



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:43 pm BST

PDB ID : 6J8M
Title : Low-dose structure of bovine heart cytochrome c oxidase in the fully oxidized state determined using 30 keV X-ray
Authors : Ueno, G.; Shimada, A.; Yamashita, E.; Hasegawa, K.; Kumasaka, T.; Shinzawa-Itoh, K.; Yoshikawa, S.; Tsukihara, T.; Yamamoto, M.
Deposited on : 2019-01-20
Resolution : 1.90 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 : 2.11
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) : 2.11

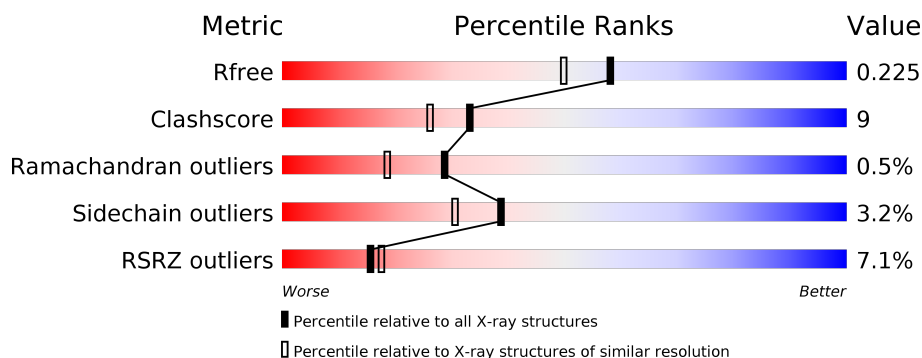
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	<div> <div style="width: 89%;"></div> <div style="width: 10%;"></div> <div style="width: 1%;"></div> </div> <div> <div style="width: 89%;"></div> <div style="width: 10%;"></div> <div style="width: 1%;"></div> </div>
1	N	514	<div> <div style="width: 87%;"></div> <div style="width: 12%;"></div> <div style="width: 1%;"></div> </div> <div> <div style="width: 87%;"></div> <div style="width: 12%;"></div> <div style="width: 1%;"></div> </div>
2	B	227	<div> <div style="width: 84%;"></div> <div style="width: 14%;"></div> <div style="width: 2%;"></div> </div> <div> <div style="width: 84%;"></div> <div style="width: 14%;"></div> <div style="width: 2%;"></div> </div>
2	O	227	<div> <div style="width: 77%;"></div> <div style="width: 21%;"></div> <div style="width: 2%;"></div> </div> <div> <div style="width: 77%;"></div> <div style="width: 21%;"></div> <div style="width: 2%;"></div> </div>
3	C	261	<div> <div style="width: 89%;"></div> <div style="width: 10%;"></div> <div style="width: 1%;"></div> </div> <div> <div style="width: 89%;"></div> <div style="width: 10%;"></div> <div style="width: 1%;"></div> </div>
3	P	261	<div> <div style="width: 89%;"></div> <div style="width: 11%;"></div> <div style="width: 1%;"></div> </div> <div> <div style="width: 89%;"></div> <div style="width: 11%;"></div> <div style="width: 1%;"></div> </div>

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
19	PER	A	607[B]	-	-	X	-
22	CHD	W	101	-	-	-	X
25	DMU	C	309	-	-	-	X
25	DMU	P	307	-	-	-	X
7	TPO	G	11	-	-	-	X
7	TPO	T	11	-	-	-	X
9	SAC	I	1	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33893 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	12	0
			4124	2753	638	693	40			
1	N	514	Total	C	N	O	S	0	13	0
			4123	2752	638	693	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	6	0
			1868	1213	288	348	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	289	348	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	8	0
			2174	1451	345	364	14			
3	P	259	Total	C	N	O	S	0	8	0
			2173	1451	344	363	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	6	0
			1249	814	206	224	5			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	197	219	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	5	0
			789	489	142	152	6			
6	S	98	Total	C	N	O	S	0	1	0
			755	468	135	147	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 706	C 454	N 133	O 117	P 1	S 1	0	3	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	1	0
			609	395	108	101	5			

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

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

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

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

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

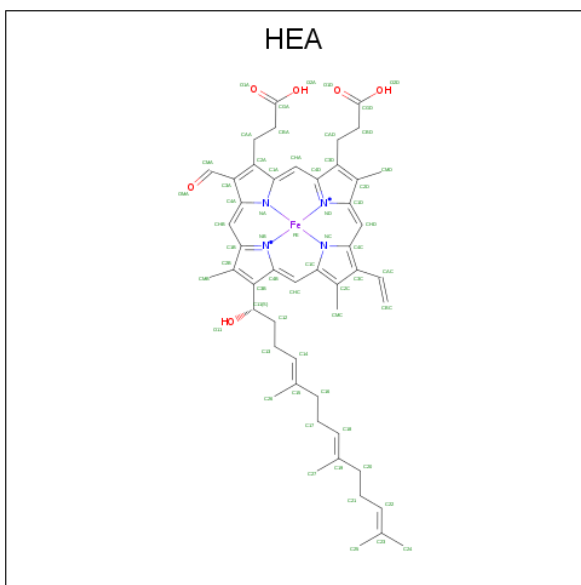
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

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
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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

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

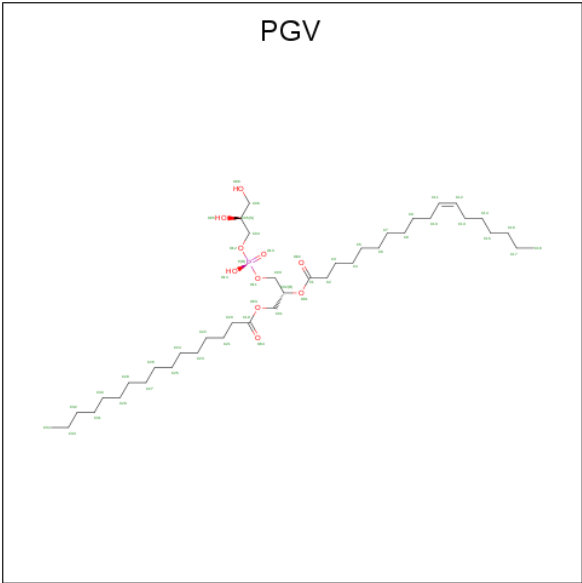
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 18 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).



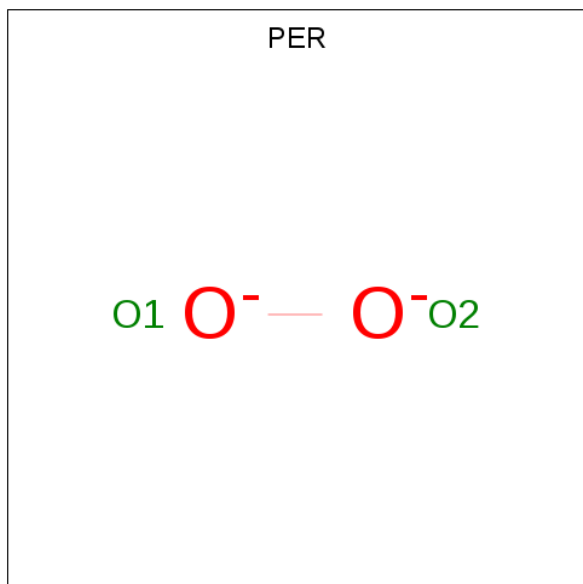
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 51 40 10 1	0	0
18	A	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	P	1	Total C O P 51 40 10 1	0	0

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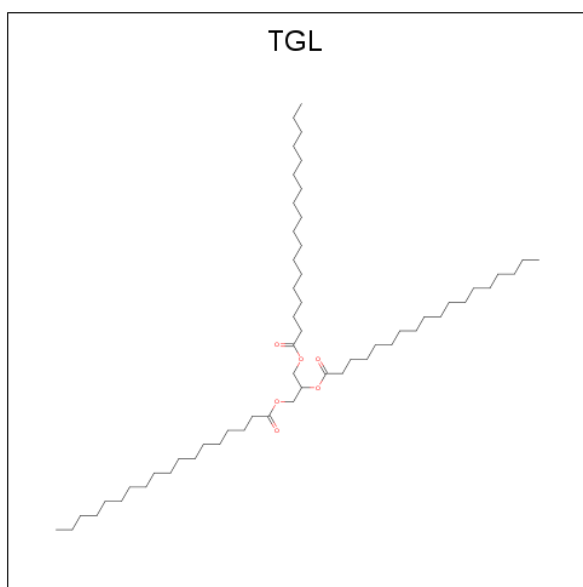
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



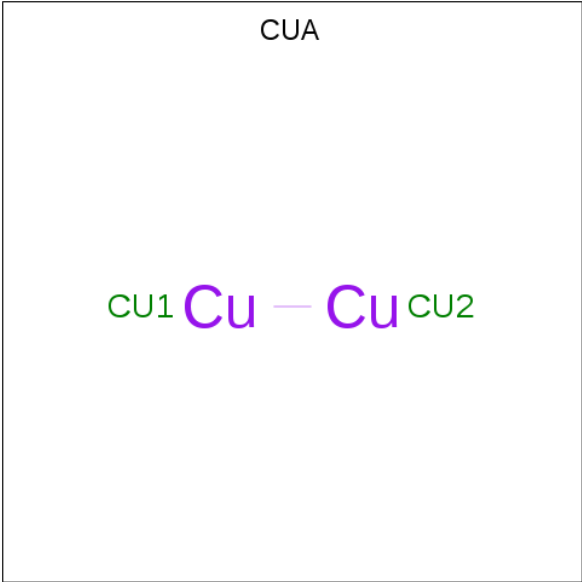
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	1
			4	4		
19	N	1	Total	O	0	1
			4	4		

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



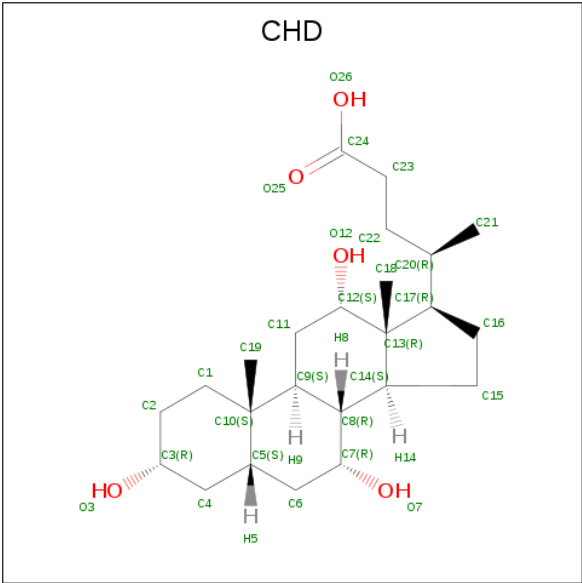
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



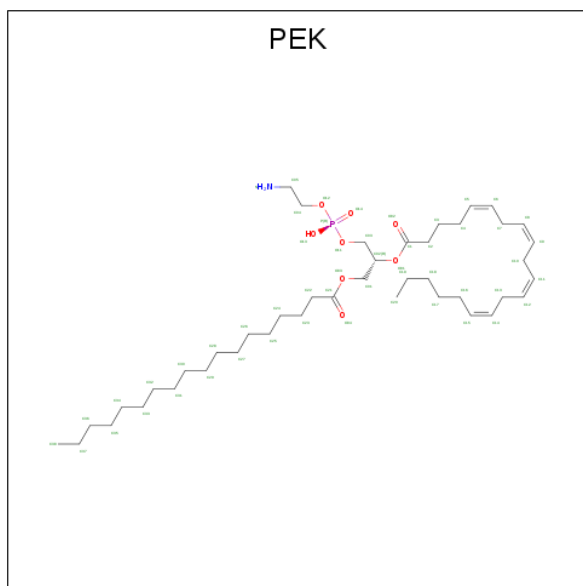
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 23 is (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).



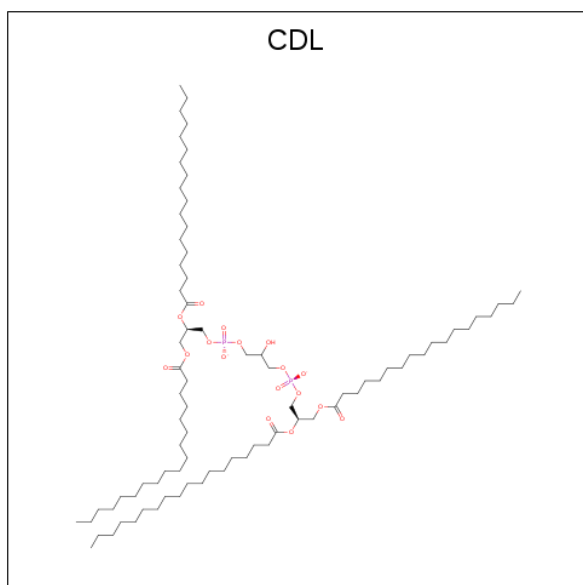
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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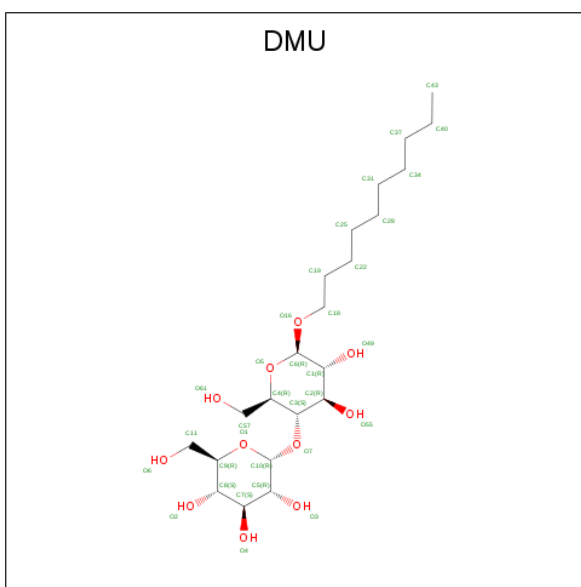
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



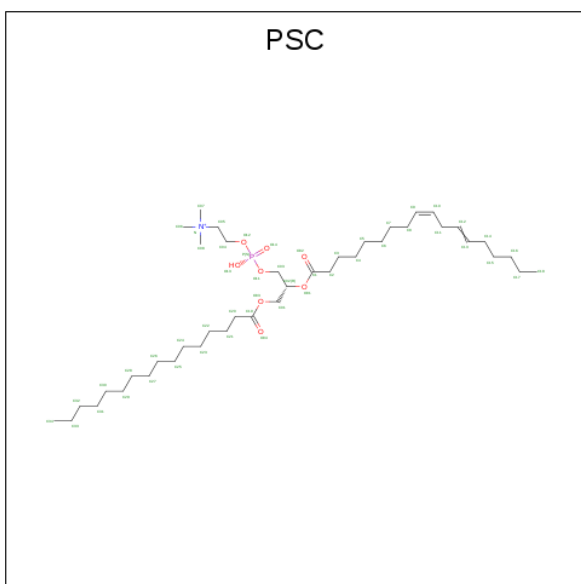
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	O	P		0	0
			100	81	17	2			
24	G	1	Total	C	O	P		0	0
			100	81	17	2			
24	P	1	Total	C	O	P		0	0
			100	81	17	2			
24	T	1	Total	C	O	P		0	0
			100	81	17	2			

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 26 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: $C_{42}H_{81}NO_8P$).



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

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	270	Total	O	0	0
			270	270		
28	B	206	Total	O	0	0
			206	206		
28	C	145	Total	O	0	0
			145	145		
28	D	167	Total	O	0	0
			167	167		
28	E	113	Total	O	0	0
			113	113		
28	F	137	Total	O	0	0
			137	137		
28	G	77	Total	O	0	0
			77	77		
28	H	83	Total	O	0	0
			83	83		
28	I	50	Total	O	0	0
			50	50		
28	J	42	Total	O	0	0
			42	42		
28	K	44	Total	O	0	0
			44	44		
28	L	36	Total	O	0	0
			36	36		
28	M	28	Total	O	0	0
			28	28		
28	N	266	Total	O	0	0
			266	266		

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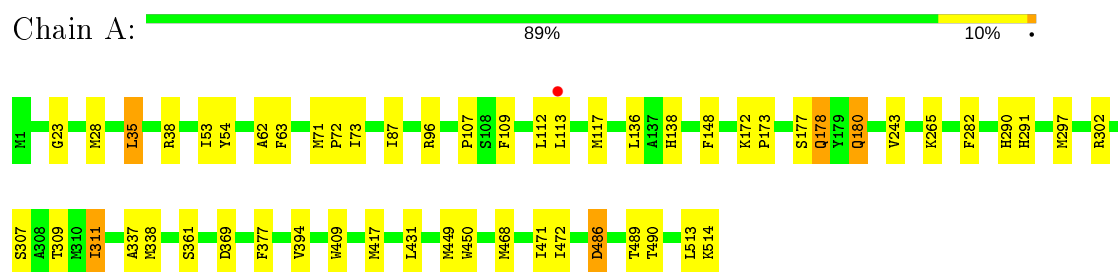
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	O	168	Total 168	O 168	0	0
28	P	138	Total 138	O 138	0	0
28	Q	84	Total 84	O 84	0	0
28	R	91	Total 91	O 91	0	0
28	S	126	Total 126	O 126	0	0
28	T	62	Total 62	O 62	0	0
28	U	68	Total 68	O 68	0	0
28	V	41	Total 41	O 41	0	0
28	W	44	Total 44	O 44	0	0
28	X	28	Total 28	O 28	0	0
28	Y	24	Total 24	O 24	0	0
28	Z	20	Total 20	O 20	0	0

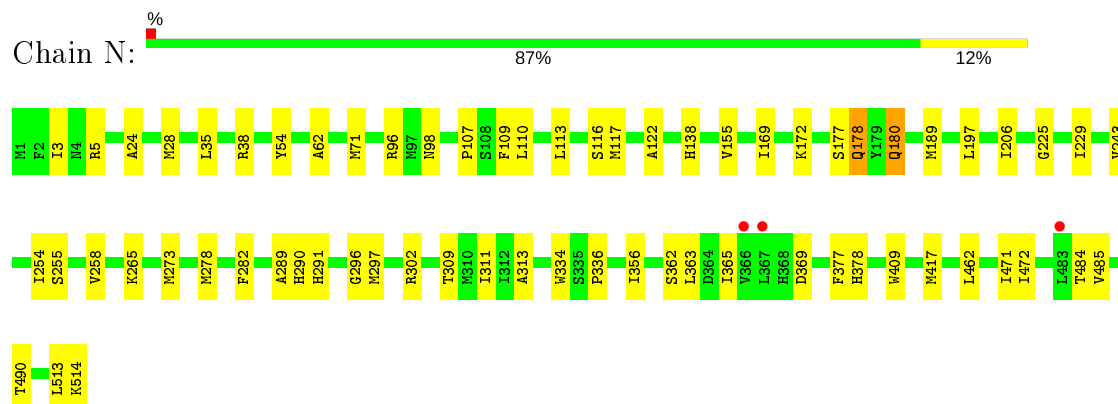
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

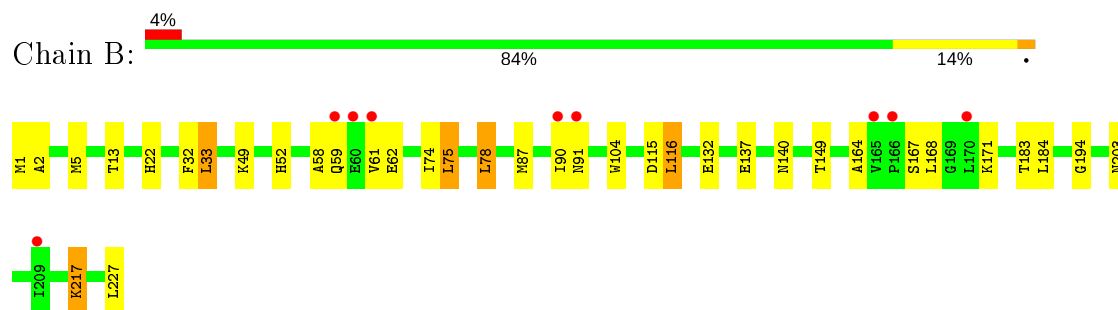
- Molecule 1: Cytochrome c oxidase subunit 1



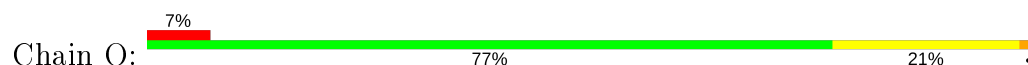
- Molecule 1: Cytochrome c oxidase subunit 1

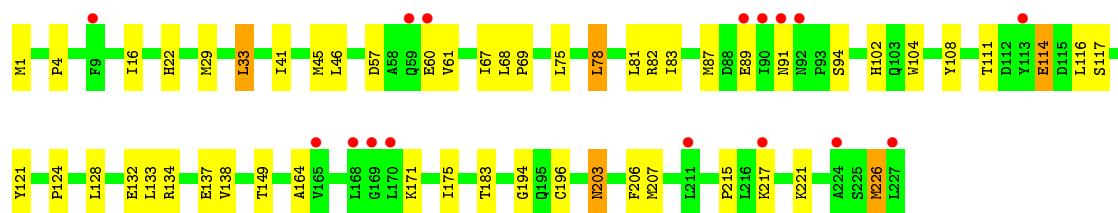


- Molecule 2: Cytochrome c oxidase subunit 2

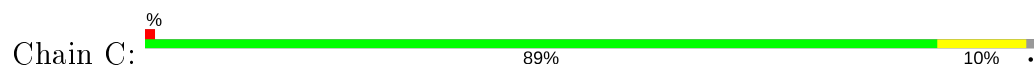


- Molecule 2: Cytochrome c oxidase subunit 2

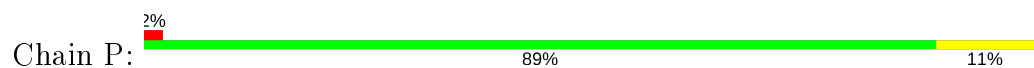




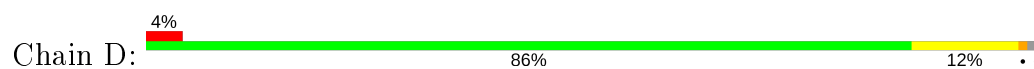
• Molecule 3: Cytochrome c oxidase subunit 3



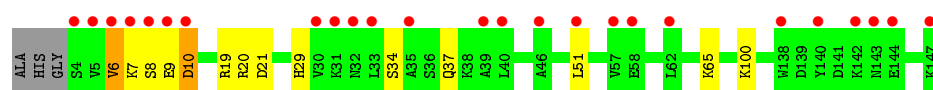
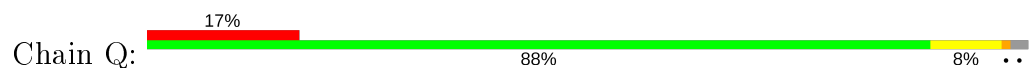
• Molecule 3: Cytochrome c oxidase subunit 3



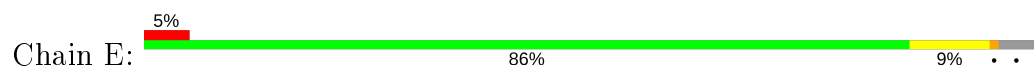
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



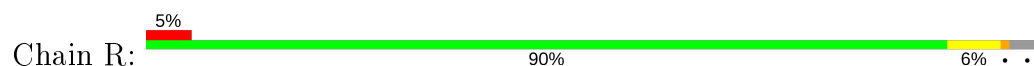
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

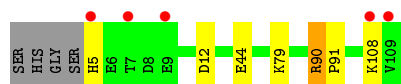


• Molecule 5: Cytochrome c oxidase subunit 5A

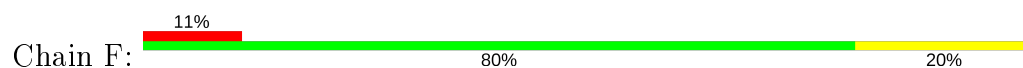


• Molecule 5: Cytochrome c oxidase subunit 5A

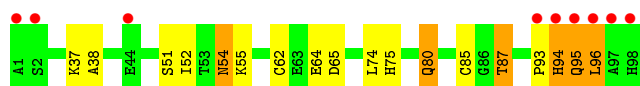
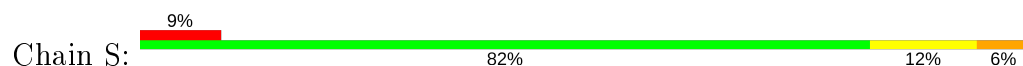




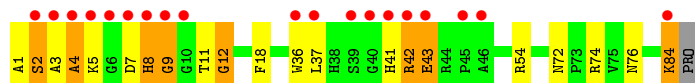
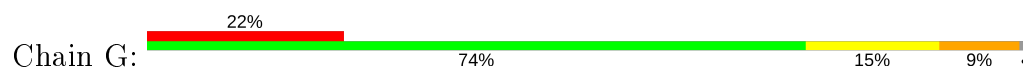
- Molecule 6: Cytochrome c oxidase subunit 5B



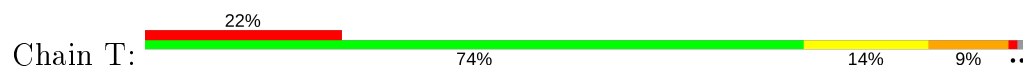
- Molecule 6: Cytochrome c oxidase subunit 5B



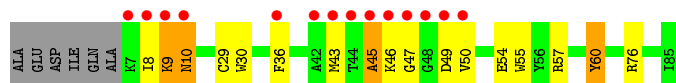
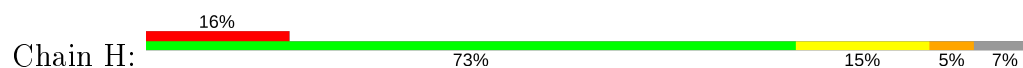
- Molecule 7: Cytochrome c oxidase subunit 6A2



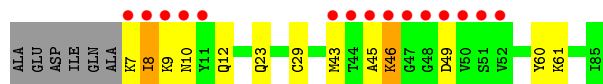
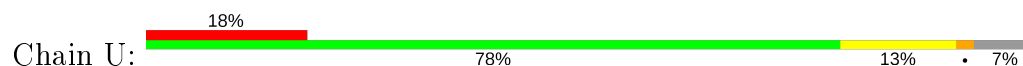
- Molecule 7: Cytochrome c oxidase subunit 6A2



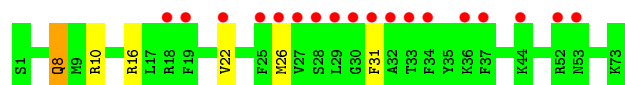
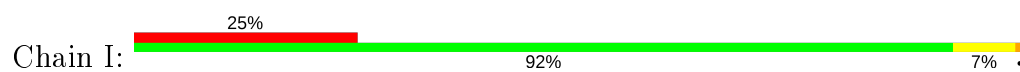
- Molecule 8: Cytochrome c oxidase subunit 6B1



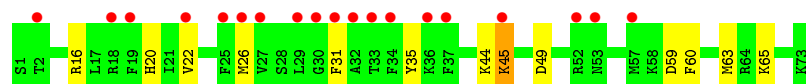
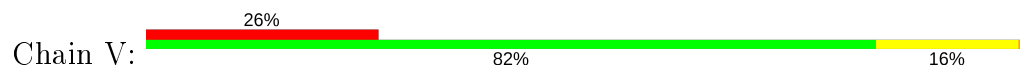
- Molecule 8: Cytochrome c oxidase subunit 6B1



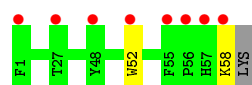
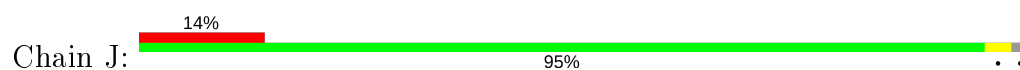
- Molecule 9: Cytochrome c oxidase subunit 6C



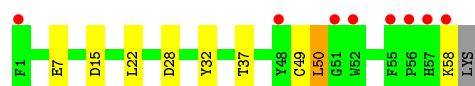
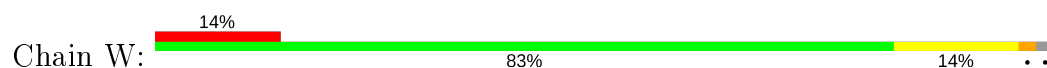
• Molecule 9: Cytochrome c oxidase subunit 6C



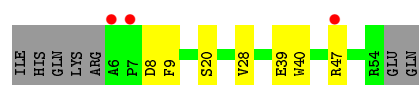
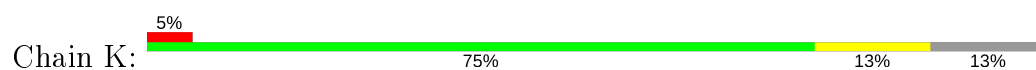
• Molecule 10: Cytochrome c oxidase subunit 7A1



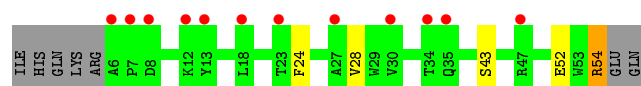
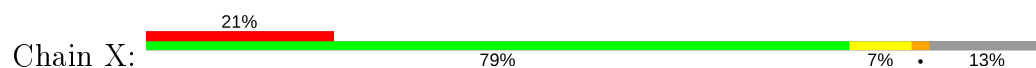
• Molecule 10: Cytochrome c oxidase subunit 7A1



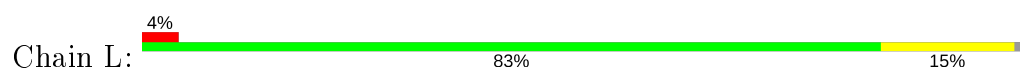
• Molecule 11: Cytochrome c oxidase subunit 7B




• Molecule 11: Cytochrome c oxidase subunit 7B

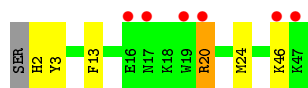


• Molecule 12: Cytochrome c oxidase subunit 7C




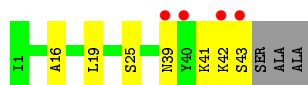
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:  13% 85% 11% ..




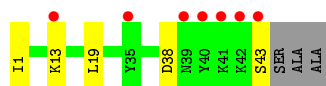
• Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:  9% 78% 15% 7%



• Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:  15% 83% 11% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.02Å 203.54Å 177.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 36.37 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (40.00-1.90) 98.1 (36.37-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.172 , 0.199 0.174 , 0.225	Depositor DCC
R_{free} test set	33115 reflections (6.58%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33893	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: ZN, TPO, CHD, TGL, CDL, PSC, PEK, MG, PER, PGV, SAC, DMU, CUA, NA, FME, CU, HEA

