



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:40 am BST

PDB ID : 3ASO
Title : Bovine heart cytochrome C oxidase in the fully oxidized state measured at 0.9 angstrom wavelength
Authors : Suga, M.; Yano, N.; Muramoto, K.; Shinzawa-Itoh, K.; Maeda, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-12-17
Resolution : 2.30 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

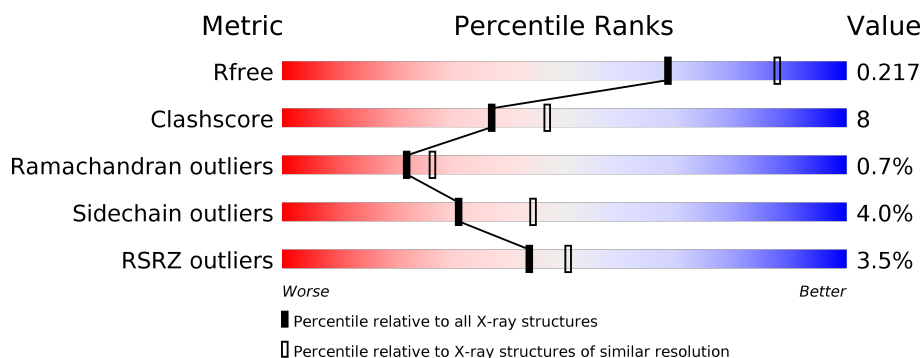
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



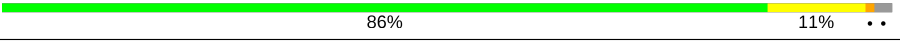

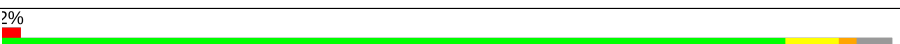
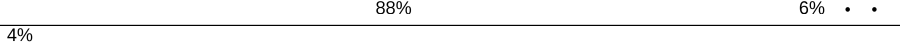
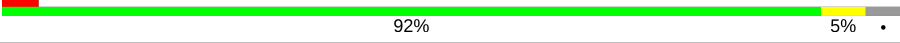


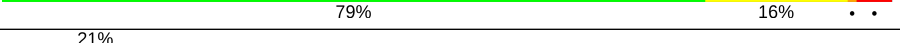


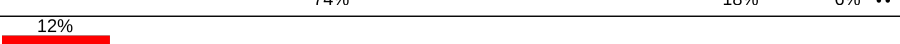







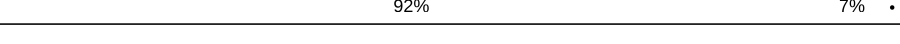

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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: 87%;"></div> <div style="width: 12%;"></div> <div style="width: 1%;"></div> </div> <div>87% 12% .</div>
1	N	514	<div> <div style="width: 85%;"></div> <div style="width: 14%;"></div> <div style="width: 1%;"></div> </div> <div>85% 14% .</div>
2	B	227	<div> <div style="width: 81%;"></div> <div style="width: 18%;"></div> <div style="width: 1%;"></div> </div> <div>81% 18% .</div>
2	O	227	<div> <div style="width: 4%;"></div> <div style="width: 78%;"></div> <div style="width: 19%;"></div> <div style="width: 1%;"></div> </div> <div>4% 78% 19% .</div>
3	C	261	<div> <div style="width: 87%;"></div> <div style="width: 11%;"></div> <div style="width: 2%;"></div> </div> <div>87% 11% .</div>
3	P	261	<div> <div style="width: 85%;"></div> <div style="width: 14%;"></div> <div style="width: 1%;"></div> </div> <div>85% 14% .</div>

Continued on next page...

Continued from previous page...

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	515	X	-	-	-
14	HEA	A	516	X	-	-	-
14	HEA	N	515	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	516	X	-	-	-
22	CHD	J	60	-	-	-	X
22	CHD	W	1059	-	-	-	X
23	UNX	C	262	-	-	-	X
24	PEK	T	263	-	-	-	X
25	CDL	T	1269	-	-	X	-
27	DMU	M	526	X	-	-	-
27	DMU	Z	1526	X	-	-	-
9	SAC	I	1	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 32377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

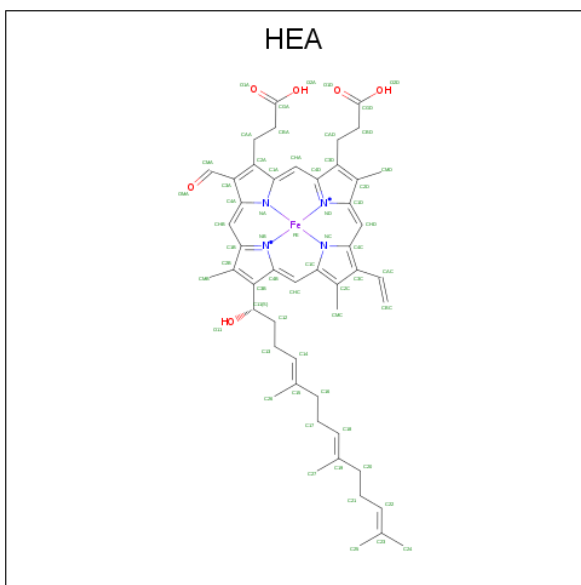
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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		

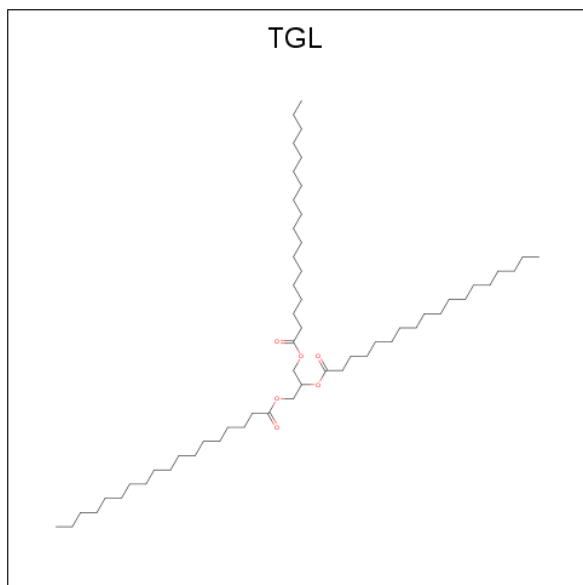
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

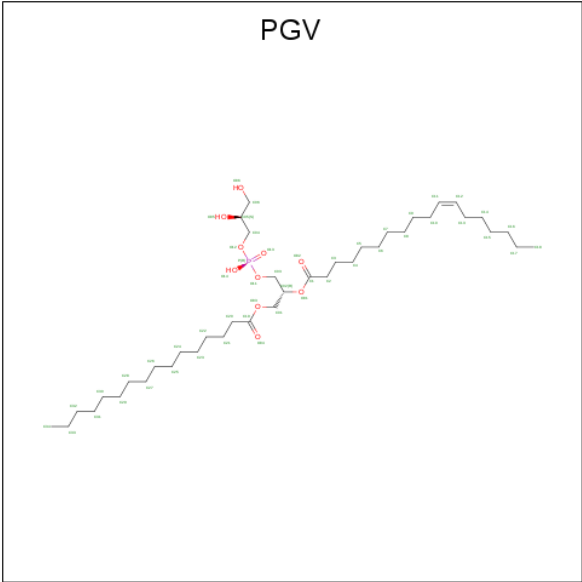
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



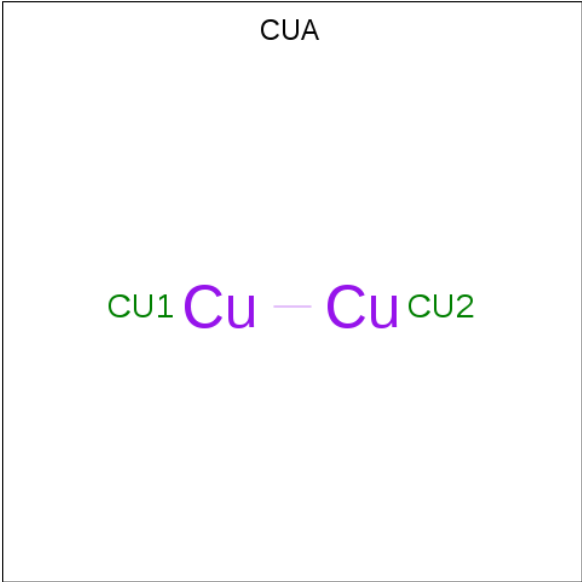
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	D	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 19 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).



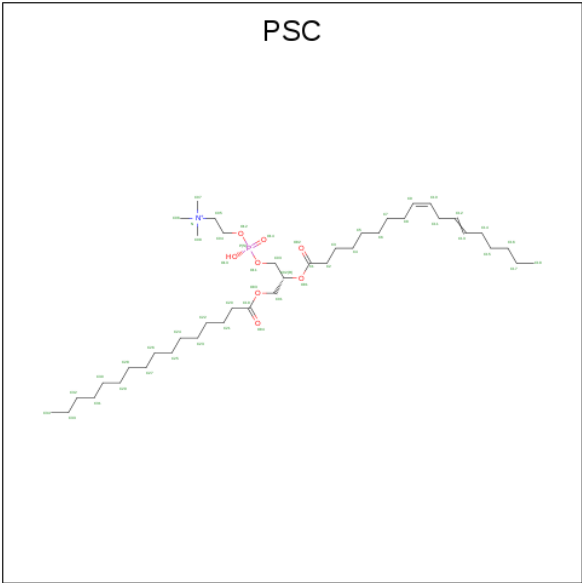
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



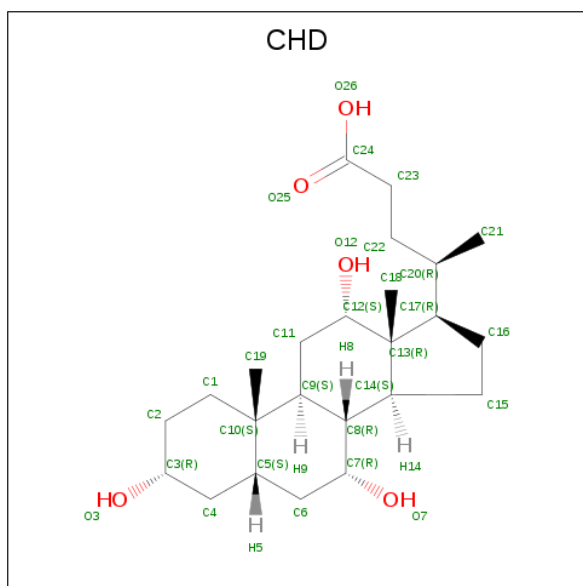
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

Continued on next page...

Continued from previous page...

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

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

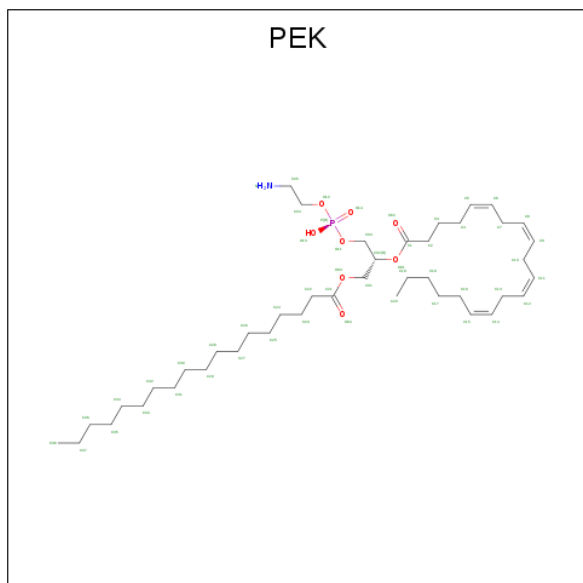


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

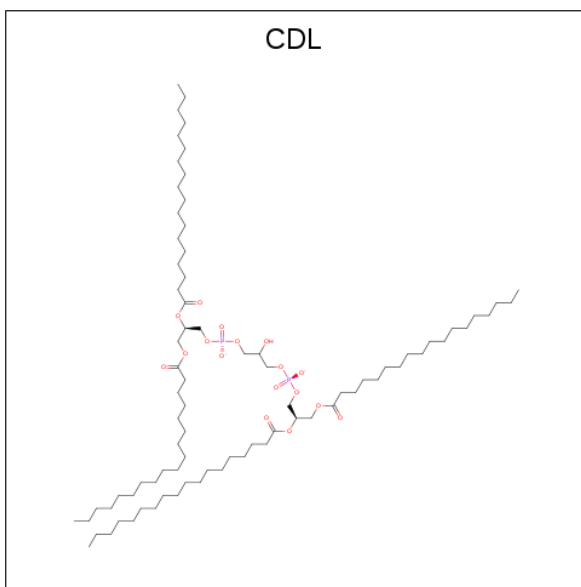
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total X 1 1	0	0
23	C	1	Total X 1 1	0	0

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



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

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).

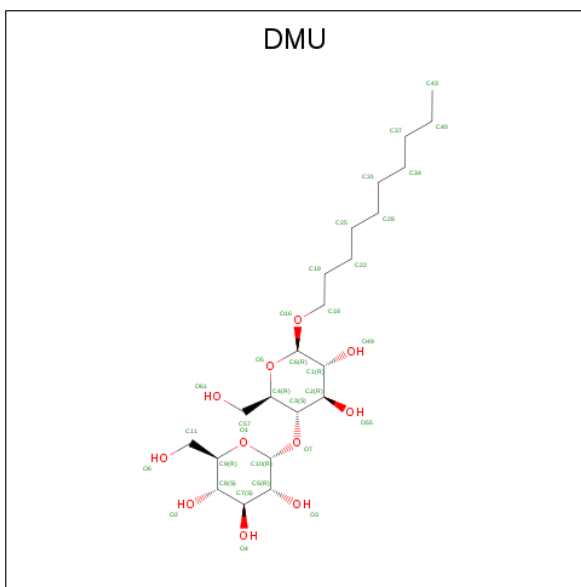


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	215	Total O 215 215	0	0
28	B	124	Total O 124 124	0	0
28	C	109	Total O 109 109	0	0
28	D	102	Total O 102 102	0	0
28	E	67	Total O 67 67	0	0
28	F	81	Total O 81 81	0	0
28	G	48	Total O 48 48	0	0
28	H	48	Total O 48 48	0	0
28	I	31	Total O 31 31	0	0
28	J	16	Total O 16 16	0	0

Continued on next page...

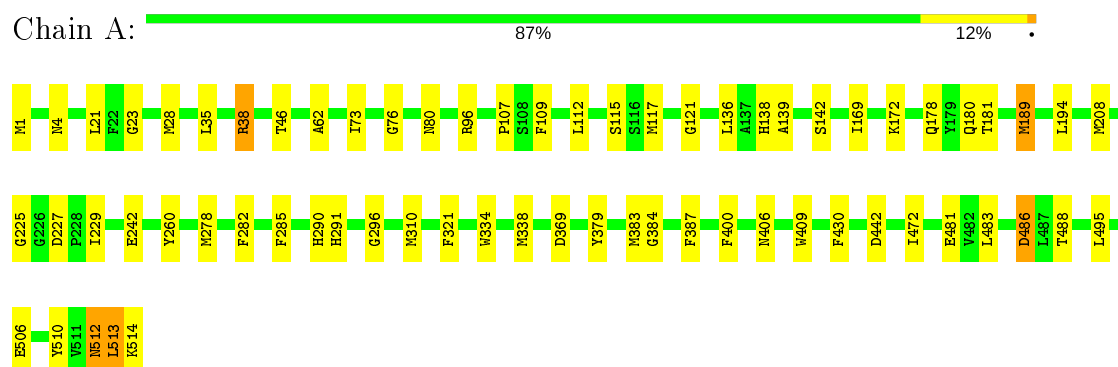
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	26	Total 26	O 26	0	0
28	L	28	Total 28	O 28	0	0
28	M	20	Total 20	O 20	0	0
28	N	220	Total 220	O 220	0	0
28	O	114	Total 114	O 114	0	0
28	P	109	Total 109	O 109	0	0
28	Q	60	Total 60	O 60	0	0
28	R	45	Total 45	O 45	0	0
28	S	77	Total 77	O 77	0	0
28	T	39	Total 39	O 39	0	0
28	U	45	Total 45	O 45	0	0
28	V	21	Total 21	O 21	0	0
28	W	16	Total 16	O 16	0	0
28	X	17	Total 17	O 17	0	0
28	Y	19	Total 19	O 19	0	0
28	Z	14	Total 14	O 14	0	0

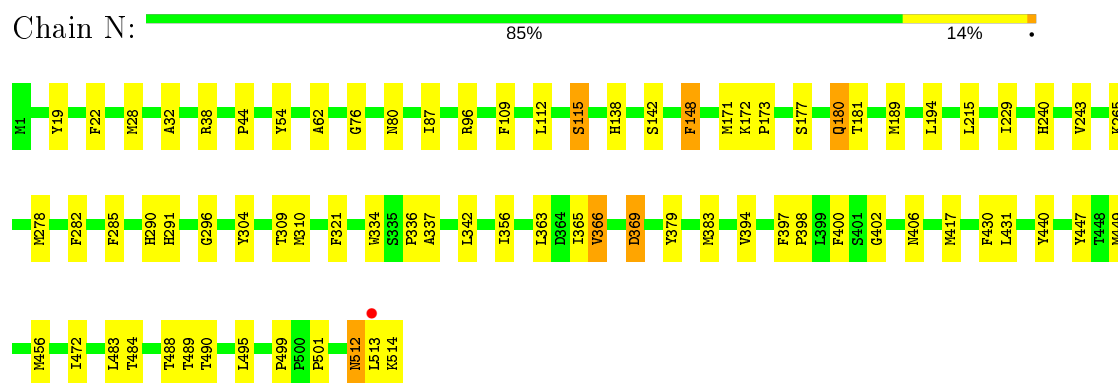
3 Residue-property plots

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 ($RSRZ > 2$). 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.

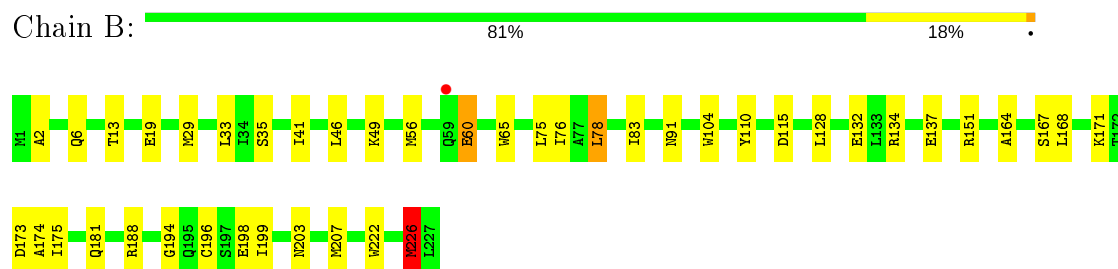
• Molecule 1: Cytochrome c oxidase subunit 1



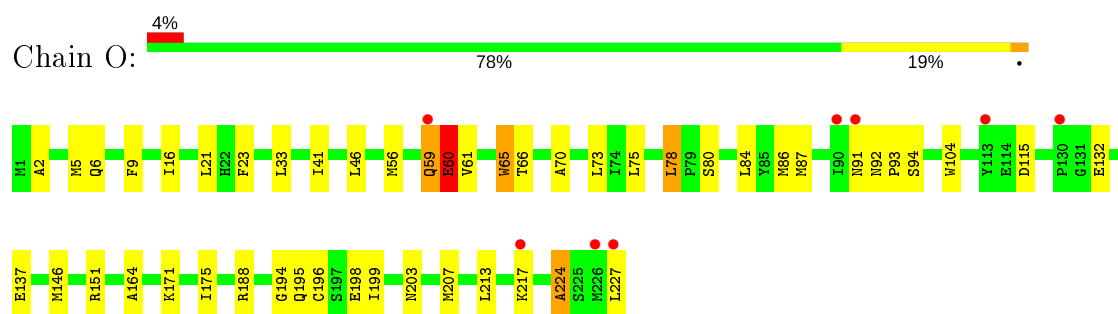
• Molecule 1: Cytochrome c oxidase subunit 1



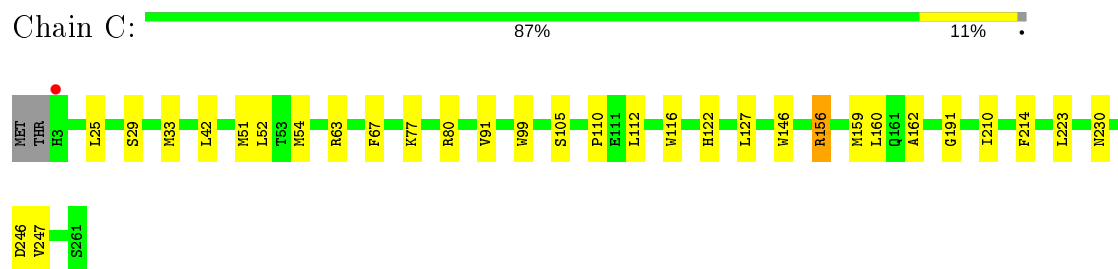
• Molecule 2: Cytochrome c oxidase subunit 2



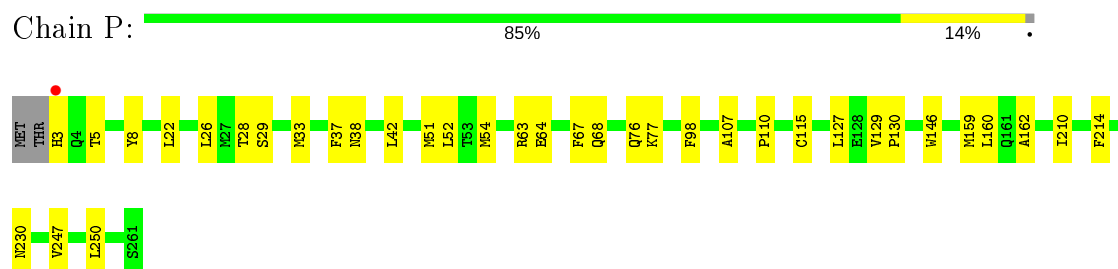
• Molecule 2: Cytochrome c oxidase subunit 2



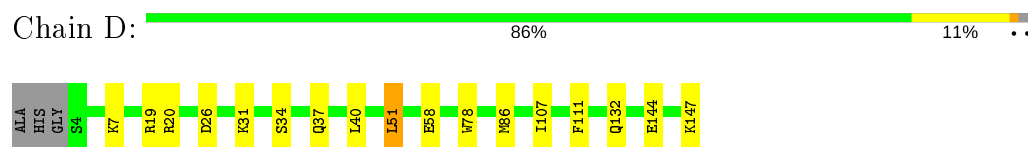
- Molecule 3: Cytochrome c oxidase subunit 3



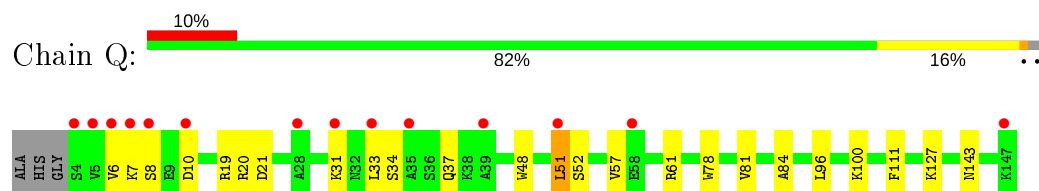
- Molecule 3: Cytochrome c oxidase subunit 3



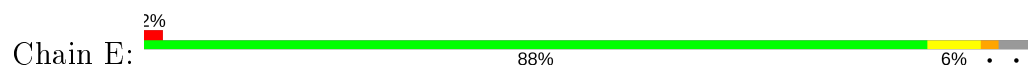
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

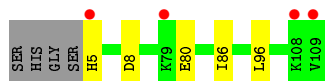
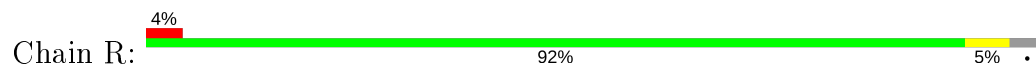


- Molecule 5: Cytochrome c oxidase subunit 5A

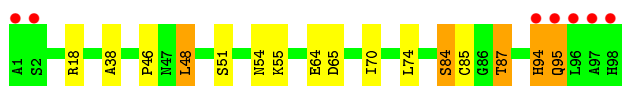
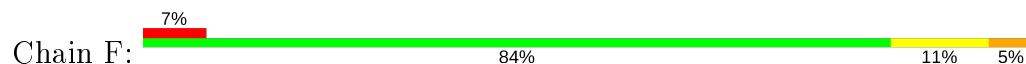




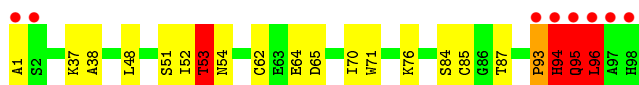
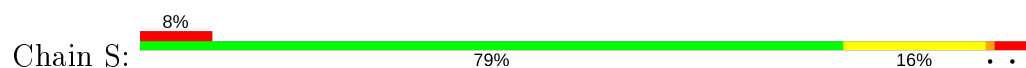
- Molecule 5: Cytochrome c oxidase subunit 5A



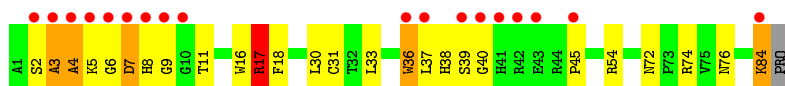
- Molecule 6: Cytochrome c oxidase subunit 5B



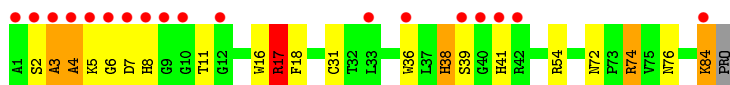
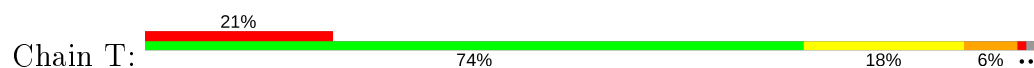
- Molecule 6: Cytochrome c oxidase subunit 5B



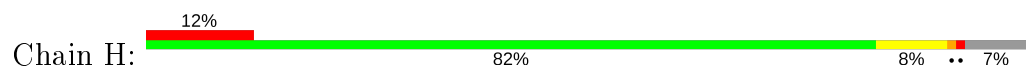
- Molecule 7: Cytochrome c oxidase subunit 6A2



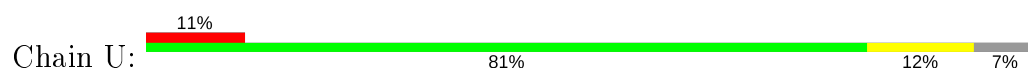
- Molecule 7: Cytochrome c oxidase subunit 6A2



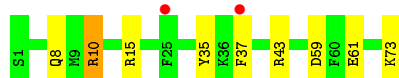
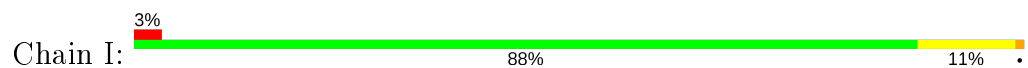
- Molecule 8: Cytochrome c oxidase subunit 6B1



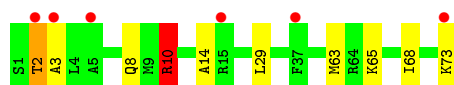
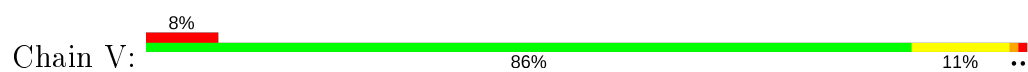
- Molecule 8: Cytochrome c oxidase subunit 6B1



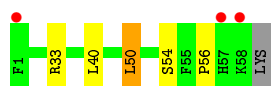
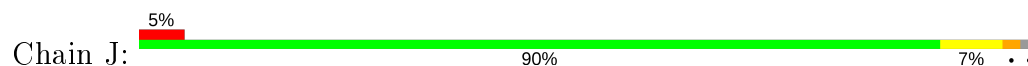
- Molecule 9: Cytochrome c oxidase subunit 6C



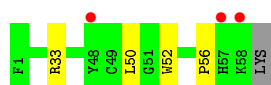
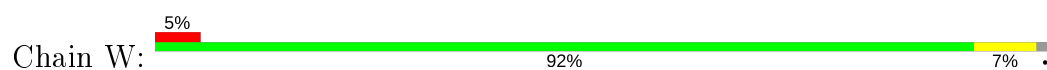
- Molecule 9: Cytochrome c oxidase subunit 6C



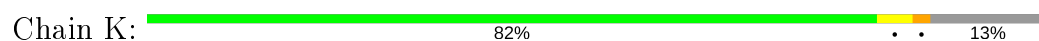
- Molecule 10: Cytochrome c oxidase subunit 7A1



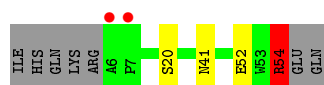
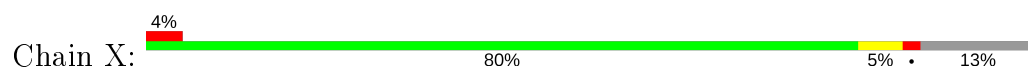
- Molecule 10: Cytochrome c oxidase subunit 7A1



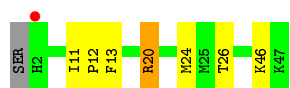
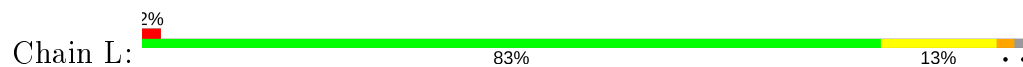
- Molecule 11: Cytochrome c oxidase subunit 7B



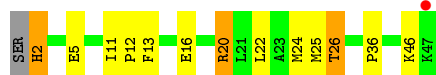
- Molecule 11: Cytochrome c oxidase subunit 7B



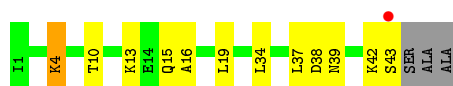
- Molecule 12: Cytochrome c oxidase subunit 7C



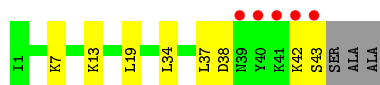
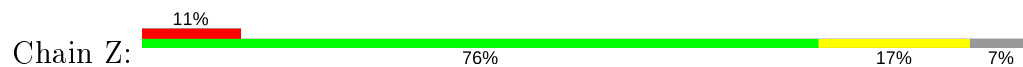
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.87Å 204.11Å 177.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 107.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.30) 99.7 (107.93-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.169 , 0.205 0.184 , 0.217	Depositor DCC
R_{free} test set	14532 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32377	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.14	4/4156 (0.1%)	0.90	15/5678 (0.3%)
1	N	1.07	2/4156 (0.0%)	0.83	3/5678 (0.1%)
2	B	1.12	2/1860 (0.1%)	0.93	3/2534 (0.1%)
2	O	0.98	2/1860 (0.1%)	0.92	1/2534 (0.0%)
3	C	1.04	0/2197	0.79	2/3005 (0.1%)
3	P	1.04	1/2197 (0.0%)	0.79	0/3005
4	D	1.07	0/1229	0.92	3/1658 (0.2%)
4	Q	0.91	0/1229	0.79	2/1658 (0.1%)
5	E	1.04	0/871	0.92	2/1182 (0.2%)
5	R	0.94	0/871	0.84	0/1182
6	F	1.03	0/765	0.95	2/1038 (0.2%)
6	S	1.08	1/765 (0.1%)	1.03	3/1038 (0.3%)
7	G	1.10	1/690 (0.1%)	0.93	1/937 (0.1%)
7	T	1.02	1/690 (0.1%)	0.89	1/937 (0.1%)
8	H	1.00	0/682	0.80	0/921
8	U	0.91	1/682 (0.1%)	0.83	1/921 (0.1%)
9	I	0.99	0/605	0.83	2/802 (0.2%)
9	V	0.94	0/605	0.90	1/802 (0.1%)
10	J	0.91	0/471	0.78	0/636
10	W	0.91	0/471	0.80	0/636
11	K	1.02	0/398	0.86	1/546 (0.2%)
11	X	0.92	0/398	0.76	1/546 (0.2%)
12	L	1.02	0/393	0.84	1/526 (0.2%)
12	Y	1.10	1/393 (0.3%)	0.74	0/526
13	M	1.03	0/345	0.85	0/470
13	Z	0.87	0/345	0.79	0/470
All	All	1.04	16/29324 (0.1%)	0.86	45/39866 (0.1%)

