 47 47	12, 27, 47, 59	0
4	Q	144/147 (97%)	1.35	29 (20%) 3 2	24, 52, 76, 185	0
5	E	105/109 (96%)	0.03	4 (3%) 44 44	15, 26, 53, 83	0
5	R	105/109 (96%)	0.52	3 (2%) 53 53	23, 40, 58, 85	0
6	F	98/98 (100%)	0.46	7 (7%) 22 20	13, 27, 78, 119	0
6	S	98/98 (100%)	1.08	13 (13%) 7 6	21, 37, 103, 151	0
7	G	83/85 (97%)	1.14	16 (19%) 3 3	15, 33, 100, 116	0
7	T	83/85 (97%)	1.40	18 (21%) 2 2	14, 43, 92, 121	0
8	H	79/85 (92%)	0.47	6 (7%) 20 18	14, 28, 73, 83	0
8	U	79/85 (92%)	1.17	14 (17%) 4 3	29, 45, 87, 128	0
9	I	72/73 (98%)	0.56	6 (8%) 17 16	18, 36, 63, 76	0
9	V	72/73 (98%)	1.10	9 (12%) 8 7	30, 51, 72, 76	0
10	J	58/59 (98%)	0.34	3 (5%) 33 32	13, 31, 64, 92	0
10	W	58/59 (98%)	1.21	12 (20%) 2 2	32, 47, 89, 127	0
11	K	49/56 (87%)	0.19	1 (2%) 65 63	15, 28, 43, 47	0
11	X	49/56 (87%)	1.23	9 (18%) 3 3	34, 46, 69, 83	0
12	L	46/47 (97%)	0.02	1 (2%) 62 61	12, 20, 35, 77	0
12	Y	46/47 (97%)	1.02	4 (8%) 16 15	25, 41, 64, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/47 (91%)	0.28	5 (11%) 9 8	14, 21, 74, 85	0
13	Z	43/47 (91%)	1.14	9 (20%) 2 2	29, 43, 73, 82	0
All	All	3550/3616 (98%)	0.42	240 (6%) 23 22	5, 28, 65, 185	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	14.0
4	Q	5	VAL	11.9
6	S	1	ALA	11.2
6	S	97	ALA	10.1
4	Q	7	LYS	8.8
8	U	8	ILE	8.7
7	T	7	ASP	8.5
6	F	96	LEU	8.5
2	O	90	ILE	7.7
7	T	5	LYS	7.5
7	G	1	ALA	7.3
6	S	98	HIS	6.8
7	G	9	GLY	6.6
6	S	96	LEU	6.3
10	W	58	LYS	6.2
7	T	9	GLY	6.2
7	G	3	ALA	6.1
7	G	2	SER	5.9
6	F	98	HIS	5.8
6	F	1	ALA	5.7
6	S	94	HIS	5.7
7	G	5	LYS	5.6
9	I	37	PHE	5.4
7	G	4	ALA	5.3
7	G	41	HIS	5.3
7	T	1	ALA	5.3
2	O	55	THR	5.1
7	T	41	HIS	5.1
8	U	7	LYS	5.1
7	T	10	GLY	4.9
2	O	227	LEU	4.9
7	G	40	GLY	4.9
11	X	6	ALA	4.7
6	S	3	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
7	T	8	HIS	4.7
4	Q	4	SER	4.7
9	V	69	PHE	4.6
9	I	33	THR	4.5
1	N	295	VAL	4.5
7	G	39	SER	4.5
10	W	56	PRO	4.4
7	T	40	GLY	4.4
7	T	36	TRP	4.4
2	B	61	VAL	4.4
1	N	296	GLY	4.3
2	B	60	GLU	4.2
9	V	25	PHE	4.1
10	W	52	TRP	4.1
1	N	120	ALA	4.1
7	G	36	TRP	4.0
10	W	57	HIS	4.0
6	S	95	GLN	4.0
6	S	93	PRO	3.9
8	U	45	ALA	3.9
7	T	6	GLY	3.9
8	U	9	LYS	3.9
13	Z	43	SER	3.8
7	T	37	LEU	3.8
3	P	3	HIS	3.8
13	M	43	SER	3.8
9	V	37	PHE	3.8
9	V	33	THR	3.7
7	T	3	ALA	3.7
4	Q	136	ALA	3.7
6	F	97	ALA	3.7
7	T	84	LYS	3.7
6	S	2	SER	3.7
7	G	10	GLY	3.7
7	T	39	SER	3.7
12	Y	20	ARG	3.6
7	G	7	ASP	3.6
8	H	44	THR	3.6
10	W	48	TYR	3.6
7	T	42	ARG	3.6
2	O	177	GLY	3.6
9	I	31	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
8	H	51	SER	3.4
13	Z	35	TYR	3.3
7	G	6	GLY	3.3
1	N	47	LEU	3.3
11	X	12	LYS	3.3
2	B	90	ILE	3.3
4	Q	134	PHE	3.3
9	V	32	ALA	3.2
11	X	37	GLY	3.2
1	N	472	ILE	3.2
3	P	37	PHE	3.2
8	U	47	GLY	3.2
9	I	62	GLU	3.2
10	J	58	LYS	3.2
6	S	38	ALA	3.1
5	R	61	PHE	3.1
2	O	213	LEU	3.1
8	H	45	ALA	3.1
13	Z	40	TYR	3.1
2	O	61	VAL	3.0
4	D	78	TRP	3.0
6	F	95	GLN	3.0
7	T	2	SER	3.0
3	P	47	LEU	2.9
2	O	225	SER	2.9
1	N	141	ALA	2.9
4	Q	111	PHE	2.9
9	I	25	PHE	2.9
3	P	62	ILE	2.9
5	E	9	GLU	2.9
2	O	113	TYR	2.9
12	L	47	LYS	2.9
8	U	27	ARG	2.8
10	W	30	ILE	2.8
13	M	39	ASN	2.8
2	O	93	PRO	2.8
9	I	32	ALA	2.8
10	W	55	PHE	2.8
4	Q	48	TRP	2.8
8	U	48	GLY	2.8
5	E	5	HIS	2.7
3	P	111	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	O	128	LEU	2.7
10	W	1	PHE	2.7
1	A	298	ASP	2.7
2	O	139	ASP	2.7
6	S	52	ILE	2.7
4	Q	8	SER	2.7
2	O	226	MET	2.7
2	B	82	ARG	2.7
4	D	102	TYR	2.7
2	B	59	GLN	2.7
3	C	125	ASN	2.7
4	D	141	ASP	2.7
3	P	195	SER	2.7
4	Q	85	ALA	2.7
4	Q	140	TYR	2.7
8	H	46	LYS	2.7
4	Q	31	LYS	2.6
5	E	109	VAL	2.6
7	G	37	LEU	2.6
7	G	38	HIS	2.6
11	X	9	PHE	2.6
8	H	47	GLY	2.6
2	O	57	ASP	2.6
12	Y	2	HIS	2.6
4	Q	59	LEU	2.6
10	W	50	LEU	2.6
11	X	54	ARG	2.6
13	Z	32	TRP	2.6
10	J	1	PHE	2.6
4	Q	41	LYS	2.6
6	F	94	HIS	2.5
2	O	218	TYR	2.5
3	P	114	GLY	2.5
9	V	30	GLY	2.5
2	O	138	VAL	2.5
11	X	45	VAL	2.5
12	Y	3	TYR	2.5
2	O	78	LEU	2.5
7	T	38	HIS	2.5
4	Q	115	TRP	2.5
4	Q	73	ARG	2.4
1	N	209	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	Q	56	LYS	2.4
10	W	53	ALA	2.4
13	Z	1	ILE	2.4
7	G	84	LYS	2.4
2	O	160	LEU	2.4
4	Q	99	GLU	2.4
11	X	33	ALA	2.4
1	N	400	PHE	2.4
13	Z	42	LYS	2.4
2	O	148	MET	2.4
1	N	462	LEU	2.4
2	O	68	LEU	2.4
2	O	217	LYS	2.4
6	F	2	SER	2.4
2	O	134	ARG	2.4
5	R	5	HIS	2.4
10	J	57	HIS	2.4
4	Q	104	TYR	2.3
9	V	72	ALA	2.3
8	U	26	THR	2.3
4	Q	103	VAL	2.3
4	Q	51	LEU	2.3
4	Q	117	ALA	2.3
13	M	41	LYS	2.3
5	R	22	PRO	2.3
4	Q	53	ILE	2.3
1	N	113	LEU	2.3
10	W	10	LYS	2.3
11	X	51	LYS	2.3
3	P	182	TYR	2.3
3	C	161	GLN	2.2
4	D	53	ILE	2.2
1	N	48	LEU	2.2
8	U	50	VAL	2.2
13	M	38	ASP	2.2
2	O	89	GLU	2.2
9	V	42	LYS	2.2
13	M	42	LYS	2.2
1	N	117	MET	2.2
1	N	368	HIS	2.2
1	N	139	ALA	2.2
11	K	19	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
13	Z	2	THR	2.2
1	N	473	TRP	2.2
4	Q	145	TRP	2.2
2	O	7	LEU	2.2
4	Q	61	ARG	2.2
8	U	42	ALA	2.2
8	U	44	THR	2.2
1	N	334	TRP	2.1
6	S	91	LEU	2.1
3	P	11	VAL	2.1
12	Y	12	PRO	2.1
4	Q	105	GLY	2.1
3	P	38	ASN	2.1
3	P	9	HIS	2.1
2	O	58	ALA	2.1
1	N	513	LEU	2.1
13	Z	37	LEU	2.1
1	N	49	GLY	2.1
4	Q	50	SER	2.1
6	S	14	THR	2.1
7	T	61	SER	2.1
2	B	58	ALA	2.1
8	H	7	LYS	2.1
2	O	21	LEU	2.1
10	W	38	LEU	2.1
2	O	15	PRO	2.1
1	N	384	GLY	2.1
8	U	79	GLY	2.1
8	U	46	LYS	2.0
4	Q	123	MET	2.0
9	V	24	ALA	2.0
13	Z	39	ASN	2.0
1	N	54	TYR	2.0
11	X	48	VAL	2.0
4	Q	64	PHE	2.0
5	E	54	ALA	2.0
8	U	66	ILE	2.0
4	D	147	LYS	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	0.61	0.27	81,114,143,143	0
7	TPO	T	11	11/12	0.74	0.27	85,108,132,134	0
1	FME	N	1	10/11	0.80	0.24	55,66,83,83	0
1	FME	A	1	10/11	0.90	0.13	31,37,45,48	0
2	FME	O	1	10/11	0.94	0.13	18,42,55,61	0
2	FME	B	1	10/11	0.96	0.08	23,25,26,26	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
28	SAC	I	101	9/10	0.64	0.23	82,90,98,99	0
26	DMU	P	302	33/33	0.67	0.20	45,87,96,102	0
23	CHD	Y	101	29/29	0.69	0.35	63,140,155,157	0
24	PEK	T	102	53/53	0.71	0.29	47,76,131,143	0
26	DMU	G	101	33/33	0.71	0.21	41,106,120,123	0
26	DMU	C	310	33/33	0.72	0.21	47,78,102,105	0
24	PEK	C	311	53/53	0.72	0.24	39,70,95,114	0
22	PSC	V	101	52/52	0.73	0.32	56,102,190,205	0
23	CHD	T	103	29/29	0.74	0.28	58,120,126,132	0
17	PGV	N	610	51/51	0.74	0.27	38,85,153,163	0
24	PEK	P	301	53/53	0.75	0.24	44,86,182,202	0
21	TGL	N	609	63/63	0.76	0.29	46,78,101,118	0
22	PSC	B	303	52/52	0.76	0.30	48,102,189,190	0
25	CDL	P	307	100/100	0.76	0.26	36,78,106,118	0
25	CDL	P	309	100/100	0.76	0.31	53,91,123,125	0
17	PGV	P	306	51/51	0.77	0.19	45,64,98,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CDL	C	308	100/100	0.77	0.27	28,85,117,123	0
25	CDL	C	306	100/100	0.78	0.24	35,69,129,133	0
24	PEK	C	304	53/53	0.79	0.26	33,89,176,203	0
21	TGL	N	604	63/63	0.79	0.25	37,73,98,109	0
17	PGV	A	604	51/51	0.79	0.24	30,60,146,150	0
26	DMU	Q	201	33/33	0.79	0.16	35,57,71,74	0
17	PGV	H	101	51/51	0.79	0.22	57,69,86,88	0
26	DMU	C	309	33/33	0.80	0.17	23,71,87,95	0
28	SAC	V	102	9/10	0.80	0.14	60,74,78,79	0
23	CHD	W	101	29/29	0.81	0.19	58,83,95,96	0
21	TGL	D	201	63/63	0.84	0.22	36,60,93,97	0
21	TGL	L	101	63/63	0.85	0.19	13,53,77,82	0
23	CHD	C	307	29/29	0.85	0.14	32,50,56,60	0
23	CHD	J	101	29/29	0.85	0.13	53,61,64,69	0
21	TGL	B	302	63/63	0.86	0.22	21,56,94,98	0
21	TGL	O	301	63/63	0.88	0.19	33,61,87,93	0
23	CHD	P	308	29/29	0.88	0.14	52,72,76,80	0
23	CHD	O	303	29/29	0.90	0.10	24,27,30,33	0
23	CHD	P	303	29/29	0.91	0.09	16,24,28,30	0
16	NA	N	603	1/1	0.91	0.08	30,30,30,30	0
17	PGV	N	605	51/51	0.93	0.16	21,34,68,73	0
17	PGV	P	305	51/51	0.94	0.13	18,31,64,74	0
26	DMU	M	101	33/33	0.94	0.07	10,23,34,36	0
17	PGV	C	301	51/51	0.94	0.10	12,25,37,40	0
24	PEK	P	304	53/53	0.94	0.14	23,49,81,83	0
24	PEK	C	303	53/53	0.94	0.15	20,44,104,113	0
23	CHD	C	302	29/29	0.94	0.08	14,17,18,20	0
23	CHD	T	101	29/29	0.95	0.08	11,13,15,17	0
17	PGV	C	305	51/51	0.95	0.12	14,26,74,81	0
18	HEA	N	607	60/60	0.96	0.11	24,29,53,58	0
18	HEA	N	606	60/60	0.97	0.08	16,20,33,37	0
16	NA	A	603	1/1	0.98	0.05	18,18,18,18	0
18	HEA	A	605	60/60	0.98	0.07	5,11,22,24	0
18	HEA	A	606	60/60	0.98	0.07	9,12,15,16	0
15	MG	A	602	1/1	0.98	0.03	15,15,15,15	0
15	MG	N	602	1/1	0.98	0.14	26,26,26,26	0
20	CUA	B	301	2/2	0.98	0.04	19,19,19,19	0
19	OH	N	608	1/1	0.99	0.04	14,14,14,14	0
20	CUA	O	302	2/2	0.99	0.02	29,29,29,34	0
14	CU	A	601	1/1	1.00	0.02	12,12,12,12	0
27	ZN	F	101	1/1	1.00	0.03	23,23,23,23	0
27	ZN	S	101	1/1	1.00	0.03	30,30,30,30	0