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	0.83	0/4253	0.78	3/5805 (0.1%)
1	N	0.77	0/4252	0.76	3/5804 (0.1%)
2	B	0.74	0/1906	0.82	1/2595 (0.0%)
2	O	0.63	0/1908	0.78	1/2599 (0.0%)
3	C	0.75	0/2261	0.68	0/3090
3	P	0.72	0/2260	0.67	0/3088
4	D	0.66	0/1284	0.80	3/1730 (0.2%)
4	Q	0.52	0/1237	0.66	0/1668
5	E	0.65	0/882	0.66	0/1196
5	R	0.55	0/871	0.68	1/1182 (0.1%)
6	F	0.67	0/806	0.80	0/1093
6	S	0.69	0/772	0.79	1/1048 (0.1%)
7	G	0.72	0/702	0.77	1/953 (0.1%)
7	T	0.67	0/724	0.85	3/984 (0.3%)
8	H	0.66	0/682	0.70	0/921
8	U	0.63	0/682	0.67	0/921
9	I	0.62	0/605	0.69	0/802
9	V	0.53	0/613	0.66	0/812
10	J	0.54	0/471	0.61	0/636
10	W	0.55	0/471	0.66	0/636
11	K	0.65	0/405	0.66	0/556
11	X	0.53	0/405	0.55	0/556
12	L	0.73	0/393	0.69	0/526
12	Y	0.65	0/393	0.60	0/526
13	M	0.64	0/345	0.67	0/470
13	Z	0.60	0/345	0.61	0/470
All	All	0.70	0/29928	0.73	17/40667 (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
6	F	0	1
6	S	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	-12.07	114.27	120.30
4	D	20	ARG	NE-CZ-NH1	10.37	125.49	120.30
7	T	17	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	35	LEU	CA-CB-CG	-9.63	93.15	115.30
1	A	96	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	N	71	MET	CG-SD-CE	-7.33	88.48	100.20
6	S	94	HIS	N-CA-C	6.12	127.51	111.00
7	G	12	GLY	N-CA-C	5.99	128.07	113.10
4	D	26	ASP	CB-CG-OD1	5.64	123.37	118.30
1	N	5	ARG	NE-CZ-NH2	-5.61	117.50	120.30
7	T	12	GLY	N-CA-C	5.60	127.09	113.10
2	B	116	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	486	ASP	CB-CG-OD2	5.26	123.04	118.30
1	N	96	ARG	NE-CZ-NH2	-5.22	117.69	120.30
5	R	90	ARG	NE-CZ-NH2	-5.22	117.69	120.30
7	T	7	ASP	N-CA-C	5.14	124.88	111.00
2	O	82	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
6	S	93	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4124	0	4102	57	0
1	N	4123	0	4098	74	0
2	B	1868	0	1864	27	0
2	O	1870	0	1867	37	0
3	C	2174	0	2082	32	0
3	P	2173	0	2083	30	0
4	D	1249	0	1242	27	1
4	Q	1203	0	1191	10	0
5	E	863	0	857	8	0
5	R	852	0	845	3	0
6	F	789	0	769	22	0
6	S	755	0	734	17	0
7	G	686	0	651	32	0
7	T	706	0	664	27	0
8	H	662	0	623	15	0
8	U	662	0	623	13	0
9	I	601	0	613	7	0
9	V	609	0	621	12	0
10	J	460	0	459	2	0
10	W	460	0	459	8	0
11	K	391	0	374	7	0
11	X	391	0	374	6	0
12	L	380	0	380	8	0
12	Y	380	0	380	9	0
13	M	335	0	352	9	0
13	Z	335	0	352	2	0
14	A	120	0	108	14	0
14	N	120	0	108	14	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	102	0	152	16	0
18	C	102	0	152	3	0
18	N	102	0	152	8	0
18	P	102	0	152	8	0
19	A	4	0	0	3	0
19	N	4	0	0	2	0
20	B	63	0	110	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	63	0	110	11	0
20	L	63	0	110	11	0
20	N	126	0	220	10	0
20	Q	63	0	110	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	1	0
22	C	58	0	78	1	0
22	J	29	0	38	0	0
22	N	29	0	39	1	0
22	O	29	0	39	1	0
22	P	29	0	39	1	0
22	W	29	0	39	5	0
23	C	106	0	154	21	0
23	G	53	0	77	7	0
23	P	53	0	77	11	0
23	T	106	0	154	8	0
24	C	100	0	156	13	0
24	G	100	0	156	17	0
24	P	100	0	156	10	0
24	T	100	0	156	20	0
25	C	33	0	42	6	0
25	M	33	0	42	0	0
25	P	33	0	42	4	0
25	Z	33	0	42	1	0
26	E	52	0	80	7	0
26	R	52	0	80	6	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	270	0	0	9	0
28	B	206	0	0	13	2
28	C	145	0	0	4	0
28	D	167	0	0	10	1
28	E	113	0	0	1	0
28	F	137	0	0	6	0
28	G	77	0	0	3	0
28	H	83	0	0	2	0
28	I	50	0	0	0	0
28	J	42	0	0	0	0
28	K	44	0	0	2	0
28	L	36	0	0	0	0
28	M	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	N	266	0	0	16	0
28	O	168	0	0	4	0
28	P	138	0	0	8	0
28	Q	84	0	0	0	0
28	R	91	0	0	2	0
28	S	126	0	0	1	0
28	T	62	0	0	2	0
28	U	68	0	0	3	0
28	V	41	0	0	1	0
28	W	44	0	0	2	0
28	X	28	0	0	0	0
28	Y	24	0	0	1	0
28	Z	20	0	0	0	0
All	All	33893	0	31868	544	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (544) 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)
4:D:4:SER:HB3	28:D:389:HOH:O	1.32	1.26
23:P:302:PEK:H383	24:T:103:CDL:C27	1.65	1.25
6:F:53:THR:HB	28:F:201:HOH:O	1.14	1.24
19:N:607[B]:PER:O2	19:N:607[B]:PER:O1	1.55	1.23
19:N:607[A]:PER:O2	19:N:607[A]:PER:O1	1.55	1.22
19:A:607[B]:PER:O2	19:A:607[B]:PER:O1	1.55	1.21
19:A:607[A]:PER:O2	19:A:607[A]:PER:O1	1.55	1.21
1:A:297[B]:MET:HB3	28:A:833:HOH:O	1.38	1.20
1:A:486:ASP:OD1	4:D:19[A]:ARG:HD2	1.45	1.14
20:L:101:TGL:HC41	20:L:101:TGL:OC1	1.45	1.11
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	1.91	1.11
20:D:201:TGL:HG31	28:D:392:HOH:O	1.48	1.11
24:T:103:CDL:HA21	24:T:103:CDL:H111	1.33	1.09
23:P:302:PEK:C38	24:T:103:CDL:H273	1.81	1.09
8:H:9:LYS:HD3	8:H:10:ASN:H	0.96	1.09
18:P:303:PGV:H172	24:P:305:CDL:H632	1.27	1.06
2:O:124:PRO:HB2	28:O:401:HOH:O	1.51	1.06
8:U:9:LYS:HG3	8:U:10:ASN:H	1.18	1.02
3:P:3:HIS:HB3	28:P:506:HOH:O	1.59	1.02
23:P:302:PEK:H383	24:T:103:CDL:H273	1.06	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:57:ASP:H	26:R:201:PSC:H211	1.25	1.00
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG2	2.02	1.00
1:N:297[B]:MET:CG	1:N:302[B]:ARG:HG3	1.90	0.99
1:N:258:VAL:N	28:N:701:HOH:O	1.96	0.99
3:C:33:MET:HE1	3:C:42:LEU:H	1.25	0.98
1:N:296:GLY:HA2	8:U:23:GLN:HE21	1.25	0.98
8:H:9:LYS:HD3	8:H:10:ASN:N	1.80	0.96
6:F:85:CYS:SG	6:F:87:THR:HG23	2.06	0.96
5:E:14[B]:ARG:O	5:E:14[B]:ARG:HD2	1.66	0.95
1:N:296:GLY:HA2	8:U:23:GLN:NE2	1.81	0.95
1:N:297[B]:MET:SD	1:N:302[B]:ARG:CG	2.55	0.94
3:P:157:LYS:NZ	23:P:302:PEK:H051	1.82	0.93
26:E:201:PSC:H071	9:I:10:ARG:HH21	1.33	0.92
7:T:72:ASN:H	7:T:76:ASN:HD22	1.17	0.92
28:N:883:HOH:O	2:O:87:MET:SD	2.27	0.92
1:A:486:ASP:OD1	4:D:19[A]:ARG:CD	2.19	0.90
3:P:157:LYS:HZ1	23:P:302:PEK:H051	1.34	0.90
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.33	0.90
24:G:101:CDL:H352	2:O:78:LEU:HD12	1.51	0.90
12:L:20:ARG:NH2	20:L:101:TGL:HC52	1.86	0.88
1:A:472:ILE:HG21	20:L:101:TGL:HA91	1.55	0.87
4:D:19[B]:ARG:HG2	4:D:21:ASP:OD1	1.74	0.87
23:C:303:PEK:C38	24:G:101:CDL:H273	2.05	0.86
1:N:297[B]:MET:HG2	1:N:302[B]:ARG:HG3	1.57	0.85
7:G:5:LYS:HG3	23:G:102:PEK:H351	1.58	0.85
23:C:303:PEK:H222	23:C:303:PEK:H32	1.59	0.84
28:B:596:HOH:O	26:E:201:PSC:H282	1.78	0.84
1:N:28:MET:HE1	14:N:601:HEA:C27	2.08	0.83
8:H:9:LYS:CD	8:H:10:ASN:H	1.88	0.83
2:B:59:GLN:HG2	28:P:496:HOH:O	1.79	0.83
1:N:206:ILE:HD11	28:N:933:HOH:O	1.78	0.83
8:U:9:LYS:CG	8:U:10:ASN:H	1.87	0.83
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.27	0.82
18:A:608:PGV:H342	23:C:302:PEK:H382	1.60	0.82
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.62	0.82
23:C:303:PEK:H383	24:G:101:CDL:H273	1.62	0.82
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.60	0.82
9:V:65:LYS:O	11:X:54:ARG:NH1	2.12	0.82
1:N:255:SER:O	28:N:701:HOH:O	1.97	0.81
1:A:113[B]:LEU:CD2	1:A:117[B]:MET:SD	2.69	0.81
4:D:78:TRP:CA	20:D:201:TGL:HB22	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:14[B]:ARG:C	5:E:14[B]:ARG:HD2	2.01	0.80
18:P:303:PGV:C17	24:P:305:CDL:H632	2.12	0.79
7:G:72:ASN:H	7:G:76:ASN:HD22	1.29	0.79
6:S:52:ILE:HA	6:S:94:HIS:HB3	1.65	0.79
1:A:112:LEU:HD13	28:A:801:HOH:O	1.82	0.79
1:N:28:MET:CE	14:N:601:HEA:C27	2.61	0.79
28:A:913:HOH:O	2:B:87:MET:SD	2.39	0.79
24:T:103:CDL:H781	24:T:103:CDL:H561	1.64	0.78
9:V:45:LYS:HD3	9:V:49:ASP:OD2	1.83	0.78
7:G:5:LYS:NZ	28:G:201:HOH:O	2.16	0.78
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.66	0.78
6:F:75:HIS:H	6:F:80[B]:GLN:HE22	1.32	0.78
3:C:188[B]:ILE:HD13	3:C:198:PHE:HB2	1.65	0.77
7:T:76:ASN:HD21	23:T:102:PEK:HN2	1.29	0.77
23:C:302:PEK:HN2	7:G:76:ASN:HD21	1.32	0.77
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG3	2.22	0.77
23:T:101:PEK:H361	24:T:103:CDL:H861	1.67	0.76
6:S:75:HIS:H	6:S:80:GLN:HE22	1.32	0.76
1:N:28:MET:CE	14:N:601:HEA:H271	2.16	0.76
1:A:513:LEU:O	1:A:514:LYS:HB2	1.86	0.76
1:A:311[B]:ILE:HG22	24:T:103:CDL:H421	1.67	0.75
1:N:365:ILE:HD11	28:N:729:HOH:O	1.86	0.75
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.15	0.75
2:O:183:THR:HG23	28:O:541:HOH:O	1.87	0.75
4:D:19[B]:ARG:CG	4:D:21:ASP:OD1	2.34	0.75
23:P:302:PEK:H383	24:T:103:CDL:H272	1.66	0.75
4:D:31:LYS:HD2	28:D:452:HOH:O	1.87	0.74
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.18	0.74
1:N:273:MET:HE2	28:N:776:HOH:O	1.87	0.73
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	1.70	0.73
12:L:20:ARG:HH21	20:L:101:TGL:HC32	1.52	0.73
18:N:606:PGV:H012	18:N:606:PGV:H222	1.70	0.73
3:P:40[B]:MET:O	3:P:44[B]:MET:HG3	1.88	0.73
11:X:54:ARG:NH2	11:X:54:ARG:HG3	1.96	0.73
1:A:113[B]:LEU:HD21	1:A:117[B]:MET:SD	2.28	0.73
6:F:92[A]:VAL:HG23	6:F:92[A]:VAL:O	1.88	0.73
20:N:611:TGL:HC32	12:Y:20:ARG:HH21	1.55	0.72
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.71	0.72
4:D:34:SER:H	4:D:37:GLN:HE21	1.38	0.72
12:L:14:SER:H	20:L:101:TGL:HC31	1.55	0.71
20:Q:201:TGL:H362	9:V:20:HIS:HE1	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:MET:CE	14:A:601:HEA:C27	2.67	0.71
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.73	0.71
18:A:608:PGV:C34	23:C:302:PEK:H382	2.20	0.71
26:E:201:PSC:C07	9:I:10:ARG:HH21	2.04	0.71
26:R:201:PSC:H011	26:R:201:PSC:O02	1.90	0.71
18:A:606:PGV:H292	13:M:16:ALA:HA	1.73	0.70
24:C:306:CDL:H212	24:C:306:CDL:H632	1.72	0.70
4:D:78:TRP:HA	20:D:201:TGL:HB22	1.72	0.70
23:P:302:PEK:H203	7:T:36[A]:TRP:HE1	1.55	0.70
24:T:103:CDL:H522	24:T:103:CDL:HB61	1.73	0.70
20:L:101:TGL:CC4	20:L:101:TGL:OC1	2.30	0.70
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.05	0.69
1:A:113[B]:LEU:HD22	1:A:117[B]:MET:SD	2.32	0.69
1:A:136[B]:LEU:HD11	28:A:963:HOH:O	1.92	0.69
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.75	0.68
1:A:28:MET:CE	14:A:601:HEA:H271	2.23	0.68
1:N:254:ILE:O	28:N:701:HOH:O	2.11	0.68
2:B:91:ASN:HB3	2:B:149:THR:HG21	1.76	0.68
18:N:606:PGV:H041	18:N:606:PGV:H02	1.75	0.68
18:A:606:PGV:H301	18:A:606:PGV:H181	1.75	0.68
2:O:57:ASP:N	26:R:201:PSC:H211	2.06	0.67
20:Q:201:TGL:HB51	20:Q:201:TGL:HA22	1.75	0.67
23:C:303:PEK:H052	6:F:1:ALA:H2	1.60	0.67
1:A:468:MET:HG3	28:A:942:HOH:O	1.93	0.67
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.91	0.67
2:B:49:LYS:HE2	28:D:441:HOH:O	1.94	0.67
4:D:78:TRP:HB3	20:D:201:TGL:HB22	1.75	0.67
8:U:9:LYS:HG3	8:U:10:ASN:N	2.02	0.67
4:D:78:TRP:CB	20:D:201:TGL:HB22	2.24	0.66
1:A:28:MET:HE1	14:A:601:HEA:C27	2.25	0.66
6:F:54[B]:ASN:ND2	28:F:201:HOH:O	2.07	0.66
1:N:297[B]:MET:HG2	1:N:302[B]:ARG:CG	2.25	0.66
7:T:5:LYS:NZ	28:T:201:HOH:O	2.23	0.66
8:U:9:LYS:CG	8:U:10:ASN:N	2.59	0.66
20:Q:201:TGL:H362	9:V:20:HIS:CE1	2.30	0.66
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.31	0.65
24:T:103:CDL:CA2	24:T:103:CDL:H111	2.21	0.65
20:N:611:TGL:HC32	12:Y:20:ARG:NH2	2.11	0.65
18:A:608:PGV:H183	23:C:302:PEK:H322	1.79	0.64
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.79	0.64
5:E:90:ARG:HD2	28:E:380:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:85:CYS:SG	6:S:87[A]:THR:CG2	2.80	0.64
7:T:12:GLY:HA3	28:T:240:HOH:O	1.97	0.64
7:T:8:HIS:CG	7:T:9:GLY:H	2.16	0.64
3:C:131:LEU:HD21	24:G:101:CDL:HB4	1.79	0.64
3:C:33:MET:HB2	25:C:309:DMU:C25	2.28	0.64
6:S:85:CYS:SG	6:S:87[B]:THR:HG22	2.38	0.64
1:N:297[B]:MET:CG	1:N:302[B]:ARG:CG	2.70	0.64
7:G:84:LYS:NZ	7:G:84:LYS:H	1.96	0.64
1:N:513:LEU:O	1:N:514:LYS:HB2	1.98	0.64
23:P:302:PEK:C38	24:T:103:CDL:C27	2.54	0.63
6:F:92[A]:VAL:HG21	28:F:328:HOH:O	1.99	0.63
7:G:9:GLY:CA	1:N:178:GLN:HE21	2.11	0.62
1:N:417[A]:MET:CE	28:N:889:HOH:O	2.46	0.62
4:Q:19:ARG:CG	4:Q:21:ASP:OD1	2.47	0.62
7:T:72:ASN:H	7:T:76:ASN:ND2	1.95	0.62
4:D:4:SER:HA	28:D:383:HOH:O	1.99	0.62
7:T:2:SER:HB2	23:T:101:PEK:H281	1.82	0.62
23:C:303:PEK:C05	6:F:1:ALA:N	2.61	0.62
2:O:89:GLU:O	2:O:91:ASN:ND2	2.32	0.62
2:O:91:ASN:HB3	2:O:149:THR:HG21	1.80	0.62
3:P:3:HIS:HA	28:P:513:HOH:O	1.99	0.61
18:A:606:PGV:H291	13:M:19:LEU:CD2	2.31	0.61
4:D:100:LYS:HE2	28:D:312:HOH:O	1.99	0.61
24:T:103:CDL:H511	24:T:103:CDL:H212	1.82	0.61
18:A:606:PGV:O02	18:A:606:PGV:P	2.58	0.61
24:G:101:CDL:H662	18:P:304:PGV:H171	1.81	0.61
6:S:94:HIS:CD2	6:S:95:GLN:O	2.53	0.61
2:B:22[B]:HIS:HD2	28:B:521:HOH:O	1.82	0.60
2:O:83:ILE:O	2:O:87:MET:HG3	2.00	0.60
1:N:28:MET:HE1	14:N:601:HEA:H273	1.83	0.60
23:C:303:PEK:H051	6:F:1:ALA:H1	1.65	0.60
12:L:20:ARG:HH22	20:L:101:TGL:HC52	1.66	0.60
1:N:113[A]:LEU:HD12	20:N:611:TGL:H291	1.84	0.60
1:N:255:SER:C	28:N:701:HOH:O	2.38	0.60
18:A:606:PGV:H291	13:M:19:LEU:HD23	1.82	0.60
6:F:54[B]:ASN:ND2	28:F:202:HOH:O	2.35	0.60
24:G:101:CDL:H212	1:N:311:ILE:HD12	1.83	0.60
8:U:61:LYS:HE3	28:U:122:HOH:O	2.01	0.60
2:B:217:LYS:HE2	28:B:578:HOH:O	2.02	0.60
7:G:72:ASN:H	7:G:76:ASN:ND2	2.00	0.59
2:B:164:ALA:O	2:B:194:GLY:HA3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:201:TGL:H352	9:V:16:ARG:HE	1.67	0.59
3:P:59:ARG:HA	24:P:305:CDL:H512	1.84	0.59
3:C:55:TYR:CE1	24:C:306:CDL:H511	2.38	0.59
1:A:177:SER:H	1:A:180:GLN:HE21	1.51	0.59
6:F:64:GLU:O	6:F:65:ASP:HB2	2.01	0.58
12:L:20:ARG:HH21	20:L:101:TGL:HC52	1.68	0.58
8:U:43:MET:HE3	8:U:49:ASP:N	2.18	0.58
6:S:64:GLU:O	6:S:65:ASP:HB2	2.02	0.58
18:A:608:PGV:C18	23:C:302:PEK:H322	2.34	0.58
3:C:33:MET:HB2	25:C:309:DMU:C22	2.34	0.58
18:C:305:PGV:H131	24:T:103:CDL:H651	1.85	0.58
18:N:606:PGV:H311	13:Z:19:LEU:HD23	1.85	0.58
23:C:303:PEK:H052	6:F:1:ALA:N	2.18	0.57
7:T:8:HIS:CG	7:T:9:GLY:N	2.72	0.57
3:C:224:LYS:CD	24:C:306:CDL:HB32	2.35	0.57
22:W:101:CHD:O12	22:W:101:CHD:H222	2.05	0.57
1:A:63:PHE:HB3	28:A:854:HOH:O	2.04	0.57
18:P:303:PGV:H182	24:P:305:CDL:H651	1.86	0.57
23:C:303:PEK:H031	28:C:426:HOH:O	2.03	0.57
7:G:3:ALA:O	7:G:4:ALA:CB	2.52	0.57
1:N:514:LYS:HA	6:S:38:ALA:CB	2.33	0.57
3:P:157:LYS:HZ2	23:P:302:PEK:H051	1.66	0.57
1:A:177:SER:H	1:A:180:GLN:NE2	2.03	0.56
2:B:183:THR:HG23	28:B:567:HOH:O	2.05	0.56
7:G:3:ALA:O	7:G:4:ALA:HB2	2.05	0.56
8:U:7:LYS:O	8:U:8:ILE:HB	2.05	0.56
24:G:101:CDL:H851	23:G:102:PEK:H361	1.87	0.56
1:A:28:MET:HE2	14:A:601:HEA:C27	2.36	0.56
1:N:169[A]:ILE:HD11	1:N:189:MET:SD	2.45	0.56
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.88	0.56
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.41	0.56
18:P:304:PGV:H032	28:P:488:HOH:O	2.04	0.56
7:T:2:SER:CB	23:T:101:PEK:H281	2.36	0.56
24:G:101:CDL:H212	1:N:311:ILE:CD1	2.36	0.56
7:T:37:LEU:HD23	24:T:103:CDL:H361	1.86	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.06	0.56
4:Q:19:ARG:HG3	4:Q:21:ASP:OD1	2.06	0.55
24:C:306:CDL:H192	28:C:541:HOH:O	2.06	0.55
8:H:43:MET:HE3	8:H:49:ASP:N	2.21	0.55
11:X:24:PHE:O	11:X:28[B]:VAL:HG23	2.05	0.55
3:P:33:MET:HE1	3:P:42:LEU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:54:ASN:HD22	6:S:54:ASN:C	2.10	0.55
18:A:606:PGV:O02	18:A:606:PGV:O14	2.24	0.55
2:B:61:VAL:HG11	28:B:596:HOH:O	2.07	0.55
3:C:51[A]:MET:SD	3:C:54[A]:MET:CE	2.95	0.55
11:K:39:GLU:HB3	28:K:123:HOH:O	2.05	0.55
9:V:45:LYS:HD2	28:V:113:HOH:O	2.07	0.55
2:B:140:ASN:HB3	28:B:504:HOH:O	2.06	0.55
3:P:157:LYS:O	3:P:161:GLN:HG3	2.07	0.55
6:S:51:SER:O	6:S:94:HIS:HB3	2.07	0.55
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.89	0.54
26:R:201:PSC:H222	26:R:201:PSC:O02	2.07	0.54
10:W:37:THR:OG1	22:W:101:CHD:H5	2.07	0.54
7:G:12:GLY:HA3	28:G:249:HOH:O	2.07	0.54
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.88	0.54
23:C:303:PEK:C22	23:C:303:PEK:H32	2.33	0.54
6:F:30:PRO:O	6:F:96:LEU:HD11	2.08	0.54
8:U:43:MET:HE3	8:U:49:ASP:H	1.73	0.53
23:C:303:PEK:C05	6:F:1:ALA:H1	2.20	0.53
3:C:33:MET:HE1	3:C:42:LEU:N	2.08	0.53
24:G:101:CDL:H222	24:G:101:CDL:H511	1.90	0.53
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.89	0.53
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.90	0.53
3:P:3:HIS:HD2	28:P:513:HOH:O	1.92	0.53
1:A:28:MET:HE2	14:A:601:HEA:H273	1.90	0.53
1:A:112:LEU:HD11	28:A:938:HOH:O	2.08	0.53
18:N:606:PGV:C22	18:N:606:PGV:H012	2.37	0.53
3:P:224:LYS:HE3	24:P:305:CDL:HB32	1.90	0.53
1:A:28:MET:HE1	14:A:601:HEA:H271	1.89	0.53
6:F:92[A]:VAL:CG2	6:F:92[A]:VAL:O	2.56	0.53
7:G:3:ALA:CB	23:G:102:PEK:H362	2.39	0.53
5:E:12:ASP:OD2	5:E:44:GLU:HG3	2.08	0.52
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.90	0.52
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.92	0.52
12:Y:2:HIS:CD2	12:Y:3:TYR:H	2.26	0.52
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.45	0.52
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.90	0.52
4:D:58:GLU:HG3	28:D:301:HOH:O	2.09	0.52
24:G:101:CDL:H351	2:O:81:LEU:HD12	1.91	0.52
26:E:201:PSC:H02	26:E:201:PSC:H212	1.91	0.52
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.40	0.52
1:N:334:TRP:HZ3	20:Q:201:TGL:HA51	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:103:CDL:H531	24:T:103:CDL:H231	1.90	0.52
12:Y:2:HIS:CG	12:Y:3:TYR:H	2.27	0.52
4:D:34:SER:H	4:D:37:GLN:NE2	2.07	0.51
1:A:409:TRP:HB3	1:A:471:ILE:HG12	1.91	0.51
2:O:164:ALA:O	2:O:194:GLY:HA3	2.10	0.51
8:H:50:VAL:HG23	28:H:147:HOH:O	2.11	0.51
2:O:1:FME:HE1	2:O:133:LEU:HD13	1.91	0.51
7:G:2:SER:OG	23:G:102:PEK:H291	2.11	0.51
20:D:201:TGL:H342	9:I:16:ARG:HE	1.76	0.51
24:G:101:CDL:C85	23:G:102:PEK:H361	2.40	0.51
7:G:42:ARG:NH1	7:G:42:ARG:HA	2.26	0.51
1:N:28:MET:CE	14:N:601:HEA:H273	2.39	0.51
2:O:41:ILE:HG21	26:R:201:PSC:H332	1.93	0.51
24:P:305:CDL:H622	24:P:305:CDL:H182	1.92	0.51
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.26	0.51
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.50
25:C:309:DMU:H4	10:J:52:TRP:CZ2	2.46	0.50
12:L:2:HIS:CG	12:L:3:TYR:H	2.29	0.50
12:Y:2:HIS:CG	28:Y:122:HOH:O	2.64	0.50
14:A:601:HEA:HBC1	14:A:601:HEA:HMC1	1.92	0.50
5:E:86:ILE:O	5:E:90:ARG:HG2	2.12	0.50
3:P:5:THR:HG22	6:S:96:LEU:CD1	2.41	0.50
23:C:303:PEK:H051	6:F:1:ALA:N	2.27	0.50
2:B:52:HIS:HE1	26:E:201:PSC:H201	1.77	0.50
1:N:116:SER:HB3	28:N:757:HOH:O	2.12	0.50
7:G:5:LYS:HB2	23:G:102:PEK:H332	1.93	0.50
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.94	0.50
1:N:472:ILE:HG21	20:N:611:TGL:HA91	1.93	0.50
9:I:8:GLN:OE1	9:I:10:ARG:O	2.30	0.50
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.94	0.50
1:N:514:LYS:HD3	28:S:270:HOH:O	2.12	0.50
24:G:101:CDL:H381	24:G:101:CDL:H142	1.94	0.49
8:H:55:TRP:H	8:U:46:LYS:HZ3	1.59	0.49
3:P:62:ILE:HD12	24:P:305:CDL:H511	1.93	0.49
3:P:5:THR:HG22	6:S:96:LEU:HD11	1.94	0.49
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.94	0.49
3:C:33:MET:HB2	25:C:309:DMU:H13	1.94	0.49
24:G:101:CDL:H191	1:N:311:ILE:HD11	1.95	0.49
20:N:611:TGL:H152	12:Y:24:MET:SD	2.53	0.49
7:T:72:ASN:N	7:T:76:ASN:HD22	1.98	0.49
2:B:75:LEU:HB3	28:B:509:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:525:HOH:O	24:T:103:CDL:H331	2.13	0.49
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.11	0.49
1:N:177:SER:H	1:N:180:GLN:NE2	2.10	0.48
1:N:334:TRP:CZ3	20:Q:201:TGL:HA51	2.48	0.48
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.28	0.48
4:D:100:LYS:CE	28:D:312:HOH:O	2.59	0.48
6:F:87:THR:HG21	28:F:310:HOH:O	2.12	0.48
20:L:101:TGL:HC82	20:L:101:TGL:HC22	1.93	0.48
3:C:224:LYS:HD2	24:C:306:CDL:HB32	1.95	0.48
1:N:417[A]:MET:HE2	28:N:889:HOH:O	2.11	0.48
8:U:12:GLN:HB2	28:U:153:HOH:O	2.13	0.48
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.96	0.48
3:C:52:LEU:HD23	24:C:306:CDL:H362	1.95	0.48
1:N:3:ILE:HG21	22:W:101:CHD:H232	1.95	0.48
1:A:311[B]:ILE:CG2	24:T:103:CDL:H421	2.38	0.48
24:G:101:CDL:C51	24:G:101:CDL:H222	2.44	0.48
4:D:78:TRP:HA	20:D:201:TGL:CB2	2.42	0.48
22:O:301:CHD:H212	22:O:301:CHD:H12	1.96	0.48
28:N:860:HOH:O	4:Q:100:LYS:HE2	2.13	0.48
20:D:201:TGL:HA91	20:D:201:TGL:H242	1.96	0.47
4:D:58:GLU:CG	28:D:301:HOH:O	2.62	0.47
3:C:67:PHE:HE2	24:C:306:CDL:H1	1.78	0.47
1:N:309:THR:CG2	14:N:602:HEA:HMB2	2.43	0.47
22:B:303:CHD:H212	22:B:303:CHD:H12	1.95	0.47
23:C:303:PEK:H222	23:C:303:PEK:C3	2.38	0.47
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.97	0.47
25:P:307:DMU:H23	10:W:50:LEU:HG	1.96	0.47
2:O:203[B]:ASN:HD22	2:O:206:PHE:HD2	1.62	0.47
7:T:41:HIS:HB3	7:T:74:ARG:HH12	1.79	0.47
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.95	0.47
3:C:224:LYS:HE3	24:C:306:CDL:CB3	2.45	0.47
2:O:16:ILE:HD12	2:O:87:MET:HG2	1.96	0.47
6:S:95:GLN:NE2	6:S:95:GLN:HA	2.24	0.47
7:T:38:HIS:HE1	24:T:103:CDL:H122	1.79	0.47
3:C:76:GLN:NE2	28:C:401:HOH:O	2.40	0.47
4:D:81:VAL:HG11	20:D:201:TGL:HB52	1.97	0.47
7:G:5:LYS:HB3	1:N:278[B]:MET:HE1	1.95	0.47
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.96	0.47
3:P:3:HIS:CD2	28:P:513:HOH:O	2.67	0.47
7:G:84:LYS:HZ2	7:G:84:LYS:H	1.60	0.47
4:D:87[B]:PHE:HZ	11:K:20:SER:HG	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:609:PGV:H262	18:P:303:PGV:H292	1.97	0.47
23:C:303:PEK:H381	24:G:101:CDL:H273	1.94	0.47
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.13	0.47
28:B:532:HOH:O	23:P:302:PEK:H301	2.13	0.47
24:P:305:CDL:H672	28:P:529:HOH:O	2.14	0.47
18:A:608:PGV:H183	23:C:302:PEK:C32	2.44	0.47
3:C:127:LEU:HD21	22:N:610:CHD:H3	1.96	0.47
7:G:11:TPO:HA	7:G:11:TPO:O3P	2.14	0.47
10:W:15:ASP:OD2	28:W:201:HOH:O	2.20	0.47
25:P:307:DMU:H11	10:W:49:CYS:HB3	1.96	0.47
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.97	0.46
1:A:307:SER:O	1:A:311[A]:ILE:HG12	2.14	0.46
2:B:1:FME:HE2	2:B:2:ALA:O	2.14	0.46
24:G:101:CDL:H662	18:P:304:PGV:C17	2.46	0.46
3:C:188[B]:ILE:CD1	3:C:195:SER:HA	2.45	0.46
4:D:109:HIS:HD2	28:D:365:HOH:O	1.98	0.46
1:N:35:LEU:HB3	25:Z:101:DMU:H24	1.97	0.46
20:N:608:TGL:HA92	20:N:608:TGL:H142	1.97	0.46
7:G:84:LYS:HZ3	7:G:84:LYS:H	1.63	0.46
2:B:13:THR:OG1	2:B:167:SER:HB2	2.16	0.46
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.51	0.46
2:O:29:MET:HG3	9:V:35:TYR:CG	2.51	0.46
3:P:51[B]:MET:SD	24:P:305:CDL:H641	2.55	0.46
1:A:87:ILE:O	1:A:173:PRO:HD3	2.15	0.46
5:R:108:LYS:HB3	28:R:385:HOH:O	2.15	0.46
10:W:7:GLU:HG3	28:W:230:HOH:O	2.14	0.46
1:A:282:PHE:HA	7:T:4:ALA:CB	2.44	0.46
2:B:90:ILE:HG13	28:B:561:HOH:O	2.15	0.46
3:C:161[B]:GLN:HG3	28:C:524:HOH:O	2.15	0.46
11:K:47:ARG:HH11	11:K:47:ARG:HG2	1.81	0.46
3:P:160:LEU:HD13	22:P:306:CHD:H181	1.97	0.46
10:W:32:TYR:OH	22:W:101:CHD:H221	2.15	0.46
24:T:103:CDL:H821	24:T:103:CDL:H791	1.40	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.98	0.45
20:N:608:TGL:H272	20:N:608:TGL:H242	1.49	0.45
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.94	0.45
1:A:297[B]:MET:CB	28:A:833:HOH:O	2.21	0.45
3:C:51[A]:MET:SD	3:C:54[A]:MET:HE1	2.56	0.45
7:G:8:HIS:O	7:G:9:GLY:C	2.55	0.45
18:N:606:PGV:C04	18:N:606:PGV:H02	2.43	0.45
28:B:443:HOH:O	7:T:17:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:201:PSC:H21	28:R:382:HOH:O	2.16	0.45
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.98	0.45
20:L:101:TGL:HA92	20:L:101:TGL:H221	1.60	0.45
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.99	0.45
7:G:4:ALA:CB	1:N:282:PHE:HA	2.47	0.45
7:G:41:HIS:HB3	7:G:74:ARG:NH1	2.32	0.45
7:G:8:HIS:O	7:G:8:HIS:CD2	2.69	0.45
9:I:22:VAL:O	9:I:26:MET:HG2	2.17	0.45
1:N:309:THR:HG22	14:N:602:HEA:HMB2	1.98	0.45
10:W:32:TYR:CE2	22:W:101:CHD:H181	2.52	0.45
24:C:306:CDL:H842	24:C:306:CDL:H812	1.66	0.45
8:H:9:LYS:NZ	8:H:9:LYS:HA	2.32	0.45
22:C:307:CHD:H231	22:C:307:CHD:H162	1.98	0.45
3:P:33:MET:HE1	3:P:41:THR:HB	2.00	0.44
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.98	0.44
3:C:37:PHE:CG	25:C:309:DMU:H8	2.52	0.44
2:O:217:LYS:HD2	28:O:567:HOH:O	2.17	0.44
1:A:309:THR:HG22	14:A:602:HEA:HMB2	2.00	0.44
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.56	0.44
2:O:111:THR:HA	2:O:114:GLU:O	2.18	0.44
18:N:606:PGV:H05	28:N:939:HOH:O	2.17	0.44
2:O:104:TRP:CG	2:O:203[B]:ASN:HB2	2.53	0.44
28:B:443:HOH:O	7:T:17:ARG:CD	2.65	0.44
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	2.53	0.44
1:N:485:VAL:HG12	13:Z:1:ILE:HG13	1.99	0.44
25:C:309:DMU:H9	25:C:309:DMU:H15	1.83	0.44
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.17	0.44
2:B:227:LEU:HD21	28:B:546:HOH:O	2.18	0.44
3:C:224:LYS:HE3	24:C:306:CDL:HB31	2.00	0.44
20:N:611:TGL:HC41	20:N:611:TGL:OC1	2.18	0.44
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.53	0.44
7:T:3:ALA:O	7:T:4:ALA:CB	2.66	0.44
7:G:5:LYS:CG	23:G:102:PEK:H351	2.39	0.44
2:O:67:ILE:HD11	28:O:545:HOH:O	2.18	0.44
8:H:60:TYR:C	8:H:60:TYR:CD1	2.91	0.43
1:A:172:LYS:HZ2	1:A:178:GLN:HE22	1.66	0.43
5:E:41:LEU:HD22	26:E:201:PSC:H072	2.00	0.43
11:K:8:ASP:HB2	28:K:120:HOH:O	2.17	0.43
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.83	0.43
7:T:5:LYS:HB2	23:T:101:PEK:H322	1.99	0.43
4:D:19[B]:ARG:NE	4:D:21:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:409:TRP:HB3	1:N:471:ILE:HG12	1.99	0.43
1:A:514:LYS:HA	6:F:38:ALA:CB	2.46	0.43
26:E:201:PSC:H201	26:E:201:PSC:H231	1.76	0.43
7:G:2:SER:H	1:N:197:LEU:HD21	1.82	0.43
2:B:58:ALA:O	2:B:61:VAL:HG12	2.18	0.43
3:C:210:ILE:HG21	18:C:304:PGV:H281	2.01	0.43
7:T:2:SER:O	23:T:101:PEK:H301	2.19	0.43
1:A:302[B]:ARG:HE	1:A:361:SER:HB2	1.83	0.43
1:A:302[B]:ARG:HH12	2:B:87:MET:CE	2.32	0.43
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.18	0.43
4:D:78:TRP:N	20:D:201:TGL:CB2	2.82	0.43
7:G:42:ARG:HG3	7:G:43:GLU:H	1.84	0.43
7:G:7:ASP:HB3	7:G:8:HIS:H	1.54	0.43
8:H:55:TRP:H	8:U:46:LYS:NZ	2.15	0.43
18:A:606:PGV:H012	11:K:9:PHE:HB2	2.01	0.43
3:C:67:PHE:CE2	24:C:306:CDL:H1	2.54	0.43
1:N:377:PHE:HB2	14:N:602:HEA:HMD3	2.00	0.43
7:T:2:SER:HB2	23:T:101:PEK:C28	2.47	0.43
1:A:282:PHE:HZ	24:T:103:CDL:H761	1.83	0.43
1:A:53:ILE:HD11	12:L:40:VAL:HG13	2.01	0.43
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.01	0.43
1:N:113[B]:LEU:HD11	1:N:117[B]:MET:SD	2.59	0.43
4:Q:29:HIS:CE1	4:Q:65:LYS:HG3	2.54	0.43
20:B:301:TGL:HA32	20:B:301:TGL:HA91	2.00	0.42
3:C:33:MET:HG2	3:C:39:SER:O	2.19	0.42
7:T:11:TPO:HA	7:T:11:TPO:O3P	2.19	0.42
9:V:59:ASP:O	9:V:63[B]:MET:HG3	2.19	0.42
20:L:101:TGL:H352	20:L:101:TGL:H321	2.00	0.42
1:N:122:ALA:HB3	28:N:712:HOH:O	2.18	0.42
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.55	0.42
12:L:26:THR:HG23	13:M:25:SER:CB	2.49	0.42
1:N:297[B]:MET:HG2	1:N:302[B]:ARG:CD	2.48	0.42
1:N:313:ALA:HB2	1:N:356:ILE:HD11	2.00	0.42
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.01	0.42
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.06	0.42
4:D:126:MET:HG3	4:D:128:VAL:HG23	2.00	0.42
2:O:102:HIS:O	2:O:104:TRP:HA	2.20	0.42
20:N:611:TGL:HC31	12:Y:13:PHE:HA	2.01	0.42
18:C:304:PGV:H132	24:C:306:CDL:H652	2.01	0.42
1:N:243:VAL:HB	14:N:602:HEA:CAC	2.50	0.42
7:G:4:ALA:HB1	1:N:282:PHE:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:2:SER:HB2	23:T:101:PEK:C29	2.49	0.42
3:C:37:PHE:CD1	10:J:52:TRP:HZ3	2.38	0.42
3:P:111:GLU:HG3	28:U:147:HOH:O	2.19	0.42
1:A:148:PHE:HB3	3:C:28:THR:HB	2.01	0.42
6:F:87:THR:HG21	28:F:226:HOH:O	2.19	0.42
8:H:76:ARG:HD2	28:H:104:HOH:O	2.19	0.42
1:A:417:MET:CE	14:A:601:HEA:H263	2.50	0.42
10:W:22:LEU:HA	10:W:28:ASP:HB3	2.02	0.42
4:D:86[A]:MET:HG2	20:D:201:TGL:H312	2.02	0.42
5:E:43:PRO:HB2	5:E:48:ILE:HD11	2.02	0.41
14:N:601:HEA:HHC	14:N:601:HEA:H122	2.01	0.41
2:O:108:TYR:O	2:O:117:SER:HA	2.20	0.41
3:P:127[A]:LEU:HD22	3:P:127[A]:LEU:N	2.35	0.41
3:P:33:MET:HG2	3:P:39:SER:O	2.19	0.41
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.55	0.41
1:A:243:VAL:HB	14:A:602:HEA:CAC	2.50	0.41
4:D:93:ALA:HB3	11:K:28[B]:VAL:HG12	2.01	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.41
6:S:64:GLU:O	6:S:65:ASP:CB	2.67	0.41
23:C:303:PEK:C05	6:F:1:ALA:H2	2.27	0.41
18:A:606:PGV:C29	13:M:16:ALA:HA	2.45	0.41
1:N:377:PHE:CE1	1:N:378:HIS:CE1	3.07	0.41
1:N:54:TYR:HB2	28:N:821:HOH:O	2.20	0.41
8:H:45:ALA:O	8:H:47:GLY:N	2.53	0.41
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.02	0.41
4:Q:19:ARG:HG2	4:Q:21:ASP:OD1	2.18	0.41
3:C:257:TYR:O	3:C:261:SER:HB3	2.20	0.41
6:S:55:LYS:HA	6:S:74:LEU:O	2.21	0.41
2:B:58:ALA:O	2:B:62:GLU:HG3	2.21	0.41
24:C:306:CDL:H352	24:C:306:CDL:H162	2.03	0.41
7:G:9:GLY:HA3	1:N:178:GLN:HE21	1.84	0.41
1:A:449[A]:MET:HB2	11:K:40:TRP:O	2.20	0.41
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.61	0.41
1:N:110:LEU:HD21	25:P:307:DMU:H24	2.02	0.41
2:B:32[B]:PHE:CD1	9:I:31:PHE:CZ	3.09	0.41
8:H:36:PHE:CE1	8:H:57:ARG:HB2	2.56	0.41
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.55	0.41
3:P:22:LEU:O	3:P:26:LEU:HG	2.20	0.41
4:Q:6:VAL:HB	4:Q:10:ASP:OD2	2.21	0.41
9:V:22:VAL:O	9:V:26:MET:HG2	2.21	0.41
1:A:54:TYR:HB2	28:A:792:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:606:PGV:H291	13:M:19:LEU:HD22	2.03	0.41
2:B:74:ILE:HG22	2:B:78:LEU:HD22	2.01	0.41
3:C:188[B]:ILE:HD12	3:C:195:SER:HA	2.03	0.41
3:C:77:LYS:HE2	3:C:81:TYR:OH	2.20	0.41
7:G:12:GLY:CA	28:G:249:HOH:O	2.68	0.41
7:G:1:ALA:HB2	18:P:304:PGV:H312	2.02	0.41
20:N:608:TGL:HB92	20:N:608:TGL:C28	2.51	0.41
1:N:155:VAL:HG21	18:N:609:PGV:H142	2.03	0.41
5:R:12:ASP:OD2	5:R:44:GLU:HG3	2.21	0.41
23:C:303:PEK:H342	23:C:303:PEK:H371	1.87	0.41
24:G:101:CDL:H541	24:G:101:CDL:H771	2.03	0.41
1:N:24:ALA:HB2	14:N:601:HEA:H253	2.02	0.41
12:Y:2:HIS:CG	12:Y:3:TYR:N	2.89	0.41
13:M:41:LYS:O	13:M:43:SER:N	2.52	0.40
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.08	0.40
2:O:121:TYR:O	2:O:138:VAL:HA	2.21	0.40
3:P:59:ARG:CA	24:P:305:CDL:H512	2.51	0.40
3:P:33:MET:HB2	25:P:307:DMU:H9	2.03	0.40
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.03	0.40
1:A:302[B]:ARG:HH12	2:B:87:MET:HE2	1.85	0.40
1:A:489:THR:HA	6:F:71:TRP:O	2.21	0.40
18:A:606:PGV:C29	13:M:19:LEU:HD23	2.49	0.40
1:N:177:SER:H	1:N:180:GLN:HE21	1.68	0.40
28:N:908:HOH:O	4:Q:20:ARG:HG3	2.20	0.40
1:A:513:LEU:O	1:A:514:LYS:CB	2.62	0.40
14:A:602:HEA:ND	19:A:607[B]:PER:O1	2.54	0.40
4:Q:10:ASP:C	4:Q:10:ASP:OD1	2.60	0.40
2:O:4:PRO:HB2	11:X:43:SER:HA	2.03	0.40
4:D:19[B]:ARG:HE	4:D:21:ASP:CG	2.25	0.40
1:A:377:PHE:HB2	14:A:602:HEA:HMD3	2.04	0.40
18:A:606:PGV:H302	13:M:19:LEU:HD23	2.03	0.40
23:P:302:PEK:H012	28:P:496:HOH:O	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:LYS:CE	28:B:402:HOH:O[2_585]	2.12	0.08
28:B:482:HOH:O	28:D:361:HOH:O[2_584]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/514 (102%)	510 (97%)	14 (3%)	0	100	100
1	N	524/514 (102%)	511 (98%)	13 (2%)	0	100	100
2	B	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
2	O	230/227 (101%)	221 (96%)	9 (4%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	148/147 (101%)	144 (97%)	4 (3%)	0	100	100
4	Q	143/147 (97%)	138 (96%)	5 (4%)	0	100	100
5	E	104/109 (95%)	104 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	101/98 (103%)	94 (93%)	3 (3%)	4 (4%)	3	0
6	S	97/98 (99%)	91 (94%)	6 (6%)	0	100	100
7	G	82/85 (96%)	71 (87%)	8 (10%)	3 (4%)	3	0
7	T	84/85 (99%)	73 (87%)	8 (10%)	3 (4%)	3	0
8	H	77/85 (91%)	73 (95%)	1 (1%)	3 (4%)	3	0
8	U	77/85 (91%)	69 (90%)	5 (6%)	3 (4%)	3	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	72/73 (99%)	70 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	6	1
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3575/3614 (99%)	3448 (96%)	109 (3%)	18 (0%)	29	18

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	T	4	ALA
8	U	8	ILE
8	U	45	ALA
8	U	46	LYS
6	F	95	GLN
8	H	46	LYS
12	Y	46	LYS
7	G	9	GLY
8	H	8	ILE
13	M	42	LYS
7	T	3	ALA
7	T	6	GLY
6	F	97	ALA
8	H	45	ALA
6	F	2	SER
7	G	8	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/426 (103%)	428 (98%)	10 (2%)	50	45
1	N	438/426 (103%)	427 (98%)	11 (2%)	47	41
2	B	215/210 (102%)	208 (97%)	7 (3%)	38	29
2	O	215/210 (102%)	203 (94%)	12 (6%)	21	11
3	C	232/226 (103%)	229 (99%)	3 (1%)	69	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	232/226 (103%)	229 (99%)	3 (1%)	69	68
4	D	134/129 (104%)	133 (99%)	1 (1%)	84	84
4	Q	129/129 (100%)	123 (95%)	6 (5%)	26	16
5	E	93/95 (98%)	91 (98%)	2 (2%)	52	47
5	R	92/95 (97%)	90 (98%)	2 (2%)	52	47
6	F	86/81 (106%)	85 (99%)	1 (1%)	71	70
6	S	82/81 (101%)	75 (92%)	7 (8%)	10	4
7	G	68/68 (100%)	59 (87%)	9 (13%)	4	1
7	T	70/68 (103%)	60 (86%)	10 (14%)	3	1
8	H	71/75 (95%)	67 (94%)	4 (6%)	21	11
8	U	71/75 (95%)	69 (97%)	2 (3%)	43	36
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	55
9	V	58/57 (102%)	57 (98%)	1 (2%)	60	57
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	51
10	W	49/50 (98%)	47 (96%)	2 (4%)	30	21
11	K	40/46 (87%)	40 (100%)	0	100	100
11	X	40/46 (87%)	38 (95%)	2 (5%)	24	15
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	39
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	39
13	M	37/38 (97%)	36 (97%)	1 (3%)	44	38
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	4
All	All	3111/3082 (101%)	3008 (97%)	103 (3%)	39	29

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	178	GLN
1	A	180	GLN
1	A	311[A]	ILE
1	A	311[B]	ILE
1	A	338	MET

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Mol	Chain	Res	Type
1	A	369	ASP
2	B	33	LEU
2	B	75	LEU
2	B	78	LEU
2	B	115	ASP
2	B	116	LEU
2	B	171	LYS
2	B	217	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
4	D	31	LYS
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
7	G	2	SER
7	G	18[A]	PHE
7	G	18[B]	PHE
7	G	36	TRP
7	G	37	LEU
7	G	42	ARG
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS
8	H	9	LYS
8	H	10	ASN
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
10	J	58	LYS
12	L	47	LYS
13	M	39	ASN
1	N	38	ARG
1	N	98	ASN
1	N	109	PHE
1	N	138	HIS
1	N	178	GLN
1	N	180	GLN
1	N	336	PRO
1	N	362	SER
1	N	363	LEU
1	N	369	ASP

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Mol	Chain	Res	Type
1	N	484	THR
2	O	33	LEU
2	O	60	GLU
2	O	61	VAL
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	114	GLU
2	O	171	LYS
2	O	203[A]	ASN
2	O	203[B]	ASN
2	O	221	LYS
2	O	226	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	6	VAL
4	Q	7	LYS
4	Q	8	SER
4	Q	9	GLU
4	Q	10	ASP
4	Q	51	LEU
5	R	5	HIS
5	R	79	LYS
6	S	37	LYS
6	S	54	ASN
6	S	80	GLN
6	S	87[A]	THR
6	S	87[B]	THR
6	S	95	GLN
6	S	96	LEU
7	T	5	LYS
7	T	17	ARG
7	T	18	PHE
7	T	33	LEU
7	T	36[A]	TRP
7	T	36[B]	TRP
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	74	ARG
8	U	29	CYS

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Mol	Chain	Res	Type
8	U	60	TYR
9	V	45	LYS
10	W	50	LEU
10	W	58	LYS
11	X	52	GLU
11	X	54	ARG
12	Y	20	ARG
13	Z	13	LYS
13	Z	38	ASP
13	Z	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	59	GLN
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	68	GLN
4	D	37	GLN
4	D	143	ASN
5	E	94	ASN
7	G	8	HIS
7	G	34	ASN
7	G	76	ASN
8	H	37	HIS
10	J	29	ASN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN

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Mol	Chain	Res	Type
3	P	76	GLN
3	P	122	HIS
4	Q	29	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
5	R	5	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	34	ASN
7	T	38	HIS
7	T	76	ASN
8	U	23	GLN
8	U	37	HIS
9	V	20	HIS
10	W	29	ASN
12	Y	2	HIS
13	Z	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	O	1	2	8,9,10	0.77	0	7,9,11	1.50	1 (14%)
7	TPO	G	11	7	8,10,11	1.52	1 (12%)	10,14,16	1.12	1 (10%)
9	SAC	V	1	9	7,8,9	1.25	1 (14%)	8,9,11	1.76	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SAC	I	1	9	7,8,9	1.52	1 (14%)	8,9,11	1.71	2 (25%)
1	FME	A	1	1	8,9,10	0.64	0	7,9,11	1.54	2 (28%)
7	TPO	T	11	7	8,10,11	1.50	1 (12%)	10,14,16	0.81	0
2	FME	B	1	2	8,9,10	1.75	1 (12%)	7,9,11	6.65	3 (42%)
1	FME	N	1	1	8,9,10	0.65	0	7,9,11	1.40	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	V	1	9	-	2/7/8/10	-
9	SAC	I	1	9	-	4/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-4.41	1.09	1.22
9	I	1	SAC	CA-N	3.95	1.51	1.46
9	V	1	SAC	CA-N	3.08	1.50	1.46
7	T	11	TPO	P-O1P	2.88	1.59	1.50
7	G	11	TPO	P-O1P	2.86	1.59	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-17.25	96.30	122.82
9	V	1	SAC	C-CA-N	4.13	117.19	109.73
9	I	1	SAC	C-CA-N	3.35	115.78	109.73
2	O	1	FME	CG-CB-CA	-2.58	105.79	112.95
1	A	1	FME	C-CA-N	2.50	114.25	109.73
1	A	1	FME	CE-SD-CG	2.26	108.16	100.40
2	B	1	FME	CG-CB-CA	-2.25	106.70	112.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	O-C-CA	-2.13	119.20	124.78
2	B	1	FME	O-C-CA	-2.09	119.30	124.78
1	N	1	FME	C-CA-N	2.09	113.50	109.73
7	G	11	TPO	O-C-CA	-2.07	119.36	124.78
9	I	1	SAC	O-C-CA	-2.03	119.46	124.78

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	C-CA-N-C1A
1	A	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	O-C-CA-CB
7	T	11	TPO	CA-CB-OG1-P
7	T	11	TPO	CG2-CB-OG1-P
2	B	1	FME	O1-CN-N-CA
1	N	1	FME	O-C-CA-CB
1	A	1	FME	CB-CG-SD-CE
9	I	1	SAC	C-CA-CB-OG
7	T	11	TPO	CB-OG1-P-O3P
1	A	1	FME	C-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 58 ligands modelled in this entry, 10 are monoatomic - leaving 48 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$
19	PER	A	607[A]	15,14	0,1,1	0.00	-	-		
22	CHD	P	306	-	29,32,32	0.53	0	48,51,51	1.56	10 (20%)
20	TGL	B	301	-	62,62,62	1.12	3 (4%)	65,65,65	1.48	7 (10%)
18	PGV	P	304	-	50,50,50	1.15	2 (4%)	53,56,56	1.03	3 (5%)
19	PER	A	607[B]	15	0,1,1	0.00	-	-		
18	PGV	N	606	-	50,50,50	1.00	2 (4%)	53,56,56	1.36	7 (13%)
18	PGV	C	305	-	50,50,50	1.08	2 (4%)	53,56,56	0.95	3 (5%)
22	CHD	C	307	-	29,32,32	0.55	0	48,51,51	2.27	18 (37%)
26	PSC	R	201	-	51,51,51	1.19	3 (5%)	57,59,59	1.02	2 (3%)
14	HEA	A	601	1	44,67,67	0.95	3 (6%)	37,103,103	2.42	16 (43%)
25	DMU	Z	101	-	34,34,34	0.50	0	45,45,45	0.85	1 (2%)
24	CDL	G	101	-	99,99,99	1.39	12 (12%)	105,111,111	1.20	6 (5%)
19	PER	N	607[A]	15,14	0,1,1	0.00	-	-		
18	PGV	A	606	-	50,50,50	0.95	2 (4%)	53,56,56	1.37	7 (13%)
23	PEK	T	102	-	52,52,52	0.91	3 (5%)	55,57,57	1.30	6 (10%)
22	CHD	N	610	-	29,32,32	0.84	0	48,51,51	1.14	3 (6%)
23	PEK	C	303	-	52,52,52	1.06	2 (3%)	55,57,57	1.00	5 (9%)
20	TGL	Q	201	-	62,62,62	1.16	3 (4%)	65,65,65	0.88	4 (6%)
23	PEK	T	101	-	52,52,52	1.07	2 (3%)	55,57,57	0.95	3 (5%)
19	PER	N	607[B]	15	0,1,1	0.00	-	-		
24	CDL	C	306	-	99,99,99	1.32	12 (12%)	105,111,111	1.25	10 (9%)
14	HEA	N	601	1	44,67,67	1.09	5 (11%)	37,103,103	1.88	15 (40%)
21	CUA	B	302	2	0,1,1	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	N	602	1,19	44,67,67	0.90	0	37,103,103	1.71	11 (29%)
24	CDL	T	103	-	99,99,99	1.33	12 (12%)	105,111,111	1.20	7 (6%)
20	TGL	N	611	-	62,62,62	1.16	3 (4%)	65,65,65	1.24	4 (6%)
14	HEA	A	602	1,19	44,67,67	1.05	2 (4%)	37,103,103	2.06	12 (32%)
23	PEK	C	302	-	52,52,52	0.85	2 (3%)	55,57,57	0.90	3 (5%)
22	CHD	C	308	-	29,32,32	0.94	1 (3%)	48,51,51	1.29	6 (12%)
22	CHD	W	101	-	29,32,32	0.55	0	48,51,51	2.38	20 (41%)
21	CUA	O	302	2	0,1,1	0.00	-	-		
18	PGV	C	304	-	50,50,50	0.83	2 (4%)	53,56,56	0.97	2 (3%)
20	TGL	N	608	-	62,62,62	1.10	3 (4%)	65,65,65	1.13	4 (6%)
25	DMU	P	307	-	34,34,34	0.74	1 (2%)	45,45,45	0.97	2 (4%)
26	PSC	E	201	-	51,51,51	1.17	3 (5%)	57,59,59	0.94	2 (3%)
22	CHD	B	303	-	29,32,32	1.00	2 (6%)	48,51,51	1.24	4 (8%)
18	PGV	P	303	-	50,50,50	0.90	3 (6%)	53,56,56	0.82	3 (5%)
22	CHD	J	101	-	29,32,32	0.49	0	48,51,51	2.01	14 (29%)
20	TGL	D	201	-	62,62,62	1.12	4 (6%)	65,65,65	0.84	4 (6%)
25	DMU	C	309	-	34,34,34	0.61	0	45,45,45	1.21	4 (8%)
23	PEK	G	102	-	52,52,52	1.04	2 (3%)	55,57,57	1.09	3 (5%)
18	PGV	A	608	-	50,50,50	0.93	2 (4%)	53,56,56	1.22	4 (7%)
20	TGL	L	101	-	62,62,62	1.17	3 (4%)	65,65,65	1.47	9 (13%)
25	DMU	M	101	-	34,34,34	0.50	0	45,45,45	1.13	3 (6%)
22	CHD	O	301	-	29,32,32	0.88	0	48,51,51	1.53	9 (18%)
24	CDL	P	305	-	99,99,99	1.36	12 (12%)	105,111,111	1.28	8 (7%)
18	PGV	N	609	-	50,50,50	0.93	2 (4%)	53,56,56	1.26	5 (9%)
23	PEK	P	302	-	52,52,52	1.07	2 (3%)	55,57,57	1.05	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	P	306	-	-	2/7/74/74	0/4/4/4
20	TGL	B	301	-	-	36/65/65/65	-
18	PGV	P	304	-	-	28/55/55/55	-
14	HEA	N	601	1	3/3/7/16	2/24/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PGV	N	606	-	-	36/55/55/55	-
18	PGV	C	305	-	-	30/55/55/55	-
22	CHD	C	307	-	-	5/7/74/74	0/4/4/4
26	PSC	R	201	-	-	22/55/55/55	-
14	HEA	A	601	1	2/2/7/16	3/24/76/76	-
25	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
24	CDL	G	101	-	-	68/110/110/110	-
18	PGV	A	606	-	-	32/55/55/55	-
23	PEK	T	102	-	-	20/56/56/56	-
22	CHD	N	610	-	-	0/7/74/74	0/4/4/4
23	PEK	C	303	-	-	32/56/56/56	-
20	TGL	Q	201	-	-	34/65/65/65	-
23	PEK	T	101	-	-	21/56/56/56	-
24	CDL	C	306	-	-	63/110/110/110	-
22	CHD	O	301	-	-	0/7/74/74	0/4/4/4
14	HEA	N	602	1,19	2/2/7/16	1/24/76/76	-
24	CDL	T	103	-	-	60/110/110/110	-
20	TGL	N	611	-	-	30/65/65/65	-
14	HEA	A	602	1,19	2/2/7/16	1/24/76/76	-
23	PEK	C	302	-	-	15/56/56/56	-
22	CHD	C	308	-	-	0/7/74/74	0/4/4/4
22	CHD	W	101	-	-	6/7/74/74	1/4/4/4
18	PGV	C	304	-	-	15/55/55/55	-
20	TGL	N	608	-	-	38/65/65/65	-
25	DMU	P	307	-	-	8/19/59/59	0/2/2/2
26	PSC	E	201	-	-	24/55/55/55	-
22	CHD	B	303	-	-	0/7/74/74	0/4/4/4
18	PGV	P	303	-	-	13/55/55/55	-
22	CHD	J	101	-	-	3/7/74/74	0/4/4/4
20	TGL	D	201	-	-	41/65/65/65	-
25	DMU	C	309	-	-	9/19/59/59	0/2/2/2
23	PEK	G	102	-	-	31/56/56/56	-
18	PGV	A	608	-	-	6/55/55/55	-
20	TGL	L	101	-	-	37/65/65/65	-
25	DMU	M	101	-	-	5/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PGV	N	609	-	-	11/55/55/55	-
24	CDL	P	305	-	-	72/110/110/110	-
23	PEK	P	302	-	-	27/56/56/56	-