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	S	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ALA	CA-CB	8.23	1.69	1.52
7	T	36	TRP	CB-CG	7.35	1.63	1.50
7	G	36	TRP	CB-CG	7.22	1.63	1.50
6	S	54	ASN	CB-CG	-7.02	1.34	1.51
1	A	260	TYR	CD1-CE1	6.95	1.49	1.39
1	A	242	GLU	CG-CD	6.85	1.62	1.51
2	O	198	GLU	C-O	6.31	1.35	1.23
12	Y	16	GLU	CG-CD	6.18	1.61	1.51
2	B	198	GLU	C-O	6.16	1.35	1.23
1	A	260	TYR	CD2-CE2	6.02	1.48	1.39
2	B	174	ALA	CA-CB	5.66	1.64	1.52
8	U	69	VAL	CB-CG1	5.44	1.64	1.52
1	N	148	PHE	CE1-CZ	5.19	1.47	1.37
3	P	115	CYS	CB-SG	5.10	1.91	1.82
1	N	366	VAL	CB-CG1	-5.08	1.42	1.52
2	O	60	GLU	CB-CG	5.02	1.61	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	90	ARG	NE-CZ-NH1	10.61	125.61	120.30
4	D	20	ARG	NE-CZ-NH2	-10.49	115.06	120.30
7	G	17	ARG	NE-CZ-NH2	-9.43	115.58	120.30
2	B	188	ARG	NE-CZ-NH2	-8.84	115.88	120.30
7	T	17	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	96	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	117	MET	CG-SD-CE	-7.65	87.96	100.20
9	V	10	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	136	LEU	CA-CB-CG	7.19	131.84	115.30
5	E	90	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	136	LEU	CB-CG-CD1	7.03	122.96	111.00
1	A	136	LEU	CB-CG-CD2	-6.89	99.28	111.00
4	D	26	ASP	CB-CG-OD1	6.64	124.28	118.30
11	K	54	ARG	NE-CZ-NH1	-6.63	116.99	120.30
4	Q	20	ARG	NE-CZ-NH2	-6.58	117.01	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	N	369	ASP	CB-CG-OD2	6.35	124.01	118.30
1	N	96	ARG	NE-CZ-NH2	-6.32	117.14	120.30
3	C	80	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	208	MET	CG-SD-CE	6.17	110.06	100.20
2	B	173	ASP	CB-CG-OD1	6.12	123.80	118.30
2	O	188	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	227	ASP	CB-CG-OD2	6.05	123.75	118.30
6	S	54	ASN	CB-CA-C	-5.92	98.57	110.40
1	A	189	MET	CG-SD-CE	-5.87	90.81	100.20
3	C	156	ARG	NE-CZ-NH2	-5.86	117.37	120.30
6	S	94	HIS	N-CA-C	5.68	126.32	111.00
9	I	10	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	486	ASP	CB-CG-OD1	5.62	123.35	118.30
12	L	20	ARG	NE-CZ-NH2	-5.54	117.53	120.30
4	D	51	LEU	CA-CB-CG	5.40	127.73	115.30
8	U	38	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	38	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	35	LEU	CA-CB-CG	-5.28	103.16	115.30
1	N	512	ASN	CB-CA-C	-5.24	99.92	110.40
11	X	54	ARG	NE-CZ-NH2	5.23	122.91	120.30
6	F	18	ARG	NE-CZ-NH2	-5.21	117.70	120.30
9	I	59	ASP	CB-CG-OD2	5.14	122.92	118.30
4	Q	20	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	B	226	MET	CB-CG-SD	5.08	127.63	112.40
1	A	442	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	512	ASN	CB-CA-C	-5.07	100.25	110.40
6	F	94	HIS	N-CA-C	5.06	124.67	111.00
1	A	169	ILE	CB-CA-C	-5.05	101.49	111.60
6	S	53	THR	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	4027	0	4001	48	0
1	N	4027	0	4001	70	0
2	B	1824	0	1833	27	0
2	O	1824	0	1833	32	0
3	C	2110	0	2027	25	0
3	P	2110	0	2027	33	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	18	0
5	E	852	0	845	3	0
5	R	852	0	845	5	0
6	F	748	0	728	9	0
6	S	748	0	728	27	0
7	G	675	0	644	27	0
7	T	675	0	644	28	0
8	H	662	0	623	7	0
8	U	662	0	623	2	0
9	I	601	0	613	8	0
9	V	601	0	613	9	0
10	J	460	0	459	7	0
10	W	460	0	459	4	0
11	K	384	0	366	1	0
11	X	384	0	366	6	0
12	L	380	0	380	10	0
12	Y	380	0	380	11	0
13	M	335	0	352	7	0
13	Z	335	0	352	3	0
14	A	120	0	108	6	0
14	N	120	0	108	9	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	63	0	110	6	0
18	D	63	0	110	6	0
18	L	63	0	110	15	0
18	N	126	0	220	21	0
18	Q	63	0	110	4	0
19	A	102	0	152	10	0
19	C	102	0	152	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	102	0	152	10	0
19	P	102	0	152	6	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	52	0	80	13	0
21	O	52	0	80	17	0
22	B	29	0	39	1	0
22	C	58	0	78	3	0
22	G	29	0	39	0	0
22	J	29	0	38	3	0
22	P	58	0	78	1	0
22	W	29	0	38	3	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	5	0
24	G	106	0	154	12	0
24	T	159	0	231	21	0
25	C	100	0	156	17	0
25	G	100	0	156	18	0
25	P	100	0	156	14	0
25	T	100	0	156	22	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	41	0	0
27	Z	33	0	40	0	0
28	A	215	0	0	7	0
28	B	124	0	0	2	0
28	C	109	0	0	2	0
28	D	102	0	0	3	0
28	E	67	0	0	1	0
28	F	81	0	0	1	0
28	G	48	0	0	5	0
28	H	48	0	0	2	0
28	I	31	0	0	1	0
28	J	16	0	0	0	0
28	K	26	0	0	2	0
28	L	28	0	0	1	0
28	M	20	0	0	0	0
28	N	220	0	0	6	0
28	O	114	0	0	0	0
28	P	109	0	0	4	0
28	Q	60	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	R	45	0	0	0	0
28	S	77	0	0	4	0
28	T	39	0	0	2	0
28	U	45	0	0	0	0
28	V	21	0	0	2	0
28	W	16	0	0	0	0
28	X	17	0	0	2	0
28	Y	19	0	0	1	0
28	Z	14	0	0	1	0
All	All	32377	0	31229	485	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (485) 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)
6:S:52:ILE:O	6:S:94:HIS:CE1	1.76	1.38
6:S:52:ILE:O	6:S:94:HIS:NE2	1.66	1.26
7:T:84:LYS:H	7:T:84:LYS:HD2	0.95	1.12
1:N:513:LEU:O	1:N:514:LYS:HB2	1.47	1.11
24:T:1265:PEK:H383	25:T:1269:CDL:C27	1.81	1.10
24:C:265:PEK:H383	25:G:269:CDL:H273	1.28	1.10
24:T:1265:PEK:H383	25:T:1269:CDL:H273	1.10	1.09
7:G:84:LYS:HD2	7:G:84:LYS:H	1.05	1.09
24:C:265:PEK:H383	25:G:269:CDL:C27	1.83	1.08
25:G:269:CDL:H541	25:G:269:CDL:H231	1.37	1.05
21:O:1229:PSC:H142	21:O:1229:PSC:H343	1.40	1.02
2:B:41:ILE:HD13	21:B:229:PSC:H342	1.42	1.02
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.22	1.01
6:S:85:CYS:SG	6:S:87:THR:HG23	2.01	1.00
7:T:5:LYS:HB2	24:T:263:PEK:H362	1.40	0.99
18:D:523:TGL:H361	28:I:4610:HOH:O	1.62	0.99
24:T:1265:PEK:C38	25:T:1269:CDL:H273	1.95	0.96
6:F:85:CYS:SG	6:F:87:THR:HG23	2.05	0.96
2:O:224:ALA:O	2:O:227:LEU:HG	1.63	0.95
7:T:72:ASN:H	7:T:76:ASN:HD22	1.14	0.94
7:T:84:LYS:N	7:T:84:LYS:HD2	1.80	0.94
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.47	0.94
6:S:52:ILE:O	6:S:94:HIS:CD2	2.22	0.93
7:T:84:LYS:H	7:T:84:LYS:CD	1.82	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:524:PGV:H311	13:M:19:LEU:HD23	1.51	0.92
24:C:265:PEK:C38	25:G:269:CDL:H273	1.99	0.92
6:S:53:THR:HA	6:S:94:HIS:CE1	2.03	0.92
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.32	0.91
28:N:4772:HOH:O	24:T:1264:PEK:H381	1.72	0.89
3:P:3:HIS:HB3	28:P:4285:HOH:O	1.72	0.89
7:G:5:LYS:HB2	24:G:1263:PEK:H362	1.55	0.89
4:D:31:LYS:HD2	28:D:4414:HOH:O	1.73	0.88
18:D:523:TGL:HC21	18:D:523:TGL:HG11	1.56	0.88
21:B:229:PSC:H072	9:I:10:ARG:HH21	1.39	0.87
21:O:1229:PSC:C34	21:O:1229:PSC:H142	2.04	0.87
7:G:84:LYS:N	7:G:84:LYS:HD2	1.90	0.86
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.56	0.86
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.12	0.84
19:C:268:PGV:H42	28:P:4823:HOH:O	1.75	0.84
7:G:72:ASN:H	7:G:76:ASN:HD22	1.23	0.84
21:B:229:PSC:C07	9:I:10:ARG:HH21	1.89	0.84
1:N:513:LEU:O	1:N:514:LYS:CB	2.21	0.84
25:T:1269:CDL:H541	25:T:1269:CDL:H231	1.59	0.84
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.44	0.83
6:S:53:THR:HA	6:S:94:HIS:HE1	1.42	0.83
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.43	0.83
1:A:1:FME:HG3	28:L:4907:HOH:O	1.78	0.82
18:N:1521:TGL:H201	18:N:1521:TGL:H241	1.62	0.81
6:S:52:ILE:C	6:S:94:HIS:CE1	2.56	0.79
21:O:1229:PSC:H343	21:O:1229:PSC:C14	2.14	0.77
7:G:76:ASN:HD21	24:G:264:PEK:HN2	1.28	0.77
12:L:13:PHE:HA	18:L:522:TGL:HC31	1.67	0.77
2:O:59:GLN:O	2:O:59:GLN:HG3	1.83	0.77
24:G:264:PEK:H161	24:G:264:PEK:H101	1.68	0.76
19:P:1268:PGV:H062	28:P:4397:HOH:O	1.84	0.76
25:G:269:CDL:C54	25:G:269:CDL:H231	2.15	0.76
7:G:84:LYS:H	7:G:84:LYS:CD	1.89	0.76
7:T:31:CYS:SG	25:T:1269:CDL:H532	2.26	0.75
1:A:112:LEU:HG	28:A:2701:HOH:O	1.87	0.74
7:T:76:ASN:HD21	24:T:1264:PEK:HN2	1.34	0.74
2:B:49:LYS:HE2	28:E:4606:HOH:O	1.87	0.74
7:T:3:ALA:HB1	24:T:263:PEK:H382	1.68	0.73
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.71	0.73
18:Q:1523:TGL:HG11	18:Q:1523:TGL:HC21	1.71	0.72
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HG21	18:L:522:TGL:HA92	1.72	0.72
19:C:267:PGV:H12	19:C:267:PGV:H161	1.72	0.72
4:D:34:SER:H	4:D:37:GLN:HE21	1.36	0.72
3:C:246:ASP:HB2	28:C:4249:HOH:O	1.89	0.71
25:C:270:CDL:PA1	25:C:270:CDL:HB22	2.30	0.71
7:T:72:ASN:H	7:T:76:ASN:ND2	1.87	0.71
18:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.72	0.70
1:A:513:LEU:O	1:A:514:LYS:HB2	1.91	0.70
6:F:54:ASN:HB2	28:F:4662:HOH:O	1.90	0.69
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.75	0.69
7:T:5:LYS:HD2	24:T:263:PEK:H371	1.74	0.69
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.75	0.69
12:L:11:ILE:CG2	18:L:522:TGL:H271	2.23	0.69
4:Q:31:LYS:HB3	28:Q:4834:HOH:O	1.92	0.68
10:W:33:ARG:HG2	22:W:1059:CHD:H151	1.75	0.68
1:A:406:ASN:HD21	19:A:524:PGV:H22	1.59	0.68
4:Q:100:LYS:HE2	28:Q:4478:HOH:O	1.94	0.68
9:V:65:LYS:O	11:X:54:ARG:NH1	2.27	0.67
6:S:95:GLN:HB2	28:S:4523:HOH:O	1.93	0.67
7:G:5:LYS:HB3	1:N:278:MET:SD	2.34	0.67
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.75	0.67
19:N:1266:PGV:H182	3:P:28:THR:HG22	1.75	0.67
28:G:4789:HOH:O	19:P:1268:PGV:H341	1.93	0.67
18:N:1521:TGL:C28	18:N:1521:TGL:H101	2.25	0.67
2:O:59:GLN:O	2:O:59:GLN:CG	2.42	0.66
1:A:406:ASN:HD21	19:A:524:PGV:C2	2.08	0.66
18:N:1521:TGL:HC22	28:V:3606:HOH:O	1.95	0.66
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.60	0.66
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.78	0.66
1:A:278:MET:SD	7:T:5:LYS:HB3	2.36	0.66
7:G:17:ARG:HD2	28:G:2446:HOH:O	1.95	0.65
1:A:486:ASP:OD2	4:D:19:ARG:HD3	1.96	0.65
21:O:1229:PSC:H222	21:O:1229:PSC:H21	1.78	0.65
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.60	0.65
2:B:56:MET:HG2	21:B:229:PSC:H211	1.78	0.65
7:G:2:SER:O	24:G:1263:PEK:H322	1.97	0.64
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.79	0.64
2:B:41:ILE:CD1	21:B:229:PSC:H342	2.25	0.63
8:H:27:ARG:HD3	28:H:4760:HOH:O	1.98	0.63
21:O:1229:PSC:C07	9:V:10:ARG:HH21	2.12	0.63
6:S:64:GLU:O	6:S:65:ASP:HB2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:210:ILE:HG12	19:C:267:PGV:H132	1.81	0.62
7:T:3:ALA:O	7:T:4:ALA:HB2	2.00	0.62
6:S:1:ALA:N	24:T:1265:PEK:H041	2.14	0.61
7:G:3:ALA:O	7:G:4:ALA:HB2	2.00	0.61
5:R:80:GLU:N	5:R:80:GLU:OE1	2.33	0.61
1:A:430:PHE:HE1	18:A:521:TGL:HB21	1.66	0.61
2:O:41:ILE:HD13	21:O:1229:PSC:H342	1.82	0.61
7:T:3:ALA:CB	24:T:263:PEK:H382	2.30	0.61
25:C:270:CDL:H642	25:C:270:CDL:H191	1.82	0.60
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.01	0.60
19:A:524:PGV:H062	28:A:2126:HOH:O	2.00	0.60
6:S:52:ILE:O	6:S:94:HIS:CG	2.54	0.60
18:A:521:TGL:H111	2:B:35:SER:OG	2.02	0.60
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.16	0.60
7:G:45:PRO:HD2	28:G:2099:HOH:O	2.01	0.60
10:W:33:ARG:HG2	22:W:1059:CHD:C15	2.32	0.60
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	2.01	0.60
18:D:523:TGL:HB62	18:D:523:TGL:HA52	1.83	0.60
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.01	0.60
1:A:483:LEU:HD21	13:M:4:LYS:HD3	1.83	0.60
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.84	0.60
2:B:78:LEU:HD12	25:T:1269:CDL:H352	1.85	0.59
19:A:524:PGV:H82	19:A:524:PGV:H262	1.84	0.59
1:N:177:SER:H	1:N:180:GLN:NE2	2.00	0.59
3:C:63:ARG:HE	25:C:270:CDL:CA2	2.14	0.59
1:N:28:MET:CE	14:N:515:HEA:C27	2.80	0.59
10:J:33:ARG:HG2	22:J:60:CHD:H151	1.84	0.59
2:O:56:MET:HG2	21:O:1229:PSC:H211	1.84	0.59
1:N:28:MET:CE	14:N:515:HEA:H271	2.32	0.58
24:C:265:PEK:H383	25:G:269:CDL:H272	1.80	0.58
7:G:31:CYS:SG	25:G:269:CDL:H552	2.44	0.58
18:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.85	0.58
7:G:3:ALA:HB1	24:G:1263:PEK:H382	1.85	0.58
4:D:34:SER:H	4:D:37:GLN:NE2	2.01	0.58
6:F:64:GLU:O	6:F:65:ASP:HB2	2.04	0.58
21:O:1229:PSC:O01	21:O:1229:PSC:H212	2.04	0.58
6:S:52:ILE:O	6:S:94:HIS:ND1	2.30	0.58
12:L:11:ILE:HG22	18:L:522:TGL:H271	1.85	0.57
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.86	0.57
4:Q:7:LYS:HA	28:Q:4706:HOH:O	2.03	0.57
28:B:3446:HOH:O	7:T:17:ARG:HD2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:CB	24:T:263:PEK:H362	2.27	0.57
6:S:87:THR:HG22	28:S:4582:HOH:O	2.04	0.57
21:B:229:PSC:H142	21:B:229:PSC:H343	1.86	0.57
1:N:400:PHE:HB3	18:N:1522:TGL:H282	1.87	0.57
12:L:20:ARG:HH22	18:L:522:TGL:HC62	1.70	0.57
18:N:1521:TGL:HA91	18:N:1521:TGL:H252	1.86	0.57
4:Q:127:LYS:HD2	28:V:3618:HOH:O	2.05	0.57
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.40	0.56
19:A:522:PGV:H183	24:G:264:PEK:H332	1.87	0.56
1:A:488:THR:HB	1:A:495:LEU:HD13	1.87	0.56
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.05	0.56
24:G:1263:PEK:H132	3:P:247:VAL:CG1	2.36	0.56
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.34	0.56
1:N:472:ILE:HG21	18:N:1522:TGL:HA91	1.88	0.55
6:S:1:ALA:H2	24:T:1265:PEK:H041	1.71	0.55
1:A:21:LEU:HD23	18:L:522:TGL:H211	1.88	0.55
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.89	0.55
3:C:210:ILE:HD13	19:C:267:PGV:H301	1.88	0.55
6:S:53:THR:CA	6:S:94:HIS:CE1	2.86	0.55
10:J:50:LEU:HD22	10:J:54:SER:HG	1.71	0.55
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.19	0.54
18:A:521:TGL:HC22	28:D:2606:HOH:O	2.06	0.54
21:B:229:PSC:H322	21:B:229:PSC:H12	1.89	0.54
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.89	0.54
3:P:52:LEU:HD21	25:P:1270:CDL:H412	1.88	0.54
1:N:430:PHE:HE1	18:N:1521:TGL:HB21	1.72	0.54
2:B:19:GLU:HG3	2:B:83:ILE:HG12	1.88	0.54
7:G:37:LEU:CD2	25:G:269:CDL:H361	2.38	0.54
9:V:2:THR:HG22	9:V:3:ALA:H	1.72	0.54
2:B:13:THR:HB	2:B:168:LEU:HD23	1.90	0.53
18:N:1521:TGL:H281	18:N:1521:TGL:H101	1.90	0.53
2:O:84:LEU:HA	2:O:87:MET:HE2	1.89	0.53
4:Q:78:TRP:HA	18:Q:1523:TGL:HB22	1.89	0.53
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.90	0.53
1:N:417:MET:CE	28:N:3166:HOH:O	2.56	0.53
21:O:1229:PSC:H071	9:V:10:ARG:HE	1.73	0.53
7:G:30:LEU:CD2	25:G:269:CDL:H462	2.39	0.53
3:C:67:PHE:CE1	25:C:270:CDL:H1	2.25	0.53
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.74	0.53
3:C:52:LEU:HD21	25:C:270:CDL:H412	1.91	0.52
1:N:321:PHE:CD2	21:O:1229:PSC:H341	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:HD2	24:T:263:PEK:C37	2.39	0.52
11:X:52:GLU:HG2	28:X:4813:HOH:O	2.09	0.52
12:Y:2:HIS:N	28:Y:4664:HOH:O	2.43	0.52
3:P:5:THR:CG2	6:S:96:LEU:HD13	2.39	0.52
14:A:515:HEA:HMC1	14:A:515:HEA:HBC1	1.90	0.52
25:T:1269:CDL:OB4	25:T:1269:CDL:H1	2.10	0.52
7:T:3:ALA:O	7:T:4:ALA:CB	2.56	0.52
12:L:12:PRO:HB2	18:L:522:TGL:HG2	1.92	0.52
1:N:28:MET:HE2	14:N:515:HEA:C27	2.40	0.52
19:A:524:PGV:H02	19:A:524:PGV:O14	2.10	0.52
3:C:54:MET:HE3	25:C:270:CDL:H612	1.92	0.52
7:G:72:ASN:H	7:G:76:ASN:ND2	1.99	0.52
18:L:522:TGL:CC6	18:L:522:TGL:HC22	2.40	0.52
12:L:20:ARG:HH12	18:L:522:TGL:HC62	1.75	0.52
18:N:1521:TGL:C10	18:N:1521:TGL:H281	2.40	0.51
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.91	0.51
19:N:1524:PGV:H011	19:N:1524:PGV:H22	1.91	0.51
25:T:1269:CDL:H111	25:T:1269:CDL:HA21	1.92	0.51
1:N:449:MET:SD	2:O:5:MET:HG2	2.50	0.51
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.91	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.45	0.51
12:L:20:ARG:HH12	18:L:522:TGL:CC6	2.23	0.51
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.40	0.51
18:D:523:TGL:H242	18:D:523:TGL:HA91	1.91	0.51
1:N:112:LEU:HG	28:N:3701:HOH:O	2.09	0.51
1:N:400:PHE:O	18:N:1522:TGL:H283	2.11	0.51
1:A:76:GLY:O	1:A:80:ASN:HB2	2.11	0.51
1:A:112:LEU:CG	28:A:2701:HOH:O	2.54	0.51
7:G:4:ALA:CB	1:N:282:PHE:HA	2.41	0.51
14:A:516:HEA:HMC1	14:A:516:HEA:HBC1	1.92	0.51
1:N:406:ASN:HD21	19:N:1524:PGV:C2	2.24	0.51
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.26	0.51
12:L:24:MET:SD	18:L:522:TGL:H161	2.51	0.51
7:G:30:LEU:HD21	25:G:269:CDL:H462	1.92	0.50
1:N:366:VAL:HG11	2:O:9:PHE:CE2	2.46	0.50
1:N:488:THR:HB	1:N:495:LEU:HD13	1.93	0.50
3:P:76:GLN:NE2	28:P:3284:HOH:O	2.37	0.50
3:P:54:MET:HE3	25:P:1270:CDL:H612	1.92	0.50
1:N:400:PHE:HB3	18:N:1522:TGL:C28	2.40	0.50
1:N:472:ILE:HD13	18:N:1522:TGL:HA91	1.94	0.50
2:O:164:ALA:O	2:O:194:GLY:HA3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:5:THR:HG22	6:S:96:LEU:CD1	2.41	0.50
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.94	0.50
7:T:2:SER:O	24:T:263:PEK:H322	2.12	0.50
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.94	0.50
2:O:146:MET:HA	2:O:213:LEU:HD12	1.94	0.50
3:P:210:ILE:HD13	19:P:1267:PGV:H301	1.93	0.50
1:A:430:PHE:CE1	18:A:521:TGL:HB21	2.47	0.50
21:O:1229:PSC:H071	9:V:10:ARG:HH21	1.77	0.50
7:G:37:LEU:HD21	25:G:269:CDL:H361	1.93	0.50
8:H:7:LYS:O	8:H:8:ILE:HB	2.11	0.50
1:N:177:SER:H	1:N:180:GLN:HE21	1.59	0.50
21:B:229:PSC:H222	21:B:229:PSC:H21	1.94	0.49
4:D:78:TRP:HA	18:D:523:TGL:HB22	1.94	0.49
1:N:172:LYS:HD2	1:N:181:THR:HG22	1.93	0.49
18:L:522:TGL:OA1	18:L:522:TGL:OG3	2.30	0.49
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.47	0.49
18:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.95	0.49
7:G:3:ALA:O	7:G:4:ALA:CB	2.60	0.49
1:A:310:MET:HE1	2:B:76:ILE:HG21	1.95	0.49
24:G:1263:PEK:H182	3:P:98:PHE:CD2	2.48	0.49
25:T:1269:CDL:H172	25:T:1269:CDL:H511	1.94	0.49
18:N:1522:TGL:H271	12:Y:11:ILE:CG2	2.43	0.49
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.11	0.48
1:A:506:GLU:HG3	28:A:4882:HOH:O	2.12	0.48
10:J:50:LEU:HD22	10:J:54:SER:OG	2.14	0.48
4:D:86:MET:CE	28:K:4688:HOH:O	2.61	0.48
24:G:1263:PEK:H132	3:P:247:VAL:HG12	1.94	0.48
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.48
2:O:41:ILE:CD1	21:O:1229:PSC:H342	2.43	0.48
25:T:1269:CDL:C57	25:T:1269:CDL:H782	2.32	0.48
1:N:112:LEU:HD23	1:N:112:LEU:C	2.34	0.48
21:O:1229:PSC:H081	5:R:8:ASP:OD1	2.14	0.48
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.53	0.48
7:T:38:HIS:NE2	25:T:1269:CDL:H111	2.29	0.48
11:K:24:PHE:O	11:K:28:VAL:HG12	2.14	0.48
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.02	0.48
3:C:91:VAL:HG22	24:T:263:PEK:H14	1.95	0.48
11:X:41:ASN:OD1	28:X:4655:HOH:O	2.20	0.48
5:E:105:GLY:O	5:E:108:LYS:HG2	2.14	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
1:A:28:MET:CE	14:A:515:HEA:H271	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:HIS:HD2	28:C:4770:HOH:O	1.97	0.47
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.15	0.47
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.14	0.47
2:B:78:LEU:CD1	25:T:1269:CDL:H352	2.44	0.47
2:B:29:MET:HG3	9:I:35:TYR:CD2	2.49	0.47
18:N:1521:TGL:C24	18:N:1521:TGL:H201	2.41	0.47
1:N:243:VAL:HB	14:N:516:HEA:CAC	2.45	0.47
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.96	0.47
28:B:3446:HOH:O	7:T:17:ARG:CD	2.63	0.47
3:C:191:GLY:HA3	28:G:2132:HOH:O	2.14	0.47
19:N:1524:PGV:H011	19:N:1524:PGV:H221	1.96	0.47
28:G:4541:HOH:O	19:P:1268:PGV:H301	2.14	0.47
25:C:270:CDL:CB3	25:C:270:CDL:HB21	2.45	0.47
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.14	0.47
18:N:1522:TGL:H302	28:N:4751:HOH:O	2.15	0.47
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.45	0.47
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.14	0.47
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	1.97	0.47
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.80	0.47
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.97	0.47
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.97	0.47
3:P:51:MET:HB3	25:P:1270:CDL:H622	1.96	0.47
25:G:269:CDL:HB32	1:N:304:TYR:HD1	1.80	0.46
1:A:379:TYR:O	1:A:383:MET:HB2	2.16	0.46
1:A:46:THR:HG23	28:A:2466:HOH:O	2.15	0.46
18:A:521:TGL:HC82	28:A:4504:HOH:O	2.14	0.46
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.97	0.46
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.79	0.46
21:B:229:PSC:C07	9:I:10:ARG:NH2	2.68	0.46
1:N:148:PHE:HB3	3:P:28:THR:HB	1.97	0.46
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.15	0.46
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.97	0.46
2:O:56:MET:HA	21:O:1229:PSC:H202	1.98	0.46
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.16	0.46
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.97	0.46
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.16	0.46
25:G:269:CDL:H1	25:G:269:CDL:OB4	2.16	0.46
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.51	0.45
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.50	0.45
24:T:1264:PEK:C10	24:T:1264:PEK:H161	2.46	0.45
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:TRP:O	2:B:226:MET:HB2	2.16	0.45
25:C:270:CDL:OA5	25:C:270:CDL:HB22	2.15	0.45
1:N:87:ILE:O	1:N:173:PRO:HD3	2.15	0.45
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.99	0.45
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.56	0.45
6:S:51:SER:O	6:S:94:HIS:HA	2.16	0.45
1:A:321:PHE:CD2	21:B:229:PSC:H341	2.51	0.45
4:D:86:MET:HE3	28:K:4688:HOH:O	2.17	0.45
7:G:38:HIS:CE1	25:G:269:CDL:H111	2.52	0.45
14:N:515:HEA:H172	14:N:515:HEA:H273	1.41	0.45
25:C:270:CDL:H741	25:C:270:CDL:H172	1.98	0.45
6:F:70:ILE:HG13	6:F:84:SER:HB3	1.98	0.45
25:T:1269:CDL:H171	28:T:4708:HOH:O	2.17	0.45
1:A:115:SER:O	1:A:121:GLY:HA2	2.17	0.45
6:F:55:LYS:HA	6:F:74:LEU:O	2.16	0.45
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.71	0.45
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.98	0.45
24:T:1264:PEK:H161	24:T:1264:PEK:H102	1.98	0.45
12:Y:22:LEU:O	12:Y:26:THR:HB	2.17	0.45
10:W:56:PRO:HD3	12:Y:46:LYS:HG2	1.98	0.45
3:C:105:SER:HA	3:C:116:TRP:CE3	2.52	0.45
8:H:60:TYR:C	8:H:60:TYR:CD1	2.89	0.45
3:P:250:LEU:HD22	25:T:1269:CDL:H662	1.98	0.45
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.82	0.44
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.52	0.44
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.52	0.44
25:C:270:CDL:H652	25:C:270:CDL:H611	2.00	0.44
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.05	0.44
1:N:309:THR:HG22	14:N:516:HEA:HMB2	1.97	0.44
18:A:521:TGL:H281	18:A:521:TGL:H101	1.99	0.44
2:O:16:ILE:HD11	2:O:86:MET:HG2	2.00	0.44
1:A:1:FME:HCN	1:A:4:ASN:H	1.82	0.44
21:B:229:PSC:H062	21:B:229:PSC:H042	1.80	0.44
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.82	0.44
18:L:522:TGL:H231	18:L:522:TGL:H202	1.41	0.44
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.83	0.44
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.48	0.44
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.99	0.44
22:B:1085:CHD:H212	22:B:1085:CHD:H12	1.99	0.44
2:B:78:LEU:HD12	25:T:1269:CDL:C35	2.48	0.44
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:1270:CDL:H242	25:P:1270:CDL:H661	1.98	0.44
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.82	0.44
10:J:40:LEU:HD12	22:J:60:CHD:H183	2.00	0.44
1:N:501:PRO:HB3	12:Y:5:GLU:OE2	2.17	0.44
1:A:481:GLU:HB2	13:M:4:LYS:HE2	2.00	0.44
5:R:80:GLU:CD	5:R:80:GLU:H	2.20	0.44
25:C:270:CDL:C19	25:C:270:CDL:H642	2.47	0.44
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.18	0.43
19:A:524:PGV:H312	13:M:16:ALA:HA	1.99	0.43
1:N:334:TRP:CZ3	18:Q:1523:TGL:HA51	2.53	0.43
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.75	0.43
13:Z:37:LEU:HA	13:Z:37:LEU:HD23	1.79	0.43
5:R:86:ILE:HA	5:R:86:ILE:HD13	1.87	0.43
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.32	0.43
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.53	0.43
3:P:64:GLU:HA	3:P:68:GLN:HE21	1.83	0.43
24:T:1265:PEK:H383	25:T:1269:CDL:H272	1.90	0.43
6:S:87:THR:HG21	28:S:3514:HOH:O	2.18	0.43
1:A:282:PHE:HA	7:T:4:ALA:CB	2.45	0.43
1:A:406:ASN:HD21	19:A:524:PGV:H21	1.80	0.43
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.53	0.43
19:C:267:PGV:H182	25:C:270:CDL:C67	2.49	0.43
2:O:65:TRP:CZ3	21:O:1229:PSC:H331	2.54	0.43
25:G:269:CDL:H352	2:O:78:LEU:HD12	2.00	0.43
3:P:63:ARG:NE	25:P:1270:CDL:HA22	2.07	0.43
1:N:215:LEU:HD11	24:T:1264:PEK:H271	2.00	0.43
19:N:1524:PGV:H132	19:N:1524:PGV:H301	2.01	0.43
1:N:472:ILE:HG21	18:N:1522:TGL:CA9	2.49	0.43
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.54	0.43
25:G:269:CDL:H451	2:O:70:ALA:HB1	2.01	0.43
21:O:1229:PSC:C07	9:V:10:ARG:HE	2.32	0.43
22:W:1059:CHD:H193	22:W:1059:CHD:H111	1.73	0.43
1:A:383:MET:O	1:A:387:PHE:HB2	2.18	0.43
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.01	0.43
4:D:132:GLN:OE1	9:I:43:ARG:HD3	2.19	0.43
10:J:33:ARG:HG2	22:J:60:CHD:C15	2.48	0.43
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.96	0.43
3:C:156:ARG:HE	22:C:271:CHD:C24	2.32	0.43
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.43
1:N:365:ILE:HD11	28:N:4859:HOH:O	2.18	0.43
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:310:MET:HB3	2:O:73:LEU:HD22	2.00	0.43
3:P:107:ALA:HB2	19:P:1268:PGV:H031	2.01	0.43
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.01	0.43
25:T:1269:CDL:H182	25:T:1269:CDL:H152	1.85	0.43
3:P:37:PHE:CD1	10:W:52:TRP:HZ3	2.36	0.43
25:P:1270:CDL:H642	25:P:1270:CDL:C19	2.49	0.42
4:D:7:LYS:HE3	28:D:4308:HOH:O	2.18	0.42
12:L:20:ARG:NH2	18:L:522:TGL:HC42	2.34	0.42
13:M:4:LYS:HG2	13:M:4:LYS:H	1.64	0.42
1:N:54:TYR:HB2	28:N:4621:HOH:O	2.19	0.42
2:B:199:ILE:HG23	2:B:199:ILE:O	2.19	0.42
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.50	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.42
3:P:29:SER:CB	3:P:42:LEU:HD13	2.48	0.42
1:N:489:THR:HA	6:S:71:TRP:O	2.19	0.42
21:B:229:PSC:H241	21:B:229:PSC:H62	2.02	0.42
1:N:115:SER:HB2	1:N:142:SER:O	2.20	0.42
2:O:199:ILE:O	2:O:199:ILE:HG23	2.19	0.42
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.18	0.42
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.01	0.42
5:E:5:HIS:HB3	5:E:6:GLU:H	1.62	0.42
7:G:31:CYS:SG	25:G:269:CDL:H532	2.59	0.42
10:J:56:PRO:HD3	12:L:46:LYS:HG2	2.01	0.42
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.55	0.42
1:N:397:PHE:HB3	1:N:398:PRO:HD3	2.01	0.42
2:O:9:PHE:HB2	2:O:21:LEU:HD21	2.01	0.42
3:C:247:VAL:CG1	24:T:263:PEK:H132	2.50	0.42
19:C:268:PGV:H341	28:T:4364:HOH:O	2.19	0.42
3:C:51:MET:HB3	25:C:270:CDL:H622	2.01	0.42
7:G:5:LYS:HD2	24:G:1263:PEK:H371	2.00	0.42
7:T:31:CYS:SG	25:T:1269:CDL:C55	3.07	0.42
4:D:78:TRP:CA	18:D:523:TGL:HB22	2.50	0.42
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.02	0.42
1:N:342:LEU:HD13	2:O:46:LEU:HD11	2.01	0.42
6:S:95:GLN:CB	28:S:4523:HOH:O	2.61	0.42
1:A:115:SER:HB2	1:A:142:SER:O	2.20	0.41
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.20	0.41
9:V:73:LYS:HE3	9:V:73:LYS:HB3	1.96	0.41
3:C:99:TRP:CE2	19:C:268:PGV:H232	2.55	0.41
19:N:1524:PGV:H322	13:Z:19:LEU:HD23	2.02	0.41
1:N:22:PHE:HA	18:N:1522:TGL:HB72	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:379:TYR:O	1:N:383:MET:HB2	2.20	0.41
2:B:29:MET:HG3	9:I:35:TYR:CG	2.55	0.41
1:N:456:MET:HG2	4:Q:96:LEU:HD13	2.01	0.41
1:N:431:LEU:HD22	1:N:447:TYR:HB3	2.03	0.41
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.56	0.41
1:N:243:VAL:HB	14:N:516:HEA:HAC	2.01	0.41
1:A:400:PHE:HB3	18:L:522:TGL:H282	2.03	0.41
6:F:46:PRO:O	6:F:48:LEU:HD13	2.21	0.41
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.35	0.41
19:N:1266:PGV:H183	24:T:1264:PEK:H332	2.03	0.41
1:A:28:MET:HE1	14:A:515:HEA:C27	2.51	0.41
21:B:229:PSC:H251	21:B:229:PSC:H221	1.79	0.41
5:E:48:ILE:O	5:E:52:LEU:HG	2.20	0.41
7:G:7:ASP:O	7:G:9:GLY:N	2.49	0.41
13:M:10:THR:HG22	13:M:15:GLN:HG3	2.02	0.41
1:N:240:HIS:C	1:N:240:HIS:CD2	2.94	0.41
1:N:76:GLY:O	1:N:80:ASN:HB2	2.20	0.41
6:S:70:ILE:HG13	6:S:84:SER:HB3	2.01	0.41
8:H:39:CYS:O	8:H:43:MET:HG2	2.21	0.41
1:N:430:PHE:CE1	18:N:1521:TGL:HB21	2.55	0.41
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.56	0.41
1:N:310:MET:HE2	1:N:356:ILE:HG23	2.02	0.41
3:P:129:VAL:N	3:P:130:PRO:CD	2.82	0.41
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.51	0.41
14:A:515:HEA:H273	14:A:515:HEA:H172	1.30	0.41
3:C:223:LEU:HD21	22:C:271:CHD:H183	2.01	0.41
24:G:264:PEK:H352	24:G:264:PEK:H382	1.72	0.41
25:P:1270:CDL:H792	25:P:1270:CDL:H821	1.86	0.41
7:T:11:TPO:O	7:T:11:TPO:CG2	2.68	0.41
25:C:270:CDL:H171	25:C:270:CDL:H202	1.87	0.41
6:F:51:SER:O	6:F:94:HIS:N	2.47	0.41
24:G:1263:PEK:H132	3:P:247:VAL:HG11	2.03	0.41
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.90	0.41
21:O:1229:PSC:H22	9:V:14:ALA:CB	2.51	0.41
13:Z:7:LYS:NZ	28:Z:4640:HOH:O	2.36	0.41
24:C:265:PEK:C38	25:G:269:CDL:C27	2.70	0.40
8:H:27:ARG:NH1	28:H:2431:HOH:O	2.53	0.40
10:J:50:LEU:HD22	10:J:50:LEU:O	2.21	0.40
19:N:1524:PGV:H92	4:Q:84:ALA:HB2	2.02	0.40
25:T:1269:CDL:HA62	25:T:1269:CDL:H322	2.02	0.40
25:T:1269:CDL:H561	25:T:1269:CDL:H592	1.63	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:TRP:CH2	19:A:524:PGV:H81	2.57	0.40
25:P:1270:CDL:H652	25:P:1270:CDL:H611	2.03	0.40
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.03	0.40
1:A:194:LEU:HD13	28:A:4206:HOH:O	2.21	0.40
2:B:196:CYS:CB	2:B:207:MET:HG3	2.52	0.40
19:C:267:PGV:H172	25:C:270:CDL:H662	2.02	0.40
3:P:22:LEU:O	3:P:26:LEU:HG	2.21	0.40
4:Q:81:VAL:HG11	18:Q:1523:TGL:HB51	2.04	0.40
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.47	0.40
1:N:402:GLY:HA3	1:N:499:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	496 (97%)	15 (3%)	1 (0%)	47	58
1	N	512/514 (100%)	499 (98%)	13 (2%)	0	100	100
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	34	42
2	O	225/227 (99%)	214 (95%)	8 (4%)	3 (1%)	12	12
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	250 (97%)	6 (2%)	1 (0%)	34	42
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	15	17
6	S	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	4	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
7	T	81/85 (95%)	66 (82%)	9 (11%)	6 (7%)	1	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	12	12
8	U	77/85 (91%)	71 (92%)	4 (5%)	2 (3%)	5	4
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	47 (100%)	0	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3371 (96%)	107 (3%)	26 (1%)	22	26

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
8	H	8	ILE
6	S	94	HIS
6	S	95	GLN
7	T	3	ALA
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
1	A	384	GLY
2	B	60	GLU
8	U	8	ILE
7	G	6	GLY
2	O	224	ALA
7	T	6	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	3	ALA
7	G	40	GLY
2	O	60	GLU
3	P	38	ASN
7	T	39	SER
8	U	10	ASN
6	S	96	LEU
2	O	92	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	418 (98%)	8 (2%)	57	73
1	N	426/426 (100%)	415 (97%)	11 (3%)	46	63
2	B	210/210 (100%)	199 (95%)	11 (5%)	23	32
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	25
3	C	224/226 (99%)	218 (97%)	6 (3%)	44	61
3	P	224/226 (99%)	218 (97%)	6 (3%)	44	61
4	D	128/129 (99%)	127 (99%)	1 (1%)	81	91
4	Q	128/129 (99%)	124 (97%)	4 (3%)	40	55
5	E	92/95 (97%)	88 (96%)	4 (4%)	29	40
5	R	92/95 (97%)	91 (99%)	1 (1%)	73	86
6	F	81/81 (100%)	78 (96%)	3 (4%)	34	48
6	S	81/81 (100%)	76 (94%)	5 (6%)	18	25
7	G	67/68 (98%)	60 (90%)	7 (10%)	7	8
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	11
8	H	71/75 (95%)	68 (96%)	3 (4%)	30	42
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	29
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	19
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	72
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	72
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	63
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	33
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	63
12	Y	39/40 (98%)	36 (92%)	3 (8%)	13	16
13	M	37/38 (97%)	30 (81%)	7 (19%)	1	1
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	4
All	All	3040/3082 (99%)	2918 (96%)	122 (4%)	31	44

