



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 09:20 PM BST

PDB ID : 5X1B
Title : CO bound cytochrome c oxidase at 20 nsec after pump laser irradiation to release CO from O₂ reduction center
Authors : Shimada, A.; Kubo, M.; Baba, S.; Yamashita, K.; Hirata, K.; Ueno, G.; Nomura, T.; Kimura, T.; Shinzawa-Itoh, K.; Baba, J.; Hatano, K.; Eto, Y.; Miyamoto, A.; Murakami, H.; Kumasaka, T.; Owada, S.; Tono, K.; Yabashi, M.; Yamaguchi, Y.; Yanagisawa, S.; Sakaguchi, M.; Ogura, T.; Komiya, R.; Yan, J.; Yamashita, E.; Yamamoto, M.; Ago, H.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2017-01-25
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

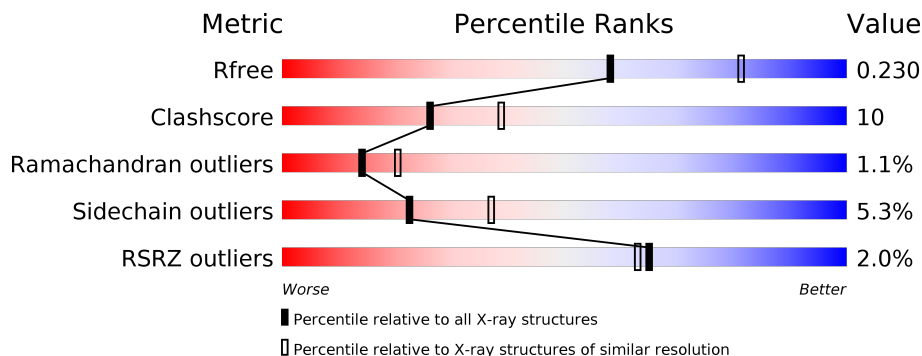
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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














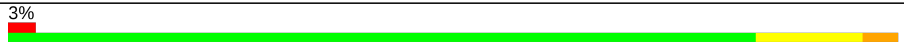




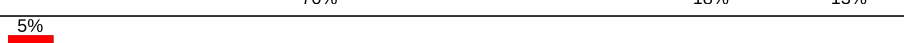

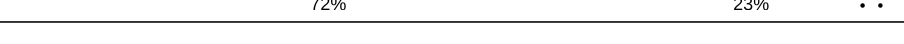
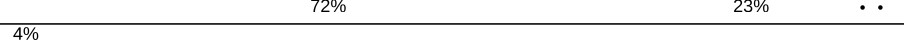
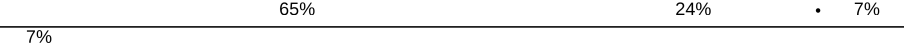
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	514	 82% 17%
1	N	514	 76% 22%
2	B	227	 77% 21%
2	O	227	 73% 25%
3	C	261	 83% 16%

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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	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601	X	-	-	-
21	EDO	A	612	-	-	-	X
21	EDO	A	614	-	-	X	-
9	SAC	V	1	-	-	-	X

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 31717 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
			Total	C	N	O	S			
1	A	514	Total	C	N	O	S	0	1	0
			4030	2694	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

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

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

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

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

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

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

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

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

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

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

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

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

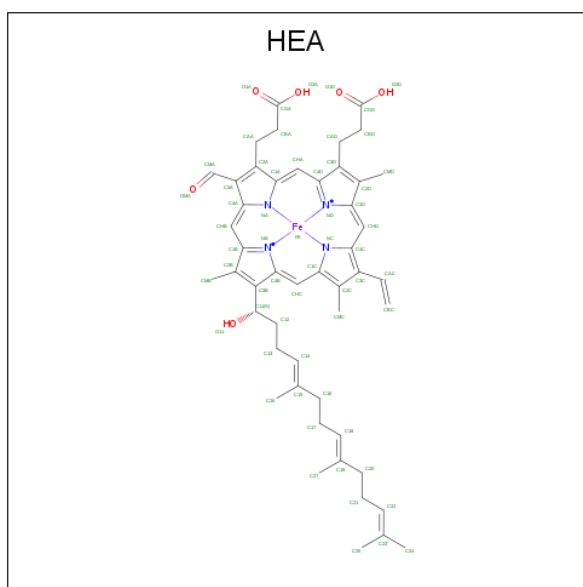
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

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

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

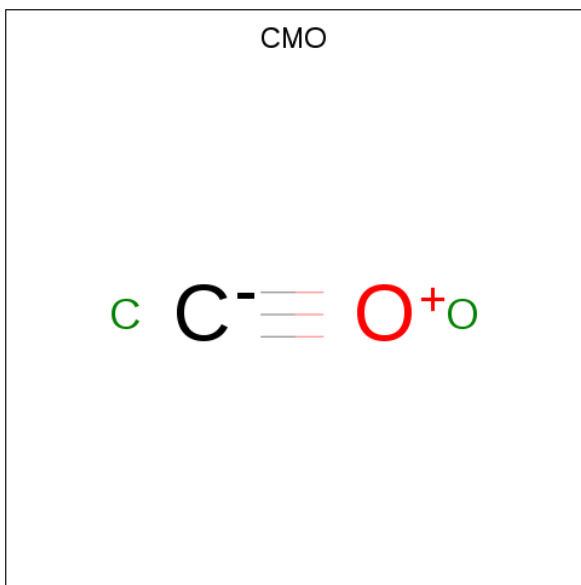
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

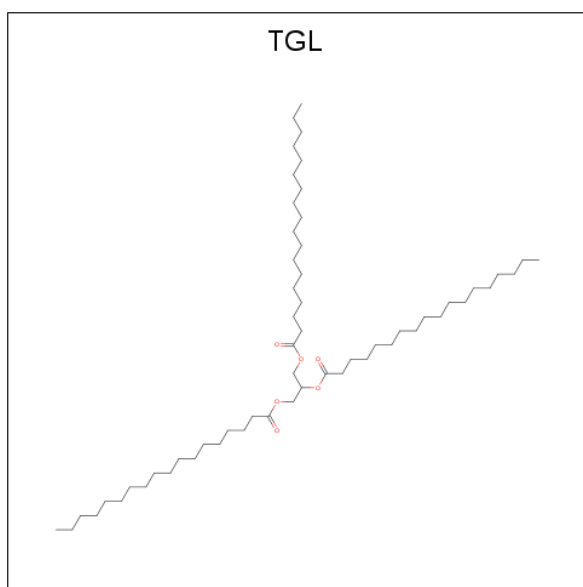
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



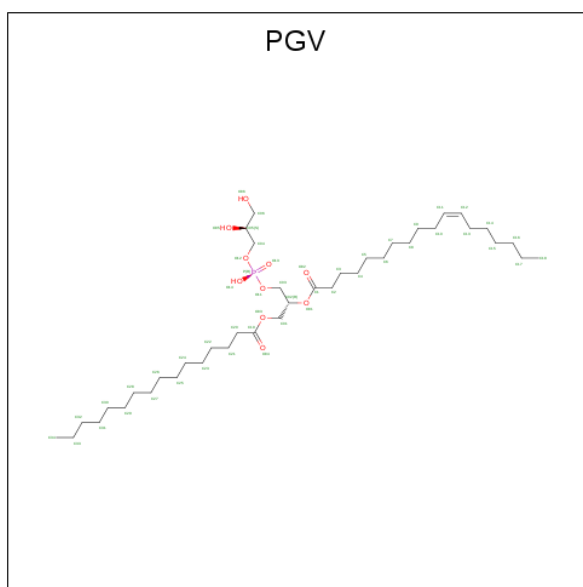
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 2 1 1	0	0
18	N	1	Total C O 2 1 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



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

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



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

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



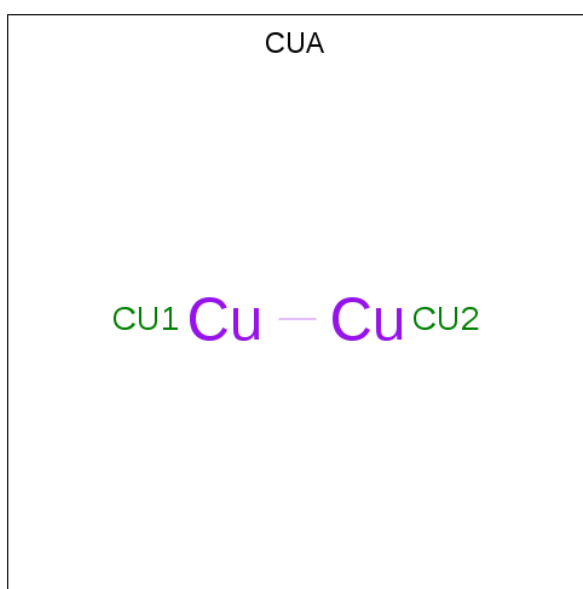
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	A	1	Total C O 4 2 2	0	0
21	B	1	Total C O 4 2 2	0	0
21	B	1	Total C O 4 2 2	0	0
21	C	1	Total C O 4 2 2	0	0
21	C	1	Total C O 4 2 2	0	0
21	C	1	Total C O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

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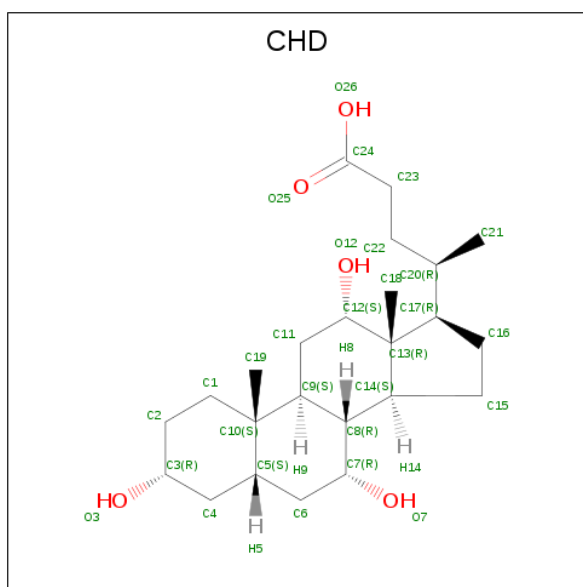
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	K	1	Total C O 4 2 2	0	0
21	L	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	T	1	Total C O 4 2 2	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



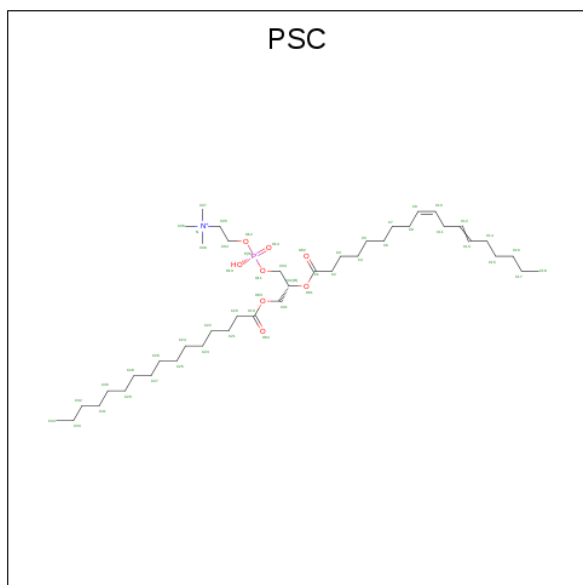
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



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

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

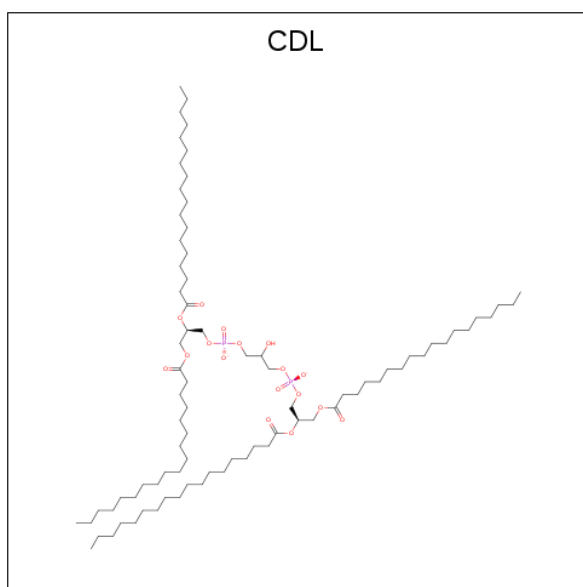


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	B	1	52	42	1	8	1	0	0
24	R	1	52	42	1	8	1	0	0

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

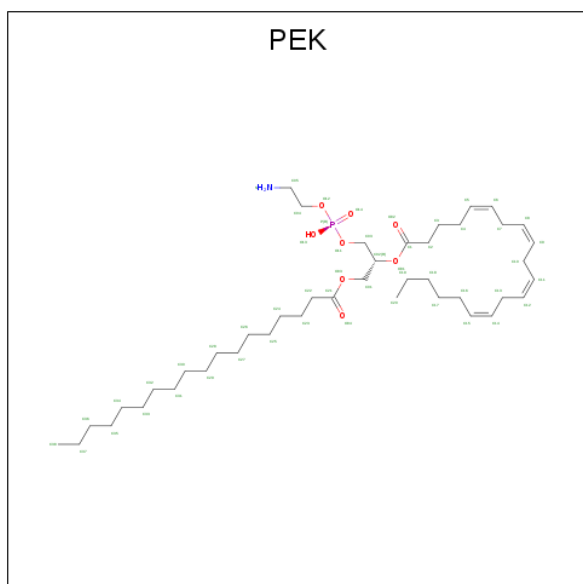
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
25	P	1	1	1	0	0
25	C	1	1	1	0	0

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 27 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).

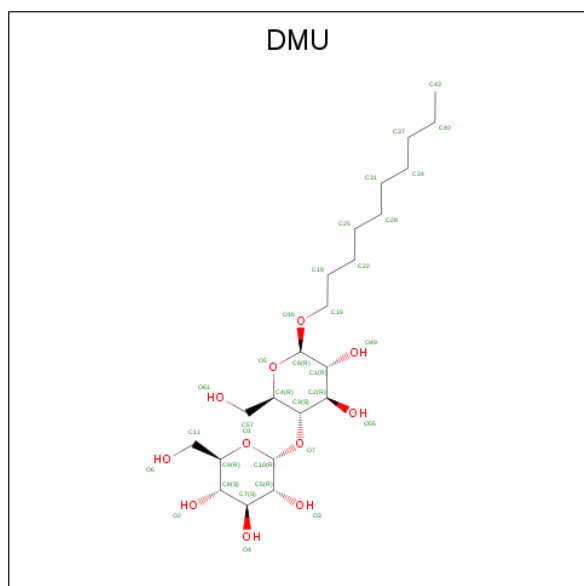


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	125	Total	O	0	0
			125	125		
30	B	77	Total	O	0	1
			78	78		
30	C	70	Total	O	0	0
			70	70		
30	D	41	Total	O	0	0
			41	41		
30	E	24	Total	O	0	0
			24	24		
30	F	36	Total	O	0	0
			36	36		
30	G	31	Total	O	0	0
			31	31		
30	H	33	Total	O	0	0
			33	33		
30	I	12	Total	O	0	0
			12	12		
30	J	19	Total	O	0	0
			19	19		
30	K	19	Total	O	0	0
			19	19		
30	L	14	Total	O	0	0
			14	14		
30	M	15	Total	O	0	0
			15	15		
30	N	117	Total	O	0	0
			117	117		
30	O	76	Total	O	0	1
			77	77		
30	P	54	Total	O	0	0
			54	54		
30	Q	29	Total	O	0	0
			29	29		
30	R	29	Total	O	0	0
			29	29		

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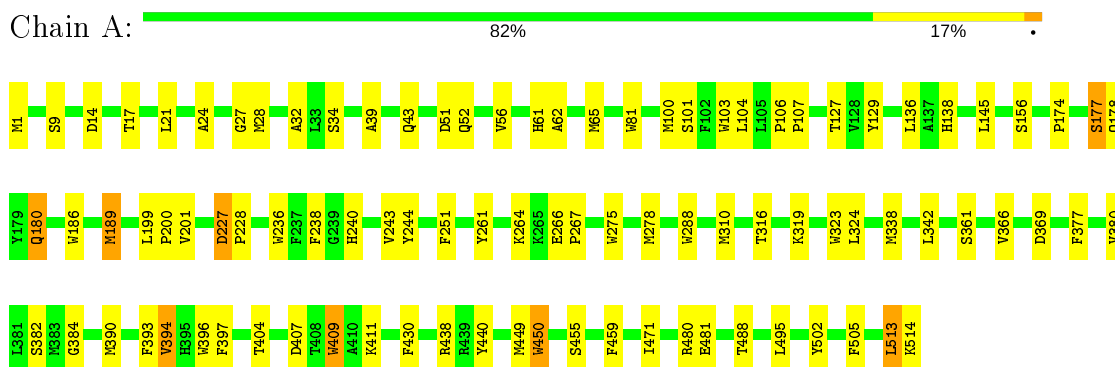
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	S	43	Total 43	O 43	0	0
30	T	20	Total 20	O 20	0	0
30	U	31	Total 31	O 31	0	0
30	V	19	Total 19	O 19	0	0
30	W	17	Total 17	O 17	0	0
30	X	9	Total 9	O 9	0	0
30	Y	6	Total 6	O 6	0	0
30	Z	4	Total 4	O 4	0	0

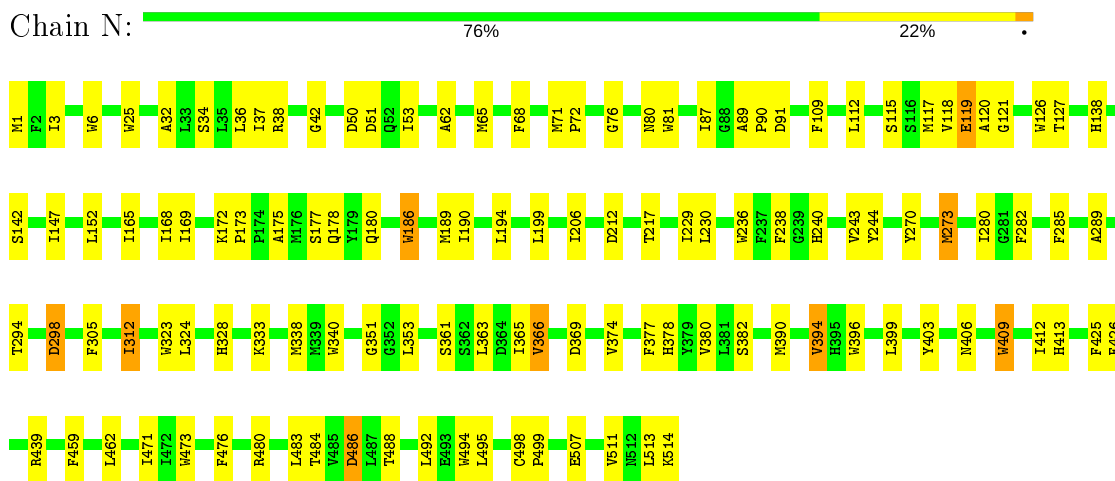
3 Residue-property plots [i](#)

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.

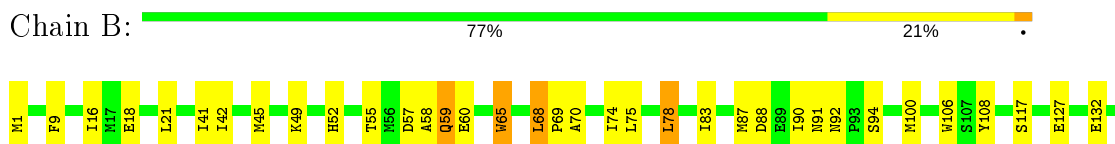
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 1: Cytochrome c oxidase subunit 1

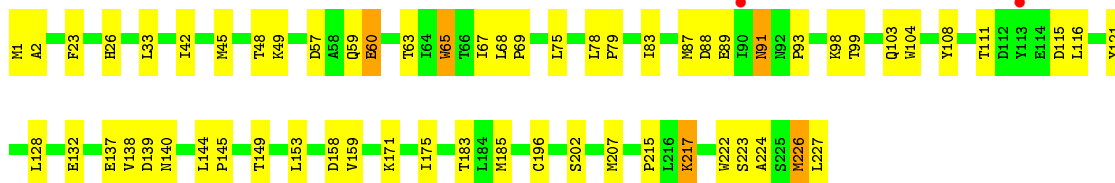
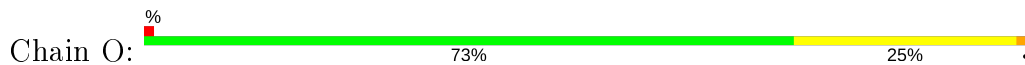


- Molecule 2: Cytochrome c oxidase subunit 2

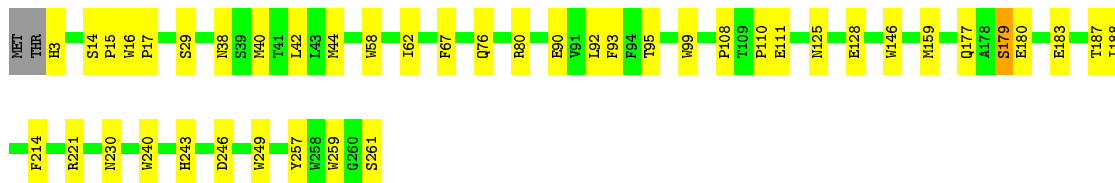
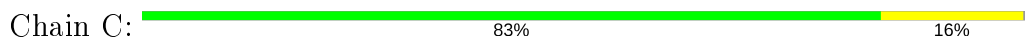




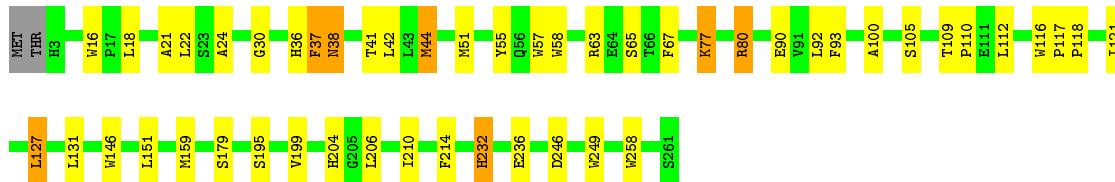
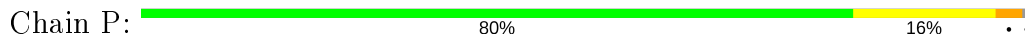
• Molecule 2: Cytochrome c oxidase subunit 2



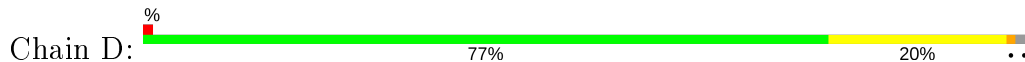
• Molecule 3: Cytochrome c oxidase subunit 3



• Molecule 3: Cytochrome c oxidase subunit 3



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

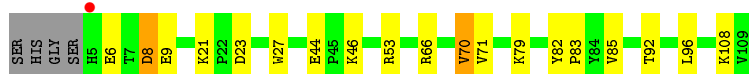
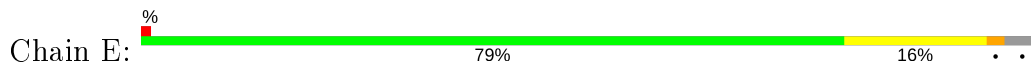


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial





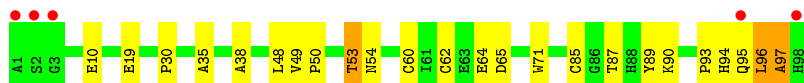
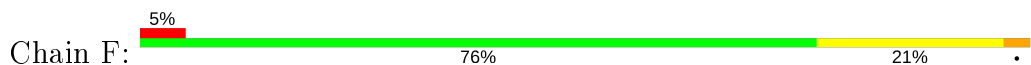
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



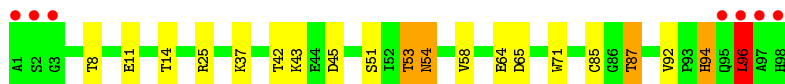
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



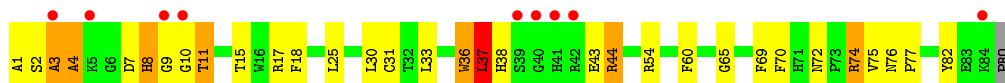
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



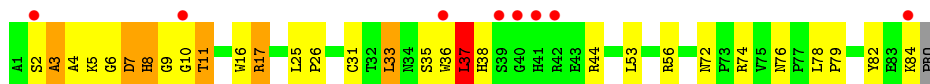
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



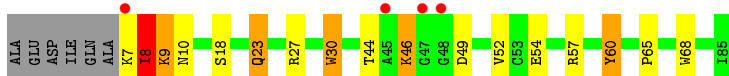
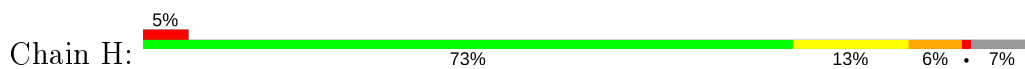
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



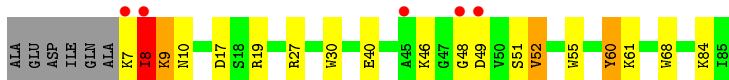
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



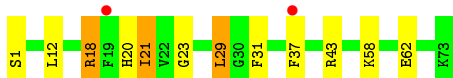
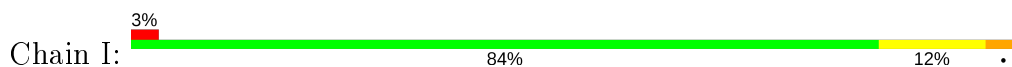
- Molecule 8: Cytochrome c oxidase subunit 6B1



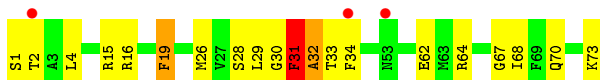
- Molecule 8: Cytochrome c oxidase subunit 6B1



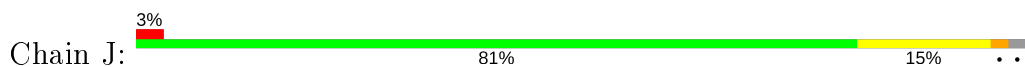
- Molecule 9: Cytochrome c oxidase subunit 6C



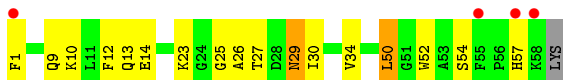
- Molecule 9: Cytochrome c oxidase subunit 6C



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



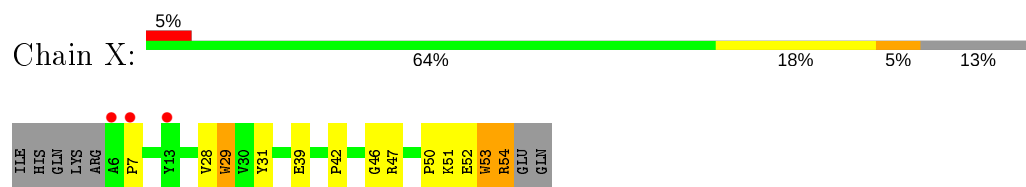
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



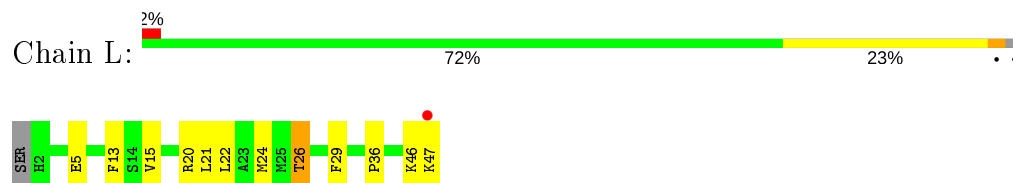
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



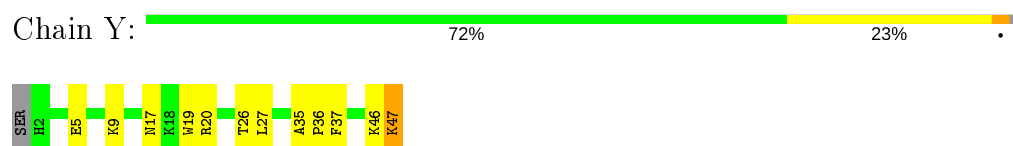
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



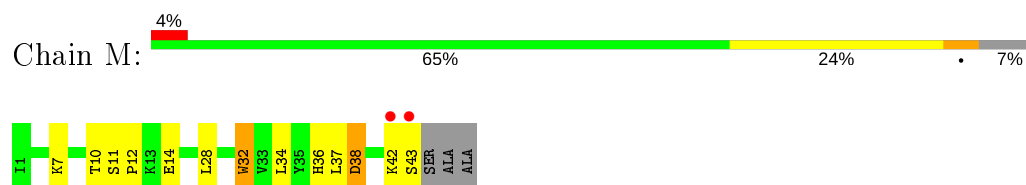
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



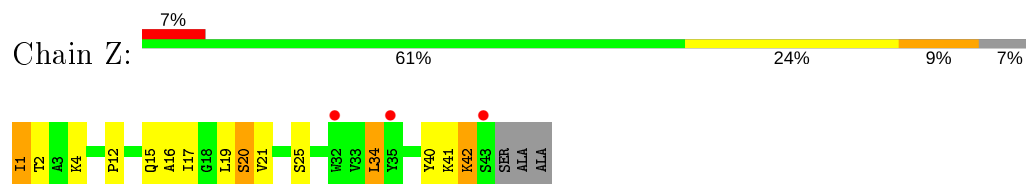
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	185.85Å 209.49Å 179.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 14.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.40) 98.2 (14.99-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.182 , 0.230 0.182 , 0.230	Depositor DCC
R_{free} test set	13569 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtrriage
Anisotropy	0.221	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.045 for l,-k,h	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31717	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, EDO, PGV, TPO, UNX, CUA, NA, FME, CU, DMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.91	10/4164 (0.2%)	0.89	4/5689 (0.1%)
1	N	0.86	11/4156 (0.3%)	0.82	0/5678
2	B	0.81	2/1860 (0.1%)	0.90	1/2534 (0.0%)
2	O	0.73	2/1860 (0.1%)	0.83	0/2534
3	C	0.92	7/2197 (0.3%)	0.81	0/3005
3	P	0.89	4/2197 (0.2%)	0.80	0/3005
4	D	0.82	4/1229 (0.3%)	0.79	0/1658
4	Q	0.76	4/1229 (0.3%)	0.74	0/1658
5	E	0.67	1/871 (0.1%)	0.80	0/1182
5	R	0.65	0/871	0.74	0/1182
6	F	0.74	1/765 (0.1%)	0.86	2/1038 (0.2%)
6	S	0.72	0/765	0.82	1/1038 (0.1%)
7	G	0.86	1/690 (0.1%)	0.87	1/937 (0.1%)
7	T	0.80	1/690 (0.1%)	0.83	1/937 (0.1%)
8	H	0.85	2/682 (0.3%)	0.86	0/921
8	U	0.79	3/682 (0.4%)	0.79	0/921
9	I	0.69	0/605	0.83	0/802
9	V	0.60	0/605	0.80	1/802 (0.1%)
10	J	0.72	0/471	0.75	0/636
10	W	0.66	1/471 (0.2%)	0.77	0/636
11	K	0.81	1/398 (0.3%)	0.76	0/546
11	X	0.80	2/398 (0.5%)	0.75	0/546
12	L	0.80	0/393	0.76	0/526
12	Y	0.75	1/393 (0.3%)	0.75	0/526
13	M	0.81	1/345 (0.3%)	0.78	0/470
13	Z	0.68	0/345	0.75	0/470
All	All	0.82	59/29332 (0.2%)	0.82	11/39877 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
7	T	0	2
All	All	0	3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	58	TRP	CD2-CE2	7.46	1.50	1.41
1	N	126	TRP	CD2-CE2	7.33	1.50	1.41
1	A	396	TRP	CD2-CE2	6.55	1.49	1.41
2	B	106	TRP	CD2-CE2	6.42	1.49	1.41
1	N	340	TRP	CD2-CE2	6.38	1.49	1.41
2	O	65	TRP	CD2-CE2	6.36	1.49	1.41
6	F	71	TRP	CD2-CE2	6.27	1.48	1.41
1	A	275	TRP	CD2-CE2	6.22	1.48	1.41
7	G	36	TRP	CD2-CE2	6.13	1.48	1.41
1	A	409	TRP	CD2-CE2	6.12	1.48	1.41
1	N	186	TRP	CD2-CE2	6.12	1.48	1.41
3	C	58	TRP	CD2-CE2	6.08	1.48	1.41
2	B	65	TRP	CD2-CE2	6.02	1.48	1.41
3	C	240	TRP	CD2-CE2	6.01	1.48	1.41
4	Q	138	TRP	CD2-CE2	5.94	1.48	1.41
1	A	81	TRP	CD2-CE2	5.93	1.48	1.41
8	U	30	TRP	CD2-CE2	5.93	1.48	1.41
1	A	323	TRP	CD2-CE2	5.84	1.48	1.41
4	Q	145	TRP	CD2-CE2	5.74	1.48	1.41
1	N	473	TRP	CD2-CE2	5.73	1.48	1.41
11	X	53	TRP	CD2-CE2	5.69	1.48	1.41
1	N	6	TRP	CD2-CE2	5.68	1.48	1.41
11	X	29	TRP	CD2-CE2	5.63	1.48	1.41
1	N	323	TRP	CD2-CE2	5.60	1.48	1.41
3	C	249	TRP	CD2-CE2	5.59	1.48	1.41
4	Q	78	TRP	CD2-CE2	5.58	1.48	1.41
1	N	236	TRP	CD2-CE2	5.54	1.48	1.41
1	A	186	TRP	CD2-CE2	5.54	1.48	1.41
11	K	53	TRP	CD2-CE2	5.53	1.48	1.41
8	H	68	TRP	CD2-CE2	5.53	1.48	1.41
5	E	27	TRP	CD2-CE2	5.52	1.48	1.41
1	A	236	TRP	CD2-CE2	5.51	1.48	1.41
3	P	16	TRP	CD2-CE2	5.46	1.48	1.41
3	C	146	TRP	CD2-CE2	5.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	36	TRP	CD2-CE2	5.38	1.47	1.41
2	O	222	TRP	CD2-CE2	5.38	1.47	1.41
1	A	103	TRP	CD2-CE2	5.37	1.47	1.41
13	M	32	TRP	CD2-CE2	5.30	1.47	1.41
8	U	68	TRP	CD2-CE2	5.29	1.47	1.41
4	D	98	TRP	CD2-CE2	5.28	1.47	1.41
12	Y	19	TRP	CD2-CE2	5.26	1.47	1.41
3	C	259	TRP	CD2-CE2	5.25	1.47	1.41
3	P	258	TRP	CD2-CE2	5.24	1.47	1.41
3	C	16	TRP	CD2-CE2	5.22	1.47	1.41
4	D	138	TRP	CD2-CE2	5.20	1.47	1.41
1	N	396	TRP	CD2-CE2	5.17	1.47	1.41
1	N	25	TRP	CD2-CE2	5.17	1.47	1.41
4	D	48	TRP	CD2-CE2	5.17	1.47	1.41
8	U	55	TRP	CD2-CE2	5.12	1.47	1.41
1	N	81	TRP	CD2-CE2	5.12	1.47	1.41
4	Q	115	TRP	CD2-CE2	5.12	1.47	1.41
4	D	78	TRP	CD2-CE2	5.11	1.47	1.41
3	P	57	TRP	CD2-CE2	5.09	1.47	1.41
3	C	99	TRP	CD2-CE2	5.06	1.47	1.41
8	H	30	TRP	CD2-CE2	5.06	1.47	1.41
1	A	450	TRP	CD2-CE2	5.01	1.47	1.41
10	W	52	TRP	CD2-CE2	5.01	1.47	1.41
1	A	288	TRP	CD2-CE2	5.01	1.47	1.41
1	N	409	TRP	CD2-CE2	5.00	1.47	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD1	7.54	125.08	118.30
1	A	438	ARG	NE-CZ-NH1	-6.50	117.05	120.30
6	S	96	LEU	CA-CB-CG	6.36	129.92	115.30
7	G	37	LEU	CA-CB-CG	6.03	129.17	115.30
6	F	48	LEU	CB-CG-CD2	-6.00	100.81	111.00
2	B	139	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	100	MET	CG-SD-CE	5.53	109.05	100.20
9	V	31	PHE	N-CA-C	-5.52	96.10	111.00
6	F	96	LEU	CA-CB-CG	5.34	127.59	115.30
7	T	37	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	310	MET	CA-CB-CG	-5.08	104.66	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	11	TPO	Peptide
7	T	10	GLY	Peptide
7	T	11	TPO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4030	0	4009	73	0
1	N	4027	0	4002	99	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	38	0
3	C	2110	0	2027	31	0
3	P	2110	0	2027	40	0
4	D	1195	0	1183	21	0
4	Q	1195	0	1183	31	0
5	E	852	0	845	8	0
5	R	852	0	845	21	0
6	F	748	0	728	13	0
6	S	748	0	728	18	0
7	G	675	0	643	29	0
7	T	675	0	643	23	0
8	H	662	0	623	13	0
8	U	662	0	623	9	0
9	I	601	0	613	8	0
9	V	601	0	613	23	0
10	J	460	0	459	8	0
10	W	460	0	459	11	0
11	K	384	0	366	6	0
11	X	384	0	366	12	0
12	L	380	0	380	12	0
12	Y	380	0	380	13	0
13	M	335	0	352	9	0
13	Z	335	0	352	15	0
14	A	120	0	108	12	0
14	N	120	0	108	13	0
15	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	0	0
19	A	63	0	110	3	0
19	D	63	0	110	1	0
19	L	63	0	110	4	0
19	N	189	0	330	11	0
20	A	102	0	152	3	0
20	C	102	0	152	0	0
20	G	51	0	76	2	0
20	N	102	0	152	8	0
20	P	51	0	76	3	0
21	A	20	0	30	9	0
21	B	8	0	12	1	0
21	C	12	0	18	0	0
21	F	4	0	6	0	0
21	G	4	0	6	0	0
21	K	12	0	18	0	0
21	L	4	0	6	0	0
21	N	4	0	6	1	0
21	T	4	0	6	1	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	1	0
23	C	58	0	78	3	0
23	J	29	0	39	1	0
23	O	29	0	39	1	0
23	P	58	0	78	2	0
23	W	29	0	38	1	0
24	B	52	0	80	12	0
24	R	52	0	80	6	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	200	0	312	15	0
26	P	100	0	156	7	0
26	T	100	0	156	13	0
27	C	53	0	77	3	0
27	G	106	0	154	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	P	53	0	77	4	0
27	T	106	0	154	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	M	33	0	42	1	0
29	Z	33	0	42	1	0
30	A	125	0	0	22	0
30	B	78	0	0	6	0
30	C	70	0	0	18	0
30	D	41	0	0	2	0
30	E	24	0	0	2	0
30	F	36	0	0	2	0
30	G	31	0	0	2	0
30	H	33	0	0	2	0
30	I	12	0	0	0	0
30	J	19	0	0	2	0
30	K	19	0	0	3	0
30	L	14	0	0	2	0
30	M	15	0	0	1	0
30	N	117	0	0	16	0
30	O	77	0	0	8	0
30	P	54	0	0	5	0
30	Q	29	0	0	7	0
30	R	29	0	0	3	0
30	S	43	0	0	4	0
30	T	20	0	0	6	0
30	U	31	0	0	3	0
30	V	19	0	0	4	0
30	W	17	0	0	1	0
30	X	9	0	0	4	0
30	Y	6	0	0	1	0
30	Z	4	0	0	0	0
All	All	31717	0	31348	645	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 10.