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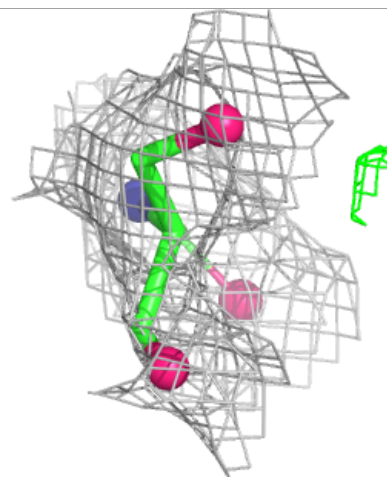
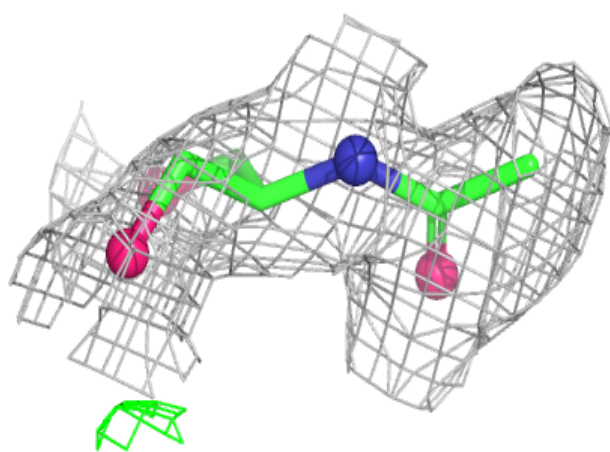
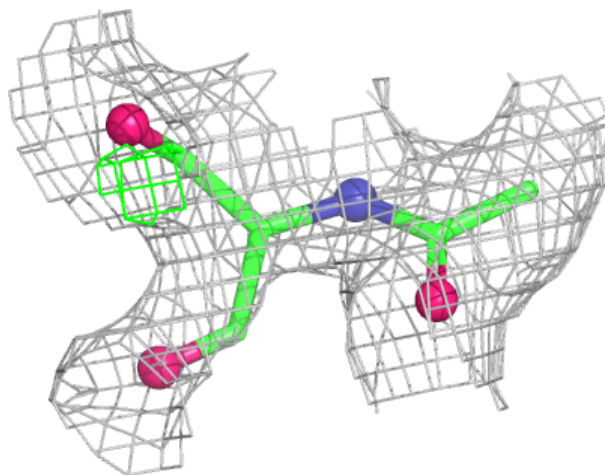
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CU	N	601	1/1	1.00	0.02	29,29,29,29	0
19	OH	A	607	1/1	1.00	0.04	9,9,9,9	0

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.

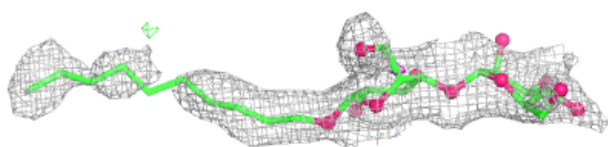
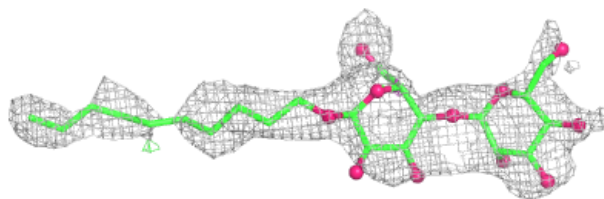
Electron density around SAC I 101:

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

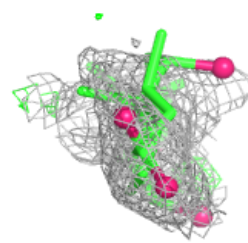
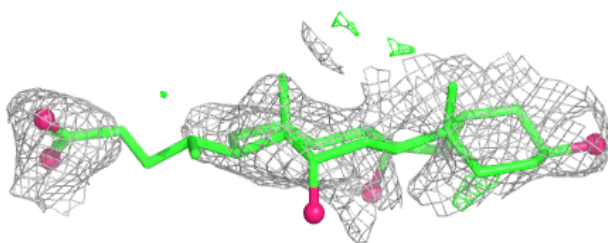
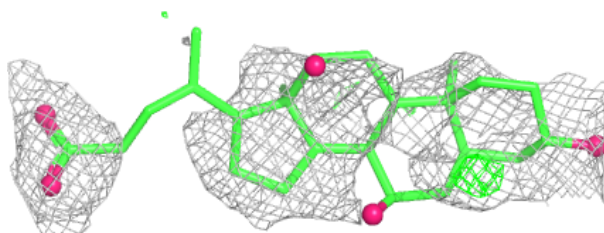


Electron density around DMU P 302:

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

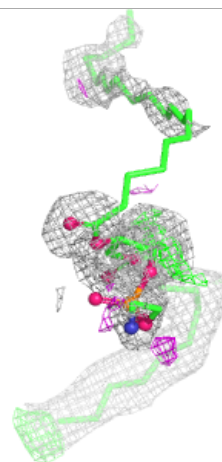
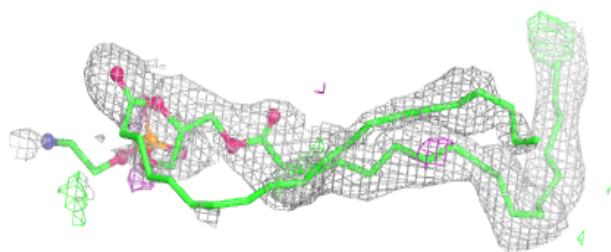
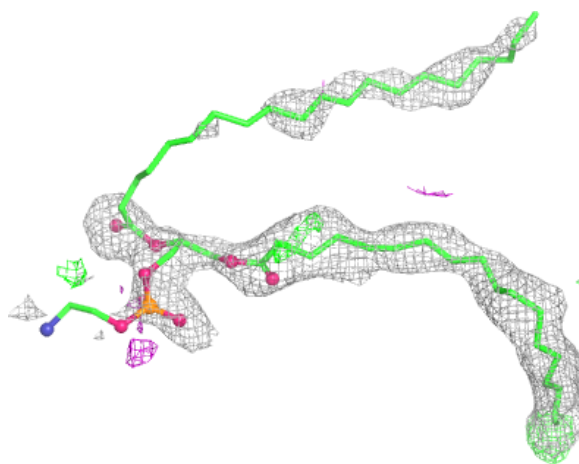
**Electron density around CHD Y 101:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