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	189	MET
1	A	338	MET
1	A	369	ASP
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	110	TYR
2	B	115	ASP
2	B	167	SER
2	B	171	LYS
2	B	226	MET
3	C	33	MET
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	51	LEU
5	E	5	HIS
5	E	31	LYS
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	84	SER
6	F	87	THR
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	8	ILE
8	H	9	LYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU
11	K	54	ARG
12	L	26	THR
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	189	MET
1	N	336	PRO
1	N	363	LEU
1	N	369	ASP
1	N	484	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	512	ASN
2	O	33	LEU
2	O	59	GLN
2	O	60	GLU
2	O	61	VAL
2	O	65	TRP
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	171	LYS
2	O	217	LYS
3	P	33	MET
3	P	77	LYS
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	51	LEU
4	Q	52	SER
4	Q	143	ASN
5	R	5	HIS
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	95	GLN
6	S	96	LEU
7	T	17	ARG
7	T	18	PHE
7	T	38	HIS
7	T	54	ARG
7	T	74	ARG
7	T	84	LYS
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
8	U	70	SER
9	V	2	THR
9	V	8	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	V	10	ARG
9	V	29	LEU
10	W	50	LEU
11	X	20	SER
11	X	54	ARG
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	178	GLN
1	A	180	GLN
1	A	360	ASN
1	A	512	ASN
2	B	52	HIS
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	71	HIS
7	G	76	ASN
10	J	29	ASN
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	3	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	50	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
5	R	94	ASN
7	T	76	ASN
10	W	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	O	1	2	8,9,10	0.92	0	7,9,11	6.06	4 (57%)
7	TPO	G	11	7	8,10,11	2.22	2 (25%)	10,14,16	1.29	1 (10%)
2	FME	B	1	2	8,9,10	1.51	1 (12%)	7,9,11	7.06	5 (71%)
9	SAC	V	1	9	7,8,9	2.51	2 (28%)	8,9,11	4.36	3 (37%)
1	FME	N	1	1	8,9,10	0.88	0	7,9,11	5.71	1 (14%)
7	TPO	T	11	7	8,10,11	1.99	2 (25%)	10,14,16	1.27	2 (20%)
9	SAC	I	1	9	7,8,9	2.61	2 (28%)	8,9,11	1.92	3 (37%)
1	FME	A	1	1	8,9,10	0.88	0	7,9,11	5.01	3 (42%)

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	-	1/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
9	SAC	V	1	9	-	1/7/8/10	-
1	FME	N	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	3/9/11/13	-
9	SAC	I	1	9	-	3/7/8/10	-
1	FME	A	1	1	-	4/7/9/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	5.47	1.35	1.23
9	V	1	SAC	CA-N	4.63	1.52	1.46
9	V	1	SAC	OAC-C1A	4.52	1.33	1.23
7	G	11	TPO	P-OG1	3.85	1.66	1.59
9	I	1	SAC	CA-N	3.72	1.51	1.46
7	T	11	TPO	P-O1P	3.35	1.61	1.50
7	G	11	TPO	P-O1P	3.27	1.61	1.50
2	B	1	FME	CA-N	3.02	1.50	1.46
7	T	11	TPO	P-OG1	2.92	1.64	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-17.00	96.68	122.82
2	O	1	FME	CA-N-CN	-14.97	99.80	122.82
1	N	1	FME	CA-N-CN	-14.72	100.18	122.82
1	A	1	FME	CA-N-CN	-12.61	103.43	122.82
9	V	1	SAC	CB-CA-N	-7.50	93.72	110.55
9	V	1	SAC	C-CA-N	7.07	122.48	109.73
9	V	1	SAC	CA-N-C1A	5.92	134.07	123.15
2	B	1	FME	CG-CB-CA	-4.57	100.25	112.95
2	B	1	FME	O1-CN-N	4.39	136.83	125.27
2	O	1	FME	CG-CB-CA	-3.71	102.64	112.95
9	I	1	SAC	C2A-C1A-N	-3.43	110.29	116.10
2	O	1	FME	C-CA-N	3.22	115.53	109.73
2	B	1	FME	C-CA-N	2.87	114.91	109.73
1	A	1	FME	CG-CB-CA	-2.64	105.62	112.95
2	B	1	FME	O-C-CA	-2.55	118.09	124.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	SAC	OAC-C1A-N	2.54	126.62	121.95
9	I	1	SAC	CA-N-C1A	2.35	127.48	123.15
1	A	1	FME	CE-SD-CG	2.30	108.29	100.40
7	T	11	TPO	O-C-CA	-2.18	119.05	124.78
7	G	11	TPO	O-C-CA	-2.06	119.39	124.78
7	T	11	TPO	CG2-CB-CA	2.06	117.22	113.16
2	O	1	FME	O-C-CA	-2.01	119.52	124.78

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 42 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
27	DMU	Z	1526	-	34,34,34	0.85	1 (2%)	45,45,45	2.50	16 (35%)
14	HEA	A	516	1	44,67,67	1.09	3 (6%)	37,103,103	2.16	10 (27%)
22	CHD	C	525	-	29,32,32	0.77	0	48,51,51	1.02	2 (4%)
18	TGL	A	521	-	62,62,62	1.27	6 (9%)	65,65,65	1.74	14 (21%)
24	PEK	C	265	-	52,52,52	1.21	2 (3%)	55,57,57	1.13	4 (7%)
19	PGV	P	1268	-	50,50,50	1.18	2 (4%)	53,56,56	1.31	5 (9%)
14	HEA	N	515	1	44,67,67	1.26	4 (9%)	37,103,103	3.19	18 (48%)
22	CHD	C	271	-	29,32,32	0.54	0	48,51,51	2.16	19 (39%)
22	CHD	P	1271	-	29,32,32	0.56	0	48,51,51	2.16	17 (35%)
19	PGV	A	524	-	50,50,50	1.18	2 (4%)	53,56,56	1.04	5 (9%)
18	TGL	N	1522	-	62,62,62	1.51	7 (11%)	65,65,65	1.57	15 (23%)
22	CHD	B	1085	-	29,32,32	1.10	3 (10%)	48,51,51	1.50	9 (18%)
22	CHD	P	1525	-	29,32,32	0.90	1 (3%)	48,51,51	1.47	7 (14%)
25	CDL	C	270	-	99,99,99	1.36	13 (13%)	105,111,111	1.30	13 (12%)
19	PGV	N	1524	-	50,50,50	1.03	2 (4%)	53,56,56	1.15	4 (7%)
22	CHD	W	1059	-	29,32,32	0.78	0	48,51,51	3.19	22 (45%)
18	TGL	Q	1523	-	62,62,62	1.32	6 (9%)	65,65,65	1.40	12 (18%)
19	PGV	A	522	-	50,50,50	0.81	2 (4%)	53,56,56	1.14	2 (3%)
25	CDL	G	269	-	99,99,99	1.38	12 (12%)	105,111,111	1.31	9 (8%)
25	CDL	T	1269	-	99,99,99	1.36	12 (12%)	105,111,111	1.26	7 (6%)
22	CHD	G	229	-	29,32,32	0.82	0	48,51,51	1.57	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CDL	P	1270	-	99,99,99	1.37	12 (12%)	105,111,111	1.36	13 (12%)
24	PEK	G	264	-	52,52,52	1.00	4 (7%)	55,57,57	1.51	9 (16%)
18	TGL	L	522	-	62,62,62	1.36	7 (11%)	65,65,65	1.54	12 (18%)
24	PEK	T	263	-	52,52,52	1.22	3 (5%)	55,57,57	1.13	5 (9%)
18	TGL	N	1521	-	62,62,62	1.23	6 (9%)	65,65,65	1.50	10 (15%)
24	PEK	T	1264	-	52,52,52	0.98	4 (7%)	55,57,57	1.39	9 (16%)
27	DMU	M	526	-	34,34,34	0.86	1 (2%)	45,45,45	2.45	17 (37%)
19	PGV	C	268	-	50,50,50	1.20	2 (4%)	53,56,56	1.28	4 (7%)
22	CHD	J	60	-	29,32,32	0.74	0	48,51,51	2.93	22 (45%)
19	PGV	P	1267	-	50,50,50	0.77	1 (2%)	53,56,56	1.13	5 (9%)
24	PEK	G	1263	-	52,52,52	1.19	2 (3%)	55,57,57	1.19	6 (10%)
24	PEK	T	1265	-	52,52,52	1.26	3 (5%)	55,57,57	1.13	5 (9%)
20	CUA	O	228	2	0,1,1	0.00	-	-	-	-
19	PGV	C	267	-	50,50,50	0.81	2 (4%)	53,56,56	1.12	5 (9%)
21	PSC	B	229	-	51,51,51	1.18	3 (5%)	57,59,59	1.04	3 (5%)
19	PGV	N	1266	-	50,50,50	0.85	2 (4%)	53,56,56	1.24	5 (9%)
14	HEA	A	515	1	44,67,67	1.06	2 (4%)	37,103,103	2.98	15 (40%)
14	HEA	N	516	1	44,67,67	0.99	1 (2%)	37,103,103	1.72	12 (32%)
18	TGL	D	523	-	62,62,62	1.29	6 (9%)	65,65,65	1.56	10 (15%)
21	PSC	O	1229	-	51,51,51	1.16	3 (5%)	57,59,59	0.97	2 (3%)
20	CUA	B	228	2	0,1,1	0.00	-	-	-	-

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
27	DMU	Z	1526	-	4/4/10/10	9/19/59/59	0/2/2/2
14	HEA	A	516	1	2/2/7/16	1/24/76/76	-
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
18	TGL	A	521	-	-	35/65/65/65	-
24	PEK	C	265	-	-	23/56/56/56	-
19	PGV	P	1268	-	-	33/55/55/55	-
14	HEA	N	515	1	3/3/7/16	2/24/76/76	-
22	CHD	C	271	-	-	4/7/74/74	0/4/4/4
22	CHD	G	229	-	-	0/7/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	A	524	-	-	33/55/55/55	-
18	TGL	N	1522	-	-	34/65/65/65	-
22	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
25	CDL	C	270	-	-	68/110/110/110	-
19	PGV	N	1524	-	-	41/55/55/55	-
22	CHD	W	1059	-	-	6/7/74/74	0/4/4/4
18	TGL	Q	1523	-	-	36/65/65/65	-
19	PGV	A	522	-	-	14/55/55/55	-
25	CDL	G	269	-	-	67/110/110/110	-
25	CDL	T	1269	-	-	51/110/110/110	-
22	CHD	P	1271	-	-	4/7/74/74	0/4/4/4
25	CDL	P	1270	-	-	68/110/110/110	-
24	PEK	G	264	-	-	25/56/56/56	-
18	TGL	L	522	-	-	39/65/65/65	-
24	PEK	T	263	-	-	34/56/56/56	-
18	TGL	N	1521	-	-	31/65/65/65	-
24	PEK	T	1264	-	-	24/56/56/56	-
27	DMU	M	526	-	2/2/10/10	8/19/59/59	0/2/2/2
19	PGV	C	268	-	-	35/55/55/55	-
22	CHD	J	60	-	-	4/7/74/74	0/4/4/4
19	PGV	P	1267	-	-	14/55/55/55	-
24	PEK	G	1263	-	-	32/56/56/56	-
24	PEK	T	1265	-	-	32/56/56/56	-
19	PGV	C	267	-	-	17/55/55/55	-
19	PGV	N	1266	-	-	15/55/55/55	-
14	HEA	A	515	1	2/2/7/16	2/24/76/76	-
14	HEA	N	516	1	2/2/7/16	3/24/76/76	-
18	TGL	D	523	-	-	37/65/65/65	-
21	PSC	O	1229	-	-	37/55/55/55	-
21	PSC	B	229	-	-	35/55/55/55	-

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	1522	TGL	OG2-CB1	6.24	1.51	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	1522	TGL	OG1-CA1	6.15	1.51	1.33
18	L	522	TGL	OG2-CB1	5.82	1.50	1.34
24	T	263	PEK	O03-C21	5.77	1.50	1.33
19	A	524	PGV	O03-C19	5.62	1.49	1.33
24	G	1263	PEK	O03-C21	5.60	1.49	1.33
19	P	1268	PGV	O01-C1	5.57	1.50	1.34
19	C	268	PGV	O01-C1	5.51	1.49	1.34
24	T	1265	PEK	O01-C1	5.42	1.49	1.34
24	C	265	PEK	O03-C21	5.42	1.49	1.33
24	T	1265	PEK	O03-C21	5.25	1.48	1.33
18	Q	1523	TGL	OG2-CB1	5.19	1.48	1.34
25	G	269	CDL	OA6-CA5	5.19	1.48	1.34
25	P	1270	CDL	OA8-CA7	5.04	1.48	1.33
25	C	270	CDL	OA8-CA7	5.01	1.48	1.33
24	C	265	PEK	O01-C1	4.94	1.48	1.34
18	A	521	TGL	OG1-CA1	4.91	1.47	1.33
25	P	1270	CDL	OA6-CA5	4.88	1.48	1.34
18	L	522	TGL	OG1-CA1	4.86	1.47	1.33
24	T	263	PEK	O01-C1	4.83	1.47	1.34
19	C	268	PGV	O03-C19	4.82	1.47	1.33
25	G	269	CDL	OB6-CB5	4.81	1.47	1.34
19	P	1268	PGV	O03-C19	4.81	1.47	1.33
24	G	1263	PEK	O01-C1	4.78	1.47	1.34
25	T	1269	CDL	OA6-CA5	4.75	1.47	1.34
19	N	1524	PGV	O03-C19	4.73	1.47	1.33
18	Q	1523	TGL	OG1-CA1	4.71	1.47	1.33
18	D	523	TGL	OG3-CC1	4.68	1.47	1.33
25	C	270	CDL	OA6-CA5	4.60	1.47	1.34
21	B	229	PSC	O01-C1	4.60	1.47	1.34
18	Q	1523	TGL	OG3-CC1	4.59	1.46	1.33
25	G	269	CDL	OB8-CB7	4.59	1.46	1.33
18	D	523	TGL	OG2-CB1	4.56	1.47	1.34
18	D	523	TGL	OG1-CA1	4.55	1.46	1.33
18	A	521	TGL	OG2-CB1	4.54	1.47	1.34
21	B	229	PSC	O03-C19	4.52	1.46	1.33
25	T	1269	CDL	OB6-CB5	4.51	1.47	1.34
25	C	270	CDL	OB8-CB7	4.46	1.46	1.33
25	T	1269	CDL	OB8-CB7	4.46	1.46	1.33
18	N	1521	TGL	OG2-CB1	4.44	1.46	1.34
21	O	1229	PSC	O01-C1	4.42	1.46	1.34
25	G	269	CDL	OA8-CA7	4.40	1.46	1.33
18	N	1521	TGL	OG3-CC1	4.37	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	O	1229	PSC	O03-C19	4.34	1.46	1.33
19	A	524	PGV	O01-C1	4.29	1.46	1.34
25	T	1269	CDL	OA8-CA7	4.27	1.45	1.33
18	N	1522	TGL	OG3-CC1	4.25	1.45	1.33
19	N	1524	PGV	O01-C1	4.06	1.45	1.34
25	P	1270	CDL	OB6-CB5	4.05	1.45	1.34
19	N	1266	PGV	O03-C19	4.01	1.45	1.33
25	P	1270	CDL	OB8-CB7	3.94	1.44	1.33
21	O	1229	PSC	C13-C12	3.89	1.54	1.31
18	N	1521	TGL	OG1-CA1	3.85	1.44	1.33
18	A	521	TGL	OG3-CC1	3.82	1.44	1.33
21	B	229	PSC	C13-C12	3.80	1.53	1.31
24	G	264	PEK	O01-C1	3.77	1.44	1.34
25	C	270	CDL	OB6-CB5	3.70	1.44	1.34
24	T	1264	PEK	O01-C1	3.65	1.44	1.34
19	P	1267	PGV	O03-C19	3.62	1.43	1.33
25	C	270	CDL	C59-C58	-3.58	1.31	1.51
18	L	522	TGL	C20-CA9	-3.56	1.31	1.51
18	N	1521	TGL	C10-CB9	-3.54	1.31	1.51
14	N	515	HEA	O11-C11	3.53	1.50	1.42
18	L	522	TGL	OG3-CC1	3.49	1.43	1.33
18	N	1522	TGL	C20-CA9	-3.47	1.32	1.51
25	P	1270	CDL	C59-C58	-3.42	1.32	1.51
25	P	1270	CDL	C79-C78	-3.36	1.32	1.51
25	T	1269	CDL	C59-C58	-3.36	1.32	1.51
25	C	270	CDL	C62-C61	-3.32	1.32	1.51
25	C	270	CDL	C79-C78	-3.30	1.33	1.51
25	G	269	CDL	C59-C58	-3.26	1.33	1.51
25	T	1269	CDL	C42-C41	-3.25	1.33	1.51
27	M	526	DMU	C3-C4	-3.23	1.44	1.52
25	P	1270	CDL	C62-C61	-3.23	1.33	1.51
18	A	521	TGL	C10-CB9	-3.23	1.33	1.51
25	T	1269	CDL	C62-C61	-3.20	1.33	1.51
24	T	1264	PEK	O01-C02	-3.19	1.38	1.46
18	L	522	TGL	C10-CB9	-3.19	1.33	1.51
25	G	269	CDL	C42-C41	-3.18	1.33	1.51
19	A	522	PGV	O03-C19	3.16	1.42	1.33
25	C	270	CDL	C82-C81	-3.13	1.34	1.51
25	P	1270	CDL	C82-C81	-3.11	1.34	1.51
25	C	270	CDL	C19-C18	-3.09	1.34	1.51
25	P	1270	CDL	C19-C18	-3.08	1.34	1.51
18	Q	1523	TGL	C20-CA9	-3.06	1.34	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	1522	TGL	C10-CB9	-3.06	1.34	1.51
18	Q	1523	TGL	C15-CC9	-3.05	1.34	1.51
25	G	269	CDL	C62-C61	-3.04	1.34	1.51
18	D	523	TGL	C20-CA9	-3.03	1.34	1.51
25	G	269	CDL	C22-C21	-3.03	1.34	1.51
25	C	270	CDL	C22-C21	-3.01	1.34	1.51
19	A	522	PGV	O01-C1	3.01	1.42	1.34
14	N	515	HEA	CAD-C3D	3.00	1.56	1.52
25	P	1270	CDL	C22-C21	-2.98	1.34	1.51
18	D	523	TGL	C15-CC9	-2.97	1.34	1.51
25	G	269	CDL	C39-C38	-2.96	1.35	1.51
25	G	269	CDL	C19-C18	-2.96	1.35	1.51
25	T	1269	CDL	C19-C18	-2.95	1.35	1.51
18	Q	1523	TGL	C10-CB9	-2.94	1.35	1.51
14	A	515	HEA	C3B-C11	-2.93	1.50	1.52
18	A	521	TGL	C20-CA9	-2.93	1.35	1.51
19	C	267	PGV	O03-C19	2.91	1.41	1.33
18	D	523	TGL	C10-CB9	-2.90	1.35	1.51
25	T	1269	CDL	C82-C81	-2.90	1.35	1.51
25	T	1269	CDL	C39-C38	-2.88	1.35	1.51
18	N	1521	TGL	C20-CA9	-2.87	1.35	1.51
24	T	1264	PEK	O03-C21	2.87	1.41	1.33
24	G	264	PEK	O03-C01	-2.86	1.38	1.45
25	T	1269	CDL	C79-C78	-2.85	1.35	1.51
25	G	269	CDL	C82-C81	-2.82	1.35	1.51
25	T	1269	CDL	C22-C21	-2.80	1.35	1.51
25	G	269	CDL	C79-C78	-2.76	1.36	1.51
25	P	1270	CDL	C39-C38	-2.75	1.36	1.51
25	C	270	CDL	C42-C41	-2.74	1.36	1.51
18	L	522	TGL	C15-CC9	-2.74	1.36	1.51
25	P	1270	CDL	C42-C41	-2.72	1.36	1.51
18	N	1521	TGL	C15-CC9	-2.71	1.36	1.51
25	C	270	CDL	C39-C38	-2.70	1.36	1.51
22	B	1085	CHD	C11-C12	2.70	1.57	1.53
18	N	1522	TGL	C15-CC9	-2.68	1.36	1.51
19	N	1266	PGV	O01-C1	2.61	1.41	1.34
27	Z	1526	DMU	C3-C4	-2.59	1.46	1.52
14	N	515	HEA	C4C-CHD	2.59	1.48	1.41
18	A	521	TGL	C15-CC9	-2.58	1.37	1.51
14	A	515	HEA	C12-C13	2.41	1.61	1.53
14	A	516	HEA	C3B-C11	-2.39	1.51	1.52
19	C	267	PGV	O01-C1	2.37	1.41	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	515	HEA	C1A-C2A	-2.33	1.37	1.42
24	T	1264	PEK	O03-C01	-2.29	1.39	1.45
25	C	270	CDL	OB6-CB4	-2.24	1.41	1.46
22	B	1085	CHD	C4-C3	2.21	1.56	1.51
22	P	1525	CHD	C11-C9	2.20	1.57	1.53
24	G	264	PEK	O03-C21	2.18	1.39	1.33
18	N	1522	TGL	CG1-CG2	2.16	1.57	1.50
14	N	516	HEA	CAD-C3D	2.14	1.55	1.52
24	G	264	PEK	O01-C02	-2.13	1.41	1.46
22	B	1085	CHD	C6-C7	2.10	1.56	1.52
18	L	522	TGL	CG1-CG2	2.09	1.57	1.50
14	A	516	HEA	CAA-C2A	2.08	1.55	1.52
24	T	263	PEK	P-O11	2.05	1.67	1.59
14	A	516	HEA	C20-C19	2.02	1.55	1.51
24	T	1265	PEK	P-O11	2.02	1.67	1.59

All (389) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	515	HEA	C17-C18-C19	-10.39	102.64	127.66
14	A	515	HEA	C17-C18-C19	-10.22	103.05	127.66
14	N	515	HEA	C17-C16-C15	8.77	141.84	112.98
14	A	515	HEA	C17-C16-C15	8.00	139.29	112.98
22	W	1059	CHD	C13-C17-C20	7.67	128.65	119.50
18	A	521	TGL	CG2-OG2-CB1	7.08	135.23	117.79
22	J	60	CHD	C6-C5-C10	7.06	120.15	112.66
22	W	1059	CHD	C11-C12-C13	6.71	118.14	111.24
22	W	1059	CHD	C17-C13-C14	-6.53	93.51	100.09
22	J	60	CHD	C13-C17-C20	6.28	127.00	119.50
27	Z	1526	DMU	O7-C3-C2	6.26	123.93	107.28
19	P	1268	PGV	O01-C1-C2	6.18	124.82	111.50
18	N	1521	TGL	CG2-OG2-CB1	6.09	132.78	117.79
22	W	1059	CHD	C6-C5-C10	6.08	119.12	112.66
14	A	516	HEA	CAD-CBD-CGD	-6.07	102.49	112.67
22	J	60	CHD	C17-C13-C14	-6.06	93.98	100.09
22	W	1059	CHD	C9-C10-C5	5.83	116.78	108.58
22	W	1059	CHD	C14-C13-C12	5.81	112.81	107.40
22	W	1059	CHD	C18-C13-C12	-5.81	103.15	109.07
22	P	1271	CHD	C1-C2-C3	5.62	117.68	110.47
19	C	268	PGV	O01-C1-C2	5.58	123.54	111.50
27	Z	1526	DMU	O1-C9-C8	5.51	119.70	109.69
14	A	516	HEA	C1B-C2B-C3B	-5.50	103.17	107.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	60	CHD	C9-C10-C5	5.45	116.24	108.58
18	D	523	TGL	OG2-CB1-CB2	5.37	123.06	111.50
27	M	526	DMU	O5-C4-C57	5.35	119.75	106.44
25	P	1270	CDL	OA6-CA5-C11	5.32	122.98	111.50
22	J	60	CHD	C10-C9-C8	5.30	117.51	111.82
25	G	269	CDL	OA6-CA5-C11	5.25	122.81	111.50
22	W	1059	CHD	C9-C11-C12	5.19	121.15	114.30
27	Z	1526	DMU	O5-C6-C1	5.13	121.22	110.35
27	M	526	DMU	C2-C3-C4	5.12	122.67	110.93
27	Z	1526	DMU	O1-C9-C11	5.09	119.09	106.44
18	Q	1523	TGL	OG2-CB1-CB2	5.06	122.41	111.50
25	G	269	CDL	OB6-CB5-C51	5.02	122.31	111.50
14	N	515	HEA	C4B-C3B-C2B	-4.96	103.40	106.87
22	C	271	CHD	C1-C2-C3	4.95	116.82	110.47
25	T	1269	CDL	OA6-CA5-C11	4.93	122.13	111.50
27	M	526	DMU	O1-C9-C8	4.90	118.59	109.69
25	C	270	CDL	OA6-CA5-C11	4.90	122.06	111.50
22	P	1271	CHD	C2-C1-C10	4.89	121.16	112.78
14	N	515	HEA	C12-C13-C14	-4.87	99.38	112.23
18	L	522	TGL	OG3-CC1-OC1	-4.86	111.33	123.59
27	M	526	DMU	O1-C9-C11	4.77	118.31	106.44
25	T	1269	CDL	OB6-CB5-C51	4.77	121.79	111.50
14	A	515	HEA	C12-C13-C14	-4.70	99.81	112.23
27	Z	1526	DMU	O5-C4-C57	4.66	118.03	106.44
27	M	526	DMU	O7-C3-C2	4.66	119.68	107.28
27	Z	1526	DMU	C8-C7-C5	4.65	118.95	110.82
22	J	60	CHD	C1-C10-C5	4.63	114.62	107.77
22	C	271	CHD	C19-C10-C1	-4.63	100.80	108.26
27	M	526	DMU	O1-C10-C5	4.60	120.08	110.35
22	J	60	CHD	C5-C4-C3	4.58	119.48	112.76
27	M	526	DMU	O5-C6-C1	4.55	119.98	110.35
19	A	522	PGV	O03-C19-O04	-4.54	112.14	123.59
18	A	521	TGL	OG2-CB1-CB2	4.47	121.12	111.50
24	G	264	PEK	O01-C1-O02	-4.45	112.94	123.70
22	G	229	CHD	C18-C13-C12	-4.43	104.55	109.07
18	N	1522	TGL	CG2-OG2-CB1	4.37	128.54	117.79
19	N	1266	PGV	O03-C19-C20	4.33	125.51	111.91
14	A	516	HEA	C13-C12-C11	-4.30	107.89	114.35
14	A	515	HEA	C4B-C3B-C2B	-4.27	103.89	106.87
19	P	1268	PGV	O03-C19-C20	4.25	125.25	111.91
24	G	264	PEK	C2-C3-C4	4.24	120.79	113.23
27	Z	1526	DMU	O5-C4-C3	4.22	118.65	109.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	1263	PEK	O03-C21-C22	4.21	125.13	111.91
22	J	60	CHD	C6-C5-C4	-4.17	106.39	111.19
22	C	271	CHD	C2-C1-C10	4.17	119.93	112.78
19	C	268	PGV	O03-C19-C20	4.13	124.87	111.91
19	N	1266	PGV	O03-C19-O04	-4.12	113.19	123.59
14	N	515	HEA	C20-C19-C18	4.11	129.43	121.12
22	J	60	CHD	C22-C20-C17	4.08	118.72	110.28
19	A	522	PGV	O03-C19-C20	4.08	124.72	111.91
22	C	271	CHD	C22-C23-C24	-4.07	104.83	113.59
27	M	526	DMU	C8-C7-C5	4.05	117.90	110.82
18	A	521	TGL	OG1-CG1-CG2	4.05	120.22	108.43
24	C	265	PEK	O03-C21-C22	4.04	124.57	111.91
21	B	229	PSC	O01-C1-C2	4.02	120.16	111.50
22	J	60	CHD	C14-C13-C12	3.97	111.10	107.40
18	D	523	TGL	OG1-CG1-CG2	3.97	119.99	108.43
14	N	515	HEA	CBA-CAA-C2A	3.93	119.71	112.48
24	T	1265	PEK	O01-C1-C2	3.87	119.85	111.50
24	T	263	PEK	O03-C21-C22	3.86	124.04	111.91
18	N	1522	TGL	OG2-CB1-CB2	3.84	119.79	111.50
22	P	1271	CHD	C19-C10-C1	-3.83	102.08	108.26
18	L	522	TGL	OG3-CC1-CC2	3.80	123.84	111.91
22	P	1271	CHD	C10-C9-C8	3.80	115.90	111.82
24	T	1264	PEK	O03-C01-C02	-3.79	97.40	108.43
22	W	1059	CHD	C18-C13-C17	3.79	117.14	111.21
18	N	1522	TGL	OG1-CA1-CA2	3.79	123.80	111.91
18	D	523	TGL	CG3-CG2-CG1	-3.77	102.87	111.79
18	N	1521	TGL	OG2-CG2-CG3	3.76	122.03	108.40
22	C	271	CHD	C10-C9-C8	3.74	115.83	111.82
22	W	1059	CHD	C22-C20-C17	3.74	118.01	110.28
14	A	515	HEA	C27-C19-C18	-3.74	114.09	123.68
22	W	1059	CHD	C5-C4-C3	3.74	118.25	112.76
22	G	229	CHD	C1-C2-C3	-3.73	105.68	110.47
22	P	1271	CHD	C18-C13-C12	-3.73	105.27	109.07
19	N	1524	PGV	O01-C1-C2	3.73	119.54	111.50
22	J	60	CHD	C16-C17-C20	3.73	117.92	112.15
27	M	526	DMU	O5-C4-C3	3.69	117.52	109.75
24	T	1265	PEK	O03-C21-C22	3.68	123.47	111.91
14	N	515	HEA	C27-C19-C18	-3.68	114.24	123.68
27	Z	1526	DMU	O1-C10-C5	3.68	118.14	110.35
22	J	60	CHD	C19-C10-C5	-3.67	104.14	110.36
22	J	60	CHD	C4-C5-C10	3.67	116.55	112.66
14	N	516	HEA	C3C-C4C-NC	3.66	113.95	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1525	CHD	C15-C14-C13	3.66	107.14	103.55
14	A	515	HEA	C20-C19-C18	3.66	128.52	121.12
18	N	1521	TGL	CG3-OG3-CC1	3.64	130.60	117.12
22	C	271	CHD	C1-C10-C5	3.63	113.14	107.77
24	T	1264	PEK	O01-C1-O02	-3.62	114.96	123.70
18	L	522	TGL	CG2-OG2-CB1	3.54	126.52	117.79
22	P	1271	CHD	C15-C14-C13	3.53	107.02	103.55
22	W	1059	CHD	C17-C13-C12	3.52	120.88	117.67
24	T	263	PEK	O01-C1-C2	3.51	119.07	111.50
22	P	1525	CHD	C22-C23-C24	-3.48	106.11	113.59
14	N	515	HEA	C12-C11-C3B	3.48	121.69	112.56
22	W	1059	CHD	C1-C10-C5	3.47	112.90	107.77
19	N	1524	PGV	O03-C19-C20	3.46	122.78	111.91
25	C	270	CDL	OB8-CB7-C71	3.45	122.73	111.91
14	N	516	HEA	CAA-CBA-CGA	-3.45	106.88	112.67
25	P	1270	CDL	OB8-CB7-C71	3.43	122.66	111.91
22	P	1271	CHD	C1-C10-C5	3.42	112.83	107.77
22	J	60	CHD	C4-C3-C2	3.41	114.62	110.55
22	W	1059	CHD	C1-C10-C9	-3.39	106.02	111.35
24	G	1263	PEK	O01-C1-C2	3.38	118.79	111.50
18	Q	1523	TGL	CG3-CG2-CG1	-3.38	103.79	111.79
24	G	1263	PEK	C02-O01-C1	3.35	126.04	117.79
22	W	1059	CHD	C5-C6-C7	3.34	118.15	114.46
22	P	1271	CHD	C22-C23-C24	-3.33	106.43	113.59
22	C	271	CHD	C18-C13-C12	-3.33	105.68	109.07
18	N	1522	TGL	CG1-OG1-CA1	3.31	129.37	117.12
22	G	229	CHD	C10-C9-C8	3.30	115.37	111.82
25	P	1270	CDL	OB8-CB7-OB9	-3.28	115.30	123.59
24	G	1263	PEK	O03-C01-C02	3.24	117.85	108.43
24	C	265	PEK	O01-C1-C2	3.23	118.47	111.50
25	T	1269	CDL	OA8-CA7-C31	3.20	121.96	111.91
18	N	1521	TGL	OG2-CB1-CB2	3.20	118.40	111.50
22	G	229	CHD	C4-C3-C2	-3.20	106.73	110.55
27	M	526	DMU	C11-C9-C8	3.20	120.50	113.00
25	G	269	CDL	C79-C78-C77	3.19	130.64	114.42
14	A	516	HEA	C17-C18-C19	3.18	135.32	127.66
18	A	521	TGL	CA3-CA2-CA1	-3.17	102.10	113.62
18	L	522	TGL	CC3-CC2-CC1	3.17	125.14	113.62
27	Z	1526	DMU	C2-C3-C4	3.15	118.15	110.93
14	A	515	HEA	C21-C20-C19	-3.14	102.66	112.98
22	W	1059	CHD	C10-C9-C8	3.13	115.19	111.82
25	P	1270	CDL	OA8-CA7-C31	3.13	121.72	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	1269	CDL	OA6-CA5-OA7	-3.12	116.15	123.70
22	W	1059	CHD	C19-C10-C5	-3.12	105.06	110.36
14	N	516	HEA	C17-C18-C19	3.12	135.17	127.66
18	D	523	TGL	OG3-CC1-CC2	3.11	121.66	111.91
24	G	264	PEK	C24-C23-C22	-3.10	102.04	113.19
27	Z	1526	DMU	C57-C4-C3	3.10	122.35	113.33
18	D	523	TGL	OG2-CB1-OB1	-3.09	116.23	123.70
22	P	1271	CHD	C16-C17-C13	3.09	106.58	103.55
22	B	1085	CHD	C4-C3-C2	3.08	114.23	110.55
18	Q	1523	TGL	OG1-CA1-CA2	3.08	121.56	111.91
22	W	1059	CHD	C6-C5-C4	-3.07	107.66	111.19
22	B	1085	CHD	C1-C10-C5	3.05	112.28	107.77
22	P	1271	CHD	C9-C10-C5	3.04	112.86	108.58
14	A	516	HEA	C25-C23-C24	3.01	121.24	114.60
18	L	522	TGL	OG2-CB1-CB2	3.00	117.97	111.50
21	O	1229	PSC	O03-C19-C20	3.00	121.33	111.91
18	D	523	TGL	CB3-CB2-CB1	2.98	124.46	113.62
22	B	1085	CHD	C19-C10-C5	-2.96	105.33	110.36
18	A	521	TGL	CG3-OG3-CC1	2.95	128.05	117.12
19	N	1266	PGV	O01-C1-O02	-2.94	116.59	123.70
22	C	271	CHD	C15-C14-C8	2.91	122.40	118.33
22	P	1271	CHD	C6-C7-C8	2.91	114.58	111.48
22	J	60	CHD	C5-C6-C7	2.91	117.67	114.46
22	C	271	CHD	C6-C7-C8	2.90	114.57	111.48
18	N	1522	TGL	OG3-CC1-CC2	2.90	121.00	111.91
22	C	271	CHD	C5-C6-C7	2.89	117.65	114.46
18	L	522	TGL	OG1-CA1-CA2	2.89	120.96	111.91
25	C	270	CDL	OA8-CA7-C31	2.88	120.94	111.91
27	Z	1526	DMU	O7-C3-C4	2.88	117.33	109.45
18	A	521	TGL	OG2-CG2-CG3	2.88	118.82	108.40
22	J	60	CHD	C1-C10-C9	-2.86	106.86	111.35
14	N	515	HEA	OMA-CMA-C3A	-2.86	118.69	124.91
14	A	515	HEA	CMC-C2C-C3C	2.84	130.00	124.68
18	A	521	TGL	OG2-CG2-CG1	2.84	118.69	108.40
24	C	265	PEK	O03-C21-O04	-2.84	116.42	123.59
25	C	270	CDL	C52-C51-CB5	-2.84	103.29	113.62
22	B	1085	CHD	C15-C14-C13	2.84	106.33	103.55
22	C	271	CHD	C23-C22-C20	-2.83	110.91	114.72
18	D	523	TGL	OG1-CA1-CA2	2.83	120.78	111.91
22	B	1085	CHD	C22-C23-C24	-2.82	107.52	113.59
14	A	515	HEA	OMA-CMA-C3A	-2.82	118.76	124.91
22	B	1085	CHD	C22-C20-C17	2.82	116.11	110.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	1059	CHD	C4-C5-C10	2.81	115.65	112.66
18	D	523	TGL	CG3-OG3-CC1	2.81	127.52	117.12
25	G	269	CDL	OA6-CA5-OA7	-2.80	116.93	123.70
25	C	270	CDL	OA8-CA6-CA4	2.80	116.58	108.43
18	N	1521	TGL	OG1-CA1-CA2	2.79	120.66	111.91
21	O	1229	PSC	O01-C1-C2	2.78	117.49	111.50
18	A	521	TGL	OG3-CC1-CC2	2.76	120.57	111.91
18	A	521	TGL	OG3-CC1-OC1	-2.76	116.64	123.59
22	G	229	CHD	C6-C5-C4	-2.75	108.02	111.19
25	G	269	CDL	OA8-CA7-C31	2.75	120.54	111.91
22	J	60	CHD	C18-C13-C12	-2.74	106.28	109.07
27	M	526	DMU	C7-C8-C9	2.74	115.12	110.24
19	P	1267	PGV	O01-C1-O02	-2.73	117.10	123.70
25	G	269	CDL	C80-C79-C78	2.73	128.30	114.42
19	A	524	PGV	O01-C02-C01	2.73	118.28	108.40
14	N	515	HEA	C21-C20-C19	-2.72	104.04	112.98
22	P	1525	CHD	C21-C20-C22	-2.72	106.10	110.36
18	D	523	TGL	CC3-CC2-CC1	-2.71	103.75	113.62
25	P	1270	CDL	OB6-CB5-C51	2.71	117.33	111.50
14	N	516	HEA	C20-C19-C18	-2.69	115.67	121.12
19	N	1524	PGV	O03-C19-O04	-2.68	116.83	123.59
18	Q	1523	TGL	OG3-CC1-CC2	2.68	120.31	111.91
18	N	1522	TGL	OB1-CB1-CB2	-2.67	113.32	123.73
24	G	264	PEK	O01-C02-C01	-2.65	98.80	108.40
14	N	516	HEA	C12-C11-C3B	2.65	119.51	112.56
24	T	1264	PEK	O13-P-O14	2.64	125.28	112.24
14	A	515	HEA	C3C-C4C-NC	2.64	112.62	109.21
18	Q	1523	TGL	CG2-OG2-CB1	2.63	124.26	117.79
24	T	263	PEK	C02-O01-C1	2.62	124.25	117.79
14	N	515	HEA	C26-C15-C16	-2.62	110.86	115.27
22	J	60	CHD	C18-C13-C17	2.61	115.30	111.21
18	N	1522	TGL	OG3-CC1-OC1	-2.61	117.00	123.59
22	P	1525	CHD	C10-C9-C8	-2.61	109.02	111.82
18	Q	1523	TGL	CG3-OG3-CC1	2.61	126.78	117.12
14	N	516	HEA	CAD-CBD-CGD	-2.61	108.30	112.67
27	M	526	DMU	C1-C2-C3	2.60	115.63	109.68
14	N	516	HEA	C27-C19-C20	2.60	119.65	115.27
24	T	1265	PEK	O03-C21-O04	-2.60	117.03	123.59
22	C	271	CHD	O7-C7-C8	2.59	115.22	109.43
19	P	1267	PGV	C27-C26-C25	-2.59	101.29	114.42
24	T	263	PEK	O03-C01-C02	2.59	115.96	108.43
14	N	515	HEA	CAA-CBA-CGA	-2.58	108.33	112.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	1522	TGL	OG1-CG1-CG2	2.58	115.94	108.43
14	N	515	HEA	C13-C14-C15	-2.58	121.45	127.66
22	J	60	CHD	C19-C10-C1	-2.58	104.11	108.26
19	A	524	PGV	O03-C19-C20	2.58	119.99	111.91
27	Z	1526	DMU	C7-C8-C9	2.58	114.83	110.24
14	N	515	HEA	C16-C15-C14	2.57	126.32	121.12
14	A	516	HEA	C3C-C4C-NC	2.57	112.53	109.21
22	W	1059	CHD	C4-C3-C2	2.56	113.61	110.55
22	C	525	CHD	C6-C7-C8	2.56	114.22	111.48
25	C	270	CDL	CA6-CA4-CA3	-2.56	105.73	111.79
27	M	526	DMU	C10-C5-C7	2.55	115.30	110.00
25	T	1269	CDL	OA8-CA7-OA9	-2.55	117.16	123.59
14	A	515	HEA	CMB-C2B-C1B	-2.54	124.56	128.46
22	C	271	CHD	C6-C5-C10	2.54	115.36	112.66
25	C	270	CDL	C39-C38-C37	2.54	127.31	114.42
24	T	1264	PEK	C24-C23-C22	-2.53	104.08	113.19
22	P	1271	CHD	C15-C14-C8	2.53	121.87	118.33
22	C	271	CHD	C9-C10-C5	2.53	112.13	108.58
14	A	515	HEA	C16-C17-C18	2.53	120.18	111.88
21	B	229	PSC	O03-C19-C20	2.52	119.81	111.91
14	N	515	HEA	C20-C21-C22	-2.52	103.61	111.88
24	T	1264	PEK	O01-C1-C2	2.52	116.92	111.50
14	A	515	HEA	C12-C11-C3B	2.52	119.16	112.56
27	Z	1526	DMU	O3-C5-C7	2.51	116.14	110.35
19	A	524	PGV	C4-C3-C2	-2.50	104.19	113.19
25	P	1270	CDL	C39-C38-C37	2.49	127.07	114.42
27	M	526	DMU	O16-C6-C1	2.49	112.19	108.30
14	A	516	HEA	C20-C19-C18	-2.49	116.08	121.12
18	Q	1523	TGL	CC3-CC2-CC1	-2.49	104.58	113.62
14	N	516	HEA	C4B-C3B-C2B	-2.48	105.13	106.87
14	A	516	HEA	C21-C22-C23	-2.48	119.28	127.75
19	N	1266	PGV	O03-C01-C02	2.47	115.62	108.43
19	C	268	PGV	O03-C19-O04	-2.46	117.38	123.59
22	C	271	CHD	C14-C13-C12	2.46	109.69	107.40
24	T	1265	PEK	C01-O03-C21	2.45	126.20	117.12
14	A	516	HEA	CMC-C2C-C3C	2.45	129.27	124.68
24	G	264	PEK	O03-C01-C02	-2.45	101.31	108.43
24	C	265	PEK	C24-C23-C22	2.44	121.95	113.19
25	C	270	CDL	OB8-CB7-OB9	-2.42	117.47	123.59
22	J	60	CHD	C14-C8-C7	2.42	115.02	111.81
25	P	1270	CDL	CB6-CB4-CB3	-2.42	106.07	111.79
24	T	1264	PEK	C30-C29-C28	-2.42	102.15	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C5-C4-C3	-2.42	109.21	112.76
25	C	270	CDL	C53-C52-C51	-2.42	104.51	113.19
19	C	267	PGV	O01-C1-C2	2.41	116.70	111.50
14	N	516	HEA	C12-C13-C14	-2.41	105.86	112.23
18	A	521	TGL	OB1-CB1-CB2	-2.40	114.36	123.73
14	A	515	HEA	C20-C21-C22	-2.40	104.00	111.88
14	N	515	HEA	C25-C23-C22	-2.40	115.72	122.65
25	P	1270	CDL	OA8-CA7-OA9	-2.40	117.55	123.59
18	N	1521	TGL	C21-C20-CA9	2.39	126.57	114.42
24	G	264	PEK	O01-C1-C2	2.38	116.63	111.50
22	G	229	CHD	O3-C3-C4	-2.38	105.11	109.85
22	C	271	CHD	C15-C14-C13	2.38	105.89	103.55
22	P	1525	CHD	C14-C8-C9	2.37	112.96	109.71
25	G	269	CDL	OB8-CB7-OB9	-2.37	117.62	123.59
18	L	522	TGL	CA8-CA7-CA6	-2.36	102.43	114.42
25	P	1270	CDL	OA4-PA1-OA3	2.36	123.91	112.24
22	C	525	CHD	C1-C2-C3	-2.35	107.44	110.47
27	Z	1526	DMU	C11-C9-C8	2.35	118.51	113.00
22	C	271	CHD	C11-C12-C13	2.33	113.64	111.24
18	N	1521	TGL	OG1-CG1-CG2	2.33	115.21	108.43
18	Q	1523	TGL	OG2-CG2-CG3	2.33	116.82	108.40
18	Q	1523	TGL	OG1-CA1-OA1	-2.32	117.73	123.59
24	G	264	PEK	C25-C24-C23	-2.32	102.64	114.42
18	N	1521	TGL	CG1-OG1-CA1	-2.31	108.56	117.12
22	P	1271	CHD	C18-C13-C14	2.31	114.83	111.21
19	P	1268	PGV	O03-C19-O04	-2.31	117.77	123.59
22	P	1271	CHD	C14-C8-C9	-2.30	106.55	109.71
18	L	522	TGL	OB1-CB1-CB2	-2.30	114.76	123.73
24	G	1263	PEK	C01-O03-C21	2.30	125.63	117.12
19	C	267	PGV	C9-C10-C11	-2.30	99.27	112.43
24	T	1264	PEK	C34-C33-C32	-2.29	102.79	114.42
19	N	1524	PGV	C4-C3-C2	-2.29	104.96	113.19
18	N	1522	TGL	C11-C10-CB9	2.29	126.04	114.42
25	P	1270	CDL	OA6-CA5-OA7	-2.29	118.18	123.70
22	P	1271	CHD	C6-C5-C10	2.28	115.08	112.66
22	C	271	CHD	C16-C17-C13	2.28	105.79	103.55
19	C	267	PGV	C4-C3-C2	-2.28	105.01	113.19
19	N	1266	PGV	O01-C1-C2	2.27	116.40	111.50
18	L	522	TGL	CB4-CB3-CB2	-2.27	105.03	113.19
22	J	60	CHD	C17-C13-C12	2.27	119.74	117.67
22	B	1085	CHD	C14-C8-C7	2.27	114.81	111.81
18	A	521	TGL	OG1-CA1-CA2	2.26	119.01	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	521	TGL	CB7-CB6-CB5	-2.26	102.93	114.42
24	T	263	PEK	C01-O03-C21	2.26	125.49	117.12
24	G	264	PEK	C27-C26-C25	-2.26	102.96	114.42
18	N	1522	TGL	OA1-CA1-CA2	-2.25	114.94	123.73
25	T	1269	CDL	C82-C81-C80	2.24	125.80	114.42
22	P	1525	CHD	C6-C5-C4	-2.24	108.61	111.19
22	W	1059	CHD	C23-C22-C20	-2.24	111.71	114.72
25	G	269	CDL	C83-C82-C81	2.23	125.77	114.42
27	M	526	DMU	O3-C5-C7	2.23	115.52	110.35
22	B	1085	CHD	O3-C3-C4	-2.23	105.41	109.85
27	Z	1526	DMU	C10-C5-C7	2.22	114.62	110.00
19	P	1268	PGV	O02-C1-C2	-2.22	115.08	123.73
14	A	515	HEA	C25-C23-C22	-2.22	116.24	122.65
19	C	267	PGV	C8-C9-C10	-2.22	104.14	113.79
14	N	515	HEA	CAD-CBD-CGD	-2.21	108.95	112.67
18	N	1522	TGL	CG3-OG3-CC1	2.21	125.31	117.12
21	B	229	PSC	O01-C1-O02	-2.21	118.36	123.70
24	G	1263	PEK	O03-C21-O04	-2.19	118.06	123.59
22	P	1271	CHD	C23-C22-C20	-2.19	111.77	114.72
18	D	523	TGL	OG1-CA1-OA1	-2.18	118.08	123.59
18	N	1522	TGL	CC3-CC2-CC1	2.18	121.56	113.62
25	G	269	CDL	OA8-CA7-OA9	-2.18	118.09	123.59
18	N	1521	TGL	CB7-CB6-CB5	-2.17	103.41	114.42
19	C	268	PGV	O02-C1-C2	-2.17	115.28	123.73
24	T	1265	PEK	O03-C01-C02	2.16	114.73	108.43
18	A	521	TGL	CB3-CB2-CB1	-2.16	105.76	113.62
18	L	522	TGL	OG1-CG1-CG2	2.16	114.72	108.43
18	N	1521	TGL	CA3-CA2-CA1	-2.16	105.77	113.62
18	N	1522	TGL	OG2-CG2-CG1	2.15	116.20	108.40
19	A	524	PGV	O03-C01-C02	2.15	114.70	108.43
14	N	516	HEA	C13-C12-C11	-2.15	111.11	114.35
25	C	270	CDL	C40-C39-C38	2.15	125.34	114.42
19	P	1268	PGV	C03-C02-C01	-2.14	106.72	111.79
18	L	522	TGL	OG2-CG2-CG1	2.14	116.16	108.40
25	T	1269	CDL	C83-C82-C81	2.14	125.29	114.42
18	L	522	TGL	C15-CC9-CC8	2.14	125.26	114.42
25	C	270	CDL	C57-C56-C55	-2.13	103.61	114.42
25	C	270	CDL	C42-C41-C40	2.13	125.21	114.42
24	G	264	PEK	C32-C31-C30	-2.12	103.65	114.42
18	N	1522	TGL	C25-C24-C23	-2.11	103.69	114.42
22	W	1059	CHD	C16-C17-C20	2.11	115.41	112.15
22	G	229	CHD	C18-C13-C14	2.11	114.51	111.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	270	CDL	OA6-CA5-OA7	-2.11	118.61	123.70
24	T	1264	PEK	C28-C27-C26	-2.10	103.75	114.42
25	P	1270	CDL	C40-C39-C38	2.10	125.10	114.42
25	P	1270	CDL	C53-C52-C51	-2.10	105.63	113.19
27	M	526	DMU	C57-C4-C3	2.10	119.44	113.33
18	Q	1523	TGL	C11-C10-CB9	2.09	125.06	114.42
18	A	521	TGL	C21-C20-CA9	2.09	125.04	114.42
14	N	516	HEA	CBD-CAD-C3D	2.09	116.34	112.49
22	G	229	CHD	C11-C9-C8	2.08	113.92	110.88
22	J	60	CHD	C21-C20-C17	-2.08	109.73	112.92
22	B	1085	CHD	C13-C17-C20	-2.07	117.02	119.50
25	P	1270	CDL	C42-C41-C40	2.07	124.93	114.42
14	N	515	HEA	CMC-C2C-C3C	2.07	128.55	124.68
22	G	229	CHD	C5-C6-C7	2.07	116.74	114.46
22	P	1525	CHD	C16-C15-C14	-2.07	101.04	105.13
14	A	516	HEA	C27-C19-C20	2.06	118.74	115.27
18	Q	1523	TGL	OG1-CG1-CG2	2.06	114.43	108.43
18	N	1522	TGL	C15-CC9-CC8	2.06	124.87	114.42
19	P	1267	PGV	C25-C24-C23	-2.06	103.99	114.42
24	T	1264	PEK	C01-O03-C21	2.05	124.72	117.12
19	C	267	PGV	O03-C19-O04	-2.05	118.42	123.59
27	Z	1526	DMU	C10-O1-C9	-2.04	109.68	113.69
14	N	516	HEA	O11-C11-C3B	-2.03	106.13	112.00
18	Q	1523	TGL	C21-C20-CA9	2.03	124.73	114.42
22	G	229	CHD	C13-C14-C8	-2.03	112.15	114.74
19	P	1267	PGV	C4-C3-C2	-2.03	105.91	113.19
19	A	524	PGV	C02-O01-C1	2.02	122.77	117.79
19	P	1267	PGV	C8-C9-C10	-2.01	105.03	113.79
27	M	526	DMU	C6-C1-C2	2.01	114.17	110.00
22	C	271	CHD	C5-C4-C3	-2.00	109.81	112.76