All (645) 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:N:240:HIS:NE2	1:N:244:TYR:CE2	1.73	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:HIS:NE2	1:A:244:TYR:HE2	1.01	1.42
1:A:240:HIS:NE2	1:A:244:TYR:CE2	1.78	1.30
1:A:240:HIS:CD2	1:A:244:TYR:HE2	1.49	1.29
1:N:240:HIS:NE2	1:N:244:TYR:HE2	0.80	1.28
5:R:50:ALA:HB3	30:R:303:HOH:O	1.43	1.18
6:S:85:CYS:SG	6:S:87:THR:CG2	2.30	1.18
9:V:26:MET:O	9:V:30:GLY:HA3	1.44	1.15
1:N:298:ASP:HB2	30:N:724:HOH:O	1.49	1.11
6:S:85:CYS:SG	6:S:87:THR:HG22	1.90	1.10
3:P:118:PRO:HD2	30:P:403:HOH:O	1.53	1.08
8:H:9:LYS:HD3	8:H:10:ASN:H	1.12	1.08
5:R:41:LEU:HD23	24:R:201:PSC:H082	1.31	1.08
26:C:307:CDL:H511	26:C:307:CDL:H221	1.12	1.05
1:A:240:HIS:CD2	1:A:244:TYR:CE2	2.33	1.03
1:N:50:ASP:HB3	1:N:53:ILE:HD12	1.39	1.02
2:O:223:SER:HA	30:O:414:HOH:O	1.61	1.01
6:F:19:GLU:HG2	30:F:231:HOH:O	1.60	1.01
24:R:201:PSC:H211	24:R:201:PSC:H031	1.44	0.99
9:V:15:ARG:HD3	30:V:113:HOH:O	1.62	0.98
1:A:104:LEU:HB2	30:A:788:HOH:O	1.64	0.97
1:N:353:LEU:HA	30:N:715:HOH:O	1.65	0.96
26:C:307:CDL:H221	26:C:307:CDL:C51	1.94	0.96
7:G:76:ASN:HD21	27:G:101:PEK:HN2	1.14	0.95
6:S:85:CYS:SG	6:S:87:THR:HG23	2.04	0.95
19:N:609:TGL:OC1	30:N:701:HOH:O	1.84	0.94
8:H:9:LYS:HD3	8:H:10:ASN:N	1.82	0.94
2:B:57:ASP:H	24:B:303:PSC:H241	1.33	0.94
12:L:47:LYS:HB2	13:M:43:SER:HB3	1.48	0.94
3:C:90:GLU:HA	30:C:413:HOH:O	1.67	0.92
1:N:240:HIS:CE1	1:N:244:TYR:HE2	1.86	0.92
14:N:601:HEA:HMC1	14:N:601:HEA:HBC1	1.52	0.92
1:N:439:ARG:NH2	30:N:702:HOH:O	2.01	0.92
6:S:54:ASN:H	6:S:54:ASN:HD22	1.18	0.91
30:A:799:HOH:O	12:L:36:PRO:HB2	1.72	0.89
1:N:240:HIS:CD2	1:N:244:TYR:HE2	1.88	0.89
19:N:609:TGL:CC1	30:N:701:HOH:O	2.19	0.89
2:B:90:ILE:HA	30:B:464:HOH:O	1.71	0.88
4:Q:107:ILE:HB	30:Q:202:HOH:O	1.73	0.88
11:K:24:PHE:O	11:K:28:VAL:HG12	1.74	0.87
11:X:42:PRO:HD2	30:X:101:HOH:O	1.72	0.87
9:V:32:ALA:O	30:V:101:HOH:O	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:607:TGL:H201	19:A:607:TGL:H361	1.55	0.86
7:G:10:GLY:HA3	1:N:177:SER:HB2	1.55	0.86
30:A:751:HOH:O	8:H:23:GLN:HG3	1.74	0.86
1:A:39:ALA:HA	21:A:614:EDO:H21	1.56	0.85
11:K:48:VAL:HB	30:K:207:HOH:O	1.77	0.84
4:Q:93:ALA:HB1	30:X:102:HOH:O	1.76	0.84
26:T:103:CDL:H531	26:T:103:CDL:H241	1.60	0.84
7:G:3:ALA:HB2	27:G:102:PEK:H292	1.60	0.84
1:A:243:VAL:HG21	18:A:606:CMO:C	2.08	0.83
1:N:240:HIS:CD2	1:N:244:TYR:CE2	2.63	0.83
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.44	0.82
19:N:611:TGL:HC42	19:N:611:TGL:OC1	1.80	0.81
19:N:611:TGL:H231	19:N:611:TGL:H282	1.62	0.81
9:V:30:GLY:C	9:V:32:ALA:N	2.28	0.81
20:N:607:PGV:H011	13:Z:15:GLN:HE22	1.43	0.81
2:O:226:MET:HB2	30:O:414:HOH:O	1.81	0.81
7:T:79:PRO:HD3	30:T:201:HOH:O	1.80	0.80
3:C:90:GLU:HG2	30:C:413:HOH:O	1.80	0.80
7:G:9:GLY:HA3	1:N:172:LYS:HZ1	1.47	0.80
26:C:307:CDL:H542	26:C:307:CDL:H771	1.64	0.80
26:T:103:CDL:H222	26:T:103:CDL:H511	1.63	0.79
1:A:513:LEU:O	1:A:514:LYS:HB2	1.82	0.79
21:A:613:EDO:H11	11:K:39:GLU:H	1.45	0.79
9:V:26:MET:O	9:V:30:GLY:CA	2.30	0.79
24:B:303:PSC:H272	24:B:303:PSC:H202	1.64	0.78
1:A:61:HIS:CD2	30:A:754:HOH:O	2.36	0.78
2:B:210:VAL:HG13	30:B:415:HOH:O	1.84	0.78
3:C:62:ILE:HG12	30:C:404:HOH:O	1.84	0.77
12:Y:17:ASN:HB3	12:Y:20:ARG:NH1	2.00	0.77
6:S:54:ASN:ND2	6:S:54:ASN:H	1.82	0.76
9:V:29:LEU:O	9:V:32:ALA:HB2	1.85	0.75
6:F:64:GLU:O	6:F:65:ASP:HB2	1.84	0.75
7:T:17:ARG:HH22	27:T:102:PEK:H041	1.51	0.75
5:R:31:LYS:HE2	30:S:229:HOH:O	1.85	0.74
12:L:47:LYS:HB2	13:M:43:SER:CB	2.18	0.74
1:N:513:LEU:O	1:N:514:LYS:HB2	1.86	0.74
11:X:29:TRP:HA	30:X:102:HOH:O	1.88	0.73
1:N:406:ASN:HD21	20:N:607:PGV:C03	2.00	0.73
13:Z:1:ILE:O	13:Z:1:ILE:HG13	1.86	0.73
10:W:30:ILE:O	10:W:34:VAL:HG23	1.88	0.73
26:T:103:CDL:H381	26:T:103:CDL:H141	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:92:VAL:HG11	30:S:240:HOH:O	1.89	0.72
3:C:221:ARG:CZ	30:C:404:HOH:O	2.38	0.72
1:A:104:LEU:CB	30:A:788:HOH:O	2.29	0.72
26:C:307:CDL:C22	26:C:307:CDL:H511	2.06	0.72
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.72	0.71
1:N:406:ASN:HD21	20:N:607:PGV:H031	1.53	0.71
7:G:44:ARG:HG2	30:G:224:HOH:O	1.90	0.71
14:A:601:HEA:HBC1	14:A:601:HEA:HMC1	1.71	0.71
6:F:93:PRO:HA	30:F:225:HOH:O	1.90	0.71
14:A:602:HEA:HMC1	14:A:602:HEA:HBC1	1.73	0.71
26:C:307:CDL:H871	27:G:102:PEK:H322	1.72	0.71
1:N:240:HIS:CE1	1:N:244:TYR:CE2	2.69	0.71
2:O:57:ASP:HB2	24:R:201:PSC:H202	1.72	0.70
12:Y:17:ASN:HB3	12:Y:20:ARG:HH12	1.54	0.70
1:N:115:SER:O	1:N:121:GLY:HA2	1.92	0.70
2:O:139:ASP:OD1	2:O:140:ASN:N	2.23	0.70
2:O:217:LYS:NZ	2:O:217:LYS:H	1.89	0.70
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.74	0.70
1:N:50:ASP:HB3	1:N:53:ILE:CD1	2.21	0.69
1:A:62:ALA:HA	30:A:754:HOH:O	1.91	0.69
8:U:9:LYS:HB2	30:U:114:HOH:O	1.92	0.69
1:N:65:MET:HB3	14:N:601:HEA:CBC	2.23	0.69
1:N:406:ASN:ND2	20:N:607:PGV:H031	2.07	0.69
3:P:18:LEU:O	3:P:22:LEU:HD12	1.93	0.68
20:A:608:PGV:H332	30:C:413:HOH:O	1.93	0.68
27:P:302:PEK:H131	20:P:303:PGV:H181	1.75	0.68
12:Y:47:LYS:HB2	13:Z:42:LYS:CD	2.23	0.68
7:T:72:ASN:H	7:T:76:ASN:HD22	1.39	0.68
9:V:30:GLY:O	9:V:31:PHE:C	2.33	0.68
10:W:9:GLN:O	10:W:13:GLN:HG3	1.94	0.68
4:D:112:GLU:HB3	30:D:328:HOH:O	1.93	0.67
6:S:54:ASN:N	6:S:54:ASN:HD22	1.86	0.67
1:A:32:ALA:HB1	30:A:799:HOH:O	1.94	0.67
2:B:18:GLU:OE1	21:B:305:EDO:O1	2.11	0.67
14:A:601:HEA:H212	30:A:743:HOH:O	1.95	0.66
9:V:29:LEU:C	9:V:32:ALA:HB2	2.15	0.66
7:G:3:ALA:HA	27:G:102:PEK:H331	1.78	0.66
26:C:307:CDL:OA7	26:C:307:CDL:H351	1.96	0.66
1:N:165:ILE:HA	30:N:805:HOH:O	1.93	0.66
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.31	0.66
1:A:156:SER:HB2	30:A:788:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:307:CDL:OB4	26:C:307:CDL:H161	1.96	0.66
2:B:127:GLU:HG2	30:B:432:HOH:O	1.95	0.65
14:N:601:HEA:HMC1	14:N:601:HEA:CBC	2.26	0.65
1:A:505:PHE:HA	30:A:702:HOH:O	1.96	0.65
4:D:109:HIS:HD2	30:D:317:HOH:O	1.79	0.65
4:Q:121:LYS:HB2	11:X:50:PRO:HB3	1.78	0.65
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.61	0.65
3:C:257:TYR:O	3:C:261:SER:HB3	1.97	0.64
2:O:217:LYS:HZ3	2:O:217:LYS:H	1.42	0.64
7:G:72:ASN:H	7:G:76:ASN:HD22	1.45	0.64
1:N:312:ILE:O	1:N:312:ILE:HD13	1.97	0.64
27:C:306:PEK:H031	30:C:412:HOH:O	1.97	0.64
9:V:28:SER:C	9:V:30:GLY:H	1.98	0.64
3:P:36:HIS:O	3:P:38:ASN:N	2.27	0.64
1:N:147:ILE:HG23	1:N:206:ILE:HD12	1.78	0.63
2:O:207:MET:HG3	30:O:402:HOH:O	1.98	0.63
1:A:455:SER:HB3	21:A:614:EDO:H12	1.79	0.63
1:N:353:LEU:HD23	30:N:715:HOH:O	1.97	0.63
1:N:488:THR:HB	1:N:495:LEU:HD13	1.79	0.63
1:A:24:ALA:HB2	30:A:723:HOH:O	1.98	0.62
3:P:36:HIS:C	3:P:38:ASN:H	2.02	0.62
26:C:307:CDL:H541	26:C:307:CDL:H752	1.79	0.62
2:O:196:CYS:HB3	30:O:402:HOH:O	1.98	0.62
13:Z:17:ILE:O	13:Z:21:VAL:HG23	1.98	0.62
9:V:30:GLY:C	9:V:32:ALA:H	2.00	0.62
1:N:484:THR:HB	13:Z:2:THR:OG1	2.00	0.62
11:X:39:GLU:HB3	30:X:106:HOH:O	1.98	0.62
1:A:240:HIS:O	1:A:243:VAL:HG22	1.98	0.61
4:Q:108:PRO:HD2	30:Q:202:HOH:O	1.98	0.61
12:Y:47:LYS:HB2	13:Z:42:LYS:HD3	1.81	0.61
7:G:17:ARG:HD3	30:O:433:HOH:O	2.00	0.61
27:P:302:PEK:HN2	7:T:76:ASN:HD21	1.48	0.61
26:C:307:CDL:H241	26:C:307:CDL:H511	1.83	0.61
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.83	0.61
6:F:85:CYS:SG	6:F:87:THR:HG23	2.41	0.60
14:N:602:HEA:C26	30:N:715:HOH:O	2.49	0.60
26:T:103:CDL:C53	26:T:103:CDL:H241	2.31	0.60
1:N:175:ALA:HB3	1:N:511:VAL:HG12	1.83	0.60
7:G:10:GLY:HA3	1:N:177:SER:CB	2.31	0.60
4:Q:78:TRP:O	4:Q:82:VAL:HG23	2.00	0.60
4:Q:26:ASP:OD1	4:Q:26:ASP:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.37	0.60
14:A:601:HEA:C1D	30:A:754:HOH:O	2.49	0.60
12:L:20:ARG:NH2	19:L:101:TGL:HC31	2.16	0.60
6:S:43:LYS:HG3	30:S:236:HOH:O	2.02	0.60
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.83	0.60
1:A:488:THR:HB	1:A:495:LEU:HD11	1.84	0.59
3:C:125:ASN:HB3	3:C:128:GLU:OE2	2.01	0.59
3:C:221:ARG:NH2	30:C:404:HOH:O	2.35	0.59
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.83	0.59
1:N:68:PHE:HE2	1:N:112:LEU:HD22	1.67	0.59
3:P:146:TRP:HB2	7:T:16:TRP:HB3	1.84	0.59
10:J:4:ARG:HD2	10:J:7:GLU:OE1	2.03	0.59
13:Z:16:ALA:O	13:Z:20:SER:OG	2.20	0.59
3:P:246:ASP:HB2	30:P:442:HOH:O	2.03	0.59
30:A:812:HOH:O	26:T:103:CDL:HB22	2.03	0.59
1:N:280:ILE:HG12	1:N:312:ILE:HD11	1.83	0.58
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.84	0.58
1:A:156:SER:CB	30:A:788:HOH:O	2.49	0.58
5:E:71:VAL:HG11	5:E:85:VAL:HG11	1.85	0.58
1:N:390:MET:O	1:N:394:VAL:HG13	2.03	0.58
7:T:31:CYS:SG	26:T:103:CDL:H532	2.42	0.58
30:B:404:HOH:O	9:I:23:GLY:HA3	2.04	0.58
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.84	0.58
5:R:80:GLU:CD	5:R:80:GLU:H	2.06	0.58
2:B:52:HIS:HE1	24:B:303:PSC:H201	1.69	0.58
5:E:8:ASP:HB2	30:E:219:HOH:O	2.04	0.58
3:C:188:ILE:HG22	27:G:101:PEK:O13	2.04	0.58
20:N:607:PGV:H202	13:Z:12:PRO:HG3	1.85	0.57
1:N:37:ILE:CG2	14:N:601:HEA:HMA	2.34	0.57
1:N:476:PHE:HZ	19:N:611:TGL:H251	1.70	0.57
1:A:27:GLY:HA3	30:A:743:HOH:O	2.02	0.57
1:A:488:THR:HB	1:A:495:LEU:CD1	2.35	0.57
8:H:7:LYS:C	8:H:8:ILE:HG13	2.26	0.56
6:S:64:GLU:HB2	30:S:230:HOH:O	2.05	0.56
10:W:9:GLN:O	10:W:13:GLN:CG	2.53	0.56
1:N:142:SER:HB2	30:N:785:HOH:O	2.03	0.56
12:Y:46:LYS:HA	30:Y:102:HOH:O	2.04	0.56
2:B:41:ILE:O	2:B:45:MET:HG2	2.06	0.56
1:A:251:PHE:CD2	1:A:319:LYS:HE2	2.41	0.56
1:A:43:GLN:HG2	4:D:104:TYR:CD1	2.40	0.56
3:P:206:LEU:HD22	27:P:302:PEK:H102	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:56:ARG:NH2	30:T:201:HOH:O	2.39	0.56
1:A:449:MET:HE2	11:K:40:TRP:HB3	1.87	0.56
9:V:31:PHE:C	9:V:31:PHE:CD1	2.78	0.56
4:Q:108:PRO:CD	30:Q:202:HOH:O	2.54	0.56
7:G:7:ASP:O	7:G:8:HIS:HB2	2.06	0.56
3:C:3:HIS:HB2	30:C:444:HOH:O	2.05	0.55
7:G:31:CYS:HA	30:G:207:HOH:O	2.05	0.55
4:Q:101:HIS:HB3	30:Q:218:HOH:O	2.06	0.55
4:Q:39:ALA:O	4:Q:42:GLU:HB2	2.05	0.55
3:P:116:TRP:HA	3:P:117:PRO:C	2.26	0.55
3:P:118:PRO:CD	30:P:403:HOH:O	2.27	0.55
7:G:8:HIS:HE1	27:G:102:PEK:H051	1.71	0.55
11:K:44:PRO:HB2	30:K:207:HOH:O	2.07	0.55
2:O:98:LYS:HG2	2:O:153:LEU:HB2	1.89	0.55
7:G:8:HIS:CE1	27:G:102:PEK:H051	2.41	0.55
19:N:609:TGL:HA71	19:N:609:TGL:H222	1.88	0.55
23:P:306:CHD:H212	23:P:306:CHD:H12	1.89	0.55
10:W:26:ALA:O	10:W:30:ILE:HD13	2.07	0.55
9:V:31:PHE:CD1	9:V:32:ALA:N	2.74	0.54
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.73	0.54
9:V:30:GLY:O	9:V:32:ALA:N	2.39	0.54
2:B:217:LYS:HG3	30:B:458:HOH:O	2.06	0.54
3:C:246:ASP:HB2	30:C:455:HOH:O	2.06	0.54
3:C:90:GLU:CA	30:C:413:HOH:O	2.37	0.54
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.90	0.54
7:T:78:LEU:HB3	7:T:79:PRO:HD2	1.90	0.54
1:A:409:TRP:HB3	1:A:471:ILE:HG12	1.89	0.54
1:A:240:HIS:CD2	1:A:244:TYR:CD2	2.94	0.54
2:B:9:PHE:HB2	2:B:21:LEU:HD21	1.90	0.54
8:U:40:GLU:HB2	30:U:105:HOH:O	2.08	0.54
9:V:64:ARG:NH1	9:V:73:LYS:O	2.40	0.54
3:P:65:SER:HB2	20:P:303:PGV:H041	1.90	0.53
26:C:307:CDL:H662	20:G:103:PGV:H172	1.90	0.53
1:N:483:LEU:HG	13:Z:4:LYS:HG2	1.90	0.53
12:Y:20:ARG:CZ	12:Y:20:ARG:HB3	2.38	0.53
1:N:127:THR:HG23	30:N:702:HOH:O	2.07	0.53
1:A:51:ASP:HB2	2:B:202:SER:O	2.09	0.53
2:O:91:ASN:HD22	2:O:93:PRO:HD3	1.72	0.53
9:V:19:PHE:CD1	9:V:19:PHE:C	2.82	0.53
3:C:67:PHE:HE2	26:C:303:CDL:H1	1.74	0.53
20:N:608:PGV:H51	20:N:608:PGV:H251	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:89:GLU:O	2:O:91:ASN:OD1	2.27	0.53
7:T:3:ALA:HB2	27:T:101:PEK:H351	1.89	0.53
4:D:110:THR:HG22	4:D:115:TRP:CE2	2.44	0.53
1:N:486:ASP:N	1:N:486:ASP:OD1	2.38	0.53
1:A:502:TYR:OH	21:A:612:EDO:H22	2.09	0.53
7:G:72:ASN:N	7:G:76:ASN:HD22	2.07	0.53
7:G:37:LEU:O	7:G:38:HIS:ND1	2.42	0.52
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.43	0.52
26:P:304:CDL:H331	26:P:304:CDL:H432	1.90	0.52
10:W:29:ASN:HD22	10:W:29:ASN:H	1.57	0.52
1:A:177:SER:H	1:A:180:GLN:NE2	2.07	0.52
1:N:365:ILE:HB	30:N:704:HOH:O	2.09	0.52
14:N:601:HEA:HBC1	14:N:601:HEA:CMC	2.31	0.52
5:R:102:GLU:N	5:R:102:GLU:OE1	2.40	0.52
23:J:101:CHD:H183	23:J:101:CHD:H212	1.91	0.52
7:T:37:LEU:HD21	26:T:103:CDL:H401	1.91	0.52
5:R:99:SER:HB2	5:R:104:LEU:HD21	1.91	0.52
26:C:307:CDL:H712	26:C:307:CDL:H522	1.92	0.52
7:G:1:ALA:H1	20:G:103:PGV:H301	1.74	0.52
1:N:87:ILE:O	1:N:173:PRO:HD3	2.09	0.52
21:A:613:EDO:O2	4:D:100:LYS:HE2	2.10	0.52
4:D:99:GLU:O	4:D:103:VAL:HB	2.09	0.52
2:B:90:ILE:H	2:B:90:ILE:HD12	1.74	0.52
2:O:63:THR:O	2:O:67:ILE:HG12	2.09	0.52
3:P:18:LEU:HG	3:P:22:LEU:CD1	2.40	0.52
5:R:108:LYS:O	5:R:109:VAL:C	2.48	0.52
10:J:54:SER:O	12:L:46:LYS:HE3	2.10	0.52
1:N:459:PHE:O	1:N:462:LEU:HB3	2.09	0.52
7:G:4:ALA:HB1	1:N:282:PHE:HA	1.91	0.51
2:O:139:ASP:O	9:V:70:GLN:NE2	2.43	0.51
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.90	0.51
8:U:7:LYS:C	8:U:8:ILE:HG13	2.30	0.51
4:D:130:PRO:HA	4:D:135:SER:HB2	1.92	0.51
3:P:63:ARG:HE	26:P:304:CDL:HA22	1.75	0.51
2:B:108:TYR:O	2:B:117:SER:HA	2.11	0.51
7:T:8:HIS:CE1	27:T:101:PEK:H312	2.46	0.51
9:V:28:SER:C	9:V:30:GLY:N	2.64	0.51
11:X:42:PRO:O	11:X:47:ARG:NH2	2.43	0.51
1:A:177:SER:H	1:A:180:GLN:HE21	1.59	0.50
7:G:60:PHE:O	7:G:65:GLY:HA2	2.12	0.50
1:A:393:PHE:O	1:A:397:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:492:LEU:HD13	6:S:71:TRP:CD2	2.47	0.50
14:A:602:HEA:HMC1	14:A:602:HEA:CBC	2.40	0.50
4:D:34:SER:H	4:D:37:GLN:NE2	2.08	0.50
2:O:83:ILE:O	2:O:87:MET:HG3	2.11	0.50
1:A:156:SER:CA	30:A:788:HOH:O	2.60	0.50
1:N:366:VAL:N	30:N:704:HOH:O	2.34	0.50
1:A:14:ASP:O	1:A:17:THR:HB	2.11	0.50
5:R:109:VAL:O	5:R:109:VAL:HG23	2.10	0.50
1:N:68:PHE:O	1:N:72:PRO:HG2	2.11	0.50
5:R:53:ARG:NH2	5:R:92:THR:HG23	2.27	0.50
1:A:201:VAL:HA	30:A:720:HOH:O	2.10	0.50
3:C:187:THR:HG22	27:G:101:PEK:H051	1.94	0.50
12:L:15:VAL:HG12	12:L:21:LEU:HD22	1.94	0.50
14:N:602:HEA:H263	30:N:715:HOH:O	2.12	0.50
1:N:76:GLY:O	1:N:80:ASN:HB2	2.11	0.50
8:H:10:ASN:HA	30:H:117:HOH:O	2.11	0.49
3:P:18:LEU:HG	3:P:22:LEU:HD12	1.94	0.49
5:E:21:LYS:HE2	5:E:23:ASP:OD1	2.12	0.49
13:M:28:LEU:HD23	29:M:101:DMU:H7	1.94	0.49
1:N:117:MET:HB3	10:W:54:SER:OG	2.12	0.49
1:N:168:ILE:HD12	30:N:805:HOH:O	2.13	0.49
1:N:186:TRP:O	1:N:190:ILE:HG13	2.12	0.49
3:P:112:LEU:HB3	3:P:118:PRO:HB3	1.93	0.49
6:S:42:THR:OG1	6:S:45:ASP:HB3	2.12	0.49
10:W:50:LEU:HD22	10:W:50:LEU:O	2.12	0.49
12:Y:26:THR:CG2	13:Z:25:SER:HB3	2.42	0.49
1:A:505:PHE:HD1	30:A:702:HOH:O	1.94	0.49
1:A:52:GLN:O	1:A:56:VAL:HG23	2.12	0.49
2:B:83:ILE:O	2:B:87:MET:HG3	2.12	0.49
1:N:37:ILE:HG22	14:N:601:HEA:HMA	1.93	0.49
4:Q:129:ALA:HB3	4:Q:134:PHE:HB3	1.94	0.49
6:F:64:GLU:O	6:F:65:ASP:CB	2.57	0.49
2:B:136:LEU:HB3	2:B:193:TYR:CD2	2.47	0.49
3:C:180:GLU:HG3	30:C:402:HOH:O	2.13	0.49
23:C:305:CHD:H212	23:C:305:CHD:H12	1.94	0.49
1:N:270:TYR:O	1:N:273:MET:HB2	2.12	0.49
10:W:12:PHE:O	10:W:23:LYS:HE2	2.12	0.49
1:A:199:LEU:N	1:A:200:PRO:CD	2.75	0.49
4:D:33:LEU:HA	4:D:37:GLN:HE21	1.77	0.49
3:P:127:LEU:HD12	3:P:131:LEU:HD22	1.95	0.49
24:R:201:PSC:H252	24:R:201:PSC:H21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:HIS:CB	30:C:444:HOH:O	2.60	0.49
3:P:67:PHE:HE2	26:P:304:CDL:H1	1.77	0.49
12:Y:5:GLU:O	12:Y:9:LYS:HG3	2.12	0.49
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.48
5:R:43:PRO:HG2	5:R:48:ILE:HD11	1.94	0.48
1:A:430:PHE:CE1	19:A:607:TGL:HB22	2.48	0.48
7:G:9:GLY:H	1:N:178:GLN:HE21	1.60	0.48
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.21	0.48
1:N:240:HIS:O	1:N:243:VAL:HG22	2.13	0.48
5:R:40:ASP:H	24:R:201:PSC:H071	1.79	0.48
1:A:380:VAL:O	1:A:384:GLY:HA3	2.14	0.48
3:C:17:PRO:HG2	30:C:445:HOH:O	2.13	0.48
26:T:103:CDL:H331	26:T:103:CDL:OA7	2.13	0.48
7:G:9:GLY:H	1:N:178:GLN:NE2	2.12	0.48
1:N:240:HIS:CD2	1:N:244:TYR:CD2	3.00	0.48
4:Q:131:ILE:HG22	4:Q:132:GLN:HG3	1.96	0.48
2:O:49:LYS:HE2	4:Q:20:ARG:CZ	2.44	0.48
10:W:25:GLY:HA2	30:W:203:HOH:O	2.13	0.48
1:A:189:MET:HG3	1:A:189:MET:O	2.10	0.48
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.48	0.48
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.26	0.48
21:A:614:EDO:H22	4:D:99:GLU:OE1	2.14	0.48
12:L:22:LEU:O	12:L:26:THR:HB	2.13	0.48
2:B:52:HIS:CE1	24:B:303:PSC:H201	2.49	0.48
7:T:78:LEU:HA	30:T:201:HOH:O	2.13	0.48
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.95	0.48
3:P:80:ARG:NH2	3:P:236:GLU:OE1	2.47	0.48
1:A:180:GLN:HB2	1:A:180:GLN:HE21	1.54	0.47
24:B:303:PSC:H011	24:B:303:PSC:H261	1.95	0.47
1:N:324:LEU:HD21	2:O:42:ILE:HG13	1.96	0.47
10:W:29:ASN:HD22	10:W:29:ASN:N	2.12	0.47
1:N:294:THR:HG22	1:N:365:ILE:HD13	1.96	0.47
5:R:72:LYS:NZ	5:R:102:GLU:OE2	2.39	0.47
1:A:21:LEU:HD23	19:L:101:TGL:H211	1.97	0.47
1:A:450:TRP:HA	1:A:450:TRP:CE3	2.50	0.47
26:C:307:CDL:H871	27:G:102:PEK:C32	2.42	0.47
1:N:328:HIS:HB2	2:O:45:MET:SD	2.54	0.47
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.61	0.47
1:N:507:GLU:OE1	6:S:51:SER:HA	2.14	0.47
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.44	0.47
3:C:38:ASN:ND2	30:C:406:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:409:TRP:HB3	1:N:471:ILE:HG12	1.96	0.47
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.50	0.47
23:W:101:CHD:H183	23:W:101:CHD:H222	1.97	0.47
23:C:304:CHD:H12	23:C:304:CHD:H212	1.95	0.47
6:F:96:LEU:O	6:F:97:ALA:HB2	2.14	0.47
1:N:378:HIS:O	1:N:382:SER:HB2	2.15	0.47
14:A:601:HEA:OMA	14:A:601:HEA:HNB	2.15	0.47
7:G:44:ARG:HD2	7:G:74:ARG:O	2.15	0.47
19:N:609:TGL:HC31	30:N:815:HOH:O	2.14	0.47
1:A:278:MET:HB3	21:T:104:EDO:H22	1.97	0.46
9:V:19:PHE:HD1	9:V:19:PHE:C	2.18	0.46
13:Z:34:LEU:HA	13:Z:34:LEU:HD12	1.77	0.46
5:E:53:ARG:NH2	5:E:92:THR:HG23	2.30	0.46
9:I:18:ARG:HB2	9:I:18:ARG:HH11	1.80	0.46
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.46	0.46
4:D:82:VAL:O	4:D:86:MET:HG3	2.14	0.46
6:F:53:THR:HB	6:F:54:ASN:H	1.56	0.46
21:N:612:EDO:C1	13:Z:1:ILE:HG21	2.46	0.46
4:Q:127:LYS:HE2	30:Q:225:HOH:O	2.15	0.46
24:B:303:PSC:C27	24:B:303:PSC:H202	2.39	0.46
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.16	0.46
20:N:608:PGV:H042	20:N:608:PGV:C03	2.45	0.46
5:R:39:TYR:HB3	24:R:201:PSC:H073	1.96	0.46
5:R:25:ASP:HB2	30:R:307:HOH:O	2.14	0.46
2:B:100:MET:HE2	2:B:157:GLU:HG3	1.97	0.46
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.98	0.46
10:J:50:LEU:HD22	10:J:50:LEU:O	2.15	0.46
13:M:38:ASP:HB3	30:M:210:HOH:O	2.15	0.46
1:N:37:ILE:HG21	14:N:601:HEA:HMA	1.97	0.46
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.16	0.46
8:H:44:THR:C	8:H:46:LYS:H	2.19	0.46
9:I:12:LEU:H	9:I:12:LEU:HD12	1.81	0.46
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.71	0.46
3:P:77:LYS:O	3:P:80:ARG:HB2	2.16	0.46
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.97	0.46
2:O:158:ASP:OD1	2:O:159:VAL:N	2.43	0.46
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.83	0.46
3:P:21:ALA:O	3:P:24:ALA:HB3	2.16	0.46
3:P:41:THR:O	3:P:44:MET:HB2	2.15	0.46
7:T:17:ARG:HD2	30:T:206:HOH:O	2.15	0.46
2:O:224:ALA:HA	30:O:466:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:302:PEK:H181	27:P:302:PEK:H101	1.97	0.45
19:A:607:TGL:HC61	19:A:607:TGL:H151	1.97	0.45
3:C:243:HIS:HD2	30:C:430:HOH:O	1.99	0.45
8:U:10:ASN:HA	30:U:115:HOH:O	2.16	0.45
1:A:316:THR:HG21	14:A:602:HEA:H14	1.98	0.45
1:A:43:GLN:HG2	4:D:104:TYR:CE1	2.52	0.45
9:I:29:LEU:HD13	9:I:29:LEU:HA	1.71	0.45
11:K:12:LYS:HB2	11:K:12:LYS:NZ	2.31	0.45
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.51	0.45
7:G:2:SER:O	7:G:3:ALA:HB2	2.16	0.45
8:H:60:TYR:C	8:H:60:TYR:CD1	2.90	0.45
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.99	0.45
4:Q:147:LYS:HA	30:Q:220:HOH:O	2.16	0.45
4:Q:29:HIS:CD2	4:Q:30:VAL:HG23	2.51	0.45
1:N:51:ASP:HB2	2:O:202:SER:O	2.16	0.45
27:C:306:PEK:H42	27:C:306:PEK:H221	1.99	0.45
2:B:145:PRO:HA	2:B:214:VAL:O	2.16	0.45
1:N:412:ILE:HD13	4:Q:84:ALA:HB3	1.99	0.45
2:O:111:THR:HG22	2:O:115:ASP:HA	1.97	0.45
2:O:226:MET:HA	2:O:226:MET:CE	2.47	0.45
2:O:128:LEU:HD22	2:O:132:GLU:HB3	1.99	0.45
2:B:74:ILE:HG22	2:B:78:LEU:HD22	1.98	0.45
7:G:77:PRO:HD3	7:G:82:TYR:CE1	2.52	0.45
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.52	0.45
4:Q:118:LYS:HA	11:X:51:LYS:O	2.17	0.45
19:N:610:TGL:HG12	19:N:610:TGL:HC42	1.98	0.44
9:I:58:LYS:O	9:I:62:GLU:HG3	2.17	0.44
19:N:611:TGL:CC4	19:N:611:TGL:OC1	2.58	0.44
4:D:130:PRO:O	4:D:136:ALA:HB2	2.18	0.44
27:G:101:PEK:H331	27:G:101:PEK:H361	1.71	0.44
1:A:28:MET:HG3	12:L:29:PHE:HD1	1.82	0.44
2:O:68:LEU:HD12	2:O:68:LEU:HA	1.78	0.44
5:R:67:ILE:O	5:R:71:VAL:HG23	2.18	0.44
7:T:25:LEU:HD23	7:T:25:LEU:HA	1.85	0.44
9:V:19:PHE:HB2	30:V:118:HOH:O	2.18	0.44
23:B:302:CHD:H12	23:B:302:CHD:H212	1.98	0.44
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.00	0.44
1:N:118:VAL:O	1:N:119:GLU:C	2.55	0.44
2:B:179:LEU:HD11	8:H:65:PRO:HD3	2.00	0.44
4:Q:8:SER:C	4:Q:10:ASP:H	2.20	0.44
7:G:25:LEU:HD23	7:G:25:LEU:HA	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:230:LEU:HD21	3:P:100:ALA:HA	1.99	0.44
1:A:127:THR:HB	1:A:129:TYR:CE1	2.52	0.44
2:B:181:GLN:O	8:H:23:GLN:HG2	2.17	0.44
30:L:210:HOH:O	13:M:32:TRP:HH2	2.00	0.44
23:P:305:CHD:H41	23:P:305:CHD:O7	2.18	0.44
7:T:7:ASP:O	7:T:9:GLY:N	2.51	0.44
8:U:17:ASP:OD2	8:U:19:ARG:NH2	2.51	0.44
1:A:390:MET:O	1:A:394:VAL:HG13	2.18	0.43
24:B:303:PSC:H272	24:B:303:PSC:C20	2.40	0.43
1:A:156:SER:HA	30:A:788:HOH:O	2.17	0.43
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.48	0.43
3:P:121:ILE:HB	30:P:403:HOH:O	2.18	0.43
6:S:53:THR:HB	6:S:54:ASN:HD22	1.83	0.43
19:N:610:TGL:H351	9:V:16:ARG:HH21	1.84	0.43
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.00	0.43
1:A:43:GLN:OE1	4:D:104:TYR:HB3	2.18	0.43
14:A:601:HEA:H11	14:A:601:HEA:HHC	1.81	0.43
3:C:14:SER:HA	3:C:15:PRO:HD3	1.87	0.43
3:P:195:SER:O	3:P:199:VAL:HG23	2.18	0.43
5:R:102:GLU:HA	5:R:107:ASP:OD1	2.19	0.43
9:V:67:GLY:HA2	30:V:102:HOH:O	2.17	0.43
26:C:307:CDL:H131	26:C:307:CDL:H1	1.99	0.43
10:J:50:LEU:HB2	30:J:215:HOH:O	2.18	0.43
13:M:10:THR:HA	13:M:14:GLU:OE2	2.19	0.43
6:S:58:VAL:O	6:S:71:TRP:HA	2.18	0.43
3:P:30:GLY:HA2	3:P:42:LEU:HB3	2.00	0.43
6:S:53:THR:HB	6:S:54:ASN:H	1.44	0.43
24:B:303:PSC:H221	24:B:303:PSC:H012	2.00	0.43
2:B:49:LYS:O	4:D:20:ARG:NH2	2.41	0.43
2:O:215:PRO:HB2	2:O:217:LYS:HE2	2.01	0.43
4:Q:108:PRO:N	30:Q:202:HOH:O	2.52	0.43
1:N:412:ILE:HD13	4:Q:84:ALA:CB	2.49	0.43
30:A:779:HOH:O	3:C:111:GLU:HB3	2.18	0.43
12:L:21:LEU:O	12:L:24:MET:HB2	2.19	0.43
6:S:94:HIS:O	6:S:96:LEU:HD13	2.19	0.43
7:T:33:LEU:HD22	7:T:33:LEU:HA	1.75	0.43
1:A:106:PRO:N	1:A:107:PRO:HD2	2.33	0.43
1:A:459:PHE:CE1	21:A:614:EDO:H11	2.54	0.43
1:A:316:THR:HG21	14:A:602:HEA:C14	2.49	0.43
2:B:70:ALA:O	2:B:74:ILE:HG13	2.18	0.43
3:C:179:SER:O	3:C:183:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:365:ILE:O	2:O:171:LYS:HD2	2.18	0.43
3:P:90:GLU:O	3:P:93:PHE:HB3	2.19	0.43
3:C:92:LEU:O	3:C:95:THR:HB	2.19	0.43
1:N:194:LEU:CD2	1:N:285:PHE:HE2	2.30	0.43
1:N:298:ASP:N	1:N:298:ASP:OD1	2.46	0.43
26:T:103:CDL:H762	26:T:103:CDL:H561	2.00	0.43
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	2.01	0.43
1:A:174:PRO:HB2	6:F:35:ALA:HB2	2.01	0.43
3:C:108:PRO:HA	30:C:446:HOH:O	2.18	0.43
4:D:120:THR:HG21	30:K:207:HOH:O	2.18	0.43
7:G:15:THR:O	7:G:18:PHE:HB3	2.18	0.43
1:N:199:LEU:HA	1:N:199:LEU:HD23	1.78	0.43
8:H:7:LYS:O	8:U:46:LYS:NZ	2.47	0.42
10:J:50:LEU:HD22	10:J:50:LEU:C	2.40	0.42
1:N:498:CYS:HA	1:N:499:PRO:HA	1.93	0.42
3:P:55:TYR:HA	26:P:304:CDL:H552	2.01	0.42
3:P:36:HIS:C	3:P:38:ASN:N	2.70	0.42
4:Q:145:TRP:CD1	11:X:46:GLY:HA2	2.54	0.42
7:G:74:ARG:HD2	7:G:75:VAL:HG13	2.01	0.42
3:P:63:ARG:HE	26:P:304:CDL:CA2	2.32	0.42
5:R:24:ILE:HG13	5:R:28:GLU:HB2	2.01	0.42
12:L:47:LYS:HA	30:L:212:HOH:O	2.18	0.42
19:N:609:TGL:H283	19:N:609:TGL:H102	2.01	0.42
8:U:49:ASP:O	8:U:52:VAL:HG23	2.19	0.42
13:Z:40:TYR:O	13:Z:42:LYS:N	2.52	0.42
1:A:407:ASP:O	1:A:411:LYS:HG3	2.19	0.42
1:N:89:ALA:HA	1:N:90:PRO:HD3	1.83	0.42
8:U:9:LYS:HA	8:U:9:LYS:HD3	1.82	0.42
1:A:227:ASP:HA	1:A:228:PRO:HD3	1.74	0.42
1:A:380:VAL:HG21	14:A:602:HEA:C4C	2.50	0.42
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.73	0.42
3:C:76:GLN:O	3:C:80:ARG:HG3	2.20	0.42
1:N:36:LEU:HD21	12:Y:37:PHE:CE1	2.54	0.42
1:N:351:GLY:HA3	1:N:380:VAL:HG13	2.01	0.42
3:P:92:LEU:HA	3:P:92:LEU:HD13	1.85	0.42
4:Q:90:GLY:O	4:Q:93:ALA:HB3	2.19	0.42
23:C:304:CHD:H12A	23:C:304:CHD:H112	1.86	0.42
7:G:30:LEU:HA	7:G:30:LEU:HD23	1.83	0.42
3:P:204:HIS:CE1	3:P:249:TRP:HB2	2.55	0.42
1:A:324:LEU:HD21	2:B:42:ILE:HG12	2.02	0.42
26:C:303:CDL:H112	26:C:303:CDL:HA4	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:30:ILE:O	10:J:34:VAL:HG23	2.19	0.42
1:N:366:VAL:HB	30:N:704:HOH:O	2.19	0.42
1:N:425:PHE:O	1:N:426:PHE:C	2.55	0.42
2:O:78:LEU:N	2:O:79:PRO:HD2	2.35	0.42
9:V:33:THR:O	9:V:34:PHE:C	2.57	0.42
20:A:609:PGV:O14	20:A:609:PGV:O02	2.37	0.42
1:A:9:SER:HA	21:A:612:EDO:H11	2.02	0.42
5:E:96:LEU:HA	5:E:96:LEU:HD23	1.77	0.42
2:O:103:GLN:HA	2:O:104:TRP:HA	1.81	0.42
2:O:144:LEU:HA	2:O:145:PRO:HD3	1.83	0.42
2:O:2:ALA:HB3	30:O:458:HOH:O	2.19	0.42
23:O:302:CHD:H161	23:O:302:CHD:H221	1.73	0.42
26:P:304:CDL:PA1	26:P:304:CDL:HB21	2.60	0.42
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.01	0.42
30:A:720:HOH:O	3:C:93:PHE:HA	2.20	0.42
6:F:60:CYS:SG	6:F:89:TYR:OH	2.73	0.42
6:S:8:THR:OG1	6:S:11:GLU:HG3	2.19	0.42
10:W:50:LEU:HD22	10:W:50:LEU:C	2.40	0.42
24:B:303:PSC:H242	24:B:303:PSC:H202	2.02	0.42
4:D:52:SER:OG	4:D:55:GLU:HG3	2.20	0.42
27:C:306:PEK:O14	7:G:17:ARG:NH2	2.52	0.42
2:O:68:LEU:HB3	2:O:69:PRO:HD3	2.01	0.42
1:A:377:PHE:HA	1:A:380:VAL:HG22	2.01	0.41
12:L:13:PHE:HA	19:L:101:TGL:HC21	2.01	0.41
4:Q:129:ALA:HB3	4:Q:134:PHE:CB	2.50	0.41
5:R:80:GLU:CD	5:R:80:GLU:N	2.73	0.41
2:B:215:PRO:O	2:B:216:LEU:C	2.57	0.41
6:F:30:PRO:O	6:F:96:LEU:HD23	2.20	0.41
30:A:825:HOH:O	19:L:101:TGL:H101	2.19	0.41
2:O:23:PHE:O	2:O:26:HIS:HB3	2.20	0.41
4:Q:91:PHE:O	4:Q:94:LEU:HB2	2.20	0.41
5:R:78:HIS:HB2	5:R:81:ILE:HD12	2.01	0.41
7:G:69:PHE:HD2	7:G:70:PHE:CE1	2.37	0.41
1:N:280:ILE:HG12	1:N:312:ILE:CD1	2.48	0.41
3:P:116:TRP:CE3	3:P:118:PRO:HD3	2.55	0.41
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.20	0.41
27:T:101:PEK:H241	27:T:101:PEK:H271	1.83	0.41
3:C:177:GLN:HA	30:C:402:HOH:O	2.21	0.41
8:H:54:GLU:CD	8:H:57:ARG:HH21	2.24	0.41
7:T:53:LEU:HA	7:T:53:LEU:HD23	1.83	0.41
1:A:404:THR:OG1	1:A:480:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ALA:O	2:B:59:GLN:C	2.58	0.41
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.65	0.41
4:Q:78:TRP:CE2	4:Q:79:LYS:HG3	2.56	0.41
4:Q:98:TRP:HE1	29:Z:101:DMU:H29	1.86	0.41
26:T:103:CDL:H111	26:T:103:CDL:H372	2.03	0.41
8:U:60:TYR:C	8:U:60:TYR:CD1	2.94	0.41
1:A:261:TYR:OH	21:A:610:EDO:H12	2.19	0.41
6:F:49:VAL:HA	6:F:50:PRO:HD2	1.87	0.41
2:B:100:MET:CE	2:B:157:GLU:HG3	2.50	0.41
1:N:68:PHE:C	1:N:72:PRO:HG2	2.41	0.41
3:P:51:MET:HG2	26:P:304:CDL:H602	2.02	0.41
7:T:44:ARG:HD2	7:T:82:TYR:CE1	2.55	0.41
7:T:44:ARG:HD3	7:T:74:ARG:O	2.19	0.41
4:D:29:HIS:CE1	4:D:65:LYS:HG3	2.56	0.41
1:N:119:GLU:HB2	1:N:120:ALA:H	1.71	0.41
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.55	0.41
4:Q:16:TYR:CE1	4:Q:25:PRO:HG2	2.56	0.41
9:V:31:PHE:CE1	9:V:32:ALA:O	2.74	0.41
24:B:303:PSC:H272	24:B:303:PSC:H242	1.82	0.41
1:N:165:ILE:O	1:N:169:ILE:HG12	2.20	0.41
1:N:3:ILE:N	1:N:3:ILE:HD12	2.35	0.41
1:N:390:MET:CE	1:N:413:HIS:HE1	2.34	0.41
1:N:65:MET:HG3	14:N:601:HEA:C2C	2.51	0.41
1:A:481:GLU:OE1	13:M:7:LYS:NZ	2.49	0.41
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.84	0.41
14:A:602:HEA:H243	2:B:69:PRO:HB3	2.03	0.41
8:H:18:SER:HB2	30:H:115:HOH:O	2.21	0.41
1:N:212:ASP:HA	1:N:217:THR:OG1	2.21	0.41
1:N:406:ASN:HD21	20:N:607:PGV:H032	1.82	0.41
2:O:99:THR:HB	2:O:108:TYR:CE1	2.56	0.41
3:P:151:LEU:HD21	3:P:232:HIS:CG	2.56	0.41
5:R:31:LYS:HD2	5:R:31:LYS:HA	1.96	0.41
7:T:25:LEU:N	7:T:26:PRO:CD	2.83	0.41
3:P:210:ILE:HG23	20:P:303:PGV:H91	2.03	0.41
5:E:66:ARG:O	5:E:70:VAL:HG12	2.21	0.40
13:M:11:SER:HB2	13:M:12:PRO:HD2	2.01	0.40
13:M:36:HIS:O	13:M:37:LEU:C	2.60	0.40
2:O:121:TYR:O	2:O:138:VAL:HA	2.21	0.40
2:O:149:THR:HG22	30:O:448:HOH:O	2.21	0.40
3:P:109:THR:HB	3:P:110:PRO:CD	2.52	0.40
3:P:37:PHE:O	3:P:38:ASN:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:103:CDL:H161	26:T:103:CDL:H402	2.03	0.40
1:A:266:GLU:HB2	1:A:267:PRO:HD2	2.02	0.40
24:B:303:PSC:C24	24:B:303:PSC:H202	2.52	0.40
19:D:201:TGL:HG31	19:D:201:TGL:HC21	1.92	0.40
1:N:403:TYR:HA	1:N:480:ARG:O	2.21	0.40
3:P:109:THR:HB	3:P:110:PRO:HD2	2.02	0.40
3:P:121:ILE:HG13	30:P:403:HOH:O	2.20	0.40
5:R:19:PHE:HB2	30:R:303:HOH:O	2.21	0.40
6:S:64:GLU:O	6:S:65:ASP:HB2	2.22	0.40
1:N:377:PHE:CE1	1:N:378:HIS:CE1	3.09	0.40
11:X:28:VAL:O	11:X:31:TYR:HB3	2.22	0.40
20:A:609:PGV:H12	20:A:609:PGV:H271	2.03	0.40
24:B:303:PSC:H221	24:B:303:PSC:H251	1.88	0.40
3:C:40:MET:O	3:C:44:MET:HG2	2.22	0.40
10:J:26:ALA:N	30:J:201:HOH:O	2.54	0.40
1:N:363:LEU:HA	1:N:363:LEU:HD23	1.94	0.40
1:N:71:MET:N	1:N:72:PRO:CD	2.85	0.40
1:A:240:HIS:HE2	1:A:244:TYR:HH	1.68	0.40
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.87	0.40
1:A:65:MET:HB3	14:A:601:HEA:CBC	2.52	0.40
3:C:187:THR:OG1	30:C:401:HOH:O	2.22	0.40
4:D:33:LEU:HA	4:D:37:GLN:NE2	2.37	0.40
5:E:44:GLU:HB3	30:E:202:HOH:O	2.22	0.40
30:B:404:HOH:O	9:I:20:HIS:HA	2.21	0.40
9:I:43:ARG:HH11	9:I:43:ARG:HD3	1.74	0.40
10:J:44:LEU:HA	10:J:44:LEU:HD23	1.85	0.40
26:T:103:CDL:H312	30:T:205:HOH:O	2.21	0.40
7:T:38:HIS:CE1	26:T:103:CDL:H142	2.56	0.40
7:T:79:PRO:CD	30:T:201:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	513/514 (100%)	494 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	488 (95%)	23 (4%)	1 (0%)	47	62
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	34	48
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	17	25
3	C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
3	P	257/261 (98%)	248 (96%)	6 (2%)	3 (1%)	13	19
4	D	142/147 (97%)	133 (94%)	9 (6%)	0	100	100
4	Q	142/147 (97%)	130 (92%)	9 (6%)	3 (2%)	7	8
5	E	103/109 (94%)	98 (95%)	4 (4%)	1 (1%)	15	23
5	R	103/109 (94%)	99 (96%)	3 (3%)	1 (1%)	15	23
6	F	96/98 (98%)	87 (91%)	7 (7%)	2 (2%)	7	8
6	S	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	15	23
7	G	81/85 (95%)	69 (85%)	8 (10%)	4 (5%)	2	1
7	T	81/85 (95%)	68 (84%)	5 (6%)	8 (10%)	0	0
8	H	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	12	17
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	1
9	I	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
9	V	71/73 (97%)	64 (90%)	6 (8%)	1 (1%)	11	15
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	8	10
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	41 (87%)	5 (11%)	1 (2%)	7	8
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
13	M	41/46 (89%)	40 (98%)	0	1 (2%)	6	6
13	Z	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	6	6
All	All	3505/3614 (97%)	3301 (94%)	167 (5%)	37 (1%)	14	20

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	97	ALA
7	G	3	ALA
7	G	4	ALA

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Mol	Chain	Res	Type
7	G	8	HIS
8	H	8	ILE
2	O	59	GLN
7	T	4	ALA
7	T	8	HIS
9	V	32	ALA
7	G	43	GLU
2	O	60	GLU
3	P	37	PHE
3	P	38	ASN
4	Q	5	VAL
4	Q	65	LYS
6	S	94	HIS
7	T	2	SER
7	T	37	LEU
13	Z	41	LYS
13	M	42	LYS
1	N	119	GLU
7	T	6	GLY
7	T	7	ASP
8	U	8	ILE
8	U	51	SER
2	B	59	GLN
5	E	8	ASP
6	F	94	HIS
3	P	232	HIS
4	Q	47	SER
5	R	101	PRO
8	U	48	GLY
10	W	57	HIS
11	X	7	PRO
7	T	3	ALA
7	T	5	LYS
8	U	9	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/426 (100%)	411 (96%)	16 (4%)	34	53
1	N	426/426 (100%)	408 (96%)	18 (4%)	30	47
2	B	210/210 (100%)	198 (94%)	12 (6%)	20	33
2	O	210/210 (100%)	198 (94%)	12 (6%)	20	33
3	C	224/226 (99%)	220 (98%)	4 (2%)	59	76
3	P	224/226 (99%)	216 (96%)	8 (4%)	35	54
4	D	128/129 (99%)	125 (98%)	3 (2%)	50	70
4	Q	128/129 (99%)	121 (94%)	7 (6%)	21	35
5	E	92/95 (97%)	86 (94%)	6 (6%)	17	27
5	R	92/95 (97%)	87 (95%)	5 (5%)	22	36
6	F	81/81 (100%)	77 (95%)	4 (5%)	25	40
6	S	81/81 (100%)	74 (91%)	7 (9%)	10	16
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	14
7	T	67/68 (98%)	63 (94%)	4 (6%)	19	31
8	H	71/75 (95%)	63 (89%)	8 (11%)	6	8
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	16
9	I	57/57 (100%)	52 (91%)	5 (9%)	10	15
9	V	57/57 (100%)	51 (90%)	6 (10%)	7	9
10	J	49/50 (98%)	46 (94%)	3 (6%)	18	30
10	W	49/50 (98%)	43 (88%)	6 (12%)	5	6
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	39
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	39
12	L	39/40 (98%)	37 (95%)	2 (5%)	24	39
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	39
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	36
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	4
All	All	3041/3082 (99%)	2880 (95%)	161 (5%)	22	37

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	SER
1	A	136	LEU
1	A	138	HIS

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Mol	Chain	Res	Type
1	A	177	SER
1	A	178	GLN
1	A	180	GLN
1	A	189	MET
1	A	238	PHE
1	A	264	LYS
1	A	338	MET
1	A	361	SER
1	A	366	VAL
1	A	369	ASP
1	A	382	SER
1	A	394	VAL
1	A	513	LEU
2	B	55	THR
2	B	60	GLU
2	B	65	TRP
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	88	ASP
2	B	91	ASN
2	B	92	ASN
2	B	94	SER
2	B	217	LYS
2	B	223	SER
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN
4	D	51	LEU
4	D	121	LYS
4	D	143	ASN
5	E	6	GLU
5	E	9	GLU
5	E	46	LYS
5	E	70	VAL
5	E	79	LYS
5	E	108	LYS
6	F	10	GLU
6	F	53	THR
6	F	90	LYS
6	F	95	GLN