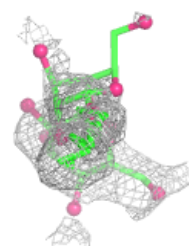
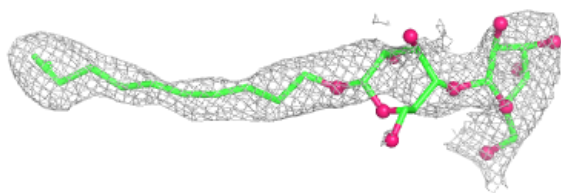
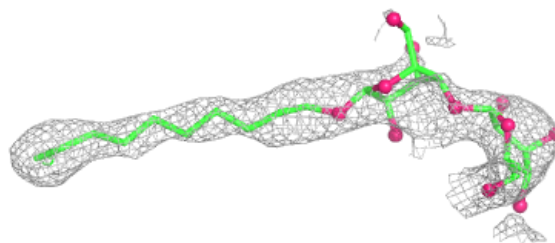
Electron density around PEK T 102:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

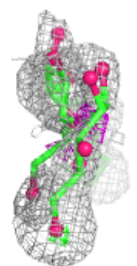
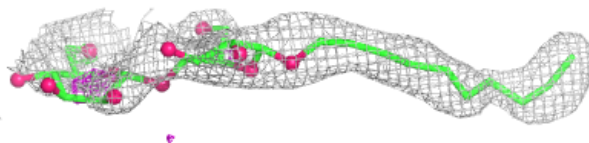
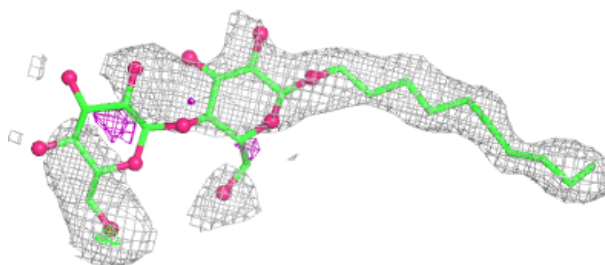


Electron density around DMU G 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

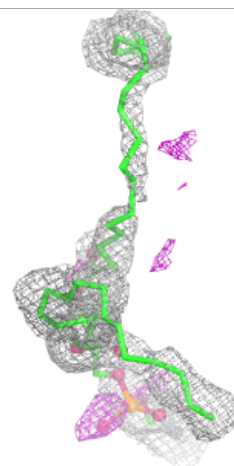
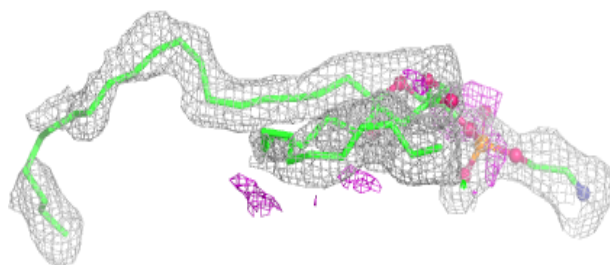
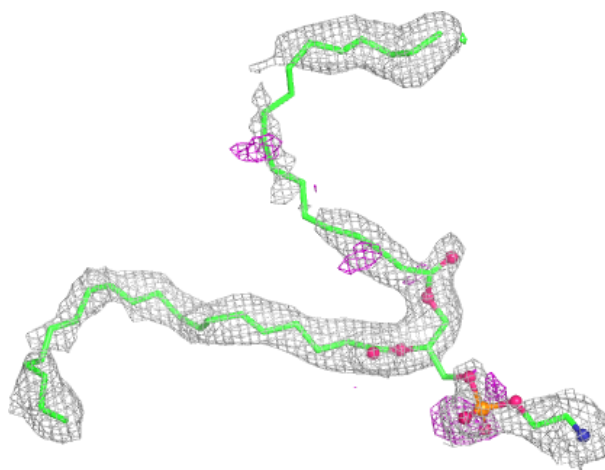
**Electron density around DMU C 310:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



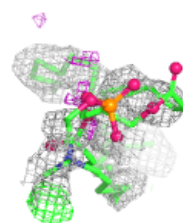
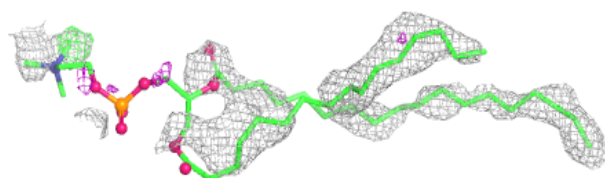
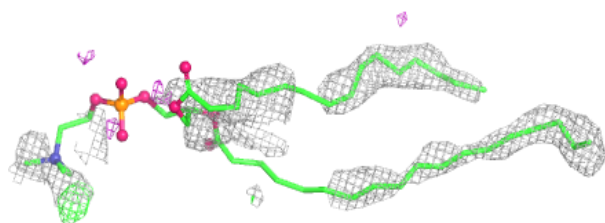
Electron density around PEK C 311:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

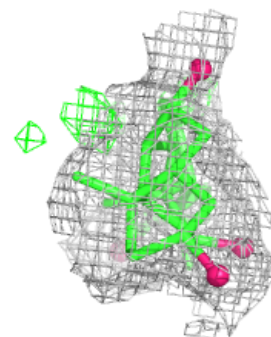
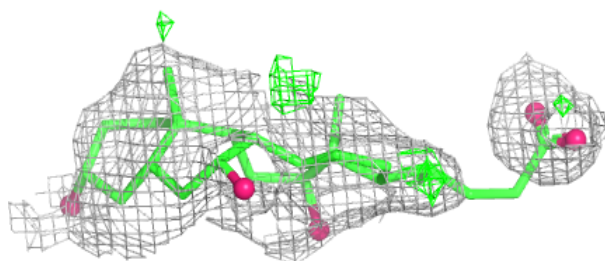


Electron density around PSC V 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

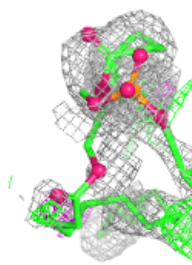
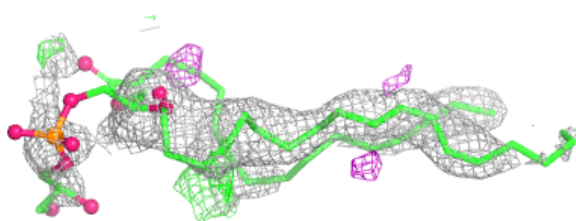
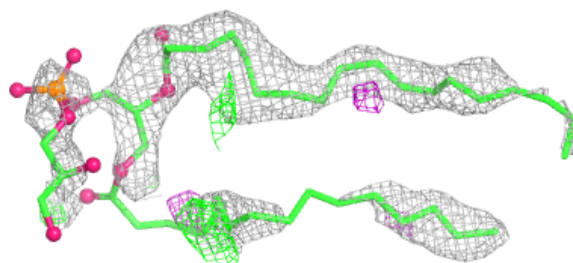
**Electron density around CHD T 103:**

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and green (positive)

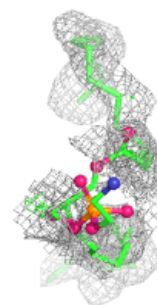
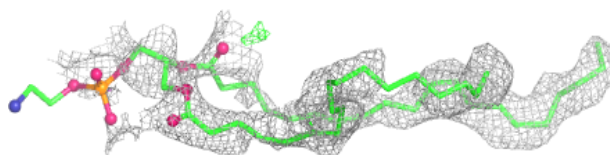
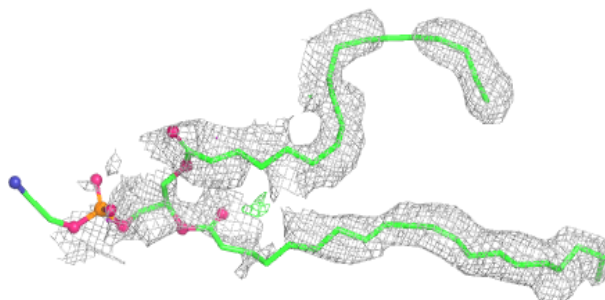


Electron density around PGV N 610:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

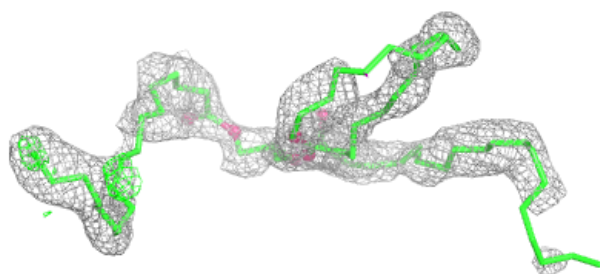
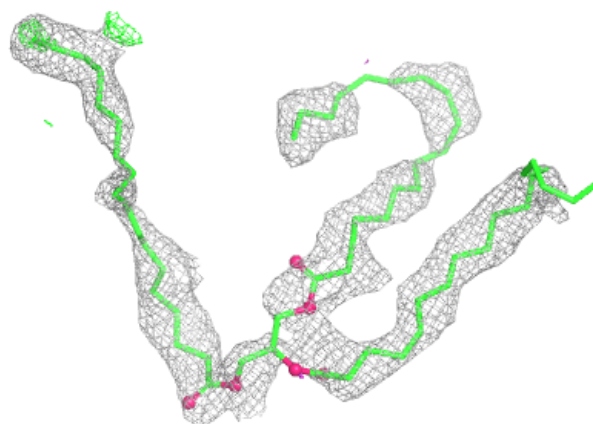
**Electron density around PEK P 301:**

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and green (positive)

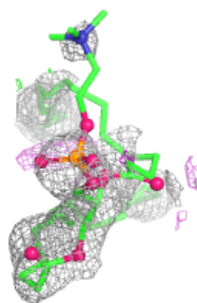
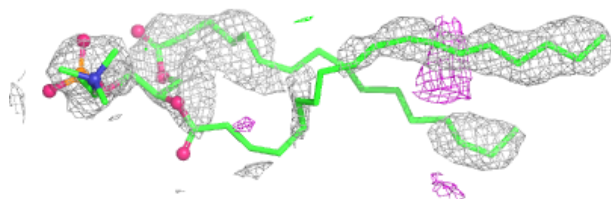
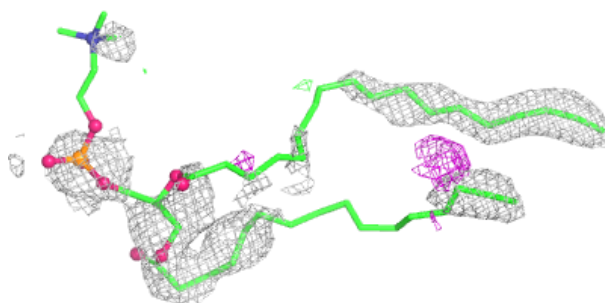