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	101	TGL	OG2-CB1	5.66	1.50	1.34
20	N	611	TGL	OG2-CB1	5.58	1.50	1.34
18	P	304	PGV	O03-C19	5.22	1.48	1.33
20	B	301	TGL	OG1-CA1	5.17	1.48	1.33
24	G	101	CDL	OB6-CB5	5.11	1.48	1.34
26	R	201	PSC	O01-C1	5.06	1.48	1.34
23	C	303	PEK	O03-C21	5.05	1.48	1.33
23	P	302	PEK	O01-C1	4.98	1.48	1.34
23	T	101	PEK	O03-C21	4.92	1.47	1.33
20	N	608	TGL	OG1-CA1	4.90	1.47	1.33
20	L	101	TGL	OG3-CC1	4.89	1.47	1.33
20	Q	201	TGL	OG3-CC1	4.89	1.47	1.33
24	P	305	CDL	OA8-CA7	4.88	1.47	1.33
20	Q	201	TGL	OG2-CB1	4.86	1.48	1.34
24	G	101	CDL	OB8-CB7	4.84	1.47	1.33
23	G	102	PEK	O03-C21	4.84	1.47	1.33
24	P	305	CDL	OB8-CB7	4.83	1.47	1.33
18	P	304	PGV	O01-C1	4.81	1.47	1.34
20	N	608	TGL	OG2-CB1	4.79	1.47	1.34
23	T	101	PEK	O01-C1	4.76	1.47	1.34
20	Q	201	TGL	OG1-CA1	4.76	1.47	1.33
20	N	611	TGL	OG3-CC1	4.76	1.47	1.33
23	P	302	PEK	O03-C21	4.75	1.47	1.33
26	E	201	PSC	O01-C1	4.75	1.47	1.34
24	T	103	CDL	OA6-CA5	4.73	1.47	1.34
18	C	305	PGV	O03-C19	4.70	1.47	1.33
18	C	305	PGV	O01-C1	4.70	1.47	1.34
24	G	101	CDL	OA6-CA5	4.69	1.47	1.34
24	T	103	CDL	OA8-CA7	4.69	1.47	1.33
24	C	306	CDL	OB8-CB7	4.61	1.46	1.33
18	N	606	PGV	O03-C19	4.61	1.46	1.33
24	C	306	CDL	OA8-CA7	4.58	1.46	1.33
23	G	102	PEK	O01-C1	4.56	1.47	1.34
24	G	101	CDL	OA8-CA7	4.52	1.46	1.33
26	E	201	PSC	O03-C19	4.50	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	201	TGL	OG1-CA1	4.46	1.46	1.33
20	B	301	TGL	OG3-CC1	4.46	1.46	1.33
20	L	101	TGL	OG1-CA1	4.44	1.46	1.33
18	A	606	PGV	O03-C19	4.42	1.46	1.33
24	P	305	CDL	OA6-CA5	4.41	1.46	1.34
24	T	103	CDL	OB6-CB5	4.38	1.46	1.34
24	P	305	CDL	OB6-CB5	4.37	1.46	1.34
24	C	306	CDL	OA6-CA5	4.36	1.46	1.34
26	R	201	PSC	O03-C19	4.36	1.46	1.33
20	N	608	TGL	OG3-CC1	4.35	1.46	1.33
20	D	201	TGL	OG2-CB1	4.34	1.46	1.34
20	N	611	TGL	OG1-CA1	4.33	1.46	1.33
20	B	301	TGL	OG2-CB1	4.32	1.46	1.34
18	P	303	PGV	O03-C19	4.26	1.45	1.33
18	N	606	PGV	O01-C1	4.26	1.46	1.34
23	C	303	PEK	O01-C1	4.24	1.46	1.34
24	T	103	CDL	OB8-CB7	4.17	1.45	1.33
20	D	201	TGL	OG3-CC1	4.14	1.45	1.33
23	T	102	PEK	O03-C21	3.98	1.45	1.33
26	R	201	PSC	C13-C12	3.94	1.54	1.31
24	C	306	CDL	OB6-CB5	3.85	1.45	1.34
18	A	606	PGV	O01-C1	3.83	1.45	1.34
26	E	201	PSC	C13-C12	3.79	1.53	1.31
23	C	302	PEK	O01-C1	3.71	1.44	1.34
18	N	609	PGV	O03-C19	3.64	1.44	1.33
18	A	608	PGV	O03-C19	3.51	1.43	1.33
24	C	306	CDL	C59-C58	-3.47	1.32	1.51
18	C	304	PGV	O03-C19	3.45	1.43	1.33
18	A	608	PGV	O01-C1	3.33	1.43	1.34
23	C	302	PEK	O03-C21	3.32	1.43	1.33
14	N	601	HEA	C3B-C11	-3.31	1.50	1.52
25	P	307	DMU	O16-C6	3.25	1.45	1.40
24	T	103	CDL	C59-C58	-3.20	1.33	1.51
24	G	101	CDL	C19-C18	-3.20	1.33	1.51
24	P	305	CDL	C79-C78	-3.18	1.33	1.51
24	C	306	CDL	C79-C78	-3.17	1.33	1.51
24	P	305	CDL	C22-C21	-3.17	1.33	1.51
24	P	305	CDL	C59-C58	-3.17	1.33	1.51
24	T	103	CDL	C82-C81	-3.16	1.33	1.51
24	G	101	CDL	C22-C21	-3.15	1.33	1.51
24	G	101	CDL	C62-C61	-3.15	1.33	1.51
24	C	306	CDL	C22-C21	-3.14	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	305	CDL	C19-C18	-3.14	1.34	1.51
24	T	103	CDL	C79-C78	-3.14	1.34	1.51
24	P	305	CDL	C39-C38	-3.12	1.34	1.51
23	T	102	PEK	O01-C1	3.11	1.43	1.34
24	T	103	CDL	C19-C18	-3.11	1.34	1.51
24	T	103	CDL	C22-C21	-3.11	1.34	1.51
24	G	101	CDL	C59-C58	-3.10	1.34	1.51
24	C	306	CDL	C19-C18	-3.10	1.34	1.51
24	P	305	CDL	C82-C81	-3.09	1.34	1.51
24	C	306	CDL	C39-C38	-3.08	1.34	1.51
24	G	101	CDL	C79-C78	-3.07	1.34	1.51
24	C	306	CDL	C62-C61	-3.07	1.34	1.51
24	G	101	CDL	C42-C41	-3.07	1.34	1.51
24	C	306	CDL	C82-C81	-3.07	1.34	1.51
24	G	101	CDL	C39-C38	-3.06	1.34	1.51
24	T	103	CDL	C42-C41	-3.06	1.34	1.51
24	G	101	CDL	C82-C81	-3.05	1.34	1.51
24	T	103	CDL	C62-C61	-3.04	1.34	1.51
24	T	103	CDL	C39-C38	-3.02	1.34	1.51
24	P	305	CDL	C42-C41	-3.01	1.34	1.51
24	P	305	CDL	C62-C61	-3.00	1.34	1.51
24	C	306	CDL	C42-C41	-2.99	1.34	1.51
18	C	304	PGV	O01-C1	2.95	1.42	1.34
18	N	609	PGV	O01-C1	2.93	1.42	1.34
18	P	303	PGV	O01-C1	2.89	1.42	1.34
14	A	602	HEA	C3C-C2C	-2.89	1.36	1.40
20	D	201	TGL	OB1-CB1	2.76	1.30	1.22
14	A	602	HEA	C3A-C2A	-2.68	1.36	1.40
14	N	601	HEA	O11-C11	2.45	1.48	1.42
14	A	601	HEA	C3B-C11	-2.35	1.51	1.52
22	C	308	CHD	C11-C9	2.34	1.57	1.53
22	B	303	CHD	C11-C12	2.26	1.57	1.53
22	B	303	CHD	C11-C9	2.22	1.57	1.53
14	N	601	HEA	C3C-C2C	-2.18	1.37	1.40
14	A	601	HEA	C3C-C2C	-2.14	1.37	1.40
14	N	601	HEA	C4D-ND	-2.13	1.31	1.36
14	A	601	HEA	C1C-NC	-2.07	1.31	1.36
23	T	102	PEK	O01-C02	-2.04	1.41	1.46
18	P	303	PGV	O01-C02	-2.02	1.41	1.46
14	N	601	HEA	C3A-C2A	-2.01	1.37	1.40

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	301	TGL	OG2-CB1-CB2	7.35	127.34	111.50
14	A	602	HEA	CAD-CBD-CGD	-6.46	101.83	112.67
22	C	307	CHD	C16-C17-C20	6.33	121.95	112.15
22	C	307	CHD	C14-C13-C12	6.16	113.13	107.40
22	J	101	CHD	C17-C13-C14	-5.92	94.13	100.09
20	N	611	TGL	OG2-CB1-CB2	5.79	123.98	111.50
22	W	101	CHD	C17-C13-C12	5.73	122.90	117.67
18	N	606	PGV	O01-C1-C2	5.69	123.77	111.50
20	L	101	TGL	OG2-CB1-CB2	5.61	123.59	111.50
24	G	101	CDL	OB6-CB5-C51	5.52	123.40	111.50
14	A	601	HEA	C1B-C2B-C3B	-5.39	103.25	107.00
22	W	101	CHD	C15-C14-C8	5.29	125.72	118.33
24	T	103	CDL	OA6-CA5-C11	5.16	122.62	111.50
22	C	307	CHD	C23-C22-C20	-5.14	107.79	114.72
18	A	606	PGV	O01-C1-C2	5.12	122.54	111.50
23	T	102	PEK	C2-C3-C4	5.10	122.33	113.23
18	N	609	PGV	O03-C19-O04	-5.07	110.80	123.59
14	A	601	HEA	CMC-C2C-C1C	-5.05	120.70	128.46
18	A	608	PGV	O03-C19-O04	-5.05	110.85	123.59
20	N	608	TGL	OG2-CB1-CB2	4.99	122.25	111.50
22	C	307	CHD	C17-C13-C14	-4.94	95.11	100.09
22	W	101	CHD	C14-C8-C7	4.86	118.25	111.81
23	P	302	PEK	O01-C1-C2	4.84	121.92	111.50
14	N	602	HEA	CAD-CBD-CGD	-4.75	104.70	112.67
23	G	102	PEK	O01-C1-C2	4.68	121.59	111.50
14	A	601	HEA	CMC-C2C-C3C	4.68	133.43	124.68
24	P	305	CDL	OA6-CA5-C11	4.63	121.48	111.50
24	G	101	CDL	OA6-CA5-C11	4.59	121.39	111.50
22	J	101	CHD	C13-C17-C20	4.58	124.96	119.50
24	C	306	CDL	OA6-CA5-C11	4.48	121.16	111.50
14	A	602	HEA	OMA-CMA-C3A	-4.45	115.21	124.91
24	P	305	CDL	OB6-CB5-C51	4.43	121.06	111.50
23	C	303	PEK	O01-C1-C2	4.40	120.99	111.50
22	W	101	CHD	C14-C8-C9	-4.39	103.68	109.71
18	N	609	PGV	O03-C19-C20	4.39	125.69	111.91
14	A	601	HEA	C13-C12-C11	-4.23	107.99	114.35
14	A	601	HEA	CMB-C2B-C3B	4.18	132.88	124.69
24	T	103	CDL	OB6-CB5-C51	4.17	120.49	111.50
22	J	101	CHD	C6-C5-C4	-4.17	106.39	111.19
23	T	101	PEK	O01-C1-C2	4.13	120.40	111.50
26	E	201	PSC	O01-C1-C2	4.13	120.39	111.50
23	T	102	PEK	O01-C1-O02	-4.11	113.76	123.70
22	W	101	CHD	C18-C13-C12	-4.11	104.88	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	304	PGV	O01-C1-C2	4.10	120.33	111.50
22	W	101	CHD	C13-C17-C20	4.05	124.33	119.50
18	A	608	PGV	O03-C19-C20	4.04	124.60	111.91
23	T	102	PEK	O03-C21-C22	4.04	124.58	111.91
20	L	101	TGL	OG3-CC1-CC2	4.03	124.55	111.91
20	B	301	TGL	OG3-CC1-CC2	3.97	124.36	111.91
22	W	101	CHD	C6-C5-C10	3.96	116.86	112.66
14	N	601	HEA	OMA-CMA-C3A	-3.92	116.36	124.91
18	C	305	PGV	O01-C1-C2	3.92	119.95	111.50
25	C	309	DMU	C7-C8-C9	3.88	117.17	110.24
14	A	601	HEA	CAA-CBA-CGA	-3.85	106.20	112.67
22	B	303	CHD	C22-C23-C24	-3.84	105.34	113.59
26	R	201	PSC	O01-C1-C2	3.80	119.68	111.50
24	P	305	CDL	OB8-CB7-C71	3.79	123.79	111.91
18	P	304	PGV	O03-C19-C20	3.77	123.74	111.91
24	C	306	CDL	OB6-CB5-C51	3.75	119.58	111.50
24	P	305	CDL	CB4-OB6-CB5	-3.73	108.61	117.79
22	O	301	CHD	C11-C12-C13	3.68	115.02	111.24
18	N	606	PGV	O03-C19-C20	3.65	123.36	111.91
20	N	608	TGL	OG1-CA1-CA2	3.52	122.96	111.91
25	C	309	DMU	O1-C9-C8	3.50	116.05	109.69
25	M	101	DMU	O16-C6-C1	3.47	113.71	108.30
23	G	102	PEK	O03-C21-C22	3.39	122.56	111.91
22	J	101	CHD	C6-C5-C10	3.39	116.26	112.66
24	C	306	CDL	OB8-CB7-C71	3.39	122.53	111.91
22	P	306	CHD	C1-C2-C3	3.37	114.79	110.47
18	C	304	PGV	O03-C19-O04	-3.36	115.11	123.59
14	A	602	HEA	C27-C19-C20	3.34	120.89	115.27
22	O	301	CHD	C22-C23-C24	-3.32	106.46	113.59
20	B	301	TGL	OG3-CC1-OC1	-3.32	115.22	123.59
20	B	301	TGL	CB3-CB2-CB1	-3.30	101.61	113.62
22	C	307	CHD	C22-C23-C24	-3.30	106.50	113.59
22	J	101	CHD	C16-C17-C20	3.30	117.25	112.15
22	P	306	CHD	C15-C14-C13	3.29	106.78	103.55
25	C	309	DMU	C10-O1-C9	3.29	120.14	113.69
22	C	308	CHD	C5-C6-C7	3.28	118.08	114.46
22	W	101	CHD	C11-C12-C13	3.27	114.61	111.24
14	A	602	HEA	C13-C12-C11	-3.27	109.43	114.35
25	M	101	DMU	C18-O16-C6	-3.22	108.50	113.84
20	N	611	TGL	OG3-CC1-CC2	3.21	121.99	111.91
22	B	303	CHD	C19-C10-C1	-3.15	103.19	108.26
25	P	307	DMU	O16-C6-C1	3.14	113.20	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	608	TGL	OG3-CC1-CC2	3.12	121.70	111.91
18	C	304	PGV	O03-C19-C20	3.10	121.64	111.91
22	O	301	CHD	O12-C12-C11	-3.10	102.81	109.12
14	N	602	HEA	CAA-CBA-CGA	-3.09	107.48	112.67
14	N	602	HEA	OMA-CMA-C3A	-3.09	118.17	124.91
18	C	305	PGV	O03-C19-C20	3.08	121.58	111.91
14	A	602	HEA	C1B-C2B-C3B	-3.07	104.86	107.00
18	A	606	PGV	O03-C19-C20	3.04	121.46	111.91
22	C	307	CHD	C19-C10-C1	-3.04	103.37	108.26
24	G	101	CDL	OB8-CB7-C71	3.03	121.41	111.91
24	G	101	CDL	OA8-CA7-C31	3.02	121.39	111.91
22	P	306	CHD	C15-C14-C8	3.02	122.56	118.33
14	N	601	HEA	C27-C19-C20	3.02	120.34	115.27
22	J	101	CHD	C22-C20-C17	3.00	116.48	110.28
26	R	201	PSC	O03-C19-C20	2.99	121.29	111.91
22	C	307	CHD	C11-C9-C10	-2.99	110.64	113.73
14	A	601	HEA	C27-C19-C20	2.99	120.30	115.27
24	C	306	CDL	CB4-OB6-CB5	-2.99	110.43	117.79
14	N	601	HEA	CMC-C2C-C1C	-2.99	123.87	128.46
14	A	601	HEA	CMB-C2B-C1B	-2.99	123.88	128.46
22	J	101	CHD	C4-C5-C10	2.98	115.82	112.66
18	A	606	PGV	O01-C1-O02	-2.98	116.51	123.70
20	Q	201	TGL	OG2-CB1-CB2	2.95	117.86	111.50
20	B	301	TGL	OG1-CA1-CA2	2.95	121.16	111.91
14	A	602	HEA	CMD-C2D-C3D	2.95	130.50	124.94
14	N	601	HEA	C13-C12-C11	-2.95	109.92	114.35
22	O	301	CHD	C18-C13-C17	-2.95	106.60	111.21
18	N	606	PGV	O03-C19-O04	-2.95	116.16	123.59
20	Q	201	TGL	OG3-CC1-CC2	2.92	121.08	111.91
14	A	601	HEA	C25-C23-C22	-2.91	114.23	122.65
14	N	601	HEA	C1B-C2B-C3B	-2.90	104.98	107.00
24	C	306	CDL	OB8-CB7-OB9	-2.89	116.30	123.59
20	L	101	TGL	CG2-OG2-CB1	2.88	124.88	117.79
23	G	102	PEK	O03-C21-O04	-2.88	116.33	123.59
18	A	606	PGV	C02-O01-C1	-2.87	110.72	117.79
22	W	101	CHD	C13-C14-C8	-2.85	111.10	114.74
14	N	601	HEA	CMC-C2C-C3C	2.84	130.00	124.68
14	N	601	HEA	C13-C14-C15	-2.82	120.86	127.66
23	T	101	PEK	O03-C21-C22	2.81	120.74	111.91
14	N	602	HEA	C13-C12-C11	-2.81	110.12	114.35
22	J	101	CHD	C23-C22-C20	-2.79	110.97	114.72
22	W	101	CHD	C9-C10-C5	2.78	112.48	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	608	PGV	O01-C1-C2	2.77	117.47	111.50
20	N	611	TGL	OG3-CC1-OC1	-2.76	116.62	123.59
24	T	103	CDL	OB8-CB7-C71	2.76	120.57	111.91
14	A	601	HEA	C20-C21-C22	-2.76	102.81	111.88
22	J	101	CHD	C1-C10-C5	2.76	111.85	107.77
20	D	201	TGL	OG3-CC1-OC1	-2.76	116.63	123.59
14	A	602	HEA	CMC-C2C-C1C	-2.76	124.22	128.46
22	W	101	CHD	C6-C5-C4	-2.75	108.03	111.19
14	A	602	HEA	C3C-C4C-NC	2.75	112.76	109.21
22	C	307	CHD	C6-C7-C8	2.74	114.41	111.48
22	N	610	CHD	C21-C20-C22	-2.74	106.07	110.36
23	C	303	PEK	O03-C21-C22	2.73	120.48	111.91
22	C	307	CHD	C1-C10-C5	2.72	111.79	107.77
20	L	101	TGL	OG1-CA1-CA2	2.71	120.43	111.91
22	C	307	CHD	C15-C14-C8	2.71	122.13	118.33
22	J	101	CHD	C15-C14-C13	2.70	106.20	103.55
24	P	305	CDL	OB8-CB7-OB9	-2.70	116.78	123.59
23	C	302	PEK	O03-C21-O04	-2.70	116.78	123.59
24	P	305	CDL	OA8-CA7-C31	2.70	120.37	111.91
22	C	308	CHD	C19-C10-C1	-2.69	103.92	108.26
22	J	101	CHD	C9-C10-C5	2.67	112.33	108.58
18	N	606	PGV	C3-C2-C1	-2.67	103.92	113.62
22	J	101	CHD	C17-C13-C12	2.66	120.09	117.67
24	T	103	CDL	OB8-CB7-OB9	-2.65	116.90	123.59
20	B	301	TGL	OB1-CB1-CB2	-2.64	113.41	123.73
14	N	602	HEA	CMB-C2B-C3B	2.64	129.86	124.69
22	W	101	CHD	C1-C10-C5	2.63	111.66	107.77
18	N	609	PGV	O01-C1-C2	2.63	117.17	111.50
22	W	101	CHD	C23-C22-C20	-2.62	111.19	114.72
22	N	610	CHD	C6-C5-C4	-2.62	108.17	111.19
18	A	606	PGV	O03-C19-O04	-2.62	116.98	123.59
20	L	101	TGL	C25-C24-C23	-2.62	101.15	114.42
14	A	602	HEA	CMC-C2C-C3C	2.61	129.56	124.68
18	N	609	PGV	O01-C1-O02	-2.61	117.40	123.70
24	T	103	CDL	OA8-CA7-C31	2.60	120.07	111.91
24	C	306	CDL	OA8-CA7-C31	2.59	120.05	111.91
14	N	601	HEA	CMB-C2B-C3B	2.58	129.75	124.69
14	A	601	HEA	C3C-C4C-NC	2.58	112.55	109.21
14	N	602	HEA	C20-C19-C18	-2.58	115.90	121.12
23	P	302	PEK	O03-C21-C22	2.57	119.98	111.91
14	A	601	HEA	O11-C11-C3B	-2.57	104.59	112.00
22	C	307	CHD	C6-C5-C10	2.55	115.37	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	CMD-C2D-C3D	2.55	129.75	124.94
22	N	610	CHD	C22-C20-C17	-2.55	105.02	110.28
18	P	304	PGV	C01-O03-C19	2.52	126.46	117.12
22	W	101	CHD	C22-C20-C17	2.52	115.49	110.28
23	C	302	PEK	O01-C1-C2	2.51	116.92	111.50
22	C	307	CHD	C6-C5-C4	-2.51	108.30	111.19
22	P	306	CHD	C10-C9-C8	2.51	114.52	111.82
22	P	306	CHD	C4-C3-C2	2.51	113.55	110.55
20	L	101	TGL	OG3-CC1-OC1	-2.49	117.31	123.59
22	O	301	CHD	C16-C17-C20	-2.49	108.30	112.15
22	W	101	CHD	C1-C2-C3	2.47	113.64	110.47
14	A	601	HEA	OMA-CMA-C3A	-2.47	119.53	124.91
18	A	606	PGV	C24-C23-C22	-2.46	101.92	114.42
22	O	301	CHD	C11-C9-C10	-2.45	111.20	113.73
26	E	201	PSC	O03-C19-C20	2.44	119.56	111.91
22	W	101	CHD	C10-C9-C8	2.43	114.43	111.82
20	Q	201	TGL	OG1-CA1-CA2	2.42	119.50	111.91
22	B	303	CHD	C4-C3-C2	2.41	113.43	110.55
22	W	101	CHD	C17-C13-C14	-2.41	97.66	100.09
22	P	306	CHD	C5-C4-C3	-2.41	109.23	112.76
14	N	602	HEA	CMB-C2B-C1B	-2.40	124.77	128.46
20	D	201	TGL	OG3-CC1-CC2	2.39	119.41	111.91
23	C	303	PEK	C01-O03-C21	2.39	125.97	117.12
22	C	307	CHD	C15-C14-C13	2.39	105.89	103.55
22	P	306	CHD	C16-C17-C13	2.38	105.89	103.55
22	W	101	CHD	C6-C7-C8	2.38	114.02	111.48
22	C	308	CHD	C6-C5-C4	-2.37	108.46	111.19
20	L	101	TGL	OG2-CB1-OB1	-2.37	117.98	123.70
24	T	103	CDL	OB8-CB6-CB4	2.37	115.33	108.43
14	N	601	HEA	CMD-C2D-C3D	2.35	129.38	124.94
14	N	602	HEA	C1B-C2B-C3B	-2.35	105.36	107.00
18	C	305	PGV	C01-O03-C19	2.35	125.83	117.12
24	G	101	CDL	OA6-CA5-OA7	-2.34	118.04	123.70
18	P	303	PGV	O03-C19-O04	-2.33	117.71	123.59
14	A	601	HEA	C4B-C3B-C2B	2.33	108.50	106.87
22	P	306	CHD	C6-C5-C10	2.32	115.12	112.66
22	W	101	CHD	C5-C6-C7	2.32	117.02	114.46
24	T	103	CDL	OA6-CA5-OA7	-2.32	118.11	123.70
24	P	305	CDL	C54-C53-C52	-2.30	102.77	114.42
25	Z	101	DMU	C18-O16-C6	-2.29	110.04	113.84
23	T	102	PEK	O03-C21-O04	-2.29	117.81	123.59
23	T	102	PEK	O01-C1-C2	2.28	116.42	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	309	DMU	O16-C6-C1	2.28	111.86	108.30
22	C	307	CHD	C17-C13-C12	-2.26	115.60	117.67
22	C	308	CHD	C11-C12-C13	2.25	113.55	111.24
22	C	307	CHD	C5-C6-C7	2.25	116.94	114.46
20	L	101	TGL	CA4-CA3-CA2	-2.24	105.13	113.19
24	G	101	CDL	OB6-CB5-OB7	-2.24	118.29	123.70
18	N	609	PGV	O03-C01-C02	2.23	114.93	108.43
20	D	201	TGL	OG1-CA1-CA2	2.23	118.91	111.91
23	C	303	PEK	O03-C21-O04	-2.23	117.97	123.59
14	N	602	HEA	C27-C19-C20	2.22	119.01	115.27
22	O	301	CHD	C11-C9-C8	2.22	114.12	110.88
14	N	601	HEA	C25-C23-C22	-2.21	116.25	122.65
18	P	303	PGV	O03-C19-C20	2.20	118.82	111.91
23	C	302	PEK	C01-O03-C21	2.20	125.27	117.12
25	P	307	DMU	C18-O16-C6	2.20	117.48	113.84
20	B	301	TGL	CG3-OG3-CC1	2.19	125.24	117.12
22	B	303	CHD	C17-C13-C12	2.19	119.67	117.67
25	M	101	DMU	C22-C19-C18	-2.18	103.82	113.49
22	C	307	CHD	C16-C17-C13	2.18	105.69	103.55
14	N	601	HEA	C3C-C4C-NC	2.17	112.01	109.21
24	C	306	CDL	OA6-CA5-OA7	-2.17	118.46	123.70
22	C	308	CHD	C18-C13-C12	2.15	111.25	109.07
22	P	306	CHD	C11-C9-C8	2.15	114.02	110.88
22	C	307	CHD	C11-C9-C8	2.14	114.02	110.88
22	C	308	CHD	C15-C14-C13	2.14	105.66	103.55
14	N	601	HEA	O11-C11-C3B	-2.14	105.83	112.00
18	N	606	PGV	C02-O01-C1	-2.14	112.53	117.79
18	A	608	PGV	O01-C1-O02	-2.14	118.54	123.70
24	C	306	CDL	OB6-CB5-OB7	-2.12	118.57	123.70
20	N	611	TGL	OG2-CB1-OB1	-2.12	118.58	123.70
22	C	307	CHD	C4-C5-C10	2.12	114.91	112.66
14	A	602	HEA	C26-C15-C16	2.11	118.82	115.27
20	Q	201	TGL	OG1-CA1-OA1	-2.11	118.27	123.59
18	P	303	PGV	O01-C1-O02	-2.10	118.61	123.70
22	J	101	CHD	C18-C13-C17	2.10	114.50	111.21
14	A	601	HEA	CBD-CAD-C3D	-2.10	108.61	112.49
22	P	306	CHD	C14-C8-C9	-2.10	106.83	109.71
24	C	306	CDL	CB6-OB8-CB7	2.10	124.89	117.12
22	W	101	CHD	C19-C10-C9	-2.10	108.30	111.18
22	J	101	CHD	C11-C12-C13	2.09	113.39	111.24
14	N	601	HEA	CMB-C2B-C1B	-2.09	125.26	128.46
14	A	602	HEA	C16-C15-C14	-2.07	116.92	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	CBA-CAA-C2A	2.07	116.30	112.48
20	N	608	TGL	OG1-CA1-OA1	-2.07	118.37	123.59
24	C	306	CDL	C83-C82-C81	2.07	124.92	114.42
23	C	303	PEK	O01-C1-O02	-2.06	118.72	123.70
23	T	101	PEK	C01-O03-C21	2.06	124.74	117.12
22	O	301	CHD	C23-C22-C20	-2.05	111.96	114.72
24	P	305	CDL	OA6-CA5-OA7	-2.04	118.77	123.70
20	D	201	TGL	CG3-OG3-CC1	2.04	124.66	117.12
14	N	602	HEA	C3C-C4C-NC	2.03	111.83	109.21
20	L	101	TGL	C23-C22-C21	-2.03	104.13	114.42
14	A	601	HEA	C25-C23-C24	2.03	119.08	114.60
14	N	601	HEA	C20-C21-C22	2.02	118.53	111.88
18	N	606	PGV	C01-O03-C19	2.02	124.59	117.12
18	A	606	PGV	O05-C05-C04	2.01	116.61	109.56
23	P	302	PEK	O03-C21-O04	-2.01	118.52	123.59
23	T	102	PEK	O13-P-O14	2.01	122.17	112.24
18	N	606	PGV	O01-C1-O02	-2.01	118.85	123.70
22	O	301	CHD	C19-C10-C1	-2.01	105.03	108.26
14	A	602	HEA	O11-C11-C3B	-2.00	106.22	112.00

All (9) chirality outliers are listed below:

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

All (892) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	P	304	PGV	C10-C11-C12-C13
18	N	606	PGV	C03-O11-P-O13
18	N	606	PGV	C03-O11-P-O14
18	N	606	PGV	C02-C03-O11-P
18	N	606	PGV	C04-C05-C06-O06
18	N	606	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
18	N	606	PGV	C20-C19-O03-C01
18	C	305	PGV	C03-O11-P-O13
18	C	305	PGV	C04-C05-C06-O06
22	C	307	CHD	C13-C17-C20-C21
26	R	201	PSC	C04-O12-P-O13
26	R	201	PSC	C01-C02-O01-C1
26	R	201	PSC	O12-C04-C05-N
24	G	101	CDL	CB2-C1-CA2-OA2
24	G	101	CDL	CA3-OA5-PA1-OA2
24	G	101	CDL	CA3-OA5-PA1-OA3
24	G	101	CDL	CA3-OA5-PA1-OA4
24	G	101	CDL	OA9-CA7-OA8-CA6
24	G	101	CDL	C31-CA7-OA8-CA6
24	G	101	CDL	CB2-OB2-PB2-OB3
24	G	101	CDL	CB3-OB5-PB2-OB2
24	G	101	CDL	CB3-OB5-PB2-OB3
24	G	101	CDL	CB3-OB5-PB2-OB4
24	G	101	CDL	C51-CB5-OB6-CB4
20	B	301	TGL	OB1-CB1-OG2-CG2
18	A	606	PGV	C03-O11-P-O12
18	A	606	PGV	C03-O11-P-O13
18	A	606	PGV	C03-O11-P-O14
18	A	606	PGV	O12-C04-C05-O05
18	A	606	PGV	C10-C11-C12-C13
23	C	303	PEK	C03-O11-P-O12
23	C	303	PEK	C03-O11-P-O13
23	C	303	PEK	C03-O11-P-O14
23	C	303	PEK	C04-O12-P-O13
23	C	303	PEK	C04-O12-P-O14
23	C	303	PEK	C2-C1-O01-C02
23	C	303	PEK	C10-C11-C12-C13
23	T	101	PEK	C03-O11-P-O14
23	T	101	PEK	O12-C04-C05-N
24	C	306	CDL	C1-CA2-OA2-PA1
24	C	306	CDL	CA2-OA2-PA1-OA4
24	C	306	CDL	CA3-OA5-PA1-OA4
24	C	306	CDL	C11-CA5-OA6-CA4
24	C	306	CDL	CB2-OB2-PB2-OB3
24	C	306	CDL	CB2-OB2-PB2-OB4
24	C	306	CDL	OB7-CB5-OB6-CB4
14	A	602	HEA	O11-C11-C12-C13
23	C	302	PEK	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	T	103	CDL	CA3-OA5-PA1-OA4
24	T	103	CDL	OA6-CA4-CA6-OA8
24	T	103	CDL	C11-CA5-OA6-CA4
24	T	103	CDL	C1-CB2-OB2-PB2
24	T	103	CDL	CB2-OB2-PB2-OB5
24	T	103	CDL	CB3-OB5-PB2-OB3
24	T	103	CDL	CB3-OB5-PB2-OB4
24	T	103	CDL	C51-CB5-OB6-CB4
22	W	101	CHD	C13-C17-C20-C21
22	W	101	CHD	C13-C17-C20-C22
22	W	101	CHD	C16-C17-C20-C21
22	W	101	CHD	C16-C17-C20-C22
25	P	307	DMU	C1-C6-O16-C18
25	P	307	DMU	O5-C6-O16-C18
26	E	201	PSC	O12-C04-C05-N
20	N	611	TGL	CB2-CB1-OG2-CG2
20	N	611	TGL	OB1-CB1-OG2-CG2
25	C	309	DMU	C1-C6-O16-C18
23	G	102	PEK	C04-O12-P-O14
23	G	102	PEK	O04-C21-O03-C01
23	G	102	PEK	C22-C21-O03-C01
23	G	102	PEK	C12-C13-C14-C15
20	L	101	TGL	CB2-CB1-OG2-CG2
20	L	101	TGL	OB1-CB1-OG2-CG2
24	P	305	CDL	O1-C1-CA2-OA2
24	P	305	CDL	C1-CA2-OA2-PA1
24	P	305	CDL	CA3-OA5-PA1-OA4
24	P	305	CDL	OA7-CA5-OA6-CA4
24	P	305	CDL	CB2-OB2-PB2-OB3
24	P	305	CDL	CB2-OB2-PB2-OB4
24	P	305	CDL	CB2-OB2-PB2-OB5
24	P	305	CDL	CB3-OB5-PB2-OB3
24	P	305	CDL	CB3-OB5-PB2-OB4
24	P	305	CDL	C51-CB5-OB6-CB4
23	P	302	PEK	C04-O12-P-O14
23	P	302	PEK	O02-C1-O01-C02
23	P	302	PEK	C2-C1-O01-C02
23	P	302	PEK	C4-C5-C6-C7
20	B	301	TGL	CC2-CC1-OG3-CG3
26	R	201	PSC	O04-C19-O03-C01
20	B	301	TGL	OC1-CC1-OG3-CG3
18	A	606	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
24	C	306	CDL	OB9-CB7-OB8-CB6
20	D	201	TGL	OC1-CC1-OG3-CG3
22	C	307	CHD	C16-C17-C20-C21
22	C	307	CHD	C13-C17-C20-C22
24	G	101	CDL	OA7-CA5-OA6-CA4
24	G	101	CDL	OB7-CB5-OB6-CB4
23	C	303	PEK	O02-C1-O01-C02
24	C	306	CDL	OA7-CA5-OA6-CA4
24	T	103	CDL	OA7-CA5-OA6-CA4
24	T	103	CDL	OB7-CB5-OB6-CB4
24	P	305	CDL	OB7-CB5-OB6-CB4
24	C	306	CDL	CB4-CB6-OB8-CB7
26	R	201	PSC	C20-C19-O03-C01
20	B	301	TGL	CB2-CB1-OG2-CG2
24	C	306	CDL	C51-CB5-OB6-CB4
24	P	305	CDL	C11-CA5-OA6-CA4
22	C	307	CHD	C16-C17-C20-C22
14	A	601	HEA	C27-C19-C20-C21
18	A	606	PGV	C20-C19-O03-C01
24	C	306	CDL	C71-CB7-OB8-CB6
20	D	201	TGL	CC2-CC1-OG3-CG3
23	T	102	PEK	C4-C5-C6-C7
23	T	102	PEK	C13-C14-C15-C16
23	C	303	PEK	C4-C5-C6-C7
26	E	201	PSC	C11-C12-C13-C14
18	N	609	PGV	C10-C11-C12-C13
23	P	302	PEK	C13-C14-C15-C16
25	C	309	DMU	C19-C22-C25-C28
22	W	101	CHD	C17-C20-C22-C23
23	C	303	PEK	C34-C35-C36-C37
18	N	606	PGV	O12-C04-C05-O05
24	G	101	CDL	O1-C1-CA2-OA2
24	G	101	CDL	O1-C1-CB2-OB2
24	G	101	CDL	C71-CB7-OB8-CB6
24	T	103	CDL	C71-CB7-OB8-CB6
24	T	103	CDL	OB9-CB7-OB8-CB6
18	N	606	PGV	C2-C1-O01-C02
24	G	101	CDL	C11-CA5-OA6-CA4
24	C	306	CDL	C37-C38-C39-C40
24	G	101	CDL	C15-C16-C17-C18
24	G	101	CDL	C78-C79-C80-C81
24	C	306	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
24	T	103	CDL	C40-C41-C42-C43
24	T	103	CDL	C79-C80-C81-C82
18	P	303	PGV	C28-C29-C30-C31
20	N	608	TGL	C24-C25-C26-C27
26	E	201	PSC	C20-C21-C22-C23
18	N	606	PGV	O02-C1-O01-C02
24	G	101	CDL	OB9-CB7-OB8-CB6
26	E	201	PSC	O04-C19-O03-C01
25	C	309	DMU	O5-C6-O16-C18
14	A	601	HEA	C15-C16-C17-C18
20	N	611	TGL	CA9-C20-C21-C22
26	E	201	PSC	C20-C19-O03-C01
25	P	307	DMU	O6-C11-C9-O1
25	P	307	DMU	O6-C11-C9-C8
18	C	305	PGV	O12-C04-C05-C06
24	G	101	CDL	CA2-C1-CB2-OB2
24	T	103	CDL	CA2-C1-CB2-OB2
25	C	309	DMU	C3-C4-C57-O61
24	G	101	CDL	C41-C42-C43-C44
20	Q	201	TGL	CC2-CC1-OG3-CG3
20	N	611	TGL	CA2-CA1-OG1-CG1
20	L	101	TGL	CA2-CA1-OG1-CG1
20	L	101	TGL	CC1-CC2-CC3-CC4
18	C	305	PGV	O01-C02-C03-O11
24	T	103	CDL	O1-C1-CB2-OB2
22	W	101	CHD	C21-C20-C22-C23
23	T	102	PEK	C1-C2-C3-C4
23	P	302	PEK	C21-C22-C23-C24
25	C	309	DMU	O5-C4-C57-O61
25	C	309	DMU	O6-C11-C9-O1
18	A	608	PGV	C26-C27-C28-C29
20	Q	201	TGL	OC1-CC1-OG3-CG3
20	L	101	TGL	OA1-CA1-OG1-CG1
20	N	608	TGL	CA2-CA1-OG1-CG1
23	T	101	PEK	C1-C2-C3-C4
23	C	303	PEK	C7-C8-C9-C10
23	C	302	PEK	C4-C5-C6-C7
25	M	101	DMU	O6-C11-C9-O1
18	N	606	PGV	C1-C2-C3-C4
18	C	305	PGV	C1-C2-C3-C4
23	G	102	PEK	C21-C22-C23-C24
24	P	305	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	E	201	PSC	C1-C2-C3-C4
22	J	101	CHD	C13-C17-C20-C21
20	N	611	TGL	OA1-CA1-OG1-CG1
24	C	306	CDL	CA5-C11-C12-C13
20	N	608	TGL	CB1-CB2-CB3-CB4
20	D	201	TGL	C21-C22-C23-C24
25	M	101	DMU	O6-C11-C9-C8
14	N	601	HEA	C19-C20-C21-C22
22	J	101	CHD	C16-C17-C20-C21
22	J	101	CHD	C13-C17-C20-C22
26	R	201	PSC	C11-C10-C9-C8
23	T	102	PEK	C10-C11-C12-C13
23	G	102	PEK	C7-C8-C9-C10
20	N	608	TGL	OA1-CA1-OG1-CG1
18	N	606	PGV	C03-O11-P-O12
26	R	201	PSC	C03-O11-P-O12
26	R	201	PSC	C04-O12-P-O11
24	G	101	CDL	CA2-OA2-PA1-OA5
18	A	606	PGV	C04-O12-P-O11
23	C	303	PEK	C04-O12-P-O11
24	C	306	CDL	CA2-OA2-PA1-OA5
24	C	306	CDL	CB2-OB2-PB2-OB5
24	C	306	CDL	CB3-OB5-PB2-OB2
24	T	103	CDL	CB3-OB5-PB2-OB2
26	E	201	PSC	C04-O12-P-O11
23	G	102	PEK	C03-O11-P-O12
23	G	102	PEK	C04-O12-P-O11
24	P	305	CDL	CB3-OB5-PB2-OB2
23	P	302	PEK	C03-O11-P-O12
18	N	606	PGV	O12-C04-C05-C06
18	A	606	PGV	O12-C04-C05-C06
24	P	305	CDL	CB2-C1-CA2-OA2
14	A	601	HEA	C18-C19-C20-C21
26	E	201	PSC	C04-C05-N-C06
26	E	201	PSC	C04-C05-N-C07
26	E	201	PSC	C04-C05-N-C08
22	P	306	CHD	C20-C22-C23-C24
24	T	103	CDL	C62-C63-C64-C65
18	N	609	PGV	C23-C24-C25-C26
18	N	606	PGV	C25-C26-C27-C28
18	C	305	PGV	C30-C31-C32-C33
26	R	201	PSC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
24	G	101	CDL	C35-C36-C37-C38
24	G	101	CDL	C60-C61-C62-C63
24	G	101	CDL	C61-C62-C63-C64
20	B	301	TGL	CC4-CC5-CC6-CC7
20	B	301	TGL	C16-C15-CC9-CC8
20	B	301	TGL	C16-C17-C18-C19
18	A	606	PGV	C30-C31-C32-C33
24	C	306	CDL	C51-C52-C53-C54
24	C	306	CDL	C80-C81-C82-C83
20	N	611	TGL	C21-C22-C23-C24
20	D	201	TGL	CC2-CC3-CC4-CC5
18	A	608	PGV	C27-C28-C29-C30
24	P	305	CDL	C57-C58-C59-C60
18	C	305	PGV	C3-C4-C5-C6
24	G	101	CDL	C51-C52-C53-C54
23	C	303	PEK	C33-C34-C35-C36
20	Q	201	TGL	C10-C11-C12-C13
20	Q	201	TGL	C13-C14-C29-C30
24	C	306	CDL	C17-C18-C19-C20
23	C	302	PEK	C32-C33-C34-C35
18	C	304	PGV	C13-C14-C15-C16
20	N	608	TGL	CB7-CB8-CB9-C10
20	N	611	TGL	CB5-CB6-CB7-CB8
20	N	611	TGL	CC3-CC4-CC5-CC6
18	P	303	PGV	C24-C25-C26-C27
20	L	101	TGL	CB5-CB6-CB7-CB8
24	P	305	CDL	C62-C63-C64-C65
24	C	306	CDL	C23-C24-C25-C26
24	T	103	CDL	C31-C32-C33-C34
24	T	103	CDL	C71-C72-C73-C74
18	C	305	PGV	C22-C23-C24-C25
26	R	201	PSC	C20-C21-C22-C23
24	G	101	CDL	C38-C39-C40-C41
23	T	101	PEK	C23-C24-C25-C26
20	N	611	TGL	C21-C20-CA9-CA8
20	N	611	TGL	C10-C11-C12-C13
20	D	201	TGL	C19-C33-C34-C35
18	C	305	PGV	O12-C04-C05-O05
20	B	301	TGL	C10-C11-C12-C13
23	C	303	PEK	C26-C27-C28-C29
24	T	103	CDL	C82-C83-C84-C85
26	E	201	PSC	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	D	201	TGL	C16-C15-CC9-CC8
23	C	303	PEK	C1-C2-C3-C4
20	D	201	TGL	CC1-CC2-CC3-CC4
18	P	304	PGV	C20-C19-O03-C01
18	P	304	PGV	C22-C23-C24-C25
24	G	101	CDL	C43-C44-C45-C46
23	T	102	PEK	C26-C27-C28-C29
23	T	101	PEK	C32-C33-C34-C35
24	T	103	CDL	C43-C44-C45-C46
20	L	101	TGL	C18-C19-C33-C34
24	G	101	CDL	C71-C72-C73-C74
24	G	101	CDL	C74-C75-C76-C77
20	B	301	TGL	CA5-CA6-CA7-CA8
23	T	102	PEK	C33-C34-C35-C36
24	C	306	CDL	C14-C15-C16-C17
24	C	306	CDL	C15-C16-C17-C18
20	L	101	TGL	C11-C10-CB9-CB8
18	P	304	PGV	C24-C25-C26-C27
24	G	101	CDL	C22-C23-C24-C25
20	Q	201	TGL	CA7-CA8-CA9-C20
24	C	306	CDL	C13-C14-C15-C16
23	C	302	PEK	C30-C31-C32-C33
23	C	302	PEK	C31-C32-C33-C34
24	T	103	CDL	C80-C81-C82-C83
20	N	608	TGL	C13-C14-C29-C30
20	N	608	TGL	C16-C15-CC9-CC8
20	N	611	TGL	C18-C19-C33-C34
20	D	201	TGL	C13-C14-C29-C30
23	G	102	PEK	C33-C34-C35-C36
20	L	101	TGL	CA3-CA4-CA5-CA6
25	M	101	DMU	C19-C22-C25-C28
24	P	305	CDL	C18-C19-C20-C21
24	P	305	CDL	C37-C38-C39-C40
18	N	606	PGV	C5-C6-C7-C8
25	Z	101	DMU	C28-C31-C34-C37
24	G	101	CDL	C83-C84-C85-C86
24	T	103	CDL	C53-C54-C55-C56
20	N	608	TGL	CB6-CB7-CB8-CB9
25	P	307	DMU	C22-C25-C28-C31
20	D	201	TGL	C21-C20-CA9-CA8
20	L	101	TGL	C21-C22-C23-C24
24	P	305	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
18	P	304	PGV	C04-C05-C06-O06
18	A	606	PGV	C04-C05-C06-O06
20	N	608	TGL	OB1-CB1-OG2-CG2
24	G	101	CDL	C21-C22-C23-C24
20	Q	201	TGL	CB4-CB5-CB6-CB7
24	C	306	CDL	C55-C56-C57-C58
23	C	302	PEK	C26-C27-C28-C29
24	T	103	CDL	C63-C64-C65-C66
18	N	606	PGV	C11-C10-C9-C8
26	E	201	PSC	C6-C7-C8-C9
20	D	201	TGL	CB1-CB2-CB3-CB4
24	P	305	CDL	CB7-C71-C72-C73
18	A	606	PGV	C13-C14-C15-C16
24	C	306	CDL	C35-C36-C37-C38
20	N	608	TGL	CA6-CA7-CA8-CA9
20	N	608	TGL	CB4-CB5-CB6-CB7
20	N	611	TGL	CB4-CB5-CB6-CB7
20	N	611	TGL	C16-C17-C18-C19
20	N	611	TGL	C19-C33-C34-C35
20	D	201	TGL	C23-C24-C25-C26
20	L	101	TGL	C13-C14-C29-C30
20	L	101	TGL	C22-C23-C24-C25
24	P	305	CDL	C22-C23-C24-C25
24	P	305	CDL	C55-C56-C57-C58
18	P	304	PGV	C20-C21-C22-C23
24	C	306	CDL	C11-C12-C13-C14
20	L	101	TGL	CB3-CB4-CB5-CB6
23	T	102	PEK	O12-C04-C05-N
18	N	606	PGV	C21-C22-C23-C24
20	B	301	TGL	C17-C18-C19-C33
24	C	306	CDL	C79-C80-C81-C82
18	C	304	PGV	C7-C8-C9-C10
26	E	201	PSC	C5-C6-C7-C8
20	L	101	TGL	C16-C15-CC9-CC8
18	N	606	PGV	C4-C5-C6-C7
18	N	606	PGV	C14-C15-C16-C17
18	C	304	PGV	C25-C26-C27-C28
20	D	201	TGL	CC5-CC6-CC7-CC8
20	D	201	TGL	C14-C29-C30-C31
24	P	305	CDL	C21-C22-C23-C24
24	P	305	CDL	C83-C84-C85-C86
23	C	303	PEK	C22-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
18	C	305	PGV	C4-C5-C6-C7
20	Q	201	TGL	CB9-C10-C11-C12
20	Q	201	TGL	CC3-CC4-CC5-CC6
24	P	305	CDL	C82-C83-C84-C85
23	P	302	PEK	C28-C29-C30-C31
25	C	309	DMU	C19-C18-O16-C6
20	Q	201	TGL	CC4-CC5-CC6-CC7
20	Q	201	TGL	C20-C21-C22-C23
20	N	611	TGL	C13-C14-C29-C30
20	B	301	TGL	C21-C20-CA9-CA8
20	Q	201	TGL	CB5-CB6-CB7-CB8
20	N	608	TGL	CA5-CA6-CA7-CA8
20	N	611	TGL	C16-C15-CC9-CC8
20	L	101	TGL	C17-C18-C19-C33
26	R	201	PSC	C11-C12-C13-C14
23	C	302	PEK	C7-C8-C9-C10
23	G	102	PEK	C4-C5-C6-C7
24	T	103	CDL	C76-C77-C78-C79
18	C	305	PGV	C2-C1-O01-C02
20	Q	201	TGL	CB2-CB1-OG2-CG2
20	N	608	TGL	CB2-CB1-OG2-CG2
18	C	304	PGV	C20-C21-C22-C23
18	C	304	PGV	C27-C28-C29-C30
18	N	606	PGV	O05-C05-C06-O06
18	A	606	PGV	O05-C05-C06-O06
20	N	608	TGL	CB9-C10-C11-C12
23	G	102	PEK	C24-C25-C26-C27
18	P	304	PGV	C12-C13-C14-C15
23	C	303	PEK	C15-C16-C17-C18
23	C	302	PEK	C15-C16-C17-C18
20	N	608	TGL	CC5-CC6-CC7-CC8
20	L	101	TGL	CC3-CC4-CC5-CC6
20	B	301	TGL	CA4-CA5-CA6-CA7
24	P	305	CDL	C56-C57-C58-C59
25	Z	101	DMU	C25-C28-C31-C34
24	C	306	CDL	C78-C79-C80-C81
24	P	305	CDL	C38-C39-C40-C41
18	P	304	PGV	O04-C19-O03-C01
18	P	304	PGV	C29-C30-C31-C32
23	P	302	PEK	C26-C27-C28-C29
18	C	305	PGV	O02-C1-O01-C02
20	N	608	TGL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
23	C	303	PEK	O04-C21-O03-C01
18	A	606	PGV	C6-C7-C8-C9
23	C	303	PEK	C29-C30-C31-C32
24	C	306	CDL	C39-C40-C41-C42
20	D	201	TGL	C10-C11-C12-C13
18	P	304	PGV	C26-C27-C28-C29
24	G	101	CDL	C79-C80-C81-C82
24	T	103	CDL	C39-C40-C41-C42
20	D	201	TGL	CC9-C15-C16-C17
24	P	305	CDL	C33-C34-C35-C36
20	Q	201	TGL	CA2-CA1-OG1-CG1
24	G	101	CDL	C40-C41-C42-C43
24	G	101	CDL	C54-C55-C56-C57
20	B	301	TGL	C11-C12-C13-C14
24	C	306	CDL	C63-C64-C65-C66
20	D	201	TGL	CB9-C10-C11-C12
24	P	305	CDL	C13-C14-C15-C16
23	P	302	PEK	C29-C30-C31-C32
24	G	101	CDL	C31-C32-C33-C34
20	B	301	TGL	C23-C24-C25-C26
20	Q	201	TGL	C21-C20-CA9-CA8
24	C	306	CDL	C61-C62-C63-C64
24	C	306	CDL	C53-C54-C55-C56
24	T	103	CDL	C14-C15-C16-C17
24	P	305	CDL	C81-C82-C83-C84
23	T	101	PEK	C10-C11-C12-C13
18	P	303	PGV	C10-C11-C12-C13
23	P	302	PEK	C10-C11-C12-C13
24	G	101	CDL	C13-C14-C15-C16
24	P	305	CDL	C35-C36-C37-C38
18	P	304	PGV	C11-C10-C9-C8
18	C	305	PGV	C12-C13-C14-C15
18	A	606	PGV	C12-C13-C14-C15
23	T	102	PEK	C2-C3-C4-C5
20	Q	201	TGL	OB1-CB1-OG2-CG2
24	T	103	CDL	C31-CA7-OA8-CA6
20	L	101	TGL	CC6-CC7-CC8-CC9
20	L	101	TGL	C19-C33-C34-C35
24	G	101	CDL	C58-C59-C60-C61
20	B	301	TGL	CA3-CA4-CA5-CA6
23	C	303	PEK	C25-C26-C27-C28
20	Q	201	TGL	CC5-CC6-CC7-CC8