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	Z	1526	DMU	C2
27	Z	1526	DMU	C3
27	Z	1526	DMU	C5
27	Z	1526	DMU	C4
14	A	516	HEA	ND
14	A	516	HEA	NB
14	N	515	HEA	ND
14	N	515	HEA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
14	N	515	HEA	NB
27	M	526	DMU	C2
27	M	526	DMU	C5
14	A	515	HEA	ND
14	A	515	HEA	NB
14	N	516	HEA	ND
14	N	516	HEA	NB

All (953) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	T	1265	PEK	C04-O12-P-O11
24	T	1265	PEK	C04-O12-P-O13
24	T	1265	PEK	C04-O12-P-O14
24	T	1265	PEK	C10-C11-C12-C13
24	T	1265	PEK	C13-C14-C15-C16
24	C	265	PEK	C5-C6-C7-C8
24	C	265	PEK	C10-C11-C12-C13
19	P	1268	PGV	C04-O12-P-O14
19	P	1268	PGV	C04-C05-C06-O06
19	P	1268	PGV	C2-C1-O01-C02
19	P	1268	PGV	C10-C11-C12-C13
19	A	524	PGV	C04-O12-P-O13
19	A	524	PGV	C04-O12-P-O14
19	A	524	PGV	C02-C03-O11-P
19	A	524	PGV	O02-C1-O01-C02
25	C	270	CDL	CA2-OA2-PA1-OA3
25	C	270	CDL	CA2-OA2-PA1-OA4
25	C	270	CDL	CA2-OA2-PA1-OA5
25	C	270	CDL	CA3-OA5-PA1-OA2
25	C	270	CDL	CA3-OA5-PA1-OA3
25	C	270	CDL	CA4-CA3-OA5-PA1
25	C	270	CDL	C11-CA5-OA6-CA4
25	C	270	CDL	CB2-OB2-PB2-OB3
25	C	270	CDL	CB2-OB2-PB2-OB4
19	N	1524	PGV	C04-O12-P-O11
19	N	1524	PGV	C04-O12-P-O13
19	N	1524	PGV	C04-O12-P-O14
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	O12-C04-C05-C06
19	N	1524	PGV	C04-C05-C06-O06
19	N	1524	PGV	O05-C05-C06-O06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	O02-C1-O01-C02
22	W	1059	CHD	C13-C17-C20-C22
22	W	1059	CHD	C16-C17-C20-C22
18	Q	1523	TGL	OC1-CC1-OG3-CG3
24	G	264	PEK	C10-C11-C12-C13
25	G	269	CDL	CB2-C1-CA2-OA2
25	G	269	CDL	CA2-C1-CB2-OB2
25	G	269	CDL	CA2-OA2-PA1-OA3
25	G	269	CDL	C11-CA5-OA6-CA4
25	G	269	CDL	C1-CB2-OB2-PB2
25	G	269	CDL	CB3-OB5-PB2-OB3
25	G	269	CDL	CB3-OB5-PB2-OB4
25	P	1270	CDL	CA2-C1-CB2-OB2
25	P	1270	CDL	CA2-OA2-PA1-OA3
25	P	1270	CDL	C11-CA5-OA6-CA4
25	P	1270	CDL	CB2-OB2-PB2-OB3
25	P	1270	CDL	CB2-OB2-PB2-OB4
24	T	263	PEK	C03-O11-P-O13
24	T	263	PEK	C03-O11-P-O14
24	T	263	PEK	O03-C01-C02-O01
24	T	263	PEK	O12-C04-C05-N
24	T	263	PEK	C7-C8-C9-C10
24	T	263	PEK	C12-C13-C14-C15
27	M	526	DMU	O5-C6-O16-C18
19	C	268	PGV	C04-O12-P-O14
19	C	268	PGV	O12-C04-C05-C06
19	C	268	PGV	C04-C05-C06-O06
24	G	1263	PEK	C03-O11-P-O14
24	G	1263	PEK	O03-C01-C02-O01
24	G	1263	PEK	O12-C04-C05-N
21	B	229	PSC	C03-O11-P-O14
21	B	229	PSC	C04-O12-P-O14
14	N	516	HEA	O11-C11-C12-C13
21	O	1229	PSC	C03-O11-P-O14
21	O	1229	PSC	C04-O12-P-O11
21	O	1229	PSC	C04-O12-P-O13
21	O	1229	PSC	C04-O12-P-O14
21	O	1229	PSC	O12-C04-C05-N
21	O	1229	PSC	C11-C10-C9-C8
21	O	1229	PSC	C11-C12-C13-C14
25	T	1269	CDL	C1-CB2-OB2-PB2
25	T	1269	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	CB3-OB5-PB2-OB4
25	T	1269	CDL	OB6-CB4-CB6-OB8
19	A	524	PGV	O04-C19-O03-C01
18	D	523	TGL	OC1-CC1-OG3-CG3
19	A	524	PGV	C20-C19-O03-C01
18	D	523	TGL	CC2-CC1-OG3-CG3
18	N	1522	TGL	OA1-CA1-OG1-CG1
19	N	1524	PGV	O04-C19-O03-C01
25	T	1269	CDL	OA9-CA7-OA8-CA6
18	A	521	TGL	OB1-CB1-OG2-CG2
19	P	1268	PGV	O02-C1-O01-C02
25	G	269	CDL	OA7-CA5-OA6-CA4
25	P	1270	CDL	OA7-CA5-OA6-CA4
25	T	1269	CDL	OA7-CA5-OA6-CA4
19	N	1524	PGV	C20-C19-O03-C01
18	Q	1523	TGL	CA2-CA1-OG1-CG1
25	G	269	CDL	C31-CA7-OA8-CA6
19	A	524	PGV	C2-C1-O01-C02
19	N	1524	PGV	C2-C1-O01-C02
25	T	1269	CDL	C11-CA5-OA6-CA4
22	J	60	CHD	C16-C17-C20-C22
18	Q	1523	TGL	CC2-CC1-OG3-CG3
18	N	1521	TGL	CA2-CA1-OG1-CG1
21	B	229	PSC	C20-C19-O03-C01
25	T	1269	CDL	C31-CA7-OA8-CA6
24	T	1265	PEK	C4-C5-C6-C7
24	T	1265	PEK	C7-C8-C9-C10
24	C	265	PEK	C4-C5-C6-C7
24	C	265	PEK	C7-C8-C9-C10
24	C	265	PEK	C13-C14-C15-C16
24	G	264	PEK	C13-C14-C15-C16
24	T	263	PEK	C4-C5-C6-C7
24	T	263	PEK	C10-C11-C12-C13
24	T	1264	PEK	C7-C8-C9-C10
24	G	1263	PEK	C4-C5-C6-C7
24	G	1263	PEK	C7-C8-C9-C10
21	B	229	PSC	C11-C10-C9-C8
21	O	1229	PSC	C22-C23-C24-C25
25	G	269	CDL	C40-C41-C42-C43
25	C	270	CDL	OA7-CA5-OA6-CA4
19	C	268	PGV	O02-C1-O01-C02
25	G	269	CDL	OA9-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	521	TGL	C21-C20-CA9-CA8
22	W	1059	CHD	C16-C17-C20-C21
25	G	269	CDL	O1-C1-CA2-OA2
25	T	1269	CDL	O1-C1-CA2-OA2
18	N	1522	TGL	CA2-CA1-OG1-CG1
18	L	522	TGL	CA2-CA1-OG1-CG1
21	O	1229	PSC	C20-C19-O03-C01
25	G	269	CDL	C77-C78-C79-C80
18	Q	1523	TGL	OA1-CA1-OG1-CG1
18	A	521	TGL	CB2-CB1-OG2-CG2
19	C	268	PGV	C2-C1-O01-C02
18	Q	1523	TGL	C16-C15-CC9-CC8
18	L	522	TGL	CC2-CC3-CC4-CC5
25	T	1269	CDL	C22-C23-C24-C25
25	C	270	CDL	C17-C18-C19-C20
18	Q	1523	TGL	C11-C10-CB9-CB8
18	N	1521	TGL	C21-C20-CA9-CA8
18	D	523	TGL	C16-C15-CC9-CC8
25	P	1270	CDL	C79-C80-C81-C82
18	D	523	TGL	CA2-CA1-OG1-CG1
18	N	1521	TGL	OA1-CA1-OG1-CG1
18	Q	1523	TGL	C21-C20-CA9-CA8
25	G	269	CDL	C22-C23-C24-C25
22	C	271	CHD	C21-C20-C22-C23
22	P	1271	CHD	C21-C20-C22-C23
21	B	229	PSC	O04-C19-O03-C01
21	O	1229	PSC	O04-C19-O03-C01
14	N	515	HEA	C15-C16-C17-C18
14	A	515	HEA	C15-C16-C17-C18
18	L	522	TGL	C21-C20-CA9-CA8
21	B	229	PSC	C20-C21-C22-C23
21	O	1229	PSC	C20-C21-C22-C23
22	J	60	CHD	C13-C17-C20-C22
22	C	271	CHD	C17-C20-C22-C23
22	P	1271	CHD	C17-C20-C22-C23
18	L	522	TGL	OA1-CA1-OG1-CG1
19	P	1268	PGV	O12-C04-C05-C06
19	A	524	PGV	O12-C04-C05-C06
25	C	270	CDL	CB2-C1-CA2-OA2
18	N	1521	TGL	OB1-CB1-OG2-CG2
18	D	523	TGL	OA1-CA1-OG1-CG1
18	A	521	TGL	CA2-CA1-OG1-CG1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	J	60	CHD	C13-C17-C20-C21
25	G	269	CDL	C57-C58-C59-C60
25	T	1269	CDL	C60-C61-C62-C63
25	T	1269	CDL	C79-C80-C81-C82
27	Z	1526	DMU	O6-C11-C9-C8
19	A	524	PGV	O12-C04-C05-O05
25	P	1270	CDL	O1-C1-CB2-OB2
19	C	268	PGV	O12-C04-C05-O05
18	A	521	TGL	OA1-CA1-OG1-CG1
18	N	1521	TGL	CC5-CC6-CC7-CC8
25	T	1269	CDL	C73-C74-C75-C76
21	B	229	PSC	O02-C1-O01-C02
18	N	1521	TGL	CB2-CB1-OG2-CG2
21	B	229	PSC	C2-C1-O01-C02
18	N	1522	TGL	CC2-CC3-CC4-CC5
27	Z	1526	DMU	C3-C4-C57-O61
19	P	1268	PGV	C1-C2-C3-C4
22	W	1059	CHD	C17-C20-C22-C23
18	D	523	TGL	C21-C22-C23-C24
25	T	1269	CDL	C15-C16-C17-C18
27	M	526	DMU	O5-C4-C57-O61
19	C	268	PGV	C20-C19-O03-C01
21	O	1229	PSC	C1-C2-C3-C4
24	G	264	PEK	C7-C8-C9-C10
19	P	1267	PGV	C10-C11-C12-C13
25	P	1270	CDL	C17-C18-C19-C20
19	C	268	PGV	O05-C05-C06-O06
24	G	264	PEK	C1-C2-C3-C4
25	G	269	CDL	CA5-C11-C12-C13
25	P	1270	CDL	CB7-C71-C72-C73
24	T	1264	PEK	C1-C2-C3-C4
21	B	229	PSC	C1-C2-C3-C4
25	T	1269	CDL	CA5-C11-C12-C13
27	M	526	DMU	O6-C11-C9-C8
27	M	526	DMU	O16-C18-C19-C22
19	A	524	PGV	C19-C20-C21-C22
18	Q	1523	TGL	CA1-CA2-CA3-CA4
25	P	1270	CDL	CA5-C11-C12-C13
18	N	1522	TGL	C21-C20-CA9-CA8
22	J	60	CHD	C16-C17-C20-C21
18	N	1521	TGL	CG2-CG3-OG3-CC1
25	C	270	CDL	CB7-C71-C72-C73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	521	TGL	C22-C23-C24-C25
19	P	1268	PGV	O12-C04-C05-O05
25	C	270	CDL	O1-C1-CA2-OA2
25	C	270	CDL	O1-C1-CB2-OB2
19	N	1524	PGV	O12-C04-C05-O05
25	G	269	CDL	O1-C1-CB2-OB2
25	T	1269	CDL	O1-C1-CB2-OB2
25	T	1269	CDL	C40-C41-C42-C43
22	W	1059	CHD	C13-C17-C20-C21
19	C	268	PGV	O04-C19-O03-C01
24	G	264	PEK	C4-C5-C6-C7
24	T	263	PEK	C13-C14-C15-C16
21	B	229	PSC	C11-C12-C13-C14
18	D	523	TGL	C11-C10-CB9-CB8
24	C	265	PEK	C04-O12-P-O11
19	P	1268	PGV	C04-O12-P-O11
19	A	524	PGV	C04-O12-P-O11
25	C	270	CDL	CB2-OB2-PB2-OB5
25	G	269	CDL	CA2-OA2-PA1-OA5
25	G	269	CDL	CB3-OB5-PB2-OB2
25	P	1270	CDL	CA2-OA2-PA1-OA5
25	P	1270	CDL	CA3-OA5-PA1-OA2
25	P	1270	CDL	CB2-OB2-PB2-OB5
24	T	263	PEK	C03-O11-P-O12
19	C	268	PGV	C04-O12-P-O11
24	G	1263	PEK	C03-O11-P-O12
21	B	229	PSC	C04-O12-P-O11
21	O	1229	PSC	C03-O11-P-O12
25	T	1269	CDL	CB3-OB5-PB2-OB2
18	A	521	TGL	CC2-CC1-OG3-CG3
27	Z	1526	DMU	O16-C18-C19-C22
25	C	270	CDL	CA2-C1-CB2-OB2
25	T	1269	CDL	CA2-C1-CB2-OB2
25	P	1270	CDL	OB7-CB5-OB6-CB4
21	O	1229	PSC	C04-C05-N-C06
19	P	1267	PGV	C11-C10-C9-C8
19	A	524	PGV	C4-C5-C6-C7
19	N	1524	PGV	C4-C5-C6-C7
19	A	522	PGV	C6-C7-C8-C9
25	P	1270	CDL	C37-C38-C39-C40
27	M	526	DMU	C25-C28-C31-C34
25	P	1270	CDL	C51-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	N	1522	TGL	C17-C18-C19-C33
25	G	269	CDL	C72-C73-C74-C75
25	P	1270	CDL	C51-C52-C53-C54
25	P	1270	CDL	C74-C75-C76-C77
18	N	1522	TGL	CC6-CC7-CC8-CC9
18	Q	1523	TGL	CC6-CC7-CC8-CC9
25	G	269	CDL	C82-C83-C84-C85
24	T	263	PEK	C34-C35-C36-C37
18	N	1521	TGL	CA5-CA6-CA7-CA8
21	O	1229	PSC	C2-C3-C4-C5
18	N	1522	TGL	OB1-CB1-OG2-CG2
21	O	1229	PSC	O02-C1-O01-C02
18	D	523	TGL	CB1-CB2-CB3-CB4
25	C	270	CDL	C18-C19-C20-C21
18	L	522	TGL	C22-C23-C24-C25
19	P	1268	PGV	C24-C25-C26-C27
18	N	1522	TGL	C20-C21-C22-C23
25	C	270	CDL	C76-C77-C78-C79
18	Q	1523	TGL	CC4-CC5-CC6-CC7
18	Q	1523	TGL	CA9-C20-C21-C22
18	L	522	TGL	C12-C13-C14-C29
21	B	229	PSC	C26-C27-C28-C29
19	C	267	PGV	C30-C31-C32-C33
18	D	523	TGL	CC4-CC5-CC6-CC7
24	T	1265	PEK	C25-C26-C27-C28
27	Z	1526	DMU	C2-C3-O7-C10
19	P	1268	PGV	C22-C23-C24-C25
18	Q	1523	TGL	CB5-CB6-CB7-CB8
24	T	1264	PEK	C23-C24-C25-C26
27	Z	1526	DMU	C25-C28-C31-C34
25	C	270	CDL	C72-C73-C74-C75
25	C	270	CDL	C73-C74-C75-C76
19	N	1524	PGV	C24-C25-C26-C27
25	G	269	CDL	C20-C21-C22-C23
25	G	269	CDL	C39-C40-C41-C42
25	P	1270	CDL	C76-C77-C78-C79
25	P	1270	CDL	C82-C83-C84-C85
24	T	1264	PEK	C24-C25-C26-C27
24	G	1263	PEK	C29-C30-C31-C32
21	B	229	PSC	C27-C28-C29-C30
19	C	267	PGV	C7-C8-C9-C10
25	T	1269	CDL	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C54-C55-C56-C57
19	N	1524	PGV	C28-C29-C30-C31
18	Q	1523	TGL	C17-C18-C19-C33
24	G	264	PEK	C22-C23-C24-C25
18	N	1521	TGL	CA4-CA5-CA6-CA7
19	C	267	PGV	C24-C25-C26-C27
19	N	1266	PGV	C6-C7-C8-C9
19	N	1266	PGV	C7-C8-C9-C10
19	N	1266	PGV	C23-C24-C25-C26
18	A	521	TGL	C16-C17-C18-C19
25	C	270	CDL	C42-C43-C44-C45
25	C	270	CDL	C74-C75-C76-C77
18	Q	1523	TGL	CB2-CB3-CB4-CB5
25	P	1270	CDL	C72-C73-C74-C75
18	L	522	TGL	CA7-CA8-CA9-C20
19	C	268	PGV	C24-C25-C26-C27
19	C	268	PGV	C27-C28-C29-C30
19	N	1266	PGV	C5-C6-C7-C8
25	T	1269	CDL	C13-C14-C15-C16
25	T	1269	CDL	C20-C21-C22-C23
18	A	521	TGL	CB3-CB4-CB5-CB6
18	N	1522	TGL	C10-C11-C12-C13
19	A	522	PGV	C26-C27-C28-C29
25	G	269	CDL	C13-C14-C15-C16
21	O	1229	PSC	C2-C1-O01-C02
18	A	521	TGL	CA5-CA6-CA7-CA8
18	A	521	TGL	C15-C16-C17-C18
18	N	1522	TGL	CB4-CB5-CB6-CB7
25	C	270	CDL	C61-C62-C63-C64
25	C	270	CDL	C82-C83-C84-C85
25	G	269	CDL	C62-C63-C64-C65
25	P	1270	CDL	C61-C62-C63-C64
24	T	263	PEK	C29-C30-C31-C32
21	B	229	PSC	C2-C3-C4-C5
25	T	1269	CDL	C72-C73-C74-C75
19	C	268	PGV	C12-C13-C14-C15
25	C	270	CDL	CA5-C11-C12-C13
19	N	1524	PGV	C19-C20-C21-C22
18	Q	1523	TGL	CB1-CB2-CB3-CB4
18	A	521	TGL	C11-C10-CB9-CB8
19	P	1268	PGV	C13-C14-C15-C16
19	P	1268	PGV	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	524	PGV	C22-C23-C24-C25
25	C	270	CDL	C51-C52-C53-C54
25	C	270	CDL	C71-C72-C73-C74
18	Q	1523	TGL	CC3-CC4-CC5-CC6
19	A	522	PGV	C7-C8-C9-C10
19	A	522	PGV	C23-C24-C25-C26
24	G	264	PEK	C31-C32-C33-C34
25	G	269	CDL	C43-C44-C45-C46
25	P	1270	CDL	C58-C59-C60-C61
25	P	1270	CDL	C59-C60-C61-C62
18	L	522	TGL	CB4-CB5-CB6-CB7
18	L	522	TGL	C11-C10-CB9-CB8
24	T	1264	PEK	C26-C27-C28-C29
24	G	1263	PEK	C34-C35-C36-C37
21	B	229	PSC	C24-C25-C26-C27
21	O	1229	PSC	C04-C05-N-C07
18	A	521	TGL	CG2-CG3-OG3-CC1
24	T	1265	PEK	C16-C17-C18-C19
25	C	270	CDL	C36-C37-C38-C39
18	L	522	TGL	C21-C22-C23-C24
24	T	263	PEK	C27-C28-C29-C30
18	D	523	TGL	CB5-CB6-CB7-CB8
25	T	1269	CDL	C43-C44-C45-C46
25	T	1269	CDL	C59-C60-C61-C62
24	C	265	PEK	O12-C04-C05-N
18	A	521	TGL	CA3-CA4-CA5-CA6
19	P	1268	PGV	C5-C6-C7-C8
18	N	1521	TGL	C11-C10-CB9-CB8
18	A	521	TGL	CB1-CB2-CB3-CB4
18	A	521	TGL	CA4-CA5-CA6-CA7
22	C	271	CHD	C20-C22-C23-C24
22	P	1271	CHD	C20-C22-C23-C24
25	P	1270	CDL	C71-C72-C73-C74
18	D	523	TGL	CB6-CB7-CB8-CB9
18	D	523	TGL	CA9-C20-C21-C22
25	T	1269	CDL	C38-C39-C40-C41
25	C	270	CDL	C13-C14-C15-C16
19	C	268	PGV	C26-C27-C28-C29
18	D	523	TGL	CC2-CC3-CC4-CC5
18	N	1522	TGL	CA7-CA8-CA9-C20
18	N	1522	TGL	CC9-C15-C16-C17
18	N	1522	TGL	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	270	CDL	C38-C39-C40-C41
25	P	1270	CDL	C38-C39-C40-C41
25	P	1270	CDL	C73-C74-C75-C76
18	L	522	TGL	CC9-C15-C16-C17
18	A	521	TGL	OC1-CC1-OG3-CG3
18	N	1522	TGL	C24-C25-C26-C27
25	P	1270	CDL	C41-C42-C43-C44
24	T	263	PEK	C25-C26-C27-C28
19	P	1267	PGV	C13-C14-C15-C16
18	D	523	TGL	CB9-C10-C11-C12
24	G	1263	PEK	C13-C14-C15-C16
27	Z	1526	DMU	C22-C25-C28-C31
18	L	522	TGL	CA5-CA6-CA7-CA8
18	L	522	TGL	C17-C18-C19-C33
24	G	1263	PEK	C27-C28-C29-C30
18	L	522	TGL	C24-C25-C26-C27
18	N	1522	TGL	CB2-CB1-OG2-CG2
27	M	526	DMU	C22-C25-C28-C31
21	O	1229	PSC	C24-C25-C26-C27
19	P	1268	PGV	O05-C05-C06-O06
18	N	1522	TGL	C16-C15-CC9-CC8
25	C	270	CDL	C41-C42-C43-C44
25	P	1270	CDL	C42-C43-C44-C45
19	P	1267	PGV	C30-C31-C32-C33
21	B	229	PSC	C29-C30-C31-C32
18	D	523	TGL	CA6-CA7-CA8-CA9
25	T	1269	CDL	C77-C78-C79-C80
24	G	264	PEK	C2-C3-C4-C5
19	C	268	PGV	C11-C10-C9-C8
19	P	1267	PGV	C12-C13-C14-C15
18	N	1521	TGL	CA3-CA4-CA5-CA6
25	P	1270	CDL	C81-C82-C83-C84
18	N	1521	TGL	C18-C19-C33-C34
19	P	1267	PGV	C7-C8-C9-C10
19	C	267	PGV	C29-C30-C31-C32
18	N	1522	TGL	CB5-CB6-CB7-CB8
25	T	1269	CDL	C16-C17-C18-C19
18	A	521	TGL	C14-C29-C30-C31
25	G	269	CDL	C79-C80-C81-C82
25	P	1270	CDL	C16-C17-C18-C19
18	L	522	TGL	CC5-CC6-CC7-CC8
18	N	1521	TGL	CB3-CB4-CB5-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	N	1521	TGL	CB6-CB7-CB8-CB9
19	C	268	PGV	C3-C4-C5-C6
19	C	268	PGV	C22-C23-C24-C25
19	P	1267	PGV	C28-C29-C30-C31
21	O	1229	PSC	C04-C05-N-C08
18	N	1521	TGL	CB1-CB2-CB3-CB4
18	N	1522	TGL	CA5-CA6-CA7-CA8
25	C	270	CDL	C23-C24-C25-C26
18	D	523	TGL	CB3-CB4-CB5-CB6
25	G	269	CDL	C71-CB7-OB8-CB6
25	C	270	CDL	C51-CB5-OB6-CB4
18	L	522	TGL	CB2-CB1-OG2-CG2
18	N	1522	TGL	C21-C22-C23-C24
21	O	1229	PSC	C27-C28-C29-C30
24	G	264	PEK	C16-C17-C18-C19
21	B	229	PSC	C23-C24-C25-C26
19	C	268	PGV	C13-C14-C15-C16
19	N	1266	PGV	C29-C30-C31-C32
25	G	269	CDL	OB9-CB7-OB8-CB6
19	A	524	PGV	C24-C25-C26-C27
25	G	269	CDL	C36-C37-C38-C39
25	P	1270	CDL	C18-C19-C20-C21
18	L	522	TGL	CC6-CC7-CC8-CC9
24	C	265	PEK	C15-C16-C17-C18
19	P	1268	PGV	C11-C10-C9-C8
18	Q	1523	TGL	CB6-CB7-CB8-CB9
25	P	1270	CDL	C75-C76-C77-C78
24	G	1263	PEK	C25-C26-C27-C28
18	A	521	TGL	CB6-CB7-CB8-CB9
25	P	1270	CDL	C13-C14-C15-C16
25	P	1270	CDL	C36-C37-C38-C39
24	T	263	PEK	C30-C31-C32-C33
18	N	1521	TGL	C17-C18-C19-C33
25	G	269	CDL	C78-C79-C80-C81
18	N	1521	TGL	CB4-CB5-CB6-CB7
18	D	523	TGL	C10-C11-C12-C13
25	C	270	CDL	C16-C17-C18-C19
25	C	270	CDL	C77-C78-C79-C80
18	L	522	TGL	C10-C11-C12-C13
27	Z	1526	DMU	O5-C6-O16-C18
24	C	265	PEK	C25-C26-C27-C28
24	T	1264	PEK	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	C	267	PGV	C13-C14-C15-C16
18	D	523	TGL	CB2-CB3-CB4-CB5
19	P	1268	PGV	C4-C5-C6-C7
18	L	522	TGL	OB1-CB1-OG2-CG2
18	Q	1523	TGL	CB7-CB8-CB9-C10
25	G	269	CDL	C61-C62-C63-C64
25	G	269	CDL	OB6-CB4-CB6-OB8
25	C	270	CDL	C58-C59-C60-C61
25	G	269	CDL	C53-C54-C55-C56
18	N	1521	TGL	C14-C29-C30-C31
24	T	1265	PEK	C15-C16-C17-C18
19	N	1266	PGV	C12-C13-C14-C15
25	T	1269	CDL	C41-C42-C43-C44
18	Q	1523	TGL	CC2-CC3-CC4-CC5
19	A	522	PGV	C25-C26-C27-C28
24	G	1263	PEK	C30-C31-C32-C33
24	C	265	PEK	C29-C30-C31-C32
18	N	1522	TGL	CC4-CC5-CC6-CC7
18	D	523	TGL	C19-C33-C34-C35
18	N	1521	TGL	OC1-CC1-OG3-CG3