Electron density around TGL N 609:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

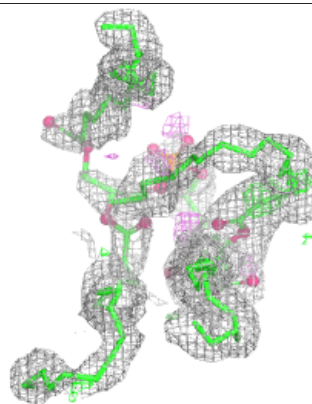
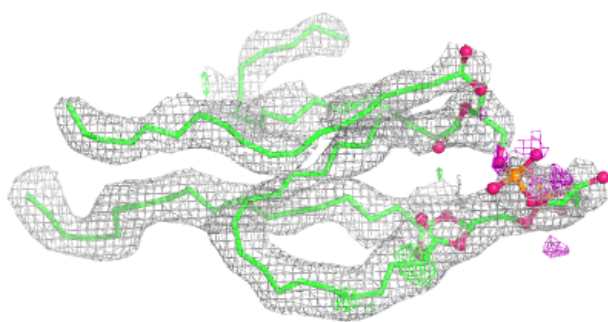
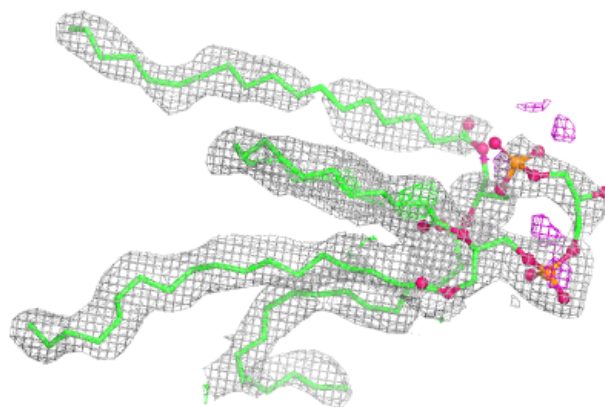
**Electron density around PSC B 303:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



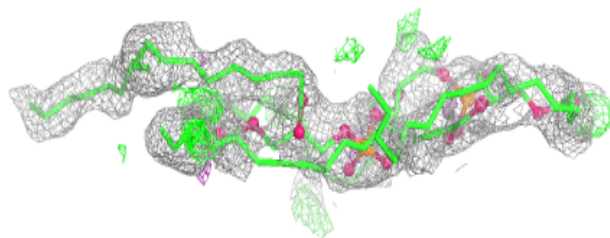
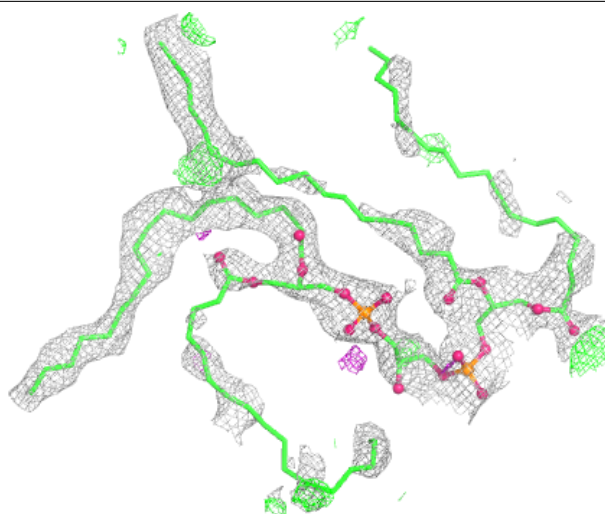
Electron density around CDL P 307:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



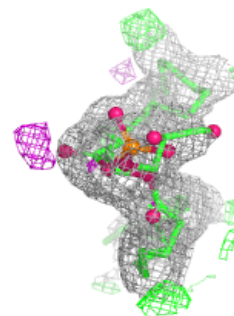
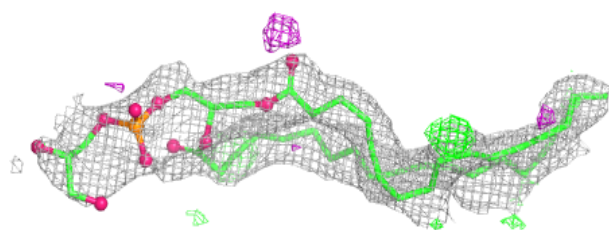
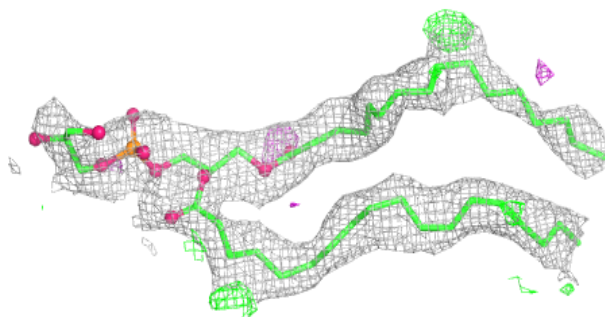
Electron density around CDL P 309:

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

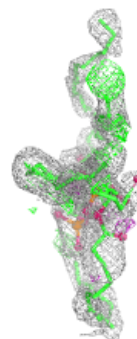
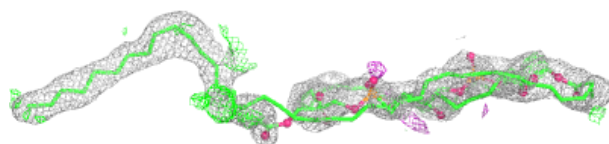
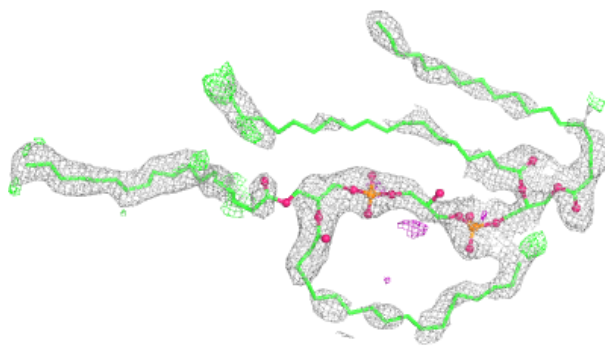


Electron density around PGV P 306:

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

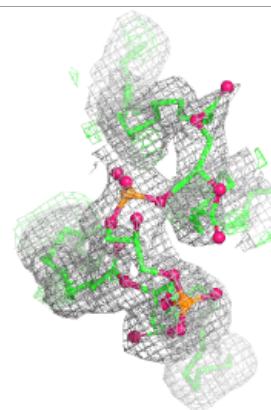
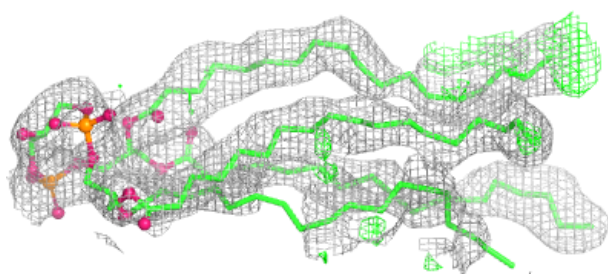
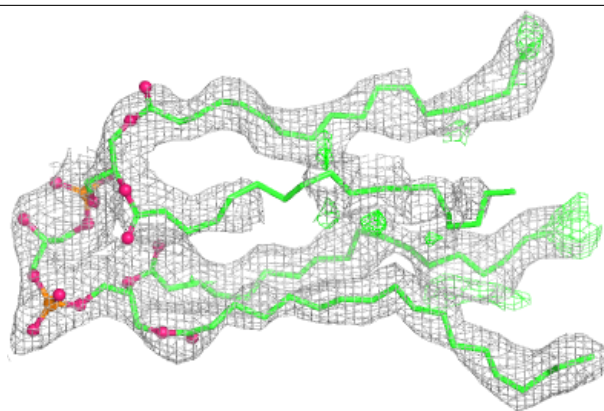
**Electron density around CDL C 308:**

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

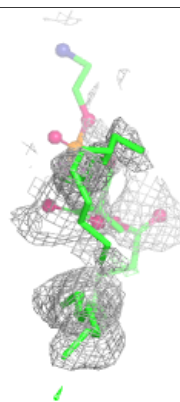
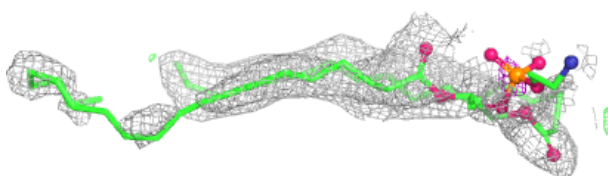
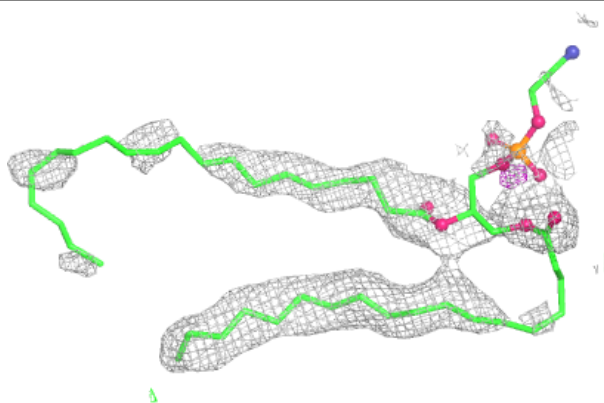