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Mol	Chain	Res	Type	Atoms
24	P	305	CDL	C72-C73-C74-C75
23	T	101	PEK	C31-C32-C33-C34
20	N	608	TGL	CB3-CB4-CB5-CB6
20	N	608	TGL	C12-C13-C14-C29
24	P	305	CDL	C11-C12-C13-C14
20	B	301	TGL	CA2-CA3-CA4-CA5
20	N	611	TGL	C15-C16-C17-C18
20	B	301	TGL	C13-C14-C29-C30
20	N	608	TGL	CC6-CC7-CC8-CC9
20	L	101	TGL	CA9-C20-C21-C22
18	N	606	PGV	C29-C30-C31-C32
24	G	101	CDL	C72-C73-C74-C75
20	N	608	TGL	C19-C33-C34-C35
18	N	606	PGV	C19-C20-C21-C22
18	A	606	PGV	C2-C1-O01-C02
23	G	102	PEK	C2-C1-O01-C02
24	C	306	CDL	OB5-CB3-CB4-OB6
24	G	101	CDL	C32-C33-C34-C35
24	T	103	CDL	C21-C22-C23-C24
20	L	101	TGL	C20-C21-C22-C23
25	M	101	DMU	C31-C34-C37-C40
23	G	102	PEK	O02-C1-O01-C02
24	G	101	CDL	C56-C57-C58-C59
20	Q	201	TGL	C22-C23-C24-C25
23	T	101	PEK	C22-C23-C24-C25
20	B	301	TGL	CB4-CB5-CB6-CB7
18	P	303	PGV	C30-C31-C32-C33
20	B	301	TGL	CA9-C20-C21-C22
20	N	611	TGL	CB7-CB8-CB9-C10
20	Q	201	TGL	OA1-CA1-OG1-CG1
18	A	606	PGV	O02-C1-O01-C02
20	N	611	TGL	CA5-CA6-CA7-CA8
25	C	309	DMU	C18-C19-C22-C25
18	C	305	PGV	C03-O11-P-O12
24	P	305	CDL	CA3-OA5-PA1-OA2
23	P	302	PEK	C04-O12-P-O11
26	R	201	PSC	C23-C24-C25-C26
18	A	606	PGV	C27-C28-C29-C30
20	N	608	TGL	C21-C20-CA9-CA8
20	N	608	TGL	C11-C10-CB9-CB8
18	N	606	PGV	C01-C02-C03-O11
18	C	305	PGV	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C01-C02-C03-O11
20	L	101	TGL	C11-C12-C13-C14
20	D	201	TGL	CA3-CA4-CA5-CA6
20	Q	201	TGL	C17-C18-C19-C33
24	T	103	CDL	C83-C84-C85-C86
26	R	201	PSC	C6-C7-C8-C9
23	G	102	PEK	C1-C2-C3-C4
18	N	606	PGV	C7-C8-C9-C10
24	T	103	CDL	C59-C60-C61-C62
23	P	302	PEK	C25-C26-C27-C28
20	D	201	TGL	CA6-CA7-CA8-CA9
24	T	103	CDL	OA9-CA7-OA8-CA6
24	G	101	CDL	CA3-CA4-CA6-OA8
20	N	611	TGL	OG1-CG1-CG2-CG3
23	G	102	PEK	O03-C01-C02-C03
20	L	101	TGL	OG1-CG1-CG2-CG3
23	T	101	PEK	C13-C14-C15-C16
26	E	201	PSC	C11-C10-C9-C8
24	G	101	CDL	C63-C64-C65-C66
20	B	301	TGL	C15-C16-C17-C18
18	C	304	PGV	C15-C16-C17-C18
26	E	201	PSC	C23-C24-C25-C26
26	E	201	PSC	C26-C27-C28-C29
23	T	102	PEK	C17-C18-C19-C20
24	C	306	CDL	C24-C25-C26-C27
20	D	201	TGL	C11-C12-C13-C14
26	R	201	PSC	C31-C32-C33-C34
23	C	302	PEK	C23-C24-C25-C26
23	G	102	PEK	C23-C24-C25-C26
18	C	304	PGV	C1-C2-C3-C4
24	P	305	CDL	C15-C16-C17-C18
24	P	305	CDL	C76-C77-C78-C79
24	P	305	CDL	C23-C24-C25-C26
18	C	305	PGV	O05-C05-C06-O06
26	R	201	PSC	C29-C30-C31-C32
24	T	103	CDL	C74-C75-C76-C77
20	D	201	TGL	CA4-CA5-CA6-CA7
18	C	304	PGV	C12-C13-C14-C15
24	G	101	CDL	C37-C38-C39-C40
24	T	103	CDL	C24-C25-C26-C27
18	N	606	PGV	C15-C16-C17-C18
20	B	301	TGL	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
24	P	305	CDL	C84-C85-C86-C87
20	B	301	TGL	CB1-CB2-CB3-CB4
23	T	101	PEK	C21-C22-C23-C24
18	P	304	PGV	C31-C32-C33-C34
20	Q	201	TGL	C16-C15-CC9-CC8
20	N	608	TGL	C25-C26-C27-C28
18	A	606	PGV	C2-C3-C4-C5
24	C	306	CDL	C33-C34-C35-C36
23	C	302	PEK	C24-C25-C26-C27
24	T	103	CDL	C78-C79-C80-C81
18	A	606	PGV	C22-C23-C24-C25
24	C	306	CDL	C60-C61-C62-C63
18	P	303	PGV	C11-C12-C13-C14
24	G	101	CDL	C1-CB2-OB2-PB2
24	C	306	CDL	C62-C63-C64-C65
20	N	608	TGL	CC2-CC1-OG3-CG3
23	G	102	PEK	O01-C02-C03-O11
20	Q	201	TGL	CB1-CB2-CB3-CB4
20	B	301	TGL	C20-C21-C22-C23
20	N	608	TGL	CA4-CA5-CA6-CA7
18	P	303	PGV	C11-C10-C9-C8
20	N	611	TGL	OG2-CG2-CG3-OG3
23	G	102	PEK	O03-C01-C02-O01
24	P	305	CDL	OB6-CB4-CB6-OB8
20	L	101	TGL	CC4-CC5-CC6-CC7
24	P	305	CDL	C61-C62-C63-C64
18	C	305	PGV	C2-C3-C4-C5
24	G	101	CDL	C44-C45-C46-C47
20	N	608	TGL	C11-C12-C13-C14
24	P	305	CDL	C36-C37-C38-C39
24	G	101	CDL	C42-C43-C44-C45
24	G	101	CDL	C57-C58-C59-C60
20	L	101	TGL	CB2-CB3-CB4-CB5
18	P	303	PGV	C7-C8-C9-C10
24	C	306	CDL	OA5-CA3-CA4-CA6
24	C	306	CDL	OB5-CB3-CB4-CB6
24	P	305	CDL	OA5-CA3-CA4-CA6
18	C	305	PGV	C14-C15-C16-C17
20	B	301	TGL	C18-C19-C33-C34
18	C	304	PGV	C28-C29-C30-C31
24	P	305	CDL	C74-C75-C76-C77
18	C	305	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
24	T	103	CDL	C58-C59-C60-C61
23	G	102	PEK	C25-C26-C27-C28
20	L	101	TGL	C15-C16-C17-C18
18	N	606	PGV	C27-C28-C29-C30
20	N	608	TGL	CC9-C15-C16-C17
20	N	611	TGL	C12-C13-C14-C29
18	P	304	PGV	C2-C3-C4-C5
20	B	301	TGL	CA7-CA8-CA9-C20
20	D	201	TGL	C11-C10-CB9-CB8
20	Q	201	TGL	C15-C16-C17-C18
18	P	303	PGV	C22-C23-C24-C25
24	T	103	CDL	C15-C16-C17-C18
24	T	103	CDL	C75-C76-C77-C78
20	N	611	TGL	CA2-CA3-CA4-CA5
24	C	306	CDL	CA3-CA4-CA6-OA8
24	T	103	CDL	CA3-CA4-CA6-OA8
24	G	101	CDL	C14-C15-C16-C17
18	A	608	PGV	C10-C11-C12-C13
24	G	101	CDL	C24-C25-C26-C27
18	N	609	PGV	C29-C30-C31-C32
18	C	305	PGV	C04-O12-P-O11
23	T	101	PEK	C5-C6-C7-C8
23	T	101	PEK	C9-C10-C11-C12
23	T	101	PEK	C11-C12-C13-C14
23	T	101	PEK	C12-C13-C14-C15
23	G	102	PEK	C5-C6-C7-C8
23	G	102	PEK	C11-C10-C9-C8
23	G	102	PEK	C11-C12-C13-C14
25	Z	101	DMU	O16-C18-C19-C22
24	P	305	CDL	C32-C33-C34-C35
18	P	304	PGV	O01-C02-C03-O11
18	N	606	PGV	O01-C02-C03-O11
23	P	302	PEK	O01-C02-C03-O11
20	B	301	TGL	CA2-CA1-OG1-CG1
18	A	608	PGV	C11-C10-C9-C8
20	N	608	TGL	OC1-CC1-OG3-CG3
20	D	201	TGL	CA1-CA2-CA3-CA4
18	N	609	PGV	C19-C20-C21-C22
18	P	304	PGV	C13-C14-C15-C16
24	C	306	CDL	C82-C83-C84-C85
18	N	609	PGV	C31-C32-C33-C34
24	P	305	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
24	P	305	CDL	OA6-CA4-CA6-OA8
20	D	201	TGL	CB2-CB3-CB4-CB5
24	P	305	CDL	C80-C81-C82-C83
18	P	304	PGV	O02-C1-O01-C02
26	R	201	PSC	C5-C6-C7-C8
18	C	304	PGV	C02-C03-O11-P
23	C	302	PEK	C25-C26-C27-C28
24	T	103	CDL	C16-C17-C18-C19
18	N	606	PGV	C13-C14-C15-C16
18	N	606	PGV	C23-C24-C25-C26
25	C	309	DMU	C28-C31-C34-C37
23	G	102	PEK	O01-C1-C2-C3
24	G	101	CDL	C75-C76-C77-C78
18	P	304	PGV	C2-C1-O01-C02
23	T	102	PEK	C2-C1-O01-C02
24	P	305	CDL	C34-C35-C36-C37
23	C	302	PEK	C22-C23-C24-C25
20	N	611	TGL	CB3-CB4-CB5-CB6
22	C	307	CHD	C21-C20-C22-C23
24	P	305	CDL	C58-C59-C60-C61
24	G	101	CDL	C20-C21-C22-C23
20	N	611	TGL	C33-C34-C35-C36
23	T	101	PEK	C4-C5-C6-C7
20	L	101	TGL	CA2-CA3-CA4-CA5
23	P	302	PEK	C31-C32-C33-C34
25	Z	101	DMU	C22-C25-C28-C31
24	T	103	CDL	C19-C20-C21-C22
20	N	608	TGL	CA7-CA8-CA9-C20
24	G	101	CDL	CB3-CB4-CB6-OB8
20	B	301	TGL	OG1-CG1-CG2-CG3
24	T	103	CDL	C1-CA2-OA2-PA1
24	P	305	CDL	CA3-CA4-CA6-OA8
24	C	306	CDL	OA5-CA3-CA4-OA6
26	E	201	PSC	O01-C02-C03-O11
25	Z	101	DMU	C19-C22-C25-C28
24	P	305	CDL	C43-C44-C45-C46
23	P	302	PEK	C33-C34-C35-C36
24	T	103	CDL	OB6-CB4-CB6-OB8
20	D	201	TGL	OG2-CG2-CG3-OG3
20	L	101	TGL	CC5-CC6-CC7-CC8
20	D	201	TGL	C16-C17-C18-C19
24	C	306	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
24	P	305	CDL	C31-C32-C33-C34
20	B	301	TGL	OA1-CA1-OG1-CG1
24	G	101	CDL	CB2-OB2-PB2-OB5
23	T	101	PEK	C03-O11-P-O12
24	T	103	CDL	C57-C58-C59-C60
18	C	304	PGV	C26-C27-C28-C29
18	P	304	PGV	C27-C28-C29-C30
23	G	102	PEK	C28-C29-C30-C31
18	A	606	PGV	C02-C03-O11-P
18	P	303	PGV	C02-C03-O11-P
20	B	301	TGL	C24-C25-C26-C27
18	C	305	PGV	C03-O11-P-O14
18	C	305	PGV	C04-O12-P-O14
26	R	201	PSC	C03-O11-P-O13
24	G	101	CDL	CA2-OA2-PA1-OA4
18	A	606	PGV	C04-O12-P-O13
18	A	606	PGV	C04-O12-P-O14
24	C	306	CDL	CA3-OA5-PA1-OA3
24	C	306	CDL	CB3-OB5-PB2-OB3
24	T	103	CDL	CB2-OB2-PB2-OB4
26	E	201	PSC	C04-O12-P-O13
23	G	102	PEK	C03-O11-P-O13
23	G	102	PEK	C03-O11-P-O14
23	G	102	PEK	C04-O12-P-O13
24	P	305	CDL	CA3-OA5-PA1-OA3
23	P	302	PEK	C03-O11-P-O14
23	P	302	PEK	C04-O12-P-O13
20	Q	201	TGL	CC1-CC2-CC3-CC4
18	P	304	PGV	C01-C02-C03-O11
23	G	102	PEK	C01-C02-C03-O11
23	P	302	PEK	C01-C02-C03-O11
20	L	101	TGL	C25-C26-C27-C28
23	C	303	PEK	C17-C18-C19-C20
24	C	306	CDL	C57-C58-C59-C60
26	R	201	PSC	C05-C04-O12-P
26	E	201	PSC	C05-C04-O12-P
23	P	302	PEK	C05-C04-O12-P
20	D	201	TGL	OG2-CB1-CB2-CB3
18	A	606	PGV	C14-C15-C16-C17
18	N	609	PGV	C12-C13-C14-C15
18	A	606	PGV	C23-C24-C25-C26
20	Q	201	TGL	CA2-CA3-CA4-CA5

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Mol	Chain	Res	Type	Atoms
24	G	101	CDL	OB5-CB3-CB4-OB6
20	B	301	TGL	CA1-CA2-CA3-CA4
18	A	606	PGV	O01-C02-C03-O11
18	P	304	PGV	C14-C15-C16-C17
24	C	306	CDL	C22-C23-C24-C25
20	D	201	TGL	C17-C18-C19-C33
20	N	611	TGL	CG1-CG2-CG3-OG3
20	D	201	TGL	CG1-CG2-CG3-OG3
24	P	305	CDL	C73-C74-C75-C76
26	R	201	PSC	O03-C01-C02-O01
20	N	611	TGL	OG1-CG1-CG2-OG2
20	L	101	TGL	OG1-CG1-CG2-OG2
18	A	606	PGV	C25-C26-C27-C28
23	C	303	PEK	C30-C31-C32-C33
20	L	101	TGL	CA5-CA6-CA7-CA8
18	P	304	PGV	C5-C6-C7-C8
24	G	101	CDL	C77-C78-C79-C80
20	Q	201	TGL	CA4-CA5-CA6-CA7
20	L	101	TGL	C24-C25-C26-C27
24	G	101	CDL	CA4-CA3-OA5-PA1
24	P	305	CDL	CA4-CA3-OA5-PA1
24	G	101	CDL	C12-C13-C14-C15
20	Q	201	TGL	C25-C26-C27-C28
18	C	305	PGV	C6-C7-C8-C9
18	N	609	PGV	C30-C31-C32-C33
18	C	305	PGV	C5-C6-C7-C8
20	L	101	TGL	C23-C24-C25-C26
14	N	601	HEA	C15-C16-C17-C18
20	N	608	TGL	CC4-CC5-CC6-CC7
25	P	307	DMU	C19-C22-C25-C28
20	N	611	TGL	CA7-CA8-CA9-C20
24	T	103	CDL	C23-C24-C25-C26
24	C	306	CDL	C42-C43-C44-C45
18	N	609	PGV	O03-C19-C20-C21
20	N	611	TGL	CC6-CC7-CC8-CC9
24	C	306	CDL	CB5-C51-C52-C53
25	P	307	DMU	C28-C31-C34-C37
18	N	606	PGV	C01-C02-O01-C1
24	P	305	CDL	C31-CA7-OA8-CA6
23	T	102	PEK	C30-C31-C32-C33
24	P	305	CDL	C78-C79-C80-C81
24	P	305	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C26-C27-C28-C29
20	B	301	TGL	CA6-CA7-CA8-CA9
23	G	102	PEK	C22-C23-C24-C25
18	C	305	PGV	C31-C32-C33-C34
20	Q	201	TGL	C23-C24-C25-C26
23	T	101	PEK	C3-C4-C5-C6
24	C	306	CDL	C12-C13-C14-C15
24	P	305	CDL	C52-C53-C54-C55
24	G	101	CDL	OA6-CA4-CA6-OA8
18	N	606	PGV	C2-C3-C4-C5
24	T	103	CDL	C11-C12-C13-C14
18	P	304	PGV	C04-O12-P-O11
18	N	606	PGV	C04-O12-P-O11
24	C	306	CDL	CA3-OA5-PA1-OA2
24	T	103	CDL	CA3-OA5-PA1-OA2
26	E	201	PSC	C03-O11-P-O12
24	T	103	CDL	CB3-CB4-CB6-OB8
20	L	101	TGL	CG1-CG2-CG3-OG3
20	Q	201	TGL	CB7-CB8-CB9-C10
20	L	101	TGL	OG1-CA1-CA2-CA3
23	P	302	PEK	C22-C23-C24-C25
26	E	201	PSC	C24-C25-C26-C27
20	D	201	TGL	CA5-CA6-CA7-CA8
18	C	305	PGV	C05-C04-O12-P
18	P	304	PGV	C23-C24-C25-C26
23	T	101	PEK	C27-C28-C29-C30
26	R	201	PSC	C7-C8-C9-C10
20	Q	201	TGL	C12-C13-C14-C29
24	C	306	CDL	C38-C39-C40-C41
24	T	103	CDL	C61-C62-C63-C64
24	T	103	CDL	C54-C55-C56-C57
20	Q	201	TGL	CA6-CA7-CA8-CA9
18	A	608	PGV	O03-C19-C20-C21
24	P	305	CDL	OA5-CA3-CA4-OA6
23	T	102	PEK	O03-C21-C22-C23
24	G	101	CDL	C52-C53-C54-C55
18	N	609	PGV	C25-C26-C27-C28
24	P	305	CDL	C16-C17-C18-C19
24	C	306	CDL	C21-C22-C23-C24
20	N	608	TGL	C23-C24-C25-C26
23	P	302	PEK	O03-C01-C02-O01
23	C	302	PEK	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	N	606	PGV	C12-C13-C14-C15
23	T	102	PEK	C15-C16-C17-C18
23	P	302	PEK	C15-C16-C17-C18
20	N	608	TGL	CA3-CA4-CA5-CA6
24	P	305	CDL	C79-C80-C81-C82
20	N	608	TGL	OG1-CG1-CG2-CG3
24	G	101	CDL	C34-C35-C36-C37
23	C	303	PEK	C27-C28-C29-C30
22	P	306	CHD	C13-C17-C20-C21
23	C	303	PEK	C5-C6-C7-C8
23	C	303	PEK	C6-C7-C8-C9
23	T	101	PEK	C11-C10-C9-C8
26	E	201	PSC	C10-C11-C12-C13
23	P	302	PEK	C6-C7-C8-C9
24	C	306	CDL	C34-C35-C36-C37
23	C	303	PEK	C23-C24-C25-C26
20	L	101	TGL	C21-C20-CA9-CA8
20	D	201	TGL	CA2-CA1-OG1-CG1
23	C	303	PEK	C31-C32-C33-C34
18	C	305	PGV	C29-C30-C31-C32
20	D	201	TGL	C15-C16-C17-C18
20	L	101	TGL	CC2-CC3-CC4-CC5
23	T	102	PEK	C23-C24-C25-C26
24	C	306	CDL	C41-C42-C43-C44
23	C	303	PEK	C13-C14-C15-C16
25	P	307	DMU	C3-C4-C57-O61
18	C	304	PGV	C30-C31-C32-C33
20	D	201	TGL	OA1-CA1-OG1-CG1
18	A	606	PGV	C24-C25-C26-C27
18	P	304	PGV	C6-C7-C8-C9
18	N	606	PGV	C20-C21-C22-C23
26	R	201	PSC	C12-C13-C14-C15
18	P	303	PGV	C1-C2-C3-C4
20	D	201	TGL	CC4-CC5-CC6-CC7
23	T	102	PEK	C16-C17-C18-C19
24	C	306	CDL	C54-C55-C56-C57
20	B	301	TGL	CC9-C15-C16-C17
23	T	102	PEK	C3-C4-C5-C6
18	A	608	PGV	C19-C20-C21-C22
24	P	305	CDL	C77-C78-C79-C80
18	A	606	PGV	C20-C21-C22-C23
26	E	201	PSC	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
20	D	201	TGL	C24-C25-C26-C27
23	C	303	PEK	O12-C04-C05-N
18	P	304	PGV	C3-C4-C5-C6
18	C	304	PGV	C05-C04-O12-P
20	L	101	TGL	OG2-CG2-CG3-OG3
24	C	306	CDL	C71-C72-C73-C74
23	C	303	PEK	C3-C4-C5-C6
18	N	609	PGV	C4-C5-C6-C7
14	N	602	HEA	C26-C15-C16-C17
24	C	306	CDL	C59-C60-C61-C62
20	Q	201	TGL	C11-C12-C13-C14
18	P	304	PGV	O01-C1-C2-C3
26	E	201	PSC	C7-C8-C9-C10
20	Q	201	TGL	C11-C10-CB9-CB8
24	P	305	CDL	C40-C41-C42-C43
23	T	102	PEK	O02-C1-O01-C02
24	G	101	CDL	C52-C51-CB5-OB6
18	P	304	PGV	C15-C16-C17-C18
23	T	102	PEK	O01-C1-C2-C3
23	T	102	PEK	C22-C23-C24-C25
18	P	303	PGV	C23-C24-C25-C26
24	T	103	CDL	C60-C61-C62-C63
24	P	305	CDL	C12-C13-C14-C15
24	P	305	CDL	CB3-CB4-CB6-OB8
20	B	301	TGL	CC5-CC6-CC7-CC8
18	C	305	PGV	C10-C11-C12-C13
20	N	608	TGL	C29-C30-C31-C32
20	D	201	TGL	CB5-CB6-CB7-CB8
20	N	608	TGL	C33-C34-C35-C36
23	T	101	PEK	O03-C21-C22-C23
24	T	103	CDL	C72-C71-CB7-OB8
24	G	101	CDL	OB5-CB3-CB4-CB6
23	C	303	PEK	C35-C36-C37-C38
18	N	606	PGV	O03-C19-C20-C21
24	T	103	CDL	C52-C51-CB5-OB6
24	C	306	CDL	OA6-CA4-CA6-OA8
23	G	102	PEK	O02-C1-C2-C3
24	T	103	CDL	C20-C21-C22-C23
20	D	201	TGL	C20-C21-C22-C23
20	D	201	TGL	OG1-CA1-CA2-CA3
18	C	305	PGV	C25-C26-C27-C28
20	B	301	TGL	C12-C13-C14-C29

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Mol	Chain	Res	Type	Atoms
23	P	302	PEK	C14-C15-C16-C17
20	D	201	TGL	CA9-C20-C21-C22
20	D	201	TGL	OG3-CC1-CC2-CC3
18	P	304	PGV	O02-C1-C2-C3
25	M	101	DMU	C34-C37-C40-C43
20	Q	201	TGL	C24-C25-C26-C27
23	T	101	PEK	O04-C21-C22-C23
24	T	103	CDL	C72-C71-CB7-OB9
26	R	201	PSC	O03-C01-C02-C03
23	P	302	PEK	O01-C1-C2-C3
20	D	201	TGL	OC1-CC1-CC2-CC3
20	N	608	TGL	C22-C23-C24-C25
24	C	306	CDL	C12-C11-CA5-OA6
18	P	303	PGV	C05-C04-O12-P
23	G	102	PEK	C02-C03-O11-P
23	T	102	PEK	O02-C1-C2-C3
18	C	304	PGV	C11-C12-C13-C14
18	C	305	PGV	C7-C8-C9-C10
18	N	606	PGV	C04-O12-P-O13
24	T	103	CDL	CA2-OA2-PA1-OA3
24	T	103	CDL	CA3-OA5-PA1-OA3
24	P	305	CDL	OB5-CB3-CB4-CB6
23	C	303	PEK	C2-C3-C4-C5
23	C	302	PEK	O03-C21-C22-C23
24	P	305	CDL	OB9-CB7-OB8-CB6
18	N	606	PGV	O04-C19-C20-C21
18	C	304	PGV	C24-C25-C26-C27
24	P	305	CDL	C71-CB7-OB8-CB6
20	B	301	TGL	OG1-CA1-CA2-CA3
18	A	606	PGV	O03-C19-C20-C21
20	N	608	TGL	OG3-CC1-CC2-CC3
24	P	305	CDL	C12-C11-CA5-OA6
20	B	301	TGL	OG3-CC1-CC2-CC3
24	C	306	CDL	CB2-C1-CA2-OA2
18	P	303	PGV	C29-C30-C31-C32
23	P	302	PEK	O02-C1-C2-C3
23	C	302	PEK	O04-C21-C22-C23
24	T	103	CDL	C52-C51-CB5-OB7
24	G	101	CDL	C36-C37-C38-C39
20	N	611	TGL	C20-C21-C22-C23
20	D	201	TGL	OA1-CA1-CA2-CA3
24	P	305	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
18	N	609	PGV	C26-C27-C28-C29
20	Q	201	TGL	CB6-CB7-CB8-CB9
20	N	608	TGL	OC1-CC1-CC2-CC3
24	G	101	CDL	C23-C24-C25-C26

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	W	101	CHD	C1-C10-C2-C3-C4-C5

43 monomers are involved in 223 short contacts:

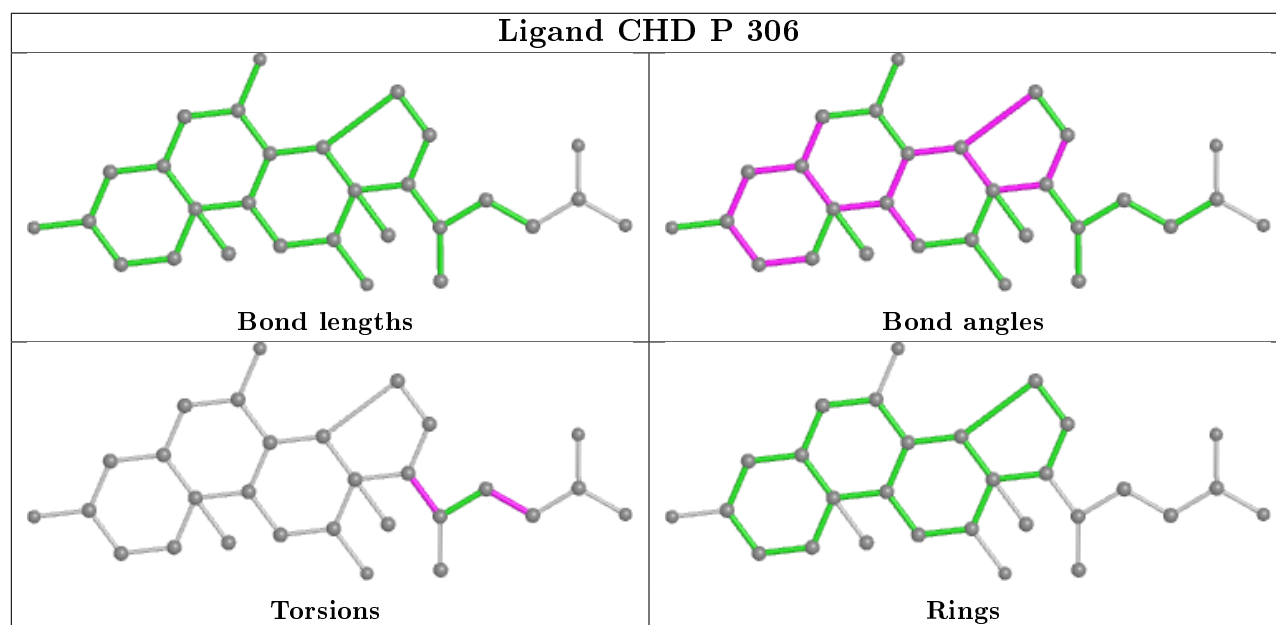
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	607[A]	PER	1	0
22	P	306	CHD	1	0
20	B	301	TGL	1	0
18	P	304	PGV	4	0
19	A	607[B]	PER	2	0
18	N	606	PGV	6	0
18	C	305	PGV	1	0
22	C	307	CHD	1	0
26	R	201	PSC	6	0
14	A	601	HEA	9	0
25	Z	101	DMU	1	0
24	G	101	CDL	17	0
19	N	607[A]	PER	1	0
18	A	606	PGV	11	0
23	T	102	PEK	1	0
22	N	610	CHD	1	0
23	C	303	PEK	15	0
20	Q	201	TGL	6	0
23	T	101	PEK	7	0
19	N	607[B]	PER	1	0
24	C	306	CDL	13	0
14	N	601	HEA	9	0
14	N	602	HEA	5	0
24	T	103	CDL	20	0
20	N	611	TGL	7	0
14	A	602	HEA	5	0
23	C	302	PEK	6	0
22	W	101	CHD	5	0
18	C	304	PGV	2	0

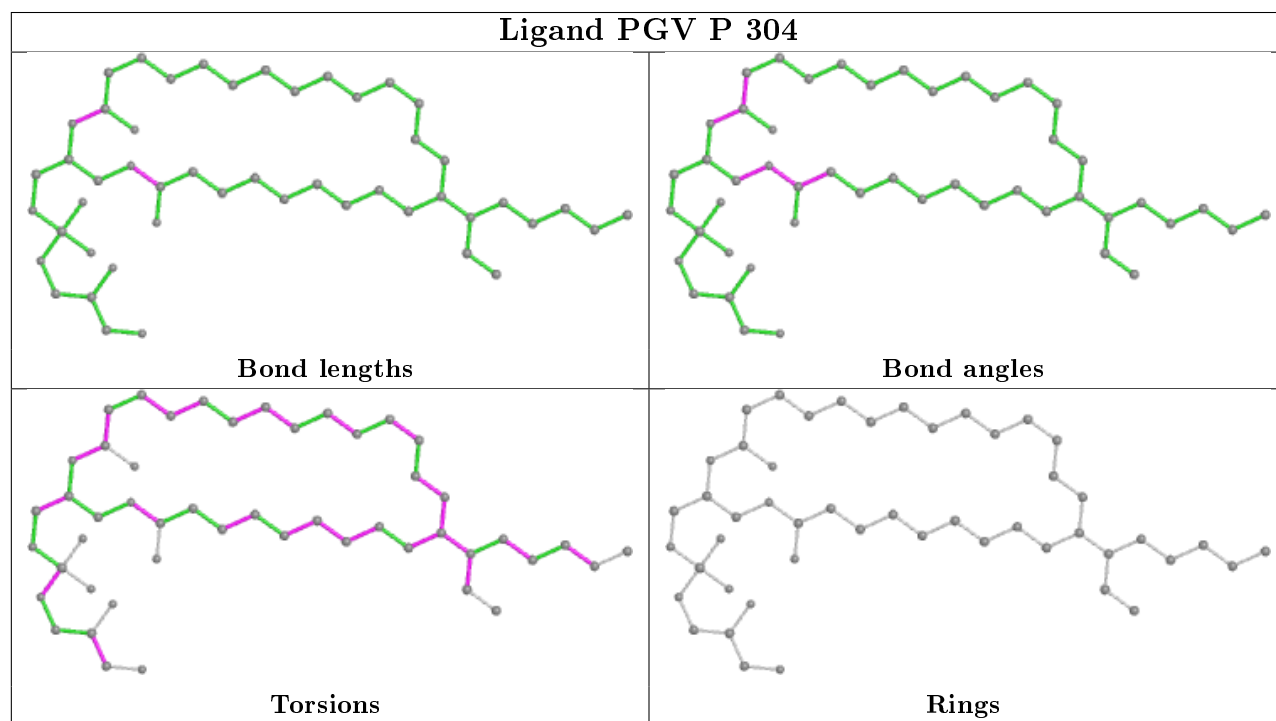
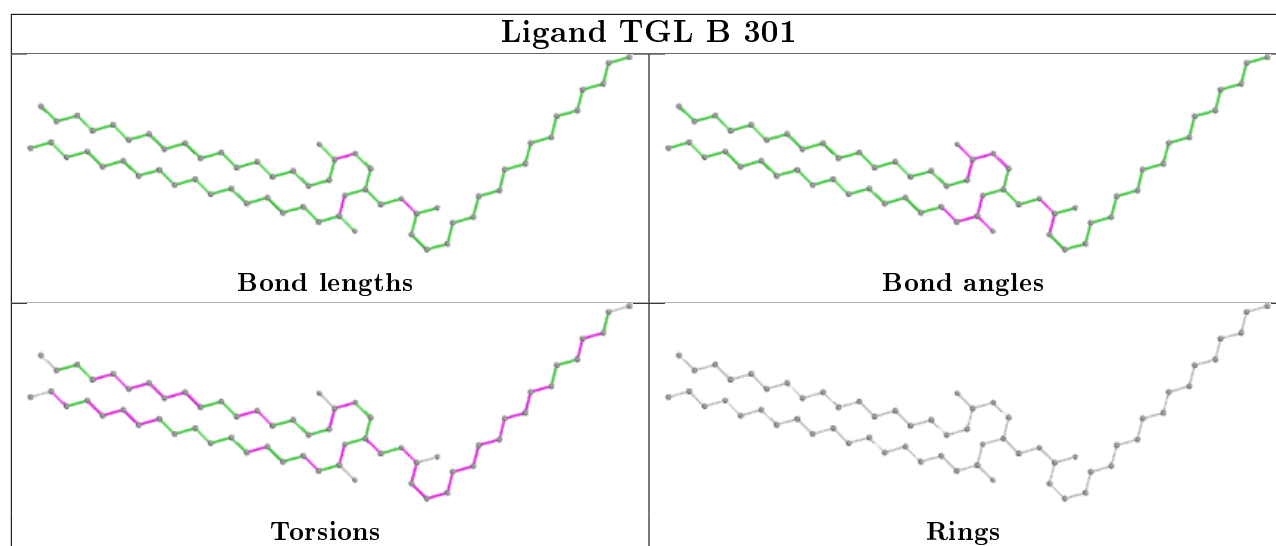
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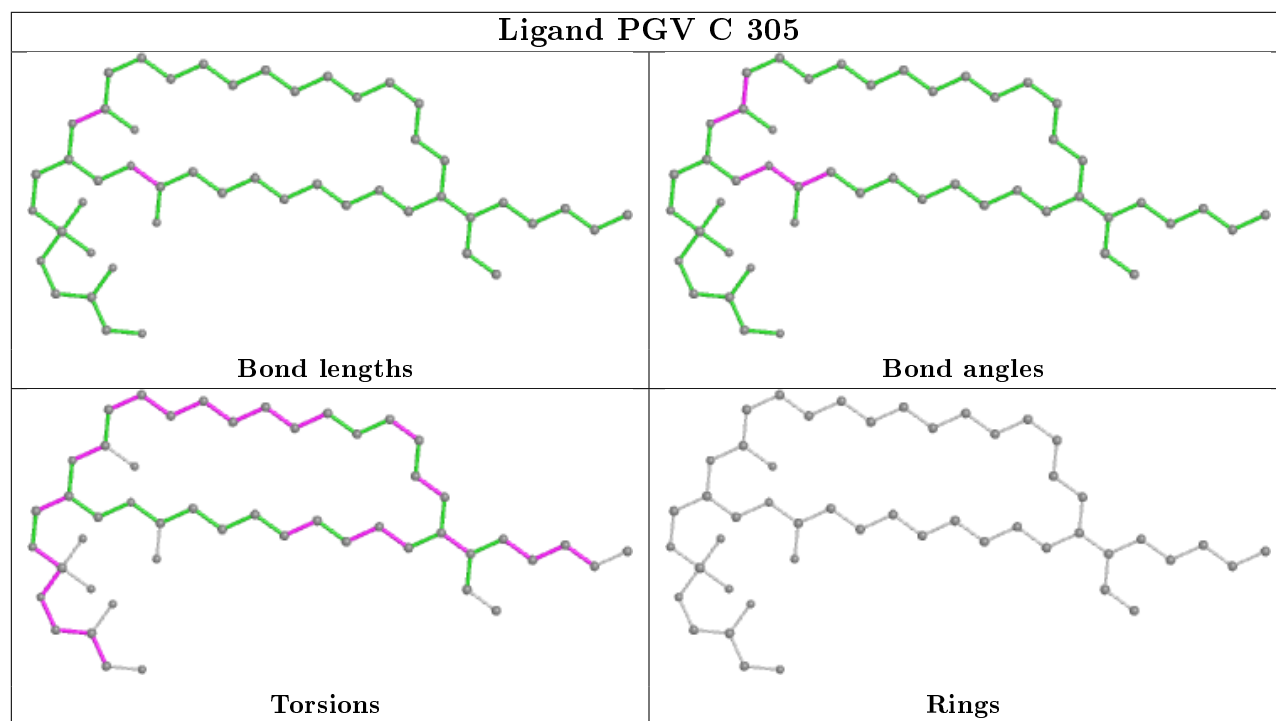
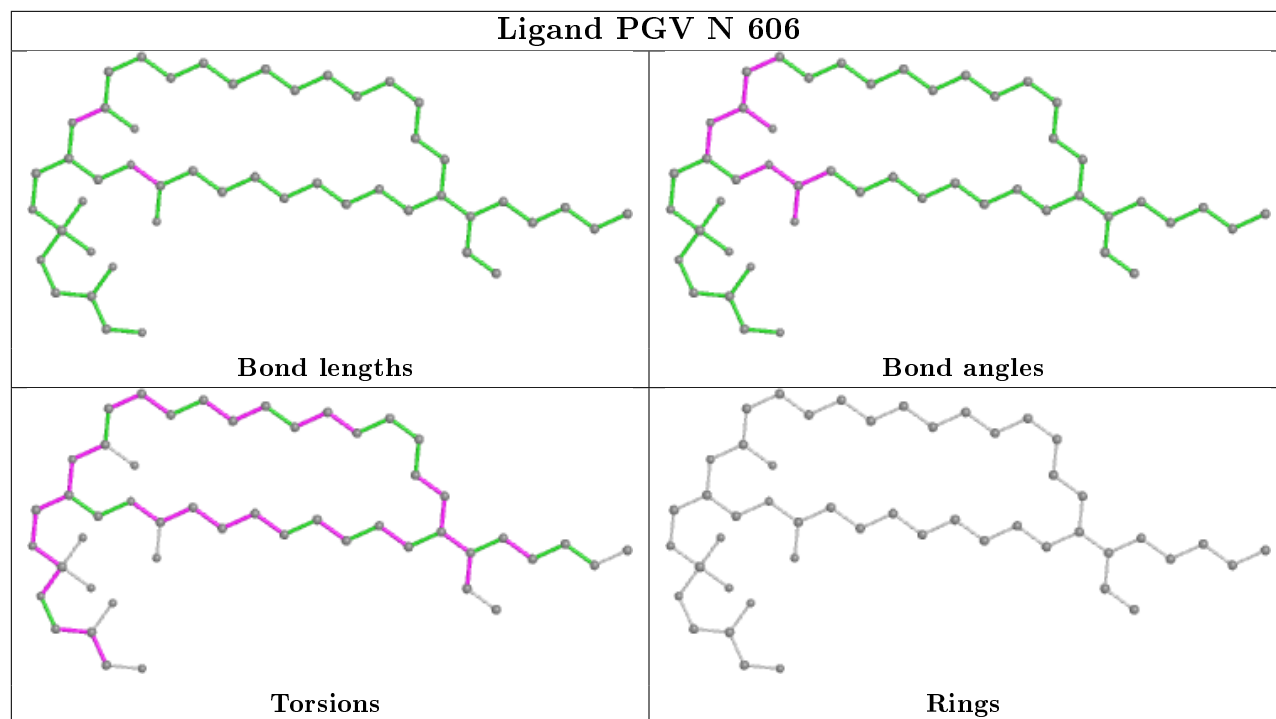
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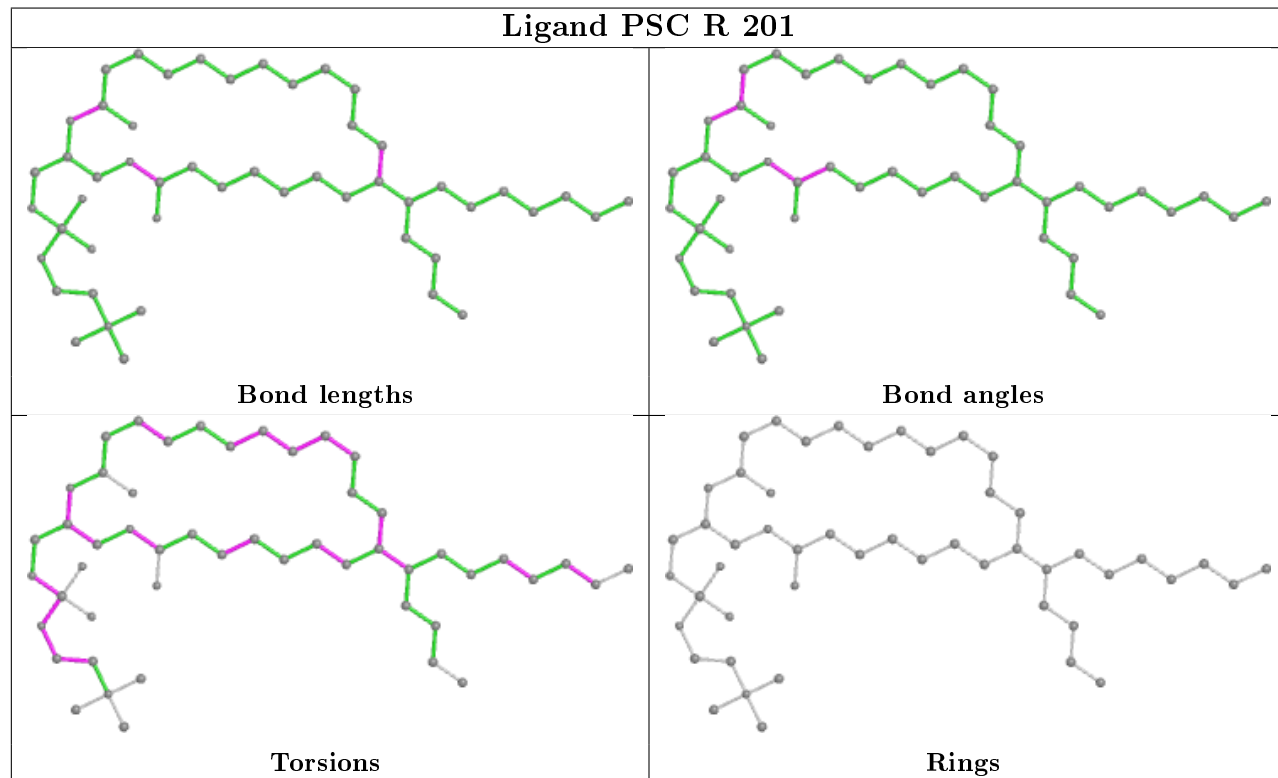
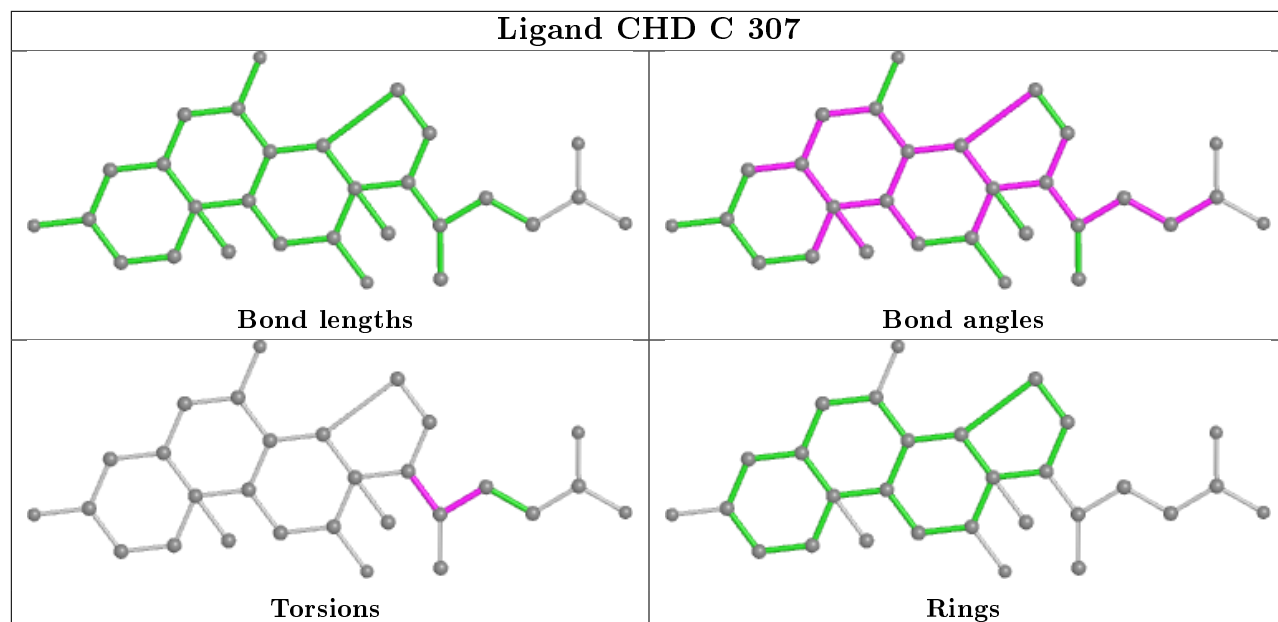
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	608	TGL	3	0
25	P	307	DMU	4	0
26	E	201	PSC	7	0
22	B	303	CHD	1	0
18	P	303	PGV	4	0
20	D	201	TGL	11	0
25	C	309	DMU	6	0
23	G	102	PEK	7	0
18	A	608	PGV	5	0
20	L	101	TGL	11	0
22	O	301	CHD	1	0
24	P	305	CDL	10	0
18	N	609	PGV	2	0
23	P	302	PEK	11	0