25	C	270	CDL	OB7-CB5-OB6-CB4
19	N	1524	PGV	C22-C23-C24-C25
25	G	269	CDL	C73-C74-C75-C76
24	T	263	PEK	C33-C34-C35-C36
18	Q	1523	TGL	CB9-C10-C11-C12
24	G	264	PEK	C23-C24-C25-C26
19	A	524	PGV	C05-C04-O12-P
24	C	265	PEK	C34-C35-C36-C37
18	N	1521	TGL	C13-C14-C29-C30
18	N	1521	TGL	CC2-CC1-OG3-CG3
25	C	270	CDL	OA5-CA3-CA4-CA6
25	C	270	CDL	OB5-CB3-CB4-CB6
25	G	269	CDL	OA5-CA3-CA4-CA6
25	P	1270	CDL	OA5-CA3-CA4-CA6
18	N	1521	TGL	C16-C17-C18-C19
19	C	268	PGV	C25-C26-C27-C28
19	C	268	PGV	C28-C29-C30-C31
25	P	1270	CDL	C15-C16-C17-C18
25	P	1270	CDL	C23-C24-C25-C26
24	T	1264	PEK	C2-C3-C4-C5
24	G	1263	PEK	C2-C3-C4-C5
19	P	1268	PGV	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	Q	1523	TGL	C16-C17-C18-C19
24	G	1263	PEK	C22-C21-O03-C01
19	P	1268	PGV	C30-C31-C32-C33
25	C	270	CDL	C59-C60-C61-C62
25	G	269	CDL	C55-C56-C57-C58
19	C	267	PGV	C28-C29-C30-C31
21	O	1229	PSC	C21-C22-C23-C24
19	P	1268	PGV	C14-C15-C16-C17
18	L	522	TGL	CB5-CB6-CB7-CB8
18	A	521	TGL	C13-C14-C29-C30
19	P	1268	PGV	C25-C26-C27-C28
18	L	522	TGL	C11-C12-C13-C14
21	O	1229	PSC	C29-C30-C31-C32
19	N	1524	PGV	O03-C01-C02-C03
19	N	1524	PGV	C14-C15-C16-C17
25	P	1270	CDL	CA3-CA4-CA6-OA8
25	P	1270	CDL	CB3-CB4-CB6-OB8
24	T	263	PEK	O03-C01-C02-C03
24	G	1263	PEK	O03-C01-C02-C03
25	T	1269	CDL	CB3-CB4-CB6-OB8
24	T	1264	PEK	C13-C14-C15-C16
19	P	1268	PGV	C31-C32-C33-C34
18	L	522	TGL	CC1-CC2-CC3-CC4
19	P	1267	PGV	C31-C32-C33-C34
25	C	270	CDL	C37-C38-C39-C40
19	A	522	PGV	C5-C6-C7-C8
25	G	269	CDL	C80-C81-C82-C83
25	C	270	CDL	C44-C45-C46-C47
18	Q	1523	TGL	C12-C13-C14-C29
25	P	1270	CDL	C44-C45-C46-C47
25	T	1269	CDL	C44-C45-C46-C47
19	A	524	PGV	C2-C3-C4-C5
18	D	523	TGL	CC3-CC4-CC5-CC6
24	G	1263	PEK	O04-C21-O03-C01
24	T	263	PEK	C26-C27-C28-C29
25	T	1269	CDL	C56-C57-C58-C59
19	P	1268	PGV	C15-C16-C17-C18
19	N	1524	PGV	C2-C3-C4-C5
19	P	1267	PGV	C15-C16-C17-C18
18	N	1522	TGL	CB6-CB7-CB8-CB9
24	G	1263	PEK	C28-C29-C30-C31
19	A	524	PGV	C03-C02-O01-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C5-C6-C7-C8
19	C	268	PGV	C31-C32-C33-C34
19	C	267	PGV	C15-C16-C17-C18
25	G	269	CDL	C15-C16-C17-C18
25	P	1270	CDL	C80-C81-C82-C83
18	N	1521	TGL	CB9-C10-C11-C12
25	T	1269	CDL	C18-C19-C20-C21
24	G	264	PEK	C22-C21-O03-C01
19	C	268	PGV	C10-C11-C12-C13
24	G	1263	PEK	C10-C11-C12-C13
19	C	267	PGV	C10-C11-C12-C13
18	D	523	TGL	CA5-CA6-CA7-CA8
25	T	1269	CDL	C71-C72-C73-C74
18	Q	1523	TGL	C24-C25-C26-C27
19	A	524	PGV	C11-C10-C9-C8
18	A	521	TGL	CA6-CA7-CA8-CA9
18	A	521	TGL	OG1-CG1-CG2-OG2
21	B	229	PSC	O03-C01-C02-O01
18	N	1522	TGL	C11-C10-CB9-CB8
24	T	1265	PEK	C29-C30-C31-C32
25	C	270	CDL	C84-C85-C86-C87
24	T	1264	PEK	C3-C4-C5-C6
25	C	270	CDL	C11-C12-C13-C14
18	Q	1523	TGL	C21-C22-C23-C24
25	P	1270	CDL	C24-C25-C26-C27
22	W	1059	CHD	C21-C20-C22-C23
18	N	1522	TGL	CB7-CB8-CB9-C10
18	A	521	TGL	CC6-CC7-CC8-CC9
19	A	524	PGV	C31-C32-C33-C34
18	Q	1523	TGL	CB3-CB4-CB5-CB6
19	N	1266	PGV	C26-C27-C28-C29
25	T	1269	CDL	C31-C32-C33-C34
18	L	522	TGL	C16-C15-CC9-CC8
25	C	270	CDL	C15-C16-C17-C18
19	A	522	PGV	C31-C32-C33-C34
19	C	268	PGV	C14-C15-C16-C17
18	Q	1523	TGL	C19-C33-C34-C35
18	L	522	TGL	CC4-CC5-CC6-CC7
21	B	229	PSC	C13-C14-C15-C16
19	A	524	PGV	C10-C11-C12-C13
19	A	522	PGV	C10-C11-C12-C13
19	C	267	PGV	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C01-C02-C03-O11
25	P	1270	CDL	OB5-CB3-CB4-CB6
25	T	1269	CDL	OA5-CA3-CA4-CA6
19	C	267	PGV	C1-C2-C3-C4
24	T	1265	PEK	O12-C04-C05-N
18	N	1522	TGL	C29-C30-C31-C32
18	N	1521	TGL	CC6-CC7-CC8-CC9
19	P	1268	PGV	C3-C4-C5-C6
18	L	522	TGL	C29-C30-C31-C32
24	G	1263	PEK	C26-C27-C28-C29
19	P	1268	PGV	C20-C19-O03-C01
24	G	1263	PEK	C24-C25-C26-C27
18	L	522	TGL	C20-C21-C22-C23
25	G	269	CDL	C16-C17-C18-C19
19	P	1268	PGV	C23-C24-C25-C26
25	T	1269	CDL	C55-C56-C57-C58
18	A	521	TGL	OG1-CG1-CG2-CG3
19	A	524	PGV	O03-C01-C02-C03
18	Q	1523	TGL	CG1-CG2-CG3-OG3
24	G	264	PEK	O03-C01-C02-C03
25	G	269	CDL	CA3-CA4-CA6-OA8
25	G	269	CDL	CB3-CB4-CB6-OB8
18	D	523	TGL	CG1-CG2-CG3-OG3
21	O	1229	PSC	O03-C01-C02-C03
19	N	1524	PGV	C10-C11-C12-C13
19	P	1268	PGV	C26-C27-C28-C29
18	N	1522	TGL	CC3-CC4-CC5-CC6
25	C	270	CDL	C78-C79-C80-C81
25	G	269	CDL	C18-C19-C20-C21
18	A	521	TGL	CC5-CC6-CC7-CC8
27	M	526	DMU	C2-C3-O7-C10
18	A	521	TGL	C17-C18-C19-C33
18	L	522	TGL	CA2-CA3-CA4-CA5
18	N	1522	TGL	C22-C23-C24-C25
25	P	1270	CDL	C62-C63-C64-C65
24	G	1263	PEK	C31-C32-C33-C34
25	T	1269	CDL	C64-C65-C66-C67
24	T	1265	PEK	C5-C6-C7-C8
24	C	265	PEK	C9-C10-C11-C12
24	G	264	PEK	C9-C10-C11-C12
25	G	269	CDL	CB2-OB2-PB2-OB5
24	T	263	PEK	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	T	263	PEK	C11-C10-C9-C8
24	T	263	PEK	C9-C10-C11-C12
24	T	1264	PEK	C11-C10-C9-C8
24	T	1264	PEK	C9-C10-C11-C12
24	G	1263	PEK	C11-C10-C9-C8
24	G	1263	PEK	C9-C10-C11-C12
21	B	229	PSC	C9-C10-C11-C12
21	O	1229	PSC	C9-C10-C11-C12
25	C	270	CDL	C14-C15-C16-C17
25	C	270	CDL	C20-C21-C22-C23
19	C	268	PGV	C7-C8-C9-C10
25	C	270	CDL	OB5-CB3-CB4-OB6
25	P	1270	CDL	OA5-CA3-CA4-OA6
24	T	263	PEK	O01-C02-C03-O11
18	N	1522	TGL	CC5-CC6-CC7-CC8
25	G	269	CDL	C54-C55-C56-C57
19	C	268	PGV	C30-C31-C32-C33
24	T	1265	PEK	O03-C01-C02-O01
25	C	270	CDL	OB6-CB4-CB6-OB8
18	Q	1523	TGL	OG2-CG2-CG3-OG3
25	P	1270	CDL	OB6-CB4-CB6-OB8
24	C	265	PEK	C32-C33-C34-C35
25	G	269	CDL	C58-C59-C60-C61
25	T	1269	CDL	CB2-C1-CA2-OA2
25	C	270	CDL	C55-C56-C57-C58
24	T	1264	PEK	C17-C18-C19-C20
19	N	1266	PGV	C31-C32-C33-C34
25	G	269	CDL	CB4-CB3-OB5-PB2
25	P	1270	CDL	CA4-CA3-OA5-PA1
19	P	1267	PGV	C02-C03-O11-P
24	T	1264	PEK	C25-C26-C27-C28
24	C	265	PEK	C31-C32-C33-C34
18	L	522	TGL	C25-C26-C27-C28
19	A	524	PGV	C11-C12-C13-C14
24	G	264	PEK	O04-C21-O03-C01
19	C	268	PGV	C1-C2-C3-C4
27	Z	1526	DMU	C34-C37-C40-C43
19	N	1524	PGV	C21-C22-C23-C24
25	P	1270	CDL	C32-C33-C34-C35
25	P	1270	CDL	C11-C12-C13-C14
24	T	1265	PEK	C01-C02-C03-O11
19	A	524	PGV	C01-C02-C03-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	P	1267	PGV	C29-C30-C31-C32
25	P	1270	CDL	C43-C44-C45-C46
24	C	265	PEK	C16-C17-C18-C19
19	A	522	PGV	C29-C30-C31-C32
18	D	523	TGL	CC6-CC7-CC8-CC9
19	N	1524	PGV	C03-C02-O01-C1
24	T	1265	PEK	C26-C27-C28-C29
19	N	1524	PGV	C31-C32-C33-C34
18	D	523	TGL	CA4-CA5-CA6-CA7
21	O	1229	PSC	C4-C5-C6-C7
24	T	1265	PEK	C31-C32-C33-C34
24	T	263	PEK	C31-C32-C33-C34
25	C	270	CDL	CB3-CB4-CB6-OB8
25	T	1269	CDL	CA3-CA4-CA6-OA8
25	C	270	CDL	OA5-CA3-CA4-OA6
24	G	1263	PEK	O01-C02-C03-O11
18	L	522	TGL	CA6-CA7-CA8-CA9
18	N	1521	TGL	C16-C15-CC9-CC8
25	G	269	CDL	CB7-C71-C72-C73
19	P	1268	PGV	O04-C19-O03-C01
19	N	1524	PGV	O03-C01-C02-O01
25	P	1270	CDL	OA6-CA4-CA6-OA8
18	D	523	TGL	OG2-CG2-CG3-OG3
19	A	524	PGV	C25-C26-C27-C28
18	N	1521	TGL	CC4-CC5-CC6-CC7
24	G	1263	PEK	C16-C17-C18-C19
25	T	1269	CDL	C51-CB5-OB6-CB4
19	N	1524	PGV	C11-C10-C9-C8
24	G	264	PEK	C25-C26-C27-C28
19	C	268	PGV	C15-C16-C17-C18
18	D	523	TGL	C29-C30-C31-C32
19	N	1524	PGV	C26-C27-C28-C29
19	A	522	PGV	C24-C25-C26-C27
18	N	1521	TGL	C15-C16-C17-C18
24	T	263	PEK	C16-C17-C18-C19
21	B	229	PSC	C3-C4-C5-C6
18	N	1522	TGL	OG2-CB1-CB2-CB3
19	P	1268	PGV	C28-C29-C30-C31
25	T	1269	CDL	C57-C58-C59-C60
25	G	269	CDL	C24-C25-C26-C27
25	T	1269	CDL	OB7-CB5-OB6-CB4
24	G	264	PEK	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	CB2-OB2-PB2-OB5
25	C	270	CDL	C1-CA2-OA2-PA1
19	C	267	PGV	C02-C03-O11-P
24	C	265	PEK	C04-O12-P-O13
25	G	269	CDL	CA2-OA2-PA1-OA4
25	P	1270	CDL	CA2-OA2-PA1-OA4
25	P	1270	CDL	CA3-OA5-PA1-OA3
24	G	1263	PEK	C03-O11-P-O13
21	B	229	PSC	C04-O12-P-O13
14	N	516	HEA	C3B-C11-C12-C13
21	O	1229	PSC	C03-O11-P-O13
18	A	521	TGL	CC4-CC5-CC6-CC7
24	T	263	PEK	C01-C02-C03-O11
24	G	1263	PEK	C01-C02-C03-O11
25	G	269	CDL	C41-C42-C43-C44
24	G	264	PEK	C15-C16-C17-C18
18	A	521	TGL	C24-C25-C26-C27
19	C	268	PGV	C4-C5-C6-C7
18	D	523	TGL	C11-C12-C13-C14
18	A	521	TGL	C20-C21-C22-C23
25	G	269	CDL	OA5-CA3-CA4-OA6
25	P	1270	CDL	OB5-CB3-CB4-OB6
25	T	1269	CDL	OA5-CA3-CA4-OA6
24	T	263	PEK	C28-C29-C30-C31
19	C	267	PGV	C22-C23-C24-C25
25	G	269	CDL	C56-C57-C58-C59
18	N	1521	TGL	C23-C24-C25-C26
24	T	1265	PEK	C21-C22-C23-C24
24	T	1265	PEK	C24-C25-C26-C27
19	A	522	PGV	C22-C23-C24-C25
18	L	522	TGL	CA3-CA4-CA5-CA6
19	N	1266	PGV	C24-C25-C26-C27
21	B	229	PSC	O03-C01-C02-C03
24	G	264	PEK	O03-C01-C02-O01
25	G	269	CDL	OA6-CA4-CA6-OA8
21	O	1229	PSC	O03-C01-C02-O01
25	T	1269	CDL	OA6-CA4-CA6-OA8
25	P	1270	CDL	C14-C15-C16-C17
21	B	229	PSC	C31-C32-C33-C34
19	N	1524	PGV	C05-C04-O12-P
18	N	1521	TGL	CA6-CA7-CA8-CA9
21	B	229	PSC	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	G	269	CDL	C81-C82-C83-C84
25	T	1269	CDL	C84-C85-C86-C87
25	G	269	CDL	C31-C32-C33-C34
25	G	269	CDL	C76-C77-C78-C79
19	A	524	PGV	C23-C24-C25-C26
18	D	523	TGL	C17-C18-C19-C33
19	C	267	PGV	C23-C24-C25-C26
18	A	521	TGL	CG1-CG2-OG2-CB1
18	Q	1523	TGL	CG1-CG2-OG2-CB1
18	D	523	TGL	CG3-CG2-OG2-CB1
21	O	1229	PSC	C03-C02-O01-C1
24	G	264	PEK	C24-C25-C26-C27
24	T	263	PEK	O04-C21-O03-C01
19	C	267	PGV	C05-C04-O12-P
25	T	1269	CDL	CB4-CB3-OB5-PB2
24	T	263	PEK	C22-C21-O03-C01
19	P	1268	PGV	O01-C02-C03-O11
19	C	268	PGV	O01-C02-C03-O11
24	T	1265	PEK	C30-C31-C32-C33
19	P	1267	PGV	C1-C2-C3-C4
24	C	265	PEK	O03-C01-C02-O01
24	C	265	PEK	C30-C31-C32-C33
24	G	264	PEK	C17-C18-C19-C20
19	A	524	PGV	C03-O11-P-O12
19	N	1524	PGV	C03-O11-P-O12
21	B	229	PSC	C03-O11-P-O12
18	Q	1523	TGL	C33-C34-C35-C36
18	L	522	TGL	C19-C33-C34-C35
25	T	1269	CDL	C24-C25-C26-C27
19	P	1268	PGV	C05-C04-O12-P
25	P	1270	CDL	C1-CA2-OA2-PA1
24	T	263	PEK	C02-C03-O11-P
18	Q	1523	TGL	C29-C30-C31-C32
19	N	1524	PGV	C11-C12-C13-C14
24	G	264	PEK	C14-C15-C16-C17
19	C	268	PGV	C9-C10-C11-C12
19	N	1266	PGV	C9-C10-C11-C12
24	T	1265	PEK	C33-C34-C35-C36
25	C	270	CDL	C35-C36-C37-C38
24	G	1263	PEK	C15-C16-C17-C18
24	T	1265	PEK	O04-C21-O03-C01
24	T	1264	PEK	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	C	267	PGV	C27-C28-C29-C30
24	T	1264	PEK	C16-C17-C18-C19
18	N	1522	TGL	OG1-CA1-CA2-CA3
19	N	1524	PGV	C12-C13-C14-C15
24	T	1265	PEK	C32-C33-C34-C35
24	T	263	PEK	C21-C22-C23-C24
19	P	1268	PGV	C02-C03-O11-P
21	B	229	PSC	C04-C05-N-C06
18	D	523	TGL	CB7-CB8-CB9-C10
19	N	1524	PGV	C25-C26-C27-C28
18	N	1521	TGL	CB2-CB3-CB4-CB5
24	T	1265	PEK	O03-C01-C02-C03
18	Q	1523	TGL	OG1-CG1-CG2-CG3
24	T	1264	PEK	O03-C01-C02-C03
24	T	1264	PEK	C10-C11-C12-C13
18	N	1521	TGL	CG3-CG2-OG2-CB1
21	B	229	PSC	C03-C02-O01-C1
18	L	522	TGL	CA9-C20-C21-C22
21	B	229	PSC	C04-C05-N-C08
18	N	1522	TGL	CA9-C20-C21-C22
25	C	270	CDL	C32-C33-C34-C35
25	C	270	CDL	C80-C81-C82-C83
22	P	1271	CHD	C16-C17-C20-C22
18	L	522	TGL	C18-C19-C33-C34
24	T	1265	PEK	C6-C7-C8-C9
24	T	1265	PEK	C11-C10-C9-C8
24	T	1265	PEK	C9-C10-C11-C12
24	C	265	PEK	C6-C7-C8-C9
24	C	265	PEK	C11-C10-C9-C8
24	T	1264	PEK	C6-C7-C8-C9
24	G	1263	PEK	C5-C6-C7-C8
24	G	1263	PEK	C12-C13-C14-C15
21	O	1229	PSC	C3-C4-C5-C6
24	C	265	PEK	C22-C23-C24-C25
19	A	522	PGV	O03-C19-C20-C21
21	B	229	PSC	C7-C8-C9-C10
24	G	264	PEK	C26-C27-C28-C29
18	A	521	TGL	C23-C24-C25-C26
25	G	269	CDL	C33-C34-C35-C36
19	A	524	PGV	C30-C31-C32-C33
18	Q	1523	TGL	C10-C11-C12-C13
24	T	1264	PEK	O03-C01-C02-O01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	524	PGV	C21-C22-C23-C24
18	N	1522	TGL	CB1-CB2-CB3-CB4
18	A	521	TGL	C21-C22-C23-C24
25	P	1270	CDL	C20-C21-C22-C23
25	G	269	CDL	C14-C15-C16-C17
18	L	522	TGL	C13-C14-C29-C30
18	L	522	TGL	OG2-CB1-CB2-CB3
14	A	515	HEA	C26-C15-C16-C17
25	C	270	CDL	C75-C76-C77-C78
27	M	526	DMU	C34-C37-C40-C43
18	D	523	TGL	C16-C17-C18-C19
19	N	1266	PGV	O03-C19-C20-C21
19	N	1524	PGV	C30-C31-C32-C33
25	P	1270	CDL	C63-C64-C65-C66
14	N	515	HEA	C26-C15-C16-C17
18	A	521	TGL	C18-C19-C33-C34
25	G	269	CDL	C11-C12-C13-C14
25	C	270	CDL	C24-C25-C26-C27
18	D	523	TGL	OB1-CB1-OG2-CG2
19	P	1268	PGV	C01-C02-C03-O11
19	C	268	PGV	C01-C02-C03-O11
24	G	1263	PEK	C21-C22-C23-C24
25	C	270	CDL	C52-C53-C54-C55
19	A	524	PGV	O03-C01-C02-O01
24	T	1265	PEK	C22-C21-O03-C01
18	D	523	TGL	C24-C25-C26-C27
19	A	522	PGV	C11-C12-C13-C14
19	P	1267	PGV	C11-C12-C13-C14
25	P	1270	CDL	C77-C78-C79-C80
25	P	1270	CDL	C12-C11-CA5-OA6
18	N	1522	TGL	OB1-CB1-CB2-CB3
14	N	516	HEA	C26-C15-C16-C17
19	N	1266	PGV	C4-C5-C6-C7
25	C	270	CDL	C43-C44-C45-C46
25	P	1270	CDL	C52-C53-C54-C55
19	C	268	PGV	C2-C3-C4-C5
22	C	271	CHD	C16-C17-C20-C22
24	T	263	PEK	C2-C3-C4-C5
24	G	264	PEK	C29-C30-C31-C32
25	P	1270	CDL	C35-C36-C37-C38
19	C	267	PGV	C9-C10-C11-C12
19	N	1524	PGV	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	G	269	CDL	OB7-CB5-OB6-CB4
25	G	269	CDL	CA7-C31-C32-C33
19	A	524	PGV	O01-C1-C2-C3
25	P	1270	CDL	C52-C51-CB5-OB6
25	P	1270	CDL	C84-C85-C86-C87
18	N	1522	TGL	OG3-CC1-CC2-CC3
24	G	264	PEK	O01-C1-C2-C3
24	T	1264	PEK	O01-C1-C2-C3
18	L	522	TGL	C23-C24-C25-C26
19	C	268	PGV	C23-C24-C25-C26
18	Q	1523	TGL	OG3-CC1-CC2-CC3
25	C	270	CDL	C81-C82-C83-C84
19	N	1266	PGV	C30-C31-C32-C33
19	N	1266	PGV	C11-C12-C13-C14
21	O	1229	PSC	C7-C8-C9-C10
25	G	269	CDL	C52-C53-C54-C55
24	T	1265	PEK	C34-C35-C36-C37
18	D	523	TGL	C21-C20-CA9-CA8
25	G	269	CDL	C19-C20-C21-C22
19	C	267	PGV	C11-C12-C13-C14
21	O	1229	PSC	C12-C13-C14-C15
21	O	1229	PSC	O01-C1-C2-C3
27	Z	1526	DMU	C19-C22-C25-C28
24	T	263	PEK	C35-C36-C37-C38
19	N	1524	PGV	O01-C1-C2-C3
19	N	1524	PGV	O03-C19-C20-C21
18	D	523	TGL	OG2-CB1-CB2-CB3
19	A	522	PGV	C9-C10-C11-C12
18	L	522	TGL	CB9-C10-C11-C12
24	T	1265	PEK	C1-C2-C3-C4
19	N	1266	PGV	C19-C20-C21-C22
25	C	270	CDL	C12-C11-CA5-OA6
25	C	270	CDL	C32-C31-CA7-OA8
18	L	522	TGL	OG1-CA1-CA2-CA3
21	B	229	PSC	O03-C19-C20-C21
19	N	1524	PGV	C15-C16-C17-C18
21	B	229	PSC	C04-C05-N-C07
24	T	1264	PEK	O02-C1-C2-C3
25	C	270	CDL	C62-C63-C64-C65
25	G	269	CDL	C71-C72-C73-C74
25	C	270	CDL	C63-C64-C65-C66
24	T	1264	PEK	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	524	PGV	O02-C1-C2-C3
18	N	1522	TGL	OC1-CC1-CC2-CC3
19	P	1267	PGV	C2-C3-C4-C5
25	C	270	CDL	C32-C31-CA7-OA9
18	Q	1523	TGL	OC1-CC1-CC2-CC3
18	D	523	TGL	OG3-CC1-CC2-CC3
19	C	268	PGV	C02-C03-O11-P
24	G	1263	PEK	C02-C03-O11-P
19	A	524	PGV	C14-C15-C16-C17
24	G	264	PEK	O02-C1-C2-C3
19	A	524	PGV	C03-O11-P-O13
25	T	1269	CDL	CA2-OA2-PA1-OA3
21	O	1229	PSC	O03-C19-C20-C21
25	P	1270	CDL	C12-C11-CA5-OA7
19	N	1524	PGV	C23-C24-C25-C26
21	O	1229	PSC	O02-C1-C2-C3
24	T	263	PEK	C3-C4-C5-C6
19	N	1524	PGV	C29-C30-C31-C32
14	A	516	HEA	C26-C15-C16-C17
25	G	269	CDL	C51-CB5-OB6-CB4
25	G	269	CDL	C44-C45-C46-C47
24	T	1264	PEK	C05-C04-O12-P
25	P	1270	CDL	C52-C51-CB5-OB7
21	B	229	PSC	O01-C1-C2-C3
24	T	1264	PEK	C30-C31-C32-C33
21	O	1229	PSC	C19-C20-C21-C22
18	A	521	TGL	CB5-CB6-CB7-CB8
21	B	229	PSC	O02-C1-C2-C3
19	N	1524	PGV	O02-C1-C2-C3
24	T	1265	PEK	O03-C21-C22-C23
18	A	521	TGL	OG1-CA1-CA2-CA3
24	T	263	PEK	O01-C1-C2-C3
18	D	523	TGL	OC1-CC1-CC2-CC3
18	L	522	TGL	OG3-CC1-CC2-CC3
21	B	229	PSC	O04-C19-C20-C21
21	O	1229	PSC	O04-C19-C20-C21
24	C	265	PEK	O01-C1-C2-C3
24	T	1265	PEK	O04-C21-C22-C23
24	C	265	PEK	O02-C1-C2-C3
18	Q	1523	TGL	OG1-CA1-CA2-CA3

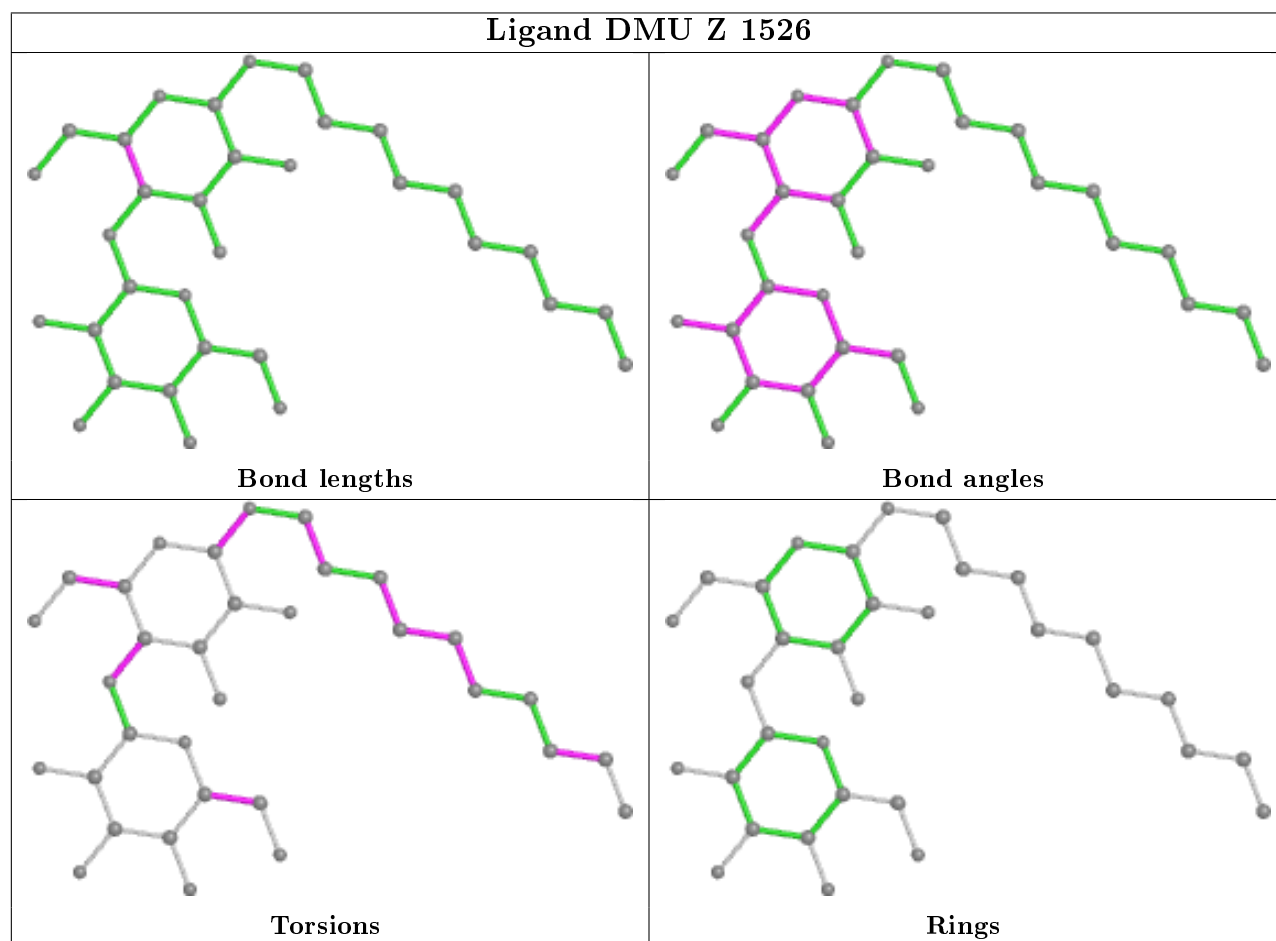
There are no ring outliers.