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Mol	Chain	Res	Type
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	44	ARG
7	G	54	ARG
7	G	74	ARG
8	H	8	ILE
8	H	9	LYS
8	H	23	GLN
8	H	27	ARG
8	H	46	LYS
8	H	49	ASP
8	H	52	VAL
8	H	60	TYR
9	I	18	ARG
9	I	21	ILE
9	I	29	LEU
9	I	31	PHE
9	I	37	PHE
10	J	14	GLU
10	J	50	LEU
10	J	58	LYS
11	K	20	SER
11	K	54	ARG
12	L	5	GLU
12	L	26	THR
13	M	34	LEU
13	M	38	ASP
1	N	38	ARG
1	N	91	ASP
1	N	109	PHE
1	N	138	HIS
1	N	152	LEU
1	N	180	GLN
1	N	189	MET
1	N	238	PHE
1	N	273	MET
1	N	298	ASP
1	N	312	ILE
1	N	333	LYS
1	N	338	MET
1	N	361	SER

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Mol	Chain	Res	Type
1	N	366	VAL
1	N	369	ASP
1	N	394	VAL
1	N	486	ASP
2	O	33	LEU
2	O	48	THR
2	O	60	GLU
2	O	65	TRP
2	O	75	LEU
2	O	88	ASP
2	O	91	ASN
2	O	183	THR
2	O	185	MET
2	O	217	LYS
2	O	226	MET
2	O	227	LEU
3	P	44	MET
3	P	77	LYS
3	P	80	ARG
3	P	105	SER
3	P	127	LEU
3	P	159	MET
3	P	179	SER
3	P	214	PHE
4	Q	6	VAL
4	Q	15	SER
4	Q	19	ARG
4	Q	26	ASP
4	Q	31	LYS
4	Q	33	LEU
4	Q	126	MET
5	R	21	LYS
5	R	36	LEU
5	R	70	VAL
5	R	79	LYS
5	R	92	THR
6	S	14	THR
6	S	25	ARG
6	S	37	LYS
6	S	53	THR
6	S	54	ASN
6	S	87	THR

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Mol	Chain	Res	Type
6	S	96	LEU
7	T	17	ARG
7	T	33	LEU
7	T	35	SER
7	T	84	LYS
8	U	8	ILE
8	U	27	ARG
8	U	52	VAL
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	2	THR
9	V	4	LEU
9	V	19	PHE
9	V	31	PHE
9	V	62	GLU
9	V	68	ILE
10	W	1	PHE
10	W	10	LYS
10	W	14	GLU
10	W	27	THR
10	W	29	ASN
10	W	50	LEU
11	X	52	GLU
11	X	54	ARG
12	Y	27	LEU
12	Y	47	LYS
13	Z	1	ILE
13	Z	19	LEU
13	Z	20	SER
13	Z	34	LEU
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	178	GLN
1	A	180	GLN
1	A	413	HIS
2	B	10	GLN
2	B	52	HIS

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Mol	Chain	Res	Type
2	B	181	GLN
3	C	68	GLN
3	C	149	HIS
4	D	29	HIS
4	D	37	GLN
5	E	78	HIS
7	G	8	HIS
7	G	71	HIS
7	G	76	ASN
8	H	12	GLN
8	H	23	GLN
8	H	37	HIS
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	291	HIS
1	N	413	HIS
1	N	512	ASN
2	O	10	GLN
2	O	59	GLN
2	O	91	ASN
2	O	181	GLN
3	P	68	GLN
3	P	70	HIS
4	Q	37	GLN
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
7	T	8	HIS
7	T	34	ASN
7	T	76	ASN
8	U	23	GLN
8	U	37	HIS
10	W	29	ASN
13	Z	15	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	N	1	1	8,9,10	0.45	0	7,9,11	1.59	2 (28%)
7	TPO	T	11	7	8,10,11	1.73	2 (25%)	10,14,16	1.02	1 (10%)
9	SAC	I	1	9	7,8,9	1.30	1 (14%)	8,9,11	0.99	0
1	FME	A	1	1	8,9,10	0.44	0	7,9,11	1.97	4 (57%)
2	FME	O	1	2	8,9,10	0.85	0	7,9,11	1.63	1 (14%)
7	TPO	G	11	7	8,10,11	1.45	1 (12%)	10,14,16	0.92	1 (10%)
2	FME	B	1	2	8,9,10	0.97	0	7,9,11	1.45	3 (42%)
9	SAC	V	1	9	7,8,9	1.70	1 (14%)	8,9,11	1.82	2 (25%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.27	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-N	3.22	1.50	1.46
7	T	11	TPO	P-O1P	2.85	1.59	1.50
7	G	11	TPO	P-O1P	2.83	1.59	1.50
7	T	11	TPO	P-OG1	2.33	1.63	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	C-CA-N	3.75	116.49	109.73
2	O	1	FME	CA-N-CN	3.70	128.51	122.82
1	N	1	FME	C-CA-N	2.76	114.71	109.73
1	A	1	FME	C-CA-N	2.75	114.69	109.73
1	A	1	FME	CE-SD-CG	2.60	109.33	100.40
1	A	1	FME	CG-CB-CA	-2.48	106.06	112.95
1	N	1	FME	O-C-CA	-2.38	118.55	124.78
7	G	11	TPO	CB-CA-N	-2.28	99.43	114.41
7	T	11	TPO	CB-CA-N	-2.23	99.75	114.41
2	B	1	FME	CG-CB-CA	-2.22	106.77	112.95
9	V	1	SAC	CA-N-C1A	2.21	127.22	123.15
1	A	1	FME	O-C-CA	-2.13	119.19	124.78
2	B	1	FME	O-C-CA	-2.01	119.50	124.78
2	B	1	FME	CA-N-CN	2.01	125.92	122.82

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	B	1	FME	CB-CG-SD-CE
7	T	11	TPO	CB-OG1-P-O3P
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 62 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	N	608	-	50,50,50	0.90	3 (6%)	53,56,56	1.17	4 (7%)
22	CUA	O	301	2	0,1,1	0.00	-	-		
19	TGL	N	609	-	62,62,62	1.12	3 (4%)	65,65,65	1.29	8 (12%)
20	PGV	A	609	-	50,50,50	1.10	2 (4%)	53,56,56	1.08	5 (9%)
27	PEK	G	102	-	52,52,52	1.21	2 (3%)	55,57,57	1.06	5 (9%)
20	PGV	C	308	-	50,50,50	1.21	2 (4%)	53,56,56	1.01	3 (5%)
23	CHD	W	101	-	29,32,32	0.83	1 (3%)	48,51,51	2.13	16 (33%)
27	PEK	P	302	-	52,52,52	0.87	2 (3%)	55,57,57	1.35	5 (9%)
23	CHD	P	305	-	29,32,32	0.50	0	48,51,51	1.87	13 (27%)
23	CHD	J	101	-	29,32,32	0.60	0	48,51,51	1.60	10 (20%)
19	TGL	D	201	-	62,62,62	1.13	3 (4%)	65,65,65	0.99	5 (7%)
21	EDO	K	101	-	3,3,3	0.47	0	2,2,2	0.33	0
21	EDO	A	610	-	3,3,3	0.52	0	2,2,2	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	602	1	44,67,67	0.91	2 (4%)	37,103,103	1.75	7 (18%)
29	DMU	Z	101	-	34,34,34	0.53	0	45,45,45	1.13	4 (8%)
23	CHD	B	302	-	29,32,32	0.79	0	48,51,51	1.25	4 (8%)
14	HEA	A	601	1	44,67,67	1.04	3 (6%)	37,103,103	1.89	9 (24%)
26	CDL	P	304	-	99,99,99	1.39	12 (12%)	105,111,111	1.16	7 (6%)
14	HEA	N	602	1	44,67,67	1.07	1 (2%)	37,103,103	1.97	11 (29%)
24	PSC	R	201	-	51,51,51	1.22	3 (5%)	57,59,59	0.99	4 (7%)
21	EDO	K	103	-	3,3,3	0.56	0	2,2,2	0.11	0
27	PEK	T	102	-	52,52,52	1.19	2 (3%)	55,57,57	1.13	4 (7%)
21	EDO	L	102	-	3,3,3	0.46	0	2,2,2	0.40	0
21	EDO	B	305	-	3,3,3	0.39	0	2,2,2	0.49	0
14	HEA	N	601	1	44,67,67	1.04	3 (6%)	37,103,103	1.72	8 (21%)
21	EDO	K	102	-	3,3,3	0.50	0	2,2,2	0.26	0
18	CMO	N	606	-	0,1,1	0.00	-	-	-	-
18	CMO	A	606	15	0,1,1	0.00	-	-	-	-
27	PEK	C	306	-	52,52,52	1.03	2 (3%)	55,57,57	0.90	3 (5%)
21	EDO	C	309	-	3,3,3	0.38	0	2,2,2	0.68	0
20	PGV	C	302	-	50,50,50	0.92	2 (4%)	53,56,56	0.93	4 (7%)
20	PGV	P	303	-	50,50,50	0.93	2 (4%)	53,56,56	1.08	5 (9%)
24	PSC	B	303	-	51,51,51	1.28	3 (5%)	57,59,59	1.07	5 (8%)
26	CDL	T	103	-	99,99,99	1.37	12 (12%)	105,111,111	1.31	11 (10%)
21	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.60	0
27	PEK	T	101	-	52,52,52	1.16	2 (3%)	55,57,57	1.06	4 (7%)
19	TGL	A	607	-	62,62,62	1.23	4 (6%)	65,65,65	1.38	10 (15%)
19	TGL	N	611	-	62,62,62	1.18	3 (4%)	65,65,65	1.24	7 (10%)
20	PGV	N	607	-	50,50,50	1.09	2 (4%)	53,56,56	1.07	4 (7%)
21	EDO	C	310	-	3,3,3	0.53	0	2,2,2	0.33	0
20	PGV	A	608	-	50,50,50	0.79	2 (4%)	53,56,56	1.44	5 (9%)
23	CHD	P	306	-	29,32,32	0.72	1 (3%)	48,51,51	1.52	11 (22%)
26	CDL	C	303	-	99,99,99	1.39	12 (12%)	105,111,111	1.22	7 (6%)
21	EDO	N	612	-	3,3,3	0.56	0	2,2,2	0.16	0
27	PEK	G	101	-	52,52,52	0.94	2 (3%)	55,57,57	1.23	4 (7%)
19	TGL	L	101	-	62,62,62	1.19	3 (4%)	65,65,65	1.25	5 (7%)
23	CHD	C	305	-	29,32,32	0.93	1 (3%)	48,51,51	1.22	7 (14%)
21	EDO	C	311	-	3,3,3	0.53	0	2,2,2	0.30	0
21	EDO	G	104	-	3,3,3	0.40	0	2,2,2	0.56	0
20	PGV	G	103	-	50,50,50	1.07	2 (4%)	53,56,56	0.95	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DMU	M	101	-	34,34,34	0.53	0	45,45,45	1.14	4 (8%)
22	CUA	B	301	2	0,1,1	0.00	-	-		
21	EDO	A	613	-	3,3,3	0.54	0	2,2,2	0.24	0
23	CHD	O	302	-	29,32,32	1.00	1 (3%)	48,51,51	1.48	8 (16%)
21	EDO	F	102	-	3,3,3	0.57	0	2,2,2	0.06	0
19	TGL	N	610	-	62,62,62	1.13	3 (4%)	65,65,65	1.13	6 (9%)
23	CHD	C	304	-	29,32,32	0.58	0	48,51,51	2.06	16 (33%)
21	EDO	A	614	-	3,3,3	0.59	0	2,2,2	0.11	0
21	EDO	T	104	-	3,3,3	0.45	0	2,2,2	0.26	0
26	CDL	C	307	-	99,99,99	1.43	13 (13%)	105,111,111	1.23	8 (7%)
21	EDO	A	611	-	3,3,3	0.37	0	2,2,2	0.61	0
21	EDO	A	612	-	3,3,3	0.52	0	2,2,2	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	N	608	-	-	22/55/55/55	-
19	TGL	N	609	-	-	37/65/65/65	-
20	PGV	A	609	-	-	31/55/55/55	-
27	PEK	G	102	-	-	35/56/56/56	-
20	PGV	C	308	-	-	32/55/55/55	-
23	CHD	W	101	-	-	4/7/74/74	0/4/4/4
27	PEK	P	302	-	-	17/56/56/56	-
23	CHD	P	305	-	-	7/7/74/74	0/4/4/4
23	CHD	J	101	-	-	7/7/74/74	0/4/4/4
19	TGL	D	201	-	-	38/65/65/65	-
21	EDO	K	101	-	-	1/1/1/1	-
21	EDO	A	610	-	-	1/1/1/1	-
14	HEA	A	602	1	1/1/7/16	1/24/76/76	-
29	DMU	Z	101	-	-	9/19/59/59	0/2/2/2
23	CHD	B	302	-	-	0/7/74/74	0/4/4/4
14	HEA	A	601	1	3/3/7/16	6/24/76/76	-
26	CDL	P	304	-	-	66/110/110/110	-
14	HEA	N	602	1	-	3/24/76/76	-
24	PSC	R	201	-	-	29/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	K	103	-	-	0/1/1/1	-
27	PEK	T	102	-	-	29/56/56/56	-
21	EDO	L	102	-	-	1/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
14	HEA	N	601	1	3/3/7/16	1/24/76/76	-
21	EDO	K	102	-	-	1/1/1/1	-
27	PEK	C	306	-	-	30/56/56/56	-
21	EDO	C	309	-	-	1/1/1/1	-
20	PGV	C	302	-	-	15/55/55/55	-
20	PGV	P	303	-	-	21/55/55/55	-
24	PSC	B	303	-	-	30/55/55/55	-
26	CDL	T	103	-	-	63/110/110/110	-
21	EDO	B	304	-	-	1/1/1/1	-
27	PEK	T	101	-	-	22/56/56/56	-
19	TGL	A	607	-	-	36/65/65/65	-
19	TGL	N	611	-	-	34/65/65/65	-
20	PGV	N	607	-	-	33/55/55/55	-
21	EDO	C	310	-	-	1/1/1/1	-
20	PGV	A	608	-	-	11/55/55/55	-
23	CHD	P	306	-	-	1/7/74/74	0/4/4/4
26	CDL	C	303	-	-	65/110/110/110	-
21	EDO	N	612	-	-	0/1/1/1	-
27	PEK	G	101	-	-	21/56/56/56	-
19	TGL	L	101	-	-	35/65/65/65	-
23	CHD	C	305	-	-	0/7/74/74	0/4/4/4
21	EDO	C	311	-	-	0/1/1/1	-
21	EDO	G	104	-	-	0/1/1/1	-
20	PGV	G	103	-	-	33/55/55/55	-
29	DMU	M	101	-	-	5/19/59/59	0/2/2/2
21	EDO	A	613	-	-	1/1/1/1	-
23	CHD	O	302	-	-	2/7/74/74	0/4/4/4
21	EDO	F	102	-	-	0/1/1/1	-
19	TGL	N	610	-	-	42/65/65/65	-
23	CHD	C	304	-	-	3/7/74/74	0/4/4/4
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	T	104	-	-	1/1/1/1	-
26	CDL	C	307	-	-	64/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	A	611	-	-	1/1/1/1	-
21	EDO	A	612	-	-	1/1/1/1	-

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG2-CB1	5.59	1.50	1.34
19	A	607	TGL	OG1-CA1	5.58	1.49	1.33
27	T	102	PEK	O01-C1	5.50	1.49	1.34
19	A	607	TGL	OG2-CB1	5.44	1.49	1.34
20	C	308	PGV	O01-C1	5.43	1.49	1.34
19	N	609	TGL	OG2-CB1	5.35	1.49	1.34
27	G	102	PEK	O01-C1	5.32	1.49	1.34
19	N	611	TGL	OG2-CB1	5.29	1.49	1.34
27	G	102	PEK	O03-C21	5.27	1.48	1.33
26	C	307	CDL	OB8-CB7	5.25	1.48	1.33
19	N	611	TGL	OG3-CC1	5.19	1.48	1.33
24	B	303	PSC	O03-C19	5.14	1.48	1.33
26	T	103	CDL	OB8-CB7	5.12	1.48	1.33
26	C	303	CDL	OB8-CB7	5.12	1.48	1.33
20	A	609	PGV	O01-C1	5.10	1.48	1.34
26	C	303	CDL	OB6-CB5	5.10	1.48	1.34
19	L	101	TGL	OG3-CC1	5.09	1.48	1.33
26	P	304	CDL	OB8-CB7	5.06	1.48	1.33
20	C	308	PGV	O03-C19	5.06	1.48	1.33
27	T	101	PEK	O01-C1	5.01	1.48	1.34
27	T	101	PEK	O03-C21	5.00	1.47	1.33
20	N	607	PGV	O01-C1	4.98	1.48	1.34
19	N	610	TGL	OG2-CB1	4.97	1.48	1.34
24	B	303	PSC	O01-C1	4.96	1.48	1.34
26	P	304	CDL	OA6-CA5	4.93	1.48	1.34
26	P	304	CDL	OA8-CA7	4.93	1.47	1.33
26	C	307	CDL	OB6-CB5	4.91	1.48	1.34
27	T	102	PEK	O03-C21	4.90	1.47	1.33
19	D	201	TGL	OG1-CA1	4.90	1.47	1.33
24	R	201	PSC	O01-C1	4.86	1.48	1.34
26	C	303	CDL	OA6-CA5	4.85	1.48	1.34
20	G	103	PGV	O01-C1	4.83	1.47	1.34
20	N	607	PGV	O03-C19	4.77	1.47	1.33
20	G	103	PGV	O03-C19	4.74	1.47	1.33
26	C	307	CDL	OA8-CA7	4.73	1.47	1.33
26	T	103	CDL	OA6-CA5	4.68	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	303	CDL	OA8-CA7	4.66	1.47	1.33
26	C	307	CDL	OA6-CA5	4.65	1.47	1.34
26	T	103	CDL	OB6-CB5	4.65	1.47	1.34
19	N	609	TGL	OG1-CA1	4.63	1.46	1.33
19	N	610	TGL	OG3-CC1	4.63	1.46	1.33
27	C	306	PEK	O01-C1	4.63	1.47	1.34
26	P	304	CDL	OB6-CB5	4.57	1.47	1.34
20	A	609	PGV	O03-C19	4.57	1.46	1.33
24	R	201	PSC	O03-C19	4.55	1.46	1.33
19	D	201	TGL	OG3-CC1	4.55	1.46	1.33
27	C	306	PEK	O03-C21	4.54	1.46	1.33
20	P	303	PGV	O03-C19	4.52	1.46	1.33
19	N	610	TGL	OG1-CA1	4.44	1.46	1.33
19	N	611	TGL	OG1-CA1	4.40	1.46	1.33
19	D	201	TGL	OG2-CB1	4.37	1.46	1.34
19	L	101	TGL	OG1-CA1	4.34	1.46	1.33
20	C	302	PGV	O03-C19	4.18	1.45	1.33
26	T	103	CDL	OA8-CA7	4.14	1.45	1.33
27	G	101	PEK	O03-C21	4.09	1.45	1.33
20	N	608	PGV	O03-C19	4.02	1.45	1.33
27	G	101	PEK	O01-C1	3.98	1.45	1.34
19	N	609	TGL	OG3-CC1	3.94	1.44	1.33
14	N	602	HEA	C3B-C11	-3.90	1.49	1.52
20	A	608	PGV	O03-C19	3.90	1.44	1.33
27	P	302	PEK	O01-C1	3.89	1.45	1.34
24	B	303	PSC	C13-C12	3.83	1.54	1.31
24	R	201	PSC	C13-C12	3.72	1.53	1.31
27	P	302	PEK	O03-C21	3.69	1.44	1.33
20	P	303	PGV	O01-C1	3.60	1.44	1.34
20	N	608	PGV	O01-C1	3.40	1.43	1.34
20	C	302	PGV	O01-C1	3.34	1.43	1.34
14	A	601	HEA	C3B-C11	-3.21	1.50	1.52
19	A	607	TGL	OG3-CC1	3.17	1.42	1.33
26	C	307	CDL	C19-C18	-3.17	1.33	1.51
26	T	103	CDL	C19-C18	-3.12	1.34	1.51
26	C	303	CDL	C59-C58	-3.12	1.34	1.51
26	C	307	CDL	C59-C58	-3.11	1.34	1.51
26	P	304	CDL	C22-C21	-3.09	1.34	1.51
26	T	103	CDL	C62-C61	-3.08	1.34	1.51
26	C	303	CDL	C79-C78	-3.07	1.34	1.51
26	C	303	CDL	C22-C21	-3.07	1.34	1.51
26	T	103	CDL	C42-C41	-3.06	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	303	CDL	C19-C18	-3.05	1.34	1.51
26	P	304	CDL	C79-C78	-3.04	1.34	1.51
26	P	304	CDL	C82-C81	-3.04	1.34	1.51
26	P	304	CDL	C39-C38	-3.04	1.34	1.51
26	T	103	CDL	C79-C78	-3.03	1.34	1.51
26	C	307	CDL	C39-C38	-3.01	1.34	1.51
26	T	103	CDL	C39-C38	-3.01	1.34	1.51
26	P	304	CDL	C59-C58	-3.01	1.34	1.51
26	P	304	CDL	C19-C18	-3.00	1.34	1.51
26	C	307	CDL	C79-C78	-3.00	1.34	1.51
26	T	103	CDL	C59-C58	-2.99	1.34	1.51
26	P	304	CDL	C42-C41	-2.99	1.34	1.51
26	C	303	CDL	C39-C38	-2.98	1.34	1.51
26	C	307	CDL	C42-C41	-2.96	1.35	1.51
14	N	601	HEA	C3B-C11	-2.96	1.50	1.52
26	C	303	CDL	C42-C41	-2.95	1.35	1.51
26	C	307	CDL	C62-C61	-2.93	1.35	1.51
26	C	303	CDL	C62-C61	-2.92	1.35	1.51
26	T	103	CDL	C22-C21	-2.92	1.35	1.51
20	A	608	PGV	O01-C1	2.91	1.42	1.34
26	P	304	CDL	C62-C61	-2.90	1.35	1.51
26	C	303	CDL	C82-C81	-2.90	1.35	1.51
26	T	103	CDL	C82-C81	-2.84	1.35	1.51
26	C	307	CDL	C22-C21	-2.84	1.35	1.51
26	C	307	CDL	C82-C81	-2.80	1.35	1.51
14	A	602	HEA	C3B-C11	-2.60	1.50	1.52
14	A	601	HEA	O11-C11	2.56	1.48	1.42
14	N	601	HEA	C1B-NB	-2.43	1.31	1.36
14	N	601	HEA	C3A-CMA	2.37	1.51	1.46
14	A	601	HEA	C4B-C3B	-2.37	1.37	1.42
26	C	307	CDL	CB3-CB4	2.21	1.57	1.50
20	N	608	PGV	O01-C02	-2.20	1.41	1.46
23	C	305	CHD	C19-C10	-2.18	1.50	1.54
23	W	101	CHD	C20-C17	2.12	1.58	1.54
14	A	602	HEA	C3A-CMA	2.11	1.51	1.46
23	P	306	CHD	C13-C14	-2.10	1.51	1.55
19	A	607	TGL	OC1-CC1	-2.07	1.16	1.22
23	O	302	CHD	C13-C17	-2.05	1.52	1.55

All (268) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	101	CHD	C13-C17-C20	5.97	126.63	119.50
19	N	611	TGL	OG2-CB1-CB2	5.80	124.01	111.50
19	N	609	TGL	OG2-CB1-CB2	5.64	123.66	111.50
26	T	103	CDL	OB6-CB5-C51	5.53	123.42	111.50
26	C	303	CDL	OA6-CA5-C11	5.44	123.22	111.50
27	G	101	PEK	O01-C1-C2	5.30	122.93	111.50
26	T	103	CDL	OA6-CA5-C11	5.15	122.60	111.50
19	N	610	TGL	OG2-CB1-CB2	5.12	122.54	111.50
19	A	607	TGL	CG3-CG2-CG1	-5.12	99.69	111.79
26	C	307	CDL	OB6-CB5-C51	5.09	122.48	111.50
23	C	304	CHD	C10-C9-C8	5.08	117.27	111.82
14	A	602	HEA	CAD-CBD-CGD	-5.06	104.18	112.67
27	T	102	PEK	O01-C1-C2	5.06	122.40	111.50
23	O	302	CHD	C15-C14-C13	5.04	108.50	103.55
14	N	602	HEA	CBD-CAD-C3D	5.01	121.72	112.49
27	P	302	PEK	O01-C1-C2	4.97	122.22	111.50
20	A	608	PGV	O03-C19-C20	4.97	127.51	111.91
19	L	101	TGL	OG2-CB1-CB2	4.96	122.20	111.50
26	P	304	CDL	OA6-CA5-C11	4.90	122.06	111.50
23	P	305	CHD	C6-C5-C4	-4.86	105.60	111.19
14	A	601	HEA	C26-C15-C16	4.71	123.20	115.27
23	W	101	CHD	C9-C10-C5	4.69	115.17	108.58
19	A	607	TGL	OG2-CB1-CB2	4.64	121.51	111.50
27	P	302	PEK	O03-C21-C22	4.62	126.42	111.91
23	W	101	CHD	C6-C5-C10	4.61	117.55	112.66
23	W	101	CHD	C22-C20-C17	4.54	119.66	110.28
23	C	304	CHD	C23-C22-C20	-4.50	108.66	114.72
14	A	601	HEA	C27-C19-C20	4.44	122.75	115.27
26	C	303	CDL	OB6-CB5-C51	4.37	120.93	111.50
26	C	307	CDL	OA6-CA5-C11	4.26	120.68	111.50
20	A	608	PGV	O03-C19-O04	-4.25	112.86	123.59
14	A	601	HEA	C3C-C4C-NC	4.22	114.66	109.21
20	A	608	PGV	O01-C1-C2	4.21	120.58	111.50
14	N	602	HEA	CAD-CBD-CGD	-4.21	105.61	112.67
27	C	306	PEK	O01-C1-C2	4.18	120.50	111.50
23	C	304	CHD	C15-C14-C8	4.12	124.10	118.33
23	C	304	CHD	C16-C17-C20	4.12	118.53	112.15
24	B	303	PSC	O01-C1-C2	4.00	120.12	111.50
20	P	303	PGV	O01-C1-C2	3.95	120.01	111.50
23	P	305	CHD	C4-C5-C10	3.94	116.85	112.66
23	C	304	CHD	C6-C5-C4	-3.89	106.72	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	609	PGV	O01-C1-C2	3.88	119.87	111.50
14	A	602	HEA	CBA-CAA-C2A	3.84	119.56	112.48
14	N	602	HEA	CMC-C2C-C3C	3.81	131.81	124.68
20	N	608	PGV	O03-C19-C20	3.80	123.83	111.91
19	N	609	TGL	OG1-CA1-CA2	3.78	123.77	111.91
23	P	305	CHD	C9-C10-C5	3.78	113.89	108.58
20	N	608	PGV	O01-C1-C2	3.76	119.61	111.50
26	P	304	CDL	OB6-CB5-C51	3.76	119.61	111.50
27	P	302	PEK	O03-C21-O04	-3.75	114.12	123.59
23	B	302	CHD	C1-C2-C3	3.74	115.27	110.47
19	A	607	TGL	OG3-CC1-CC2	3.72	123.59	111.91
20	G	103	PGV	O01-C1-C2	3.71	119.49	111.50
19	L	101	TGL	OG3-CC1-CC2	3.68	123.46	111.91
27	T	101	PEK	O01-C1-C2	3.68	119.43	111.50
14	N	601	HEA	C13-C12-C11	-3.67	108.83	114.35
14	N	601	HEA	CBA-CAA-C2A	3.67	119.23	112.48
14	N	602	HEA	C27-C19-C20	3.64	121.39	115.27
23	P	305	CHD	C15-C14-C13	3.63	107.12	103.55
24	B	303	PSC	O03-C19-C20	3.63	123.30	111.91
23	W	101	CHD	C10-C9-C8	3.56	115.64	111.82
20	N	607	PGV	O01-C1-C2	3.54	119.14	111.50
19	A	607	TGL	OG3-CC1-OC1	-3.53	114.69	123.59
20	G	103	PGV	O03-C19-C20	3.51	122.92	111.91
29	M	101	DMU	C6-O5-C4	3.51	120.57	113.69
27	T	101	PEK	O03-C01-C02	3.50	118.61	108.43
14	N	601	HEA	CMB-C2B-C1B	-3.49	123.09	128.46
24	R	201	PSC	O03-C19-C20	3.49	122.87	111.91
23	J	101	CHD	C21-C20-C22	-3.49	104.90	110.36
23	J	101	CHD	C1-C2-C3	3.49	114.94	110.47
27	G	102	PEK	O01-C1-C2	3.42	118.88	111.50
20	N	607	PGV	O03-C19-C20	3.41	122.61	111.91
27	G	102	PEK	O03-C01-C02	3.40	118.32	108.43
20	C	308	PGV	O03-C19-C20	3.39	122.56	111.91
24	R	201	PSC	O01-C1-C2	3.39	118.81	111.50
23	W	101	CHD	C17-C13-C12	3.36	120.74	117.67
19	N	611	TGL	OG3-CC1-CC2	3.36	122.45	111.91
26	C	307	CDL	OA8-CA7-C31	3.36	122.44	111.91
26	C	303	CDL	OB8-CB7-C71	3.35	122.43	111.91
14	A	602	HEA	C1B-C2B-C3B	-3.34	104.67	107.00
23	B	302	CHD	C13-C17-C20	-3.32	115.54	119.50
23	C	304	CHD	C4-C5-C10	3.30	116.16	112.66
14	N	601	HEA	C12-C11-C3B	3.29	121.20	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C13-C12-C11	-3.27	109.44	114.35
14	A	602	HEA	CBD-CAD-C3D	3.25	118.47	112.49
23	P	306	CHD	C13-C17-C20	-3.24	115.63	119.50
19	N	611	TGL	OG2-CB1-OB1	-3.23	115.89	123.70
27	P	302	PEK	O01-C1-O02	-3.23	115.89	123.70
19	A	607	TGL	OG1-CA1-CA2	3.21	121.99	111.91
14	N	601	HEA	CMB-C2B-C3B	3.21	130.97	124.69
14	A	602	HEA	C27-C19-C20	3.21	120.67	115.27
23	C	305	CHD	C6-C7-C8	3.20	114.89	111.48
20	C	308	PGV	O01-C1-C2	3.19	118.39	111.50
27	T	102	PEK	O03-C21-C22	3.18	121.89	111.91
19	N	609	TGL	CG3-CG2-CG1	-3.18	104.27	111.79
20	A	609	PGV	O03-C19-C20	3.18	121.88	111.91
23	O	302	CHD	C14-C8-C9	-3.17	105.35	109.71
27	G	101	PEK	O01-C1-O02	-3.17	116.05	123.70
19	N	610	TGL	OG3-CC1-CC2	3.15	121.80	111.91
27	G	102	PEK	O03-C21-C22	3.13	121.75	111.91
23	C	304	CHD	C15-C14-C13	3.13	106.62	103.55
20	A	608	PGV	O01-C1-O02	-3.12	116.16	123.70
19	N	610	TGL	OG2-CB1-OB1	-3.09	116.24	123.70
23	J	101	CHD	C22-C23-C24	-3.07	106.98	113.59
19	N	610	TGL	OG1-CA1-CA2	3.06	121.52	111.91
26	T	103	CDL	OB8-CB7-C71	3.02	121.39	111.91
23	W	101	CHD	C6-C5-C4	-3.02	107.71	111.19
14	N	602	HEA	CMC-C2C-C1C	-3.02	123.82	128.46
23	J	101	CHD	C6-C7-C8	3.02	114.70	111.48
14	N	601	HEA	C4B-C3B-C2B	-3.02	104.76	106.87
20	A	608	PGV	C02-O01-C1	-3.01	110.37	117.79
14	N	602	HEA	CMB-C2B-C3B	3.01	130.58	124.69
19	N	609	TGL	OG3-CC1-CC2	3.01	121.34	111.91
29	M	101	DMU	O2-C8-C7	-2.99	103.43	110.35
20	N	608	PGV	O03-C19-O04	-2.99	116.05	123.59
20	P	303	PGV	O03-C19-C20	2.97	121.24	111.91
19	D	201	TGL	OG3-CC1-CC2	2.96	121.21	111.91
23	P	305	CHD	C16-C17-C13	2.95	106.44	103.55
27	G	101	PEK	O03-C01-C02	-2.93	99.90	108.43
20	P	303	PGV	O01-C1-O02	-2.92	116.65	123.70
23	P	306	CHD	O12-C12-C11	-2.91	103.19	109.12
14	A	601	HEA	C27-C19-C18	-2.91	116.22	123.68
23	C	304	CHD	C1-C10-C5	2.89	112.04	107.77
19	N	611	TGL	OG3-CG3-CG2	2.87	116.79	108.43
20	C	308	PGV	C01-O03-C19	2.87	127.74	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	201	TGL	OG1-CA1-CA2	2.86	120.89	111.91
23	C	304	CHD	C9-C11-C12	-2.86	110.52	114.30
23	P	305	CHD	C11-C12-C13	2.83	114.15	111.24
27	G	102	PEK	C02-O01-C1	2.83	124.76	117.79
19	D	201	TGL	OG2-CB1-CB2	2.82	117.57	111.50
19	D	201	TGL	CG2-OG2-CB1	-2.81	110.87	117.79
23	P	306	CHD	C16-C15-C14	-2.81	99.56	105.13
14	N	602	HEA	CMB-C2B-C1B	-2.80	124.16	128.46
23	W	101	CHD	C1-C2-C3	2.80	114.06	110.47
14	A	601	HEA	CAA-C2A-C3A	2.78	133.72	126.86
23	P	305	CHD	C10-C9-C8	2.78	114.80	111.82
23	O	302	CHD	C1-C10-C5	2.77	111.87	107.77
26	P	304	CDL	OB8-CB7-C71	2.76	120.58	111.91
23	P	305	CHD	C19-C10-C1	-2.76	103.82	108.26
26	C	307	CDL	OB8-CB7-C71	2.73	120.49	111.91
14	N	602	HEA	C20-C19-C18	-2.73	115.59	121.12
19	L	101	TGL	OG3-CG3-CG2	2.73	116.38	108.43
20	N	607	PGV	O03-C19-O04	-2.71	116.76	123.59
23	J	101	CHD	C21-C20-C17	2.67	117.01	112.92
26	P	304	CDL	OA8-CA7-C31	2.66	120.25	111.91
26	T	103	CDL	OA8-CA7-C31	2.65	120.24	111.91
20	A	609	PGV	C02-O01-C1	2.65	124.32	117.79
14	N	601	HEA	C3C-C4C-NC	2.65	112.64	109.21
23	P	306	CHD	C18-C13-C14	-2.65	107.06	111.21
23	C	304	CHD	C22-C23-C24	-2.64	107.91	113.59
26	T	103	CDL	OB6-CB5-OB7	-2.62	117.36	123.70
26	C	303	CDL	OA6-CA5-OA7	-2.61	117.39	123.70
23	B	302	CHD	C6-C5-C4	-2.60	108.20	111.19
19	N	610	TGL	OG3-CC1-OC1	-2.58	117.07	123.59
29	Z	101	DMU	C10-O1-C9	2.58	118.74	113.69
29	M	101	DMU	O1-C9-C11	2.57	112.83	106.44
23	J	101	CHD	C5-C4-C3	2.54	116.49	112.76
14	N	602	HEA	O11-C11-C3B	-2.53	104.70	112.00
23	P	306	CHD	C14-C13-C12	2.53	109.75	107.40
26	C	307	CDL	CB6-OB8-CB7	2.52	126.45	117.12
23	O	302	CHD	C6-C5-C4	-2.52	108.29	111.19
23	P	306	CHD	C9-C11-C12	-2.52	110.98	114.30
19	N	609	TGL	OG1-CA1-OA1	-2.51	117.26	123.59
23	C	305	CHD	C9-C10-C5	2.51	112.11	108.58
14	A	602	HEA	C20-C19-C18	-2.50	116.06	121.12
20	C	302	PGV	O03-C19-C20	2.50	119.74	111.91
14	N	602	HEA	C1B-C2B-C3B	-2.49	105.26	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	305	CHD	C1-C10-C5	2.49	111.44	107.77
26	C	307	CDL	OB6-CB5-OB7	-2.48	117.70	123.70
19	L	101	TGL	OG3-CC1-OC1	-2.48	117.33	123.59
26	T	103	CDL	CB6-OB8-CB7	2.48	126.30	117.12
26	P	304	CDL	OB8-CB7-OB9	-2.47	117.35	123.59
27	T	101	PEK	O03-C21-C22	2.47	119.67	111.91
27	P	302	PEK	C03-C02-C01	-2.47	105.94	111.79
27	T	102	PEK	O03-C01-C02	2.47	115.62	108.43
14	N	602	HEA	CAA-CBA-CGA	2.46	116.80	112.67
14	A	601	HEA	C1B-C2B-C3B	-2.46	105.29	107.00
23	P	306	CHD	O12-C12-C13	2.44	115.15	111.03
23	J	101	CHD	C10-C9-C8	2.43	114.43	111.82
19	N	611	TGL	OG1-CA1-CA2	2.43	119.53	111.91
23	C	305	CHD	C19-C10-C1	-2.43	104.35	108.26
24	R	201	PSC	O03-C19-O04	-2.42	117.48	123.59
29	M	101	DMU	C18-O16-C6	-2.42	109.83	113.84
19	N	609	TGL	OG3-CC1-OC1	-2.41	117.52	123.59
23	W	101	CHD	C22-C23-C24	2.40	118.75	113.59
26	C	303	CDL	OA8-CA7-C31	2.40	119.43	111.91
26	C	307	CDL	OA8-CA6-CA4	2.39	115.39	108.43
19	N	611	TGL	CG2-OG2-CB1	2.39	123.67	117.79
23	J	101	CHD	C4-C3-C2	2.39	113.40	110.55
19	D	201	TGL	OG3-CC1-OC1	-2.39	117.57	123.59
20	C	302	PGV	O01-C1-C2	2.39	116.64	111.50
20	N	607	PGV	O03-C01-C02	2.38	115.36	108.43
23	W	101	CHD	C18-C13-C14	-2.38	107.49	111.21
23	O	302	CHD	C22-C20-C17	-2.38	105.38	110.28
26	T	103	CDL	CA6-CA4-CA3	-2.38	106.17	111.79
26	T	103	CDL	OA6-CA5-OA7	-2.38	117.96	123.70
14	A	601	HEA	CMC-C2C-C3C	2.37	129.11	124.68
23	P	305	CHD	C15-C14-C8	2.36	121.64	118.33
23	W	101	CHD	C4-C5-C10	2.36	115.16	112.66
23	P	306	CHD	C18-C13-C12	2.36	111.47	109.07
20	C	302	PGV	C03-C02-C01	-2.35	106.22	111.79
14	N	601	HEA	C3A-C4A-NA	2.35	115.38	110.94
23	W	101	CHD	C19-C10-C9	-2.33	107.97	111.18
29	Z	101	DMU	O1-C9-C11	2.33	112.22	106.44
20	A	609	PGV	O03-C19-O04	-2.31	117.75	123.59
23	W	101	CHD	C4-C3-C2	2.30	113.30	110.55
27	C	306	PEK	C01-O03-C21	2.30	125.64	117.12
23	C	305	CHD	C6-C5-C4	-2.30	108.54	111.19
29	Z	101	DMU	C18-O16-C6	-2.29	110.04	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	102	PEK	C01-O03-C21	2.29	125.59	117.12
24	B	303	PSC	O03-C01-C02	2.29	115.09	108.43
19	A	607	TGL	CG2-OG2-CB1	2.28	123.41	117.79
23	W	101	CHD	C16-C17-C20	2.28	115.67	112.15
23	W	101	CHD	C18-C13-C12	-2.27	106.76	109.07
19	N	610	TGL	OG1-CA1-OA1	-2.26	117.89	123.59
23	C	304	CHD	C19-C10-C1	-2.26	104.62	108.26
20	P	303	PGV	O03-C19-O04	-2.25	117.92	123.59
23	C	304	CHD	C11-C9-C10	-2.25	111.41	113.73
23	C	304	CHD	C14-C13-C12	2.25	109.50	107.40
23	P	305	CHD	C14-C8-C9	-2.24	106.63	109.71
14	A	602	HEA	C26-C15-C16	2.21	118.99	115.27
27	T	102	PEK	O03-C21-O04	-2.20	118.03	123.59
23	O	302	CHD	C21-C20-C22	2.20	113.81	110.36
23	P	305	CHD	C5-C4-C3	2.19	115.98	112.76
23	P	306	CHD	C6-C7-C8	2.18	113.81	111.48
19	A	607	TGL	OB1-CB1-CB2	-2.18	115.23	123.73
26	T	103	CDL	C83-C82-C81	2.18	125.48	114.42
23	C	304	CHD	C1-C2-C3	2.16	113.24	110.47
23	B	302	CHD	C22-C20-C17	2.15	114.74	110.28
23	C	305	CHD	C22-C23-C24	-2.15	108.97	113.59
24	B	303	PSC	C01-O03-C19	2.15	125.07	117.12
23	W	101	CHD	C14-C8-C7	2.14	114.65	111.81
29	Z	101	DMU	C6-O5-C4	-2.14	109.48	113.69
27	T	101	PEK	O01-C02-C01	2.14	116.15	108.40
20	N	608	PGV	O01-C1-O02	-2.14	118.53	123.70
19	N	609	TGL	OB1-CB1-CB2	-2.13	115.42	123.73
23	P	305	CHD	C13-C17-C20	-2.11	116.98	119.50
23	C	305	CHD	C4-C3-C2	2.11	113.07	110.55
19	A	607	TGL	OG1-CA1-OA1	-2.10	118.29	123.59
19	A	607	TGL	OG1-CG1-CG2	2.10	114.55	108.43
14	A	601	HEA	C26-C15-C14	-2.10	118.29	123.68
27	C	306	PEK	O03-C21-C22	2.10	118.49	111.91
23	J	101	CHD	C19-C10-C1	-2.09	104.89	108.26
26	C	307	CDL	OA6-CA5-OA7	-2.09	118.66	123.70
23	C	304	CHD	C9-C10-C5	2.09	111.51	108.58
20	P	303	PGV	C03-C02-C01	-2.08	106.87	111.79
19	A	607	TGL	CG1-OG1-CA1	2.08	124.81	117.12
23	P	306	CHD	C11-C12-C13	2.07	113.37	111.24
26	C	303	CDL	CA6-CA4-CA3	-2.07	106.90	111.79
23	O	302	CHD	C9-C10-C5	2.07	111.48	108.58
23	J	101	CHD	C13-C17-C20	2.06	121.95	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	611	TGL	OG3-CC1-OC1	-2.06	118.39	123.59
26	P	304	CDL	CA6-OA8-CA7	2.06	124.75	117.12
19	N	609	TGL	OG3-CG3-CG2	2.05	114.41	108.43
26	T	103	CDL	OA8-CA7-OA9	-2.05	118.41	123.59
27	G	101	PEK	C02-O01-C1	-2.05	112.74	117.79
26	T	103	CDL	OB8-CB7-OB9	-2.05	118.42	123.59
19	L	101	TGL	CG3-CG2-CG1	-2.05	106.95	111.79
23	P	306	CHD	C21-C20-C17	-2.05	109.79	112.92
26	C	303	CDL	OA8-CA7-OA9	-2.05	118.43	123.59
24	B	303	PSC	O01-C1-O02	-2.04	118.77	123.70
26	P	304	CDL	OA6-CA5-OA7	-2.03	118.80	123.70
23	C	305	CHD	C18-C13-C14	-2.01	108.06	111.21
24	R	201	PSC	C08-N-C06	-2.01	103.81	108.97
20	A	609	PGV	O03-C01-C02	2.01	114.27	108.43
23	O	302	CHD	C1-C10-C9	-2.00	108.20	111.35
20	C	302	PGV	O03-C19-O04	-2.00	118.54	123.59
23	C	304	CHD	C2-C1-C10	2.00	116.21	112.78

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	602	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	601	HEA	NB
14	N	601	HEA	ND
14	N	601	HEA	NA
14	N	601	HEA	NB