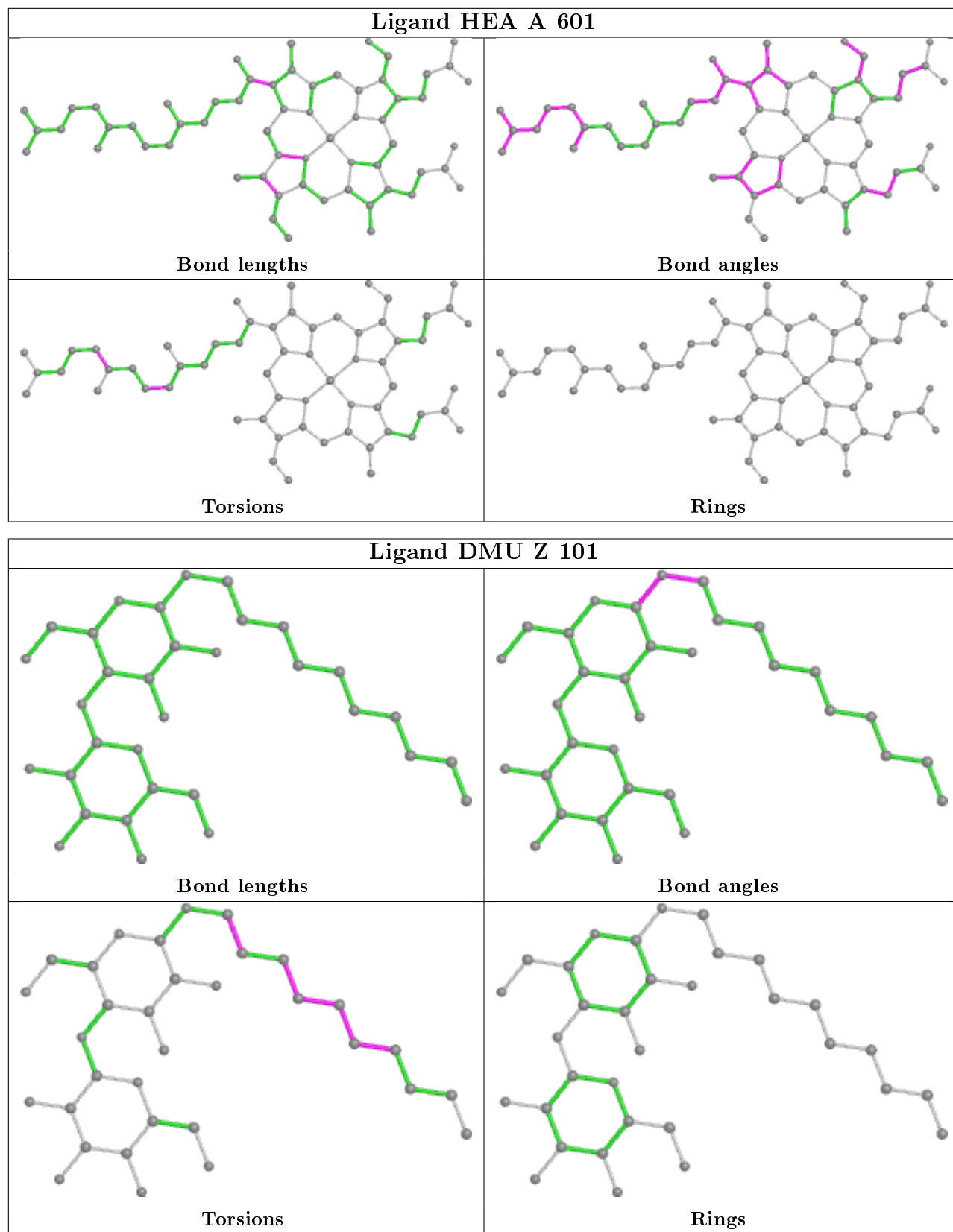
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

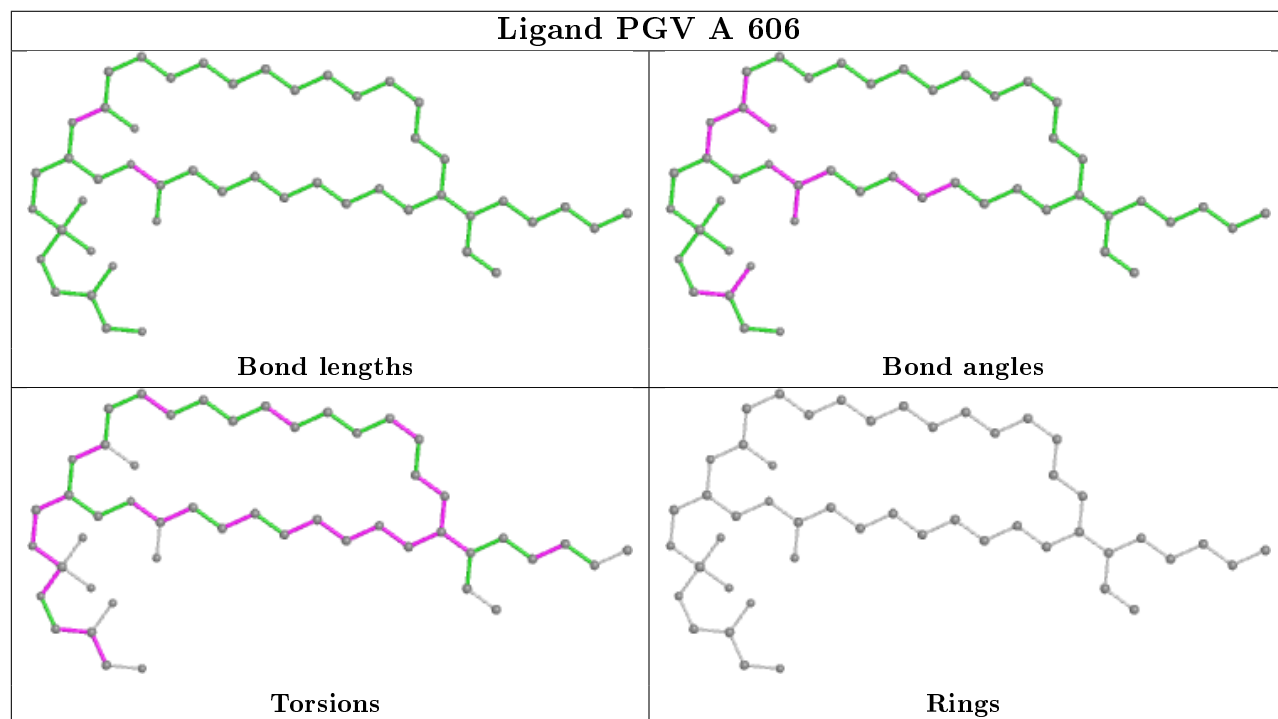
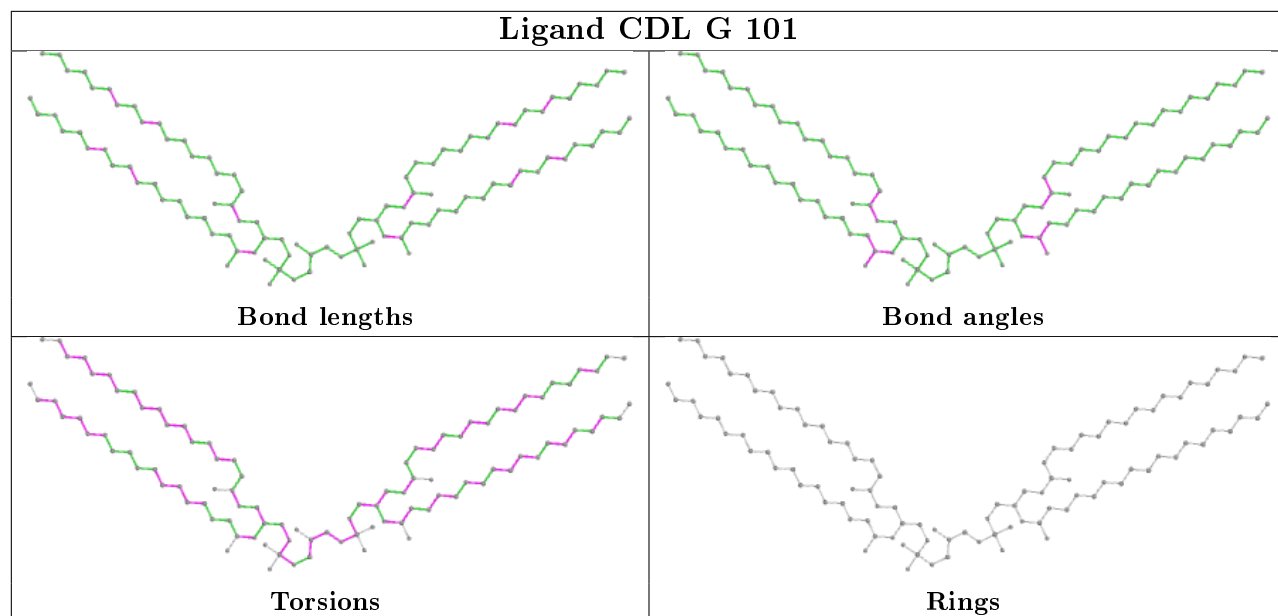




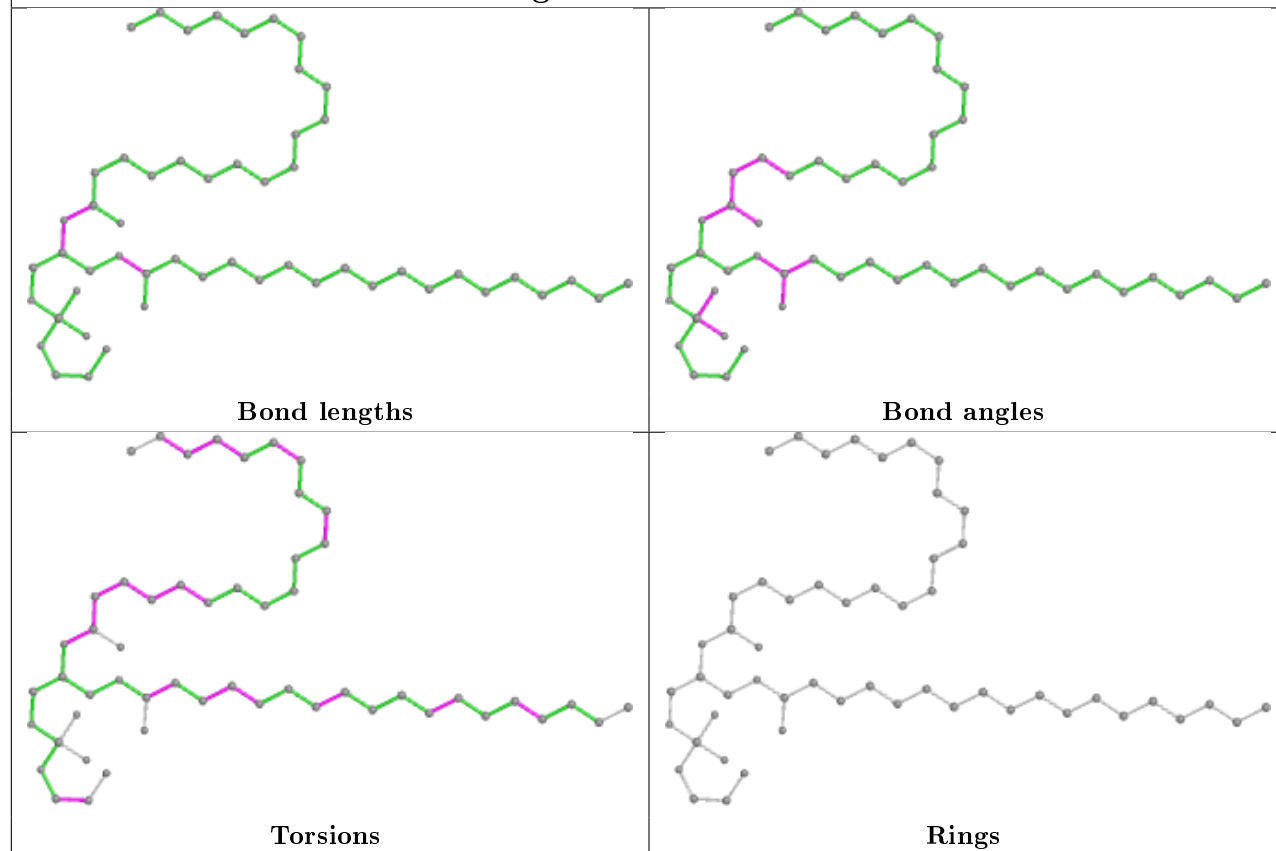




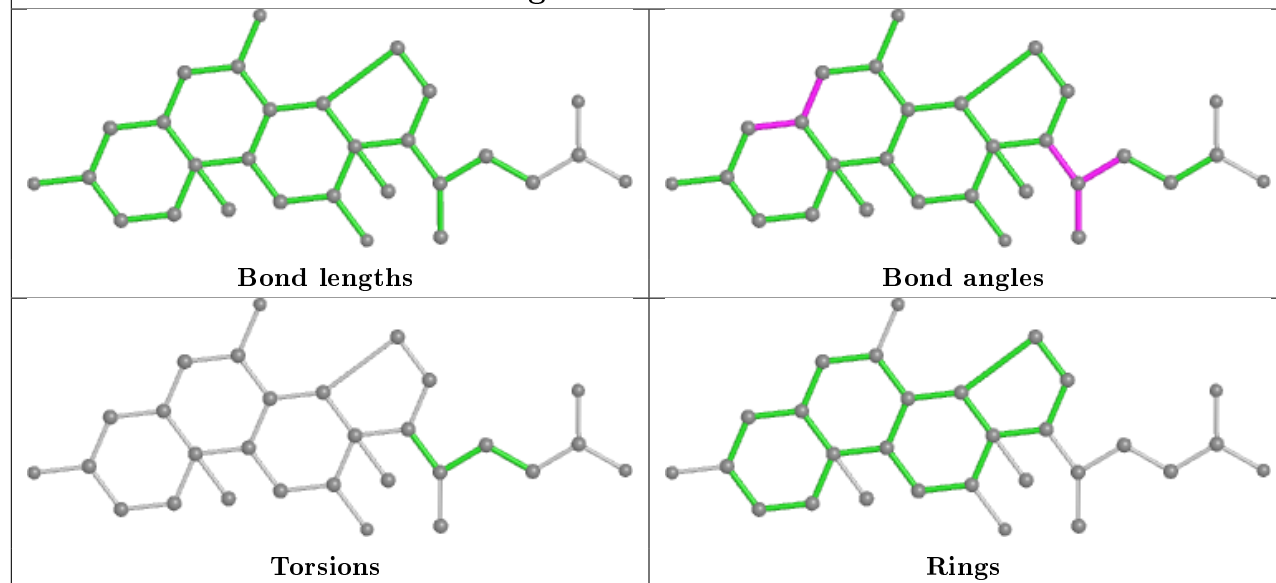




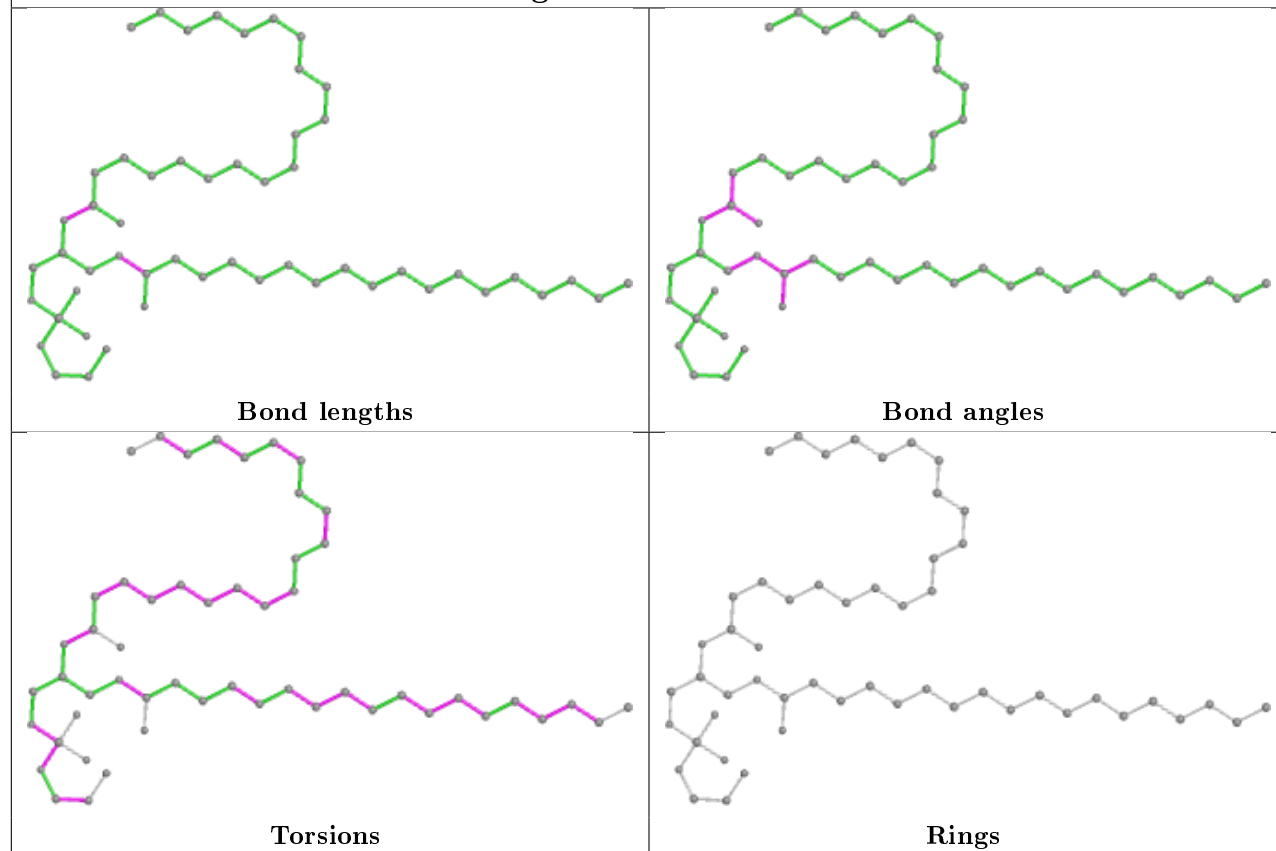
Ligand PEK T 102



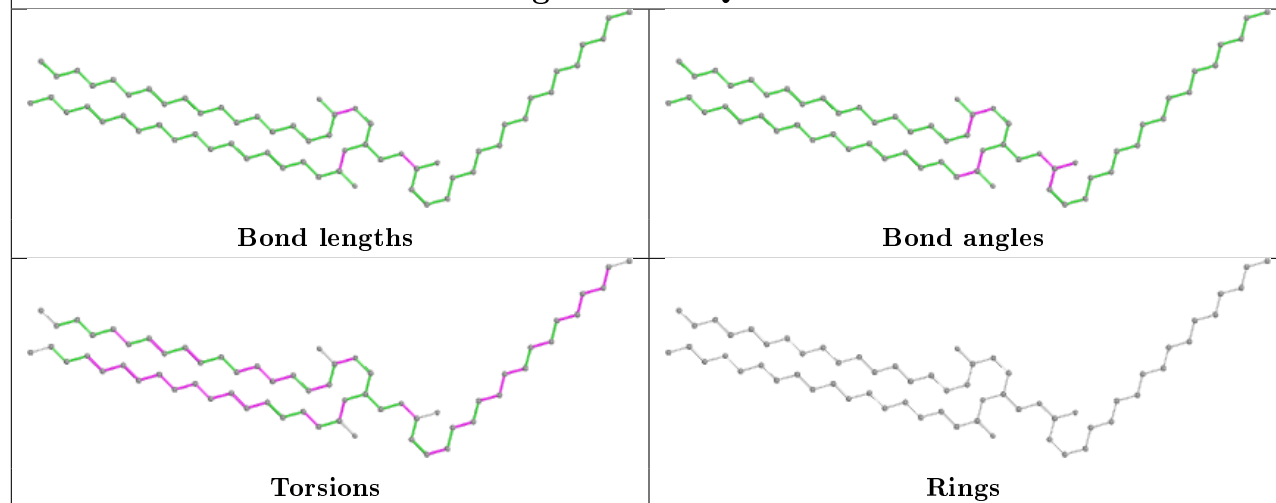
Ligand CHD N 610

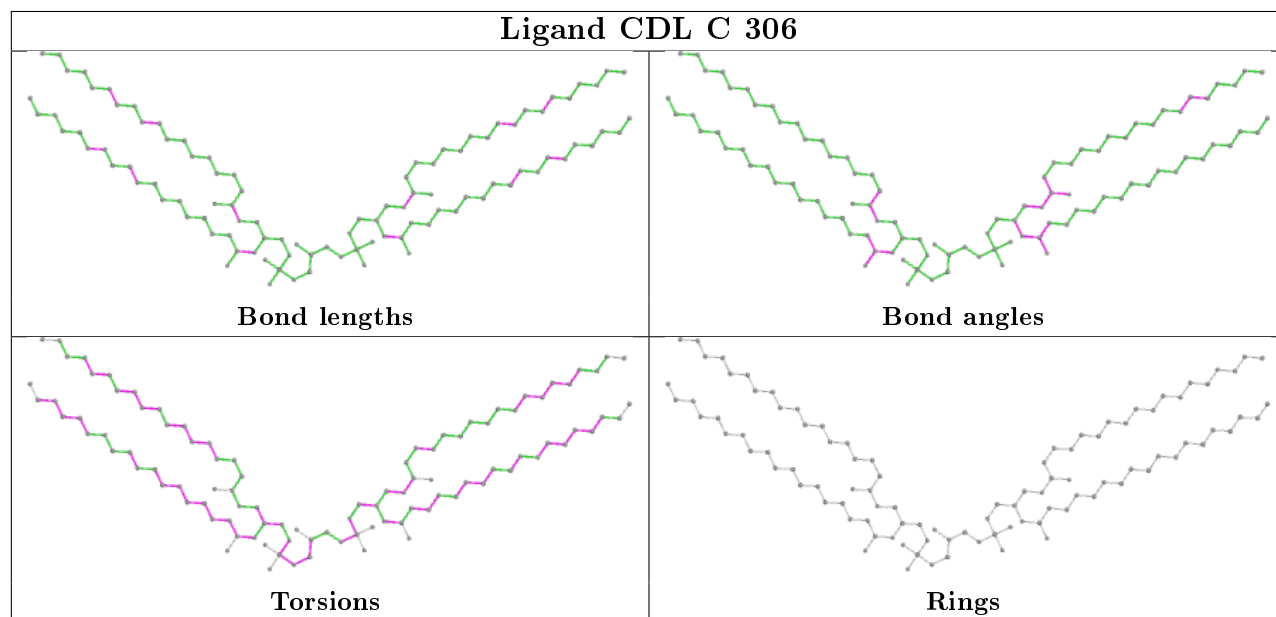
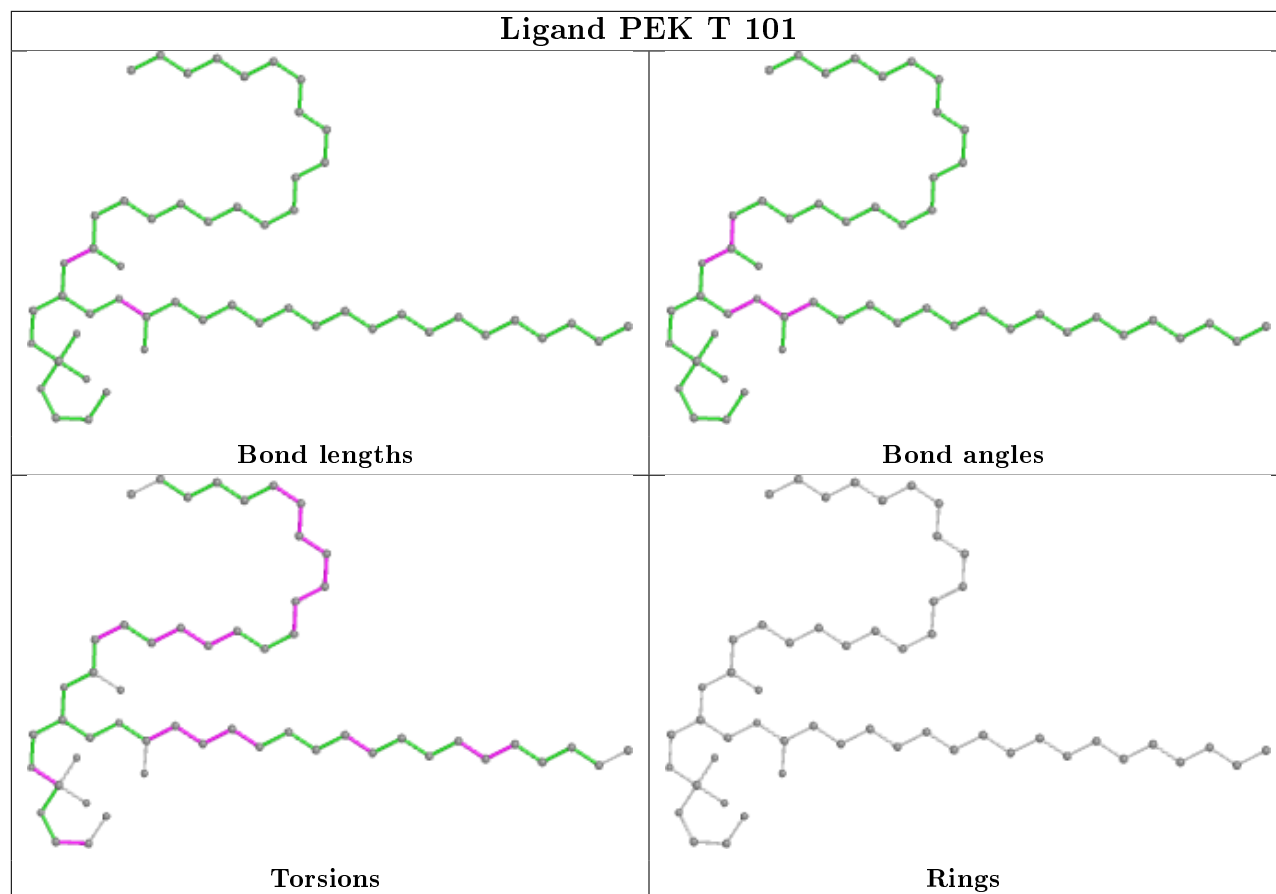


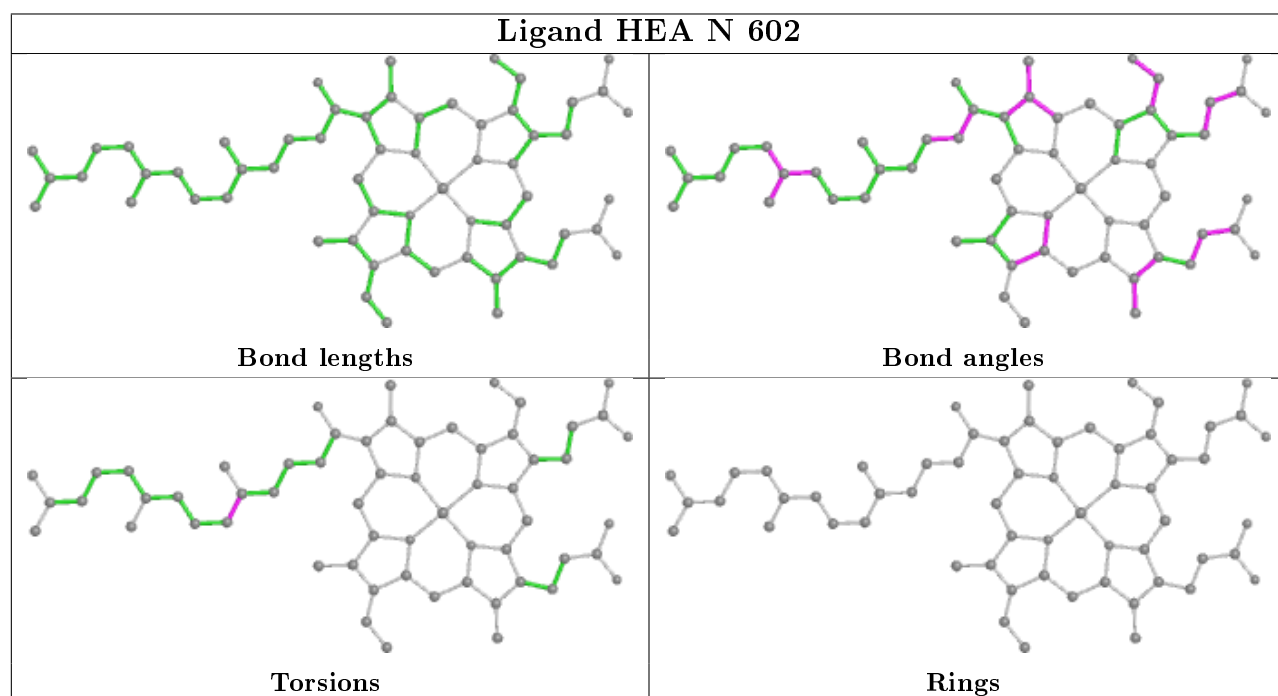
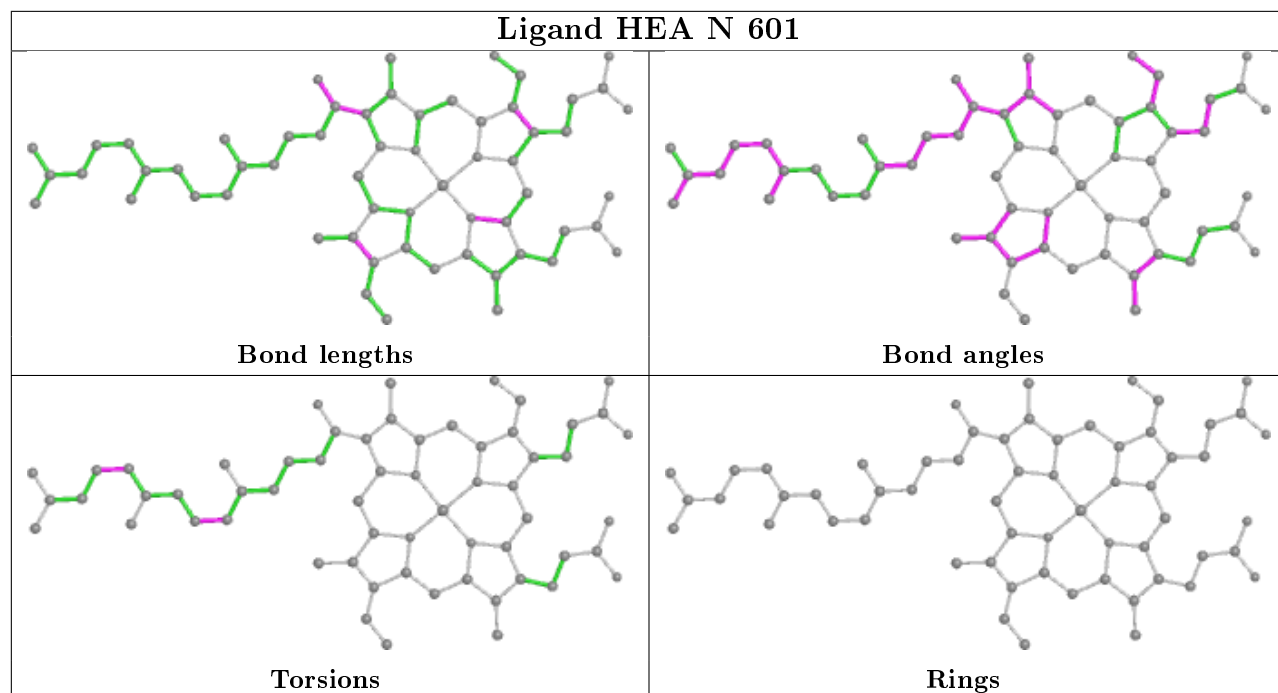
Ligand PEK C 303

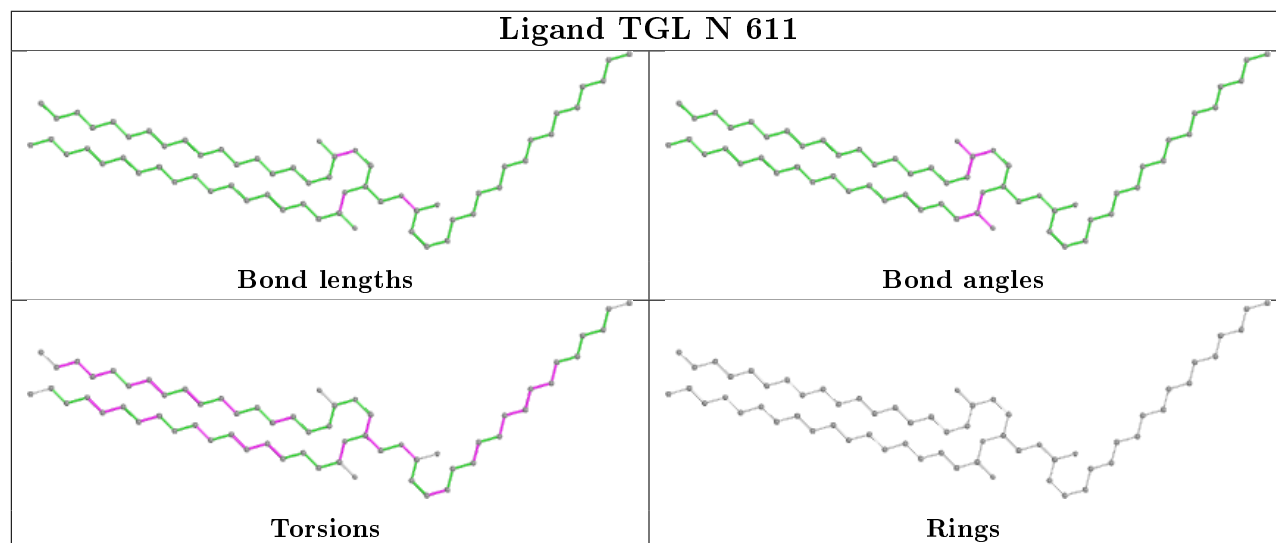
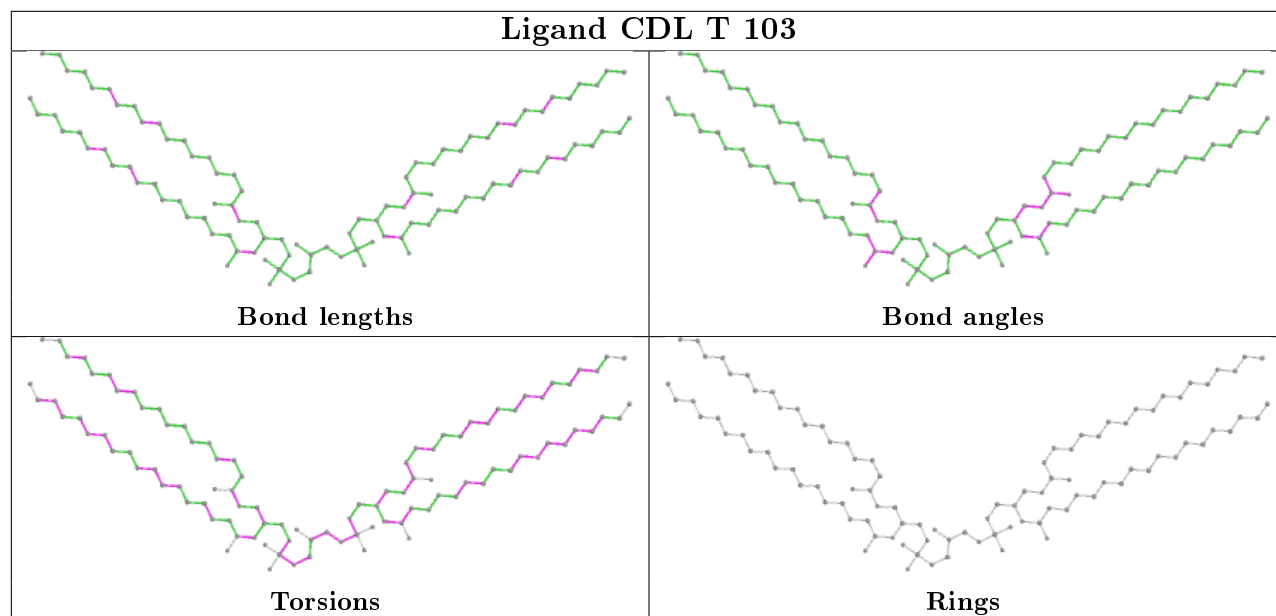