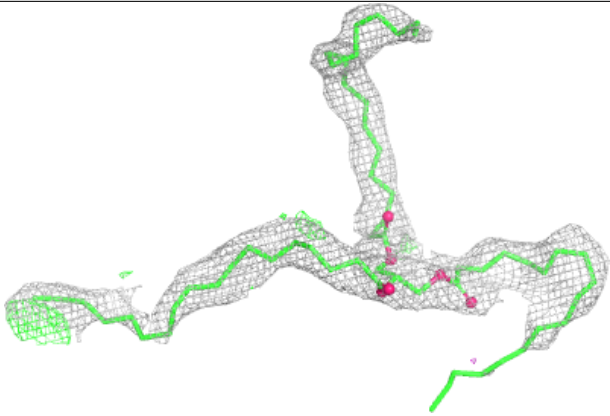
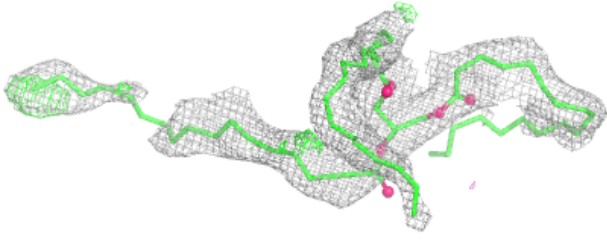
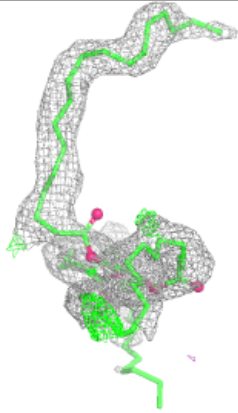
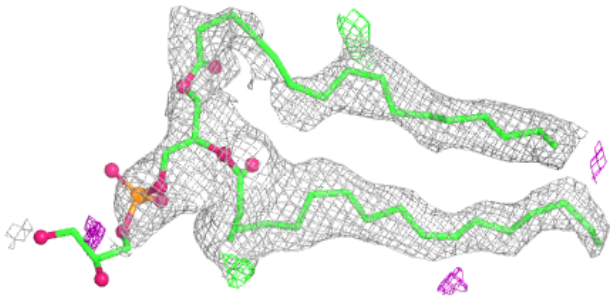
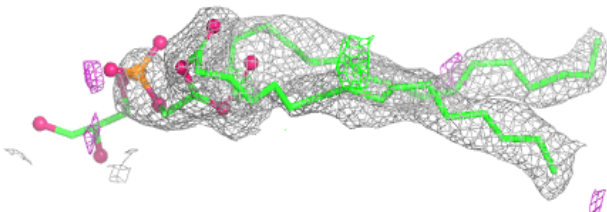
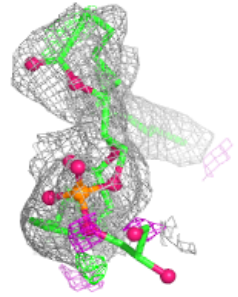
Electron density around CDL C 306:

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

**Electron density around PEK C 304:**

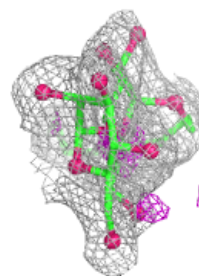
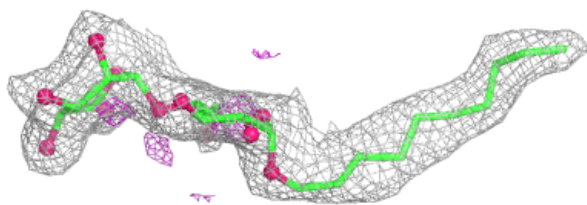
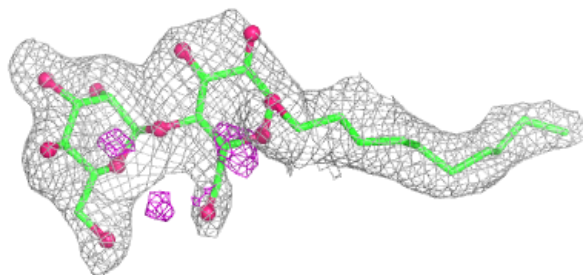
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



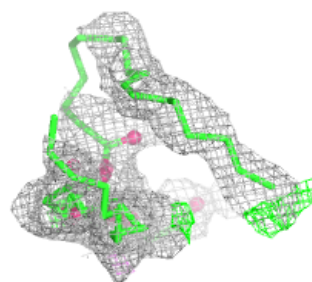
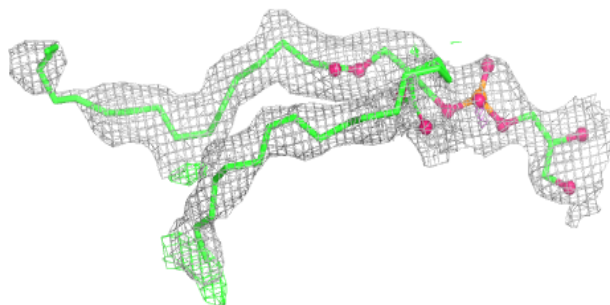
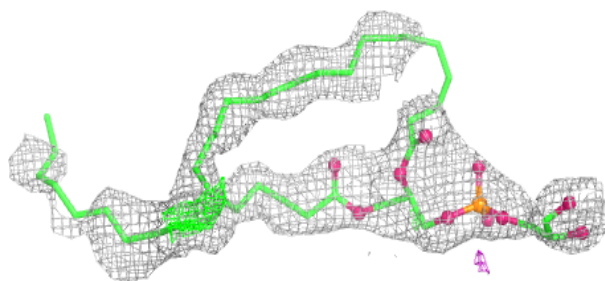
Electron density around TGL N 604: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	 A 3D visualization of the electron density map for TGL N 604. The map is shown as a gray mesh. The protein backbone is represented by a green line, and the side chains are shown as red spheres. The density map is shown in a perspective view, highlighting the overall shape and the fit of the model.
 A 3D visualization of the electron density map for TGL N 604, showing a different view or a different part of the molecule. The map is shown as a gray mesh, and the protein backbone is represented by a green line. The side chains are shown as red spheres. The density map is shown in a perspective view, highlighting the overall shape and the fit of the model.	 A 3D visualization of the electron density map for TGL N 604, showing a different view or a different part of the molecule. The map is shown as a gray mesh, and the protein backbone is represented by a green line. The side chains are shown as red spheres. The density map is shown in a perspective view, highlighting the overall shape and the fit of the model.
Electron density around PGV A 604: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	 A 3D visualization of the electron density map for PGV A 604. The map is shown as a gray mesh. The protein backbone is represented by a green line, and the side chains are shown as red spheres. The density map is shown in a perspective view, highlighting the overall shape and the fit of the model.
 A 3D visualization of the electron density map for PGV A 604, showing a different view or a different part of the molecule. The map is shown as a gray mesh, and the protein backbone is represented by a green line. The side chains are shown as red spheres. The density map is shown in a perspective view, highlighting the overall shape and the fit of the model.	 A 3D visualization of the electron density map for PGV A 604, showing a different view or a different part of the molecule. The map is shown as a gray mesh, and the protein backbone is represented by a green line. The side chains are shown as red spheres. The density map is shown in a perspective view, highlighting the overall shape and the fit of the model.

Electron density around DMU Q 201:

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

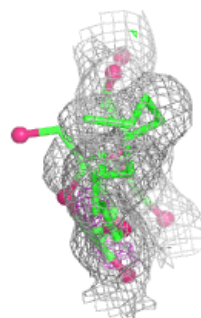
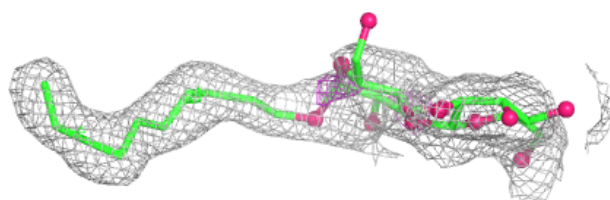
**Electron density around PGV H 101:**

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

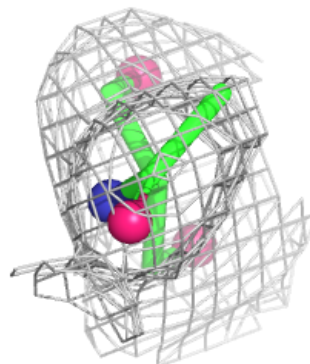
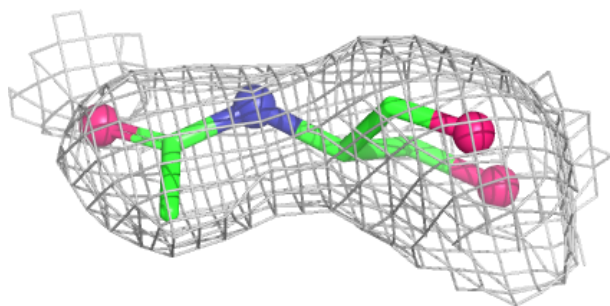
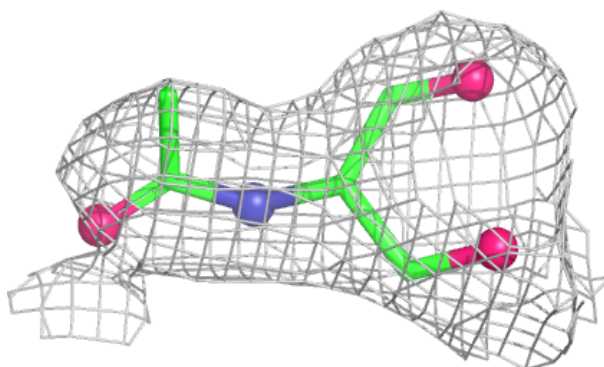


Electron density around DMU C 309:

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

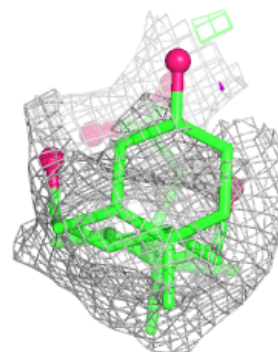
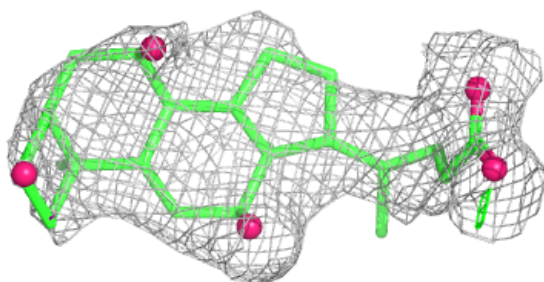
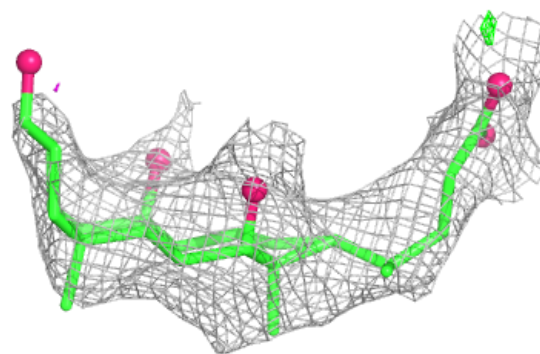
**Electron density around SAC V 102:**