All (951) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	N	608	PGV	C10-C11-C12-C13
20	A	609	PGV	C03-O11-P-O12
20	A	609	PGV	C03-O11-P-O13
20	A	609	PGV	C03-O11-P-O14
20	A	609	PGV	C04-C05-C06-O06
20	A	609	PGV	C2-C1-O01-C02
27	G	102	PEK	C03-O11-P-O13
20	C	308	PGV	C03-O11-P-O12
20	C	308	PGV	C03-O11-P-O13
20	C	308	PGV	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
20	C	308	PGV	C04-O12-P-O11
20	C	308	PGV	O12-C04-C05-C06
23	W	101	CHD	C13-C17-C20-C22
23	W	101	CHD	C16-C17-C20-C22
24	R	201	PSC	C03-O11-P-O12
24	R	201	PSC	C03-O11-P-O13
24	R	201	PSC	C03-O11-P-O14
24	R	201	PSC	C04-O12-P-O14
19	D	201	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	OC1-CC1-OG3-CG3
14	A	601	HEA	C1A-C2A-CAA-CBA
14	A	601	HEA	C3A-C2A-CAA-CBA
26	P	304	CDL	CA2-OA2-PA1-OA4
26	P	304	CDL	CA3-OA5-PA1-OA3
26	P	304	CDL	CA3-OA5-PA1-OA4
26	P	304	CDL	OA7-CA5-OA6-CA4
26	P	304	CDL	CB3-OB5-PB2-OB3
14	N	602	HEA	C2D-C3D-CAD-CBD
14	N	602	HEA	C4D-C3D-CAD-CBD
14	N	602	HEA	O11-C11-C12-C13
27	T	102	PEK	C04-O12-P-O13
27	T	102	PEK	C2-C1-O01-C02
27	C	306	PEK	C03-O11-P-O13
27	C	306	PEK	C03-O11-P-O14
27	C	306	PEK	O12-C04-C05-N
26	T	103	CDL	CB2-C1-CA2-OA2
26	T	103	CDL	CA2-OA2-PA1-OA3
26	T	103	CDL	CA2-OA2-PA1-OA4
26	T	103	CDL	CA3-OA5-PA1-OA3
26	T	103	CDL	OA6-CA4-CA6-OA8
26	T	103	CDL	C11-CA5-OA6-CA4
24	B	303	PSC	O12-C04-C05-N
24	B	303	PSC	C2-C1-O01-C02
24	B	303	PSC	O04-C19-O03-C01
24	B	303	PSC	C11-C10-C9-C8
19	N	611	TGL	CB2-CB1-OG2-CG2
19	N	611	TGL	OB1-CB1-OG2-CG2
20	N	607	PGV	C03-O11-P-O14
20	N	607	PGV	C04-C05-C06-O06
20	N	607	PGV	C20-C19-O03-C01
26	C	303	CDL	CA2-C1-CB2-OB2
26	C	303	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
26	C	303	CDL	CA2-OA2-PA1-OA3
26	C	303	CDL	CA2-OA2-PA1-OA4
26	C	303	CDL	CA2-OA2-PA1-OA5
26	C	303	CDL	CA3-OA5-PA1-OA2
26	C	303	CDL	CA3-OA5-PA1-OA3
26	C	303	CDL	OA7-CA5-OA6-CA4
26	C	303	CDL	C11-CA5-OA6-CA4
26	C	303	CDL	CB2-OB2-PB2-OB3
19	L	101	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	OB1-CB1-OG2-CG2
20	G	103	PGV	C03-O11-P-O13
20	G	103	PGV	C04-O12-P-O11
20	G	103	PGV	C04-O12-P-O13
20	G	103	PGV	C04-O12-P-O14
20	G	103	PGV	O03-C01-C02-O01
20	G	103	PGV	O12-C04-C05-C06
19	N	610	TGL	OB1-CB1-OG2-CG2
26	C	307	CDL	CB2-C1-CA2-OA2
26	C	307	CDL	C11-CA5-OA6-CA4
26	C	307	CDL	CB2-OB2-PB2-OB3
26	C	307	CDL	CB2-OB2-PB2-OB4
26	C	307	CDL	CB3-OB5-PB2-OB3
26	C	307	CDL	CB3-OB5-PB2-OB4
26	C	307	CDL	OB5-CB3-CB4-OB6
26	C	307	CDL	C51-CB5-OB6-CB4
27	T	101	PEK	C04-O12-P-O14
27	T	101	PEK	O12-C04-C05-N
26	P	304	CDL	OB9-CB7-OB8-CB6
20	N	607	PGV	O04-C19-O03-C01
19	L	101	TGL	OA1-CA1-OG1-CG1
19	N	610	TGL	OC1-CC1-OG3-CG3
26	P	304	CDL	C71-CB7-OB8-CB6
19	N	610	TGL	CC2-CC1-OG3-CG3
20	A	609	PGV	O04-C19-O03-C01
20	A	609	PGV	O02-C1-O01-C02
26	T	103	CDL	OA7-CA5-OA6-CA4
26	C	307	CDL	OA7-CA5-OA6-CA4
26	C	307	CDL	OB7-CB5-OB6-CB4
20	A	609	PGV	C20-C19-O03-C01
19	L	101	TGL	CA2-CA1-OG1-CG1
19	L	101	TGL	CC2-CC1-OG3-CG3
26	P	304	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
19	N	610	TGL	CB2-CB1-OG2-CG2
23	O	302	CHD	C21-C20-C22-C23
19	N	609	TGL	OC1-CC1-OG3-CG3
19	N	609	TGL	CC2-CC1-OG3-CG3
27	G	102	PEK	C22-C21-O03-C01
24	B	303	PSC	C20-C19-O03-C01
19	N	611	TGL	CA2-CA1-OG1-CG1
27	C	306	PEK	C4-C5-C6-C7
27	P	302	PEK	C4-C5-C6-C7
27	P	302	PEK	C10-C11-C12-C13
27	P	302	PEK	C13-C14-C15-C16
27	G	101	PEK	C4-C5-C6-C7
27	G	101	PEK	C13-C14-C15-C16
24	B	303	PSC	C24-C25-C26-C27
26	P	304	CDL	OB7-CB5-OB6-CB4
27	T	102	PEK	O02-C1-O01-C02
24	B	303	PSC	O02-C1-O01-C02
27	G	102	PEK	O04-C21-O03-C01
19	A	607	TGL	OC1-CC1-OG3-CG3
23	C	304	CHD	C20-C22-C23-C24
23	J	101	CHD	C13-C17-C20-C21
29	M	101	DMU	O6-C11-C9-O1
20	C	308	PGV	O12-C04-C05-O05
26	P	304	CDL	O1-C1-CA2-OA2
26	T	103	CDL	O1-C1-CA2-OA2
26	C	303	CDL	O1-C1-CB2-OB2
26	C	307	CDL	O1-C1-CA2-OA2
27	C	306	PEK	C22-C21-O03-C01
26	T	103	CDL	C31-CA7-OA8-CA6
19	A	607	TGL	CC2-CC1-OG3-CG3
19	L	101	TGL	OC1-CC1-OG3-CG3
29	Z	101	DMU	O5-C4-C57-O61
29	Z	101	DMU	C3-C4-C57-O61
26	P	304	CDL	C51-CB5-OB6-CB4
27	T	101	PEK	C2-C1-O01-C02
27	T	101	PEK	C24-C25-C26-C27
19	N	611	TGL	CC1-CC2-CC3-CC4
24	R	201	PSC	C20-C19-O03-C01
26	T	103	CDL	OA9-CA7-OA8-CA6
19	N	611	TGL	OA1-CA1-OG1-CG1
20	A	608	PGV	C26-C27-C28-C29
23	C	304	CHD	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
24	R	201	PSC	O04-C19-O03-C01
27	C	306	PEK	O04-C21-O03-C01
23	J	101	CHD	C16-C17-C20-C22
23	P	305	CHD	C17-C20-C22-C23
23	C	304	CHD	C17-C20-C22-C23
20	C	302	PGV	C27-C28-C29-C30
26	P	304	CDL	CB2-C1-CA2-OA2
27	T	101	PEK	O02-C1-O01-C02
29	M	101	DMU	O6-C11-C9-C8
19	N	609	TGL	CA2-CA1-OG1-CG1
20	C	308	PGV	C20-C19-O03-C01
26	C	303	CDL	C71-CB7-OB8-CB6
23	J	101	CHD	C20-C22-C23-C24
27	G	102	PEK	C1-C2-C3-C4
19	A	607	TGL	CB1-CB2-CB3-CB4
19	L	101	TGL	CA1-CA2-CA3-CA4
20	G	103	PGV	C1-C2-C3-C4
27	G	101	PEK	C33-C34-C35-C36
23	J	101	CHD	C17-C20-C22-C23
20	N	608	PGV	O12-C04-C05-O05
20	G	103	PGV	O12-C04-C05-O05
23	P	306	CHD	C21-C20-C22-C23
26	C	303	CDL	OB9-CB7-OB8-CB6
23	W	101	CHD	C16-C17-C20-C21
27	G	102	PEK	C2-C1-O01-C02
19	D	201	TGL	CB2-CB1-OG2-CG2
20	A	609	PGV	C19-C20-C21-C22
26	C	303	CDL	CA7-C31-C32-C33
26	C	307	CDL	CB5-C51-C52-C53
19	N	609	TGL	OA1-CA1-OG1-CG1
23	O	302	CHD	C17-C20-C22-C23
23	P	305	CHD	C21-C20-C22-C23
26	T	103	CDL	CB7-C71-C72-C73
26	C	303	CDL	CA5-C11-C12-C13
20	C	308	PGV	C10-C11-C12-C13
20	A	608	PGV	C10-C11-C12-C13
20	C	302	PGV	C1-C2-C3-C4
20	P	303	PGV	C1-C2-C3-C4
27	G	102	PEK	O02-C1-O01-C02
19	D	201	TGL	OB1-CB1-OG2-CG2
23	J	101	CHD	C21-C20-C22-C23
26	C	303	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
19	N	609	TGL	CA1-CA2-CA3-CA4
26	P	304	CDL	CA5-C11-C12-C13
20	P	303	PGV	C19-C20-C21-C22
19	N	611	TGL	CA1-CA2-CA3-CA4
19	N	610	TGL	CA1-CA2-CA3-CA4
21	B	304	EDO	O1-C1-C2-O2
20	C	308	PGV	O04-C19-O03-C01
14	A	601	HEA	C19-C20-C21-C22
19	D	201	TGL	CB1-CB2-CB3-CB4
20	P	303	PGV	C10-C11-C12-C13
20	G	103	PGV	C10-C11-C12-C13
29	Z	101	DMU	O6-C11-C9-C8
19	N	609	TGL	CB2-CB1-OG2-CG2
20	N	608	PGV	C04-O12-P-O11
20	A	609	PGV	C04-O12-P-O11
27	G	102	PEK	C03-O11-P-O12
24	R	201	PSC	C04-O12-P-O11
26	P	304	CDL	CA2-OA2-PA1-OA5
26	P	304	CDL	CA3-OA5-PA1-OA2
27	T	102	PEK	C04-O12-P-O11
27	C	306	PEK	C03-O11-P-O12
26	T	103	CDL	CA2-OA2-PA1-OA5
26	T	103	CDL	CB3-OB5-PB2-OB2
20	N	607	PGV	C03-O11-P-O12
26	C	303	CDL	CB2-OB2-PB2-OB5
26	C	307	CDL	CB2-OB2-PB2-OB5
26	C	307	CDL	CB3-OB5-PB2-OB2
20	C	308	PGV	C19-C20-C21-C22
23	W	101	CHD	C13-C17-C20-C21
20	N	608	PGV	O12-C04-C05-C06
19	N	609	TGL	OB1-CB1-OG2-CG2
26	T	103	CDL	C79-C80-C81-C82
27	T	102	PEK	C22-C21-O03-C01
23	P	305	CHD	C20-C22-C23-C24
27	G	102	PEK	C30-C31-C32-C33
20	C	308	PGV	C26-C27-C28-C29
27	P	302	PEK	C26-C27-C28-C29
26	C	303	CDL	C35-C36-C37-C38
26	C	303	CDL	C63-C64-C65-C66
19	L	101	TGL	C21-C22-C23-C24
19	N	610	TGL	C11-C10-CB9-CB8
26	C	307	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
26	T	103	CDL	C51-CB5-OB6-CB4
19	N	609	TGL	CA2-CA3-CA4-CA5
19	N	609	TGL	CB9-C10-C11-C12
19	N	609	TGL	C24-C25-C26-C27
20	C	308	PGV	C4-C5-C6-C7
19	D	201	TGL	C14-C29-C30-C31
26	T	103	CDL	C36-C37-C38-C39
19	A	607	TGL	C11-C12-C13-C14
19	N	611	TGL	C24-C25-C26-C27
27	G	101	PEK	C29-C30-C31-C32
26	C	307	CDL	C57-C58-C59-C60
20	N	608	PGV	C2-C3-C4-C5
20	N	608	PGV	C13-C14-C15-C16
19	N	609	TGL	CA5-CA6-CA7-CA8
19	N	609	TGL	CC6-CC7-CC8-CC9
20	A	609	PGV	C20-C21-C22-C23
27	T	102	PEK	C29-C30-C31-C32
26	T	103	CDL	C54-C55-C56-C57
27	G	101	PEK	C26-C27-C28-C29
29	Z	101	DMU	C25-C28-C31-C34
20	G	103	PGV	C6-C7-C8-C9
19	N	610	TGL	C16-C15-CC9-CC8
20	C	308	PGV	O02-C1-O01-C02
26	T	103	CDL	OB7-CB5-OB6-CB4
20	A	609	PGV	C21-C22-C23-C24
24	R	201	PSC	C20-C21-C22-C23
26	P	304	CDL	C20-C21-C22-C23
27	C	306	PEK	C16-C17-C18-C19
26	T	103	CDL	C42-C43-C44-C45
20	P	303	PGV	C20-C21-C22-C23
24	B	303	PSC	C28-C29-C30-C31
19	A	607	TGL	CC2-CC3-CC4-CC5
19	L	101	TGL	CB5-CB6-CB7-CB8
26	C	307	CDL	C17-C18-C19-C20
20	C	308	PGV	C7-C8-C9-C10
19	D	201	TGL	CC6-CC7-CC8-CC9
26	P	304	CDL	C81-C82-C83-C84
26	T	103	CDL	C12-C13-C14-C15
26	T	103	CDL	C57-C58-C59-C60
26	C	303	CDL	C12-C13-C14-C15
29	Z	101	DMU	C28-C31-C34-C37
19	N	610	TGL	CA2-CA3-CA4-CA5

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Mol	Chain	Res	Type	Atoms
20	N	607	PGV	O12-C04-C05-O05
27	G	102	PEK	C23-C24-C25-C26
20	C	308	PGV	C23-C24-C25-C26
24	R	201	PSC	C3-C4-C5-C6
20	P	303	PGV	C7-C8-C9-C10
26	C	303	CDL	C33-C34-C35-C36
19	L	101	TGL	C12-C13-C14-C29
19	N	610	TGL	C18-C19-C33-C34
19	N	610	TGL	C19-C33-C34-C35
26	C	307	CDL	C33-C34-C35-C36
26	T	103	CDL	C52-C53-C54-C55
19	N	611	TGL	CB5-CB6-CB7-CB8
27	P	302	PEK	C28-C29-C30-C31
26	C	303	CDL	C80-C81-C82-C83
19	L	101	TGL	CA6-CA7-CA8-CA9
20	G	103	PGV	C22-C23-C24-C25
26	C	307	CDL	C22-C23-C24-C25
20	N	608	PGV	C23-C24-C25-C26
19	D	201	TGL	C10-C11-C12-C13
19	D	201	TGL	C15-C16-C17-C18
20	N	607	PGV	C29-C30-C31-C32
19	L	101	TGL	C16-C17-C18-C19
26	C	307	CDL	C35-C36-C37-C38
24	R	201	PSC	C4-C5-C6-C7
19	D	201	TGL	C12-C13-C14-C29
26	P	304	CDL	C43-C44-C45-C46
27	C	306	PEK	C34-C35-C36-C37
26	T	103	CDL	C40-C41-C42-C43
20	A	608	PGV	C22-C23-C24-C25
19	L	101	TGL	CA2-CA3-CA4-CA5
19	L	101	TGL	C21-C20-CA9-CA8
19	N	610	TGL	CA3-CA4-CA5-CA6
26	C	307	CDL	C58-C59-C60-C61
26	C	307	CDL	C61-C62-C63-C64
27	T	101	PEK	C28-C29-C30-C31
27	G	102	PEK	C31-C32-C33-C34
20	C	308	PGV	C6-C7-C8-C9
24	R	201	PSC	C5-C6-C7-C8
26	T	103	CDL	C41-C42-C43-C44
26	C	303	CDL	C20-C21-C22-C23
19	N	610	TGL	C17-C18-C19-C33
20	C	308	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
19	N	609	TGL	CA4-CA5-CA6-CA7
19	D	201	TGL	C18-C19-C33-C34
20	P	303	PGV	C25-C26-C27-C28
19	A	607	TGL	C14-C29-C30-C31
19	N	611	TGL	CA7-CA8-CA9-C20
19	L	101	TGL	CB3-CB4-CB5-CB6
19	L	101	TGL	C20-C21-C22-C23
27	G	102	PEK	C15-C16-C17-C18
19	N	610	TGL	CB1-CB2-CB3-CB4
19	N	609	TGL	C21-C20-CA9-CA8
19	N	609	TGL	CB2-CB3-CB4-CB5
20	A	609	PGV	C30-C31-C32-C33
20	C	308	PGV	C3-C4-C5-C6
26	P	304	CDL	C31-C32-C33-C34
26	P	304	CDL	C37-C38-C39-C40
26	T	103	CDL	C18-C19-C20-C21
26	T	103	CDL	C59-C60-C61-C62
20	P	303	PGV	C29-C30-C31-C32
19	A	607	TGL	C24-C25-C26-C27
19	N	611	TGL	CB3-CB4-CB5-CB6
26	C	303	CDL	C81-C82-C83-C84
27	G	101	PEK	C30-C31-C32-C33
20	G	103	PGV	C4-C5-C6-C7
20	G	103	PGV	C24-C25-C26-C27
26	C	307	CDL	C62-C63-C64-C65
27	G	102	PEK	C32-C33-C34-C35
24	R	201	PSC	C21-C22-C23-C24
19	D	201	TGL	CA3-CA4-CA5-CA6
26	P	304	CDL	C35-C36-C37-C38
26	P	304	CDL	C56-C57-C58-C59
27	T	102	PEK	C26-C27-C28-C29
19	A	607	TGL	CA3-CA4-CA5-CA6
19	A	607	TGL	CC3-CC4-CC5-CC6
19	N	611	TGL	C17-C18-C19-C33
26	C	307	CDL	C23-C24-C25-C26
19	N	609	TGL	CC2-CC3-CC4-CC5
26	P	304	CDL	C36-C37-C38-C39
27	C	306	PEK	C25-C26-C27-C28
26	T	103	CDL	C73-C74-C75-C76
24	B	303	PSC	C27-C28-C29-C30
19	A	607	TGL	C17-C18-C19-C33
27	G	101	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	CC2-CC3-CC4-CC5
19	L	101	TGL	CC7-CC8-CC9-C15
20	N	608	PGV	C19-C20-C21-C22
27	T	102	PEK	O04-C21-O03-C01
19	N	609	TGL	CB4-CB5-CB6-CB7
20	C	302	PGV	C30-C31-C32-C33
26	C	303	CDL	C42-C43-C44-C45
19	N	610	TGL	CC5-CC6-CC7-CC8
19	N	609	TGL	C21-C22-C23-C24
20	C	308	PGV	C2-C3-C4-C5
19	A	607	TGL	CA5-CA6-CA7-CA8
27	P	302	PEK	C25-C26-C27-C28
26	C	303	CDL	C77-C78-C79-C80
19	N	610	TGL	C21-C20-CA9-CA8
23	J	101	CHD	C13-C17-C20-C22
19	A	607	TGL	CA9-C20-C21-C22
19	N	611	TGL	CC5-CC6-CC7-CC8
19	L	101	TGL	C18-C19-C33-C34
20	G	103	PGV	C23-C24-C25-C26
19	N	610	TGL	C20-C21-C22-C23
24	B	303	PSC	C1-C2-C3-C4
26	P	304	CDL	C38-C39-C40-C41
19	A	607	TGL	CB9-C10-C11-C12
19	A	607	TGL	CC9-C15-C16-C17
19	A	607	TGL	C21-C22-C23-C24
26	C	307	CDL	C14-C15-C16-C17
26	C	307	CDL	C16-C17-C18-C19
24	R	201	PSC	C11-C12-C13-C14
27	C	306	PEK	C10-C11-C12-C13
27	G	101	PEK	C7-C8-C9-C10
27	C	306	PEK	C29-C30-C31-C32
19	N	611	TGL	C21-C22-C23-C24
19	L	101	TGL	CA4-CA5-CA6-CA7
20	G	103	PGV	C13-C14-C15-C16
20	G	103	PGV	C26-C27-C28-C29
19	N	610	TGL	C12-C13-C14-C29
19	D	201	TGL	C21-C20-CA9-CA8
26	C	303	CDL	C19-C20-C21-C22
20	G	103	PGV	C3-C4-C5-C6
19	N	609	TGL	CC4-CC5-CC6-CC7
26	C	303	CDL	C62-C63-C64-C65
27	G	101	PEK	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
20	A	609	PGV	O05-C05-C06-O06
19	D	201	TGL	CA9-C20-C21-C22
20	P	303	PGV	C21-C22-C23-C24
27	P	302	PEK	C22-C23-C24-C25
19	N	610	TGL	C15-C16-C17-C18
26	T	103	CDL	C22-C23-C24-C25
26	C	303	CDL	C37-C38-C39-C40
26	T	103	CDL	CA7-C31-C32-C33
20	N	607	PGV	O12-C04-C05-C06
19	L	101	TGL	CA7-CA8-CA9-C20
26	C	307	CDL	C54-C55-C56-C57
26	C	307	CDL	C59-C60-C61-C62
24	R	201	PSC	O02-C1-O01-C02
26	P	304	CDL	C1-CA2-OA2-PA1
26	T	103	CDL	C1-CA2-OA2-PA1
26	P	304	CDL	C21-C22-C23-C24
24	B	303	PSC	C14-C15-C16-C17
24	B	303	PSC	C19-C20-C21-C22
21	L	102	EDO	O1-C1-C2-O2
21	A	613	EDO	O1-C1-C2-O2
21	T	104	EDO	O1-C1-C2-O2
21	A	612	EDO	O1-C1-C2-O2
19	N	609	TGL	C14-C29-C30-C31
19	D	201	TGL	CB9-C10-C11-C12
19	A	607	TGL	CB4-CB5-CB6-CB7
24	R	201	PSC	C2-C1-O01-C02
19	N	609	TGL	CC5-CC6-CC7-CC8
20	A	608	PGV	C15-C16-C17-C18
27	T	102	PEK	C1-C2-C3-C4
27	C	306	PEK	C1-C2-C3-C4
19	L	101	TGL	CC1-CC2-CC3-CC4
26	P	304	CDL	C52-C53-C54-C55
26	C	303	CDL	C58-C59-C60-C61
27	G	102	PEK	C13-C14-C15-C16
24	R	201	PSC	C11-C10-C9-C8
27	T	101	PEK	C7-C8-C9-C10
20	C	308	PGV	C24-C25-C26-C27
19	D	201	TGL	CC7-CC8-CC9-C15
27	C	306	PEK	C32-C33-C34-C35
26	C	303	CDL	C16-C17-C18-C19
27	G	102	PEK	C34-C35-C36-C37
26	C	307	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	CA1-CA2-CA3-CA4
27	G	101	PEK	C21-C22-C23-C24
27	G	102	PEK	C16-C17-C18-C19
19	D	201	TGL	C21-C22-C23-C24
27	G	101	PEK	C23-C24-C25-C26
26	C	307	CDL	C52-C53-C54-C55
26	P	304	CDL	C16-C17-C18-C19
26	P	304	CDL	C19-C20-C21-C22
27	T	102	PEK	C30-C31-C32-C33
26	T	103	CDL	C11-C12-C13-C14
26	T	103	CDL	C55-C56-C57-C58
19	A	607	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	CB2-CB3-CB4-CB5
20	N	607	PGV	C25-C26-C27-C28
20	A	608	PGV	C20-C21-C22-C23
20	N	608	PGV	C6-C7-C8-C9
26	P	304	CDL	C42-C43-C44-C45
26	T	103	CDL	C43-C44-C45-C46
19	N	610	TGL	CA9-C20-C21-C22
20	P	303	PGV	C11-C10-C9-C8
24	B	303	PSC	C6-C7-C8-C9
27	P	302	PEK	C2-C3-C4-C5
20	A	608	PGV	C11-C10-C9-C8
27	G	101	PEK	C15-C16-C17-C18
14	A	601	HEA	C27-C19-C20-C21
20	A	609	PGV	C5-C6-C7-C8
19	D	201	TGL	C23-C24-C25-C26
26	T	103	CDL	C60-C61-C62-C63
19	N	610	TGL	CC2-CC3-CC4-CC5
26	C	307	CDL	C56-C57-C58-C59
19	N	609	TGL	C20-C21-C22-C23
20	N	607	PGV	C7-C8-C9-C10
19	N	611	TGL	C11-C12-C13-C14
27	P	302	PEK	C16-C17-C18-C19
26	C	303	CDL	C36-C37-C38-C39
19	N	610	TGL	CB7-CB8-CB9-C10
19	N	610	TGL	CA6-CA7-CA8-CA9
27	T	102	PEK	C03-O11-P-O12
20	G	103	PGV	C2-C3-C4-C5
26	P	304	CDL	OA5-CA3-CA4-CA6
26	P	304	CDL	OB5-CB3-CB4-CB6
26	T	103	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
26	T	103	CDL	OB5-CB3-CB4-CB6
20	C	308	PGV	C25-C26-C27-C28
19	N	610	TGL	CA5-CA6-CA7-CA8
27	P	302	PEK	C1-C2-C3-C4
19	D	201	TGL	C16-C17-C18-C19
20	N	607	PGV	C3-C4-C5-C6
26	C	303	CDL	C83-C84-C85-C86
27	P	302	PEK	C27-C28-C29-C30
19	A	607	TGL	C22-C23-C24-C25
26	C	307	CDL	C32-C33-C34-C35
20	N	607	PGV	C12-C13-C14-C15
19	N	610	TGL	CB6-CB7-CB8-CB9
27	T	101	PEK	C29-C30-C31-C32
19	A	607	TGL	OB1-CB1-OG2-CG2
24	B	303	PSC	C23-C24-C25-C26
19	A	607	TGL	C19-C33-C34-C35
19	L	101	TGL	CC6-CC7-CC8-CC9
20	G	103	PGV	C25-C26-C27-C28
26	C	307	CDL	C76-C77-C78-C79
19	D	201	TGL	C11-C10-CB9-CB8
19	D	201	TGL	CC2-CC3-CC4-CC5
19	N	609	TGL	CC3-CC4-CC5-CC6
26	T	103	CDL	C77-C78-C79-C80
19	N	611	TGL	OG1-CG1-CG2-CG3
26	C	303	CDL	CB3-CB4-CB6-OB8
27	G	101	PEK	O03-C01-C02-C03
20	G	103	PGV	O03-C01-C02-C03
26	C	307	CDL	CA3-CA4-CA6-OA8
19	D	201	TGL	C20-C21-C22-C23
19	L	101	TGL	CA9-C20-C21-C22
27	G	101	PEK	C35-C36-C37-C38
26	P	304	CDL	C64-C65-C66-C67
19	L	101	TGL	CB9-C10-C11-C12
20	N	608	PGV	O03-C19-C20-C21
27	C	306	PEK	C17-C18-C19-C20
19	A	607	TGL	C10-C11-C12-C13
27	G	101	PEK	C17-C18-C19-C20
20	N	608	PGV	C31-C32-C33-C34
24	R	201	PSC	C30-C31-C32-C33
20	N	607	PGV	O05-C05-C06-O06
27	T	102	PEK	C23-C24-C25-C26
27	C	306	PEK	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
19	N	609	TGL	C12-C13-C14-C29
19	D	201	TGL	CA7-CA8-CA9-C20
19	L	101	TGL	CC4-CC5-CC6-CC7
24	R	201	PSC	C29-C30-C31-C32
19	L	101	TGL	C22-C23-C24-C25
26	T	103	CDL	C71-CB7-OB8-CB6
20	A	609	PGV	C03-C02-O01-C1
27	G	102	PEK	C27-C28-C29-C30
26	P	304	CDL	C58-C59-C60-C61
26	T	103	CDL	C58-C59-C60-C61
26	P	304	CDL	C18-C19-C20-C21
26	P	304	CDL	C73-C74-C75-C76
26	T	103	CDL	C81-C82-C83-C84
19	A	607	TGL	C12-C13-C14-C29
20	N	607	PGV	C5-C6-C7-C8
26	C	303	CDL	C31-C32-C33-C34
26	C	307	CDL	C21-C22-C23-C24
20	C	308	PGV	C05-C04-O12-P
20	G	103	PGV	C05-C04-O12-P
26	P	304	CDL	C23-C24-C25-C26
26	P	304	CDL	C61-C62-C63-C64
19	N	610	TGL	CA2-CA1-OG1-CG1
29	Z	101	DMU	O6-C11-C9-O1
27	G	102	PEK	C4-C5-C6-C7
20	G	103	PGV	C19-C20-C21-C22
19	D	201	TGL	CA2-CA3-CA4-CA5
26	C	303	CDL	C73-C74-C75-C76
26	C	307	CDL	C53-C54-C55-C56
20	C	302	PGV	C31-C32-C33-C34
26	T	103	CDL	C38-C39-C40-C41
27	T	101	PEK	C30-C31-C32-C33
27	G	102	PEK	C35-C36-C37-C38
20	A	609	PGV	C22-C23-C24-C25
19	D	201	TGL	CB7-CB8-CB9-C10
20	G	103	PGV	C31-C32-C33-C34
26	T	103	CDL	C32-C33-C34-C35
26	P	304	CDL	C33-C34-C35-C36
20	N	607	PGV	C15-C16-C17-C18
24	R	201	PSC	C1-C2-C3-C4
26	C	307	CDL	CA7-C31-C32-C33
26	P	304	CDL	C63-C64-C65-C66
20	A	608	PGV	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
20	N	608	PGV	C7-C8-C9-C10
19	N	609	TGL	C29-C30-C31-C32
19	N	609	TGL	C19-C33-C34-C35
26	T	103	CDL	C71-C72-C73-C74
19	N	609	TGL	CA9-C20-C21-C22
20	P	303	PGV	C24-C25-C26-C27
26	C	303	CDL	C38-C39-C40-C41
24	B	303	PSC	C4-C5-C6-C7
29	M	101	DMU	C3-C4-C57-O61
20	A	609	PGV	C14-C15-C16-C17
24	R	201	PSC	C13-C14-C15-C16
26	C	303	CDL	C57-C58-C59-C60
26	C	303	CDL	C78-C79-C80-C81
19	L	101	TGL	CA5-CA6-CA7-CA8
20	A	609	PGV	C01-C02-C03-O11
27	C	306	PEK	C01-C02-C03-O11
26	C	303	CDL	OB5-CB3-CB4-CB6
20	G	103	PGV	C01-C02-C03-O11
26	C	307	CDL	OB5-CB3-CB4-CB6
20	A	609	PGV	C2-C3-C4-C5
23	P	305	CHD	C16-C17-C20-C21
26	C	303	CDL	C56-C57-C58-C59
26	C	307	CDL	C74-C75-C76-C77
19	N	611	TGL	CB2-CB3-CB4-CB5
26	C	307	CDL	C37-C38-C39-C40
26	T	103	CDL	OB9-CB7-OB8-CB6
26	P	304	CDL	C80-C81-C82-C83
20	A	608	PGV	C24-C25-C26-C27
19	N	611	TGL	CC2-CC1-OG3-CG3
26	T	103	CDL	C39-C40-C41-C42
26	C	307	CDL	C1-CB2-OB2-PB2
20	P	303	PGV	C31-C32-C33-C34
26	C	303	CDL	C53-C54-C55-C56
19	N	609	TGL	CB5-CB6-CB7-CB8
24	B	303	PSC	C29-C30-C31-C32
26	T	103	CDL	C75-C76-C77-C78
19	A	607	TGL	CG1-CG2-CG3-OG3
20	N	607	PGV	O03-C01-C02-C03
26	C	303	CDL	CA3-CA4-CA6-OA8
27	T	101	PEK	O03-C01-C02-C03
27	G	102	PEK	C17-C18-C19-C20
26	P	304	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
27	C	306	PEK	C13-C14-C15-C16
20	P	303	PGV	C26-C27-C28-C29
24	B	303	PSC	C3-C4-C5-C6
19	A	607	TGL	CB5-CB6-CB7-CB8
19	L	101	TGL	C24-C25-C26-C27
20	A	609	PGV	C3-C4-C5-C6
27	G	102	PEK	C5-C6-C7-C8
27	G	102	PEK	C11-C10-C9-C8
24	R	201	PSC	C9-C10-C11-C12
24	R	201	PSC	C10-C11-C12-C13
27	T	102	PEK	C5-C6-C7-C8
27	T	102	PEK	C6-C7-C8-C9
27	T	102	PEK	C11-C10-C9-C8
27	T	102	PEK	C9-C10-C11-C12
27	C	306	PEK	C6-C7-C8-C9
27	C	306	PEK	C9-C10-C11-C12
24	B	303	PSC	C9-C10-C11-C12
24	B	303	PSC	C10-C11-C12-C13
27	P	302	PEK	C5-C6-C7-C8
27	T	101	PEK	C12-C13-C14-C15
27	T	102	PEK	C34-C35-C36-C37
19	N	610	TGL	C33-C34-C35-C36
20	C	308	PGV	O01-C02-C03-O11
26	T	103	CDL	OB5-CB3-CB4-OB6
23	P	305	CHD	C16-C17-C20-C22
20	G	103	PGV	C11-C10-C9-C8
19	N	610	TGL	OA1-CA1-OG1-CG1
19	D	201	TGL	C13-C14-C29-C30
20	P	303	PGV	C13-C14-C15-C16
19	N	609	TGL	CA3-CA4-CA5-CA6
19	D	201	TGL	CA6-CA7-CA8-CA9
19	D	201	TGL	C25-C26-C27-C28
20	G	103	PGV	C20-C21-C22-C23
26	C	303	CDL	C18-C19-C20-C21
19	L	101	TGL	CC5-CC6-CC7-CC8
20	A	609	PGV	O03-C01-C02-O01
20	C	308	PGV	O03-C01-C02-O01
20	N	607	PGV	O03-C01-C02-O01
27	T	101	PEK	O03-C01-C02-O01
19	N	611	TGL	C29-C30-C31-C32
26	C	307	CDL	C77-C78-C79-C80
26	C	303	CDL	C64-C65-C66-C67

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Mol	Chain	Res	Type	Atoms
20	C	308	PGV	C27-C28-C29-C30
20	C	302	PGV	C26-C27-C28-C29
27	G	101	PEK	C34-C35-C36-C37
26	P	304	CDL	C11-C12-C13-C14
26	P	304	CDL	C54-C55-C56-C57
20	A	609	PGV	C02-C03-O11-P
20	C	302	PGV	C12-C13-C14-C15
19	N	610	TGL	C22-C23-C24-C25
21	A	610	EDO	O1-C1-C2-O2
27	G	102	PEK	C24-C25-C26-C27
19	N	609	TGL	CC9-C15-C16-C17
20	C	308	PGV	C30-C31-C32-C33
26	P	304	CDL	C82-C83-C84-C85
26	T	103	CDL	C78-C79-C80-C81
20	P	303	PGV	C27-C28-C29-C30
27	G	102	PEK	C2-C3-C4-C5
19	N	610	TGL	CB3-CB4-CB5-CB6
26	T	103	CDL	C16-C17-C18-C19
20	N	607	PGV	C22-C23-C24-C25
20	N	607	PGV	C02-C01-O03-C19
27	P	302	PEK	C34-C35-C36-C37
20	P	303	PGV	C20-C19-O03-C01
27	G	102	PEK	C33-C34-C35-C36
19	N	609	TGL	C16-C15-CC9-CC8
20	C	308	PGV	C22-C23-C24-C25
19	D	201	TGL	C16-C15-CC9-CC8
19	N	611	TGL	CC3-CC4-CC5-CC6
19	N	609	TGL	C25-C26-C27-C28
19	N	610	TGL	CC1-CC2-CC3-CC4
19	D	201	TGL	C24-C25-C26-C27
20	A	609	PGV	O03-C01-C02-C03
27	G	102	PEK	O03-C01-C02-C03
26	P	304	CDL	CA3-CA4-CA6-OA8
26	T	103	CDL	CB3-CB4-CB6-OB8
20	P	303	PGV	O03-C01-C02-C03
24	B	303	PSC	O03-C01-C02-C03
19	A	607	TGL	OG1-CG1-CG2-CG3
27	C	306	PEK	O01-C02-C03-O11
26	C	303	CDL	OB5-CB3-CB4-OB6
27	T	101	PEK	O01-C02-C03-O11
24	R	201	PSC	O03-C19-C20-C21
27	C	306	PEK	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	CC6-CC7-CC8-CC9
19	N	611	TGL	C25-C26-C27-C28
20	P	303	PGV	O04-C19-O03-C01
19	N	611	TGL	OC1-CC1-OG3-CG3
20	A	608	PGV	O04-C19-O03-C01
26	C	303	CDL	C84-C85-C86-C87
26	C	307	CDL	C72-C73-C74-C75
26	T	103	CDL	OB6-CB4-CB6-OB8
20	P	303	PGV	O03-C01-C02-O01
19	A	607	TGL	OG2-CG2-CG3-OG3
26	C	303	CDL	OA6-CA4-CA6-OA8
26	C	303	CDL	OB6-CB4-CB6-OB8
19	L	101	TGL	OG1-CG1-CG2-OG2
23	J	101	CHD	C16-C17-C20-C21
26	P	304	CDL	C78-C79-C80-C81
27	P	302	PEK	C30-C31-C32-C33
26	C	307	CDL	C24-C25-C26-C27
20	C	302	PGV	O05-C05-C06-O06
27	C	306	PEK	C22-C23-C24-C25
19	N	610	TGL	C13-C14-C29-C30
26	T	103	CDL	C56-C57-C58-C59
19	N	609	TGL	C16-C17-C18-C19
27	T	102	PEK	C25-C26-C27-C28
20	C	302	PGV	C04-C05-C06-O06
20	N	607	PGV	C20-C21-C22-C23
27	T	101	PEK	C25-C26-C27-C28
26	P	304	CDL	C74-C75-C76-C77
19	N	610	TGL	C29-C30-C31-C32
26	T	103	CDL	CA3-OA5-PA1-OA2
24	B	303	PSC	C03-O11-P-O12
24	B	303	PSC	C04-O12-P-O11
20	G	103	PGV	C03-O11-P-O12
19	A	607	TGL	C25-C26-C27-C28
27	P	302	PEK	C17-C18-C19-C20
26	P	304	CDL	CA4-CA3-OA5-PA1
20	C	302	PGV	C02-C03-O11-P
20	C	302	PGV	C05-C04-O12-P
26	T	103	CDL	C1-CB2-OB2-PB2
20	P	303	PGV	C02-C03-O11-P
19	N	609	TGL	CB7-CB8-CB9-C10
20	N	608	PGV	C04-O12-P-O13
20	N	608	PGV	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
20	A	609	PGV	C04-O12-P-O13
20	A	609	PGV	C04-O12-P-O14
20	C	308	PGV	C04-O12-P-O14
24	R	201	PSC	C04-O12-P-O13
27	T	102	PEK	C03-O11-P-O13
27	T	102	PEK	C03-O11-P-O14
27	T	102	PEK	C04-O12-P-O14
26	T	103	CDL	CB3-OB5-PB2-OB3
20	N	607	PGV	C03-O11-P-O13
26	C	303	CDL	CB2-OB2-PB2-OB4
27	T	101	PEK	C01-C02-C03-O11
21	C	309	EDO	O1-C1-C2-O2
26	C	303	CDL	C54-C55-C56-C57
26	C	303	CDL	C21-C22-C23-C24
27	T	102	PEK	C33-C34-C35-C36
26	C	307	CDL	C81-C82-C83-C84
19	A	607	TGL	CB2-CB3-CB4-CB5
20	N	608	PGV	C4-C5-C6-C7
27	G	102	PEK	C26-C27-C28-C29
20	C	308	PGV	C31-C32-C33-C34
26	P	304	CDL	C60-C61-C62-C63
26	T	103	CDL	C17-C18-C19-C20
20	A	609	PGV	O01-C02-C03-O11
26	P	304	CDL	OA5-CA3-CA4-OA6
26	T	103	CDL	OA5-CA3-CA4-OA6
20	G	103	PGV	O01-C02-C03-O11
20	A	609	PGV	C9-C10-C11-C12
20	N	607	PGV	C23-C24-C25-C26
26	C	307	CDL	C73-C74-C75-C76
19	A	607	TGL	CA4-CA5-CA6-CA7
26	C	303	CDL	O1-C1-CA2-OA2
19	N	611	TGL	CA2-CA3-CA4-CA5
26	C	307	CDL	C12-C13-C14-C15
24	R	201	PSC	O12-C04-C05-N
26	T	103	CDL	CA3-CA4-CA6-OA8
27	G	102	PEK	O03-C01-C02-O01
26	P	304	CDL	OA6-CA4-CA6-OA8
24	B	303	PSC	O03-C01-C02-O01
19	N	611	TGL	OG1-CG1-CG2-OG2
29	Z	101	DMU	C22-C25-C28-C31
27	P	302	PEK	C7-C8-C9-C10
20	A	609	PGV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	CC4-CC5-CC6-CC7
27	G	102	PEK	C28-C29-C30-C31
23	P	305	CHD	C13-C17-C20-C22
26	P	304	CDL	C40-C41-C42-C43
19	N	611	TGL	CA4-CA5-CA6-CA7
23	P	305	CHD	C13-C17-C20-C21
27	C	306	PEK	C28-C29-C30-C31
20	G	103	PGV	C27-C28-C29-C30
26	P	304	CDL	C13-C14-C15-C16
19	N	610	TGL	CB4-CB5-CB6-CB7
26	C	303	CDL	C14-C15-C16-C17
26	T	103	CDL	C33-C34-C35-C36
29	M	101	DMU	C34-C37-C40-C43
24	R	201	PSC	C28-C29-C30-C31
26	C	307	CDL	C39-C40-C41-C42
27	T	101	PEK	C35-C36-C37-C38
26	C	303	CDL	OB7-CB5-OB6-CB4
27	G	101	PEK	C1-C2-C3-C4
20	G	103	PGV	C14-C15-C16-C17
26	C	303	CDL	C1-CB2-OB2-PB2
26	P	304	CDL	OB5-CB3-CB4-OB6
20	P	303	PGV	C23-C24-C25-C26
21	K	102	EDO	O1-C1-C2-O2
26	C	303	CDL	OA9-CA7-OA8-CA6
19	A	607	TGL	OG1-CG1-CG2-OG2
27	G	101	PEK	O03-C01-C02-O01
20	G	103	PGV	C7-C8-C9-C10
26	C	303	CDL	C31-CA7-OA8-CA6
26	P	304	CDL	CB3-OB5-PB2-OB2
26	C	307	CDL	CA3-OA5-PA1-OA2
27	T	101	PEK	C04-O12-P-O11
29	Z	101	DMU	O16-C18-C19-C22
27	G	102	PEK	C21-C22-C23-C24
19	L	101	TGL	OG1-CG1-CG2-CG3
19	N	611	TGL	C19-C33-C34-C35
20	N	608	PGV	C5-C6-C7-C8
27	C	306	PEK	O02-C1-O01-C02
19	N	611	TGL	CA6-CA7-CA8-CA9
26	C	307	CDL	C75-C76-C77-C78
24	R	201	PSC	C23-C24-C25-C26
19	N	610	TGL	C21-C22-C23-C24
19	N	609	TGL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	G	101	PEK	C2-C3-C4-C5
26	P	304	CDL	C62-C63-C64-C65
20	A	608	PGV	C9-C10-C11-C12
20	C	302	PGV	C24-C25-C26-C27
24	B	303	PSC	C22-C23-C24-C25
26	C	303	CDL	OA5-CA3-CA4-CA6
27	T	102	PEK	O01-C02-C03-O11
27	T	102	PEK	O01-C1-C2-C3
26	C	303	CDL	C59-C60-C61-C62
20	N	608	PGV	C27-C28-C29-C30
29	M	101	DMU	C19-C22-C25-C28
20	N	608	PGV	O04-C19-C20-C21
19	N	610	TGL	CC3-CC4-CC5-CC6
19	N	611	TGL	CC7-CC8-CC9-C15
26	T	103	CDL	C37-C38-C39-C40
24	B	303	PSC	C12-C13-C14-C15
19	A	607	TGL	CB7-CB8-CB9-C10
26	P	304	CDL	C22-C23-C24-C25
19	N	611	TGL	C23-C24-C25-C26
24	R	201	PSC	C19-C20-C21-C22
24	B	303	PSC	C03-C02-O01-C1
27	G	101	PEK	C27-C28-C29-C30
27	T	102	PEK	C3-C4-C5-C6
27	C	306	PEK	C26-C27-C28-C29
26	C	303	CDL	C13-C14-C15-C16
27	G	102	PEK	C9-C10-C11-C12
27	G	102	PEK	C11-C12-C13-C14
27	T	102	PEK	C11-C12-C13-C14
27	T	102	PEK	C12-C13-C14-C15
27	C	306	PEK	C12-C13-C14-C15
27	T	101	PEK	C9-C10-C11-C12
19	N	611	TGL	C33-C34-C35-C36
19	A	607	TGL	CA6-CA7-CA8-CA9
20	C	302	PGV	C20-C21-C22-C23
20	C	302	PGV	C13-C14-C15-C16
26	C	307	CDL	C83-C84-C85-C86
26	C	307	CDL	OA6-CA4-CA6-OA8
26	T	103	CDL	C61-C62-C63-C64
19	N	611	TGL	CC4-CC5-CC6-CC7
27	T	102	PEK	C02-C03-O11-P
26	P	304	CDL	C55-C56-C57-C58
19	D	201	TGL	OG1-CG1-CG2-CG3

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Mol	Chain	Res	Type	Atoms
29	Z	101	DMU	C19-C22-C25-C28
19	N	611	TGL	CA9-C20-C21-C22
20	N	607	PGV	O01-C02-C03-O11
20	N	607	PGV	C31-C32-C33-C34
19	N	610	TGL	CA4-CA5-CA6-CA7
20	N	608	PGV	C15-C16-C17-C18
26	T	103	CDL	C13-C14-C15-C16
26	C	303	CDL	C51-CB5-OB6-CB4
26	C	307	CDL	C18-C19-C20-C21
19	L	101	TGL	C15-C16-C17-C18
20	N	607	PGV	O01-C1-C2-C3
24	B	303	PSC	C20-C21-C22-C23
20	N	607	PGV	C9-C10-C11-C12
20	N	607	PGV	C04-O12-P-O11
14	A	601	HEA	C18-C19-C20-C21
20	N	607	PGV	O03-C19-C20-C21
26	C	307	CDL	C12-C11-CA5-OA6
20	N	608	PGV	C11-C12-C13-C14
27	G	102	PEK	C14-C15-C16-C17
20	C	302	PGV	C9-C10-C11-C12
26	P	304	CDL	CB3-CB4-OB6-CB5
26	P	304	CDL	CB6-CB4-OB6-CB5
24	B	303	PSC	C01-C02-O01-C1
20	A	609	PGV	C24-C25-C26-C27
20	A	609	PGV	C7-C8-C9-C10
20	C	308	PGV	C14-C15-C16-C17
19	N	610	TGL	C10-C11-C12-C13
26	C	307	CDL	C13-C14-C15-C16
19	L	101	TGL	OG1-CA1-CA2-CA3
27	T	101	PEK	O03-C21-C22-C23
19	N	611	TGL	CC2-CC3-CC4-CC5
26	P	304	CDL	C14-C15-C16-C17
14	N	601	HEA	C26-C15-C16-C17
27	G	102	PEK	O01-C1-C2-C3
26	P	304	CDL	C12-C11-CA5-OA6
26	P	304	CDL	C77-C78-C79-C80
20	P	303	PGV	C9-C10-C11-C12
20	C	302	PGV	C11-C10-C9-C8
26	C	303	CDL	C22-C23-C24-C25
20	N	607	PGV	C14-C15-C16-C17
19	D	201	TGL	OG1-CA1-CA2-CA3
19	N	610	TGL	OG1-CA1-CA2-CA3

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Mol	Chain	Res	Type	Atoms
21	K	101	EDO	O1-C1-C2-O2
21	C	310	EDO	O1-C1-C2-O2
21	A	611	EDO	O1-C1-C2-O2
14	A	602	HEA	C26-C15-C16-C17
20	C	308	PGV	C11-C10-C9-C8
20	N	607	PGV	C01-C02-C03-O11
26	C	307	CDL	C64-C65-C66-C67
19	A	607	TGL	OG3-CC1-CC2-CC3
27	C	306	PEK	C3-C4-C5-C6
24	B	303	PSC	O03-C19-C20-C21
20	G	103	PGV	O01-C1-C2-C3
26	C	307	CDL	C32-C31-CA7-OA8
19	A	607	TGL	C20-C21-C22-C23
20	A	608	PGV	C21-C22-C23-C24
27	G	102	PEK	C3-C4-C5-C6
20	C	308	PGV	C9-C10-C11-C12
27	C	306	PEK	C2-C1-O01-C02
19	N	611	TGL	C14-C29-C30-C31
14	A	601	HEA	O11-C11-C12-C13
26	P	304	CDL	C59-C60-C61-C62
20	N	607	PGV	O02-C1-C2-C3
19	N	610	TGL	CB5-CB6-CB7-CB8
26	C	307	CDL	C31-C32-C33-C34
27	T	101	PEK	C13-C14-C15-C16
19	D	201	TGL	OA1-CA1-CA2-CA3
26	C	307	CDL	C12-C11-CA5-OA7
27	T	101	PEK	O04-C21-C22-C23
20	N	608	PGV	O02-C1-O01-C02
27	G	102	PEK	O02-C1-C2-C3
20	N	607	PGV	O04-C19-C20-C21
19	N	611	TGL	C13-C14-C29-C30
19	N	609	TGL	CA7-CA8-CA9-C20
20	N	607	PGV	C04-O12-P-O13
26	C	307	CDL	CA2-OA2-PA1-OA3
19	N	610	TGL	OA1-CA1-CA2-CA3
27	T	102	PEK	O12-C04-C05-N
27	P	302	PEK	O12-C04-C05-N
24	B	303	PSC	O04-C19-C20-C21
26	C	307	CDL	C32-C31-CA7-OA9
19	D	201	TGL	C19-C33-C34-C35
27	T	101	PEK	C31-C32-C33-C34
27	C	306	PEK	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
27	G	101	PEK	C05-C04-O12-P
24	R	201	PSC	O04-C19-C20-C21
26	P	304	CDL	C12-C11-CA5-OA7
20	G	103	PGV	O02-C1-C2-C3
19	D	201	TGL	C11-C12-C13-C14
26	C	307	CDL	C52-C51-CB5-OB6
19	N	610	TGL	CB9-C10-C11-C12
20	N	608	PGV	C26-C27-C28-C29
19	D	201	TGL	OG3-CC1-CC2-CC3
26	C	307	CDL	C72-C71-CB7-OB8
26	C	303	CDL	CB2-C1-CA2-OA2
19	A	607	TGL	OC1-CC1-CC2-CC3
19	N	609	TGL	CA6-CA7-CA8-CA9
26	C	303	CDL	C12-C11-CA5-OA6
26	C	307	CDL	C72-C71-CB7-OB9
19	N	610	TGL	CB2-CB3-CB4-CB5
26	T	103	CDL	C32-C31-CA7-OA8

There are no ring outliers.