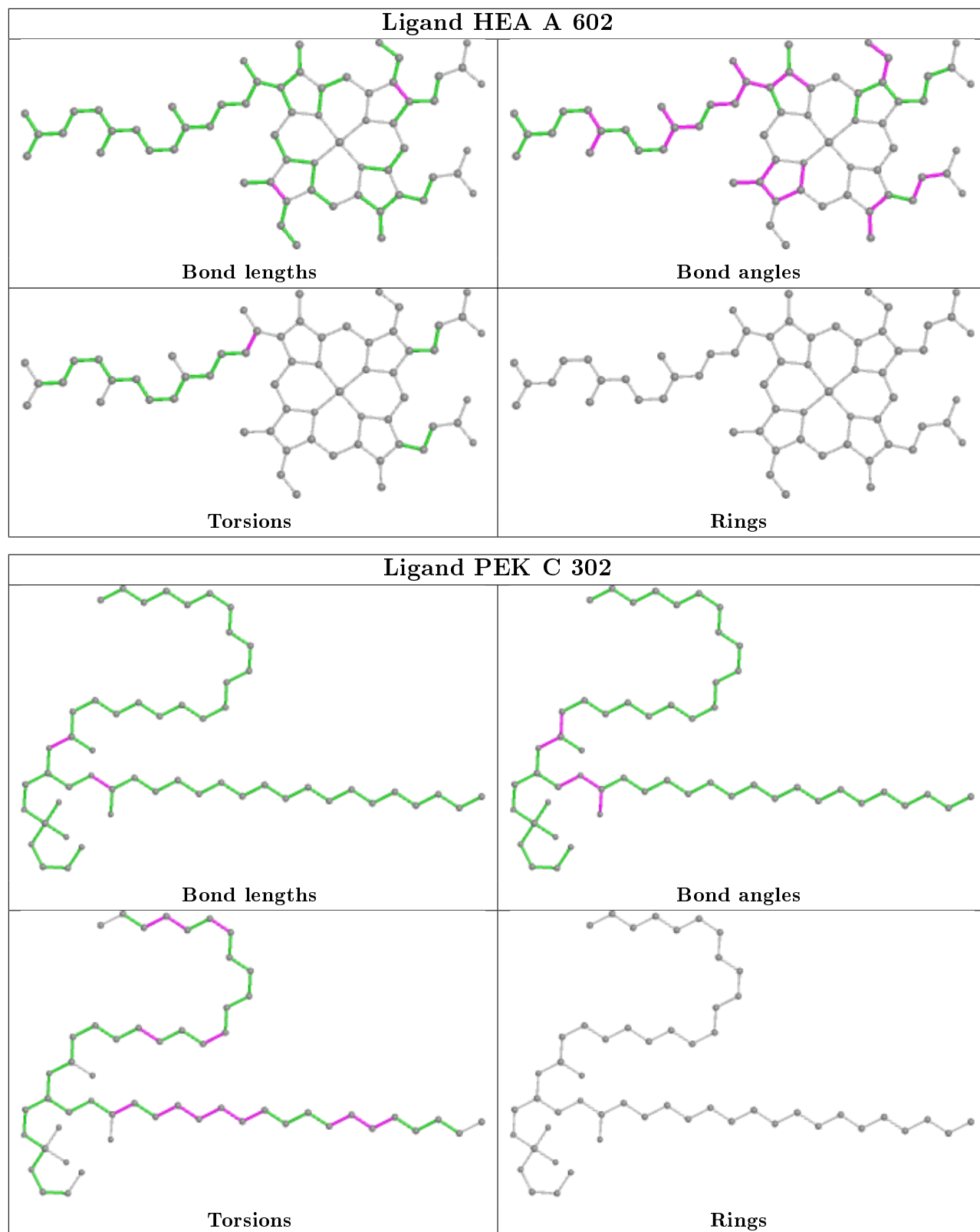
Ligand TGL Q 201

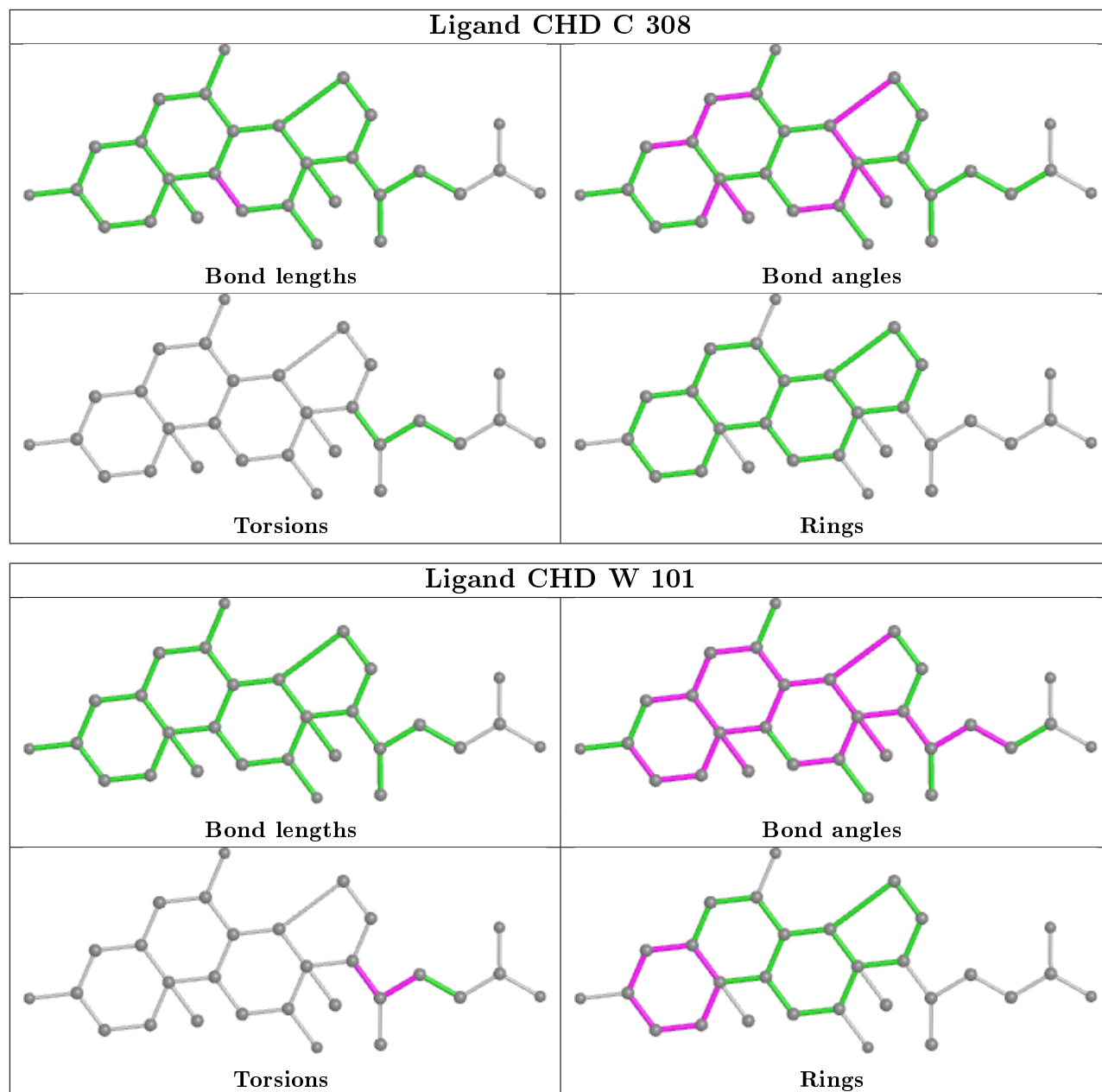


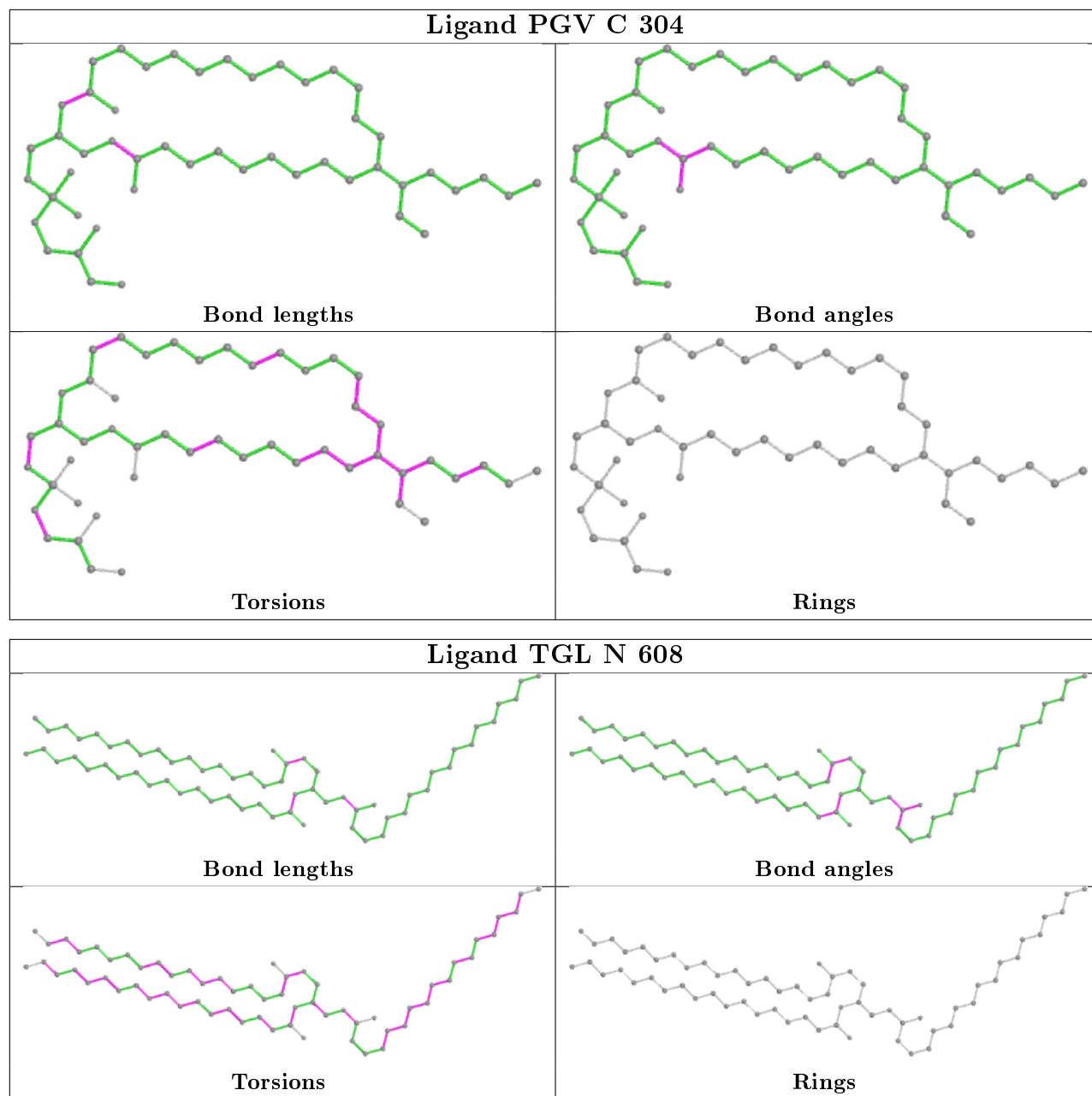




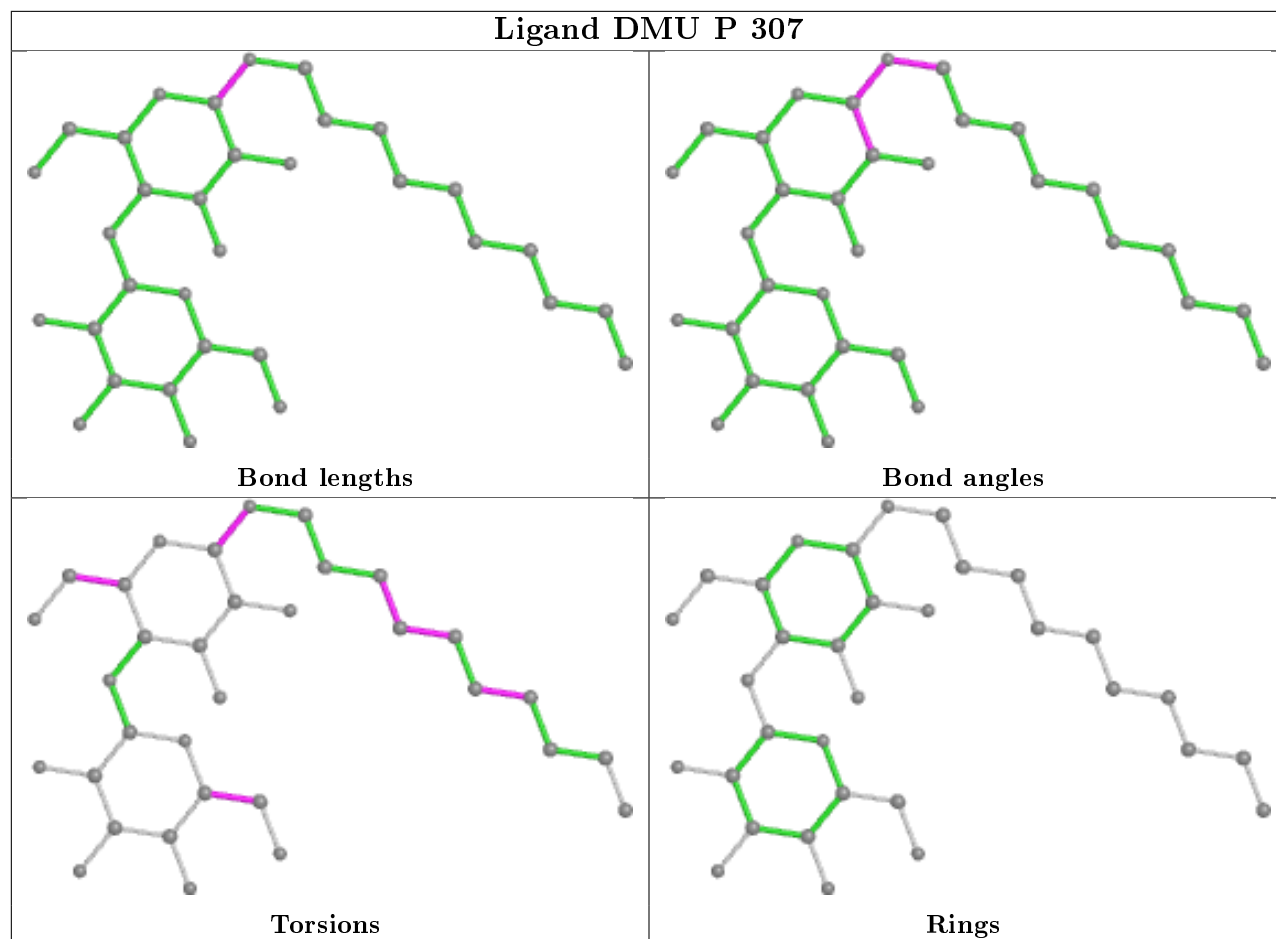




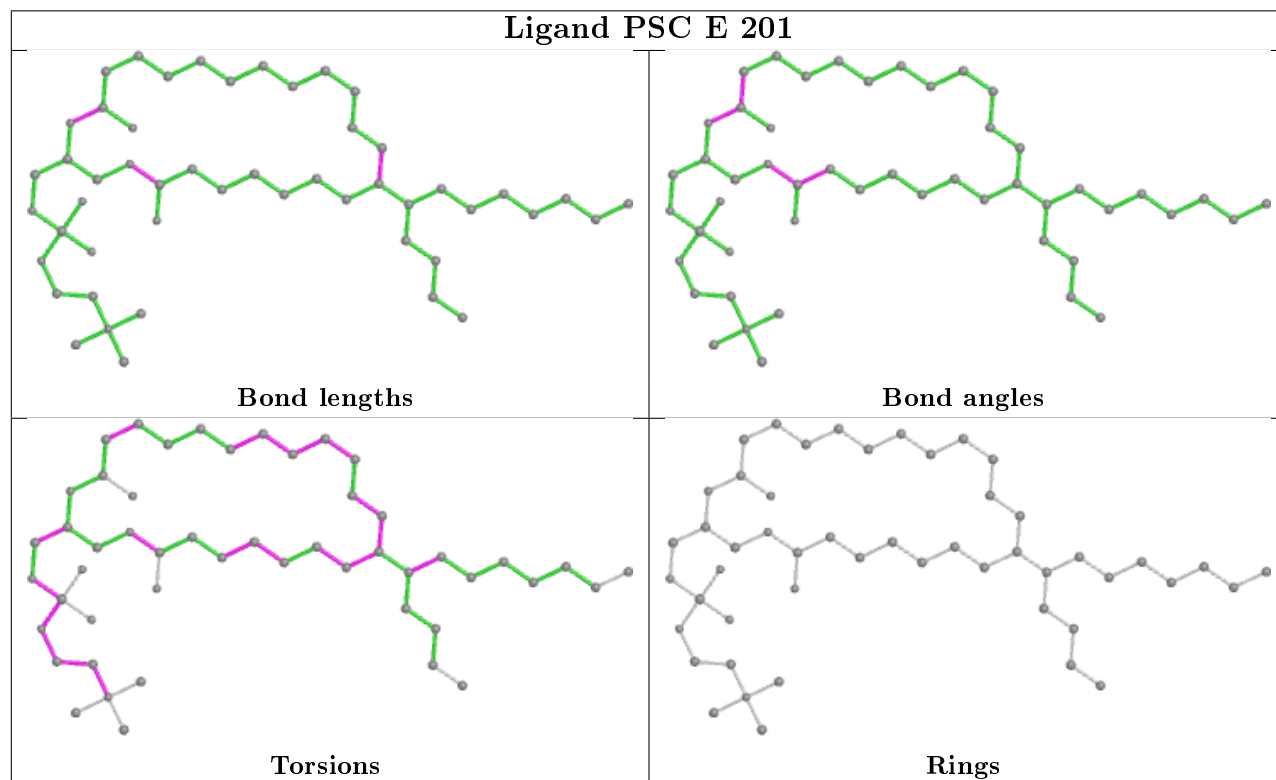


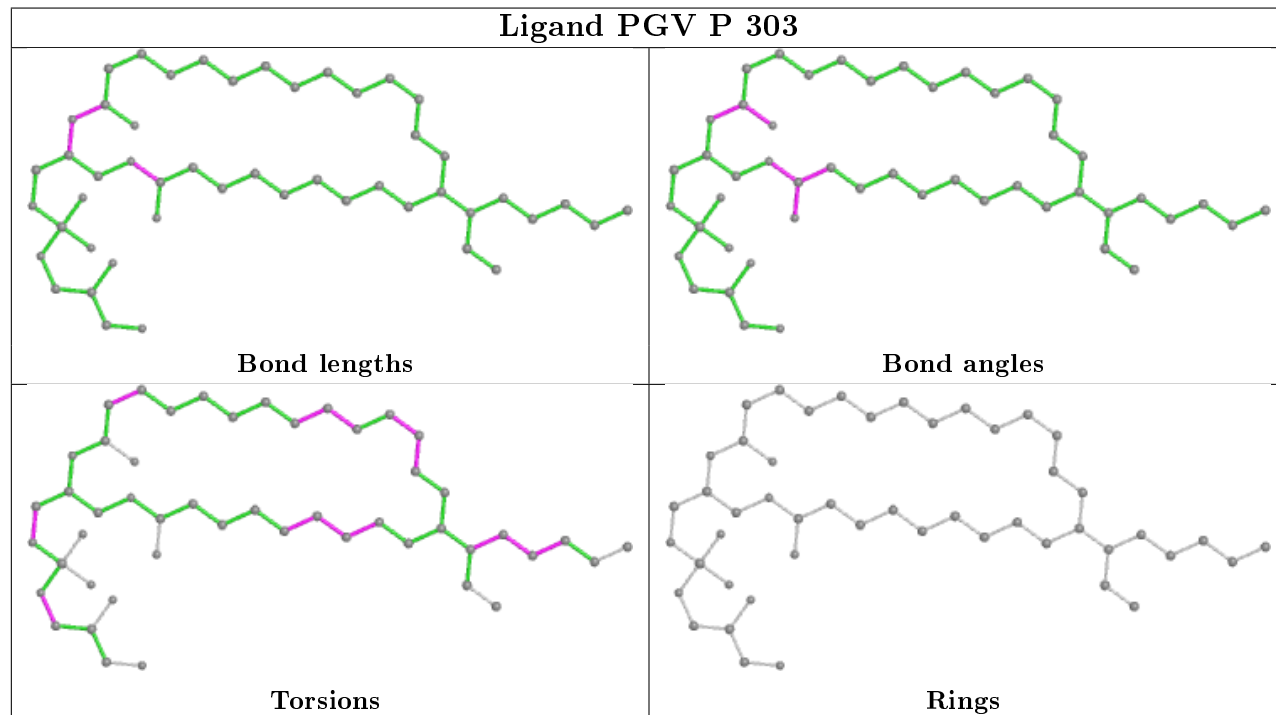
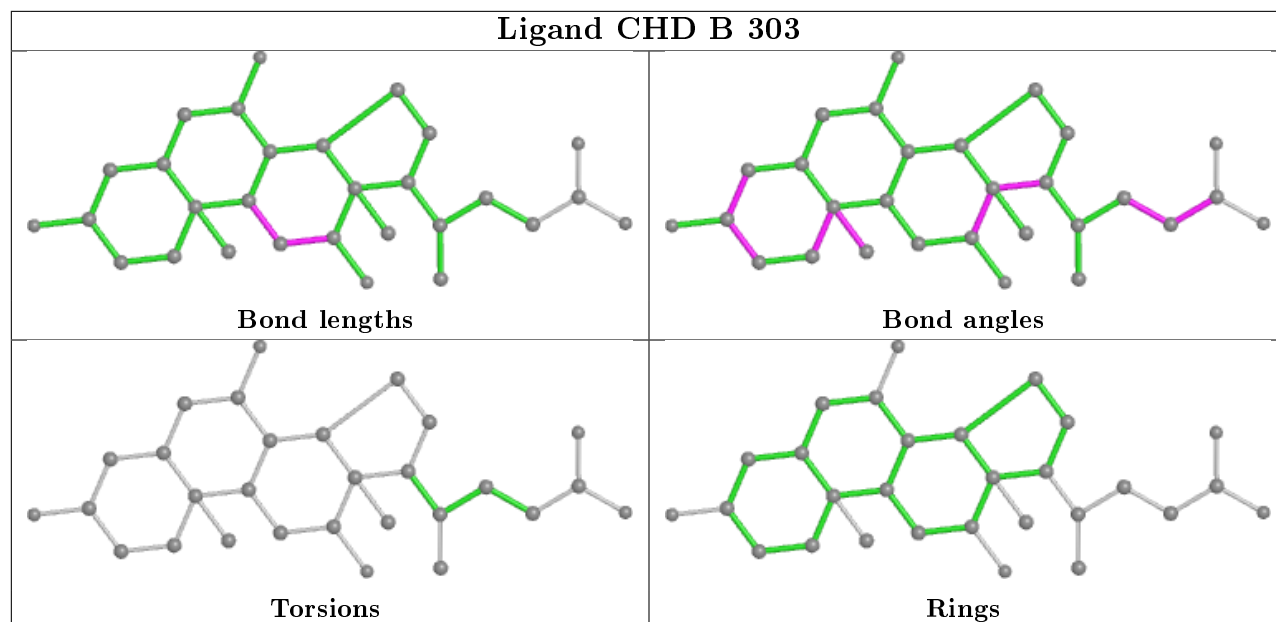


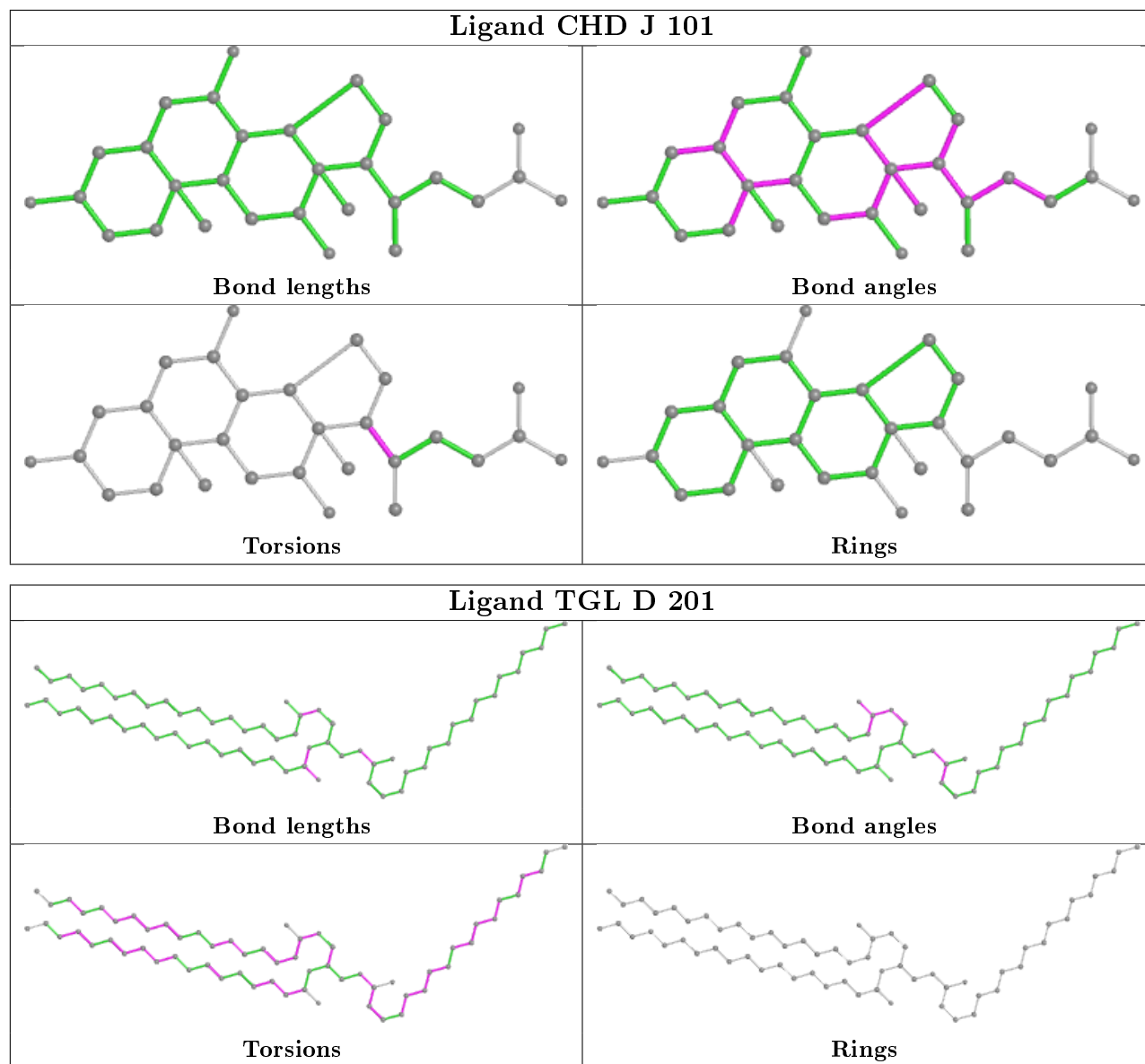
Ligand DMU P 307

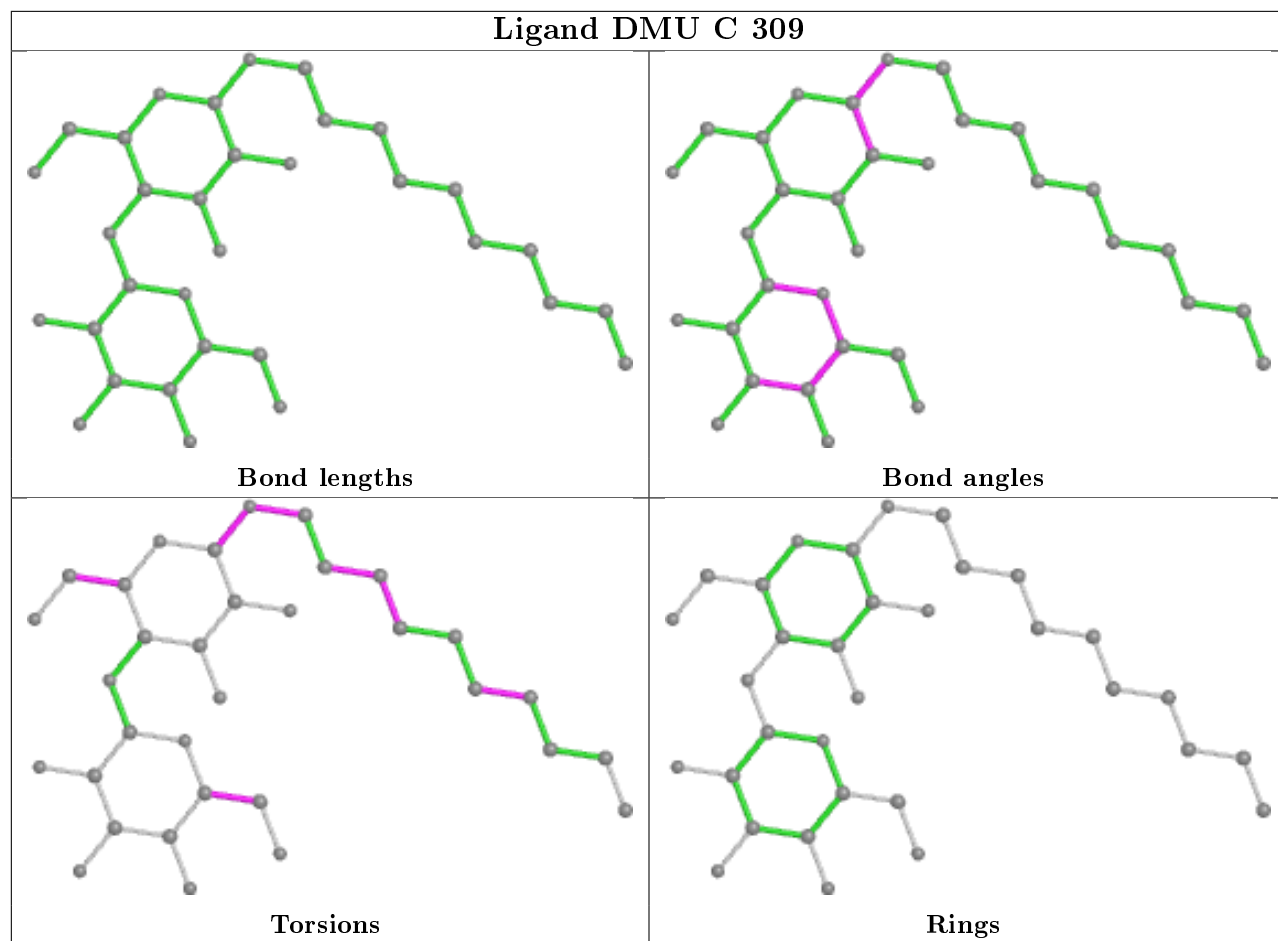


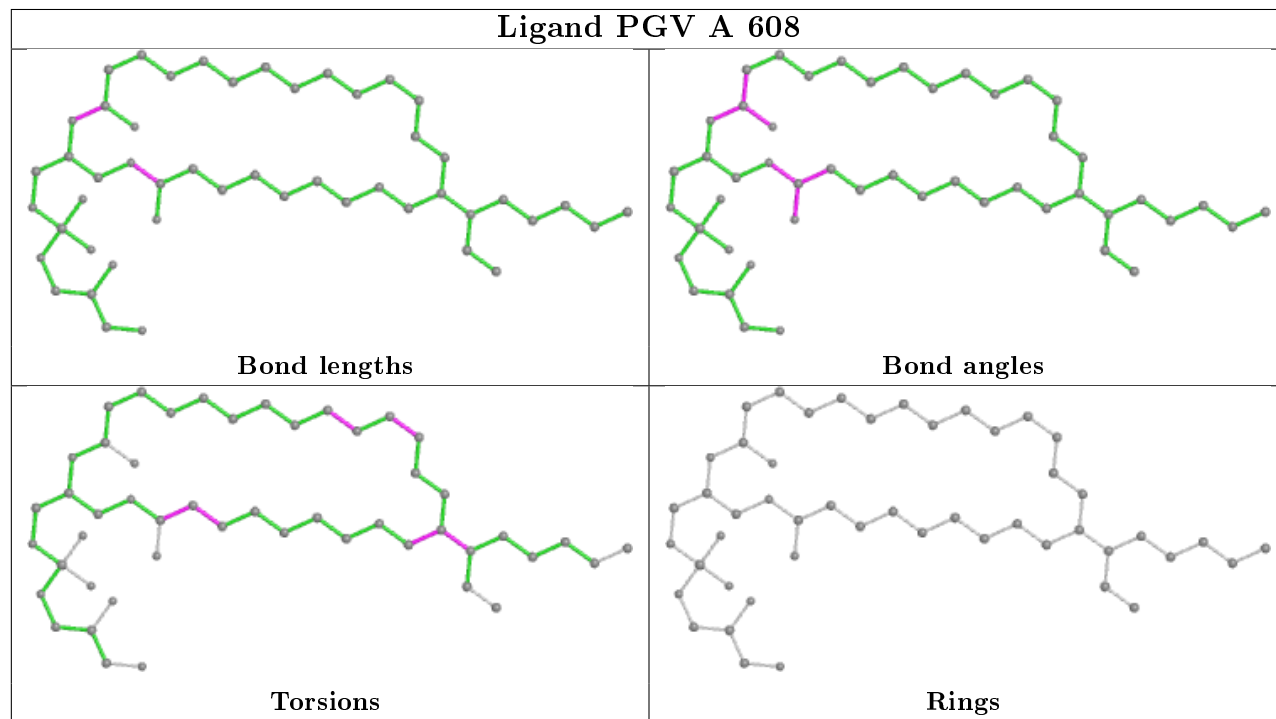
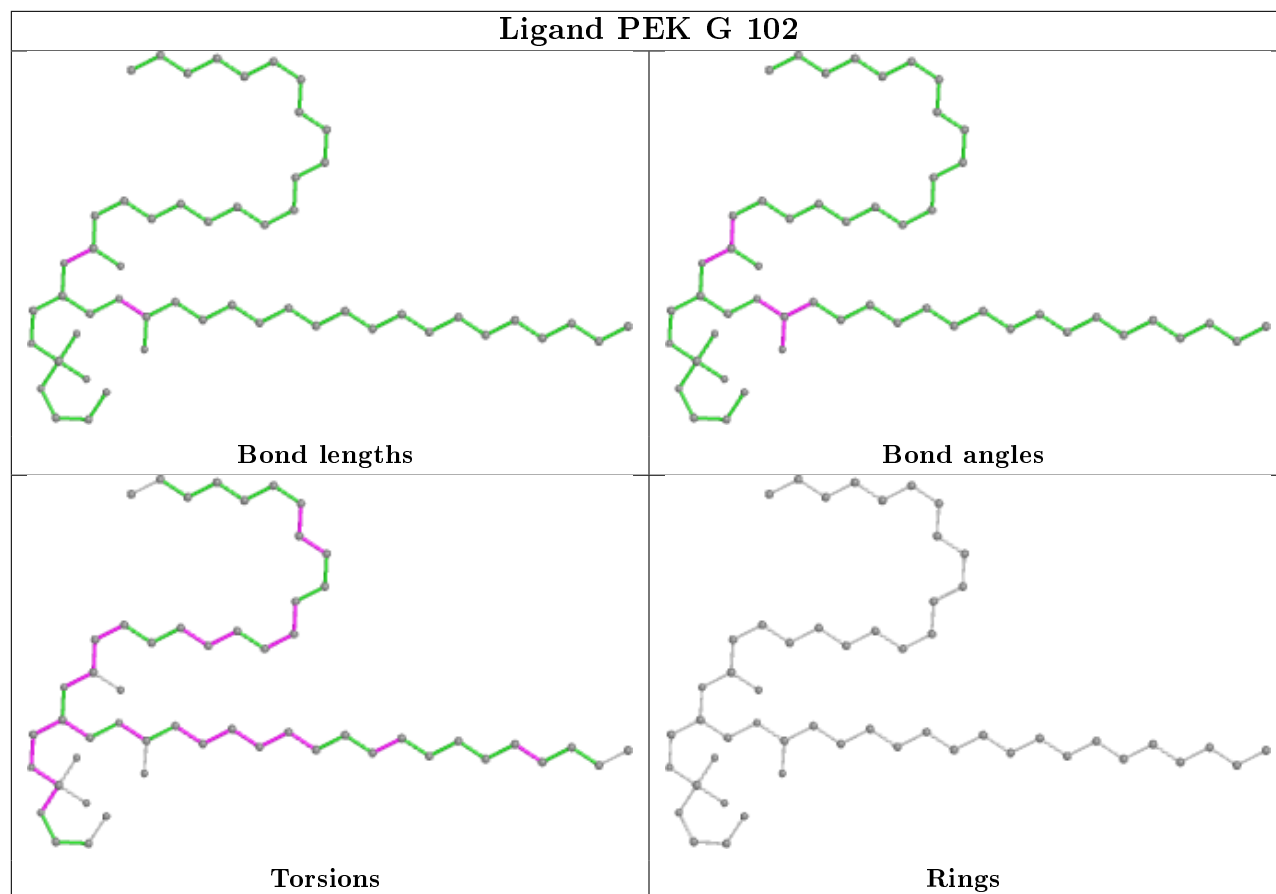
Ligand PSC E 201

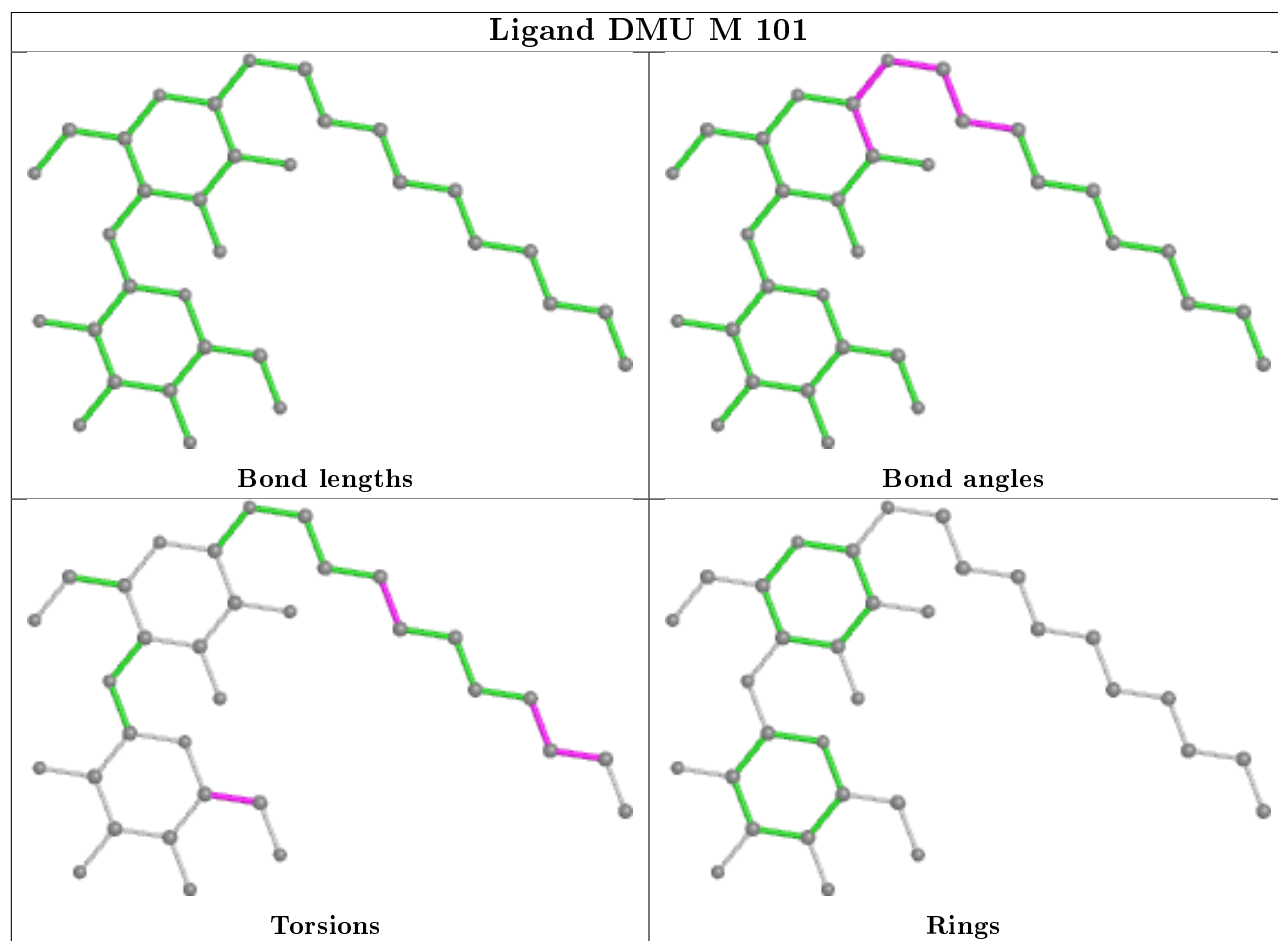
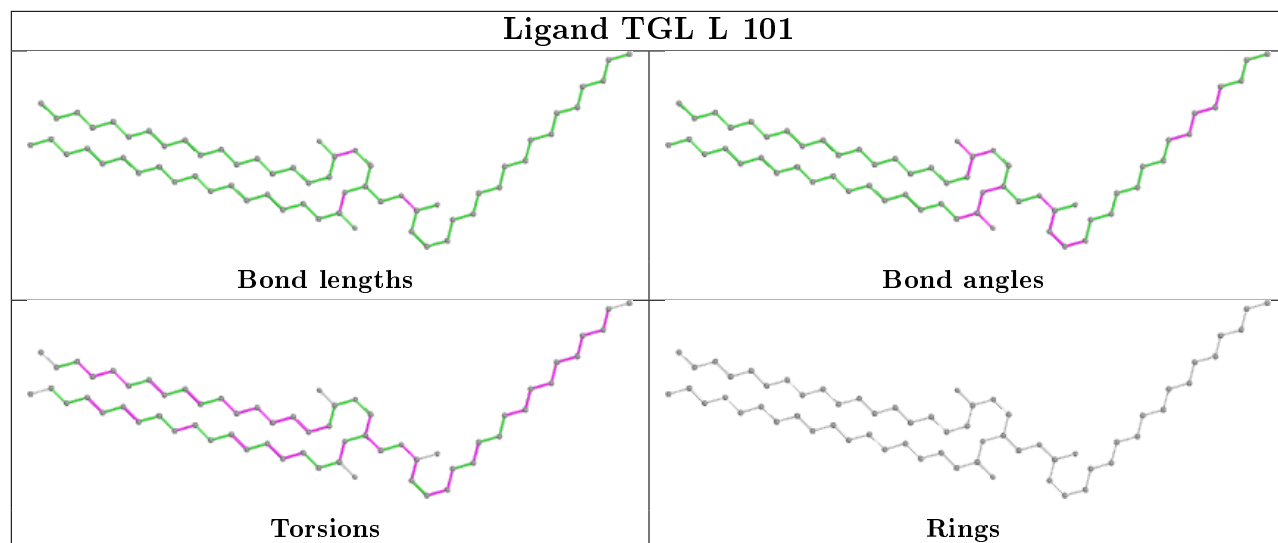


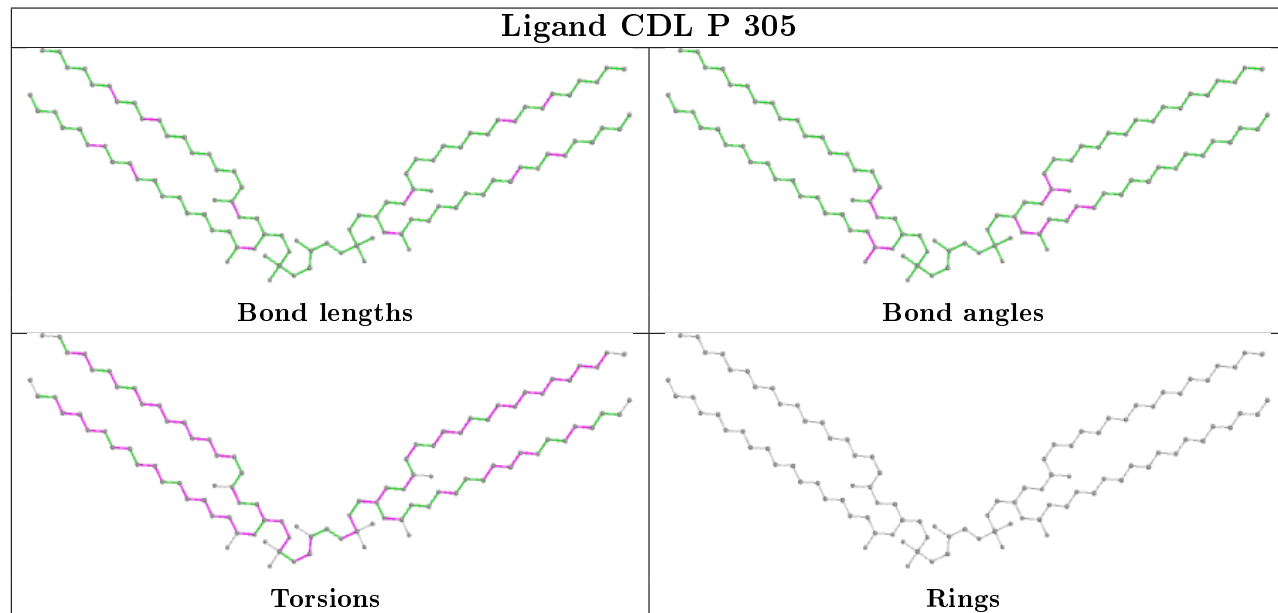
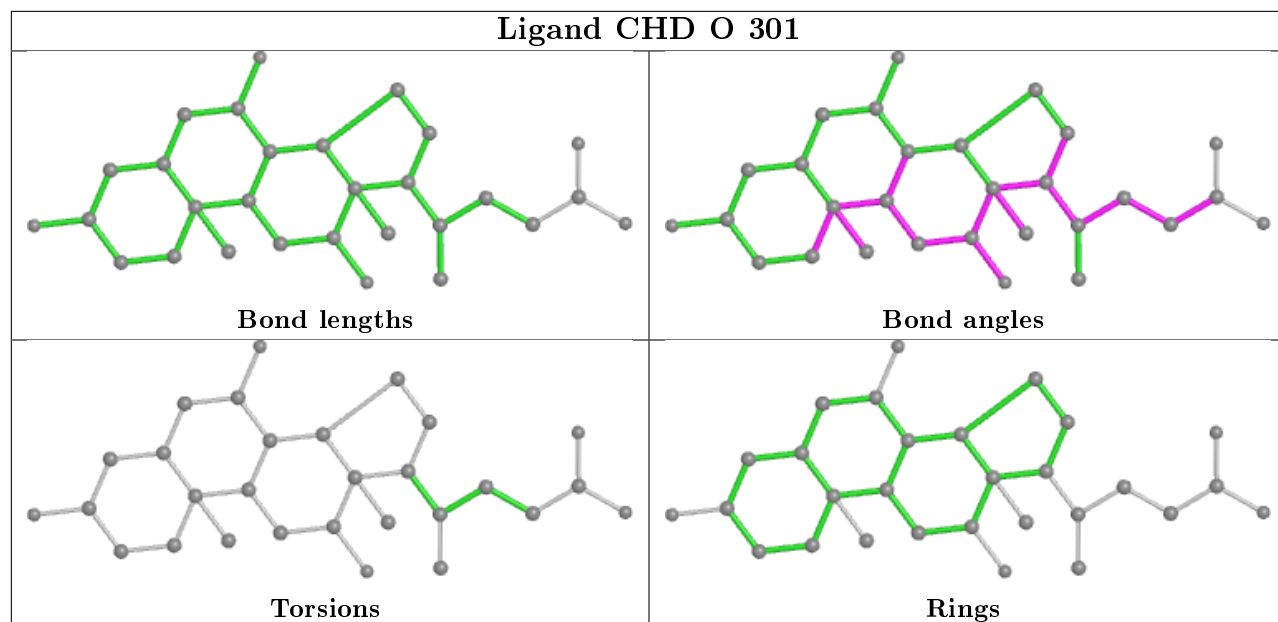