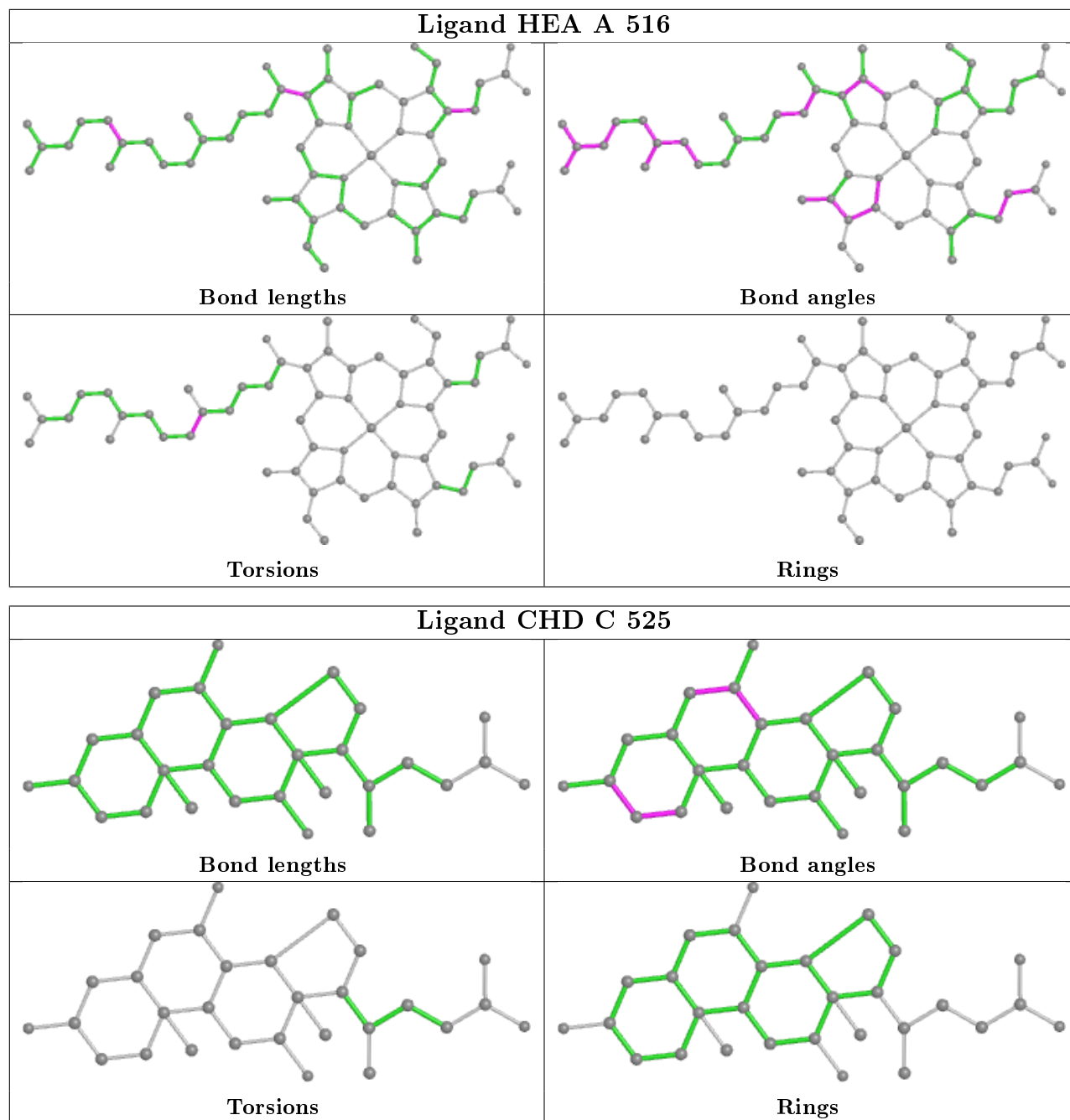
35 monomers are involved in 238 short contacts:

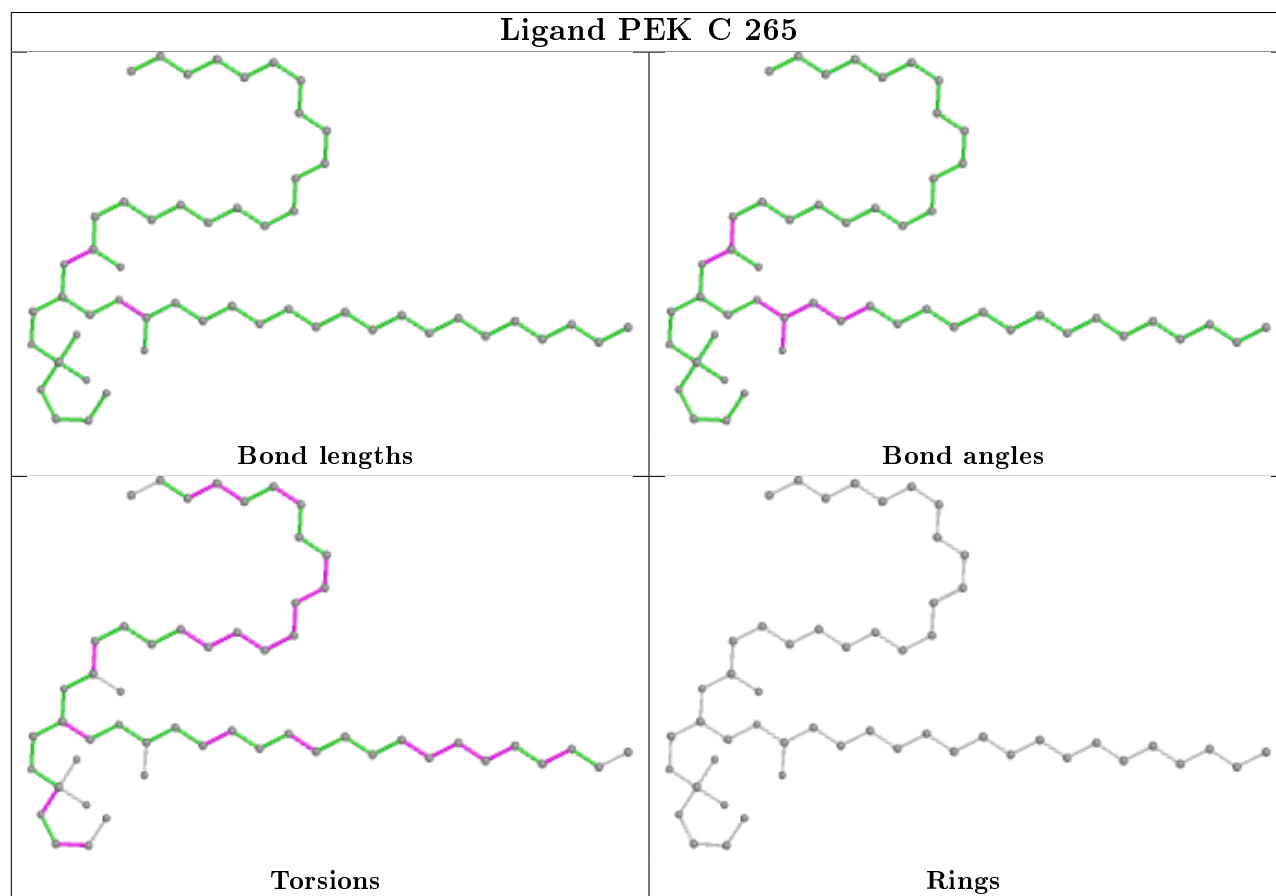
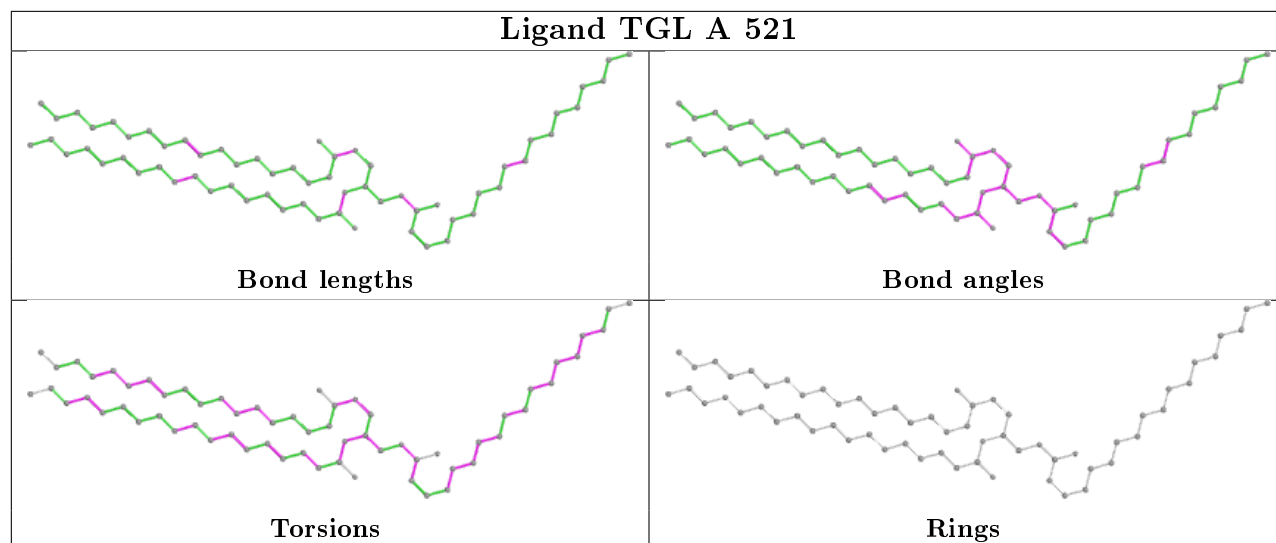
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	516	HEA	1	0
18	A	521	TGL	6	0
24	C	265	PEK	5	0
19	P	1268	PGV	4	0
14	N	515	HEA	6	0
22	C	271	CHD	3	0
22	P	1271	CHD	1	0
19	A	524	PGV	9	0
18	N	1522	TGL	12	0
22	B	1085	CHD	1	0
25	C	270	CDL	17	0
19	N	1524	PGV	8	0
22	W	1059	CHD	3	0
18	Q	1523	TGL	4	0
19	A	522	PGV	1	0
25	G	269	CDL	18	0
25	T	1269	CDL	22	0
25	P	1270	CDL	14	0
24	G	264	PEK	4	0
18	L	522	TGL	15	0
24	T	263	PEK	9	0
18	N	1521	TGL	9	0
24	T	1264	PEK	6	0
19	C	268	PGV	3	0
22	J	60	CHD	3	0
19	P	1267	PGV	2	0
24	G	1263	PEK	8	0
24	T	1265	PEK	6	0
19	C	267	PGV	5	0
21	B	229	PSC	13	0
19	N	1266	PGV	2	0
14	A	515	HEA	5	0
14	N	516	HEA	3	0
18	D	523	TGL	6	0
21	O	1229	PSC	17	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

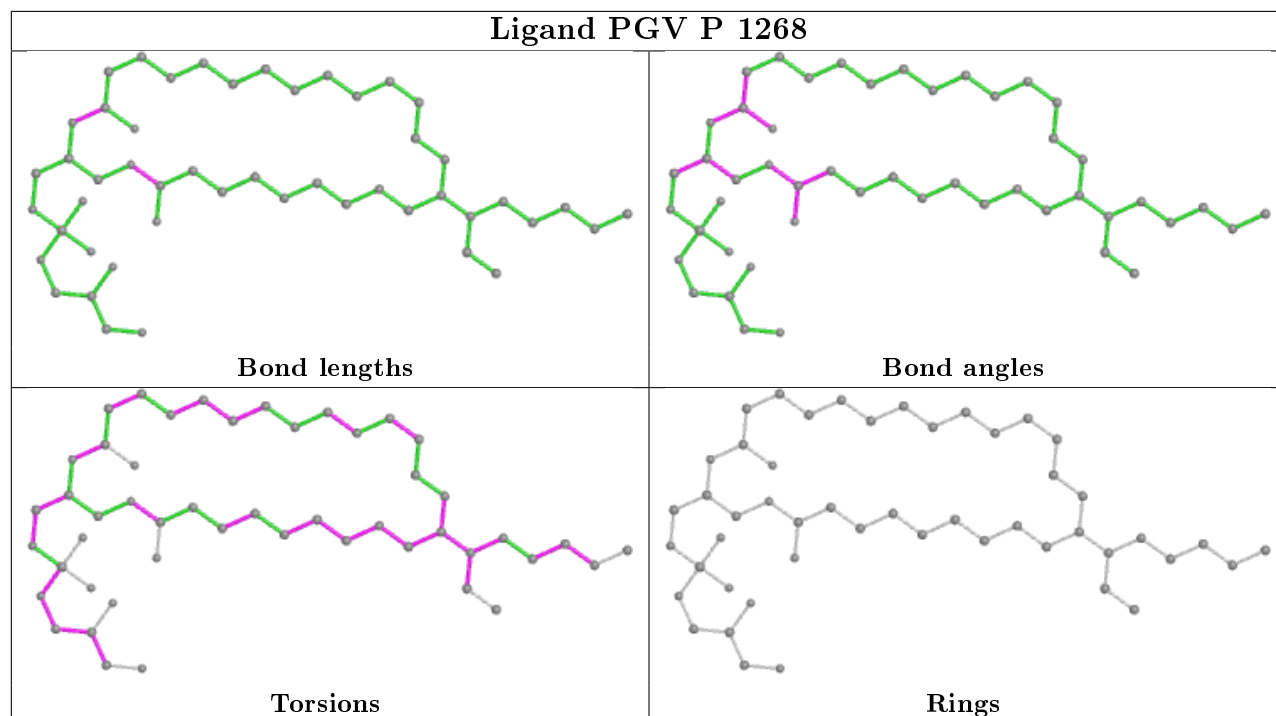
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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



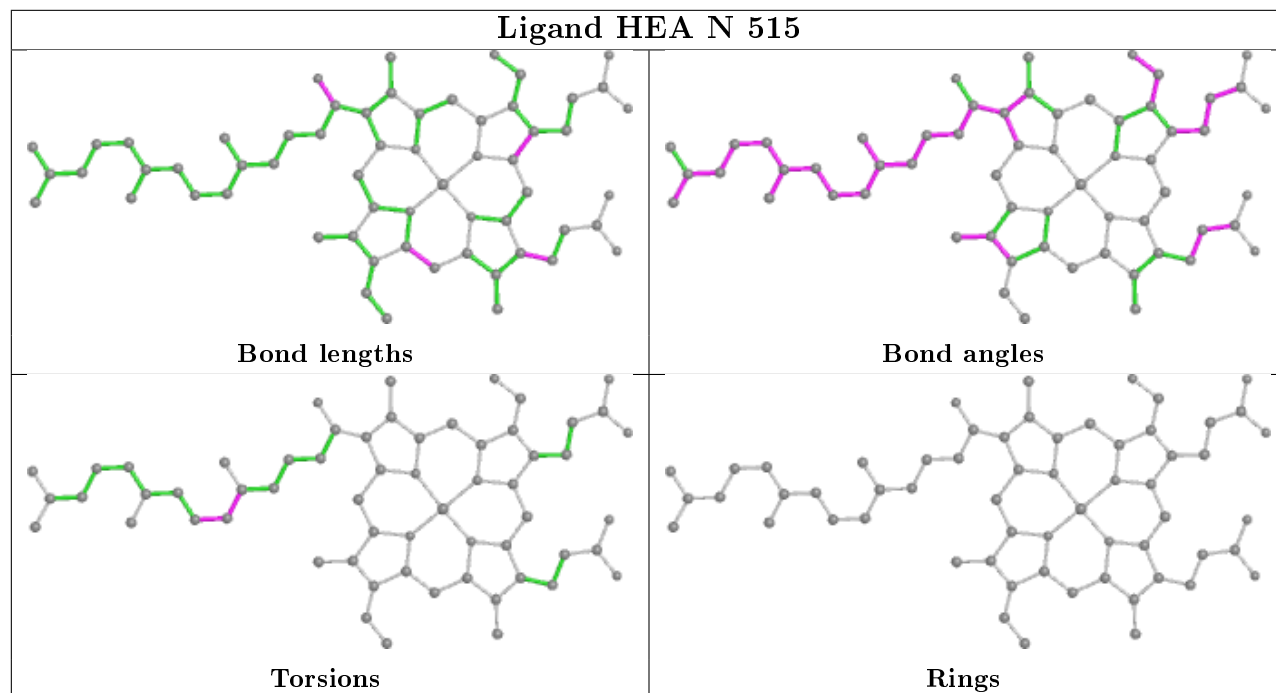


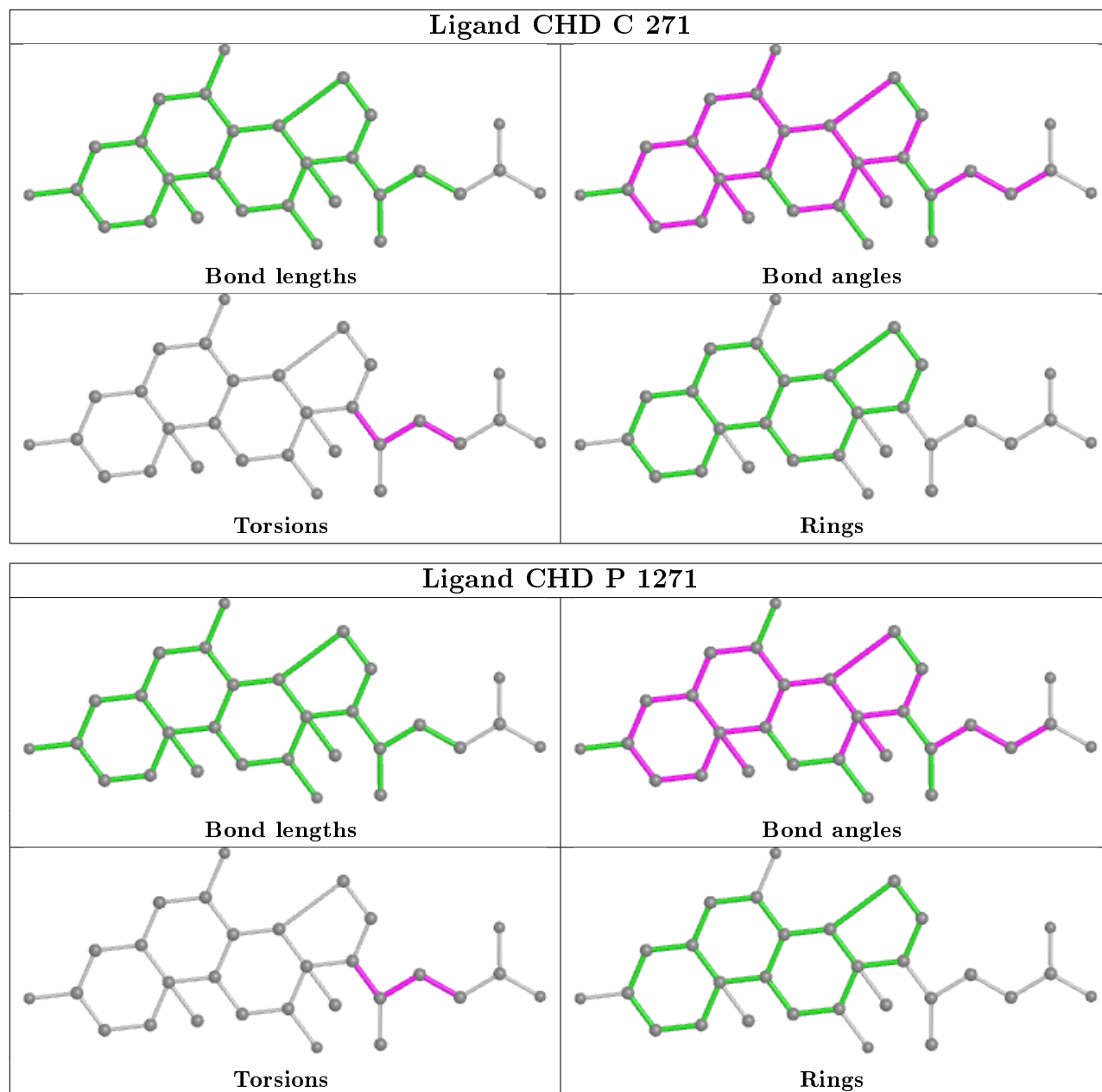


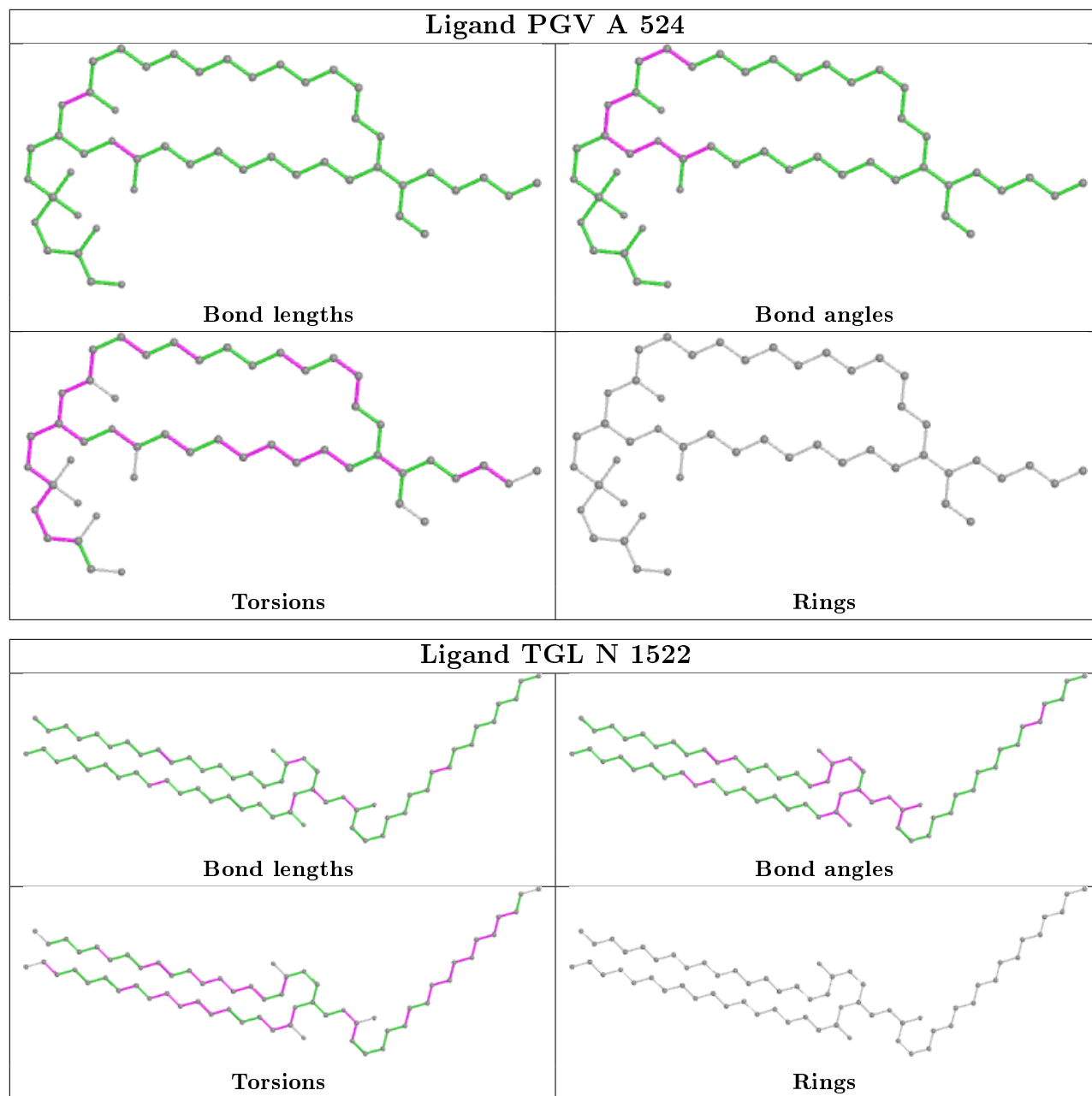
Ligand PGV P 1268



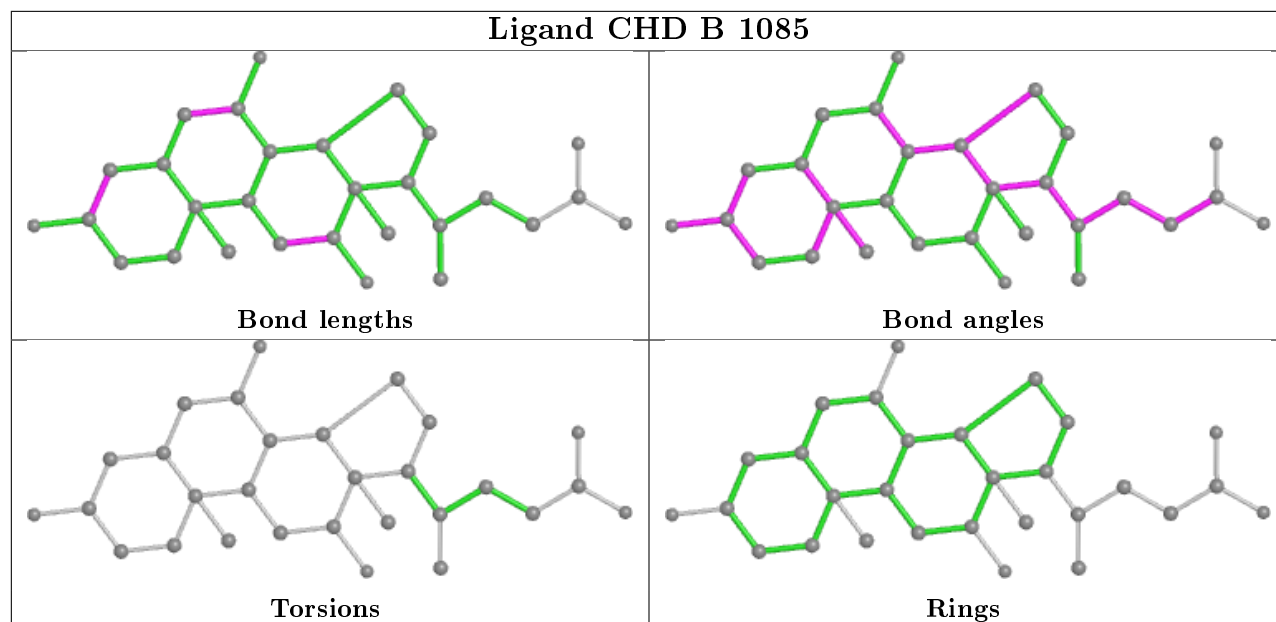
Ligand HEA N 515



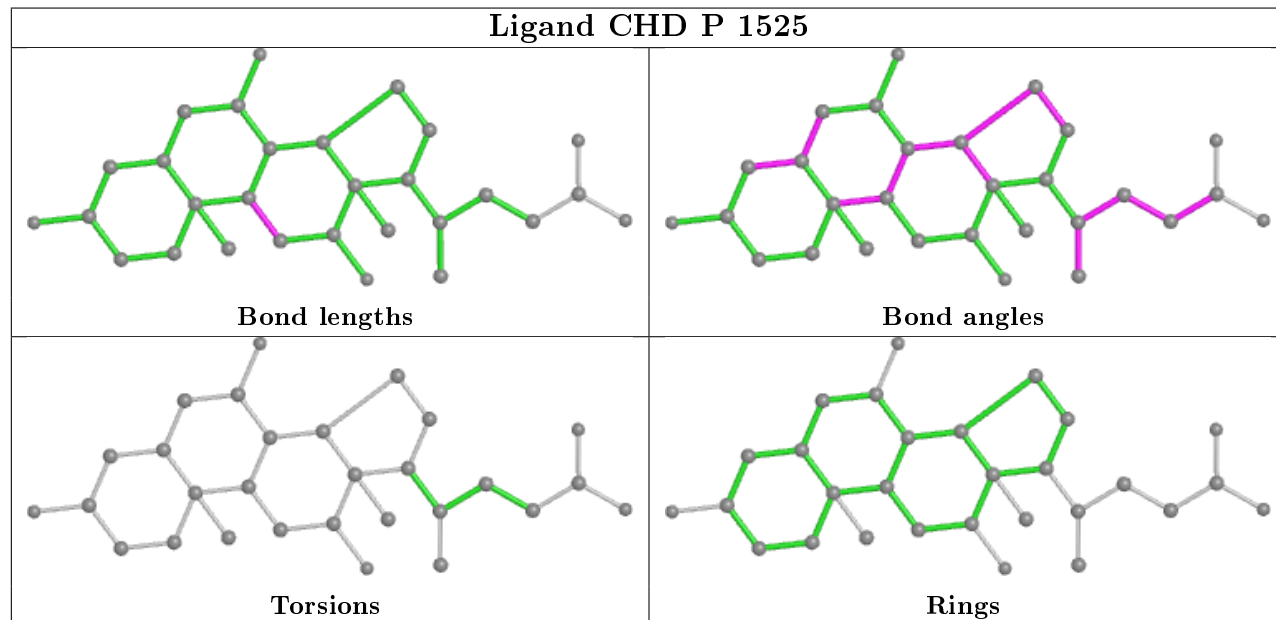


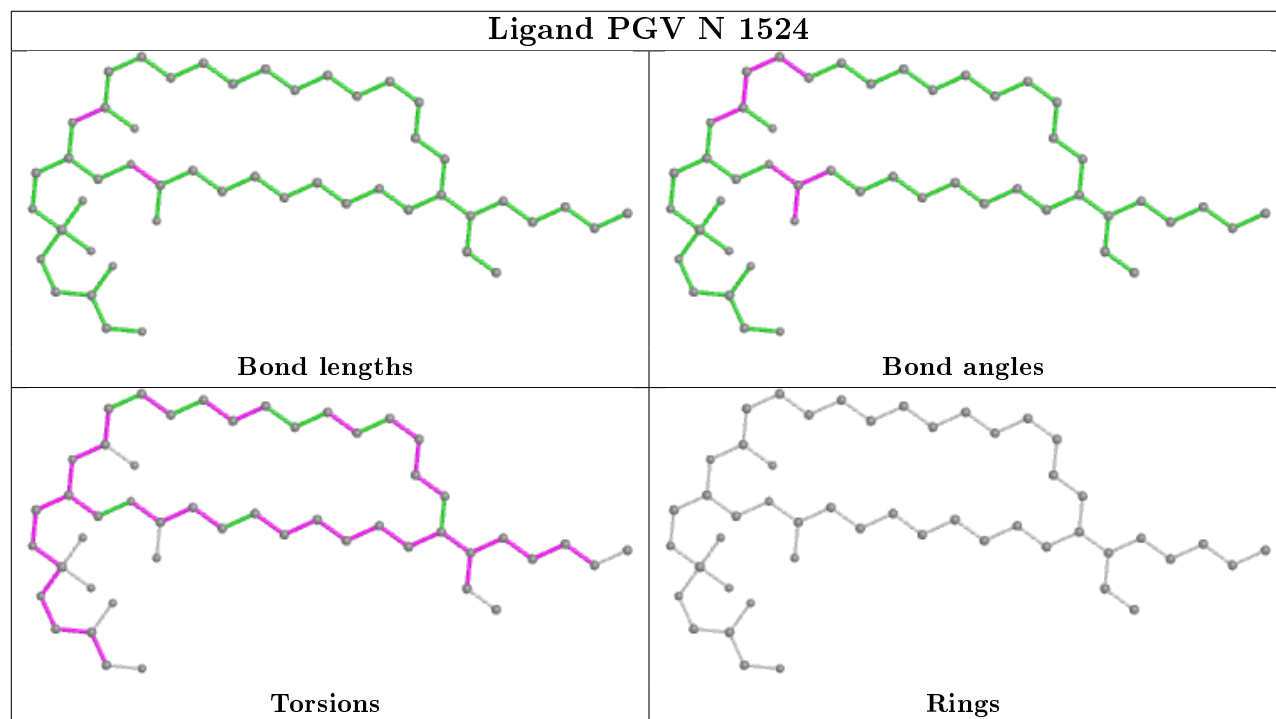
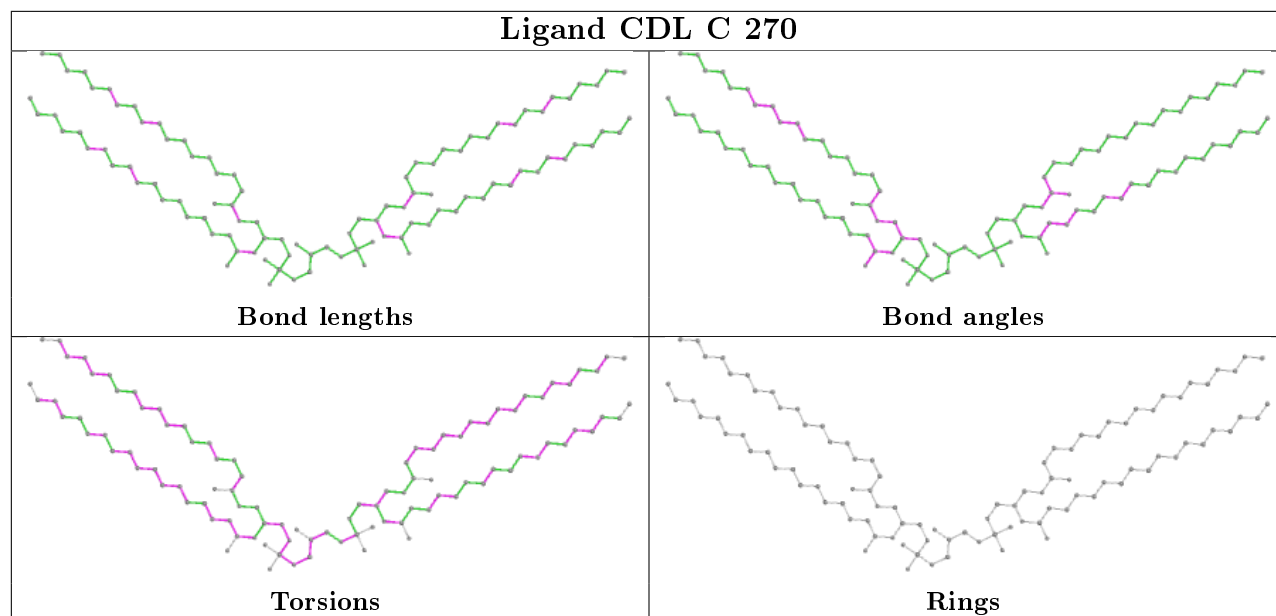