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



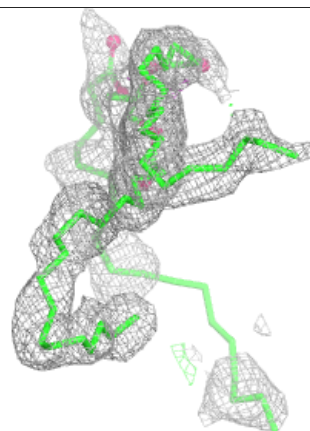
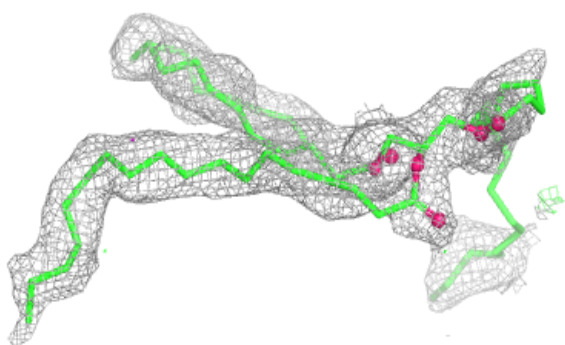
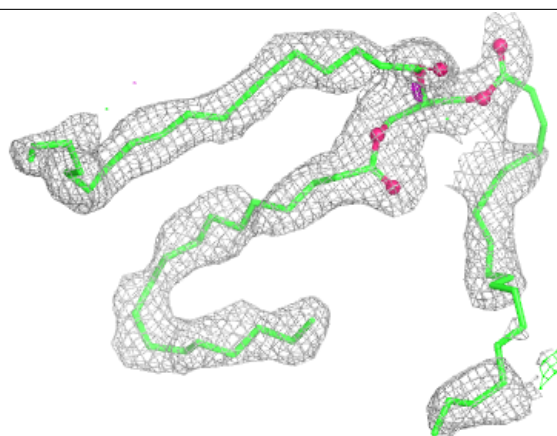
Electron density around CHD W 101:

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



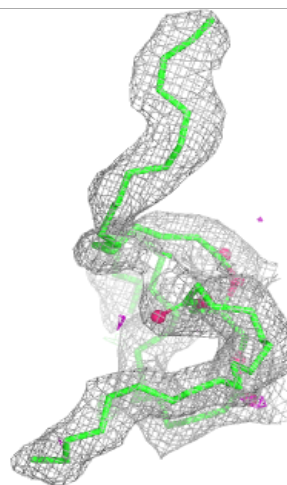
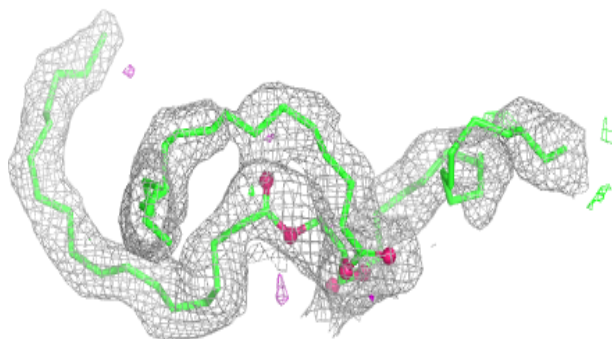
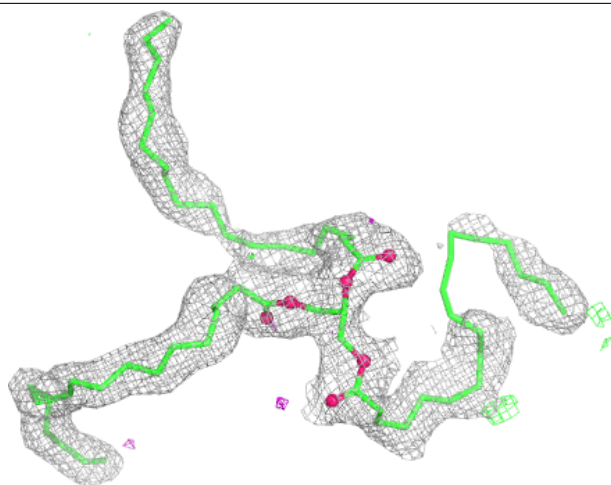
Electron density around TGL D 201:

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



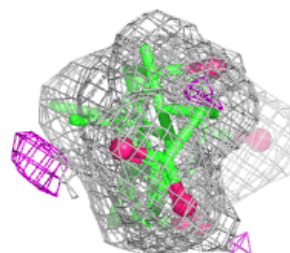
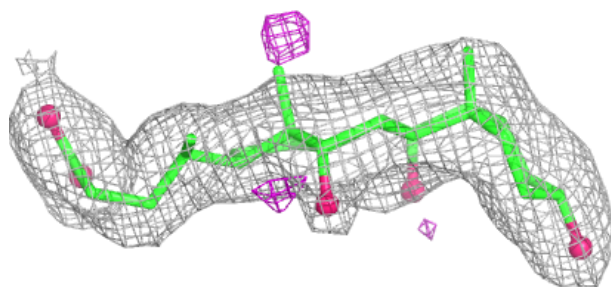
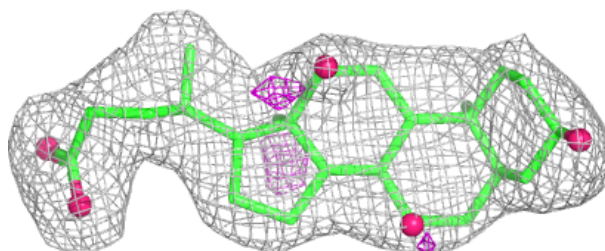
Electron density around TGL L 101:

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

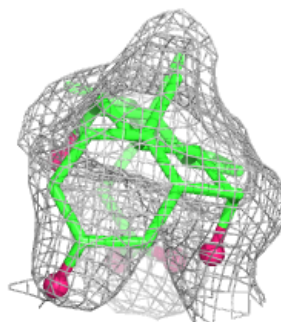
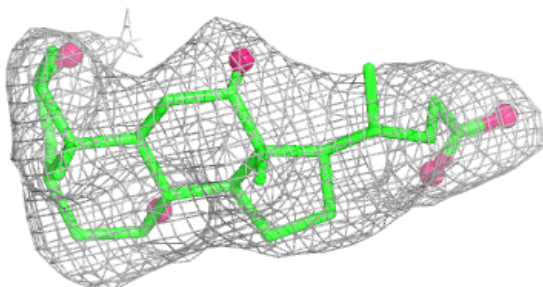
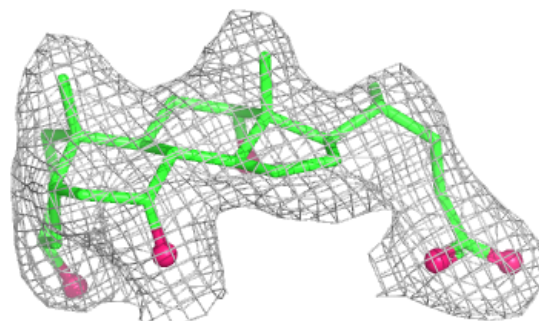


Electron density around CHD C 307:

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

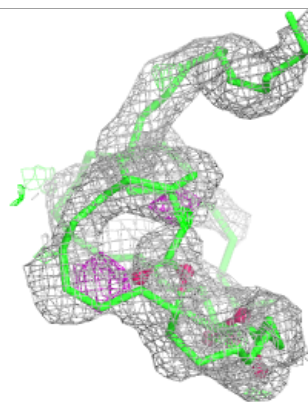
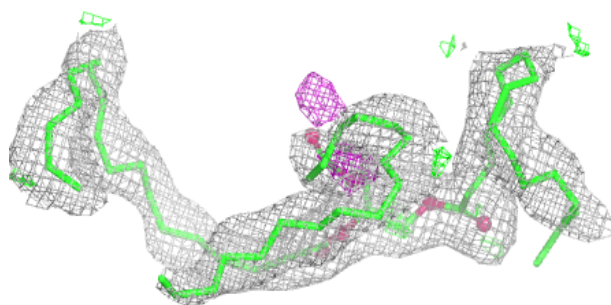
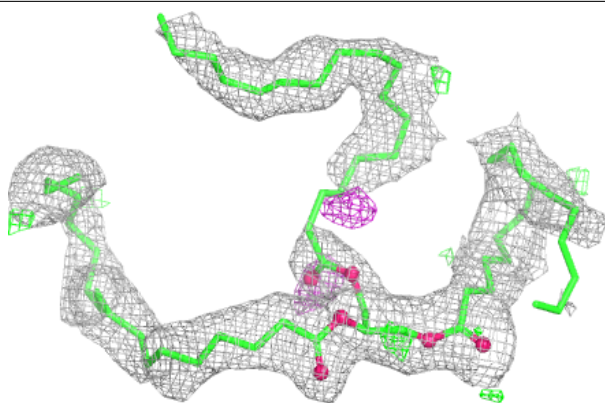
**Electron density around CHD J 101:**

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

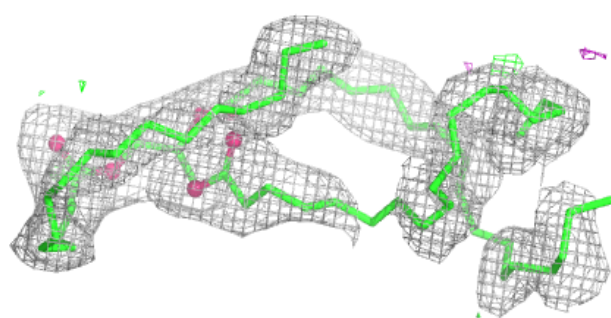
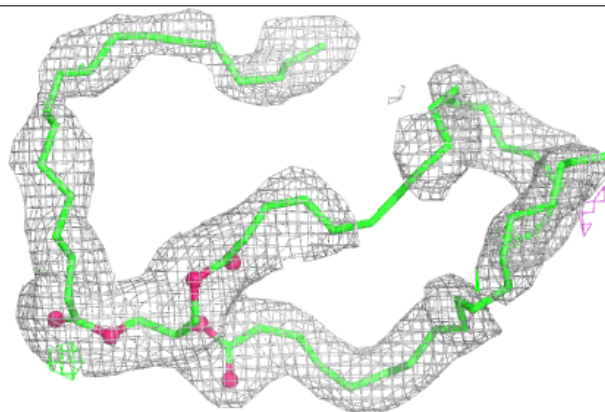


Electron density around TGL B 302:

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

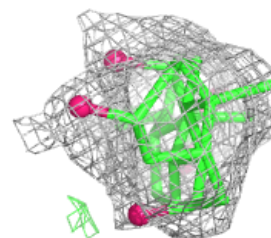
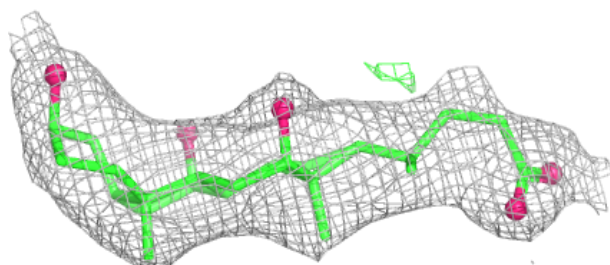
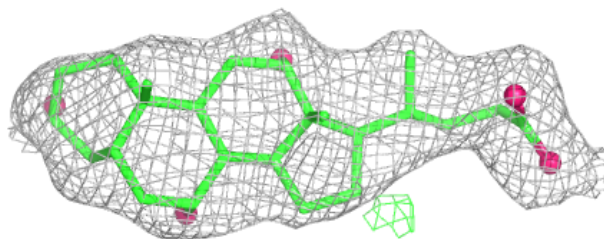
**Electron density around TGL O 301:**

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

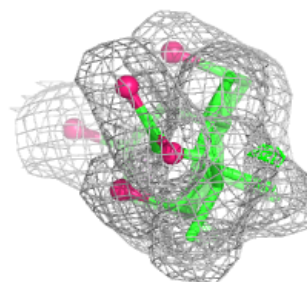
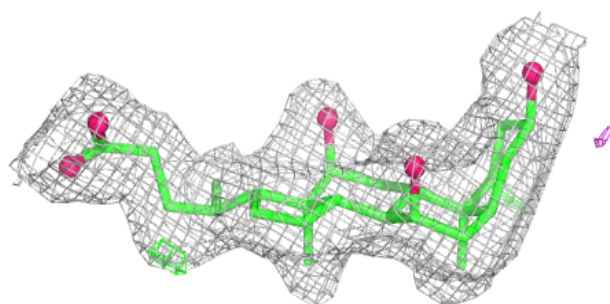
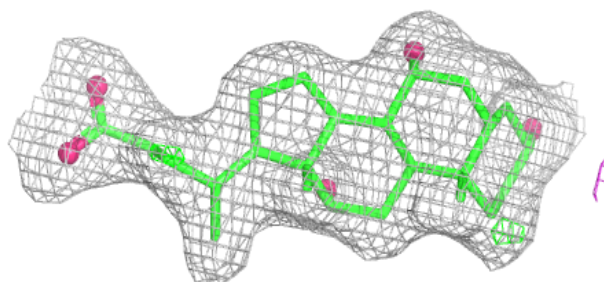


Electron density around CHD P 308:

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

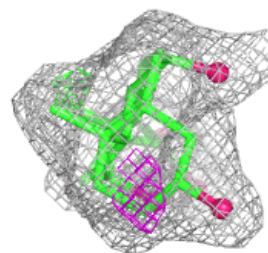
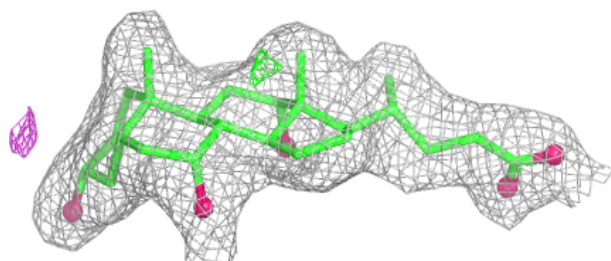
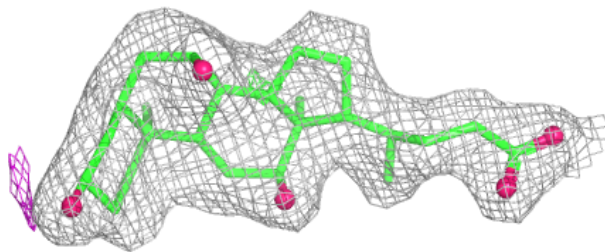
**Electron density around CHD O 303:**

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

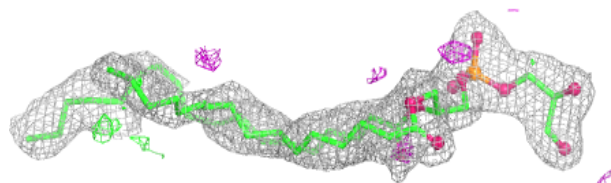
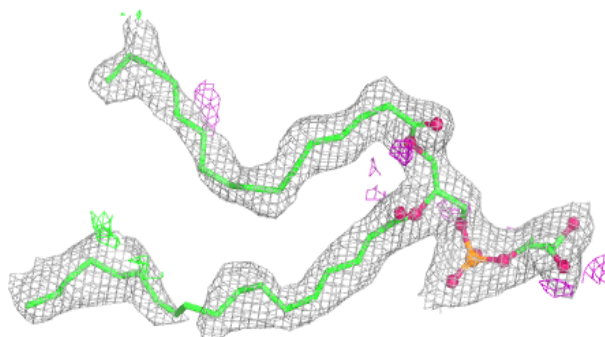


Electron density around CHD P 303:

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

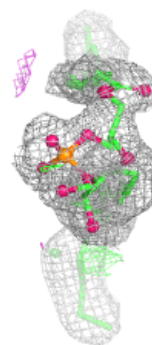
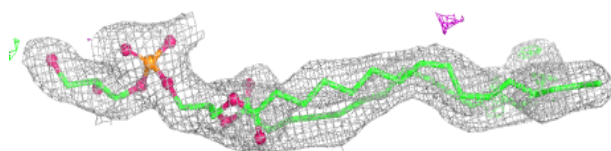
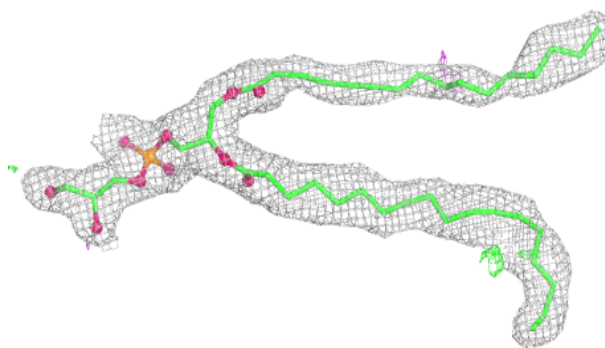
**Electron density around PGV N 605:**

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

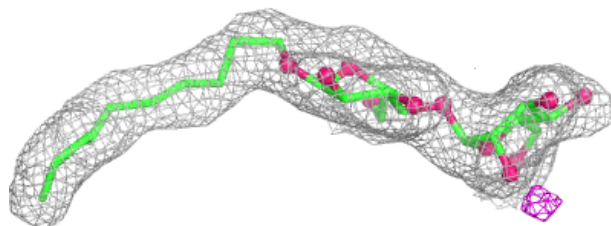
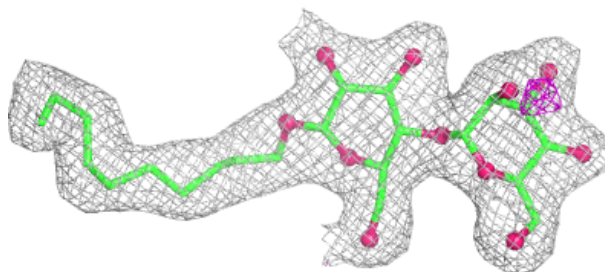


Electron density around PGV P 305:

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

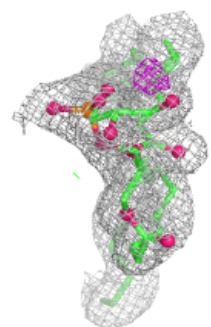
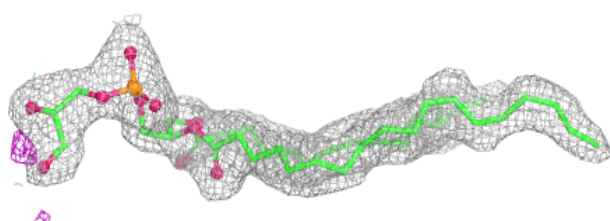
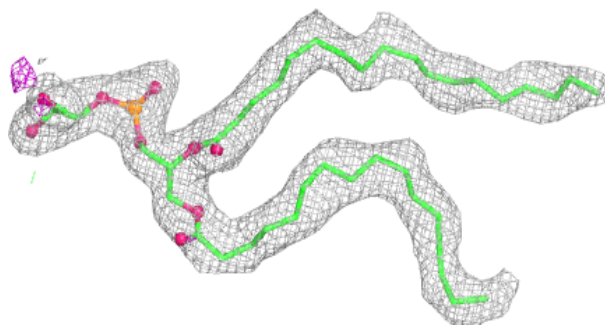
**Electron density around DMU M 101:**

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

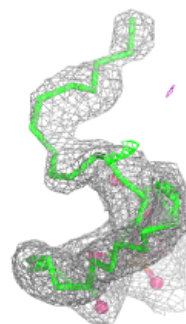
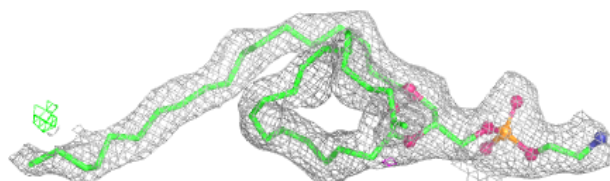
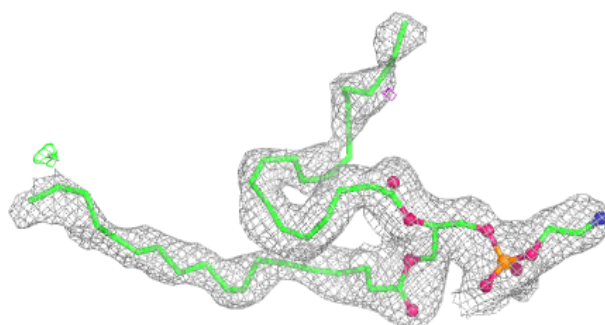


Electron density around PGV C 301:

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

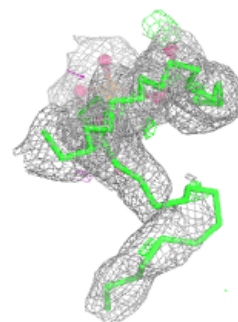
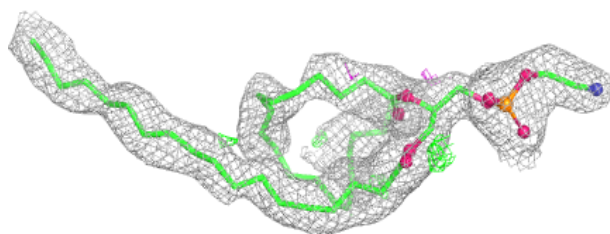
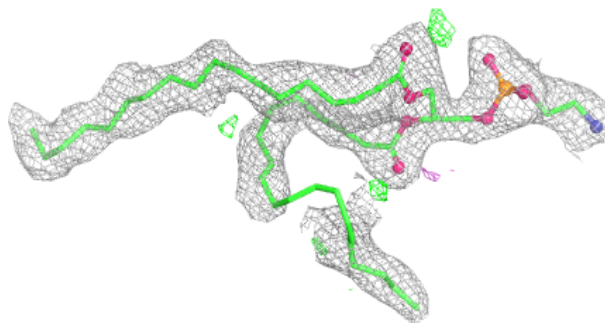
**Electron density around PEK P 304:**