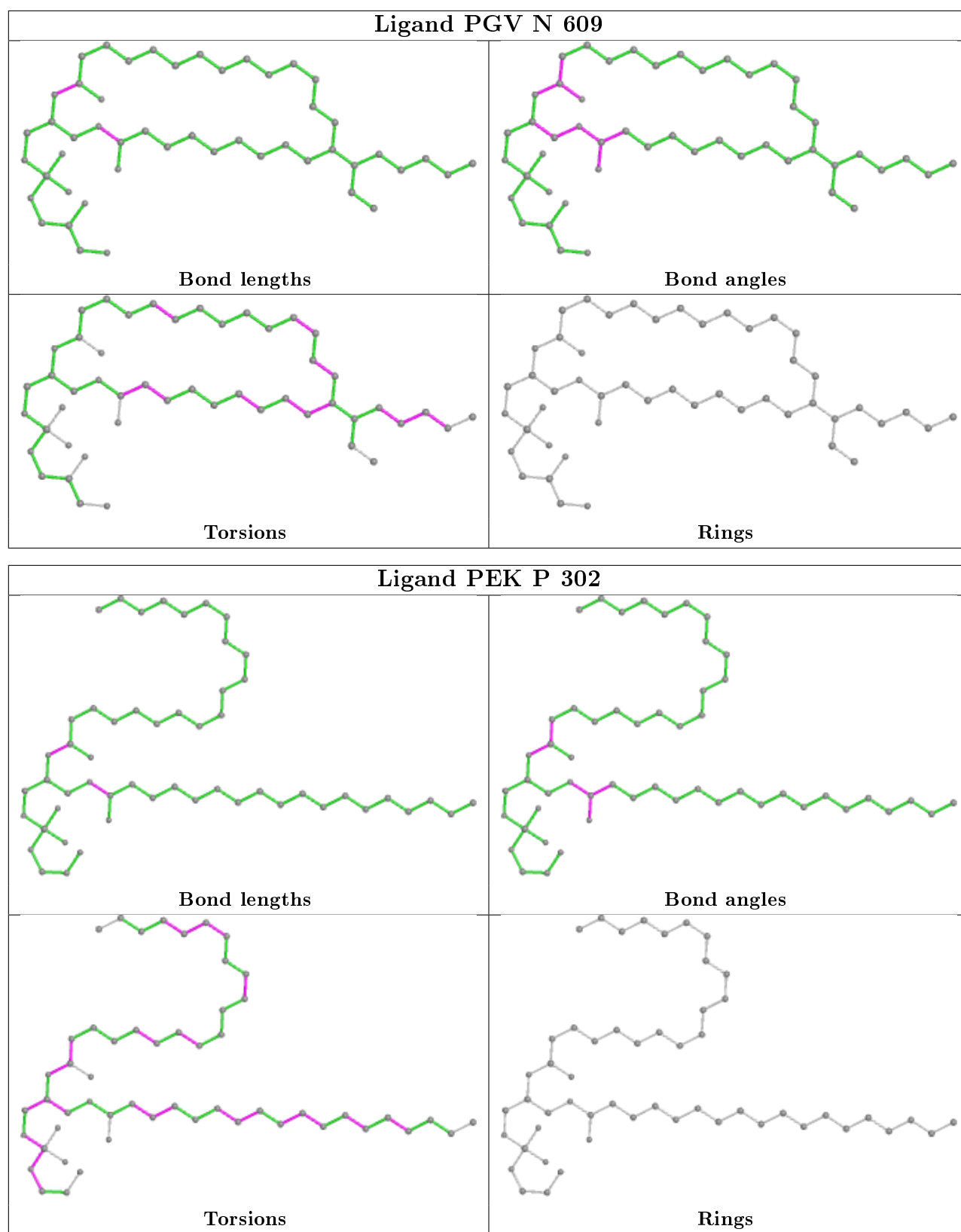












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.07	1 (0%) 95 95	24, 28, 36, 71	0
1	N	513/514 (99%)	-0.07	3 (0%) 89 90	24, 31, 40, 70	0
2	B	226/227 (99%)	0.01	9 (3%) 38 41	26, 35, 56, 91	1 (0%)
2	O	226/227 (99%)	0.02	16 (7%) 16 17	31, 40, 63, 84	0
3	C	259/261 (99%)	-0.35	3 (1%) 79 81	26, 32, 43, 78	0
3	P	259/261 (99%)	-0.32	4 (1%) 73 76	25, 32, 45, 76	0
4	D	144/147 (97%)	-0.06	6 (4%) 36 39	30, 37, 57, 76	0
4	Q	144/147 (97%)	1.01	25 (17%) 1 1	37, 49, 78, 148	0
5	E	105/109 (96%)	-0.02	5 (4%) 30 33	31, 37, 58, 103	0
5	R	105/109 (96%)	0.14	5 (4%) 30 33	34, 45, 63, 113	0
6	F	98/98 (100%)	0.63	11 (11%) 5 6	28, 38, 93, 145	0
6	S	98/98 (100%)	0.84	9 (9%) 9 10	27, 37, 97, 149	0
7	G	83/85 (97%)	1.03	19 (22%) 0 0	30, 41, 104, 128	0
7	T	83/85 (97%)	1.06	19 (22%) 0 0	31, 42, 105, 134	0
8	H	79/85 (92%)	0.89	14 (17%) 1 1	32, 41, 95, 109	0
8	U	79/85 (92%)	0.92	15 (18%) 1 1	36, 46, 96, 121	0
9	I	72/73 (98%)	1.16	18 (25%) 0 0	35, 47, 74, 86	0
9	V	72/73 (98%)	1.35	19 (26%) 0 0	34, 55, 73, 91	0
10	J	58/59 (98%)	0.52	8 (13%) 2 3	32, 43, 65, 107	0
10	W	58/59 (98%)	0.54	8 (13%) 2 3	34, 44, 70, 109	0
11	K	49/56 (87%)	0.53	3 (6%) 21 24	33, 41, 54, 60	0
11	X	49/56 (87%)	1.37	12 (24%) 0 0	42, 51, 69, 79	0
12	L	46/47 (97%)	-0.20	2 (4%) 35 38	30, 34, 54, 88	0
12	Y	46/47 (97%)	0.22	6 (13%) 3 3	33, 41, 61, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.20	4 (9%) 8 10	29, 34, 65, 99	0
13	Z	43/46 (93%)	0.63	7 (16%) 1 1	36, 42, 75, 108	0
All	All	3550/3614 (98%)	0.21	251 (7%) 16 17	24, 36, 67, 149	1 (0%)

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	29.1
4	Q	6	VAL	18.0
4	Q	5	VAL	16.2
6	S	1	ALA	15.6
6	S	98	HIS	12.7
4	Q	4	SER	12.5
4	Q	7	LYS	12.5
6	F	98	HIS	11.3
6	F	97	ALA	11.0
7	G	10	GLY	10.5
8	U	7	LYS	9.8
6	F	96	LEU	9.8
9	V	37	PHE	9.6
9	I	37	PHE	9.3
8	U	8	ILE	8.9
7	T	10	GLY	8.3
6	F	1	ALA	8.3
7	T	3	ALA	8.1
10	J	58	LYS	8.0
6	S	2	SER	7.9
5	R	109	VAL	7.7
8	U	44	THR	7.5
8	U	46	LYS	7.5
10	W	57	HIS	7.5
5	R	5	HIS	7.3
13	M	42	LYS	7.2
9	I	25	PHE	7.1
7	G	3	ALA	7.1
13	Z	43	SER	7.1
8	H	44	THR	7.0
8	H	47	GLY	6.9
7	G	2	SER	6.9
10	W	58	LYS	6.8
9	V	34	PHE	6.7

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Mol	Chain	Res	Type	RSRZ
13	M	43	SER	6.6
4	Q	8	SER	6.4
9	V	29	LEU	6.4
11	X	6	ALA	6.4
6	F	2	SER	6.4
7	T	40	GLY	6.2
9	I	29	LEU	6.2
8	H	45	ALA	6.2
5	E	5	HIS	6.2
2	O	90	ILE	6.2
5	E	109	VAL	6.2
7	G	8	HIS	6.0
7	T	2	SER	6.0
7	T	42	ARG	6.0
6	F	95	GLN	6.0
11	X	7	PRO	6.0
9	V	25	PHE	6.0
7	G	42	ARG	5.9
10	J	57	HIS	5.9
8	H	7	LYS	5.9
12	Y	47	LYS	5.8
6	S	95	GLN	5.8
10	W	52	TRP	5.7
9	I	26	MET	5.7
9	V	33	THR	5.6
7	T	36[A]	TRP	5.6
8	U	10	ASN	5.6
6	S	94	HIS	5.5
8	H	8	ILE	5.5
7	T	9	GLY	5.5
4	Q	147	LYS	5.4
10	J	52	TRP	5.4
9	I	33	THR	5.4
8	H	46	LYS	5.4
7	G	36	TRP	5.3
7	G	84	LYS	5.3
13	Z	42	LYS	5.3
8	U	45	ALA	5.2
8	H	48	GLY	5.1
9	I	34	PHE	5.1
11	X	13	TYR	5.0
2	B	60	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
9	V	26	MET	5.0
8	U	48	GLY	5.0
2	O	113	TYR	5.0
7	T	41	HIS	4.9
8	H	10	ASN	4.9
10	J	1	PHE	4.9
7	T	84	LYS	4.9
4	Q	51	LEU	4.8
7	G	41	HIS	4.8
7	T	1	ALA	4.8
8	H	50	VAL	4.8
13	M	40	TYR	4.8
7	G	9	GLY	4.7
9	V	30	GLY	4.7
10	J	56	PRO	4.7
8	U	47	GLY	4.7
2	B	59	GLN	4.7
2	O	59	GLN	4.6
6	S	96	LEU	4.6
9	I	30	GLY	4.6
10	W	1	PHE	4.5
7	T	43	GLU	4.5
7	T	8	HIS	4.5
4	D	147	LYS	4.4
9	V	19	PHE	4.4
7	G	40	GLY	4.4
10	W	55	PHE	4.3
7	T	38	HIS	4.3
7	G	5	LYS	4.2
13	M	39	ASN	4.2
3	P	37	PHE	4.2
7	G	7	ASP	4.2
8	H	42	ALA	4.2
11	X	12	LYS	4.1
7	T	39	SER	4.1
7	G	43	GLU	4.1
11	K	7	PRO	4.0
2	O	227	LEU	4.0
3	P	3	HIS	4.0
9	V	2	THR	3.9
10	J	55	PHE	3.9
7	T	5	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
11	K	6	ALA	3.9
7	G	37	LEU	3.9
13	Z	40	TYR	3.9
7	T	6	GLY	3.8
2	B	90	ILE	3.7
13	Z	39	ASN	3.7
4	Q	30	VAL	3.7
7	G	4	ALA	3.7
6	F	94	HIS	3.7
7	T	4	ALA	3.7
9	V	31	PHE	3.7
8	H	43	MET	3.6
7	G	39	SER	3.6
9	I	32	ALA	3.6
7	G	45	PRO	3.5
4	Q	33	LEU	3.5
2	O	91	ASN	3.5
9	I	31	PHE	3.4
8	H	49	ASP	3.4
7	G	6	GLY	3.4
4	D	4	SER	3.4
9	V	22	VAL	3.4
5	E	7	THR	3.3
12	L	2	HIS	3.3
8	U	52	VAL	3.2
10	W	48	TYR	3.2
4	Q	142	LYS	3.2
4	Q	58	GLU	3.1
4	Q	46	ALA	3.1
8	U	50	VAL	3.1
9	I	19	PHE	3.1
4	D	143	ASN	3.1
9	V	53	ASN	3.1
2	O	60	GLU	3.1
2	O	165	VAL	3.1
9	I	27	VAL	3.1
3	C	37	PHE	3.1
11	X	23	THR	3.0
9	V	32	ALA	3.0
4	Q	32	ASN	3.0
8	U	9	LYS	3.0
4	Q	31	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	P	38	ASN	2.9
11	X	47	ARG	2.9
8	U	49	ASP	2.9
8	U	43	MET	2.9
4	Q	138	TRP	2.9
9	I	22	VAL	2.9
3	C	38	ASN	2.9
6	F	44	GLU	2.8
8	H	36	PHE	2.8
9	I	18	ARG	2.8
9	I	53	ASN	2.8
4	Q	140	TYR	2.8
9	V	45	LYS	2.8
6	S	93	PRO	2.7
10	W	56	PRO	2.7
6	F	3	GLY	2.7
8	U	11	TYR	2.7
13	Z	41	LYS	2.7
11	X	34	THR	2.7
4	Q	39	ALA	2.7
9	V	27	VAL	2.7
12	Y	20	ARG	2.7
2	O	211	LEU	2.6
5	R	108	LYS	2.6
4	Q	62	LEU	2.6
5	R	7	THR	2.6
2	O	224	ALA	2.6
8	H	9	LYS	2.6
7	T	46	ALA	2.6
4	D	142	LYS	2.6
11	K	47	ARG	2.6
4	D	5	VAL	2.6
2	O	168	LEU	2.5
4	Q	10	ASP	2.5
2	O	92	ASN	2.5
3	P	33	MET	2.5
9	V	57	MET	2.5
2	O	89	GLU	2.5
5	E	9	GLU	2.5
7	T	7	ASP	2.5
2	O	217	LYS	2.5
10	J	48	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
6	F	25	ARG	2.4
4	Q	144	GLU	2.4
10	J	27	THR	2.4
2	B	170	LEU	2.4
11	X	8	ASP	2.4
4	Q	9	GLU	2.4
2	O	170	LEU	2.4
12	Y	19	TRP	2.4
2	B	209	ILE	2.4
9	V	52	ARG	2.3
10	W	51	GLY	2.3
9	I	52	ARG	2.3
1	N	366	VAL	2.3
11	X	30	VAL	2.3
6	F	37[A]	LYS	2.3
1	N	367	LEU	2.3
9	I	28	SER	2.3
11	X	27	ALA	2.3
8	U	51	SER	2.2
7	G	46	ALA	2.2
2	B	165	VAL	2.2
9	I	44	LYS	2.2
9	V	18	ARG	2.2
4	Q	143	ASN	2.2
9	V	36	LYS	2.2
4	Q	57	VAL	2.2
5	E	10	GLU	2.1
4	Q	35	ALA	2.1
2	B	166	PRO	2.1
13	Z	13	LYS	2.1
2	B	91	ASN	2.1
5	R	9	GLU	2.1
1	N	483	LEU	2.1
4	Q	40	LEU	2.1
4	D	141	ASP	2.1
12	Y	17	ASN	2.1
13	Z	35	TYR	2.1
9	I	36	LYS	2.1
11	X	35	GLN	2.1
12	Y	16	GLU	2.0
2	B	61	VAL	2.0
1	A	113[A]	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
11	X	18	LEU	2.0
6	S	44	GLU	2.0
2	O	9	PHE	2.0
2	O	169	GLY	2.0
12	L	45	LEU	2.0
12	Y	46	LYS	2.0
3	C	41	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.11	0.53	106,116,133,137	0
7	TPO	T	11	11/12	0.14	0.62	110,123,134,135	0
9	SAC	V	1	9/10	0.43	0.64	117,122,125,126	0
9	SAC	I	1	9/10	0.65	0.43	85,97,109,115	0
1	FME	A	1	10/11	0.94	0.21	41,46,68,84	0
1	FME	N	1	10/11	0.94	0.17	43,49,71,73	0
2	FME	B	1	10/11	0.96	0.14	32,34,43,57	0
2	FME	O	1	10/11	0.98	0.14	40,41,51,57	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	PEK	C	303	53/53	0.49	0.32	50,79,121,126	0
26	PSC	E	201	52/52	0.49	0.33	49,98,155,160	0
25	DMU	C	309	33/33	0.53	0.47	45,99,129,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CDL	G	101	100/100	0.55	0.27	63,90,131,148	0
23	PEK	P	302	53/53	0.55	0.30	51,74,133,139	0
23	PEK	G	102	53/53	0.57	0.37	49,105,138,154	0
23	PEK	T	101	53/53	0.58	0.34	52,96,152,157	0
20	TGL	Q	201	63/63	0.59	0.27	58,81,112,118	0
24	CDL	T	103	100/100	0.59	0.28	61,90,141,150	0
22	CHD	W	101	29/29	0.59	0.42	96,123,135,140	0
25	DMU	P	307	33/33	0.59	0.43	48,98,126,136	0
24	CDL	P	305	100/100	0.60	0.32	46,83,127,140	0
24	CDL	C	306	100/100	0.63	0.28	50,82,111,115	0
20	TGL	N	611	63/63	0.65	0.29	51,77,104,121	0
18	PGV	N	606	51/51	0.66	0.31	55,79,121,126	0
18	PGV	P	304	51/51	0.68	0.24	60,80,108,116	0
22	CHD	J	101	29/29	0.69	0.29	62,80,116,123	0
26	PSC	R	201	52/52	0.70	0.27	43,73,150,161	0
18	PGV	C	305	51/51	0.72	0.23	53,79,113,119	0
18	PGV	A	606	51/51	0.74	0.29	41,78,96,100	0
20	TGL	L	101	63/63	0.74	0.26	39,68,100,105	0
20	TGL	D	201	63/63	0.76	0.19	47,70,96,99	0
20	TGL	N	608	63/63	0.77	0.24	53,78,123,143	0
25	DMU	Z	101	33/33	0.80	0.23	51,56,65,65	0
20	TGL	B	301	63/63	0.82	0.20	46,70,96,102	0
25	DMU	M	101	33/33	0.82	0.17	41,46,55,61	0
22	CHD	C	307	29/29	0.86	0.22	55,60,71,81	0
22	CHD	P	306	29/29	0.89	0.23	48,59,64,70	0
23	PEK	T	102	53/53	0.93	0.21	35,47,81,85	0
17	NA	P	301	1/1	0.93	0.08	47,47,47,47	0
17	NA	C	301	1/1	0.94	0.13	49,49,49,49	0
22	CHD	C	308	29/29	0.95	0.08	30,33,38,41	0
23	PEK	C	302	53/53	0.95	0.20	31,48,80,85	0
22	CHD	N	610	29/29	0.96	0.08	30,33,38,44	0
18	PGV	N	609	51/51	0.96	0.19	29,41,63,69	0
18	PGV	C	304	51/51	0.96	0.22	29,36,75,80	0
18	PGV	P	303	51/51	0.96	0.20	28,38,72,76	0
16	MG	N	604	1/1	0.97	0.11	36,36,36,36	0
18	PGV	A	608	51/51	0.97	0.21	28,39,64,70	0
22	CHD	O	301	29/29	0.97	0.07	26,30,34,41	0
22	CHD	B	303	29/29	0.97	0.08	28,30,34,43	0
14	HEA	N	602	60/60	0.98	0.12	25,28,33,36	0
14	HEA	N	601	60/60	0.98	0.14	26,31,52,58	0
14	HEA	A	602	60/60	0.98	0.11	23,26,33,34	0
14	HEA	A	601	60/60	0.98	0.12	22,26,51,55	0

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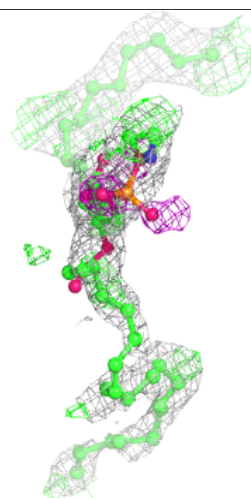
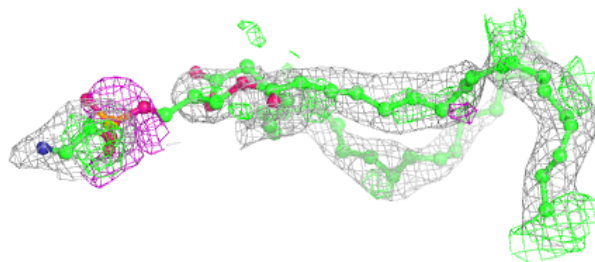
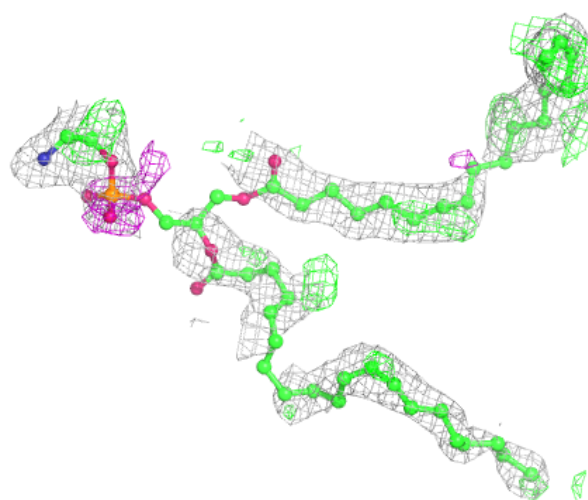
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	PER	N	607[A]	2/2	0.99	0.17	21,21,21,25	0
16	MG	A	604	1/1	0.99	0.08	29,29,29,29	0
19	PER	N	607[B]	2/2	0.99	0.17	19,19,19,19	2
17	NA	A	605	1/1	0.99	0.05	30,30,30,30	0
15	CU	N	603	1/1	1.00	0.12	29,29,29,29	0
19	PER	A	607[A]	2/2	1.00	0.13	19,19,19,25	0
17	NA	N	605	1/1	1.00	0.07	35,35,35,35	0
21	CUA	O	302	2/2	1.00	0.07	34,34,34,35	0
27	ZN	S	101	1/1	1.00	0.06	34,34,34,34	0
19	PER	A	607[B]	2/2	1.00	0.13	15,15,15,15	2
21	CUA	B	302	2/2	1.00	0.09	29,29,29,30	0
15	CU	A	603	1/1	1.00	0.09	27,27,27,27	0
27	ZN	F	101	1/1	1.00	0.05	33,33,33,33	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.

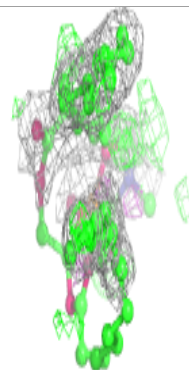
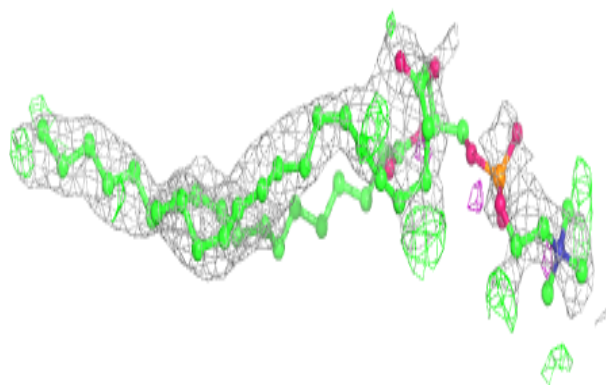
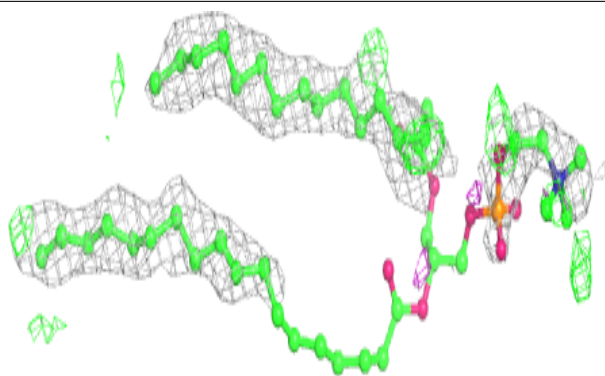
Electron density around PEK C 303:

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

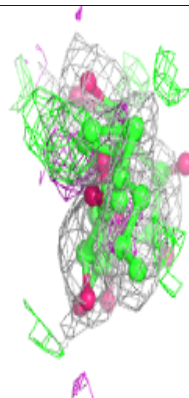
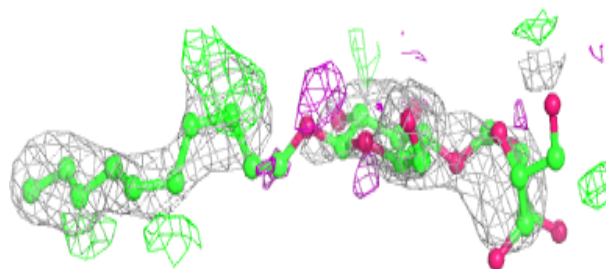
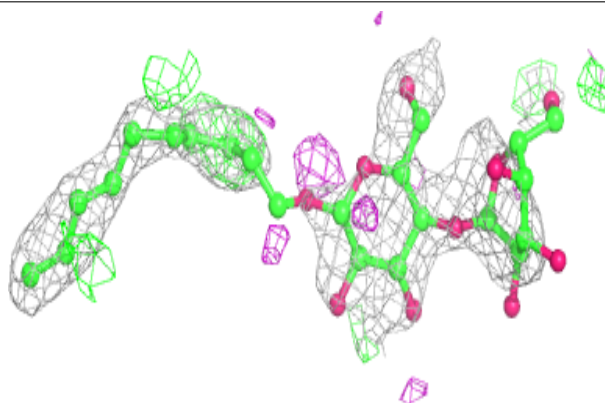


Electron density around PSC E 201:

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

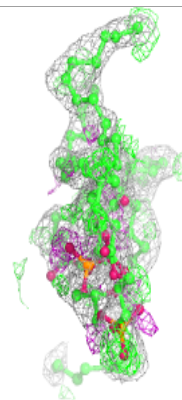
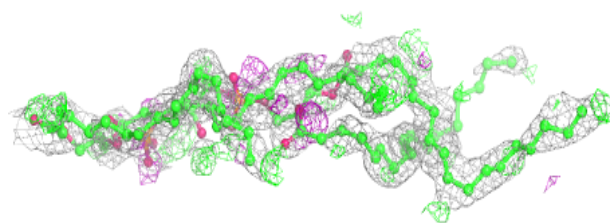
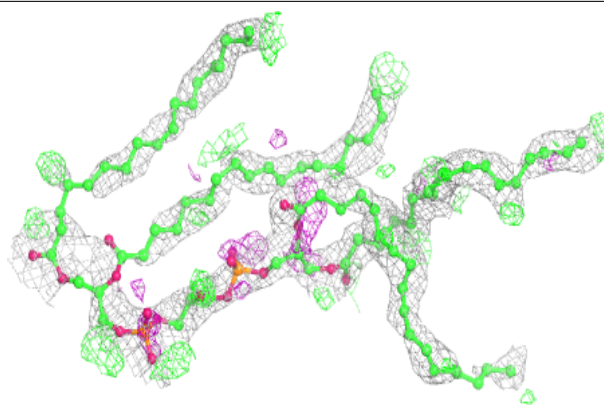
**Electron density around DMU C 309:**

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

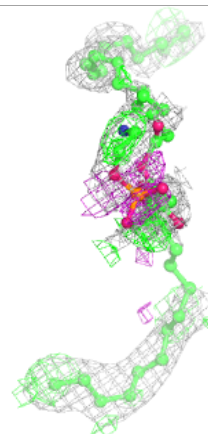
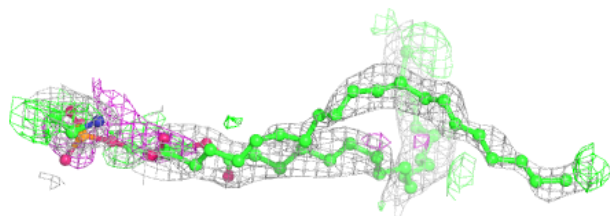
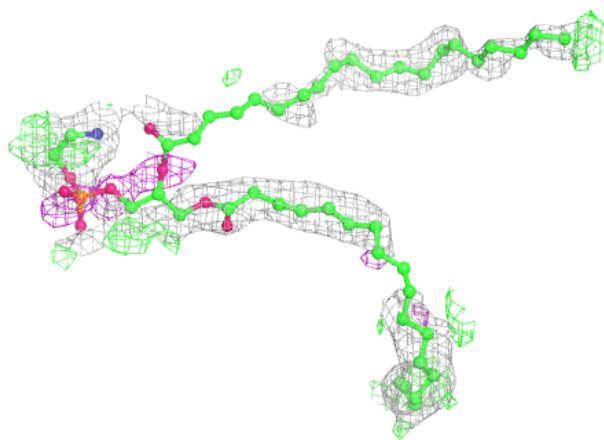


Electron density around CDL G 101:

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

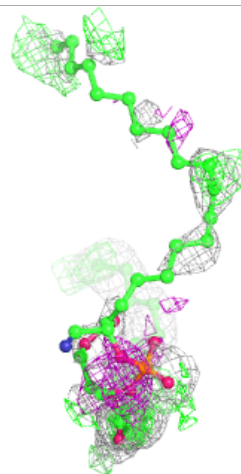
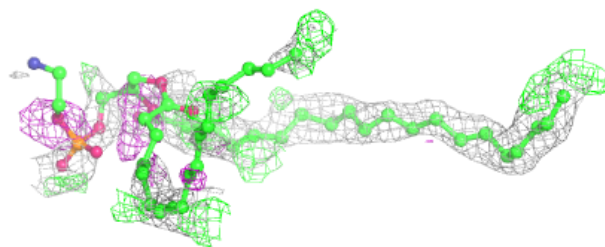
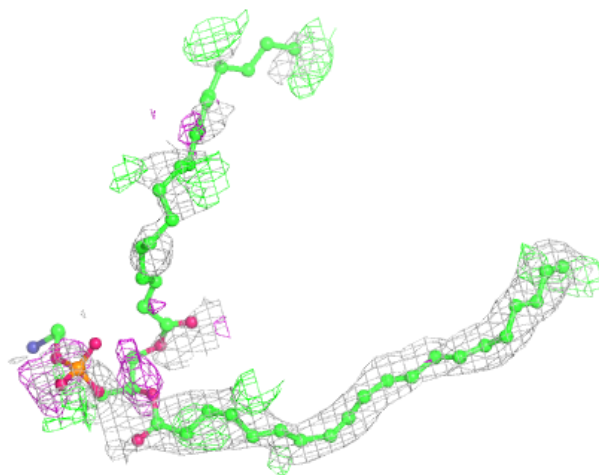
**Electron density around PEK P 302:**

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



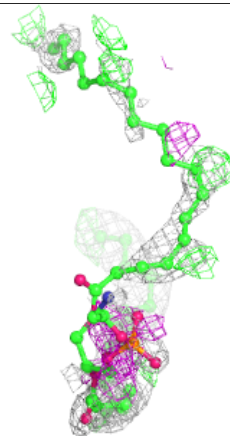
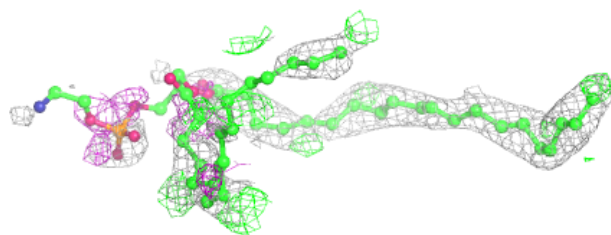
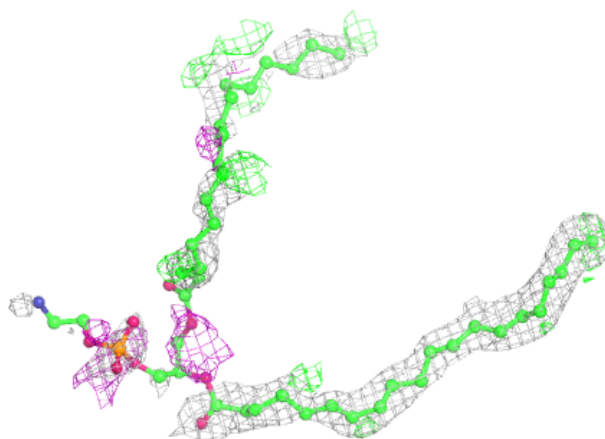
Electron density around PEK G 102:

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

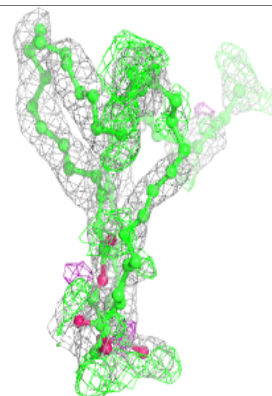
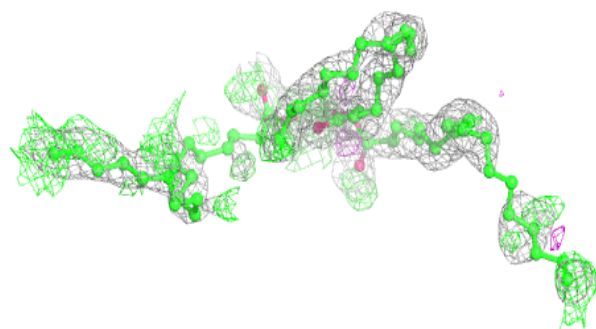
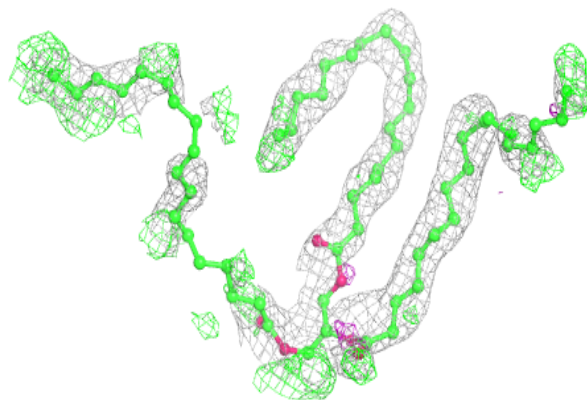


Electron density around PEK T 101:

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

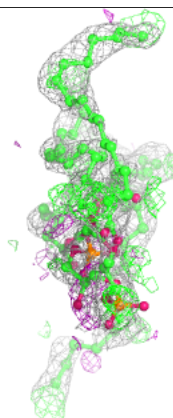
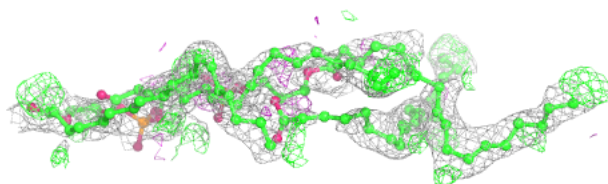
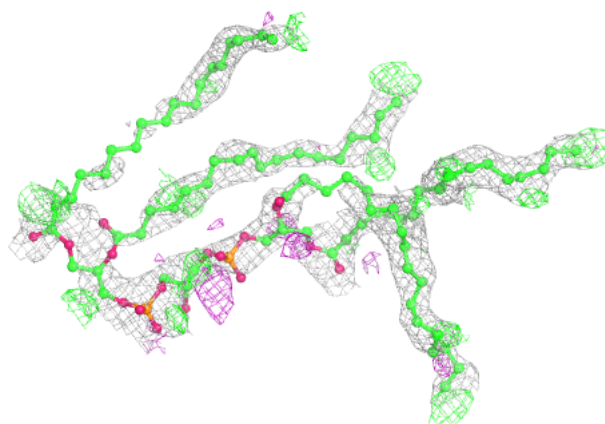
**Electron density around TGL Q 201:**

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

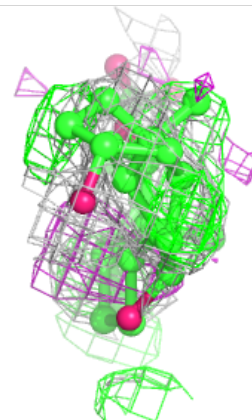
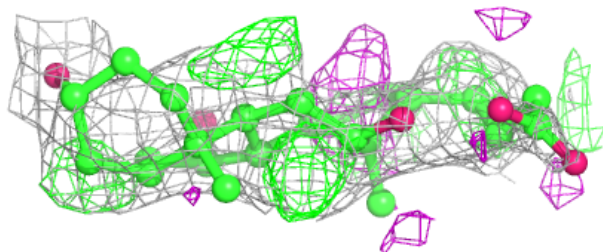
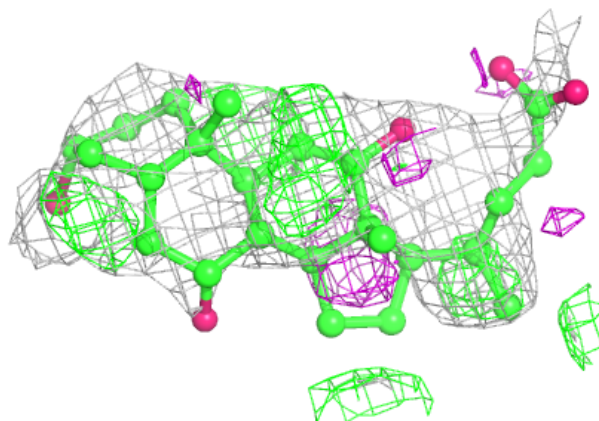


Electron density around CDL T 103:

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

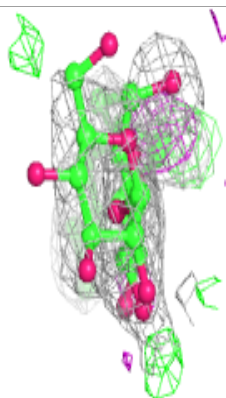
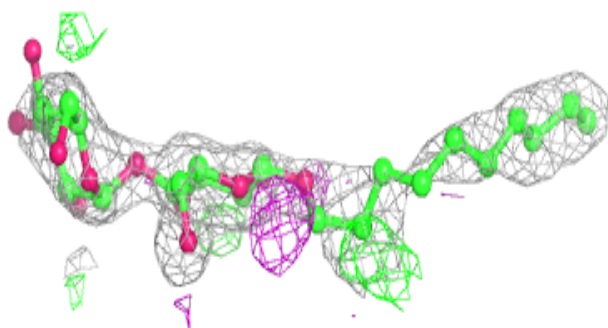
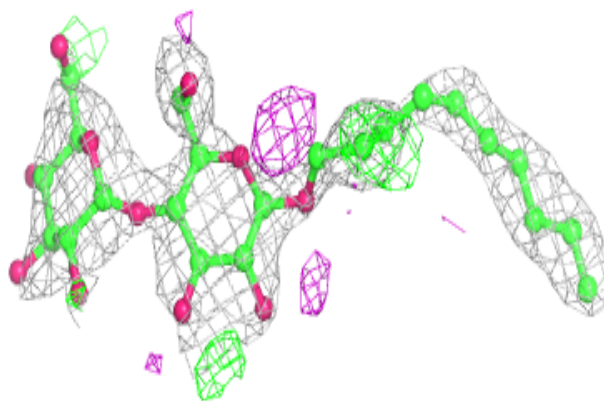
**Electron density around CHD W 101:**

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

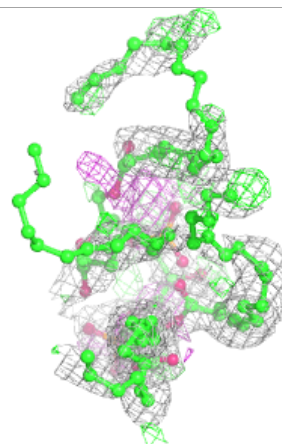
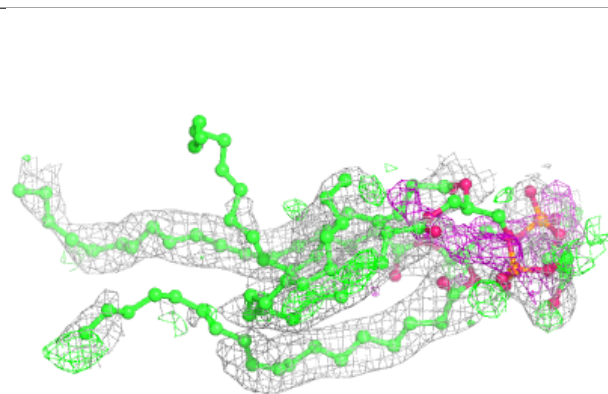
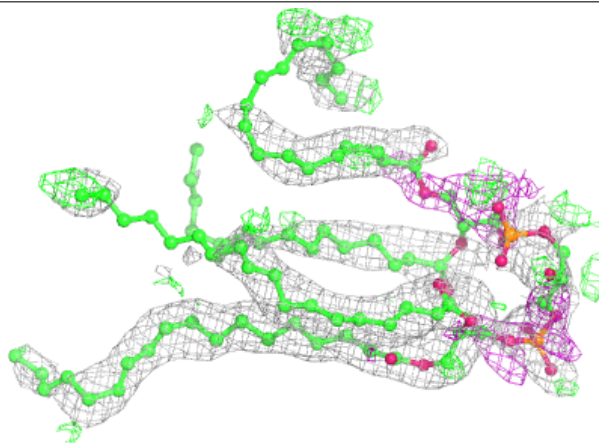


Electron density around DMU P 307:

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

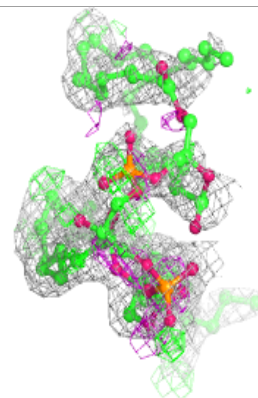
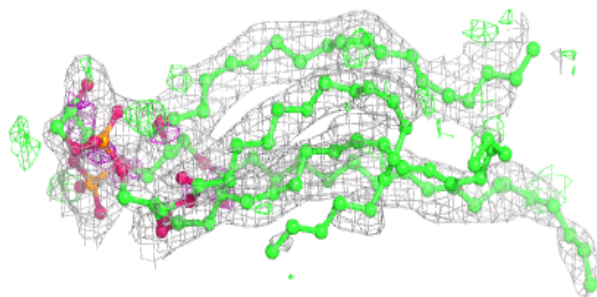
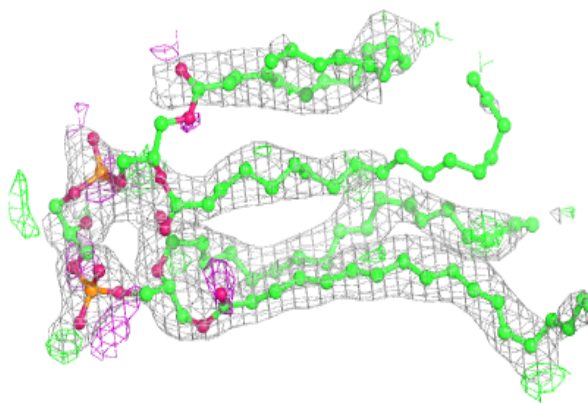
**Electron density around CDL P 305:**

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



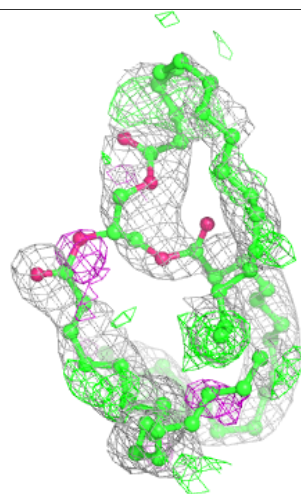
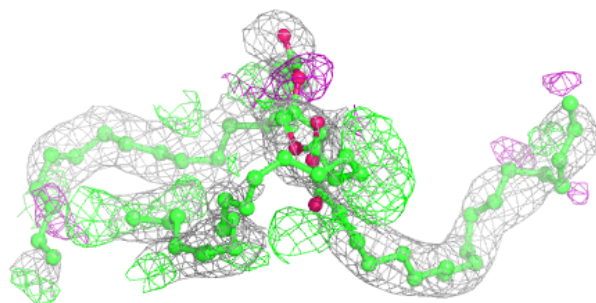
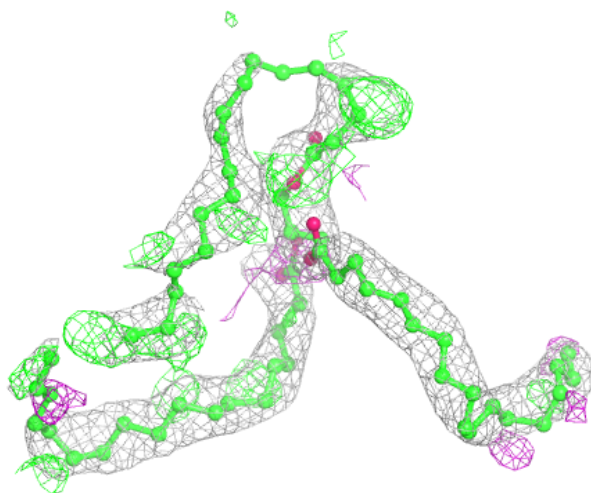
Electron density around CDL C 306:

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



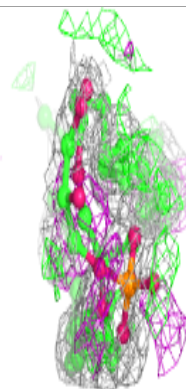
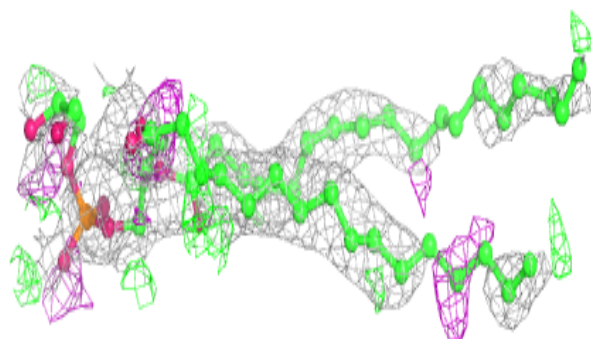
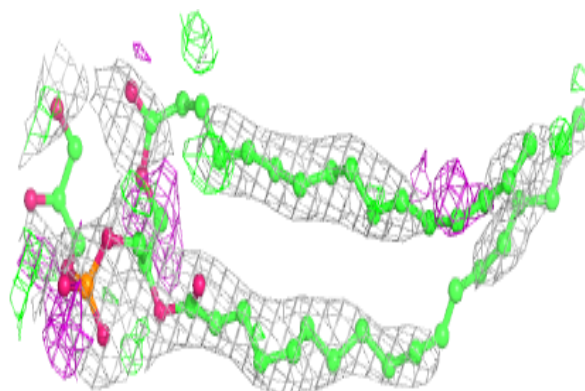
Electron density around TGL N 611:

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

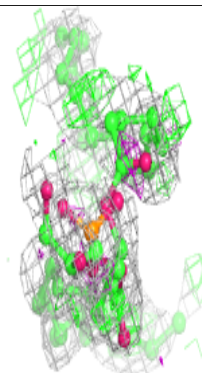
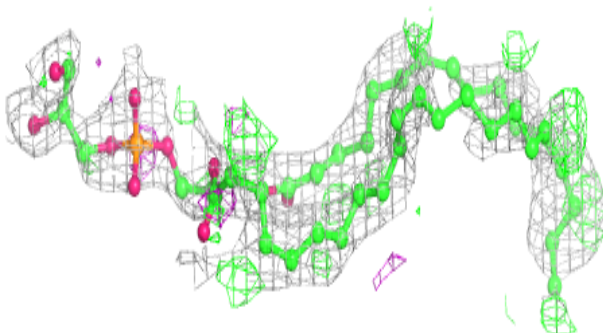
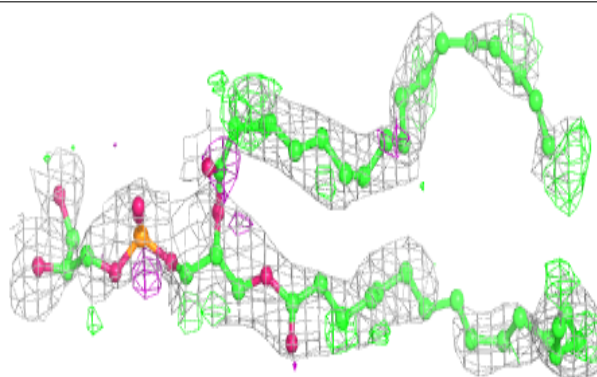


Electron density around PGV N 606:

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

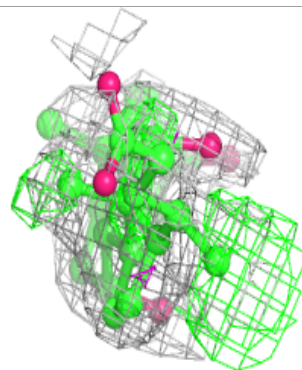
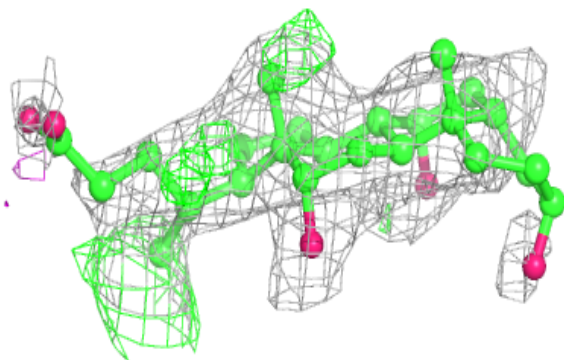
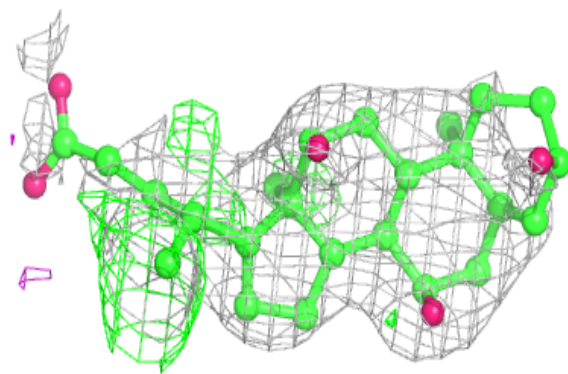
**Electron density around PGV P 304:**

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

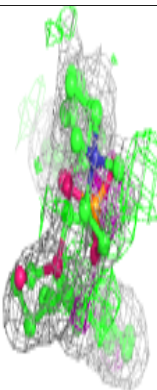
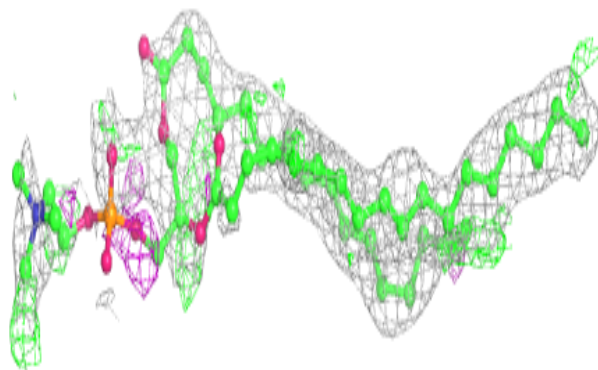
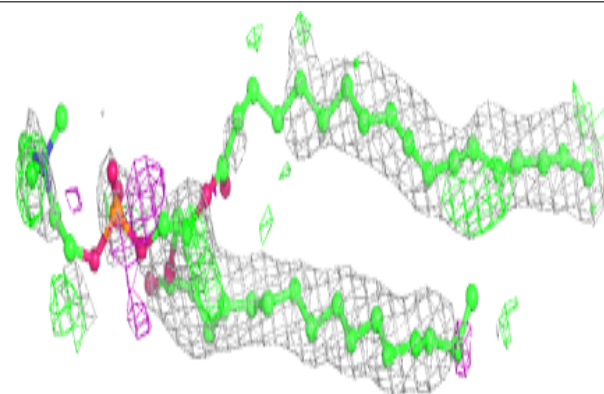


Electron density around CHD J 101:

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

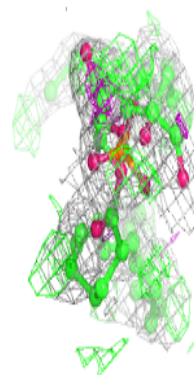
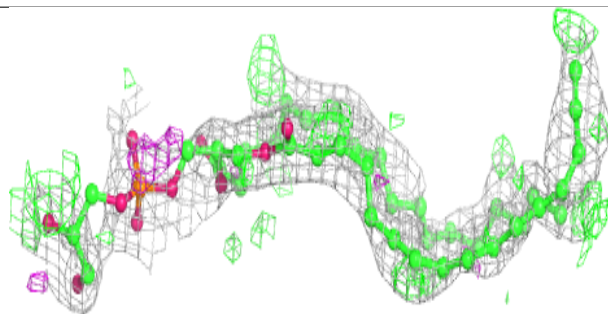
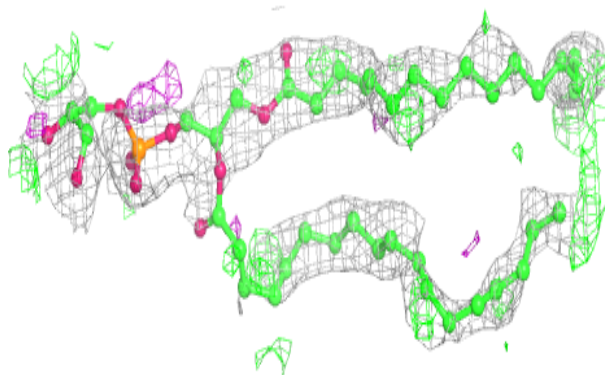
**Electron density around PSC R 201:**

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

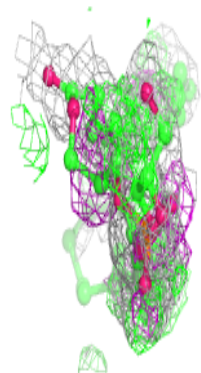
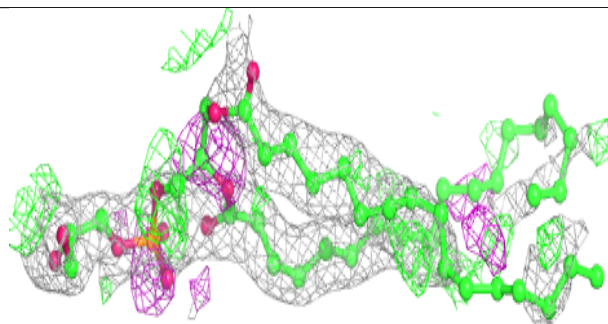
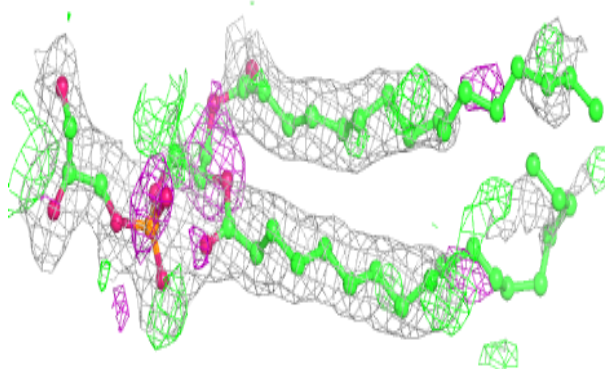


Electron density around PGV C 305:

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

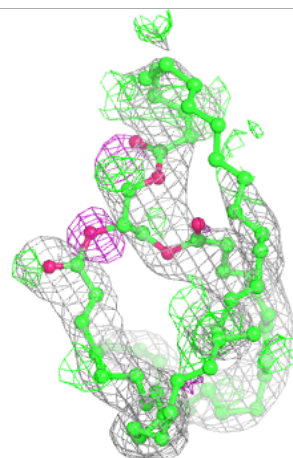
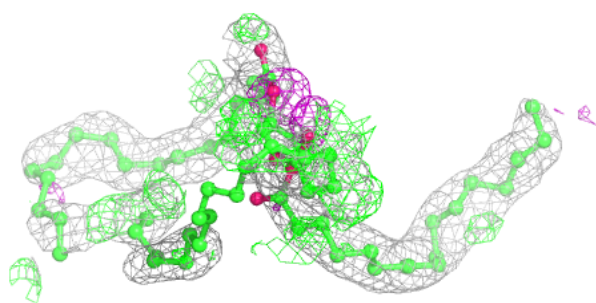
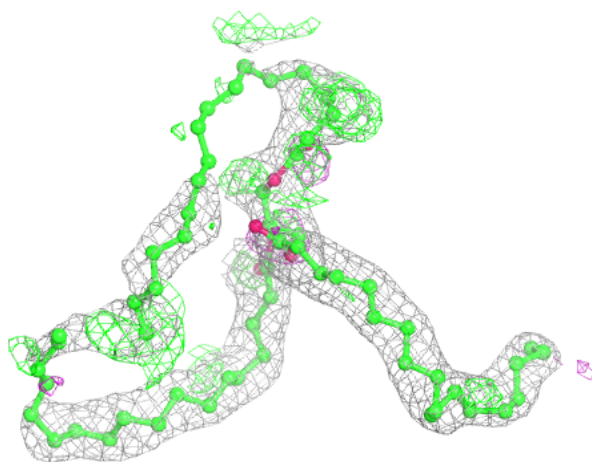
**Electron density around PGV A 606:**

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



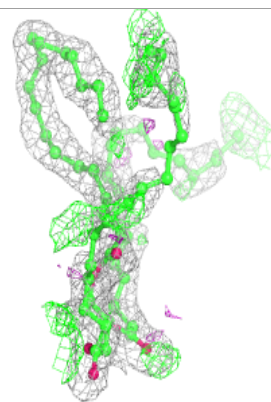
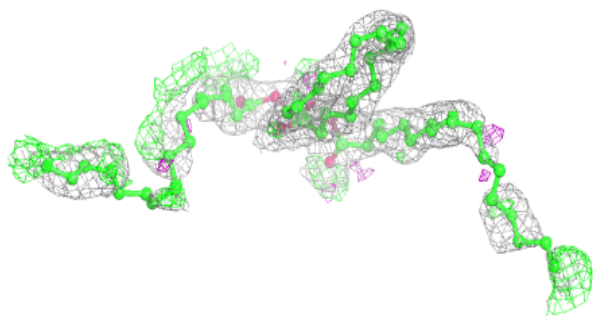
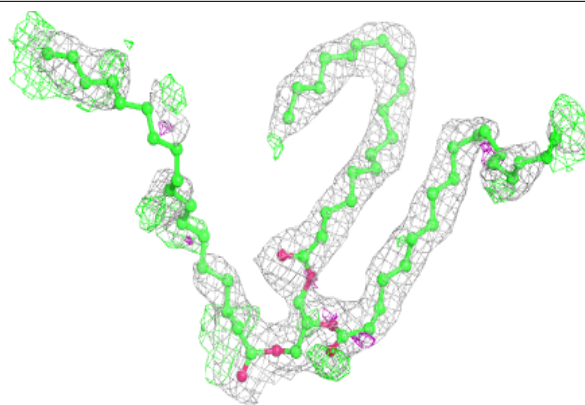
Electron density around TGL L 101:

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

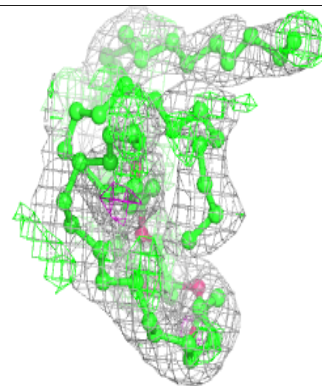
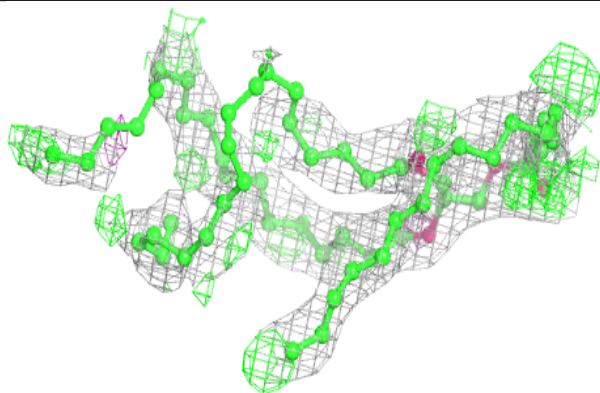
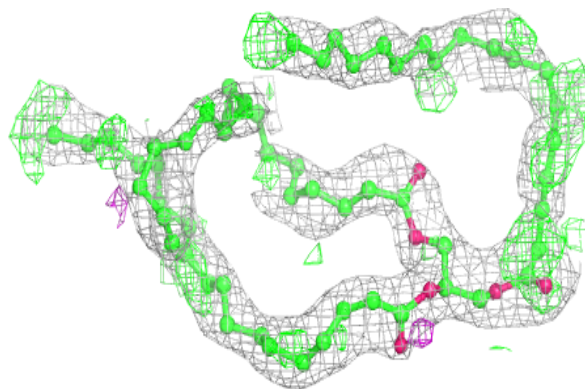


Electron density around TGL D 201:

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

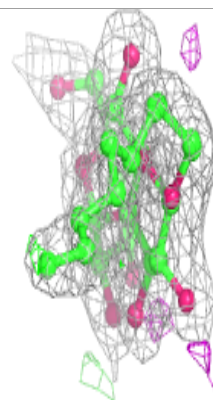
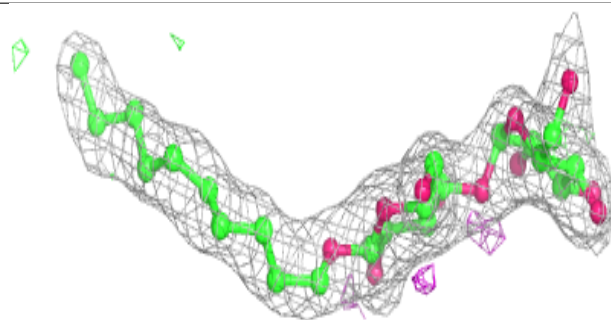
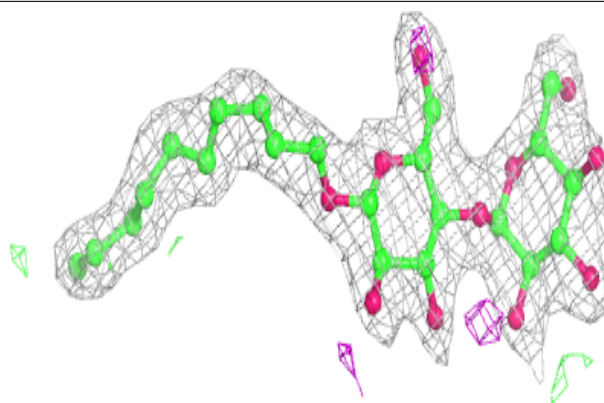
**Electron density around TGL N 608:**

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

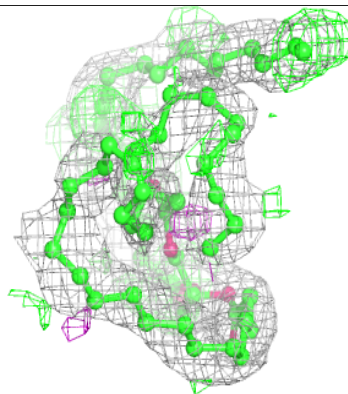
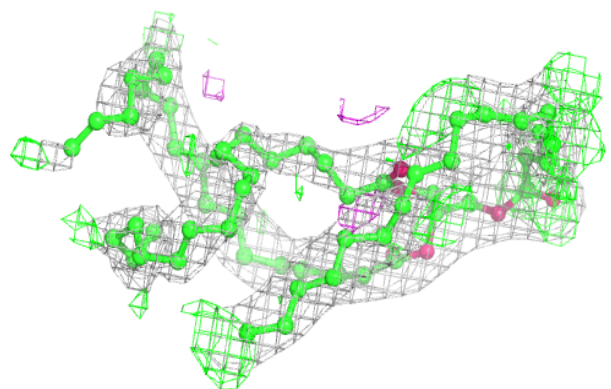
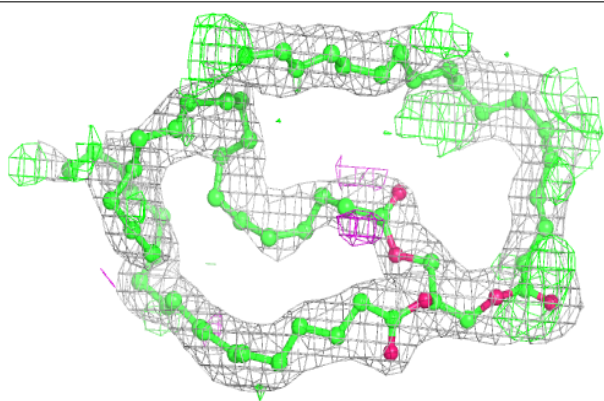


Electron density around DMU Z 101:

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

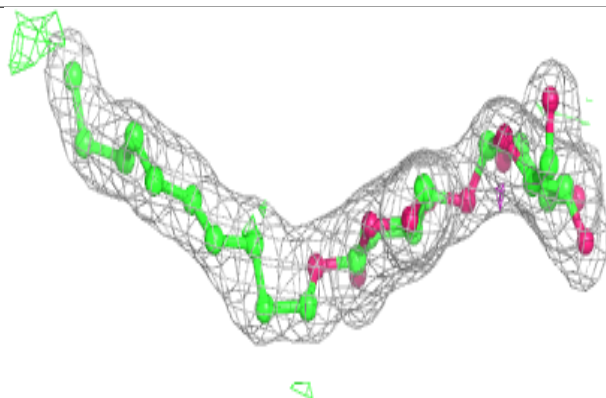
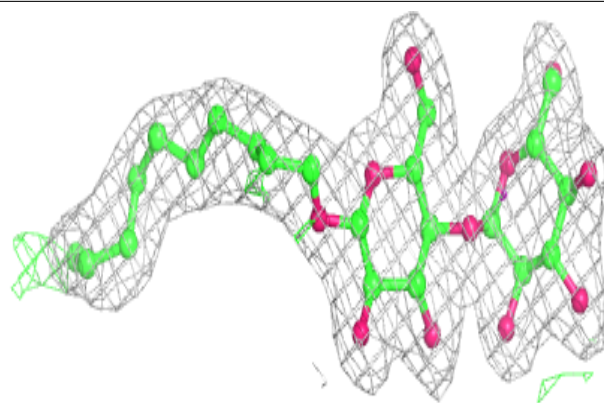
**Electron density around TGL B 301:**

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

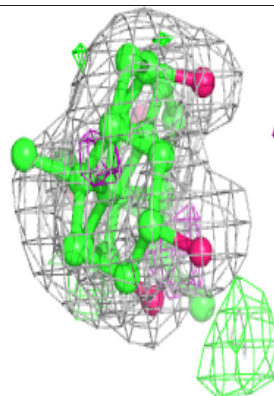
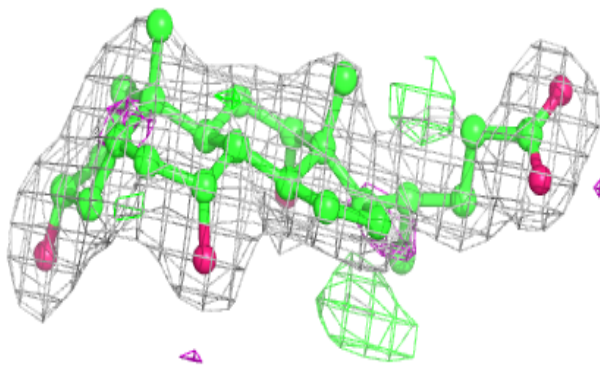
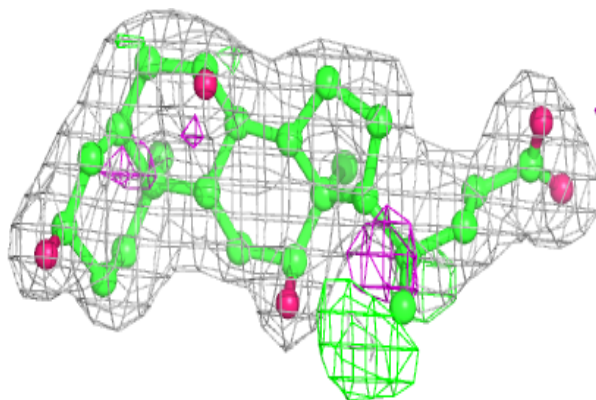


Electron density around DMU M 101:

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

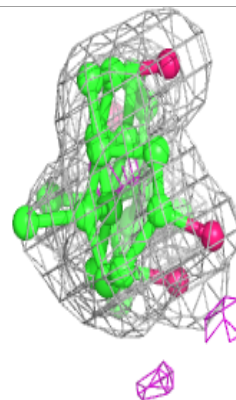
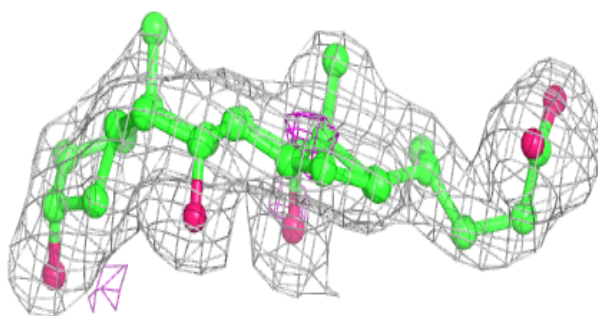
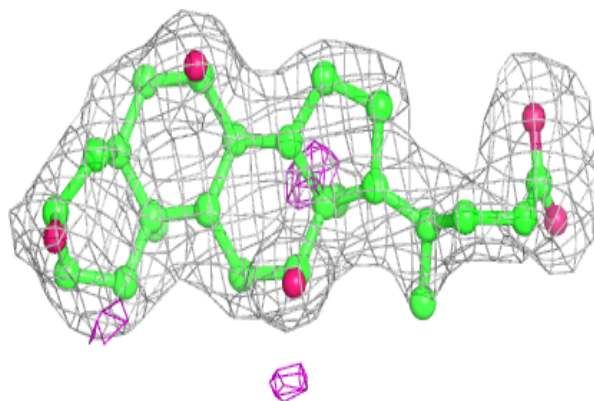
**Electron density around CHD C 307:**

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

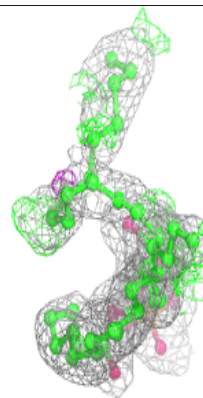
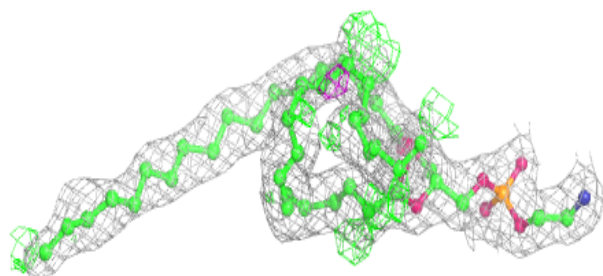
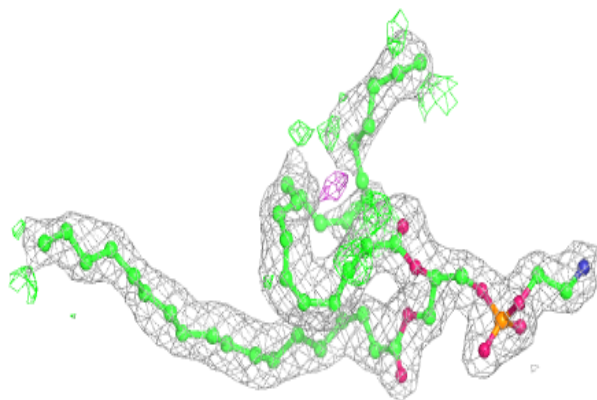


Electron density around CHD P 306:

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

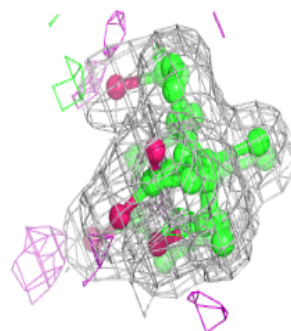
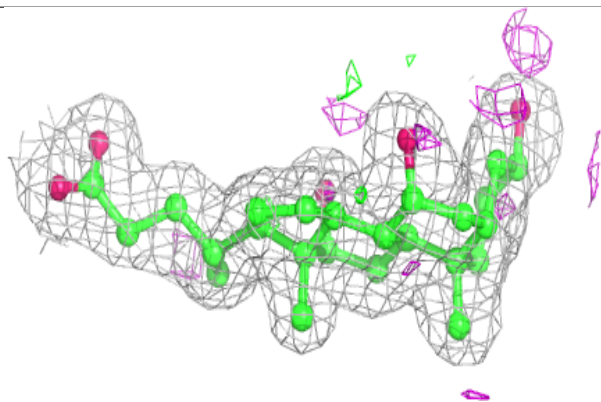
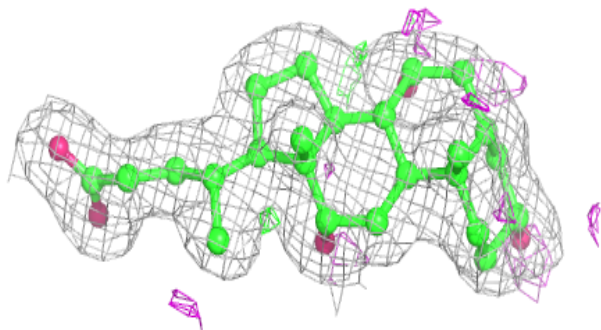
**Electron density around PEK T 102:**

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

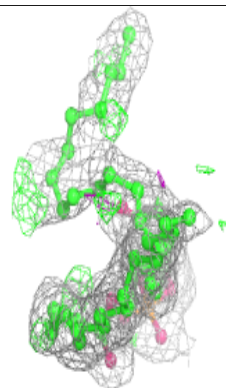
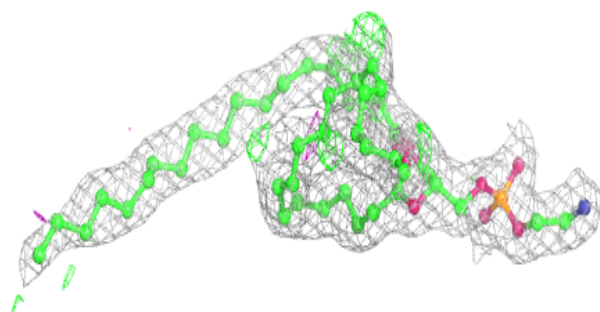
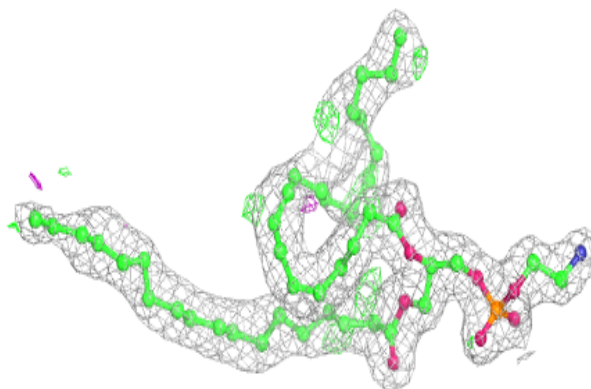


Electron density around CHD C 308:

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

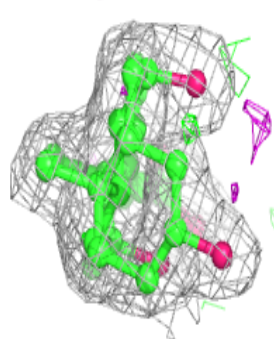
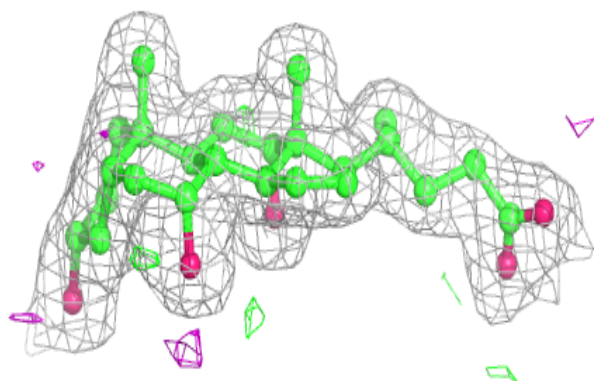
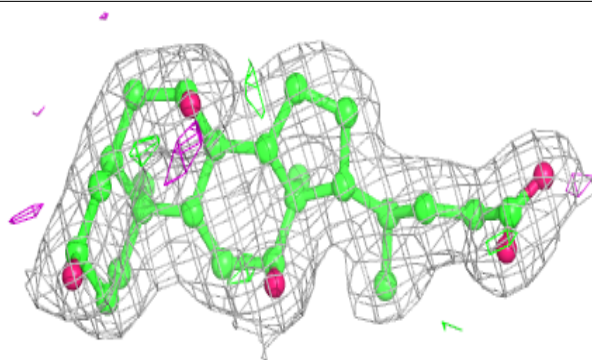
**Electron density around PEK C 302:**

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

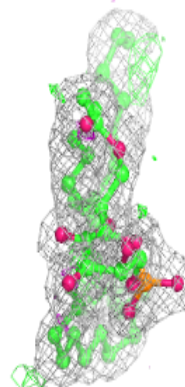
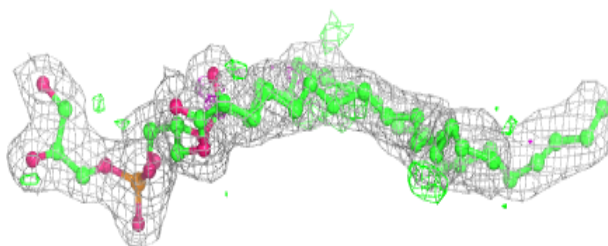
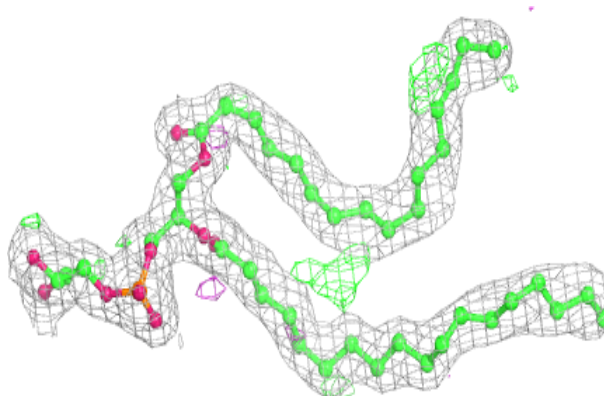


Electron density around CHD N 610:

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

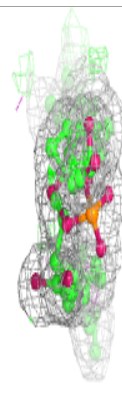
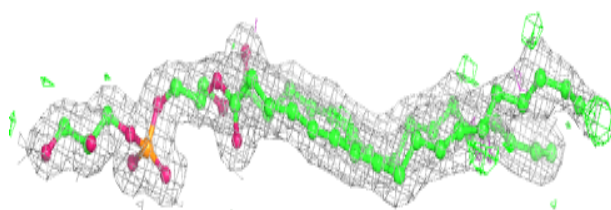
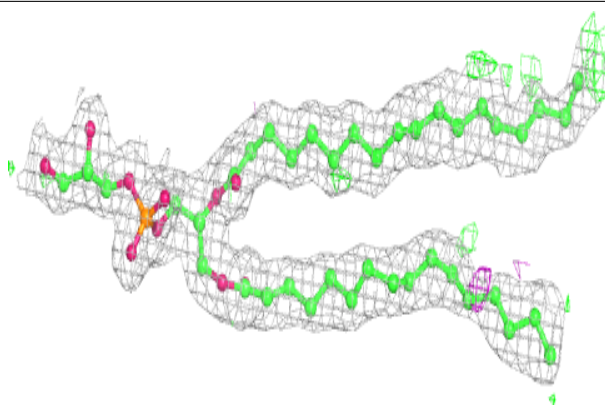
**Electron density around PGV N 609:**

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

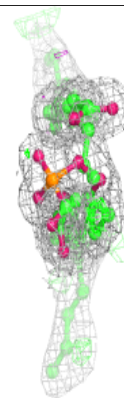
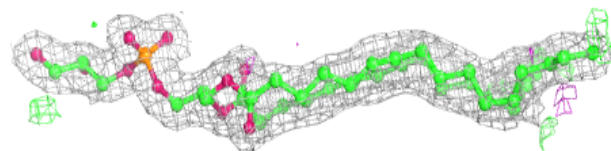
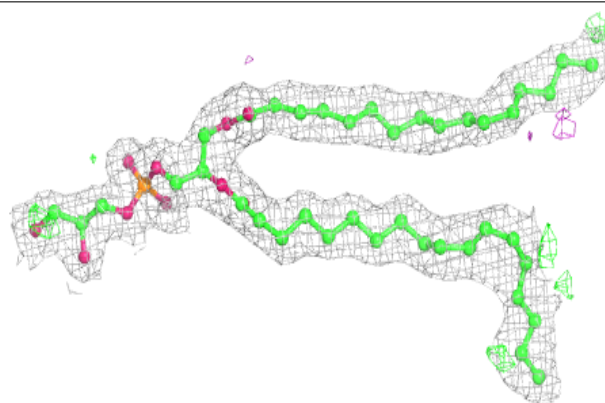


Electron density around PGV C 304:

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

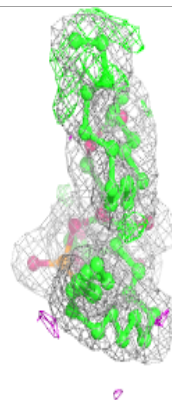
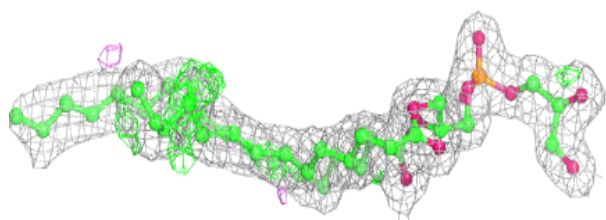
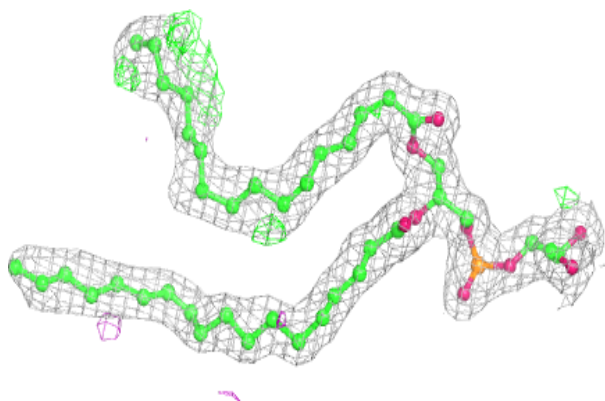
**Electron density around PGV P 303:**

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

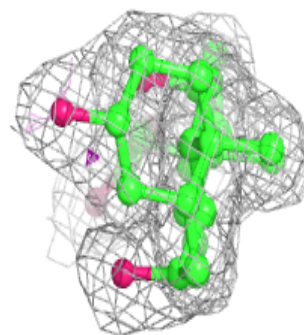
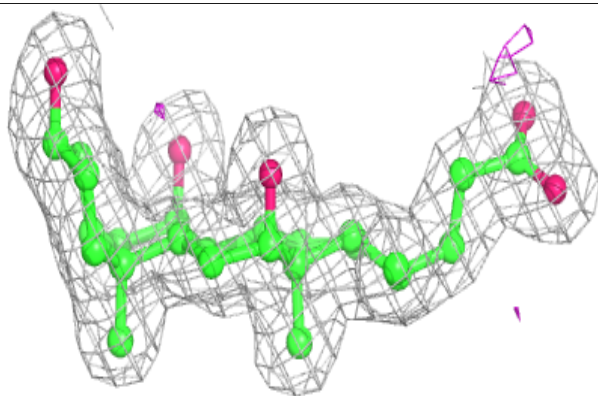
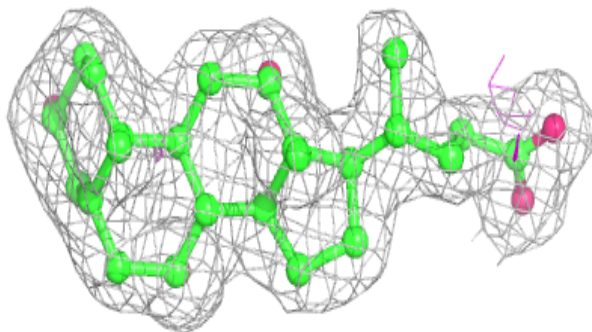


Electron density around PGV A 608:

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

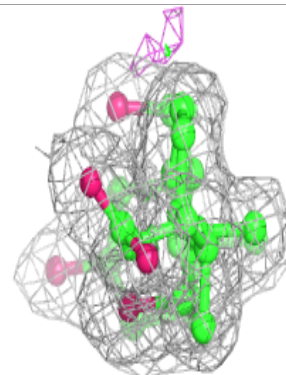
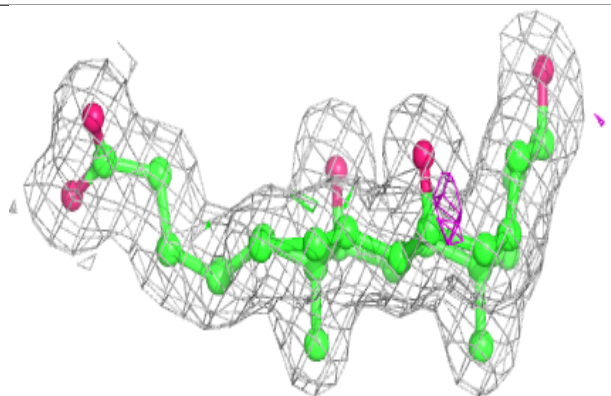
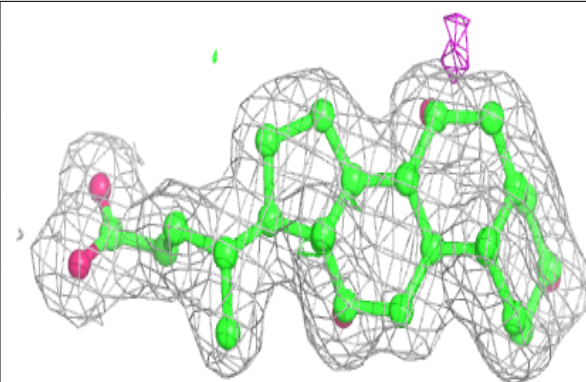
**Electron density around CHD O 301:**

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

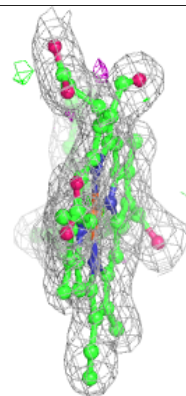
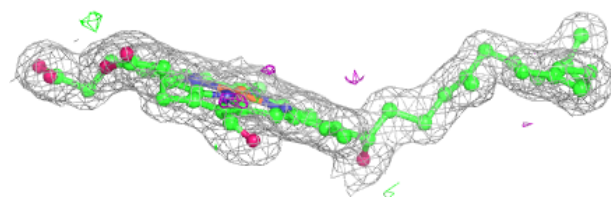
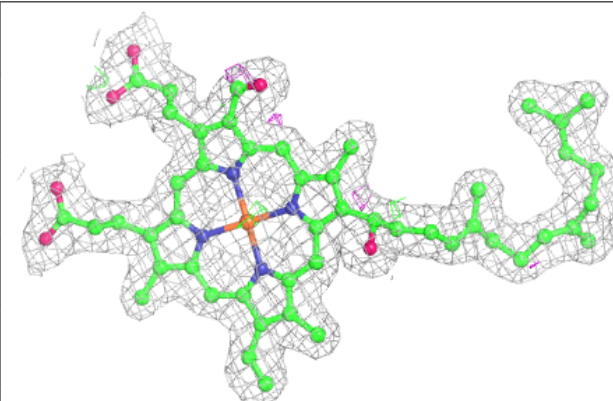


Electron density around CHD B 303:

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

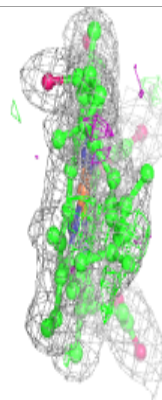
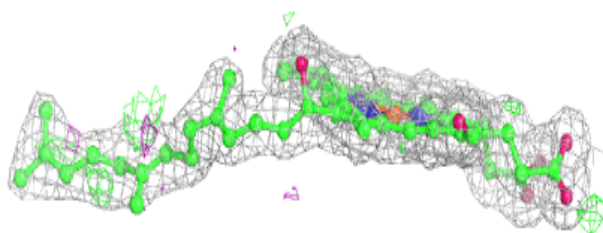
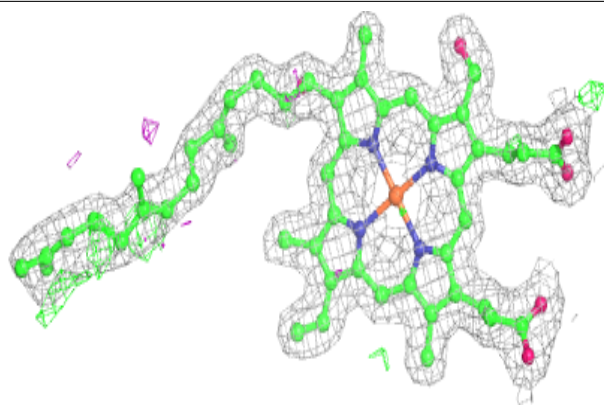
**Electron density around HEA N 602:**

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

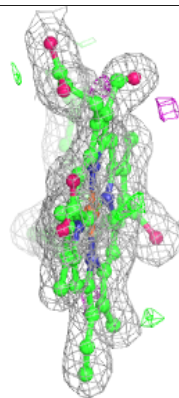
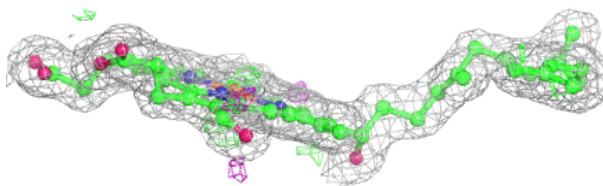
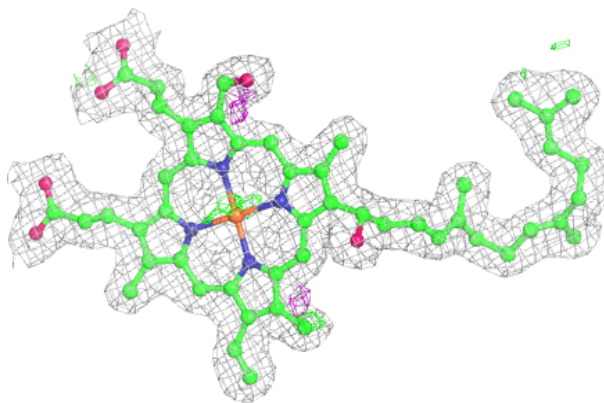


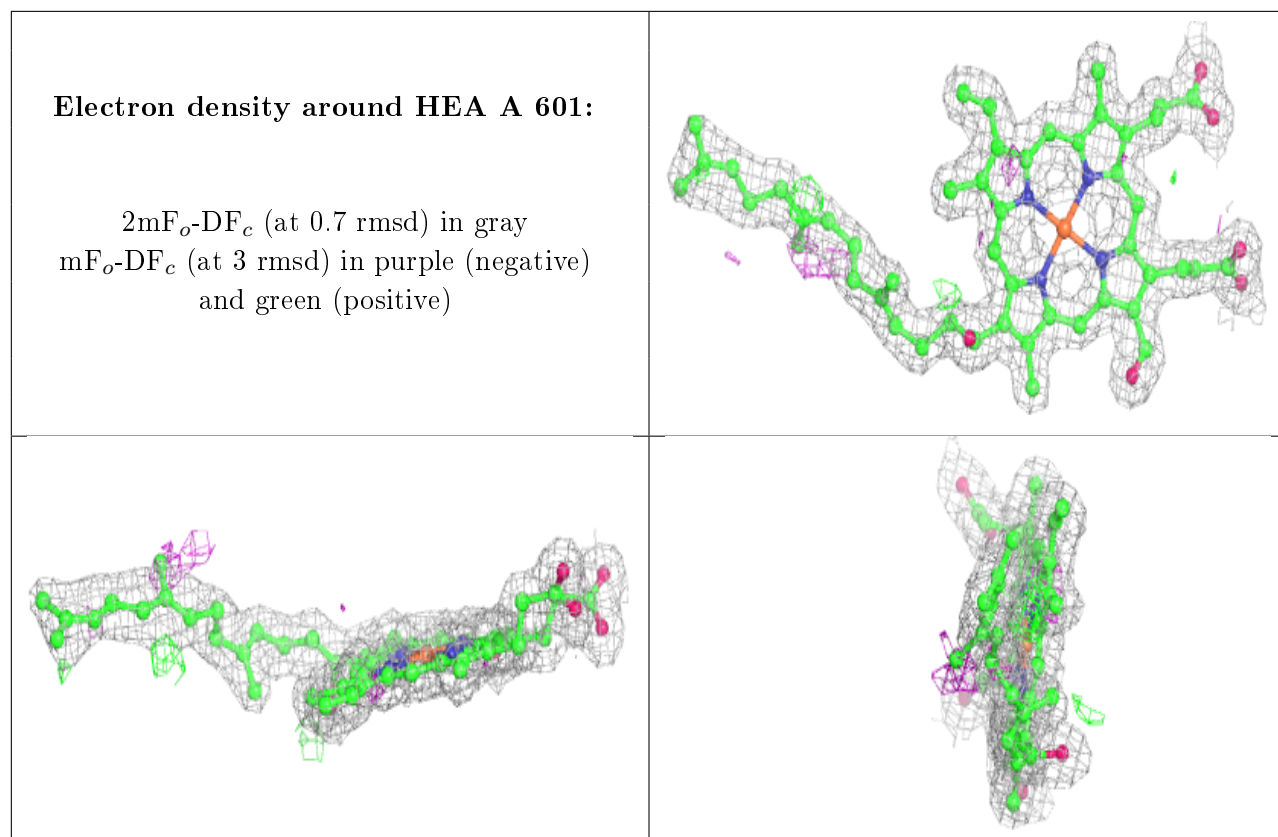
Electron density around HEA N 601:

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

**Electron density around HEA A 602:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.