Ligand CHD B 1085

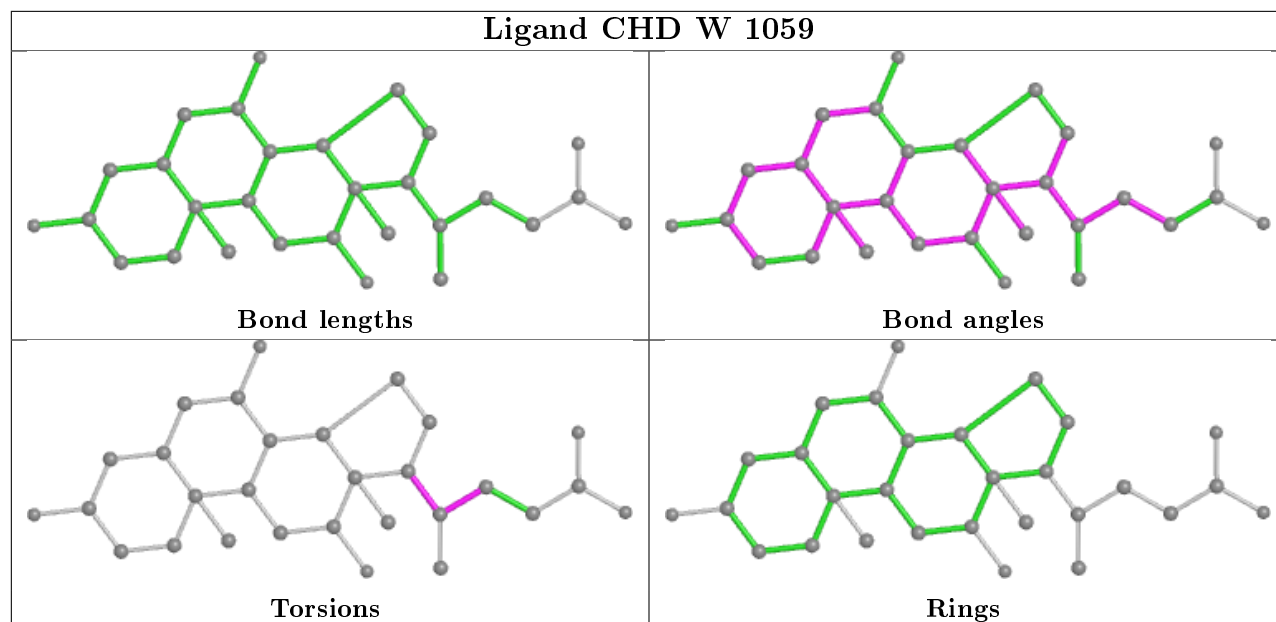


Ligand CHD P 1525

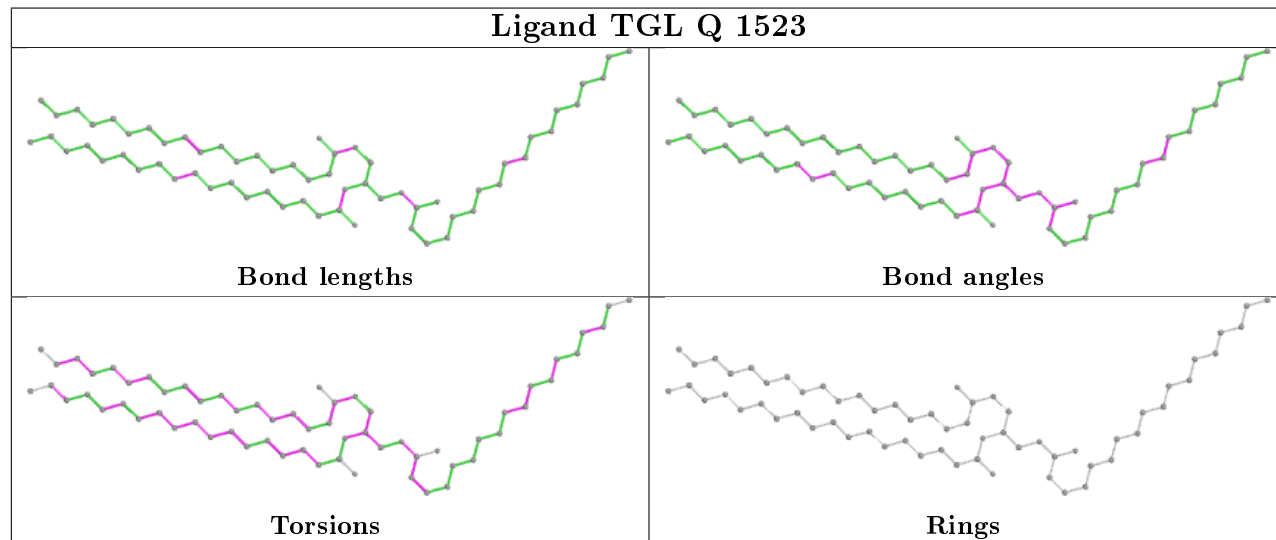


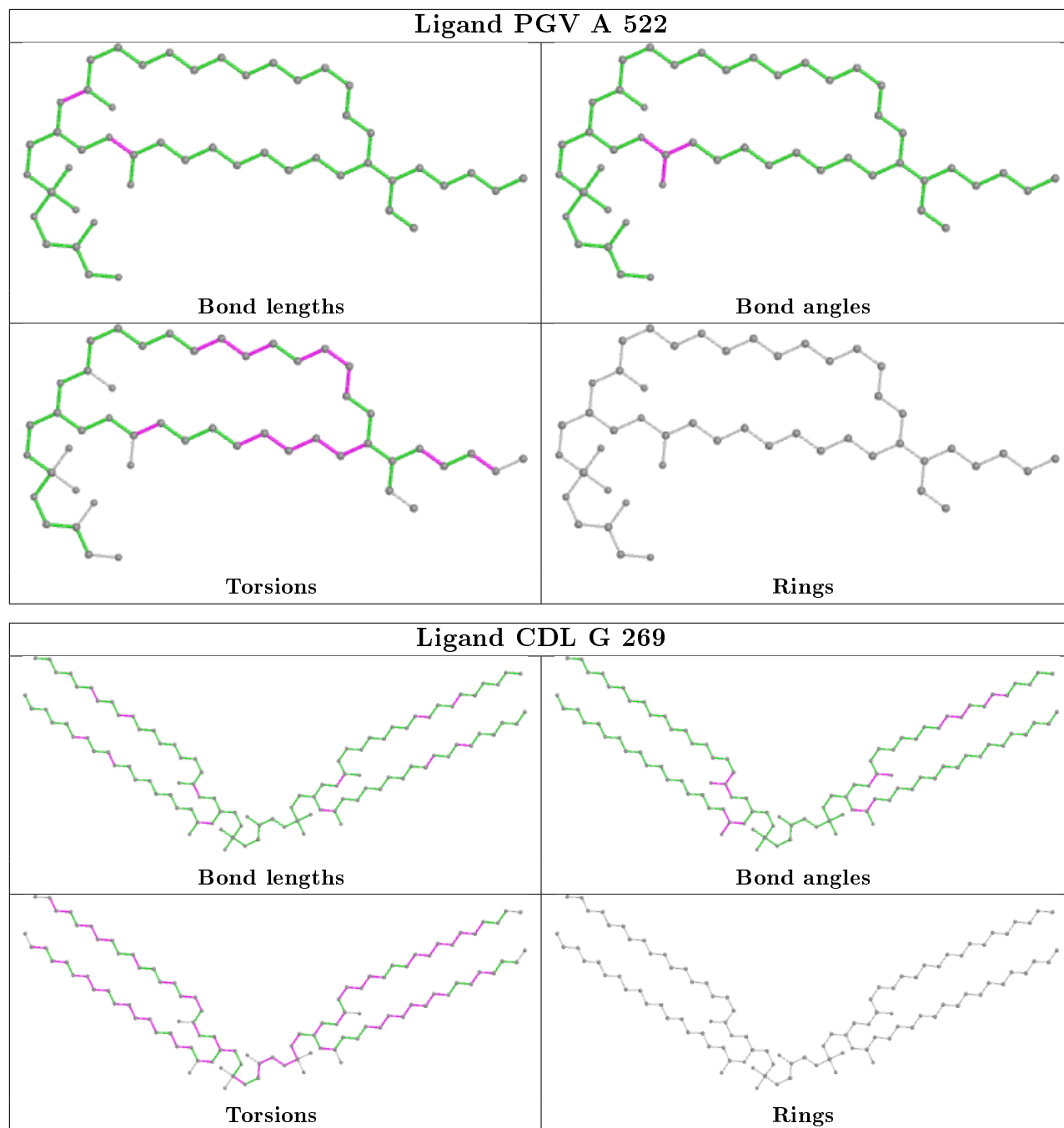


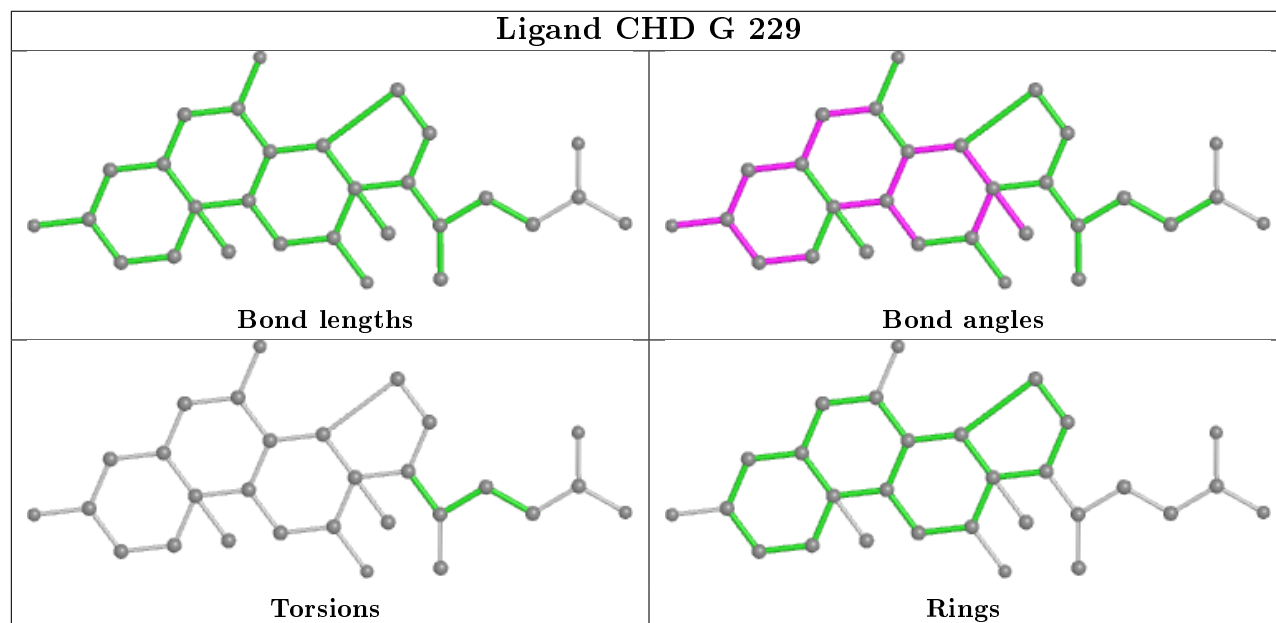
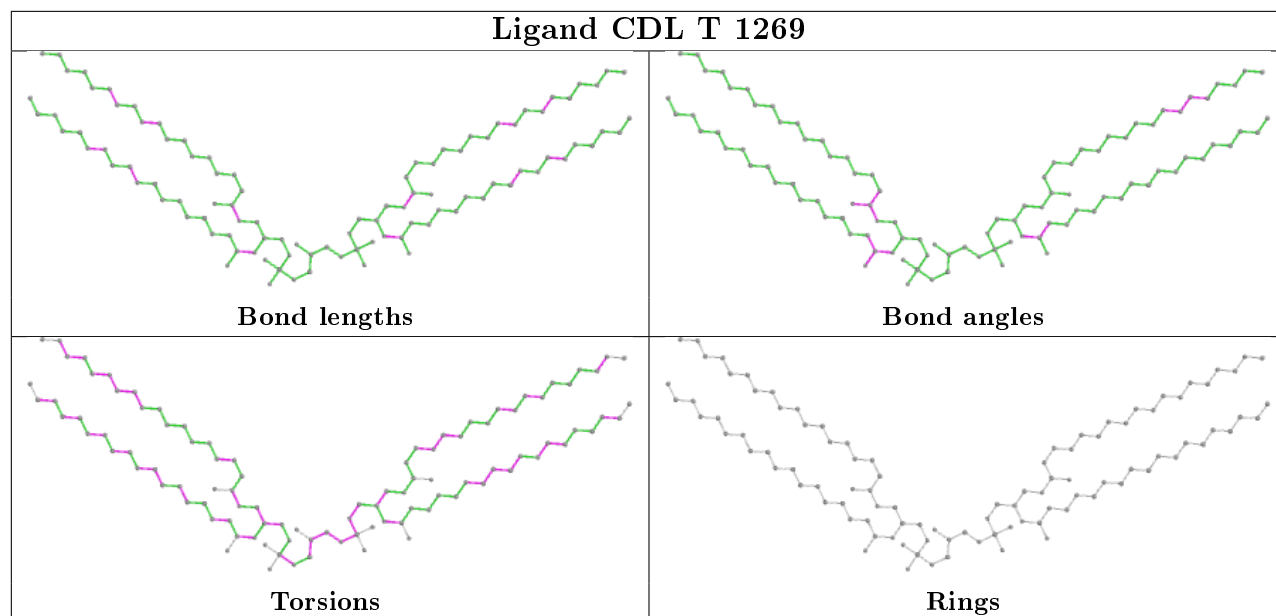
Ligand CHD W 1059

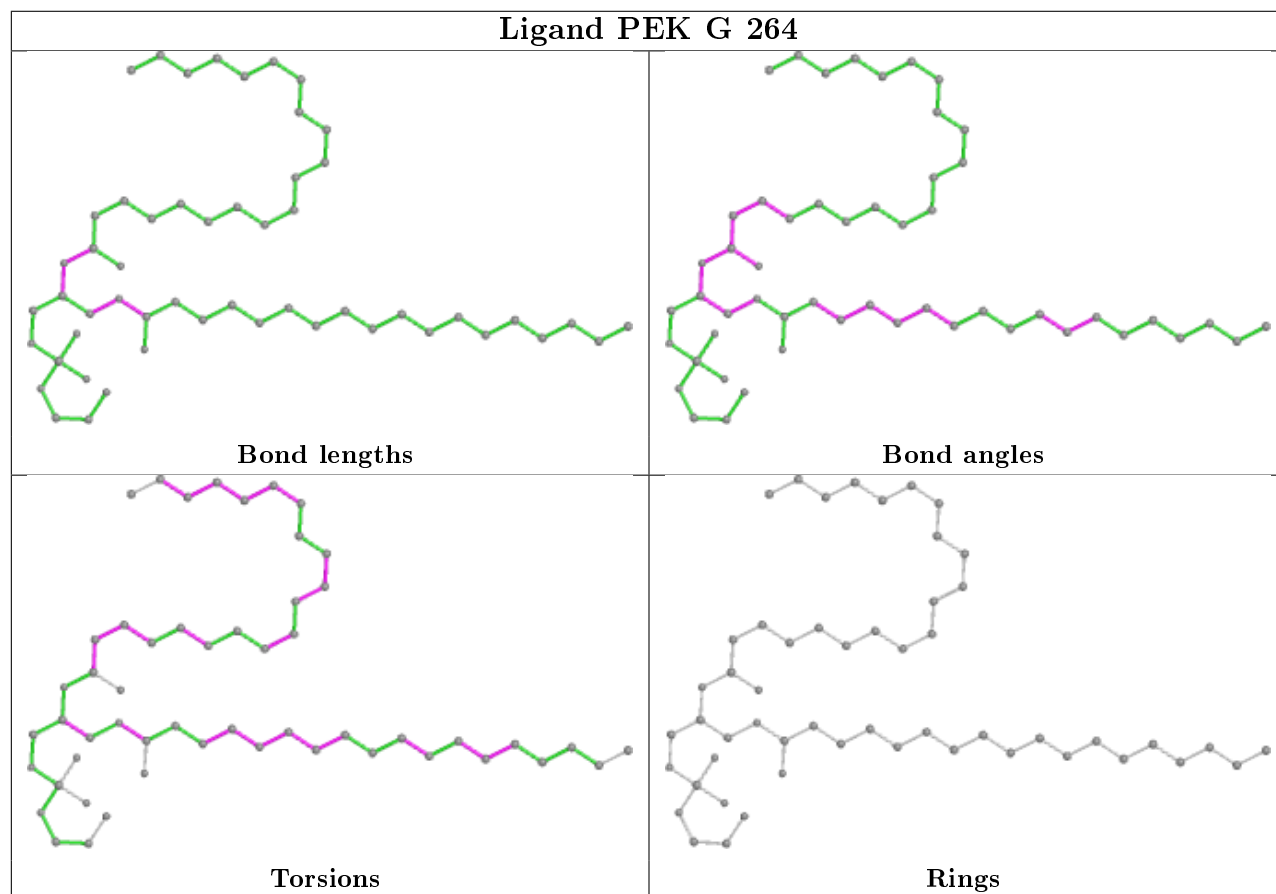
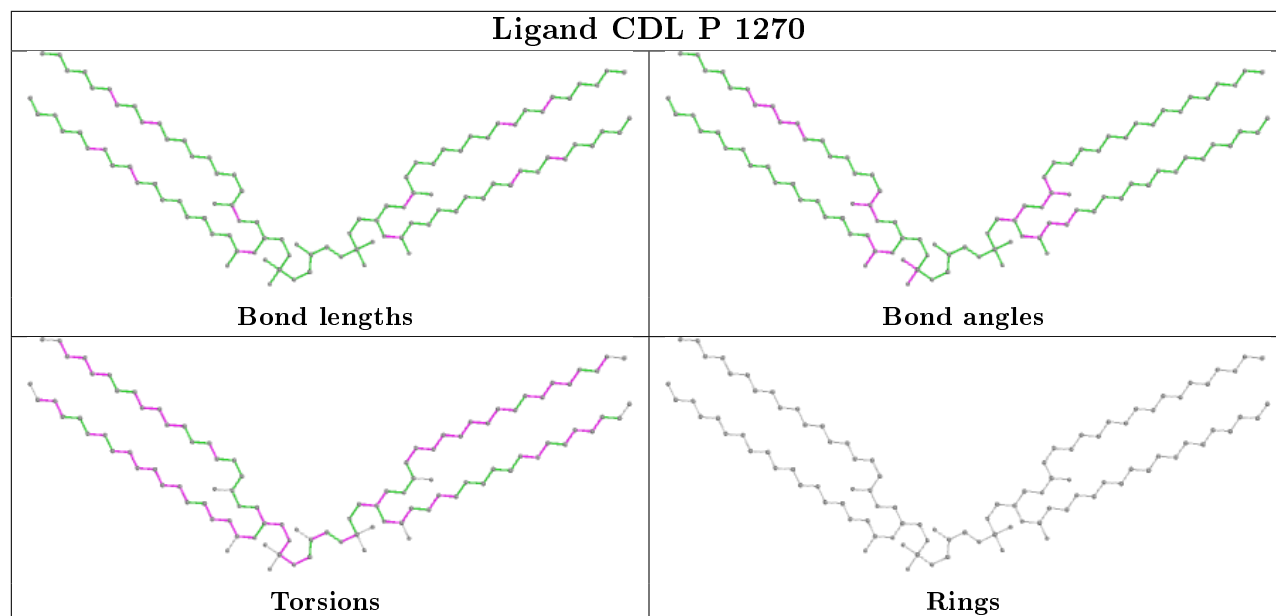


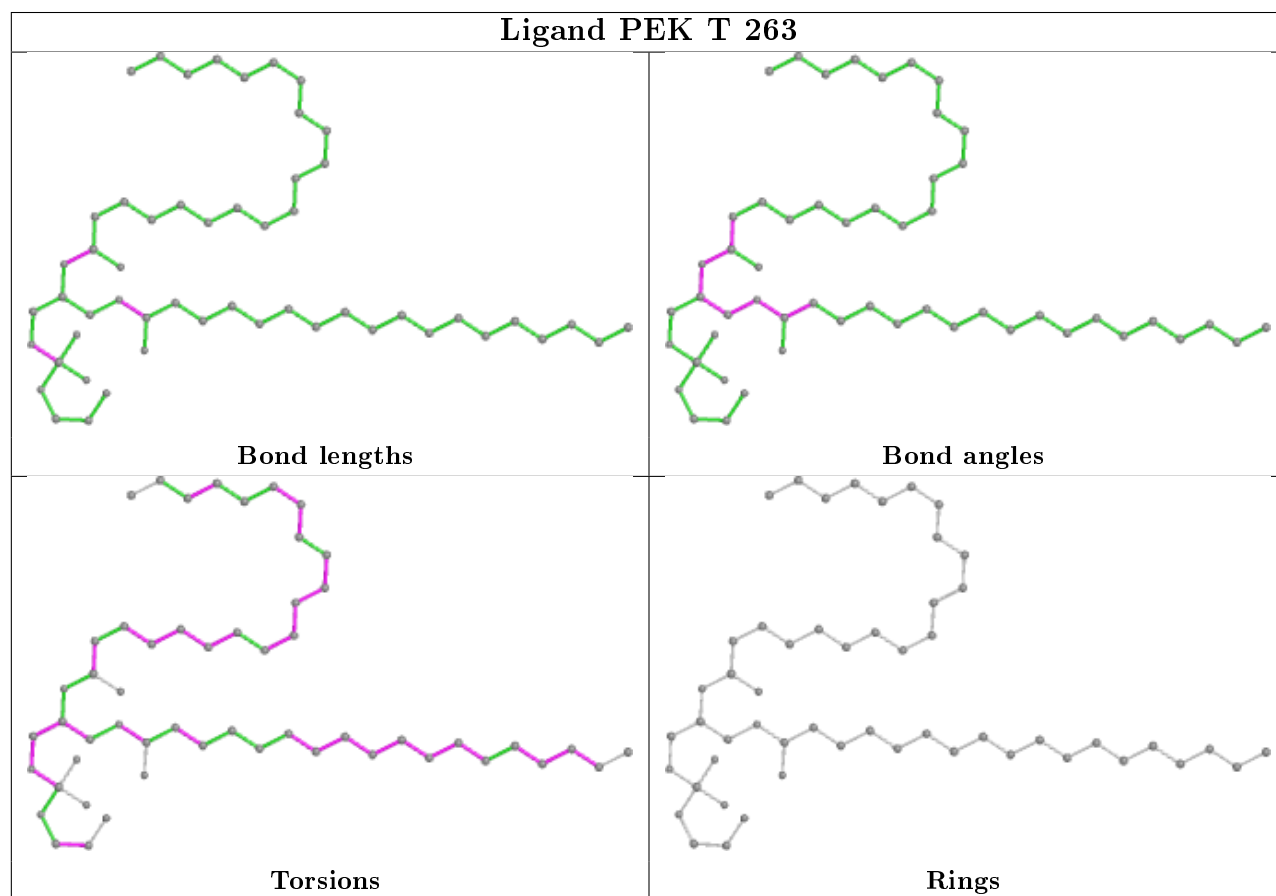
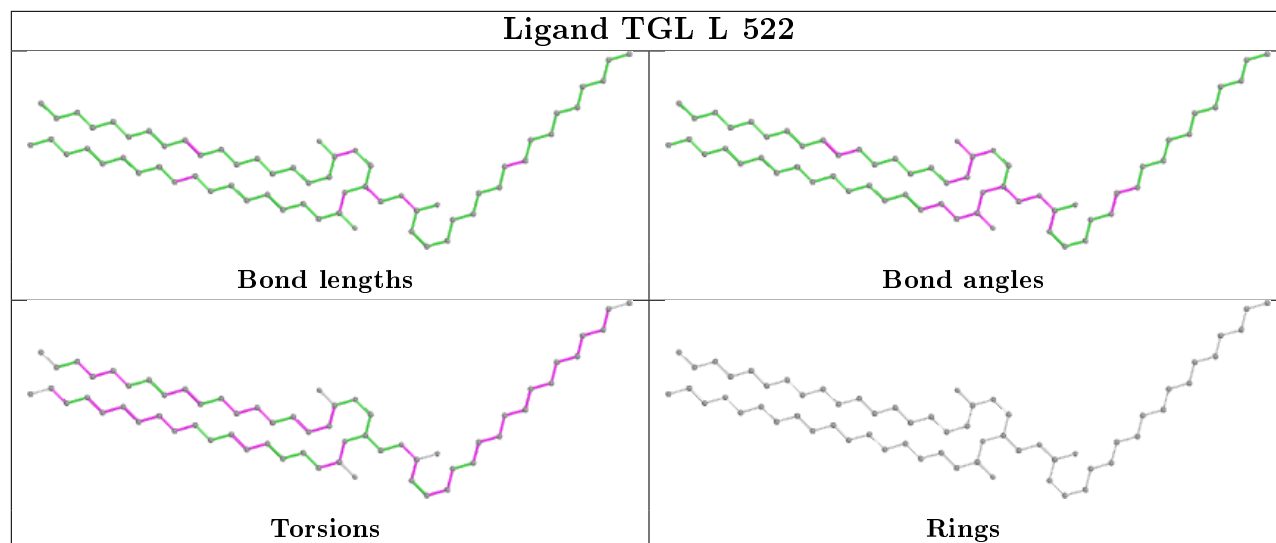
Ligand TGL Q 1523

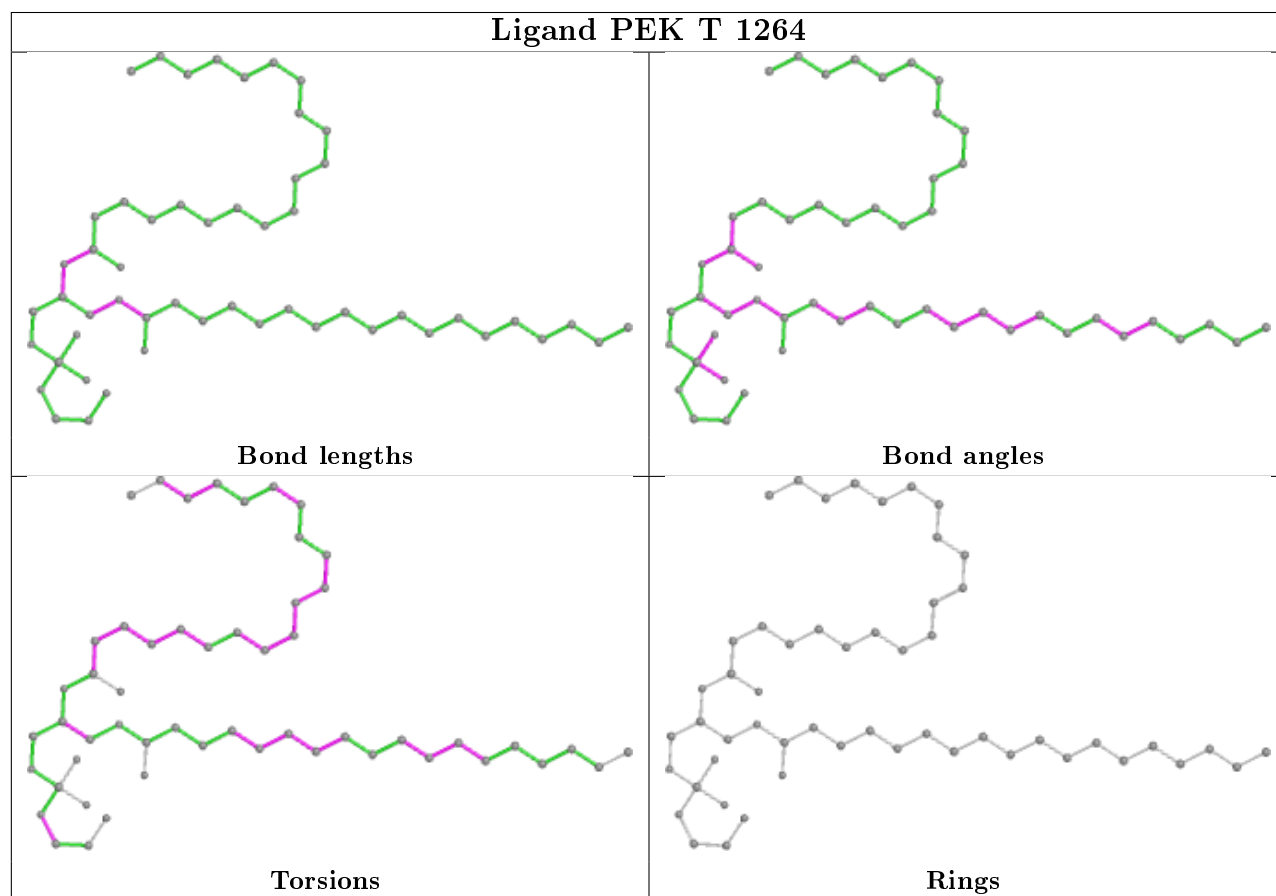
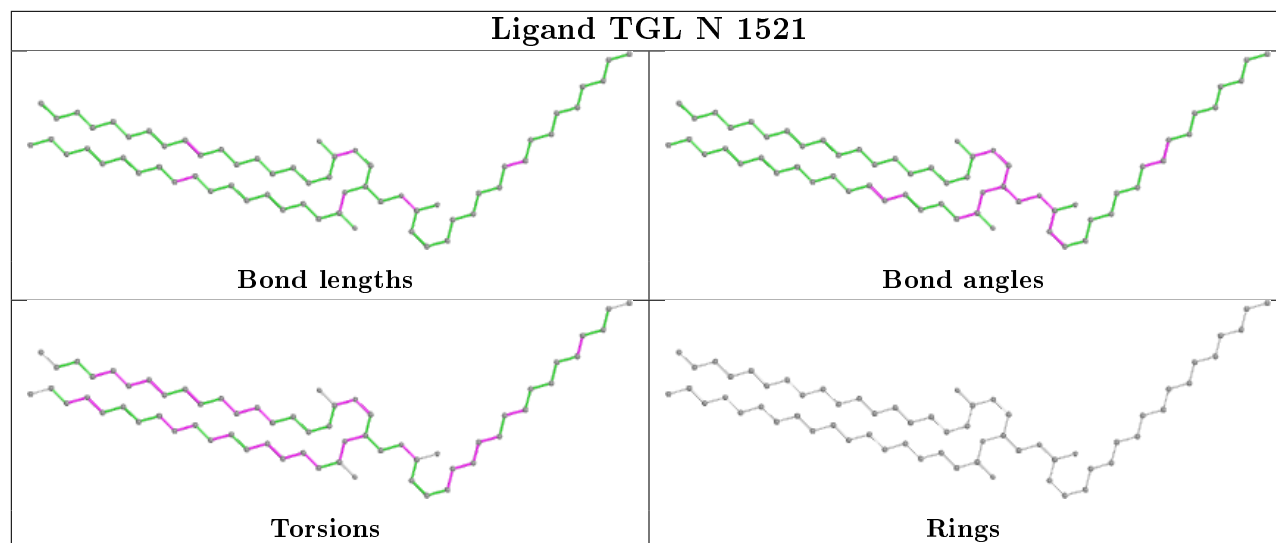




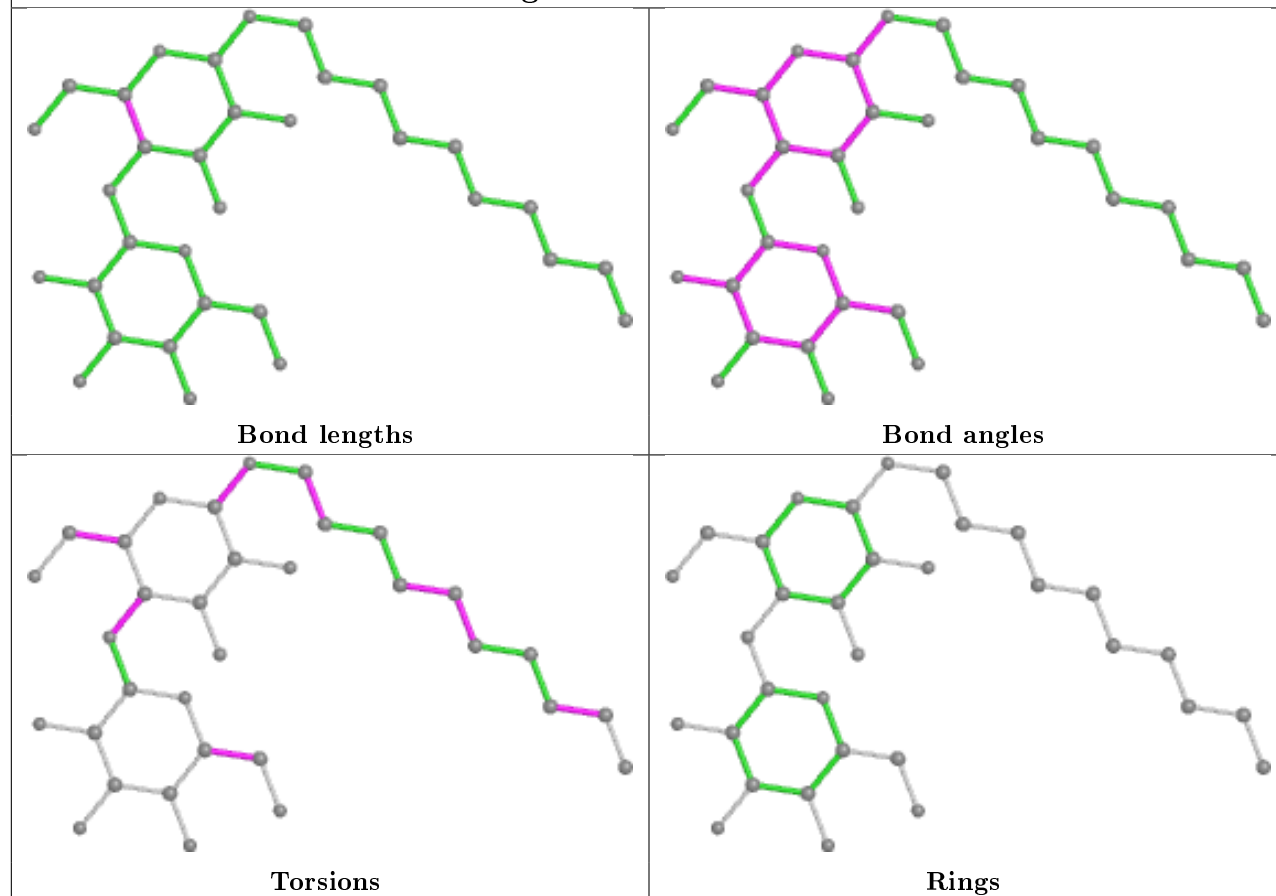




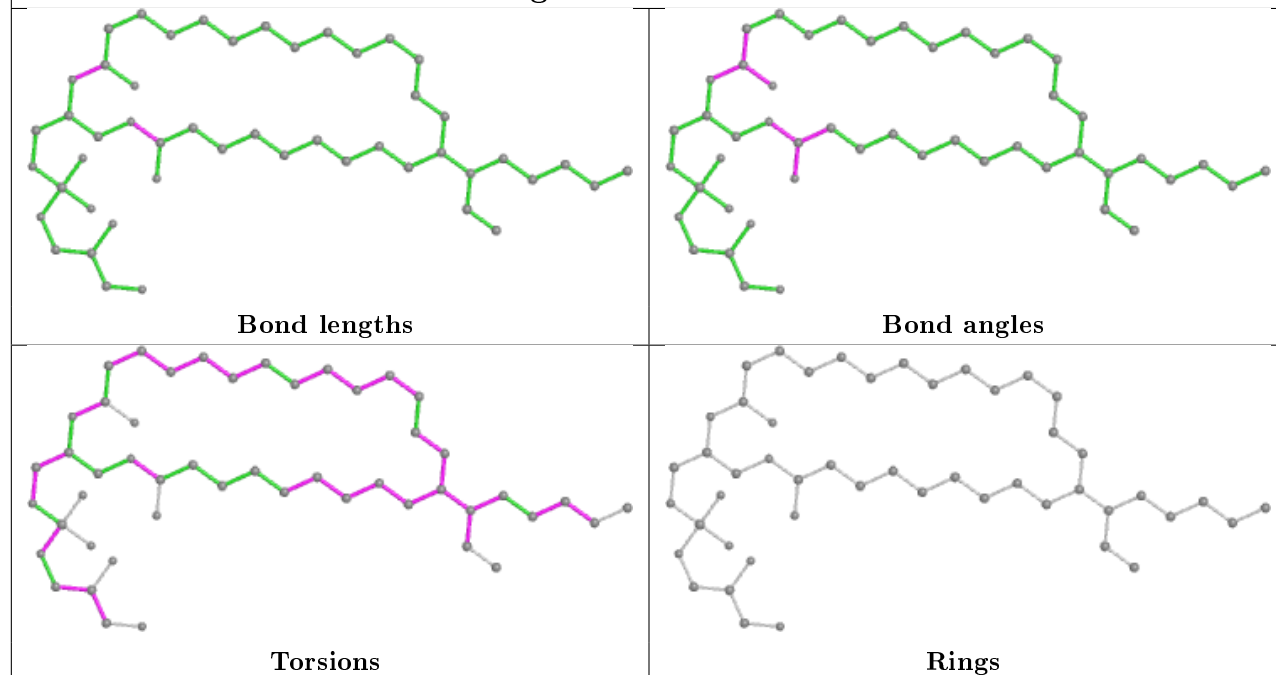


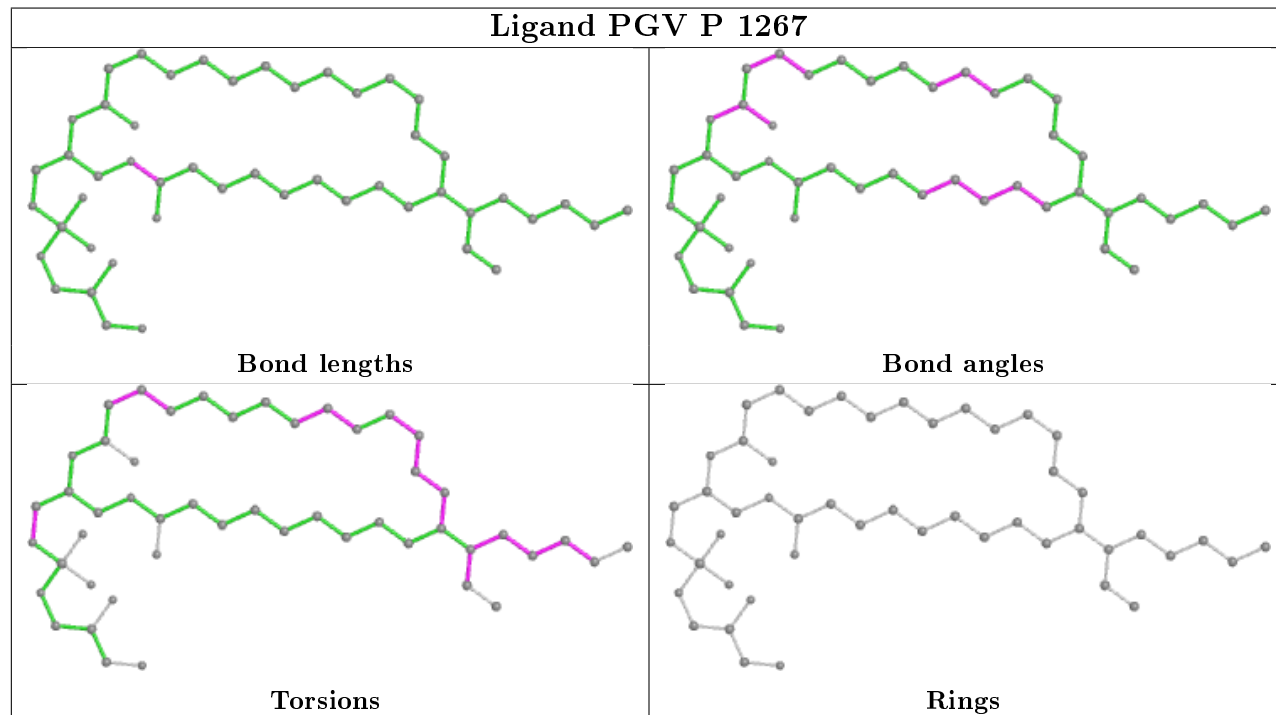
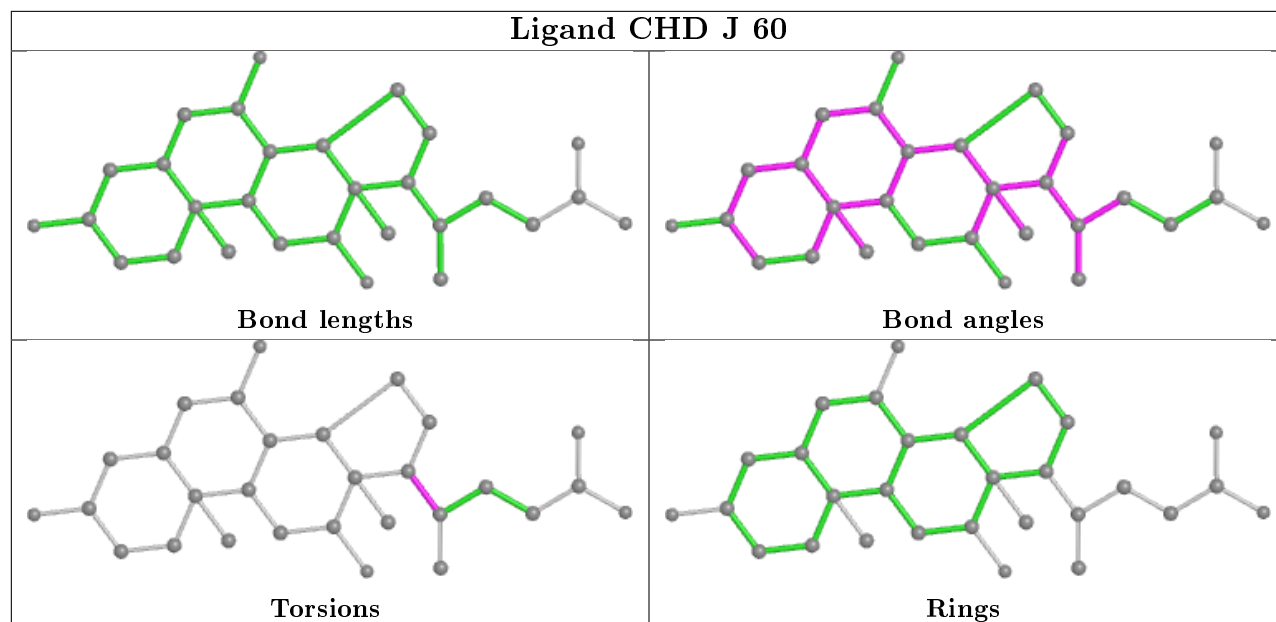