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

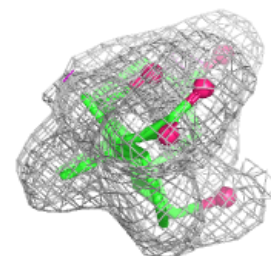
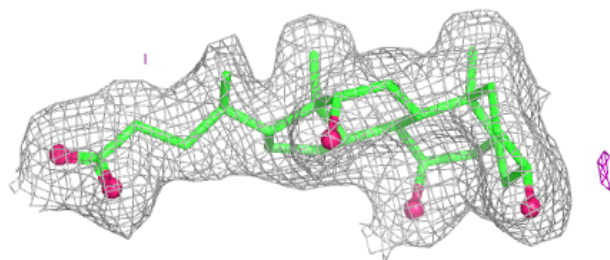
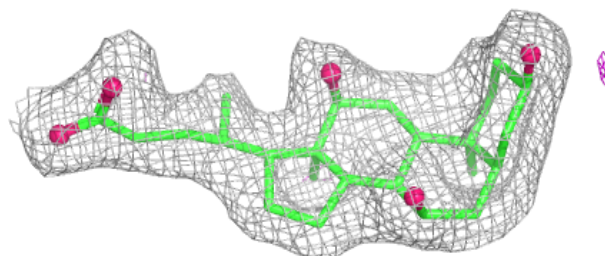


Electron density around PEK C 303:

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

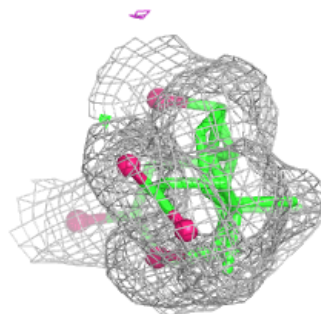
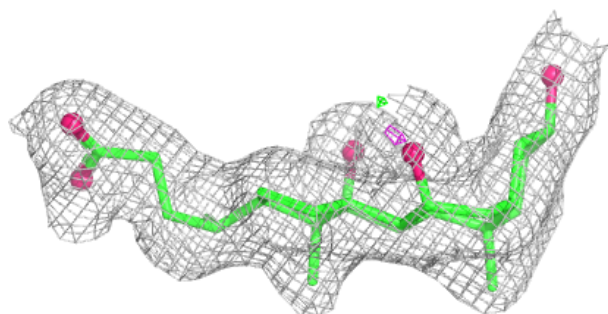
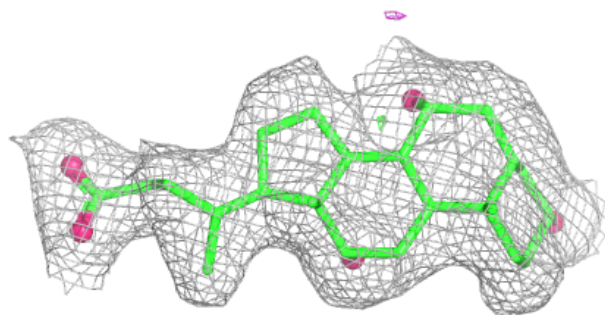
**Electron density around CHD C 302:**

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

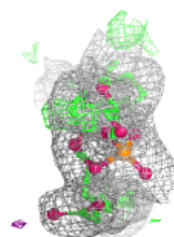
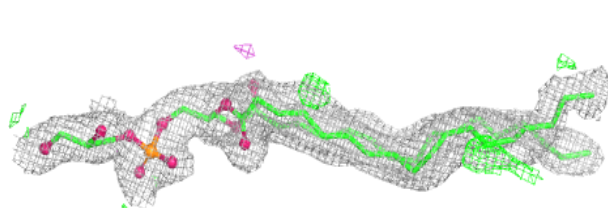
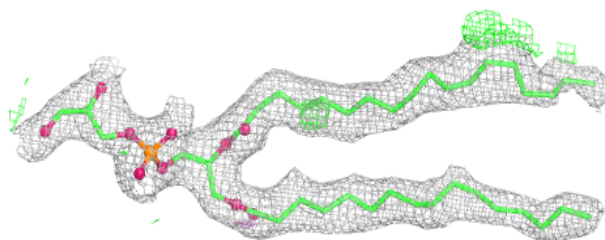


Electron density around CHD T 101:

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

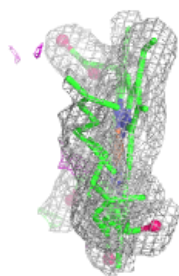
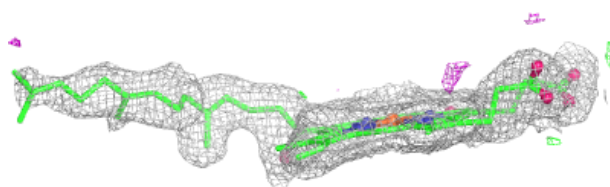
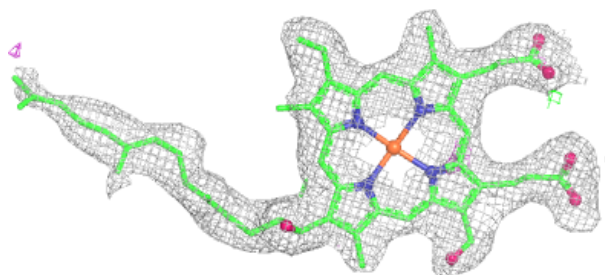
**Electron density around PGV C 305:**

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

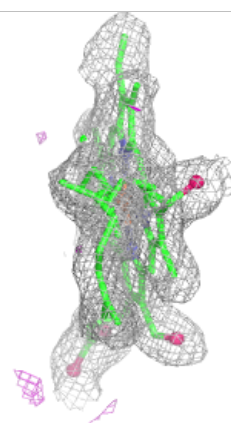
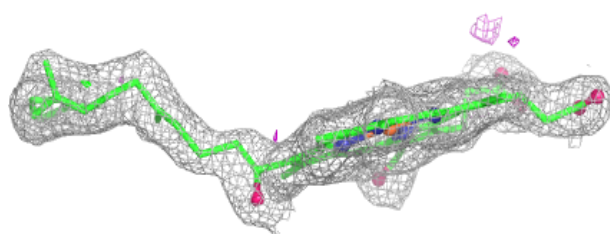
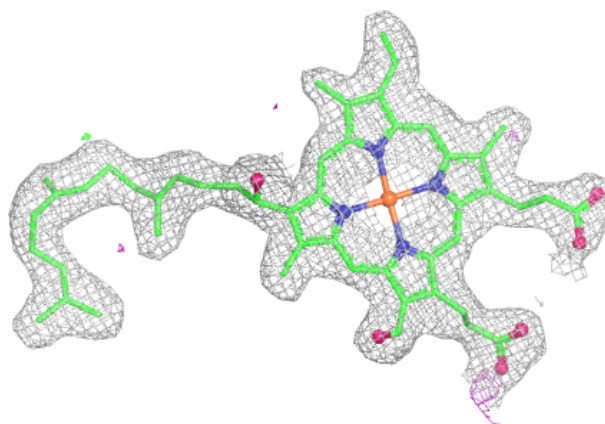


Electron density around HEA N 607:

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

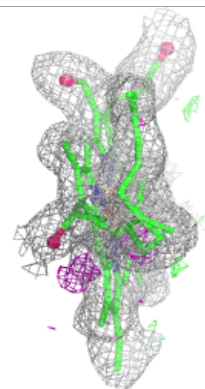
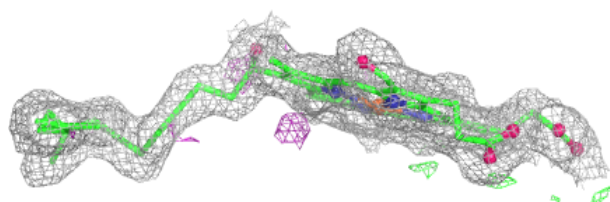
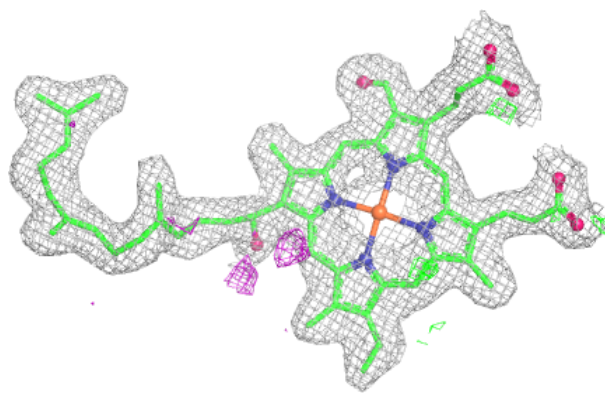
**Electron density around HEA N 606:**

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

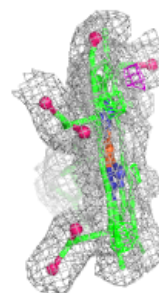
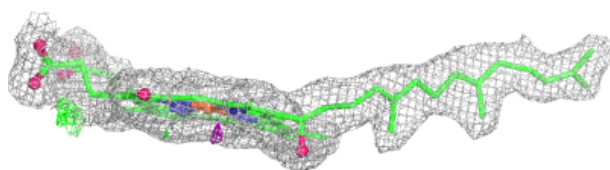
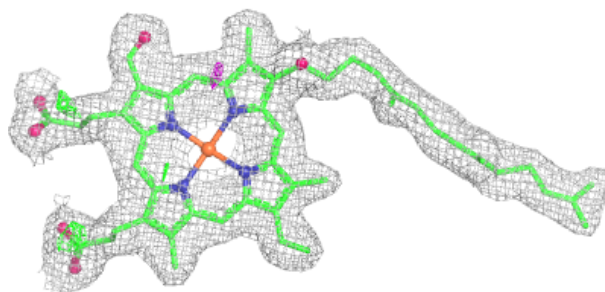


Electron density around HEA A 605:

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

**Electron density around HEA A 606:**

$2mF_o-DF_c$ (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.