46 monomers are involved in 154 short contacts:

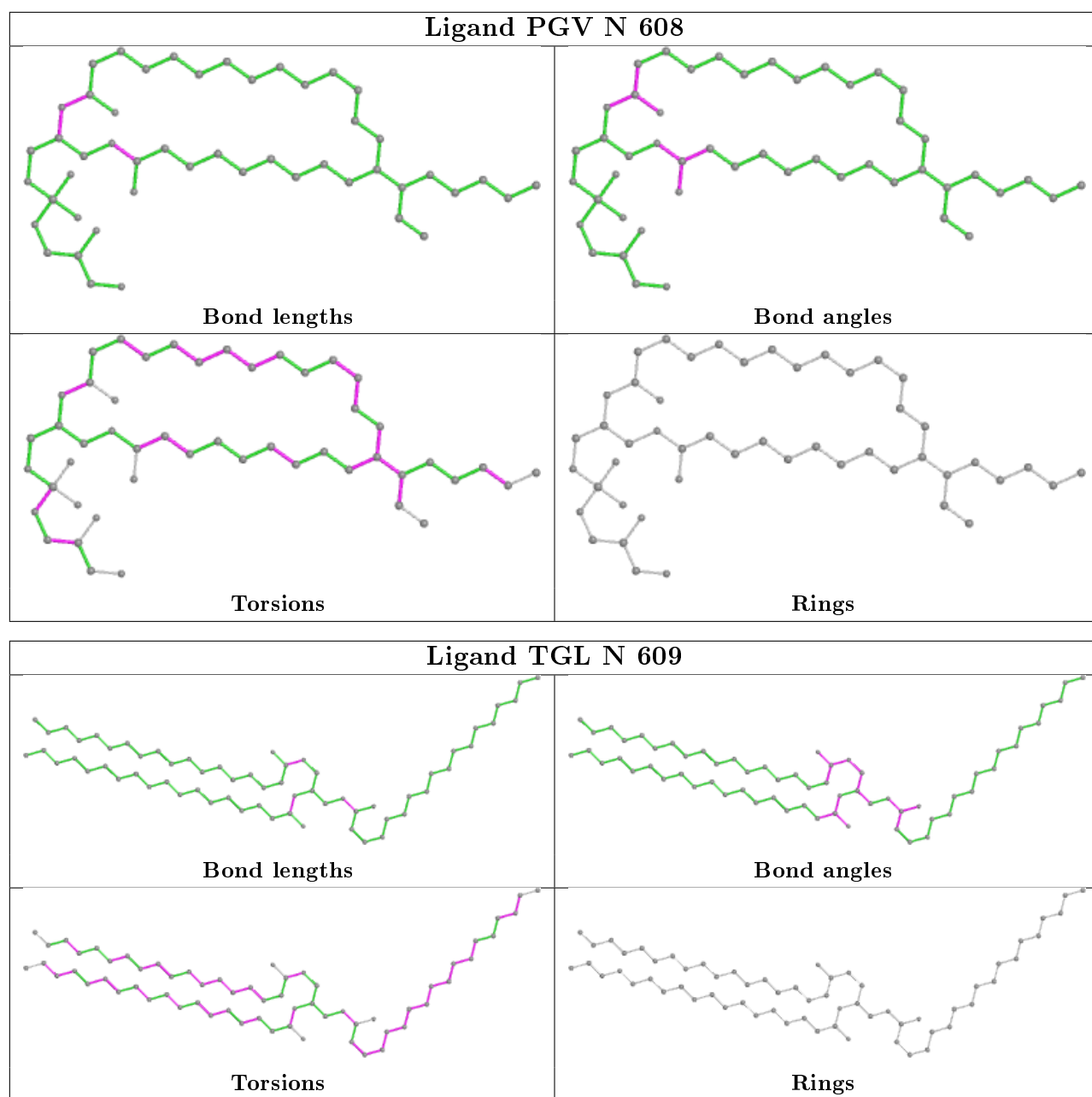
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	608	PGV	2	0
19	N	609	TGL	5	0
20	A	609	PGV	2	0
27	G	102	PEK	6	0
23	W	101	CHD	1	0
27	P	302	PEK	4	0
23	P	305	CHD	1	0
23	J	101	CHD	1	0
19	D	201	TGL	1	0
21	A	610	EDO	1	0
14	A	602	HEA	6	0
29	Z	101	DMU	1	0
23	B	302	CHD	1	0
14	A	601	HEA	6	0
26	P	304	CDL	7	0
14	N	602	HEA	3	0
24	R	201	PSC	6	0
27	T	102	PEK	1	0
21	B	305	EDO	1	0
14	N	601	HEA	10	0

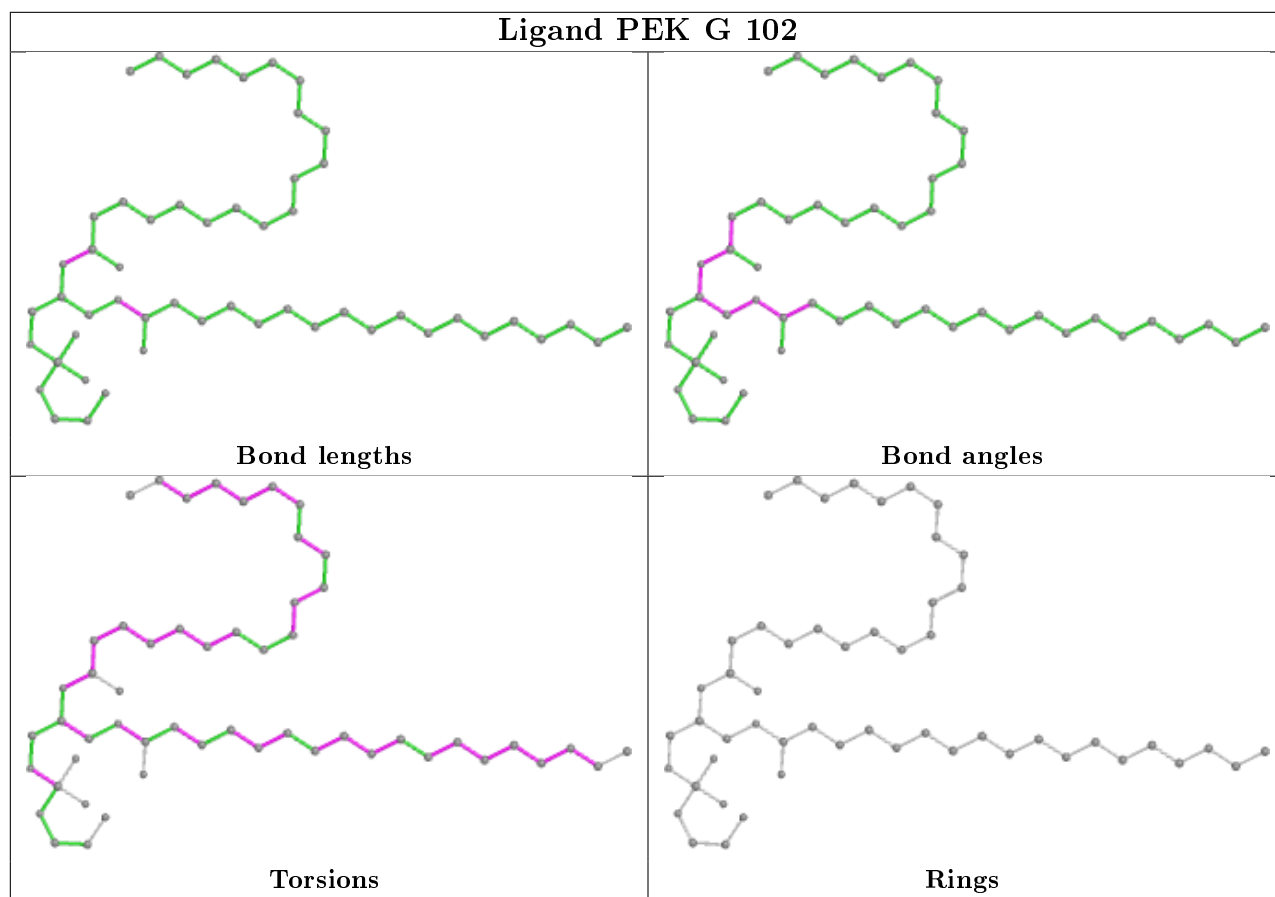
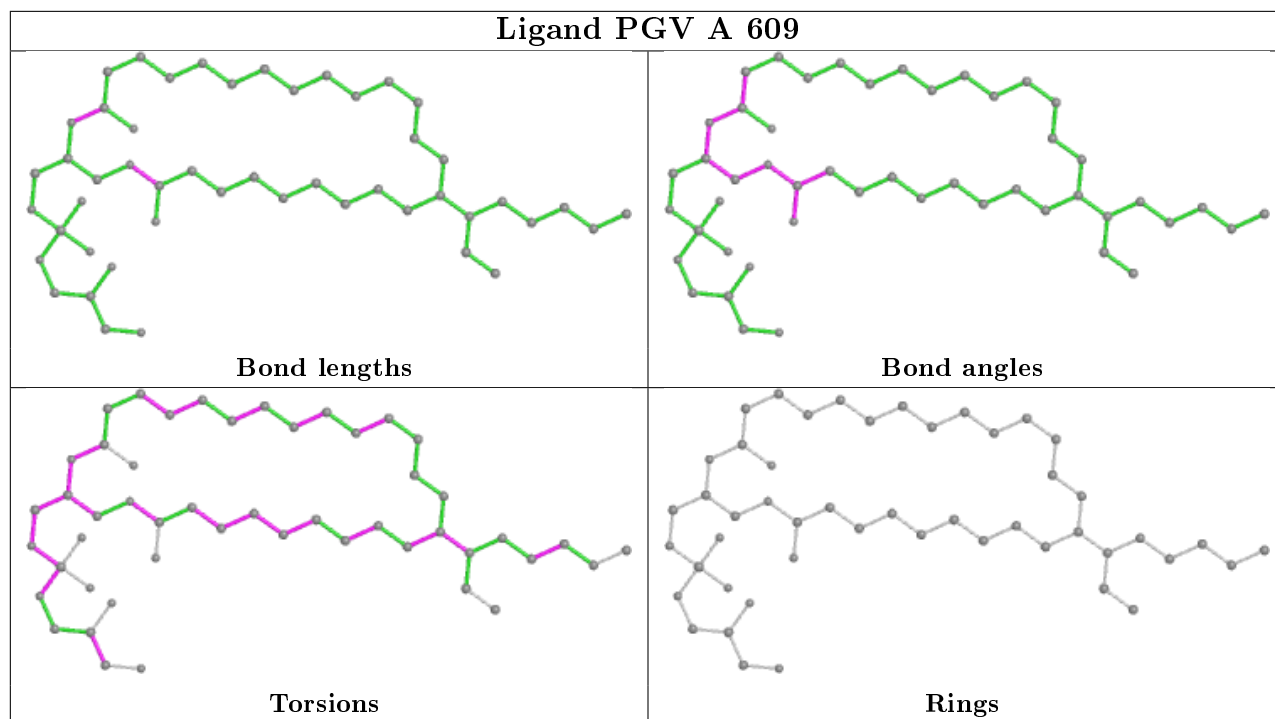
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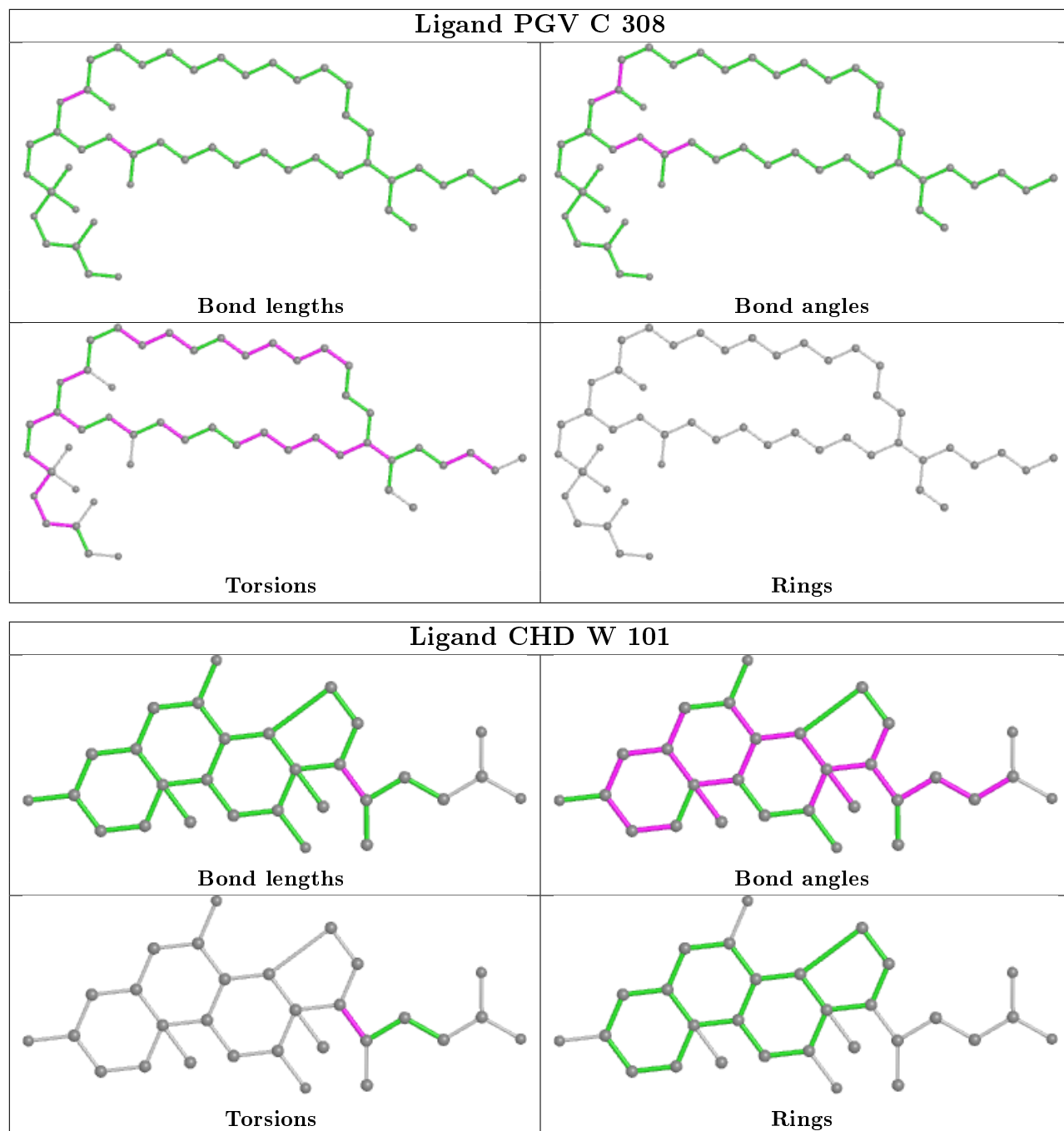
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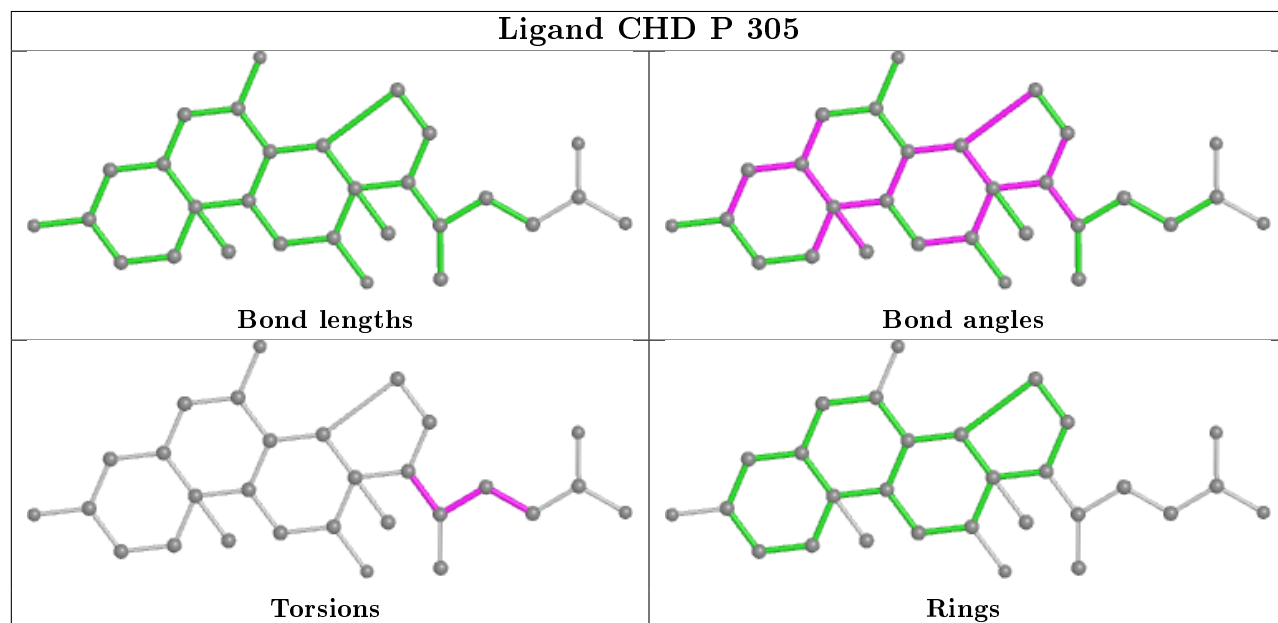
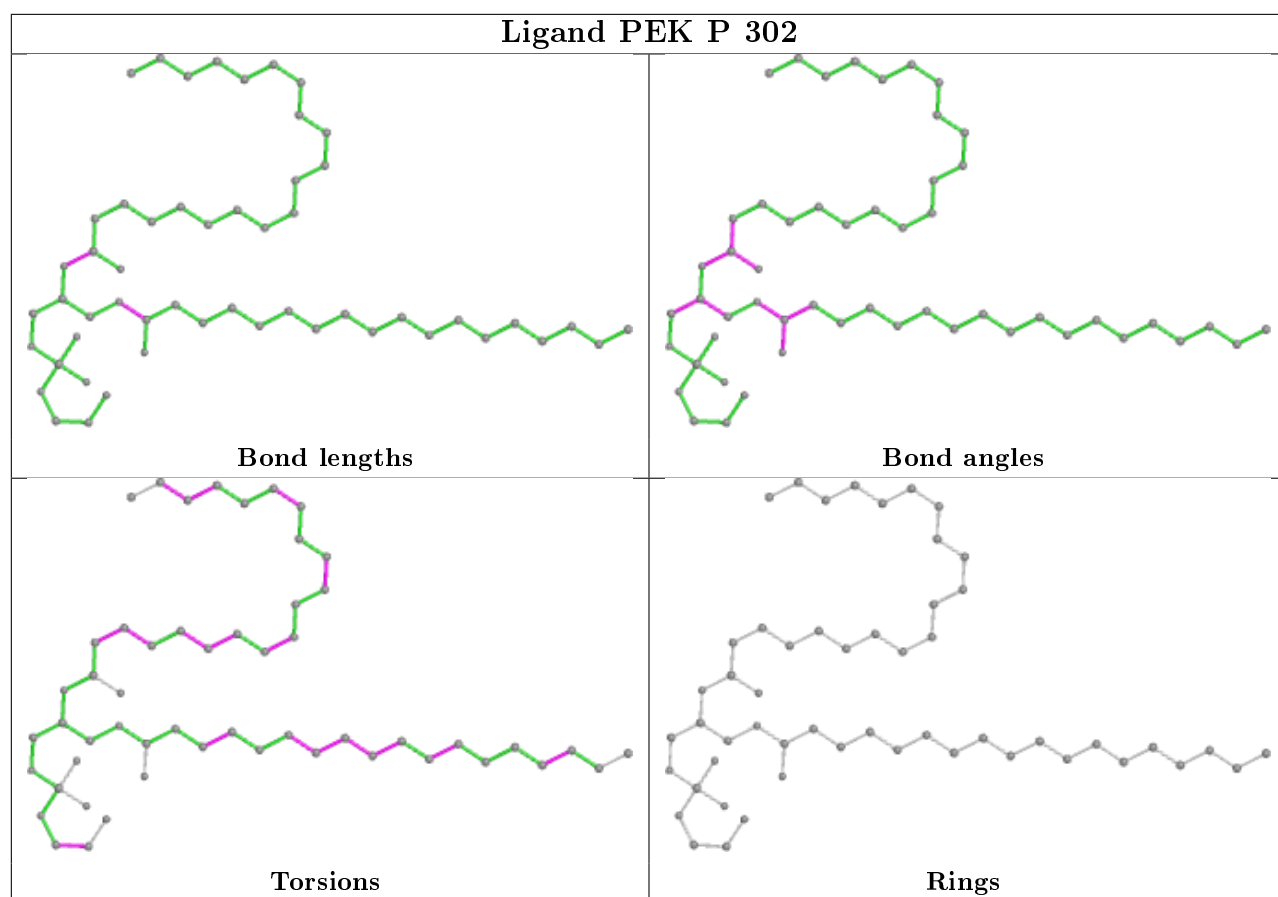
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	606	CMO	1	0
27	C	306	PEK	3	0
20	P	303	PGV	3	0
24	B	303	PSC	12	0
26	T	103	CDL	13	0
27	T	101	PEK	3	0
19	A	607	TGL	3	0
19	N	611	TGL	4	0
20	N	607	PGV	6	0
20	A	608	PGV	1	0
23	P	306	CHD	1	0
26	C	303	CDL	2	0
21	N	612	EDO	1	0
27	G	101	PEK	4	0
19	L	101	TGL	4	0
23	C	305	CHD	1	0
20	G	103	PGV	2	0
29	M	101	DMU	1	0
21	A	613	EDO	2	0
23	O	302	CHD	1	0
19	N	610	TGL	2	0
23	C	304	CHD	2	0
21	A	614	EDO	4	0
21	T	104	EDO	1	0
26	C	307	CDL	13	0
21	A	612	EDO	2	0

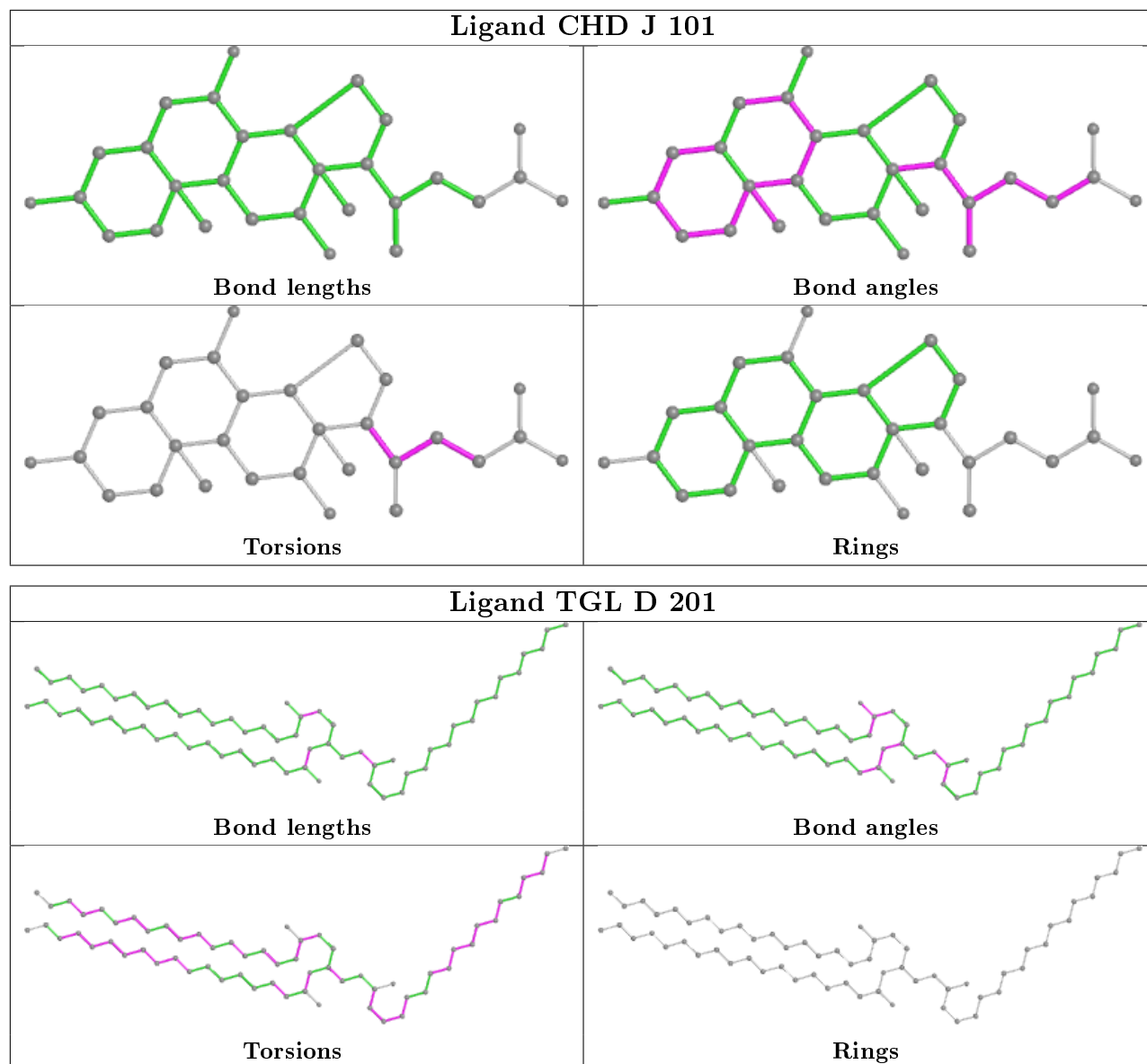
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

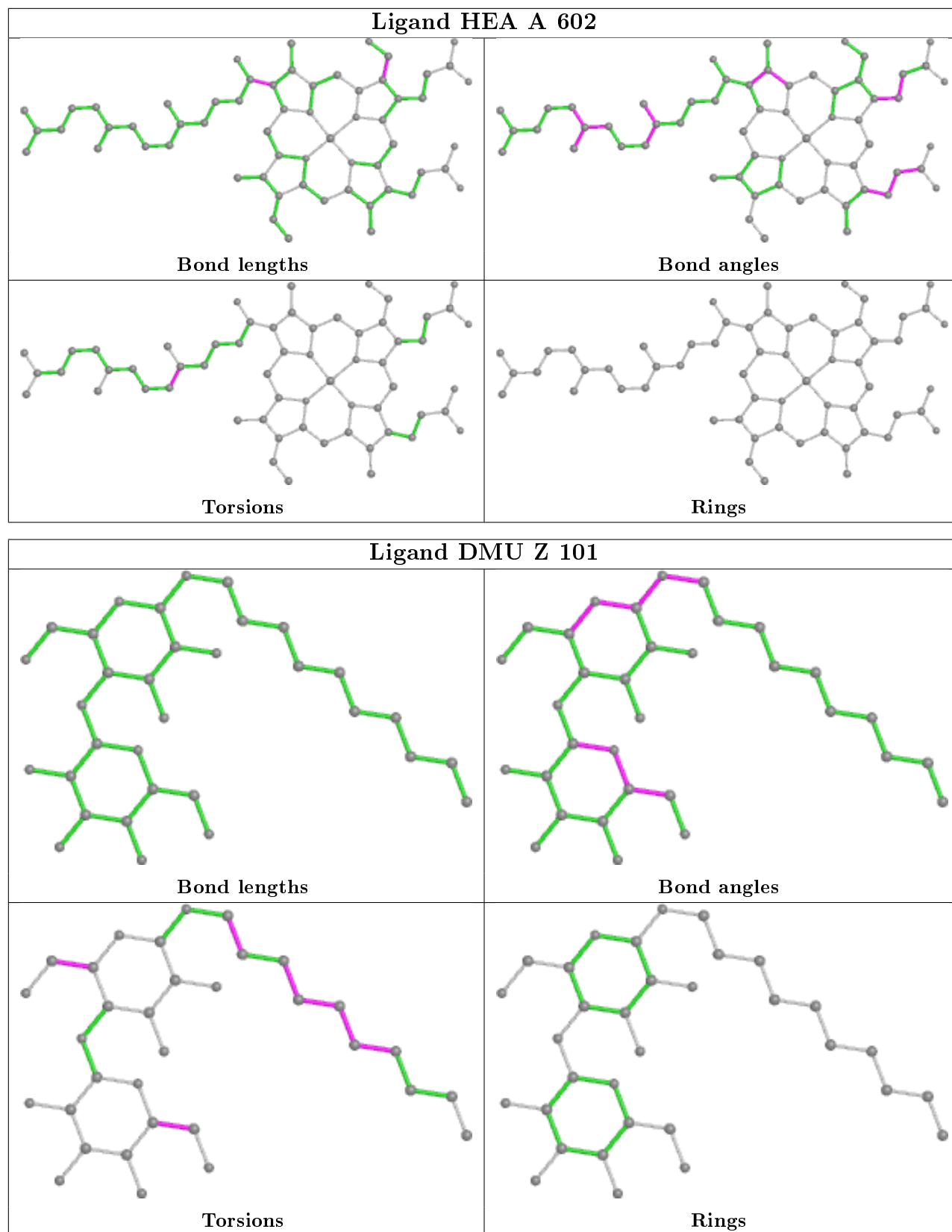


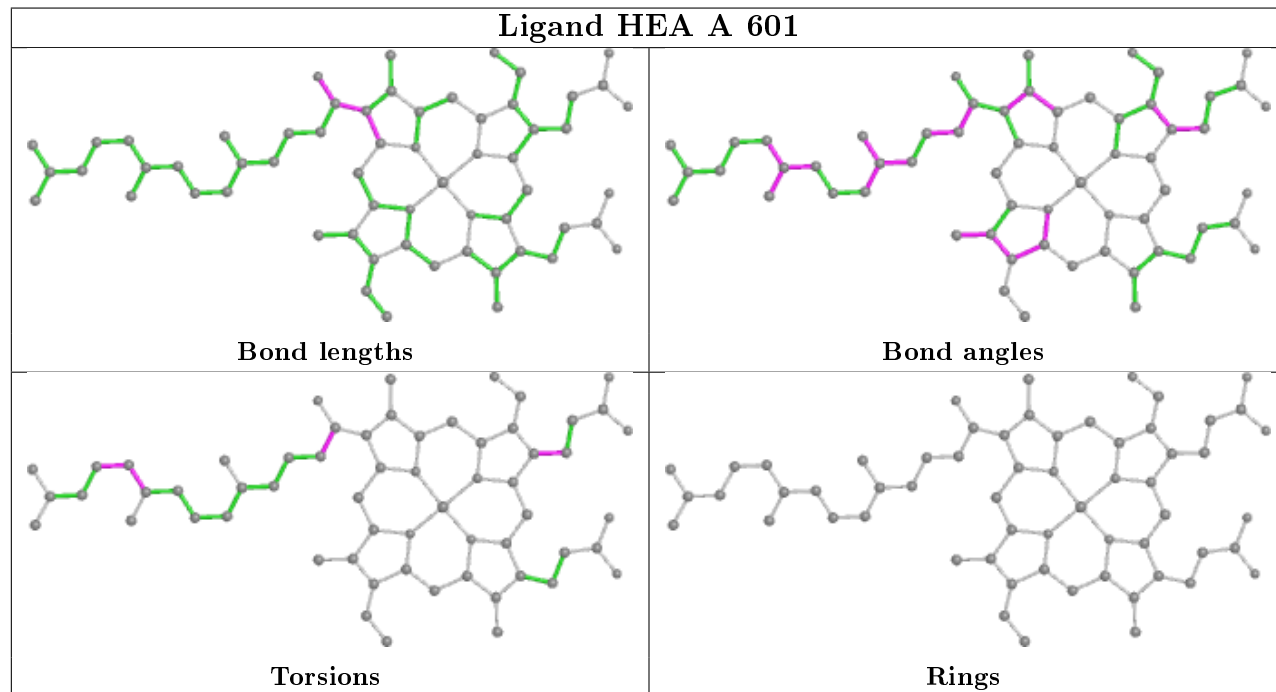
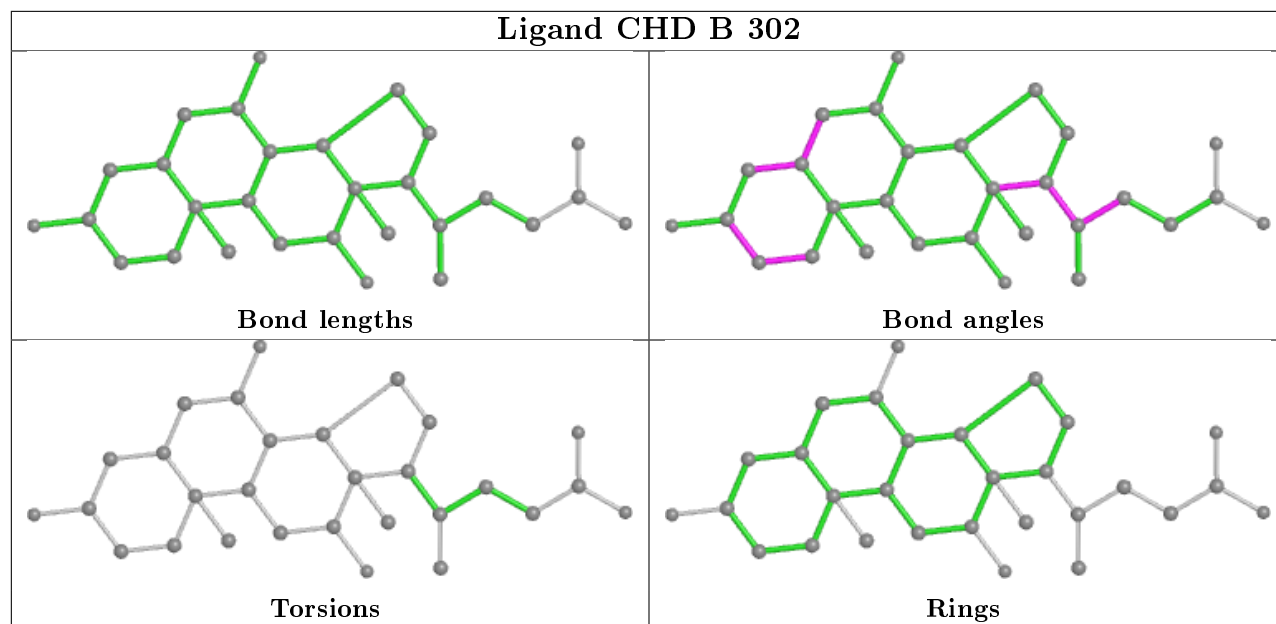


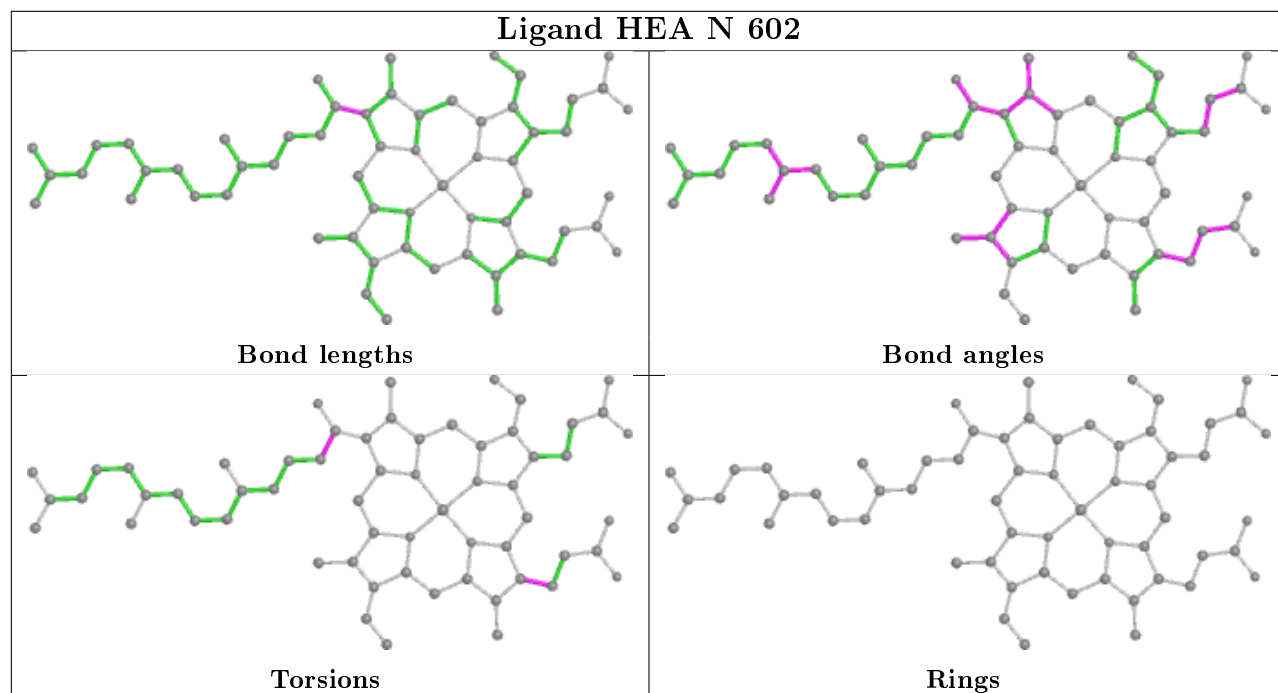
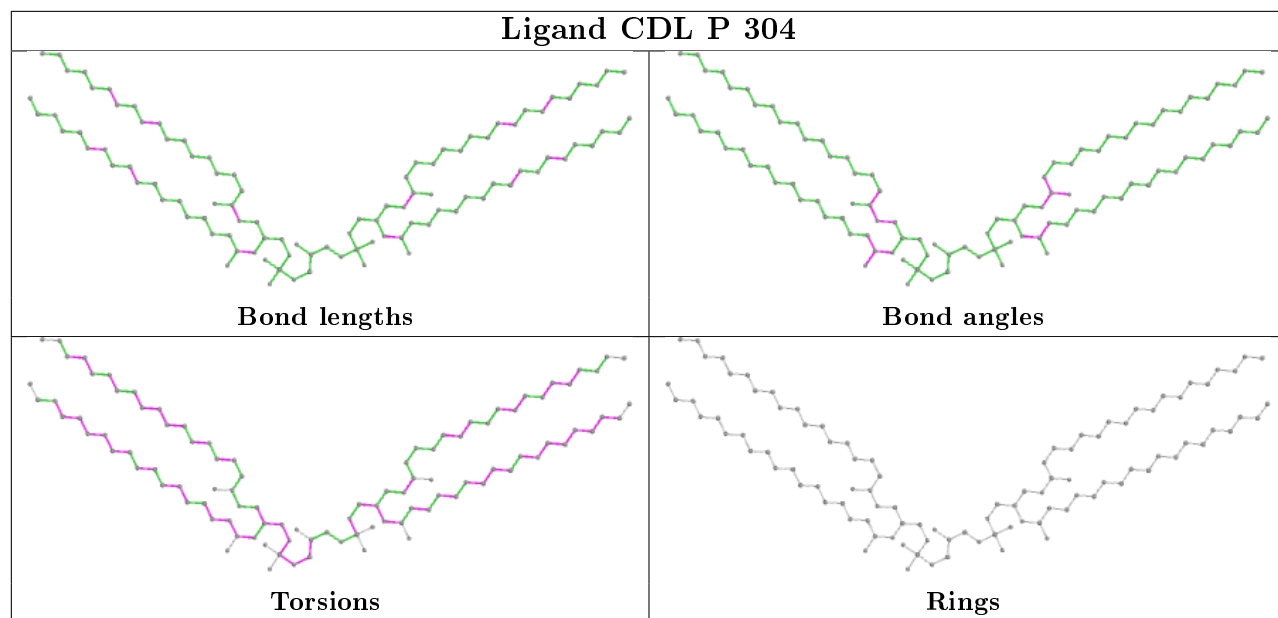


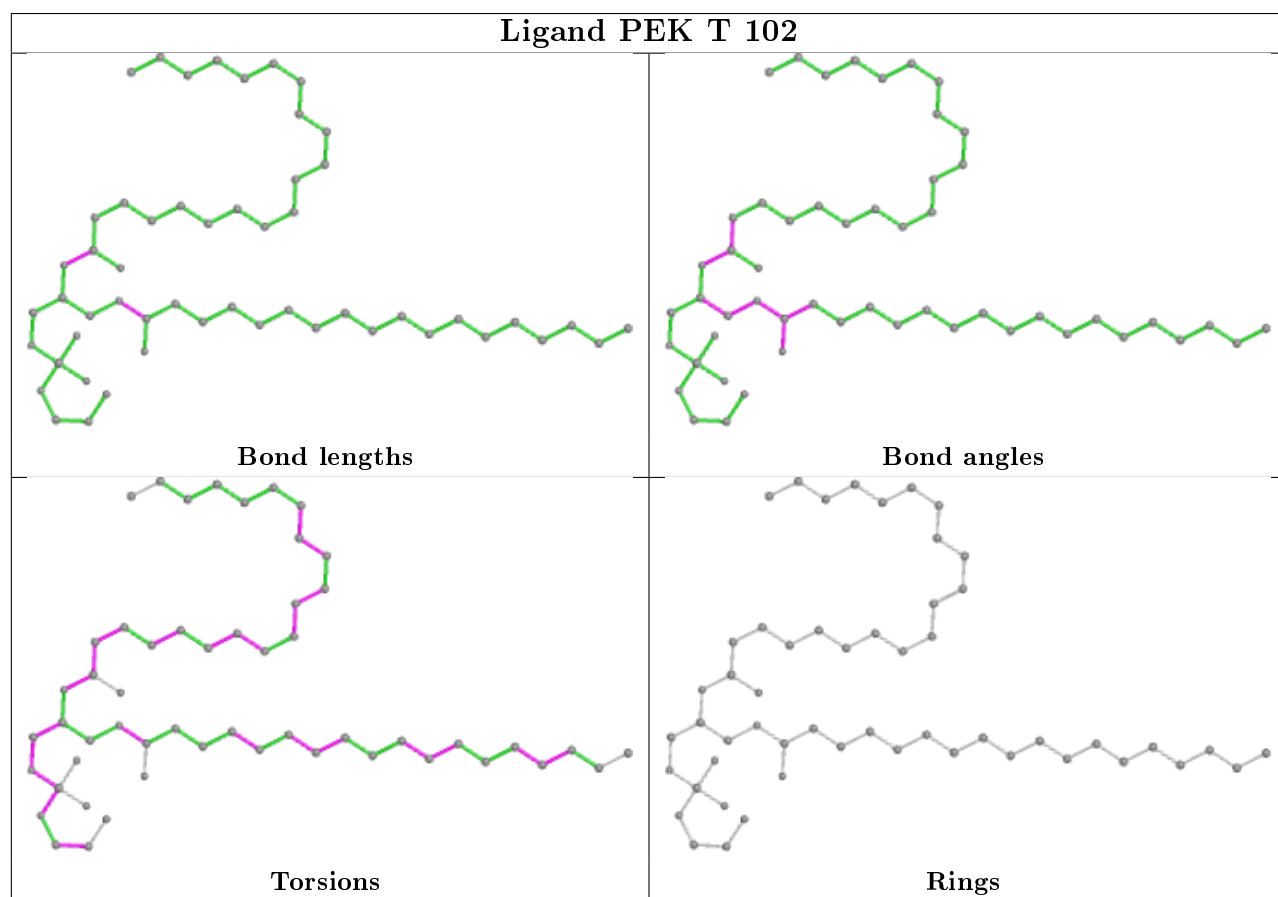
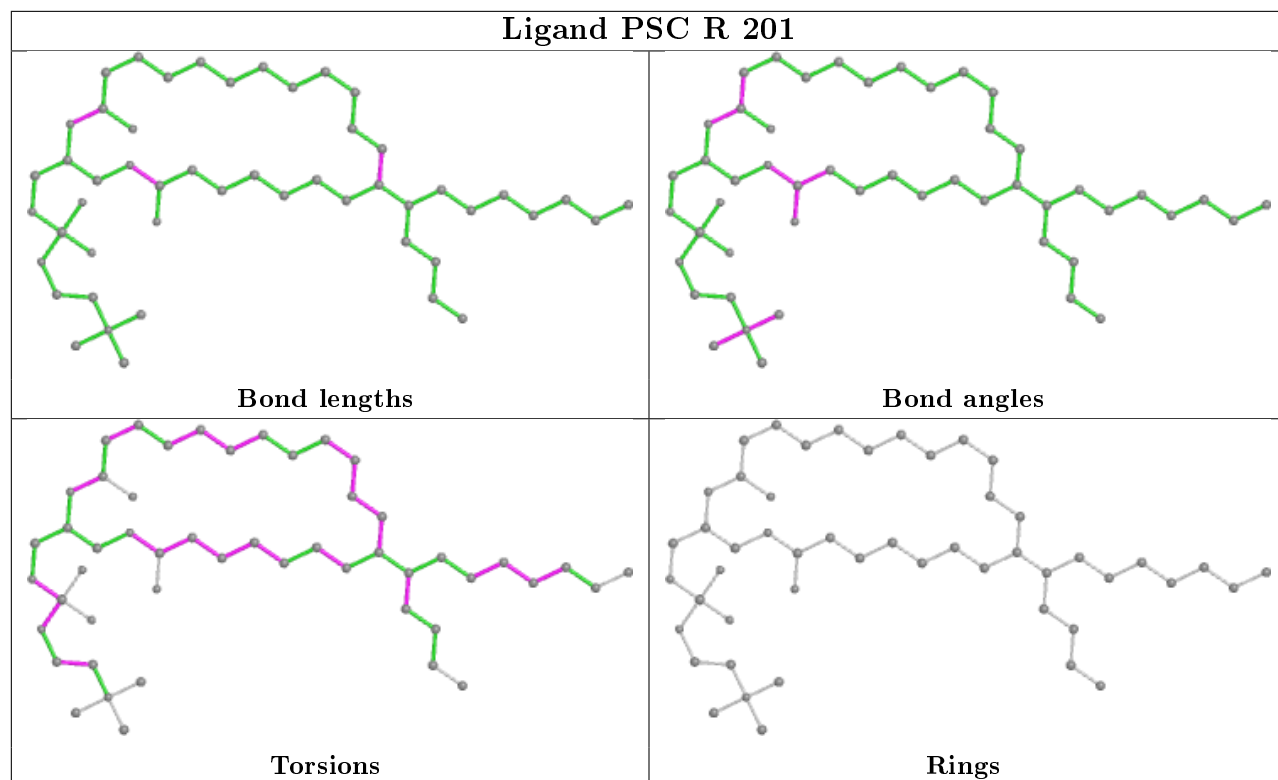


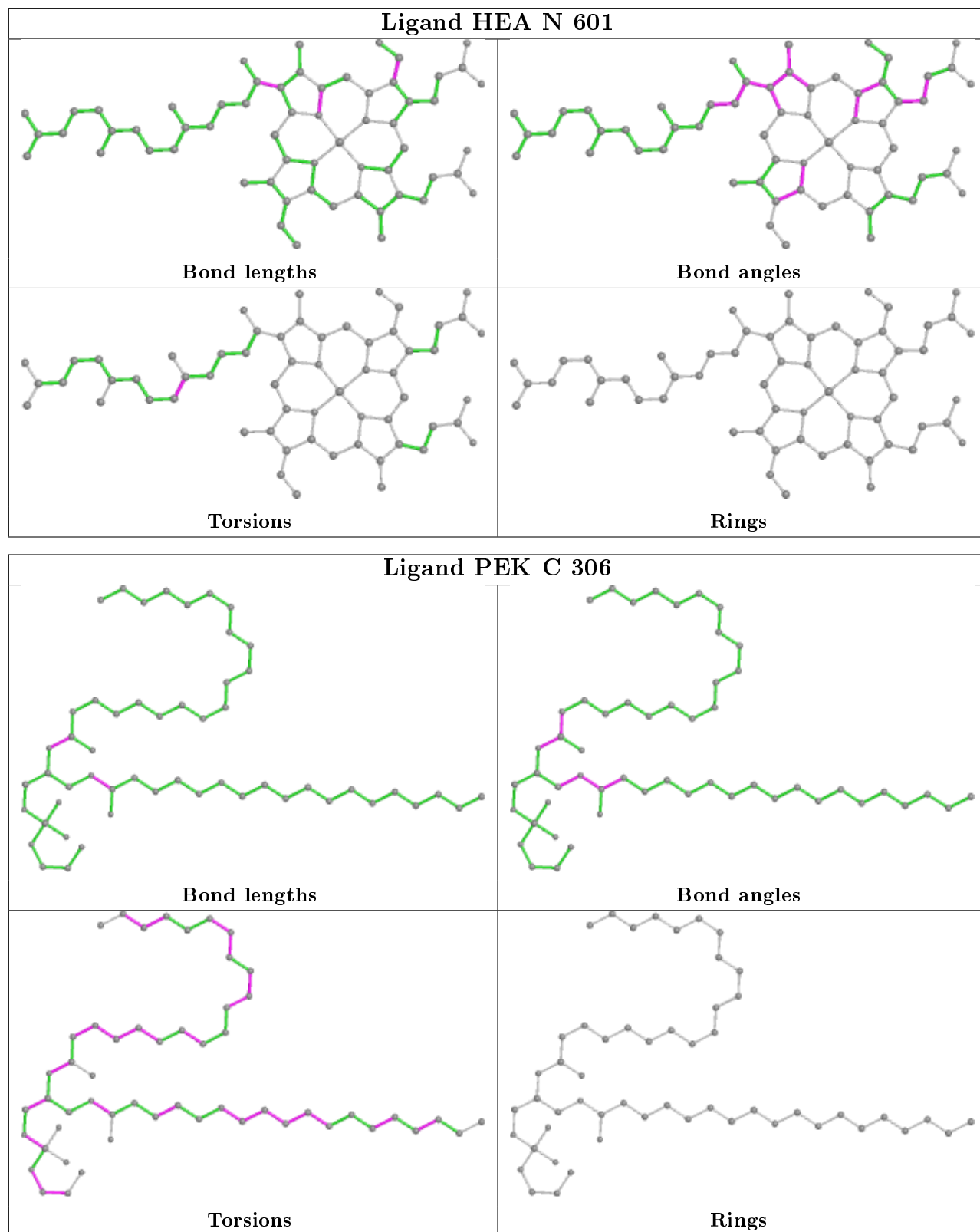


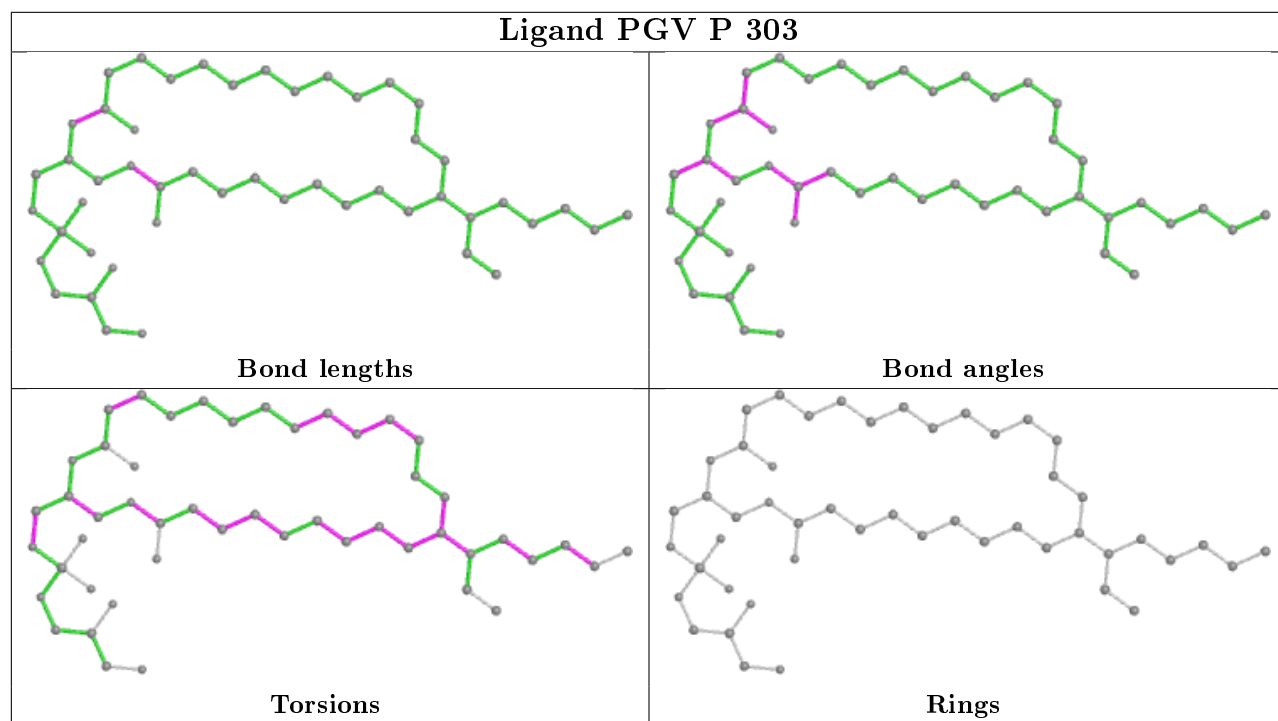
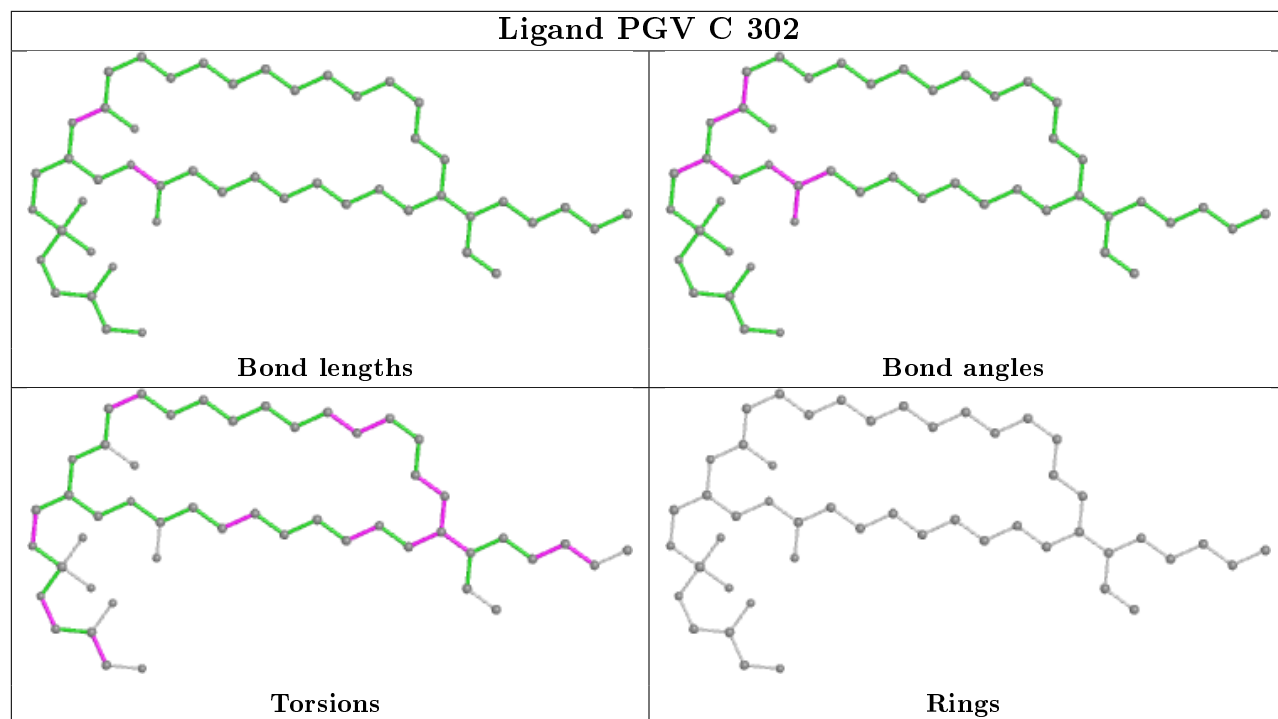


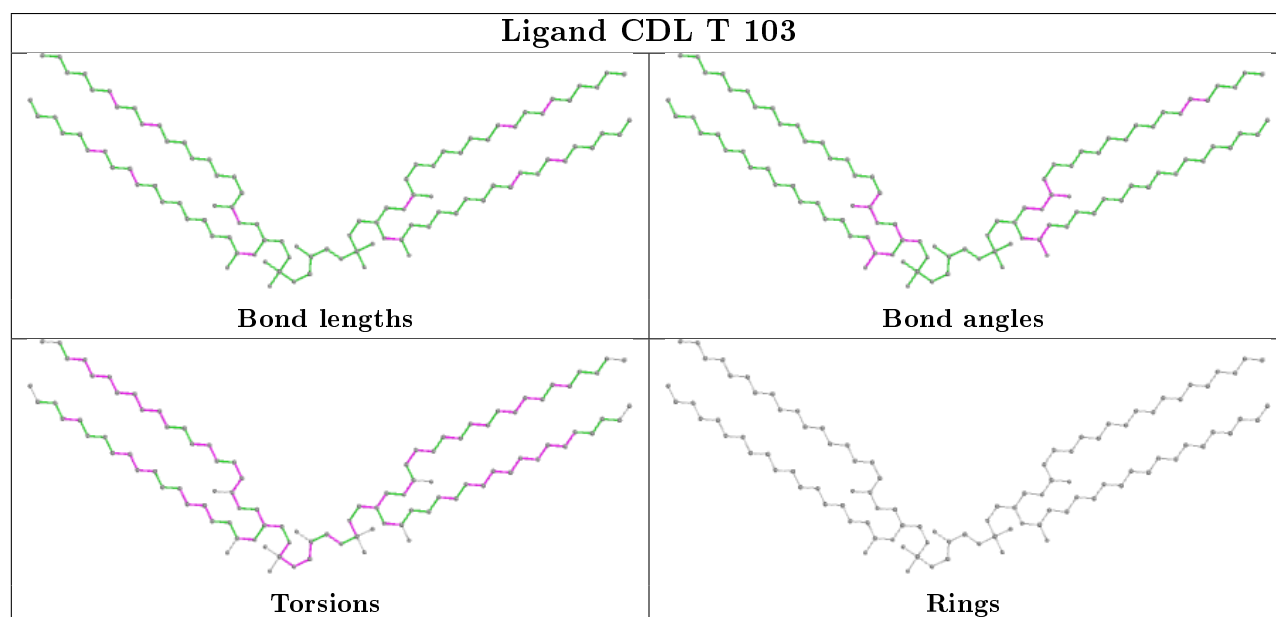
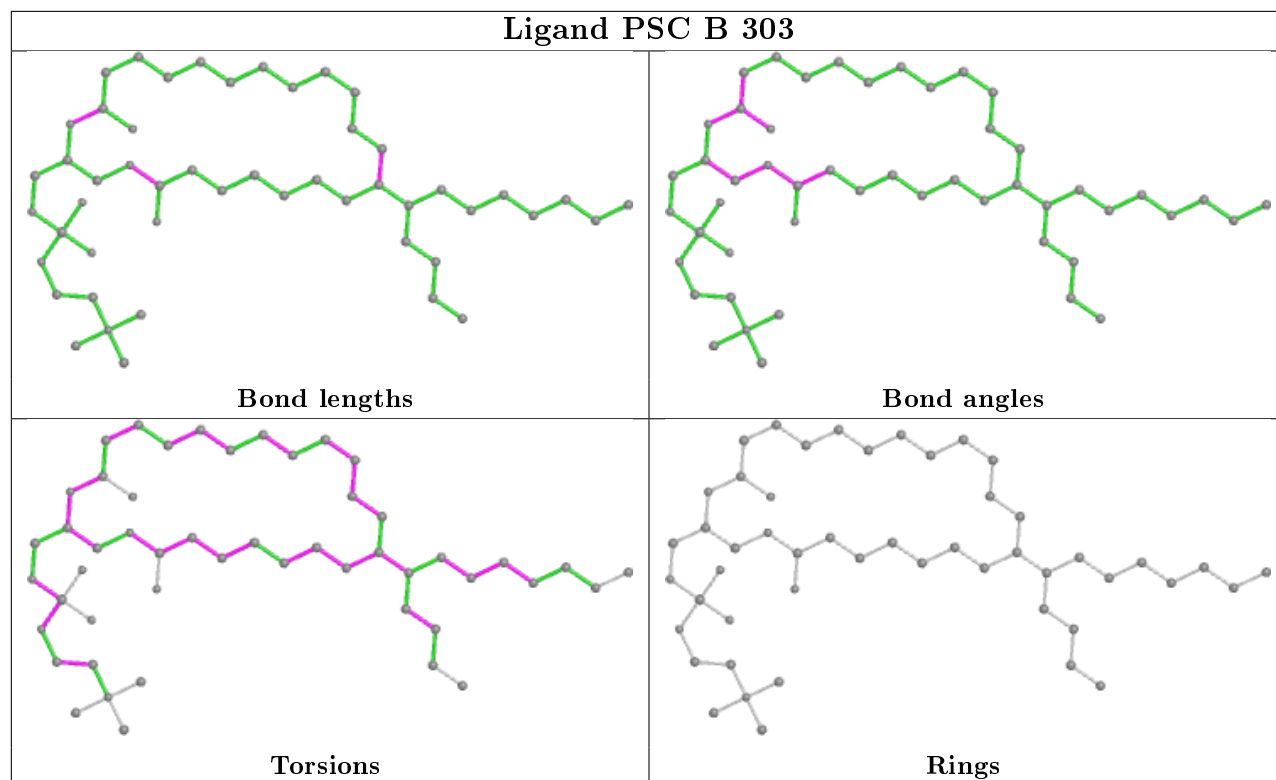


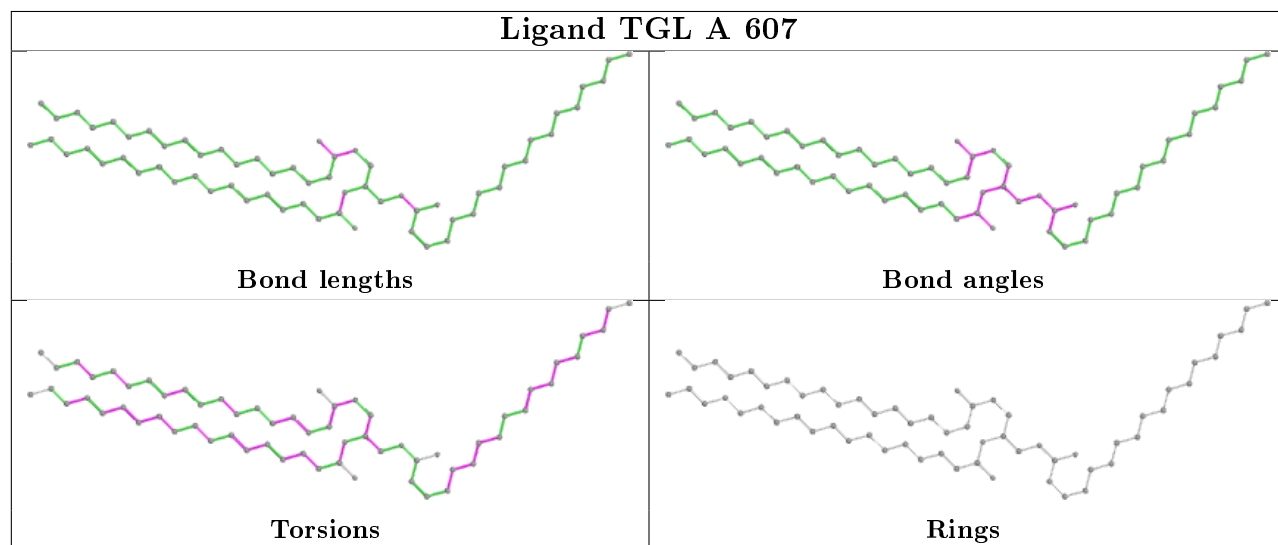
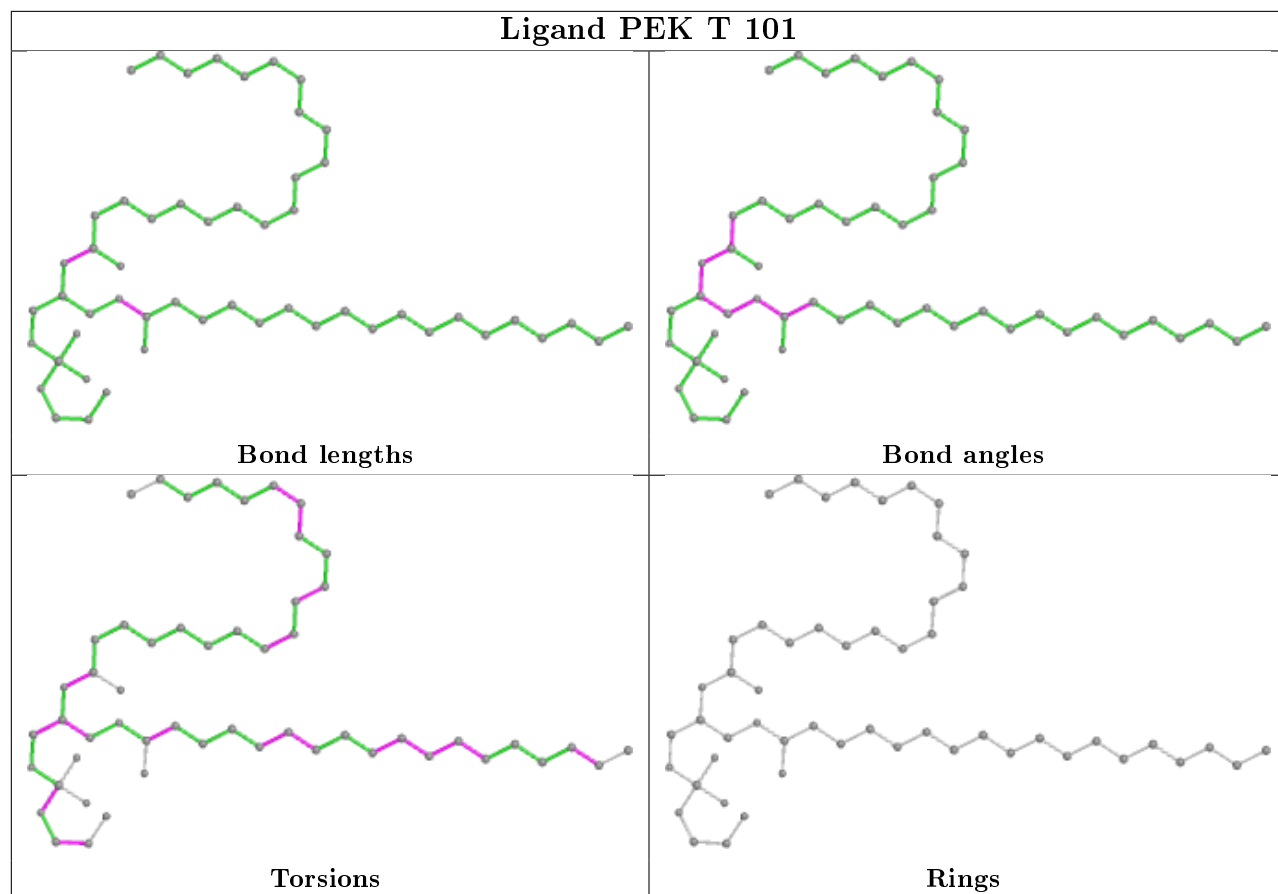


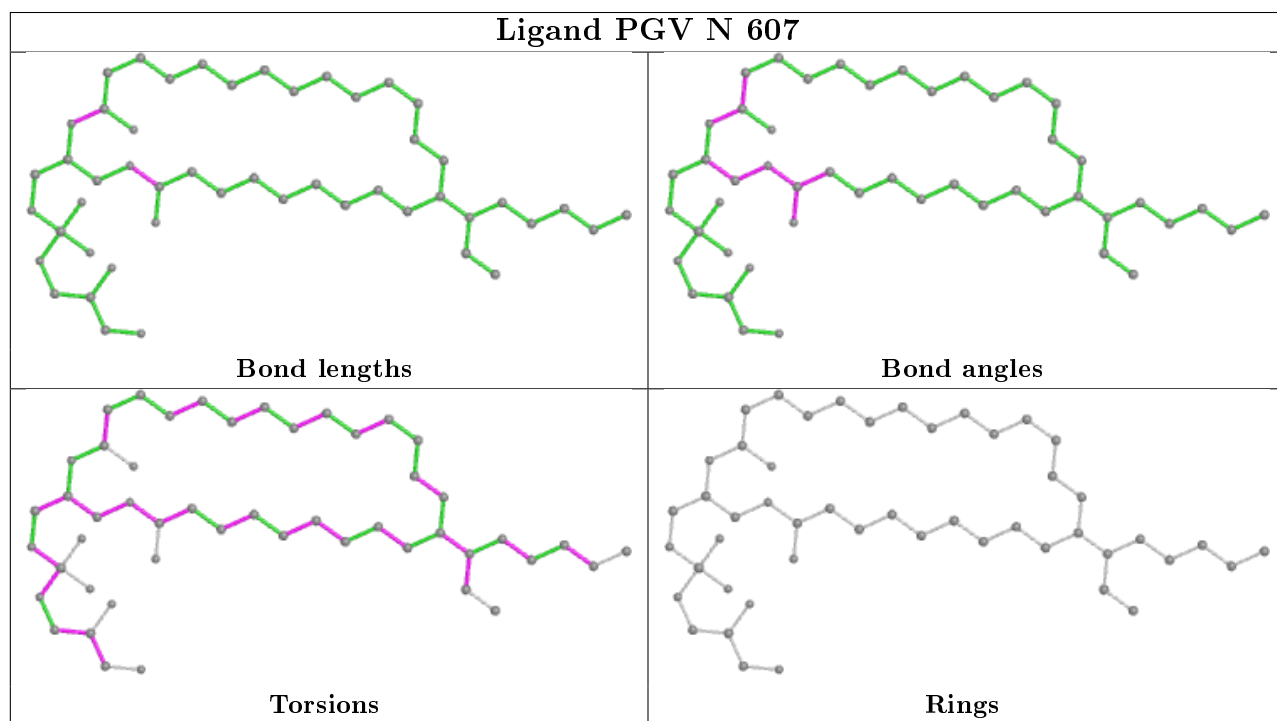
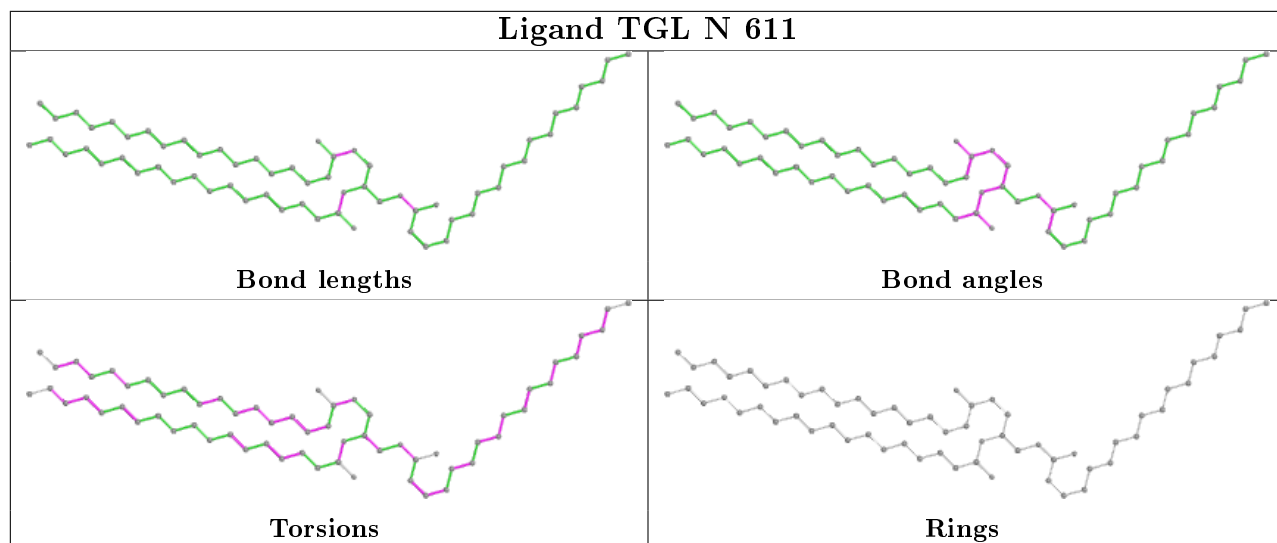


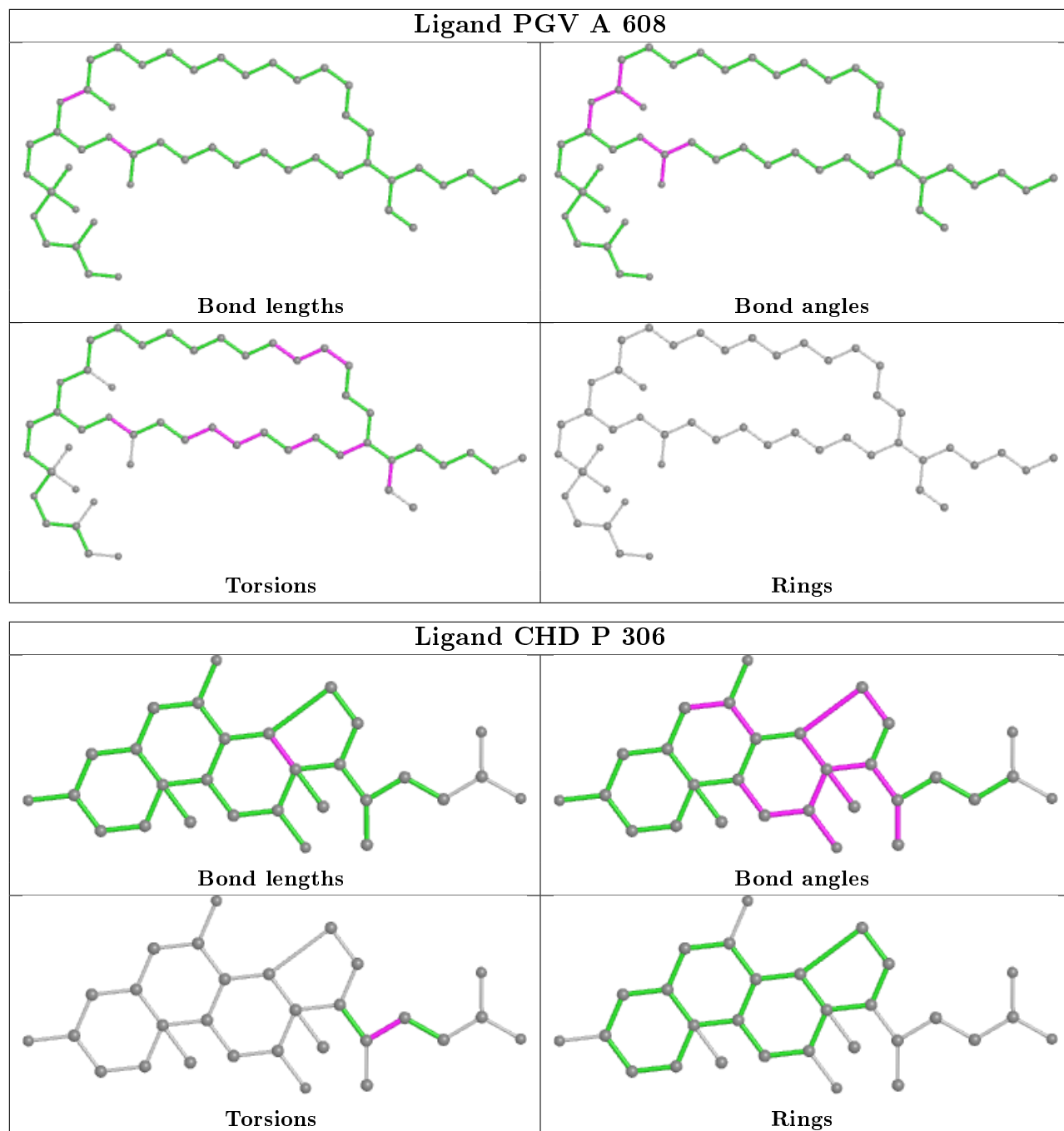


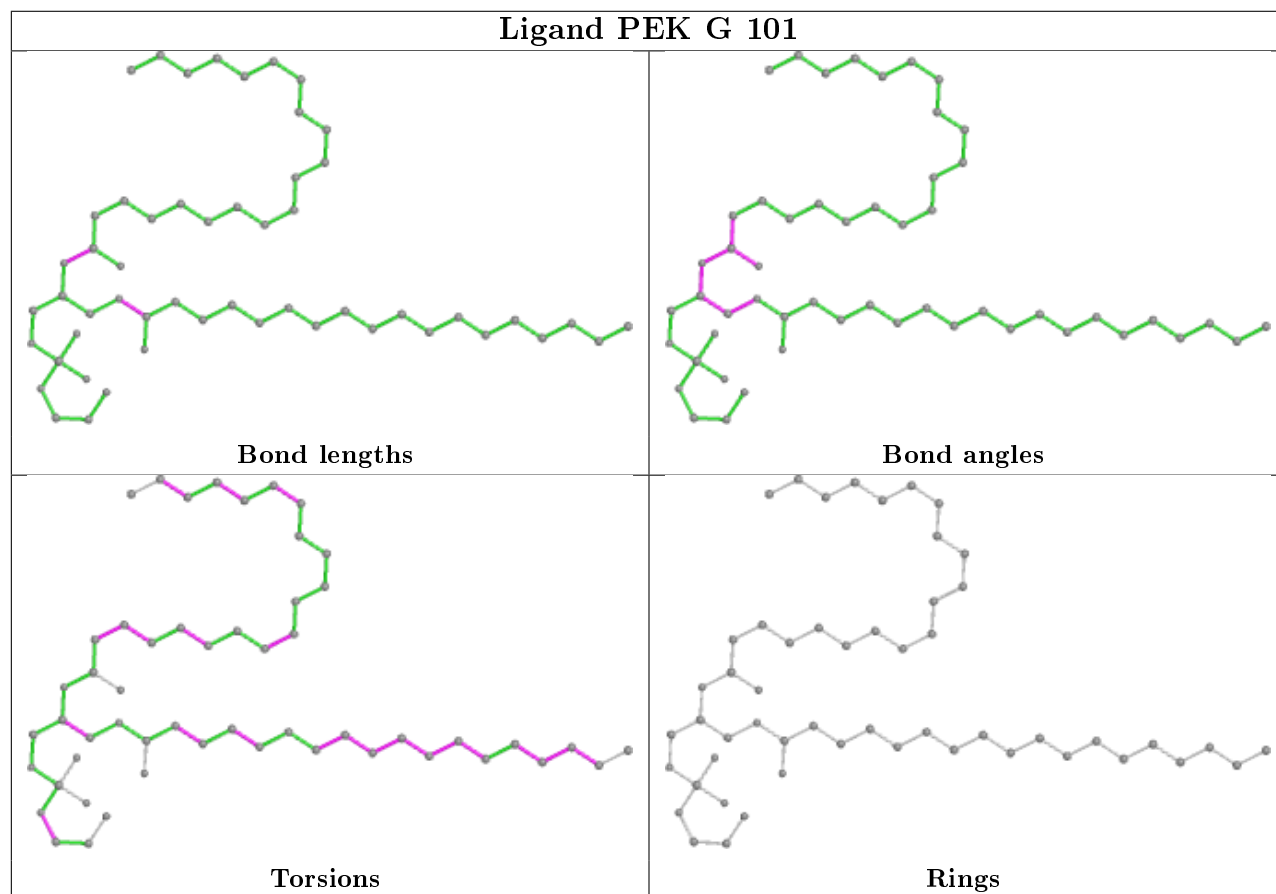
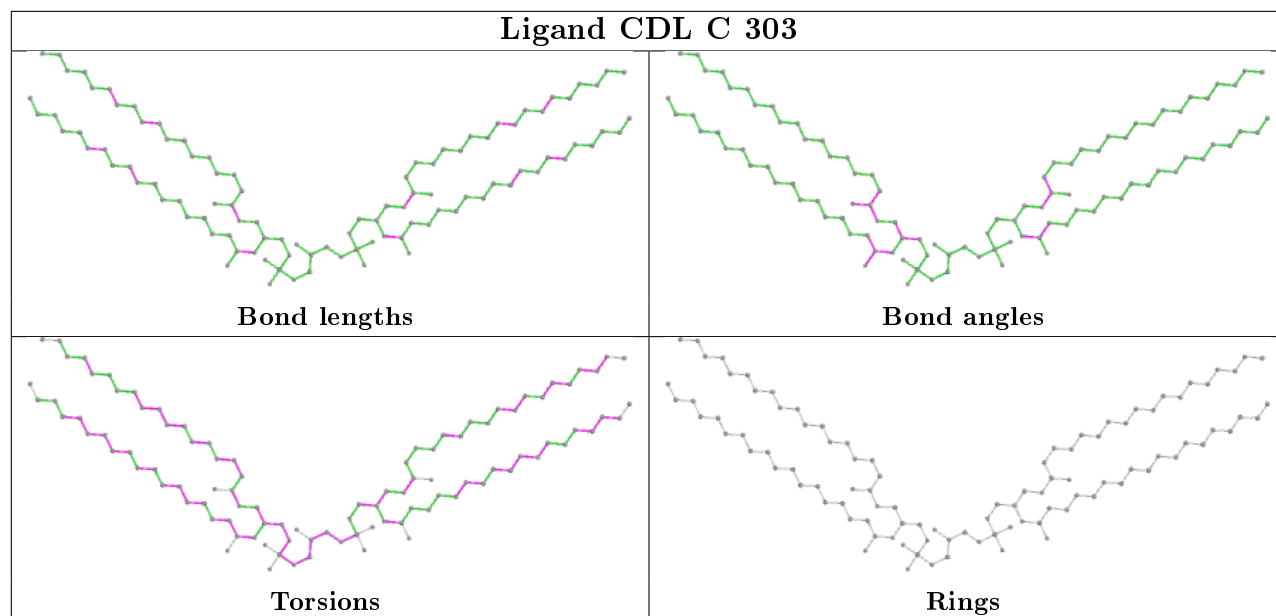


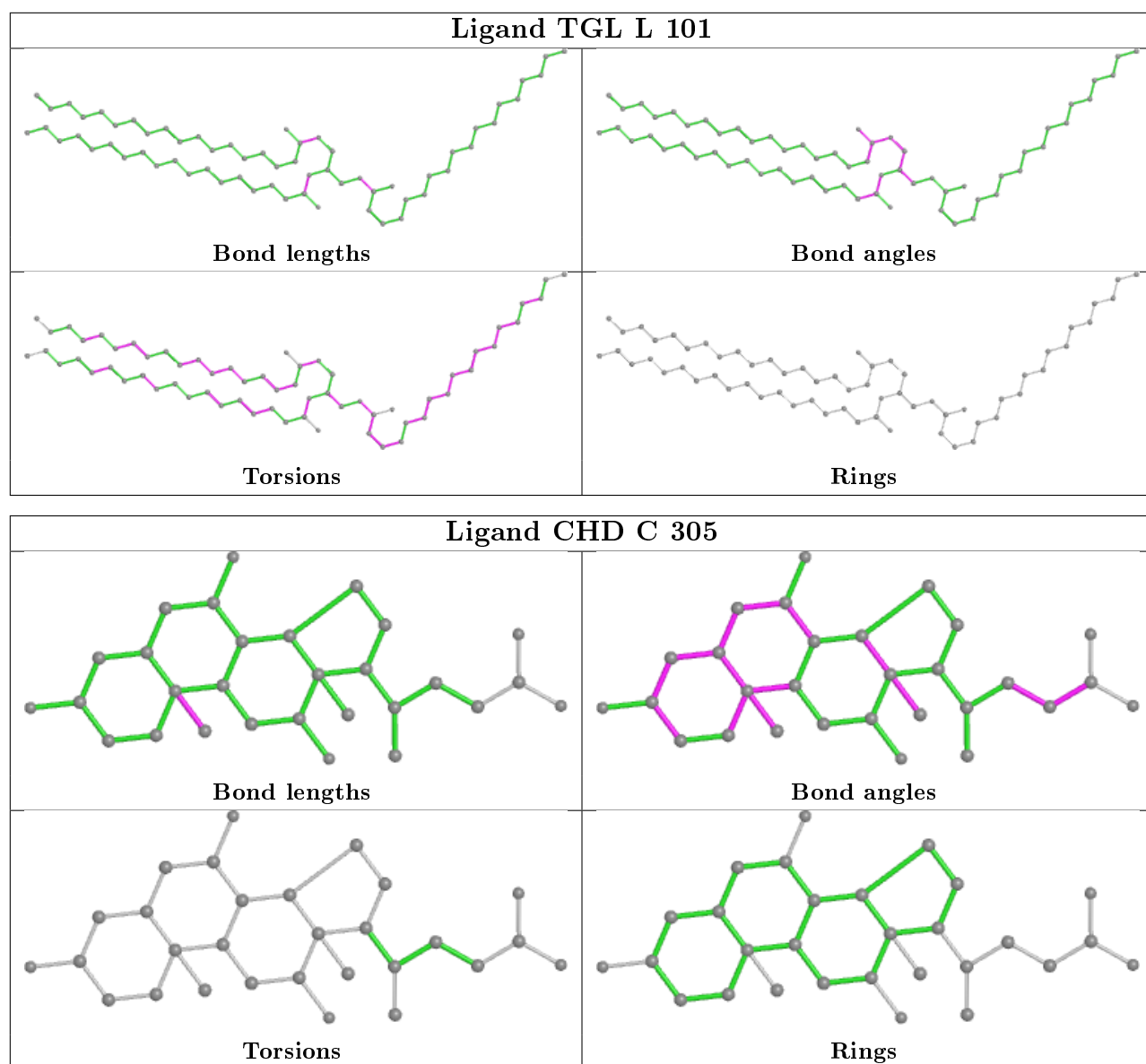


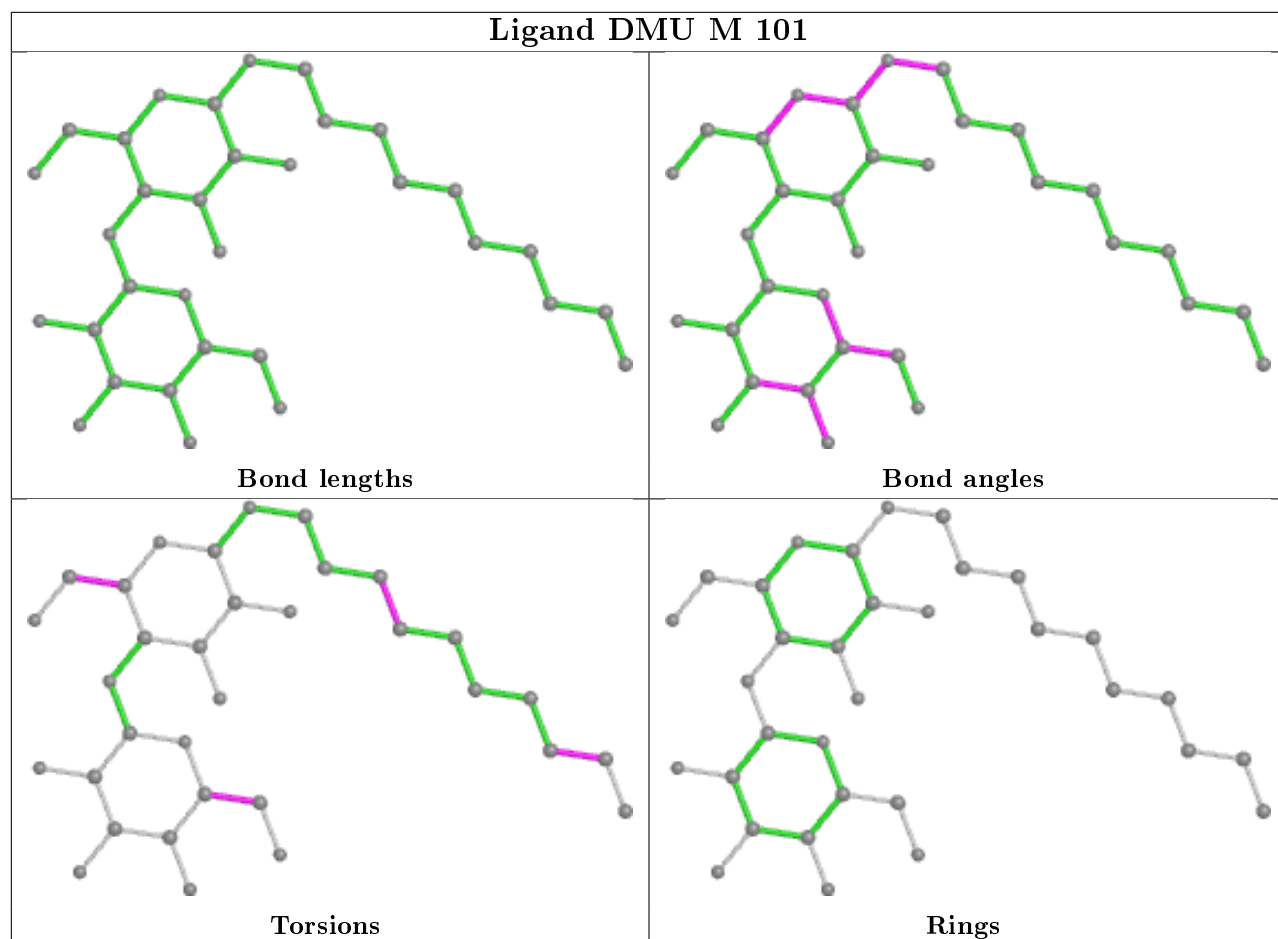
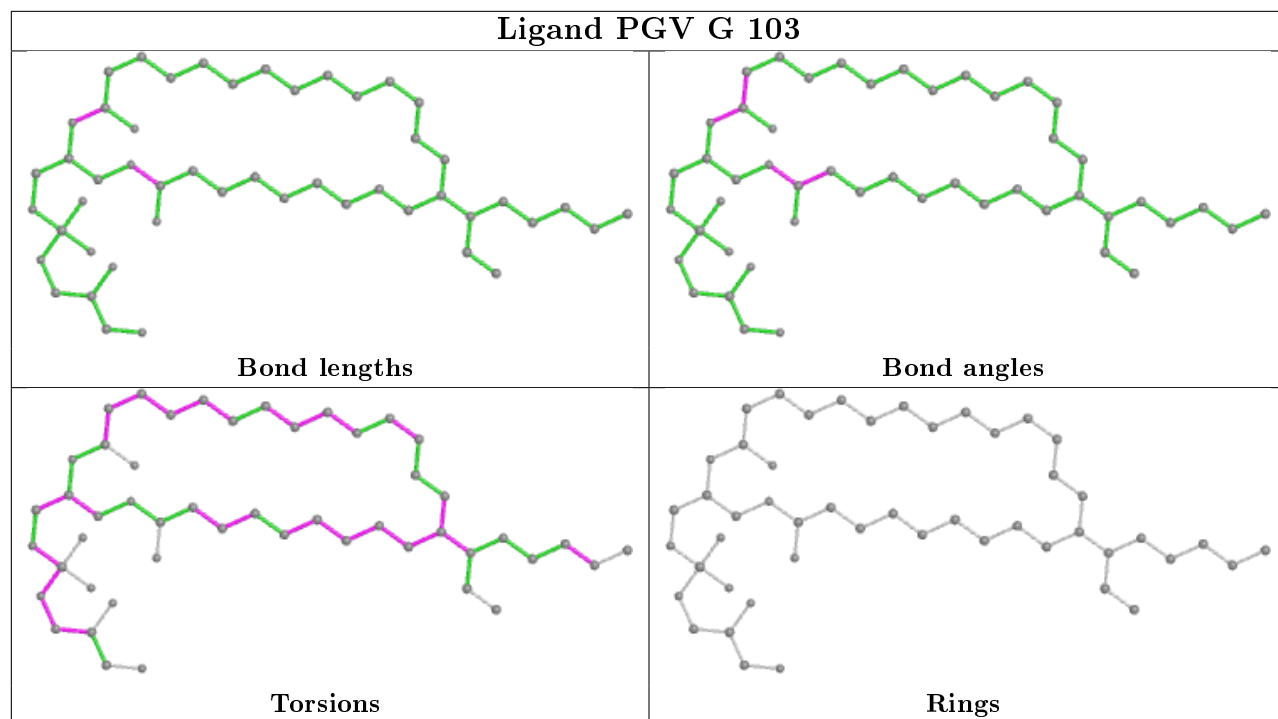


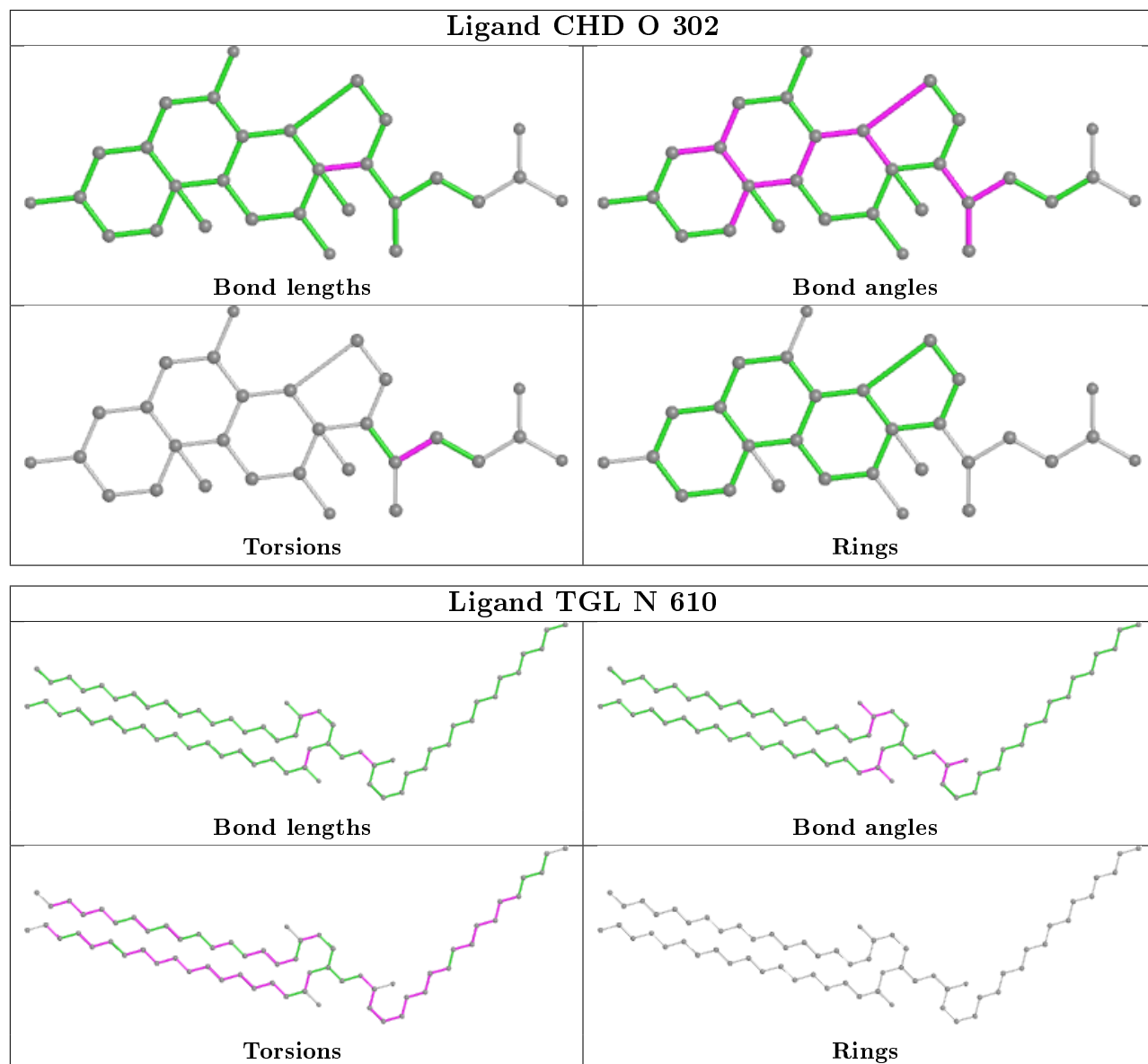


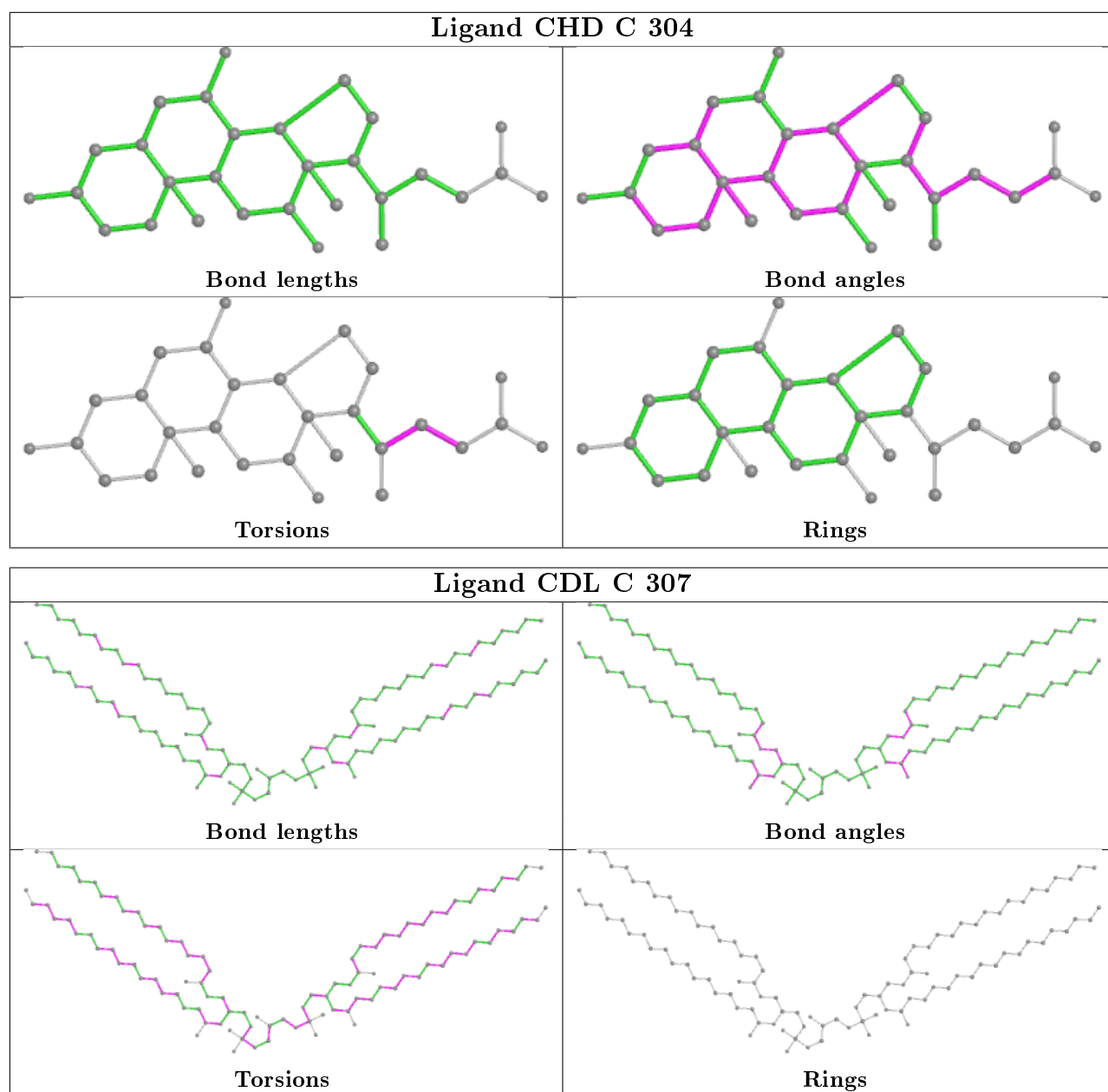












5.7 Other polymers [i](#)

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 i

6.1 Protein, DNA and RNA chains i

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%)	-1.13	0 100 100	41, 53, 66, 101	0
1	N	513/514 (99%)	-1.08	0 100 100	43, 60, 76, 104	0
2	B	226/227 (99%)	-0.99	0 100 100	46, 59, 91, 128	0
2	O	226/227 (99%)	-0.81	2 (0%) 84 82	54, 69, 104, 151	0
3	C	259/261 (99%)	-0.90	0 100 100	46, 57, 75, 115	0
3	P	259/261 (99%)	-0.90	0 100 100	46, 62, 81, 121	0
4	D	144/147 (97%)	-0.68	1 (0%) 87 86	52, 66, 89, 117	0
4	Q	144/147 (97%)	-0.23	8 (5%) 24 23	64, 83, 125, 160	0
5	E	105/109 (96%)	-0.86	1 (0%) 82 80	50, 65, 92, 147	0
5	R	105/109 (96%)	-0.76	1 (0%) 82 80	62, 79, 105, 154	0
6	F	98/98 (100%)	-0.36	5 (5%) 28 26	52, 66, 134, 154	0
6	S	98/98 (100%)	-0.20	7 (7%) 16 14	58, 74, 145, 162	0
7	G	83/85 (97%)	-0.28	9 (10%) 5 5	55, 66, 143, 159	0
7	T	83/85 (97%)	-0.21	8 (9%) 8 7	53, 73, 147, 158	0
8	H	79/85 (92%)	-0.49	4 (5%) 28 26	54, 69, 141, 156	0
8	U	79/85 (92%)	-0.30	5 (6%) 20 18	61, 80, 139, 153	0
9	I	72/73 (98%)	-0.55	2 (2%) 53 51	58, 73, 101, 114	0
9	V	72/73 (98%)	-0.29	3 (4%) 36 35	59, 84, 114, 142	0
10	J	58/59 (98%)	-0.51	2 (3%) 45 44	57, 70, 111, 144	0
10	W	58/59 (98%)	-0.27	4 (6%) 16 15	66, 82, 123, 158	0
11	K	49/56 (87%)	-0.35	1 (2%) 65 63	59, 72, 93, 119	0
11	X	49/56 (87%)	-0.12	3 (6%) 21 20	70, 84, 119, 127	0
12	L	46/47 (97%)	-0.77	1 (2%) 62 60	49, 60, 80, 122	0
12	Y	46/47 (97%)	-0.64	0 100 100	60, 75, 102, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.43	2 (4%) 31 30	50, 63, 99, 147	0
13	Z	43/46 (93%)	-0.01	3 (6%) 16 15	70, 79, 121, 164	0
All	All	3550/3614 (98%)	-0.76	72 (2%) 65 63	41, 64, 107, 164	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	Z	43	SER	10.6
2	O	90	ILE	9.5
6	F	1	ALA	9.2
7	G	40	GLY	6.7
6	S	2	SER	6.2
7	T	40	GLY	6.1
6	S	98	HIS	6.0
6	S	1	ALA	5.9
4	Q	8	SER	5.3
7	G	10	GLY	5.3
4	Q	6	VAL	5.3
4	Q	5	VAL	5.2
4	Q	7	LYS	5.1
8	U	8	ILE	4.9
7	T	39	SER	4.8
4	Q	4	SER	4.8
6	S	96	LEU	4.6
7	G	41	HIS	4.5
10	W	58	LYS	4.5
6	S	97	ALA	4.4
6	F	2	SER	4.4
8	H	48	GLY	4.3
4	Q	147	LYS	4.1
9	V	2	THR	3.9
10	J	58	LYS	3.9
10	J	1	PHE	3.8
8	U	45	ALA	3.8
8	U	7	LYS	3.8
7	T	42	ARG	3.7
11	K	6	ALA	3.7
2	O	113	TYR	3.6
8	H	45	ALA	3.6
5	E	5	HIS	3.5
13	M	42	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
6	F	98	HIS	3.4
5	R	5	HIS	3.4
10	W	1	PHE	3.3
7	G	39	SER	3.3
6	S	95	GLN	3.3
8	U	48	GLY	3.3
9	V	53	ASN	3.2
13	M	43	SER	3.1
7	T	84	LYS	3.1
10	W	57	HIS	3.0
7	G	9	GLY	3.0
7	T	41	HIS	2.9
6	F	3	GLY	2.9
9	I	19	PHE	2.9
11	X	7	PRO	2.9
7	G	5	LYS	2.8
7	G	84	LYS	2.8
4	Q	35	ALA	2.8
6	S	3	GLY	2.8
8	H	47	GLY	2.7
13	Z	32	TRP	2.7
11	X	6	ALA	2.5
7	T	36	TRP	2.5
4	Q	101	HIS	2.4
8	H	7	LYS	2.4
6	F	95	GLN	2.4
7	T	2	SER	2.4
10	W	55	PHE	2.3
7	G	42	ARG	2.2
7	T	10	GLY	2.2
4	D	147	LYS	2.2
9	V	34	PHE	2.1
7	G	3	ALA	2.1
9	I	37	PHE	2.1
11	X	13	TYR	2.1
8	U	49	ASP	2.0
13	Z	35	TYR	2.0
12	L	47	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
9	SAC	V	1	9/10	0.43	0.49	138,151,167,167	0
7	TPO	T	11	11/12	0.64	0.31	101,147,160,160	0
9	SAC	I	1	9/10	0.72	0.37	116,134,157,165	0
7	TPO	G	11	11/12	0.76	0.27	102,140,157,157	0
1	FME	N	1	10/11	0.92	0.31	80,86,125,151	0
1	FME	A	1	10/11	0.95	0.29	74,86,128,147	0
2	FME	B	1	10/11	0.98	0.07	58,65,72,72	0
2	FME	O	1	10/11	0.99	0.08	64,71,76,79	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
24	PSC	B	303	52/52	0.53	0.35	75,147,150,150	0
27	PEK	G	102	53/53	0.59	0.32	100,135,150,150	0
20	PGV	N	607	51/51	0.64	0.32	99,137,150,150	0
20	PGV	A	609	51/51	0.65	0.26	69,115,159,161	0
19	TGL	N	610	63/63	0.65	0.29	90,134,149,150	0
27	PEK	T	101	53/53	0.66	0.36	79,136,150,150	0
24	PSC	R	201	52/52	0.67	0.29	76,137,150,150	0
27	PEK	T	102	53/53	0.67	0.31	78,133,150,150	0
29	DMU	Z	101	33/33	0.68	0.30	80,128,149,150	0
23	CHD	W	101	29/29	0.69	0.40	107,145,150,150	0
26	CDL	C	307	100/100	0.71	0.30	89,138,150,150	0
26	CDL	P	304	100/100	0.72	0.25	71,140,150,150	0
21	EDO	C	310	4/4	0.72	0.24	94,105,106,112	0
19	TGL	N	611	63/63	0.73	0.25	90,126,148,150	0

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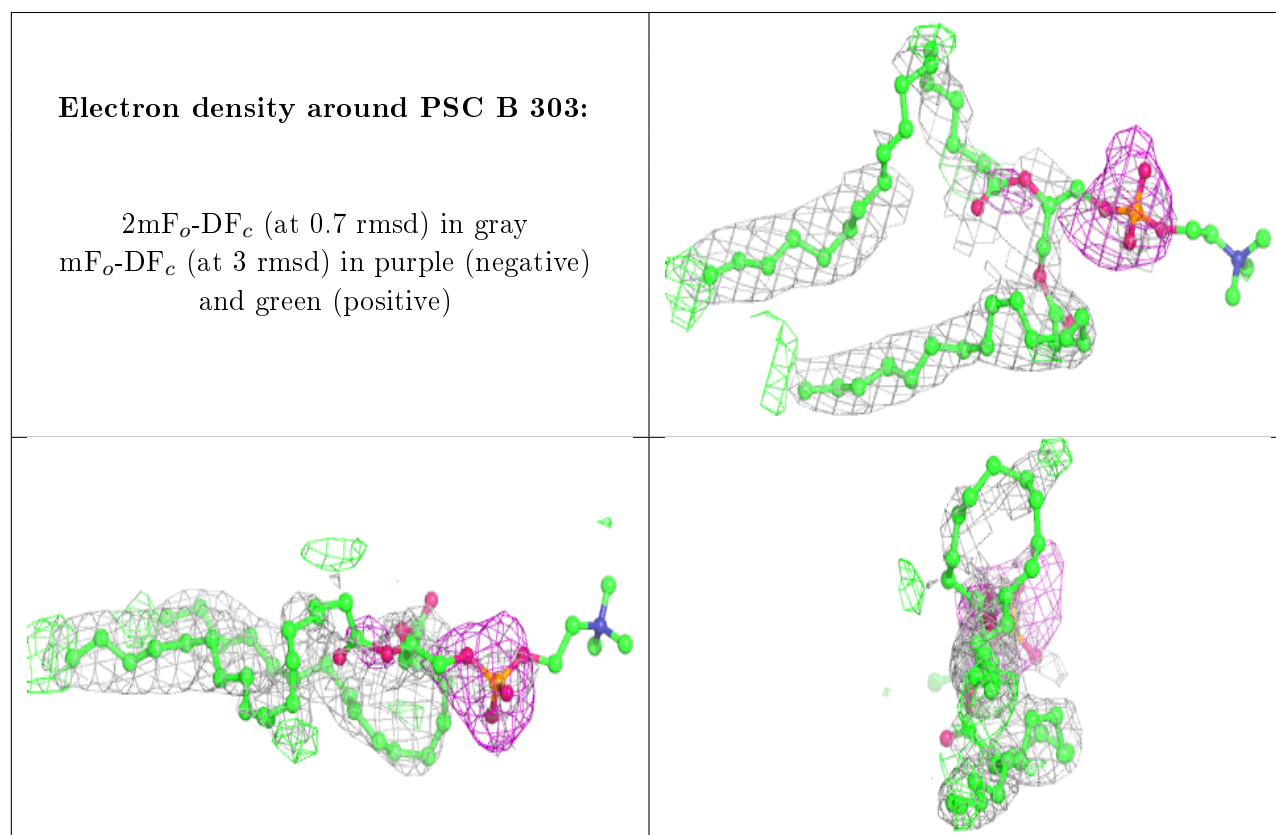
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	TGL	D	201	63/63	0.75	0.24	87,126,147,150	0
21	EDO	A	612	4/4	0.75	0.51	88,115,122,127	0
21	EDO	K	101	4/4	0.76	0.18	86,107,118,131	0
20	PGV	C	308	51/51	0.76	0.22	75,125,150,150	0
26	CDL	T	103	100/100	0.77	0.26	76,140,150,150	0
19	TGL	L	101	63/63	0.79	0.23	67,113,143,150	0
27	PEK	C	306	53/53	0.79	0.26	71,132,149,150	0
20	PGV	G	103	51/51	0.80	0.20	96,127,150,150	0
23	CHD	J	101	29/29	0.81	0.36	123,142,150,150	0
26	CDL	C	303	100/100	0.82	0.22	66,123,153,155	0
21	EDO	C	311	4/4	0.83	0.26	80,95,109,118	0
19	TGL	A	607	63/63	0.84	0.18	54,97,122,132	0
25	UNX	P	301	1/1	0.84	0.41	15,15,15,15	1
21	EDO	A	614	4/4	0.84	0.58	133,137,141,148	0
19	TGL	N	609	63/63	0.85	0.18	60,120,149,150	0
21	EDO	K	103	4/4	0.85	0.23	90,92,99,101	0
21	EDO	G	104	4/4	0.86	0.21	97,101,102,105	0
23	CHD	C	304	29/29	0.87	0.26	93,117,125,127	0
21	EDO	F	102	4/4	0.88	0.28	80,88,96,96	0
21	EDO	K	102	4/4	0.89	0.21	101,108,112,116	0
29	DMU	M	101	33/33	0.90	0.16	70,102,129,136	0
23	CHD	P	305	29/29	0.90	0.20	120,135,145,147	0
25	UNX	C	301	1/1	0.93	0.36	26,26,26,26	1
21	EDO	A	611	4/4	0.93	0.13	86,94,107,113	0
21	EDO	A	613	4/4	0.93	0.19	112,112,121,122	0
27	PEK	P	302	53/53	0.94	0.13	59,91,150,150	0
27	PEK	G	101	53/53	0.94	0.12	57,72,126,136	0
21	EDO	B	305	4/4	0.94	0.20	105,110,115,123	0
21	EDO	T	104	4/4	0.94	0.32	124,129,131,132	0
23	CHD	C	305	29/29	0.96	0.09	47,61,71,81	0
23	CHD	B	302	29/29	0.96	0.10	48,64,74,77	0
21	EDO	N	612	4/4	0.96	0.09	79,80,82,84	0
21	EDO	L	102	4/4	0.97	0.06	83,84,84,90	0
21	EDO	A	610	4/4	0.97	0.10	75,75,78,81	0
23	CHD	O	302	29/29	0.97	0.09	50,57,67,72	0
21	EDO	C	309	4/4	0.97	0.16	76,86,100,122	0
20	PGV	N	608	51/51	0.98	0.11	47,76,117,142	0
20	PGV	A	608	51/51	0.98	0.10	51,66,79,86	0
23	CHD	P	306	29/29	0.98	0.09	57,65,72,73	0
20	PGV	P	303	51/51	0.98	0.10	51,72,132,148	0
17	NA	N	605	1/1	0.98	0.11	70,70,70,70	0
16	MG	N	604	1/1	0.98	0.07	57,57,57,57	0

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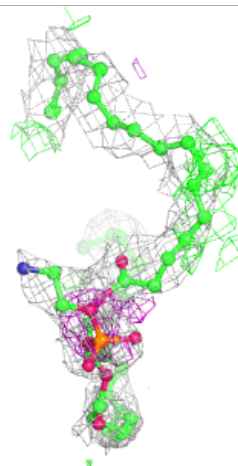
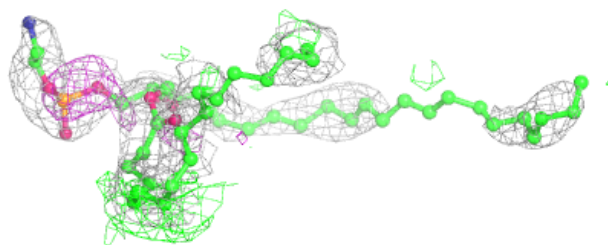
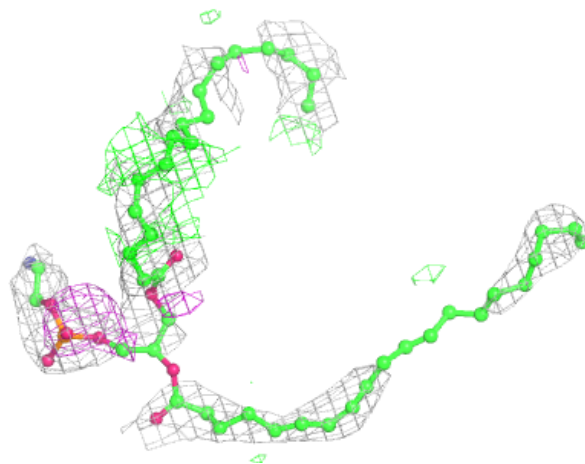
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	EDO	B	304	4/4	0.98	0.09	71,75,75,75	0
20	PGV	C	302	51/51	0.98	0.08	49,58,90,99	0
18	CMO	N	606	2/2	0.99	0.15	77,77,77,80	0
14	HEA	A	602	60/60	0.99	0.06	45,51,60,62	0
14	HEA	N	602	60/60	0.99	0.08	47,57,69,75	0
16	MG	A	604	1/1	0.99	0.06	51,51,51,51	0
22	CUA	O	301	2/2	0.99	0.06	66,66,66,67	0
14	HEA	N	601	60/60	0.99	0.09	47,56,78,84	0
17	NA	A	605	1/1	0.99	0.16	59,59,59,59	0
22	CUA	B	301	2/2	0.99	0.07	54,54,54,58	0
14	HEA	A	601	60/60	0.99	0.07	34,46,65,70	0
28	ZN	F	101	1/1	1.00	0.04	64,64,64,64	0
18	CMO	A	606	2/2	1.00	0.06	55,55,55,55	0
15	CU	N	603	1/1	1.00	0.03	55,55,55,55	0
15	CU	A	603	1/1	1.00	0.01	55,55,55,55	0
28	ZN	S	101	1/1	1.00	0.07	70,70,70,70	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.



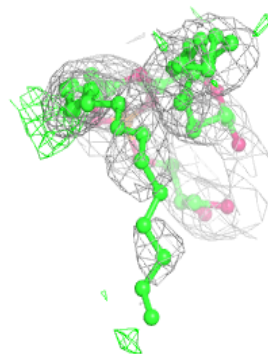
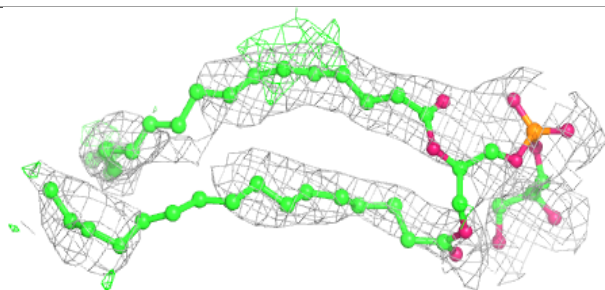
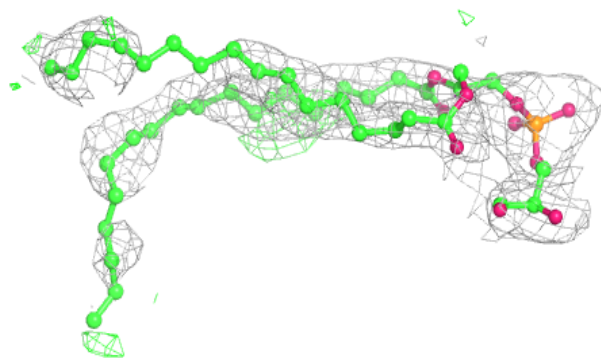
Electron density around PEK G 102:

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

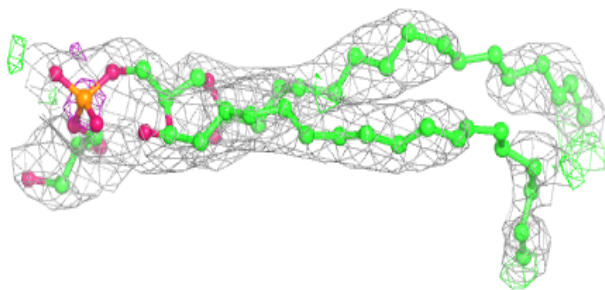
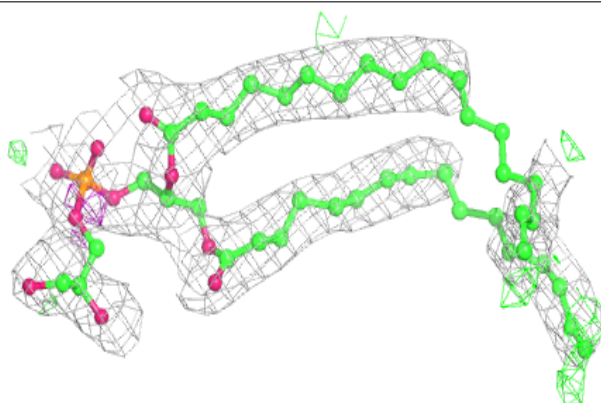


Electron density around PGV N 607:

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

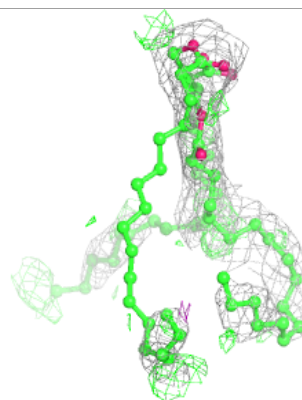
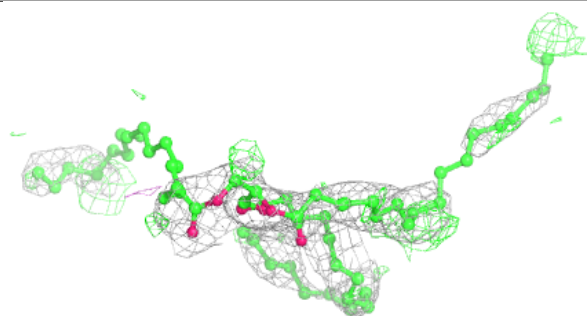
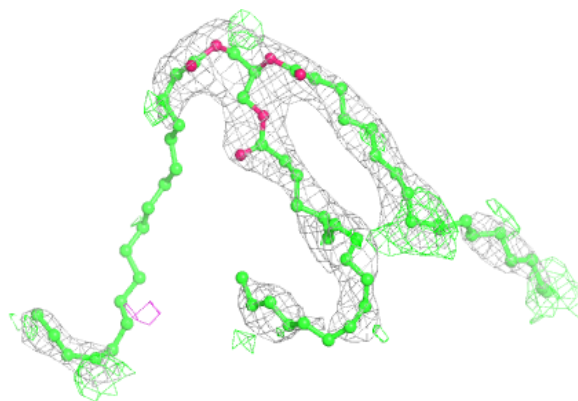
**Electron density around PGV A 609:**

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

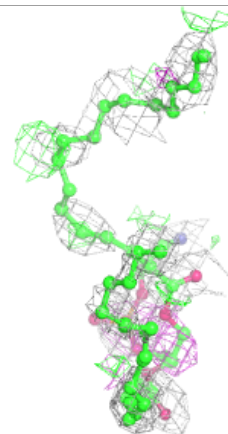
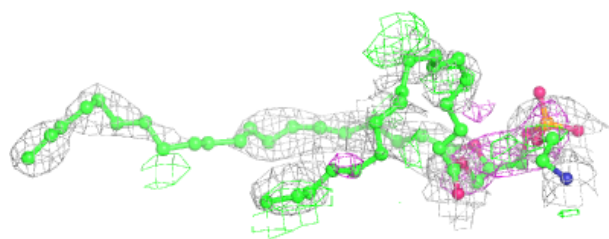
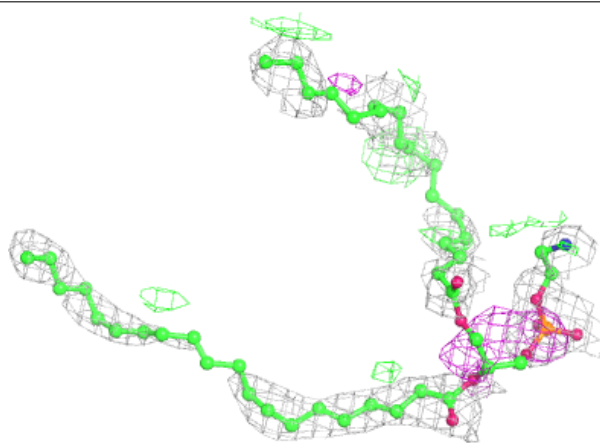


Electron density around TGL N 610:

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

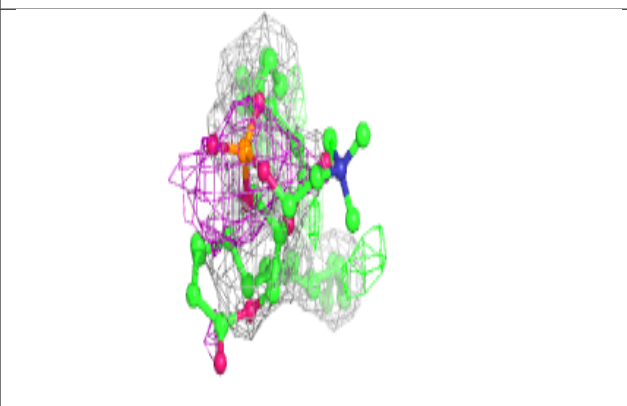
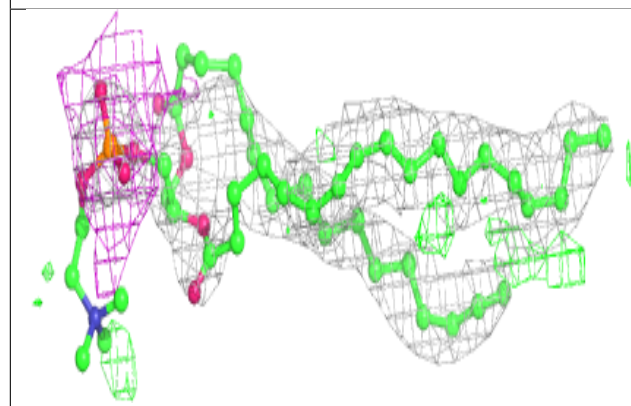
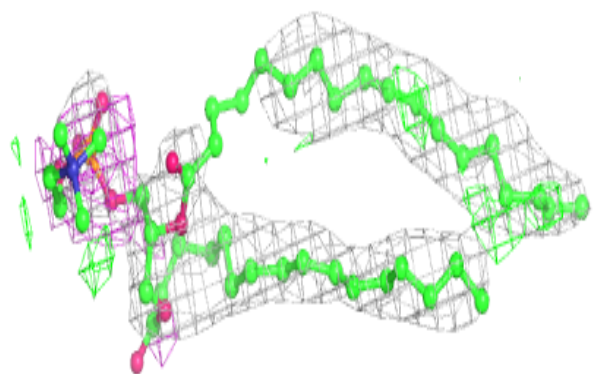
**Electron density around PEK T 101:**

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

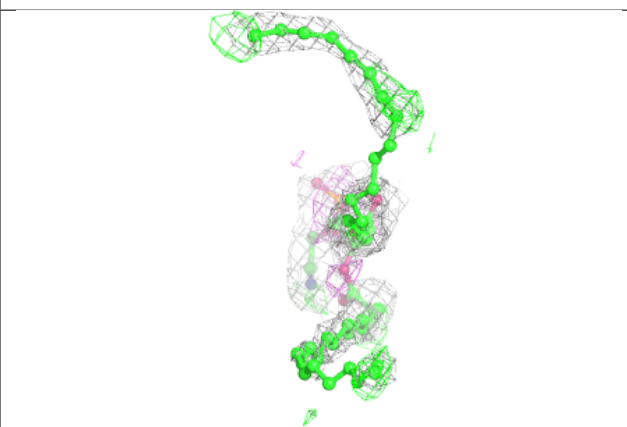
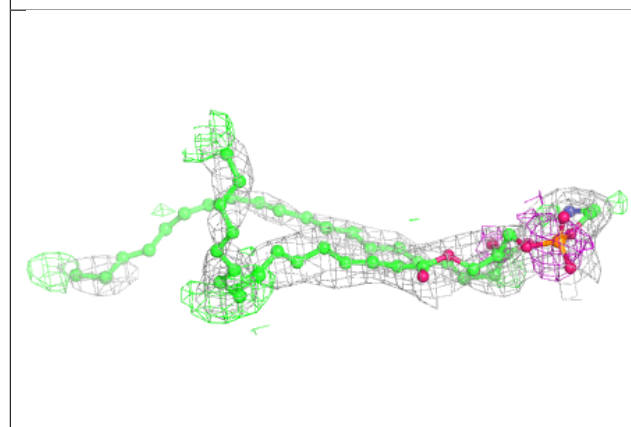
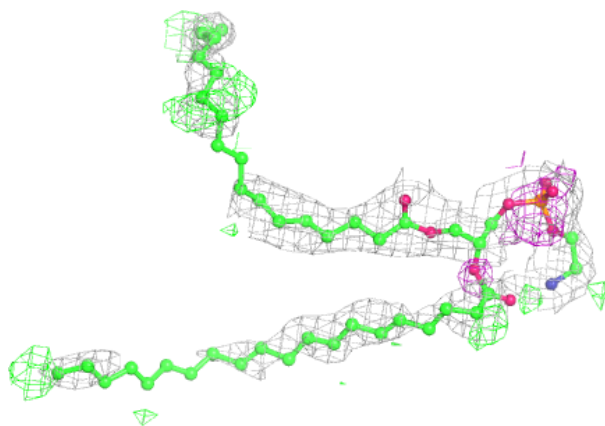


Electron density around PSC R 201:

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

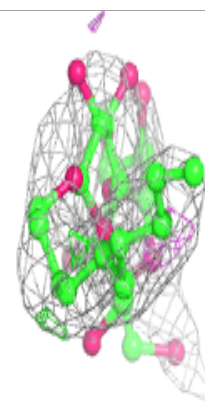
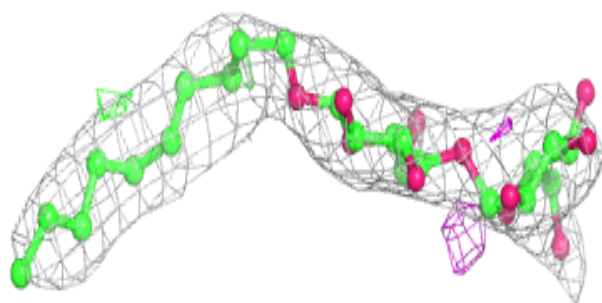
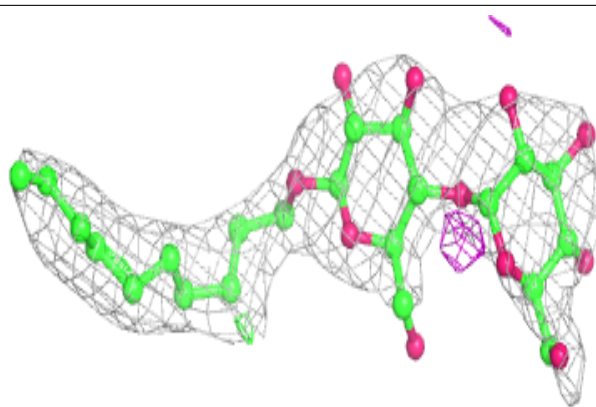
**Electron density around PEK T 102:**

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

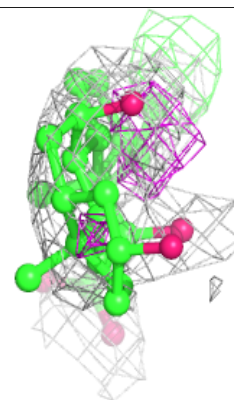
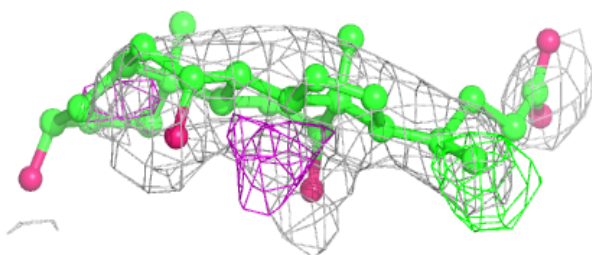
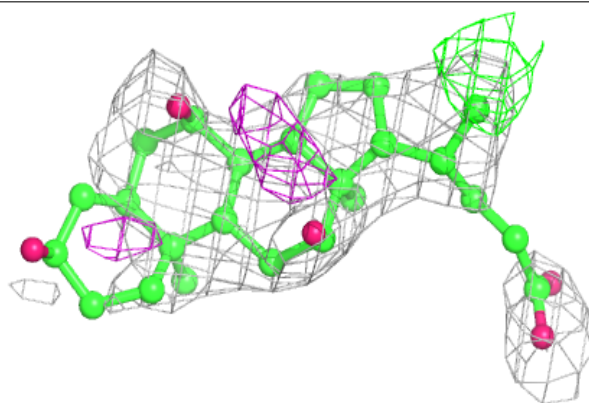


Electron density around DMU Z 101:

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

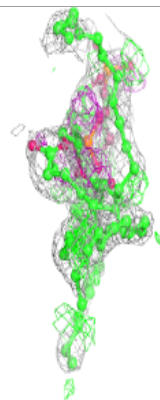
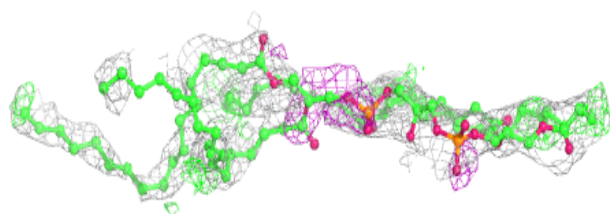
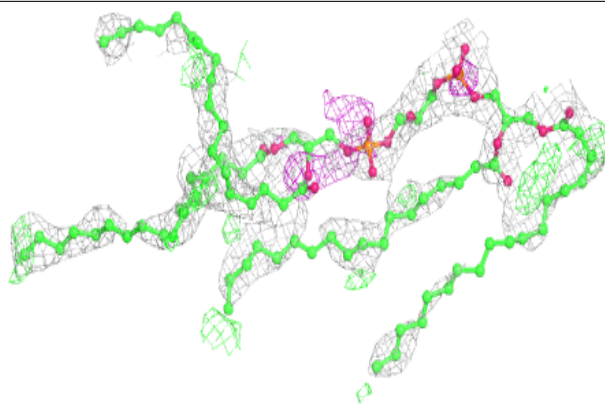
**Electron density around CHD W 101:**

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

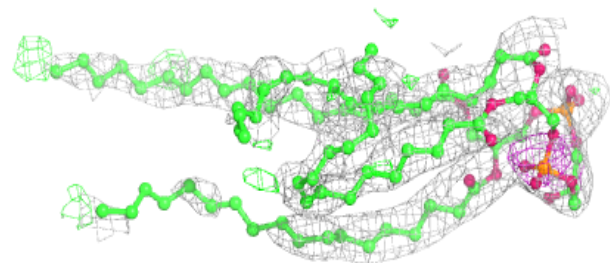
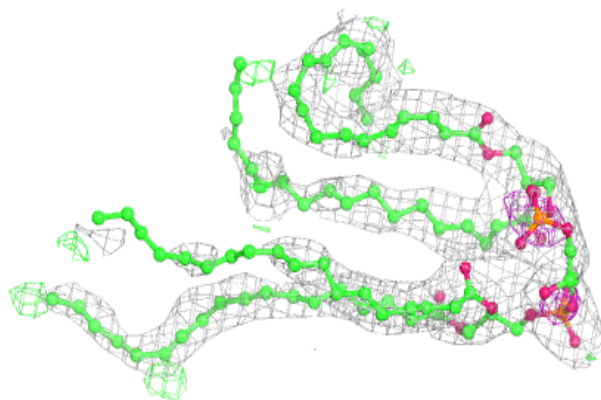


Electron density around CDL C 307:

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

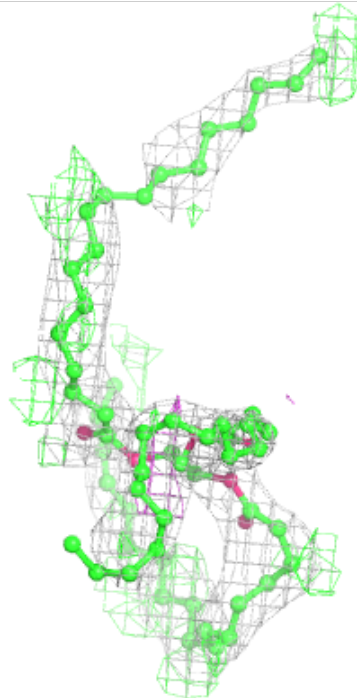
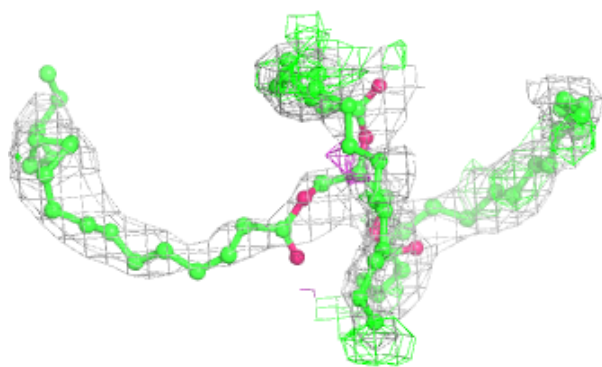
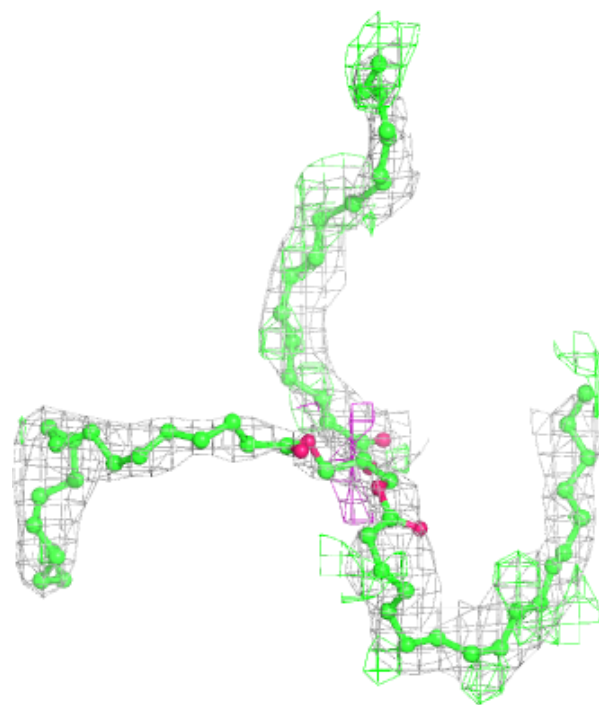
**Electron density around CDL P 304:**

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



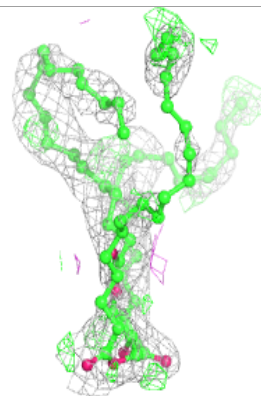
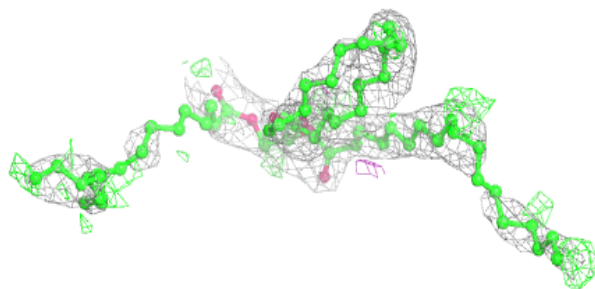
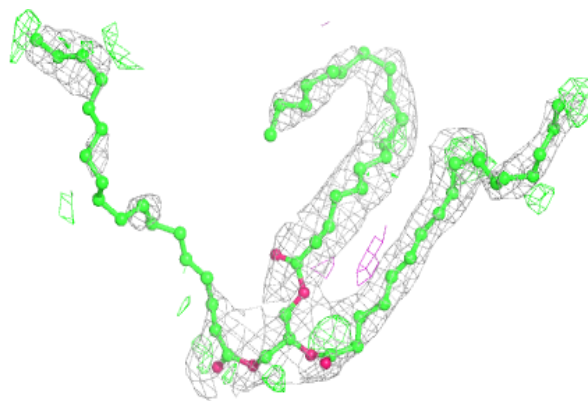
Electron density around TGL N 611:

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

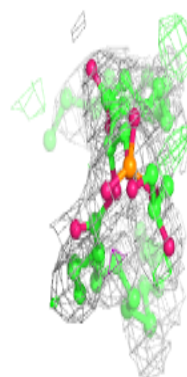
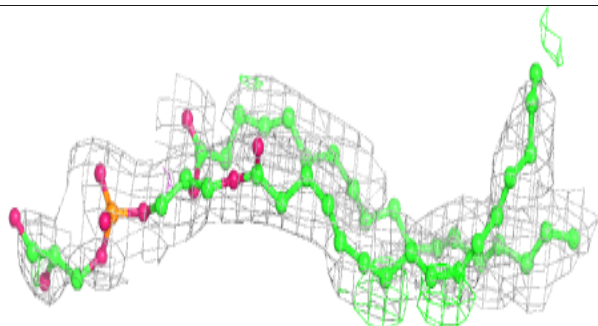
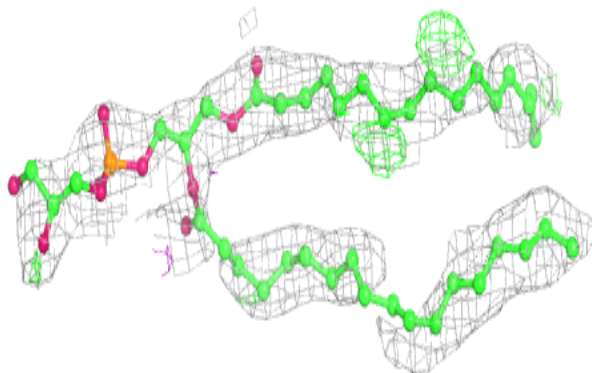


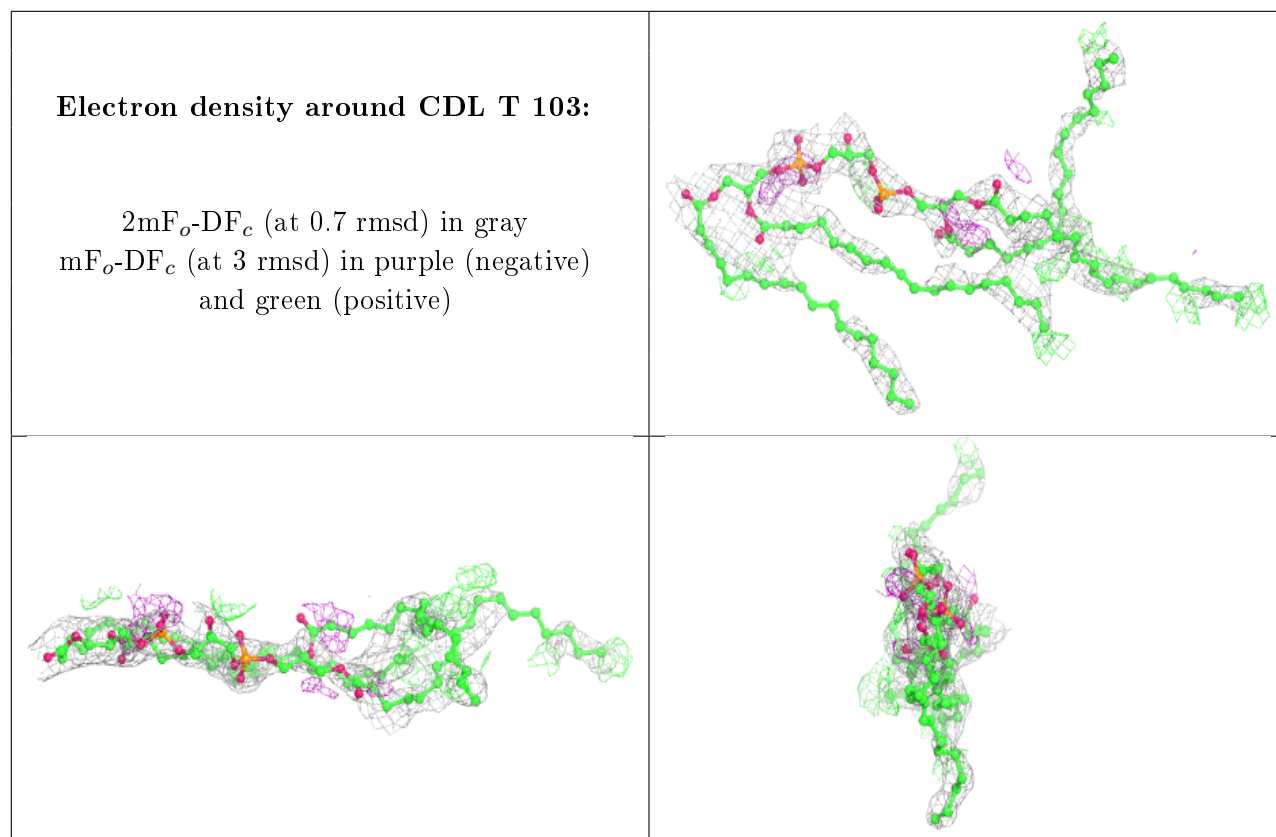
Electron density around TGL D 201:

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

**Electron density around PGV C 308:**

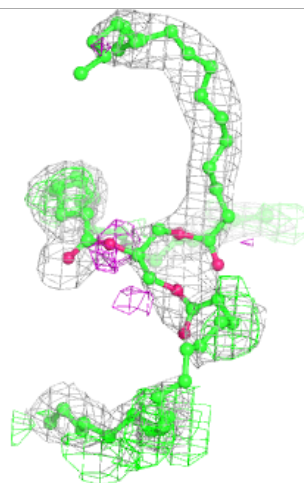
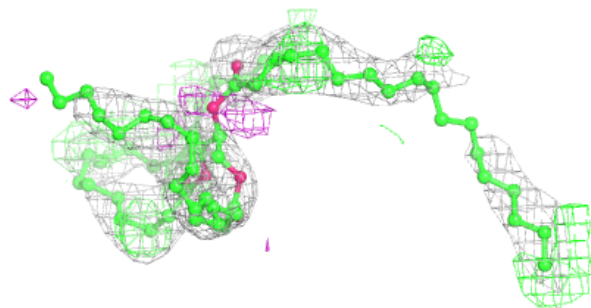
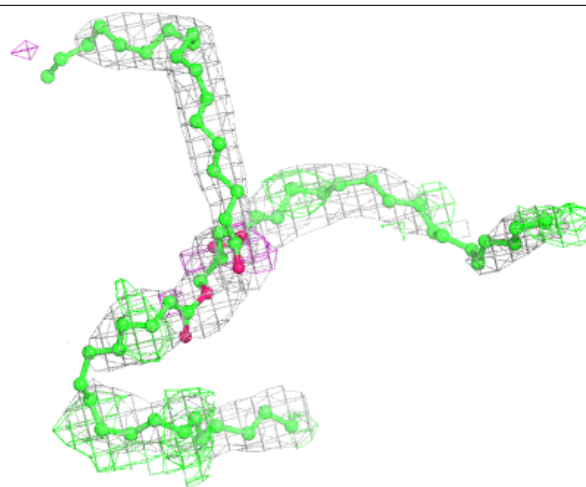
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)

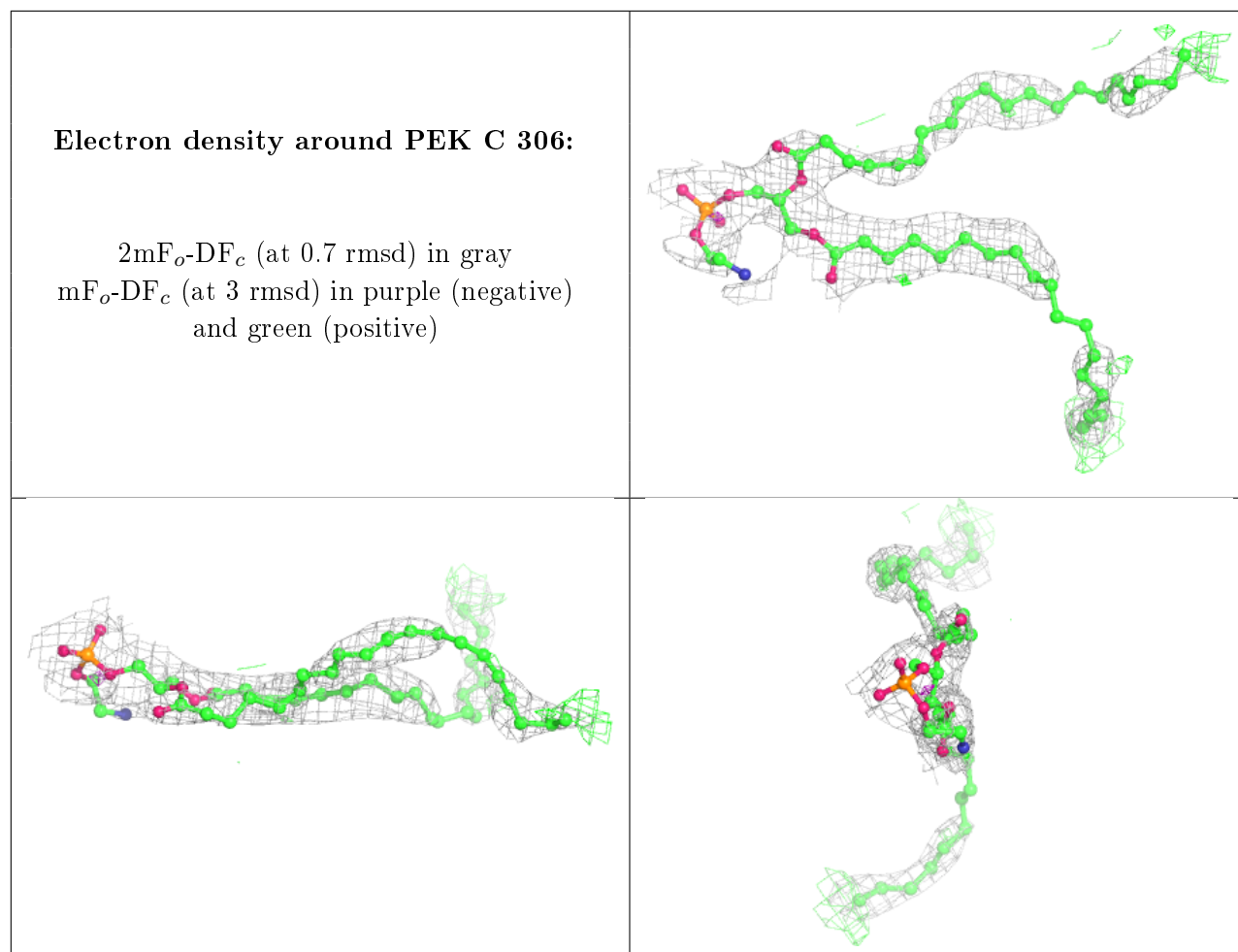




Electron density around TGL L 101:

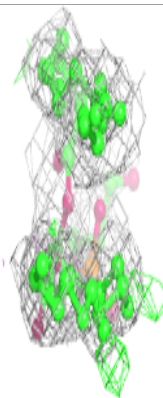
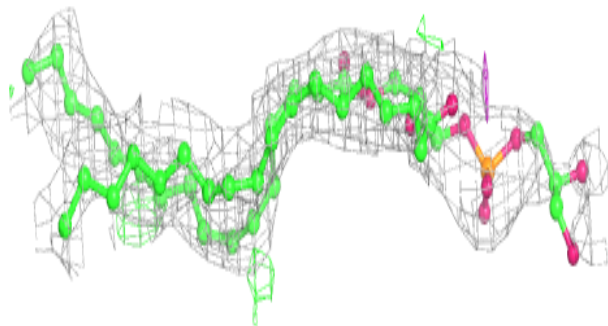
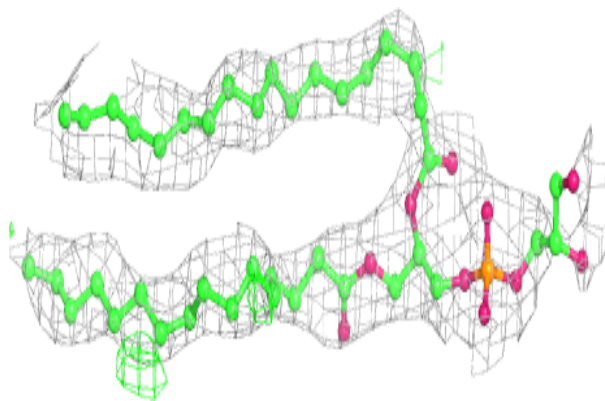
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



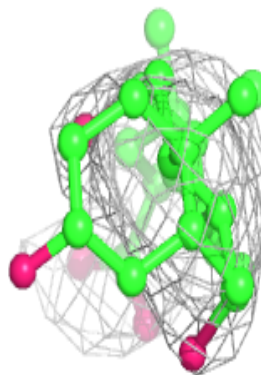
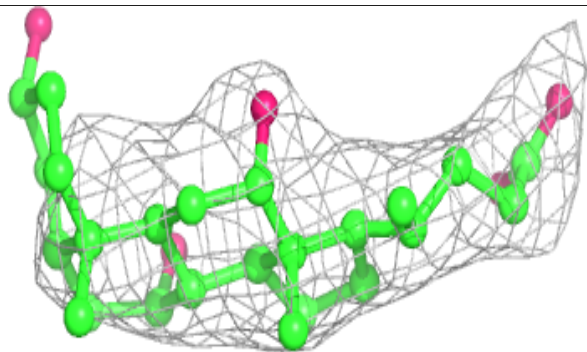
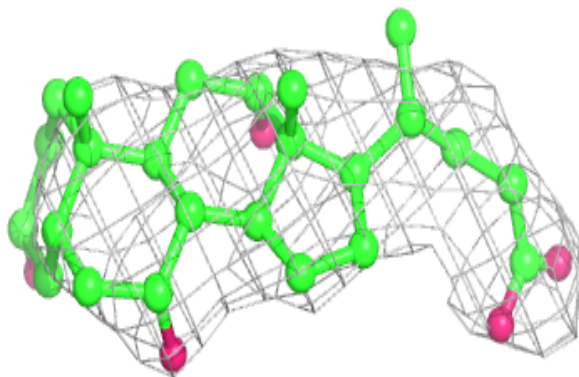


Electron density around PGV G 103:

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

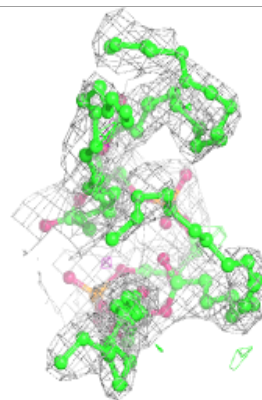
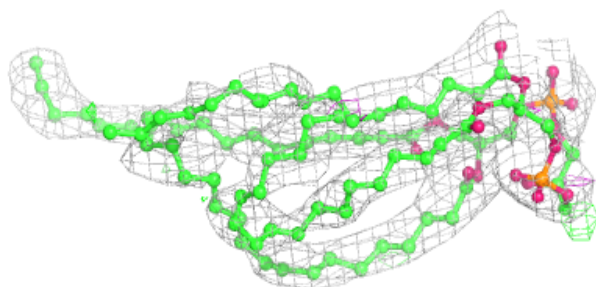
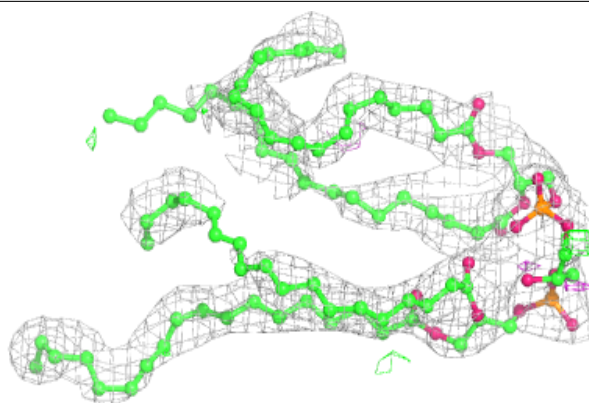
**Electron density around CHD J 101:**

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

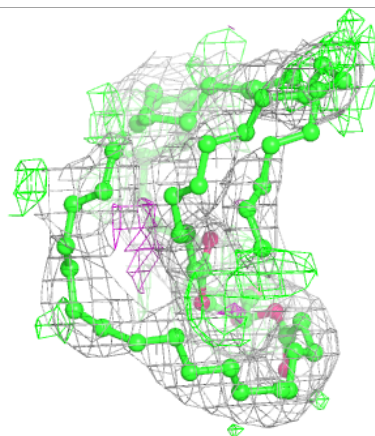
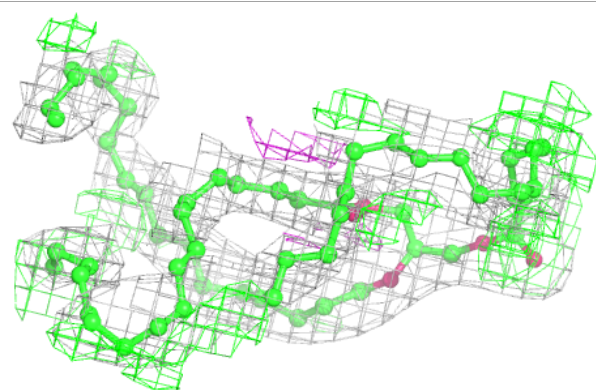
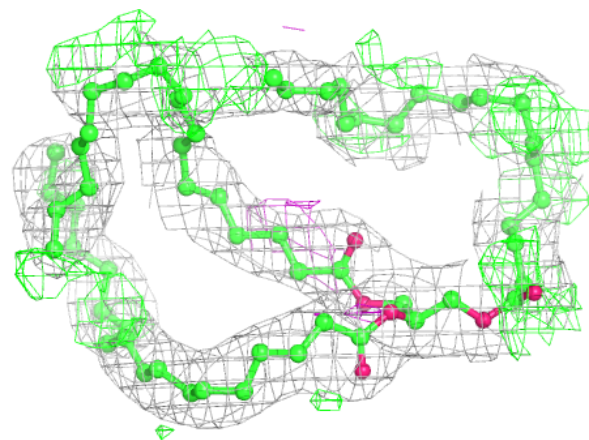


Electron density around CDL C 303:

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

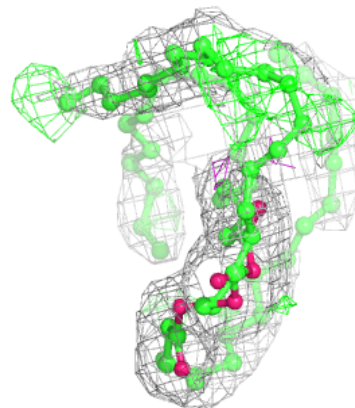
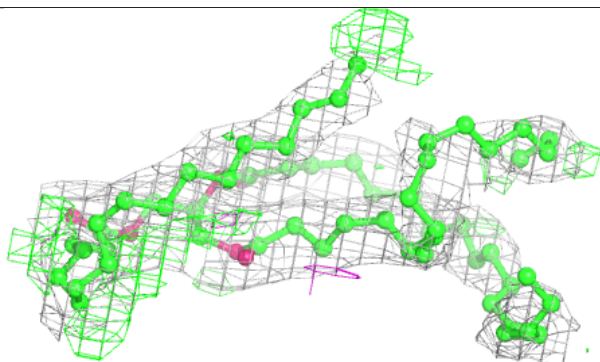
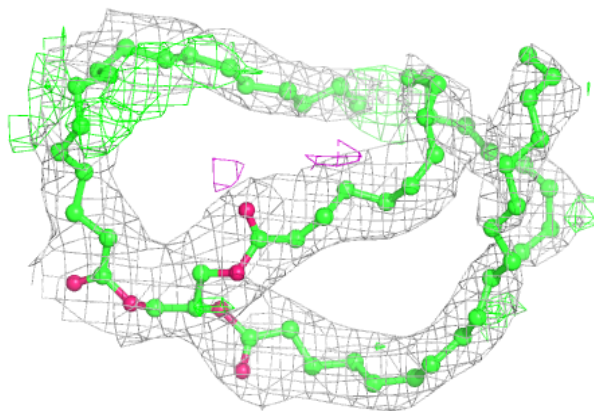
**Electron density around TGL A 607:**

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

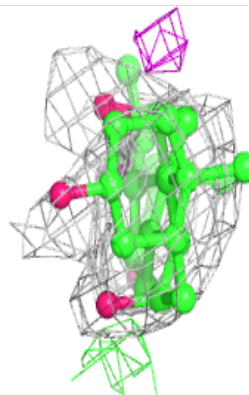
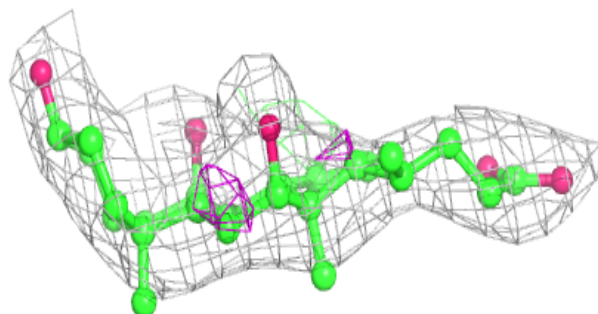
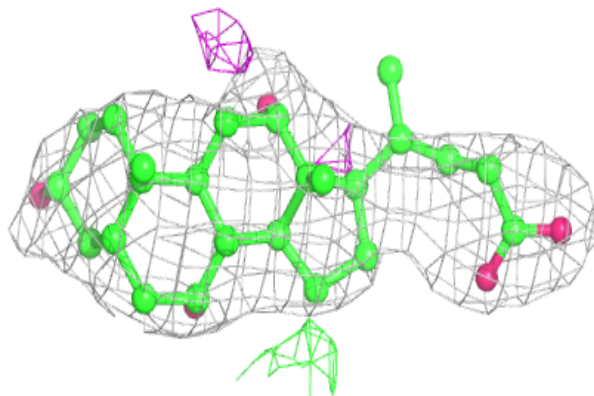


Electron density around TGL N 609:

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

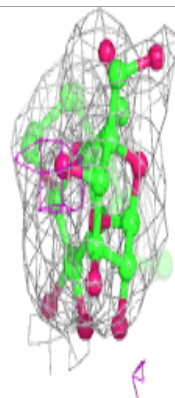
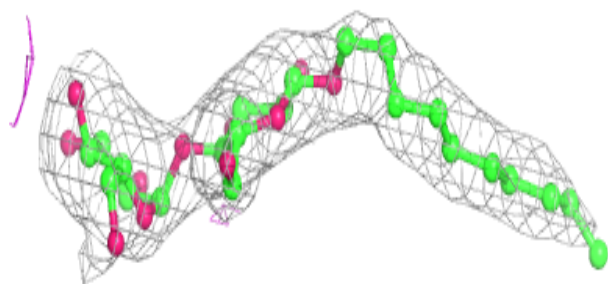
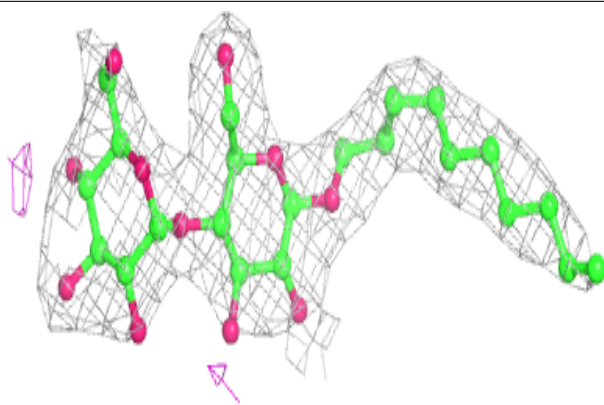
**Electron density around CHD C 304:**

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

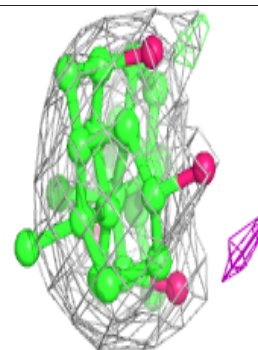
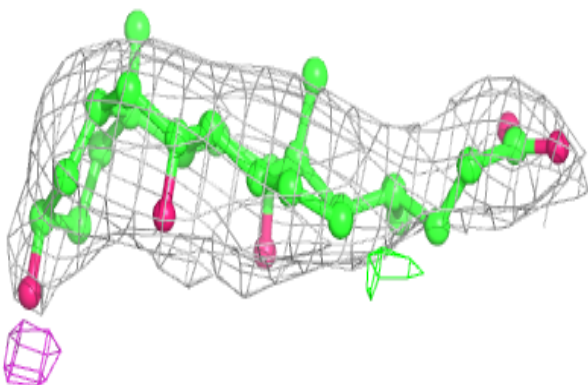
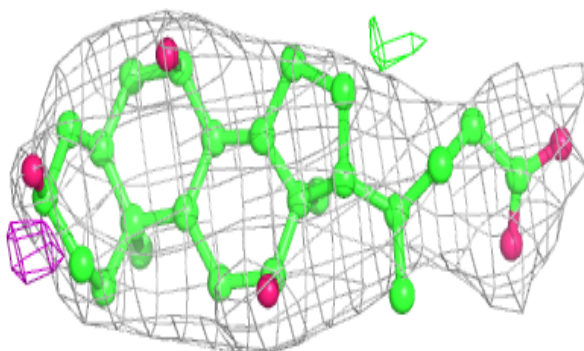


Electron density around DMU M 101:

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

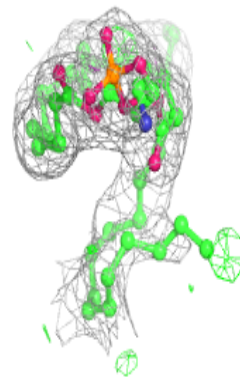
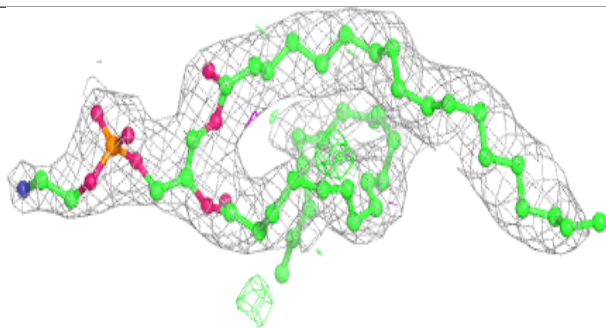
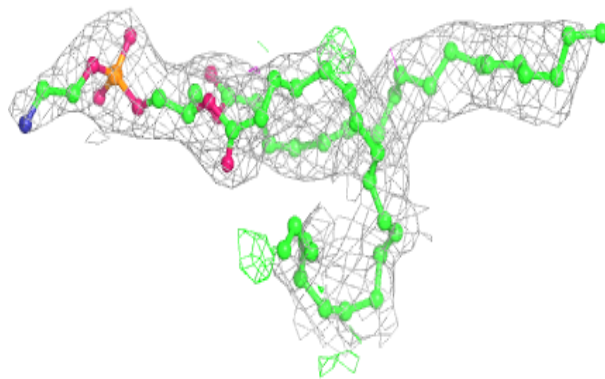
**Electron density around CHD P 305:**

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

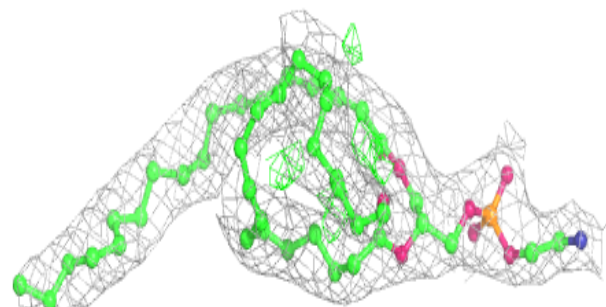
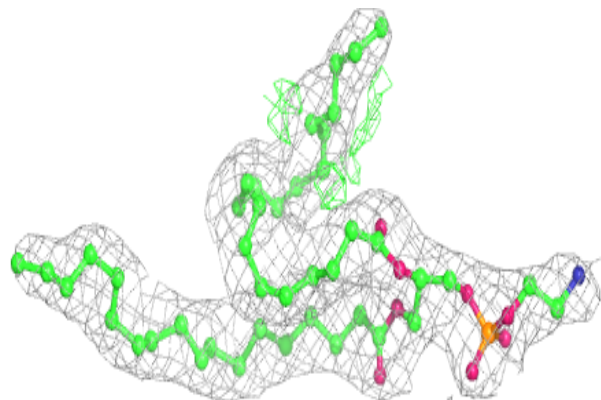


Electron density around PEK P 302:

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

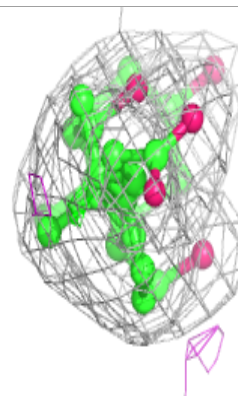
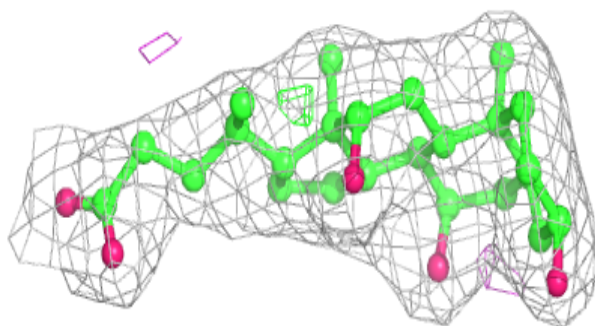
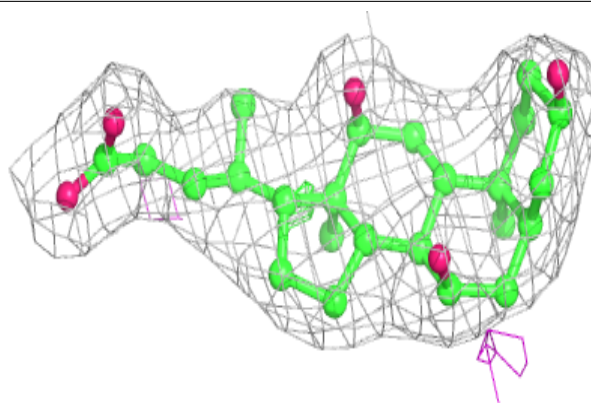
**Electron density around PEK G 101:**

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

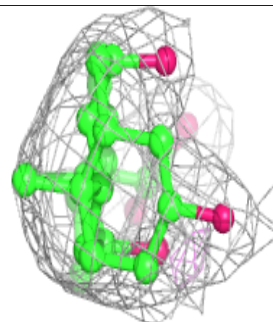
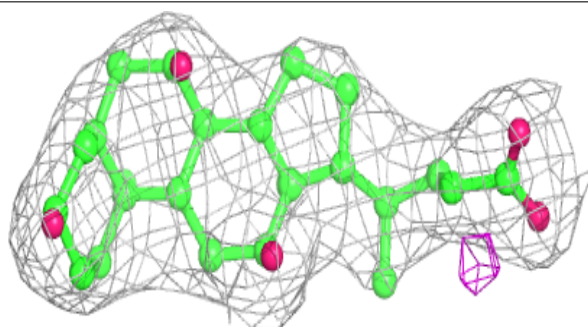


Electron density around CHD C 305:

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

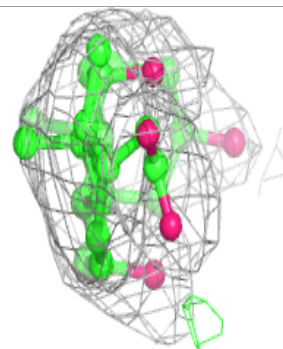
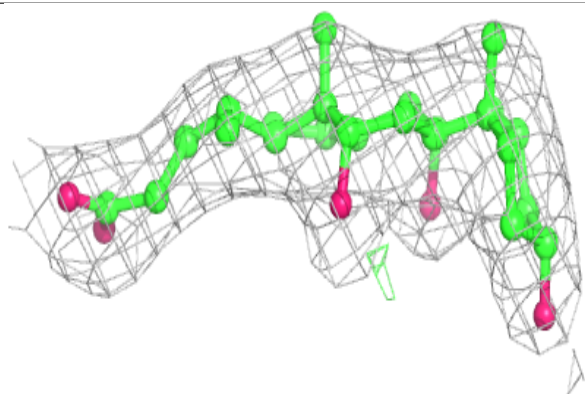
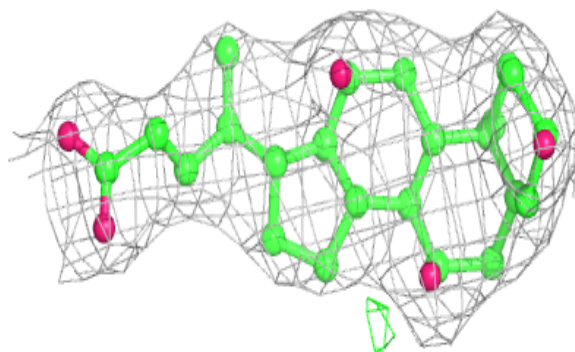
**Electron density around CHD B 302:**

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

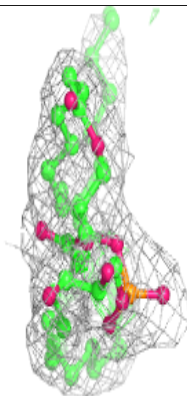
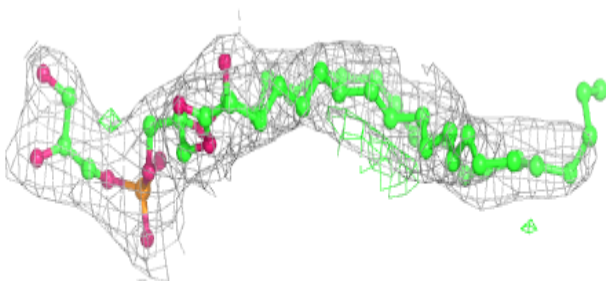
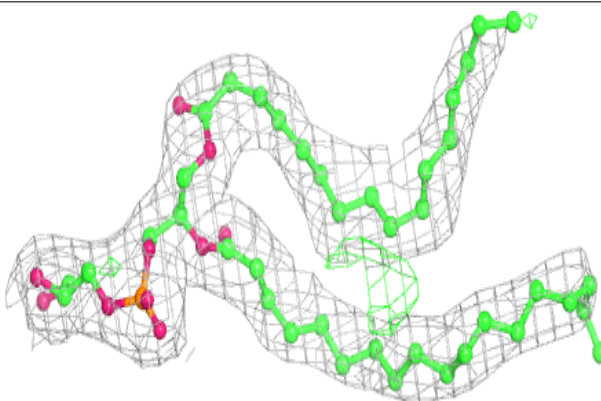


Electron density around CHD O 302:

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

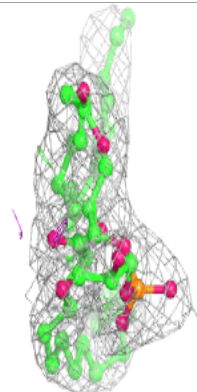
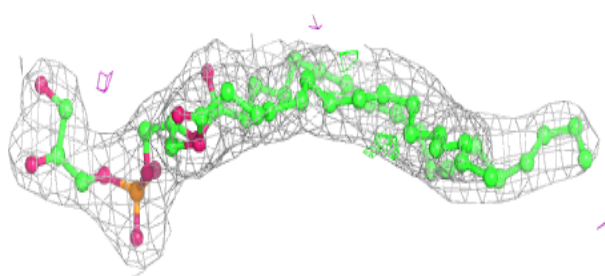
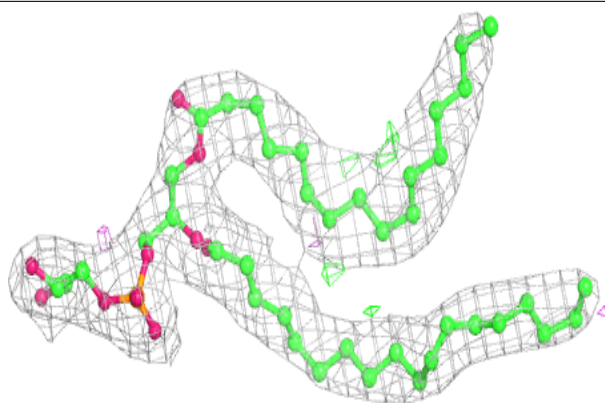
**Electron density around PGV N 608:**

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

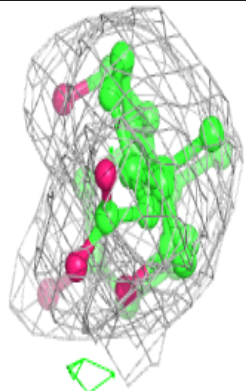
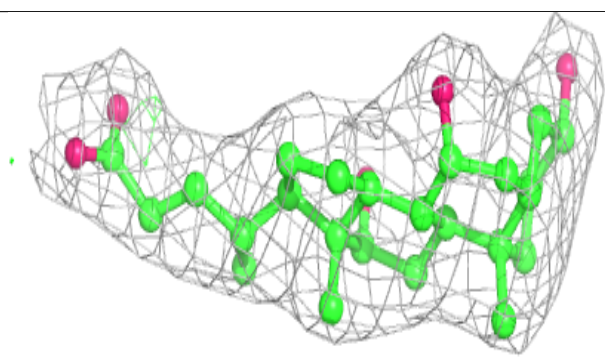
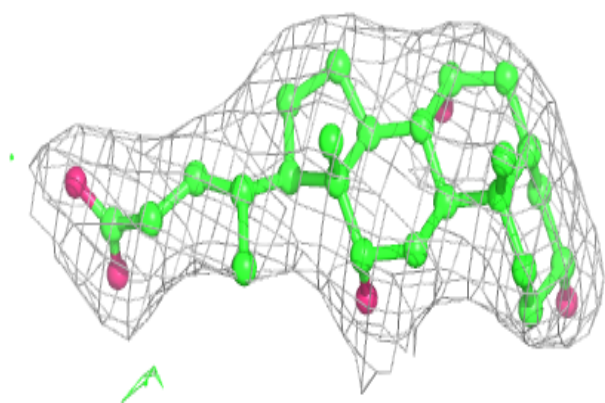


Electron density around PGV A 608:

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

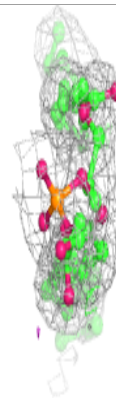
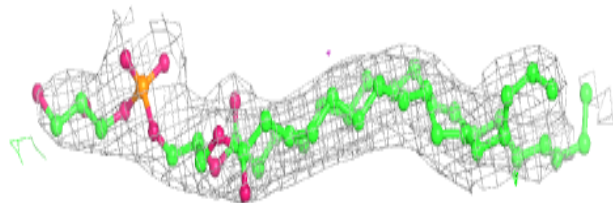
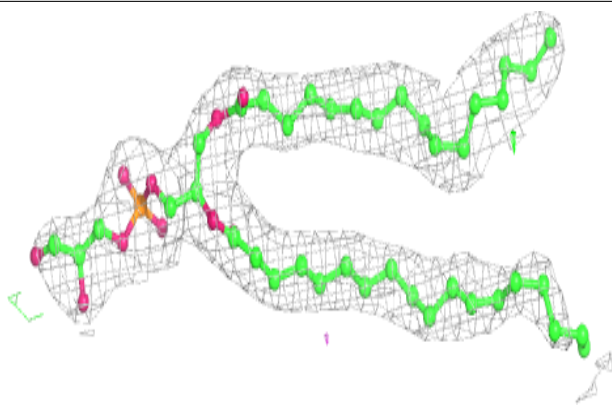
**Electron density around CHD P 306:**

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

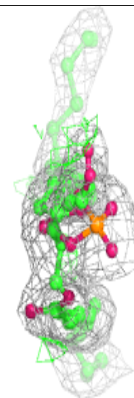
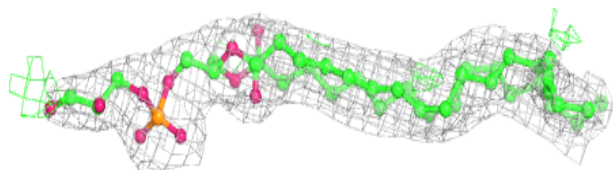
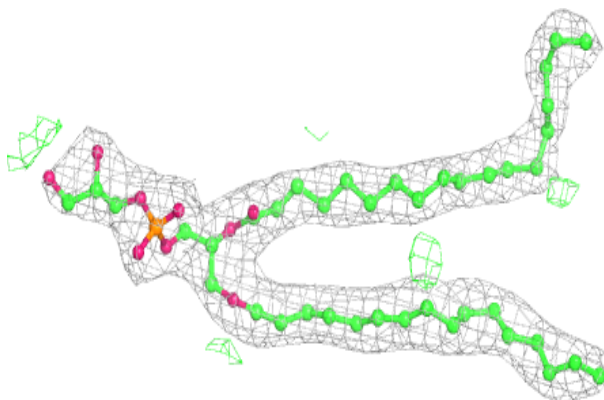


Electron density around PGV P 303:

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

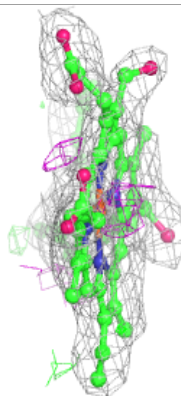
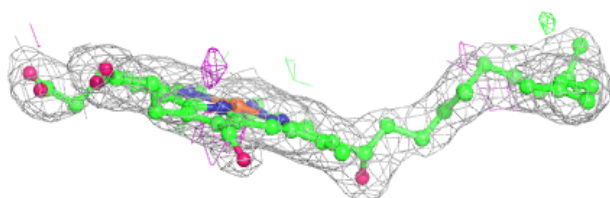
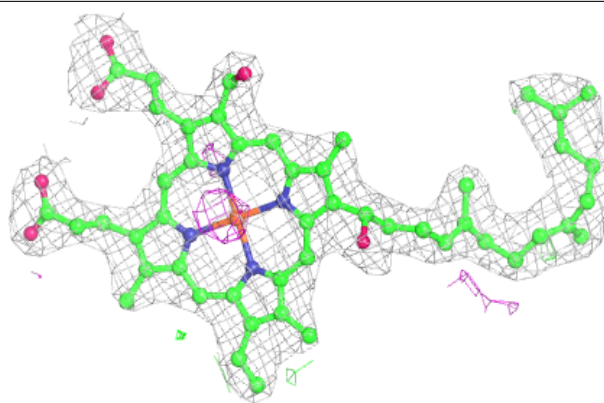
**Electron density around PGV C 302:**

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

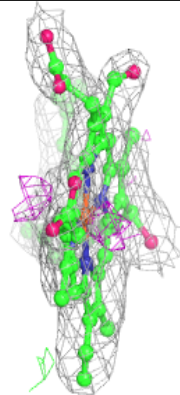
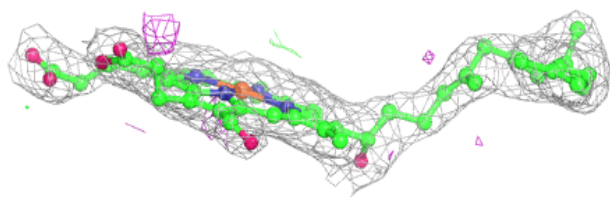
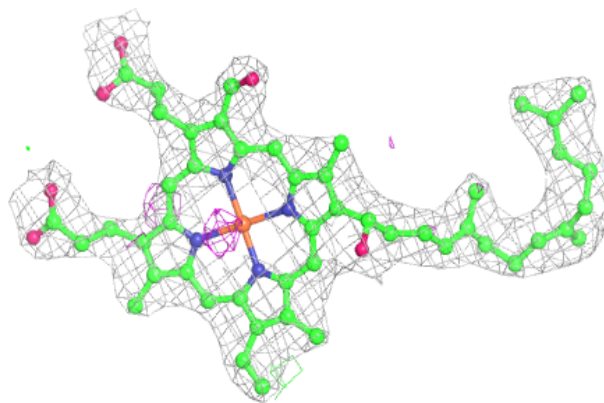


Electron density around HEA A 602:

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

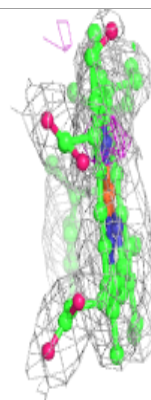
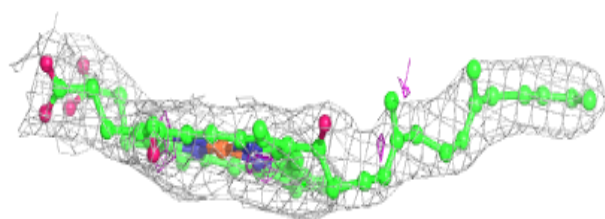
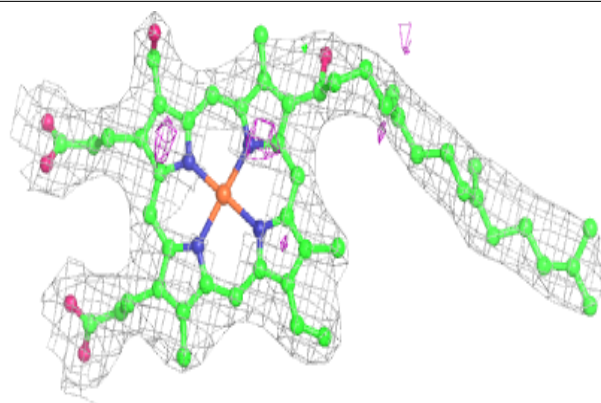
**Electron density around HEA N 602:**

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

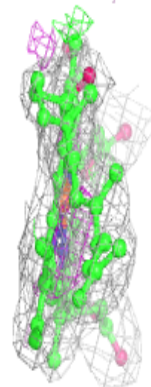
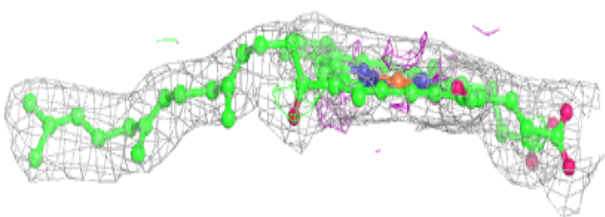
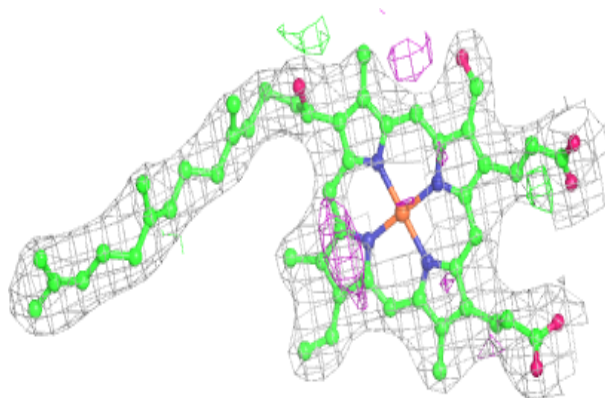


Electron density around HEA N 601:

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

**Electron density around HEA A 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.