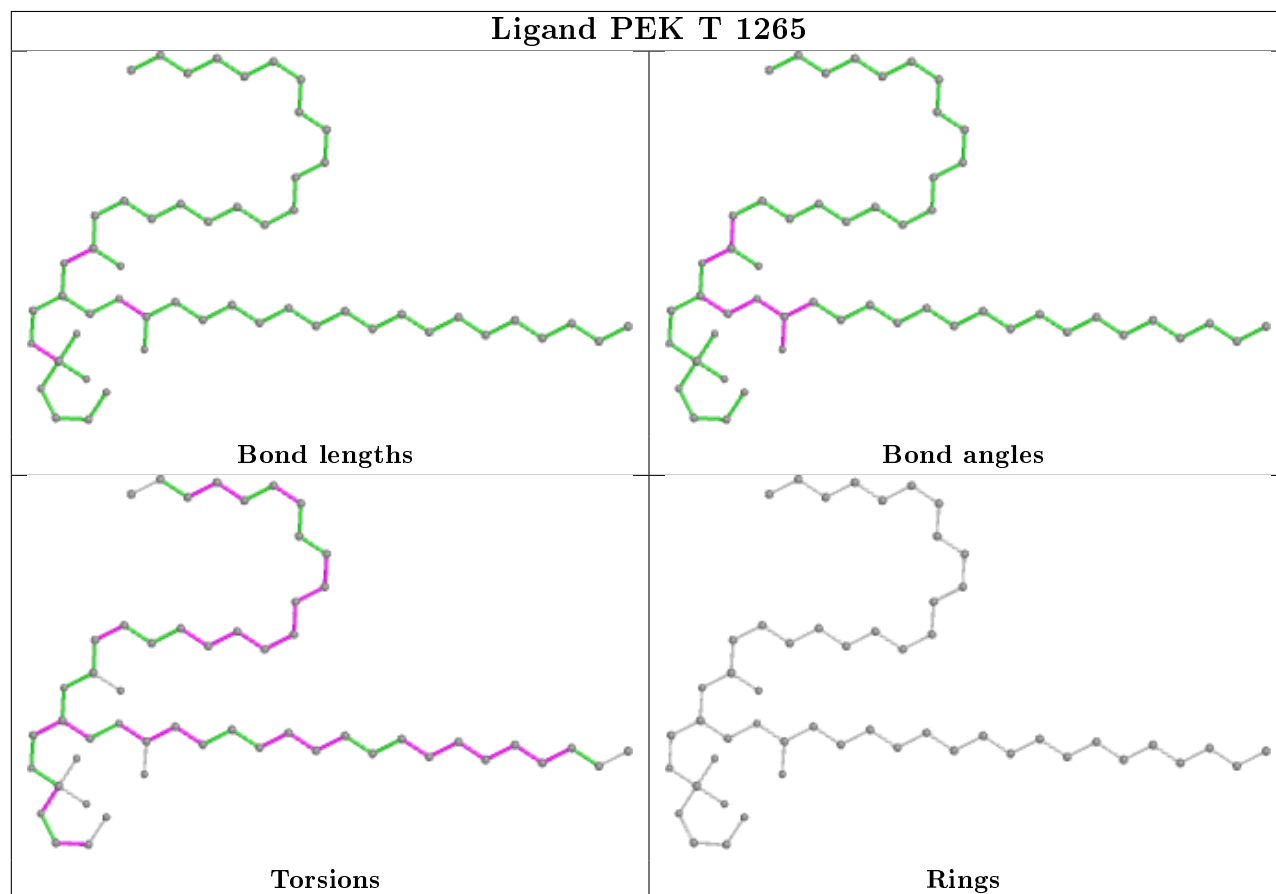
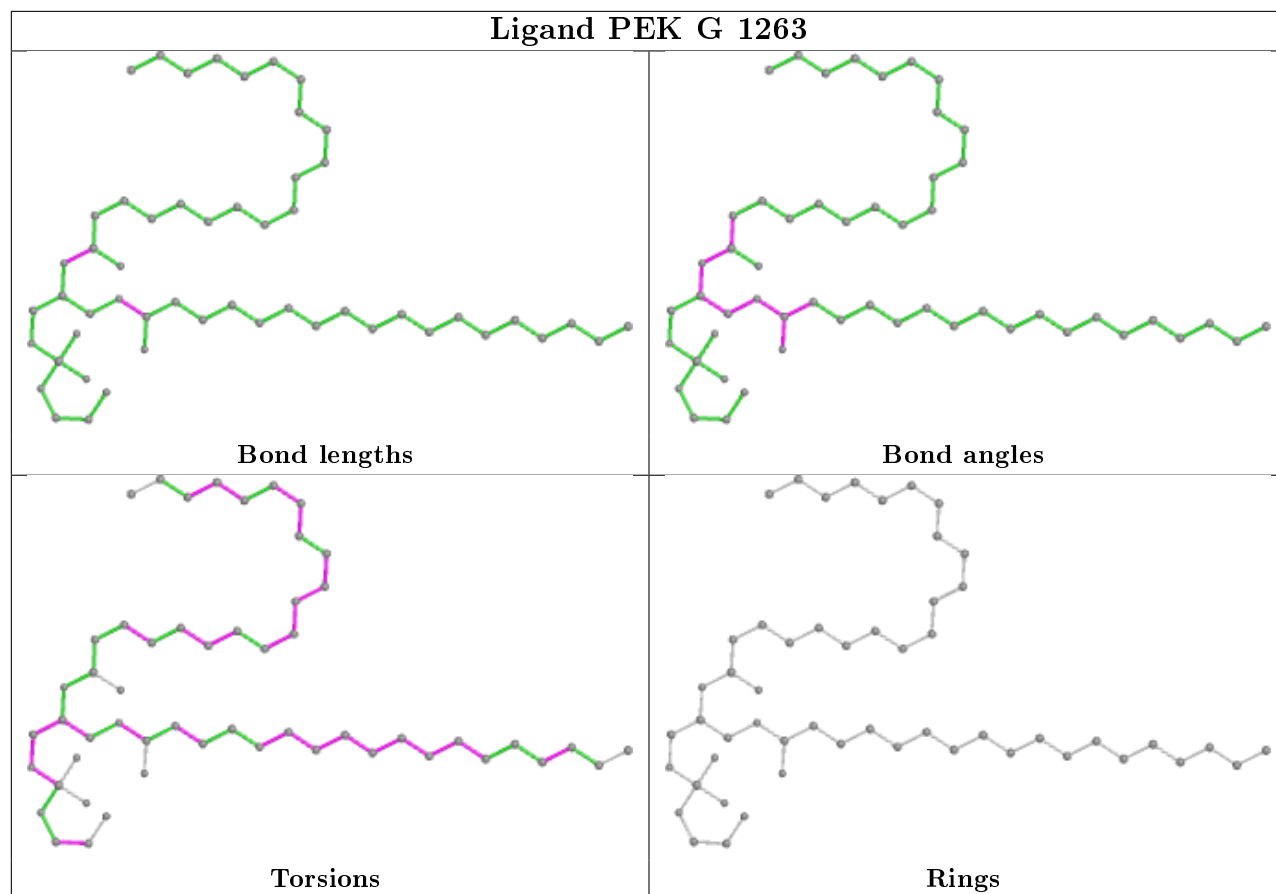
Ligand DMU M 526

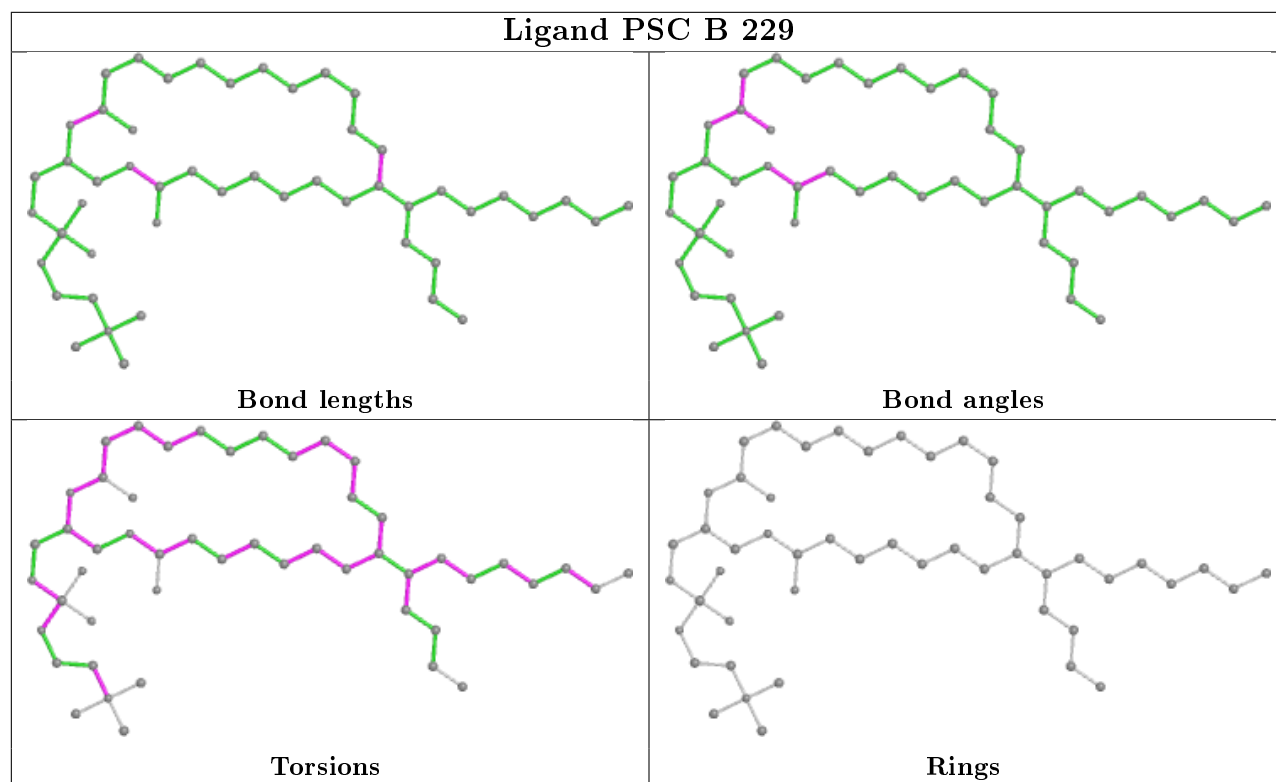
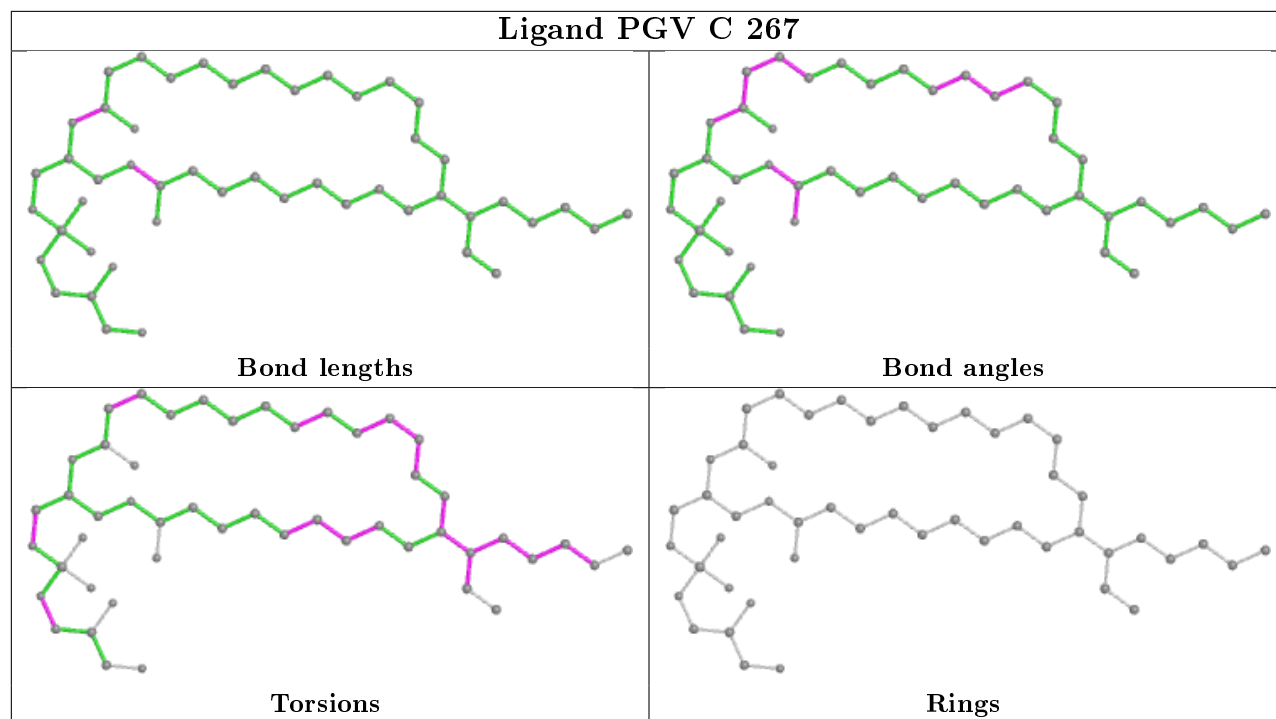


Ligand PGV C 268

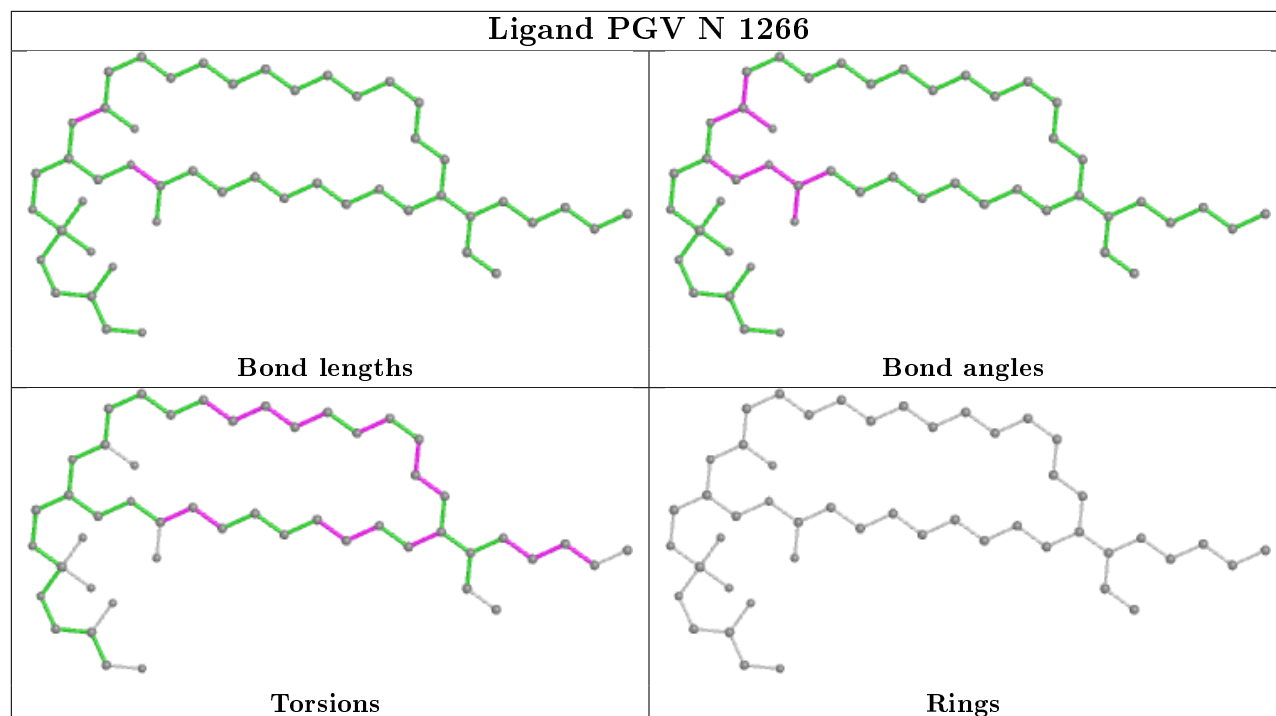




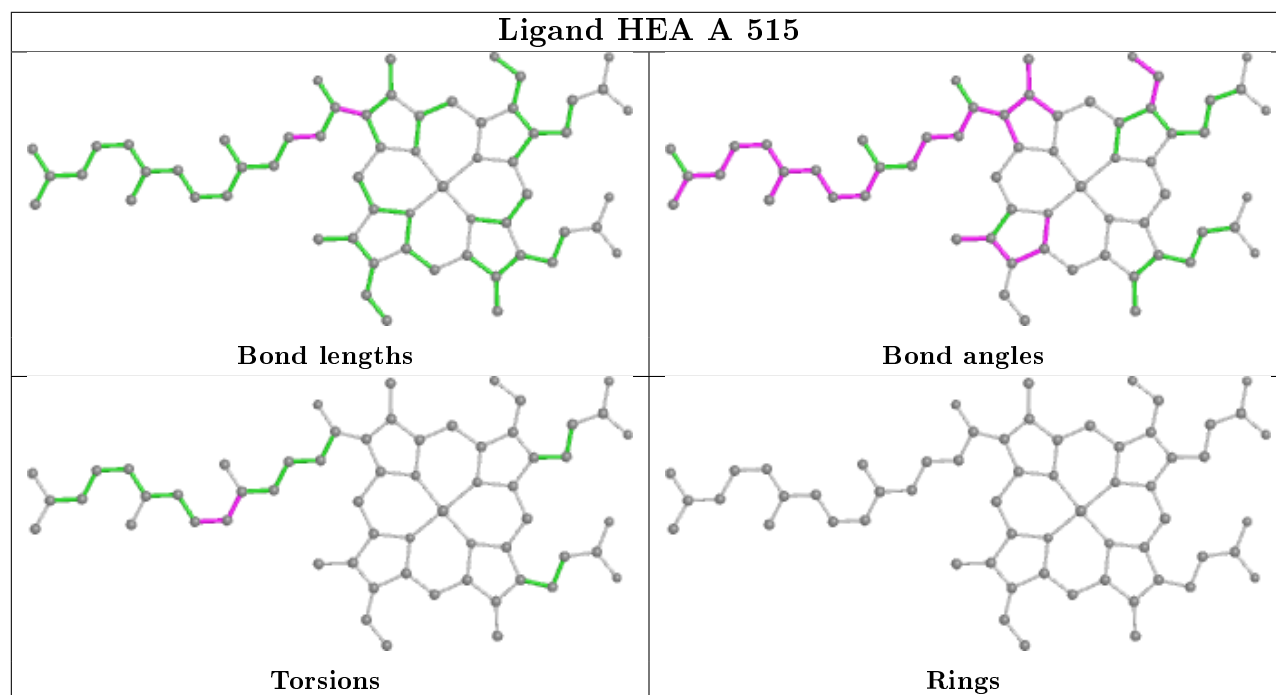


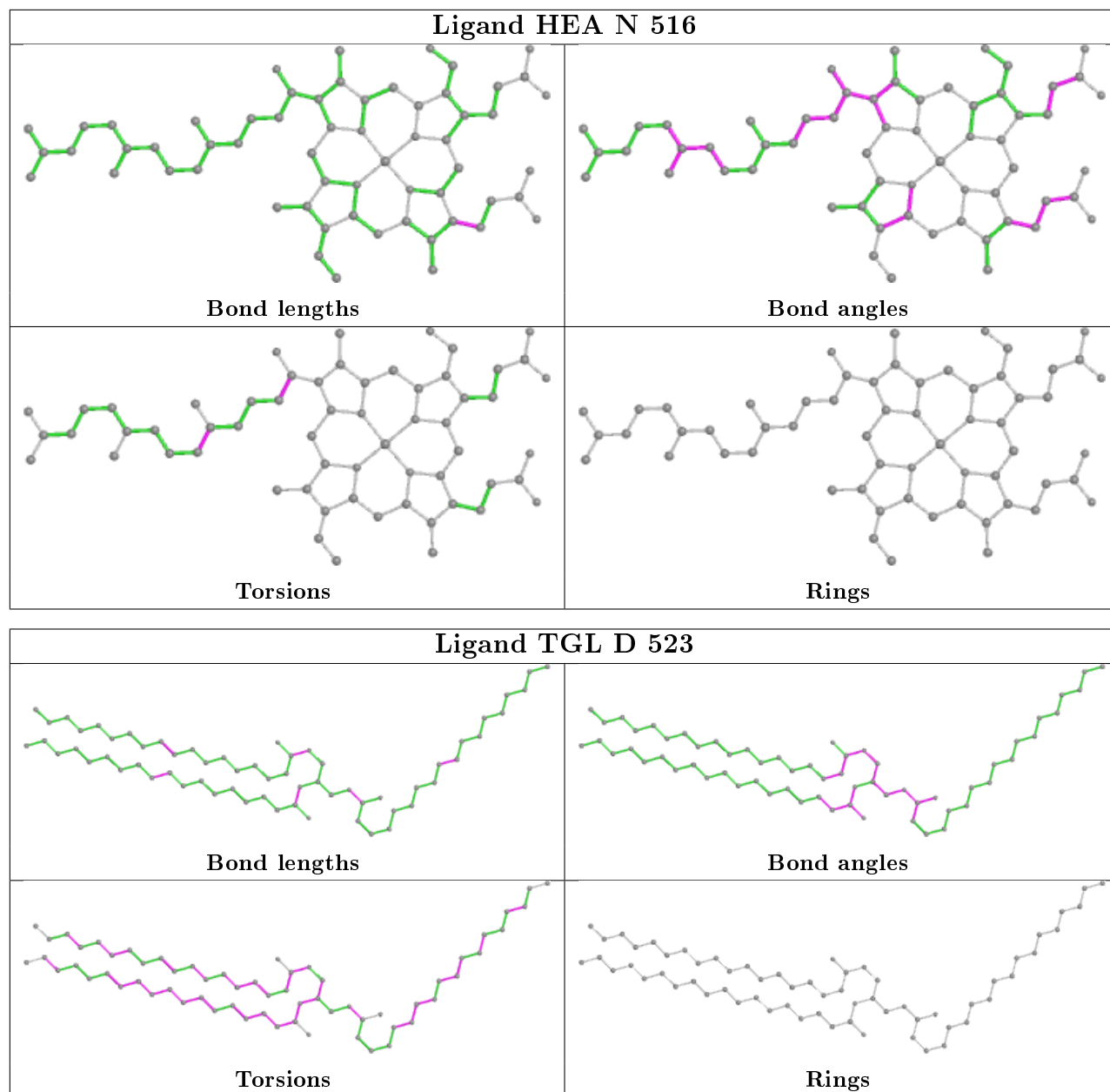


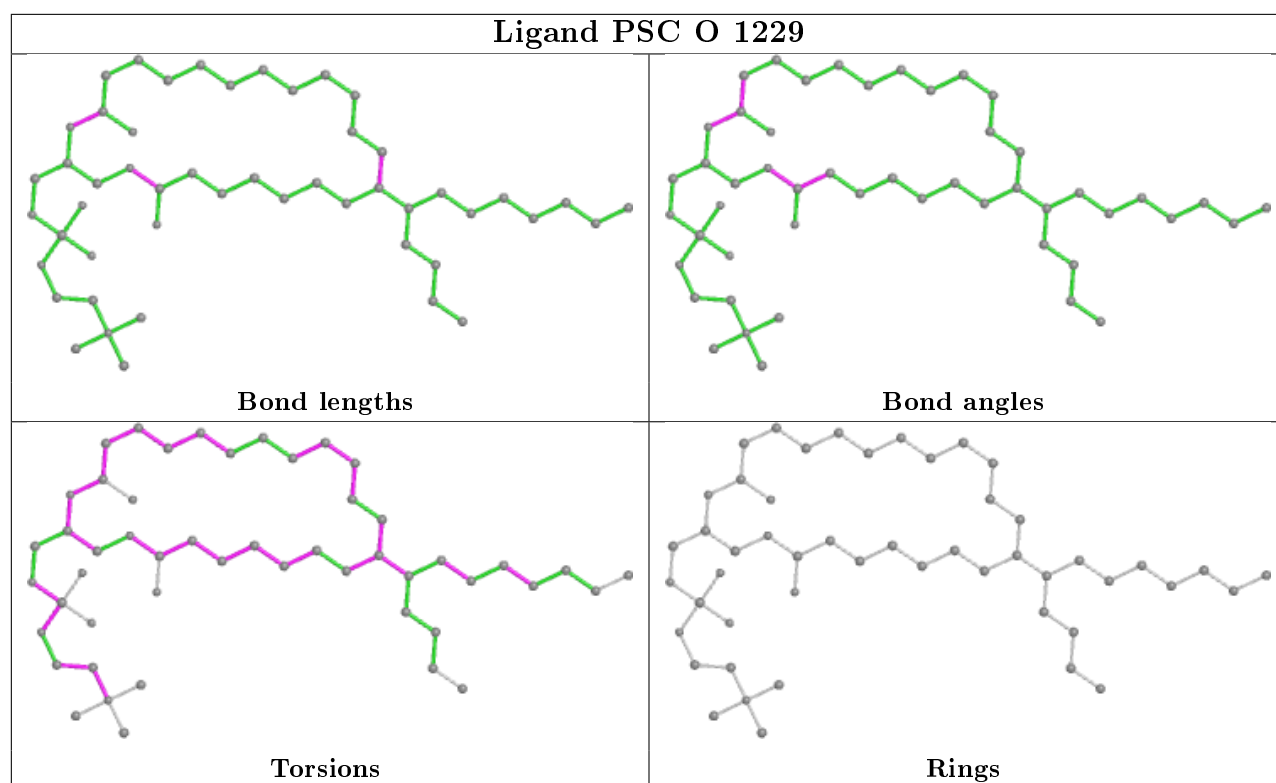
Ligand PGV N 1266



Ligand HEA A 515







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.01	0 100 100	15, 20, 27, 56	0
1	N	513/514 (99%)	-0.10	1 (0%) 95 96	17, 22, 29, 55	0
2	B	226/227 (99%)	-0.09	1 (0%) 92 95	14, 24, 51, 74	0
2	O	226/227 (99%)	0.01	8 (3%) 44 51	19, 27, 54, 72	0
3	C	259/261 (99%)	-0.01	1 (0%) 92 95	16, 22, 33, 52	0
3	P	259/261 (99%)	-0.05	1 (0%) 92 95	17, 23, 36, 55	0
4	D	144/147 (97%)	-0.32	0 100 100	17, 25, 44, 70	0
4	Q	144/147 (97%)	0.72	14 (9%) 7 10	24, 35, 59, 101	0
5	E	105/109 (96%)	-0.33	2 (1%) 66 73	16, 23, 51, 89	0
5	R	105/109 (96%)	0.13	4 (3%) 40 47	20, 27, 60, 91	0
6	F	98/98 (100%)	0.32	7 (7%) 16 21	18, 28, 75, 110	0
6	S	98/98 (100%)	0.54	8 (8%) 11 15	16, 26, 79, 108	0
7	G	83/85 (97%)	0.77	18 (21%) 0 1	16, 28, 95, 99	0
7	T	83/85 (97%)	0.93	18 (21%) 0 1	18, 29, 96, 100	0
8	H	79/85 (92%)	0.43	10 (12%) 3 5	20, 31, 79, 104	0
8	U	79/85 (92%)	0.54	9 (11%) 5 7	22, 32, 80, 105	0
9	I	72/73 (98%)	0.14	2 (2%) 53 60	19, 34, 58, 67	0
9	V	72/73 (98%)	0.27	6 (8%) 11 15	20, 39, 59, 83	0
10	J	58/59 (98%)	0.18	3 (5%) 27 34	22, 31, 60, 94	0
10	W	58/59 (98%)	0.21	3 (5%) 27 34	21, 32, 65, 99	0
11	K	49/56 (87%)	-0.16	0 100 100	23, 30, 40, 54	0
11	X	49/56 (87%)	0.23	2 (4%) 37 44	28, 36, 51, 66	0
12	L	46/47 (97%)	-0.02	1 (2%) 62 69	19, 26, 50, 74	0
12	Y	46/47 (97%)	0.04	1 (2%) 62 69	21, 28, 54, 78	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.04	1 (2%) 60 67	18, 24, 67, 94	0
13	Z	43/46 (93%)	0.28	5 (11%) 4 6	25, 31, 77, 98	0
All	All	3550/3614 (98%)	0.09	126 (3%) 44 51	14, 24, 55, 110	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	23.7
4	Q	5	VAL	22.0
4	Q	4	SER	17.7
4	Q	6	VAL	17.7
6	F	97	ALA	10.6
6	S	98	HIS	9.5
13	Z	43	SER	9.3
6	F	96	LEU	9.3
6	F	98	HIS	8.6
4	Q	8	SER	8.5
7	T	8	HIS	8.4
6	S	94	HIS	8.4
6	F	1	ALA	8.2
10	W	58	LYS	8.1
10	J	58	LYS	7.3
13	Z	42	LYS	7.0
7	G	8	HIS	7.0
9	I	37	PHE	6.9
4	Q	7	LYS	6.8
5	R	5	HIS	6.8
5	R	109	VAL	6.7
8	U	7	LYS	6.7
3	P	3	HIS	6.5
6	S	1	ALA	6.5
8	H	7	LYS	5.9
2	O	226	MET	5.8
11	X	6	ALA	5.7
7	T	2	SER	5.7
7	T	42	ARG	5.6
6	F	95	GLN	5.6
6	S	96	LEU	5.5
7	T	3	ALA	5.5
7	T	40	GLY	5.5
8	H	47	GLY	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	46	LYS	5.3
10	J	1	PHE	5.3
7	G	3	ALA	5.2
7	T	7	ASP	5.0
6	S	95	GLN	4.9
8	U	8	ILE	4.8
9	V	2	THR	4.8
7	T	5	LYS	4.8
7	T	10	GLY	4.7
7	T	36	TRP	4.7
7	G	42	ARG	4.7
5	E	5	HIS	4.6
2	O	227	LEU	4.5
7	G	5	LYS	4.5
7	G	36	TRP	4.5
7	G	6	GLY	4.4
7	G	4	ALA	4.4
10	W	57	HIS	4.3
2	O	90	ILE	4.3
12	L	2	HIS	4.2
12	Y	47	LYS	4.2
7	T	84	LYS	4.2
6	S	2	SER	4.2
7	G	2	SER	4.1
7	T	1	ALA	4.0
8	H	45	ALA	3.9
7	G	39	SER	3.9
8	U	45	ALA	3.9
2	O	113	TYR	3.9
4	Q	35	ALA	3.9
13	Z	41	LYS	3.8
8	H	8	ILE	3.7
8	U	47	GLY	3.5
5	E	109	VAL	3.5
7	T	4	ALA	3.5
6	F	94	HIS	3.5
8	H	48	GLY	3.5
7	G	7	ASP	3.4
2	O	91	ASN	3.4
13	M	43	SER	3.3
6	F	2	SER	3.2
7	T	39	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	V	37	PHE	3.2
8	U	46	LYS	3.1
7	G	43	GLU	3.1
8	U	48	GLY	3.1
4	Q	39	ALA	3.1
4	Q	10	ASP	3.0
6	S	93	PRO	2.9
4	Q	58	GLU	2.8
5	R	108	LYS	2.8
9	V	3	ALA	2.8
7	G	41	HIS	2.8
8	H	10	ASN	2.7
2	O	59	GLN	2.7
4	Q	33	LEU	2.7
8	U	44	THR	2.7
7	G	40	GLY	2.7
8	H	49	ASP	2.7
8	H	44	THR	2.6
7	T	12	GLY	2.6
9	I	25	PHE	2.5
9	V	5	ALA	2.5
11	X	7	PRO	2.5
13	Z	40	TYR	2.5
10	J	57	HIS	2.5
7	G	9	GLY	2.4
7	G	10	GLY	2.4
4	Q	31	LYS	2.4
7	G	84	LYS	2.4
2	B	59	GLN	2.4
7	T	41	HIS	2.4
7	T	9	GLY	2.4
8	U	49	ASP	2.4
4	Q	28	ALA	2.3
9	V	73	LYS	2.3
9	V	15	ARG	2.3
7	T	33	LEU	2.3
8	H	9	LYS	2.2
2	O	217	LYS	2.2
3	C	3	HIS	2.2
8	U	52	VAL	2.2
4	Q	51	LEU	2.2
1	N	513	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	45	PRO	2.2
13	Z	39	ASN	2.1
7	G	37	LEU	2.1
4	Q	147	LYS	2.0
2	O	130	PRO	2.0
10	W	48	TYR	2.0
7	T	6	GLY	2.0
5	R	79	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.44	0.36	63,71,87,88	0
9	SAC	V	1	9/10	0.48	0.58	88,90,91,91	0
7	TPO	T	11	11/12	0.52	0.36	66,73,89,89	0
9	SAC	I	1	9/10	0.56	0.44	76,79,82,83	0
1	FME	A	1	10/11	0.89	0.17	36,39,58,66	0
1	FME	N	1	10/11	0.94	0.21	37,41,58,60	0
2	FME	B	1	10/11	0.95	0.17	23,24,33,45	0
2	FME	O	1	10/11	0.97	0.20	25,26,33,38	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	PEK	T	263	53/53	0.47	0.42	51,91,109,111	0
22	CHD	W	1059	29/29	0.48	0.42	95,105,107,107	0

Continued on next page...

Continued from previous page...

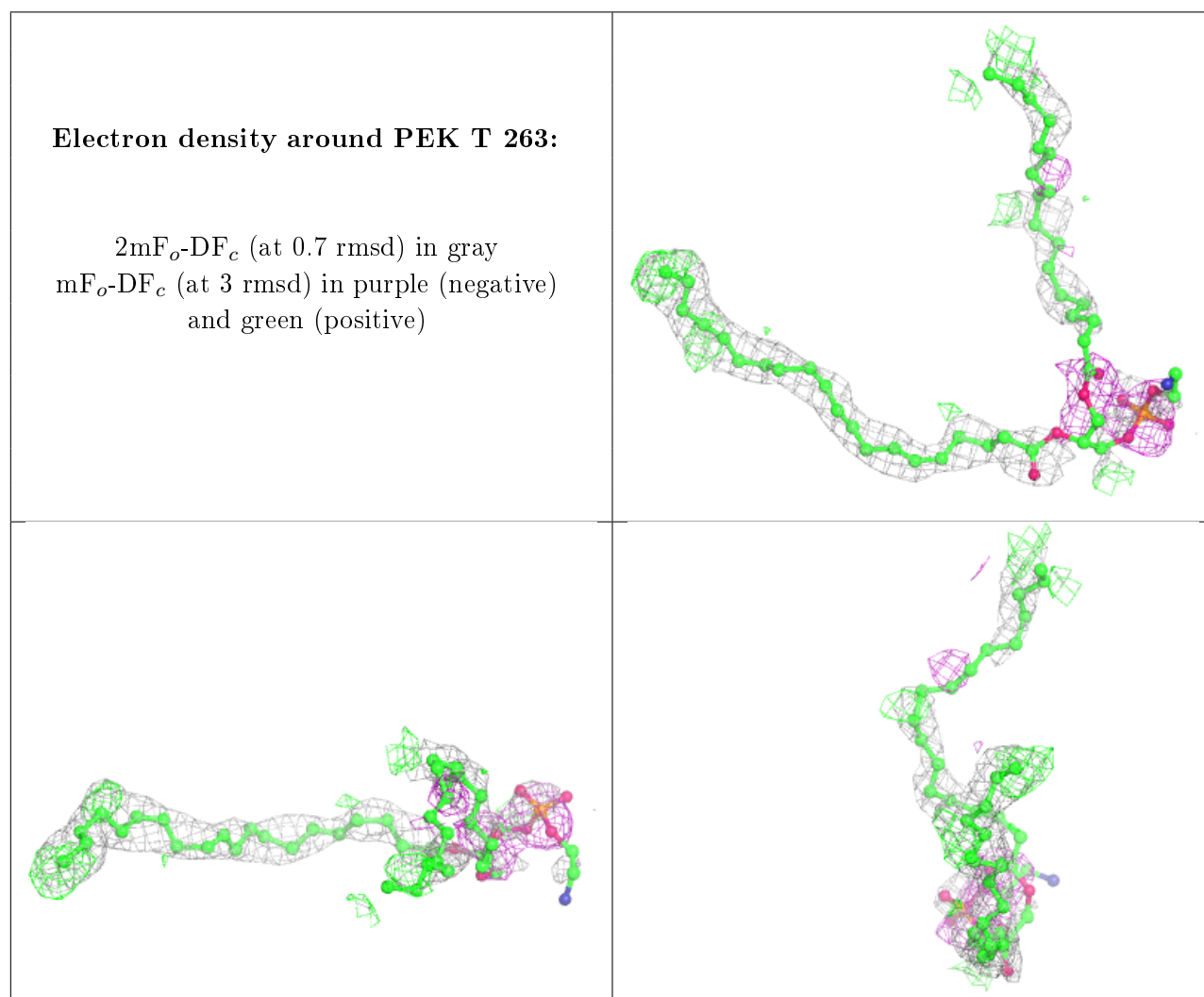
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CHD	J	60	29/29	0.52	0.41	99,107,110,111	0
24	PEK	C	265	53/53	0.53	0.32	43,91,99,100	0
23	UNX	P	262	1/1	0.54	0.28	44,44,44,44	0
24	PEK	T	1265	53/53	0.54	0.34	42,90,101,102	0
25	CDL	T	1269	100/100	0.56	0.36	56,86,108,109	0
24	PEK	G	1263	53/53	0.58	0.36	55,94,110,110	0
19	PGV	P	1268	51/51	0.59	0.34	77,90,102,103	0
25	CDL	G	269	100/100	0.61	0.36	65,85,106,111	0
19	PGV	C	268	51/51	0.61	0.32	63,88,101,102	0
18	TGL	Q	1523	63/63	0.64	0.28	49,74,91,92	0
18	TGL	N	1522	63/63	0.64	0.32	47,71,84,86	0
23	UNX	C	262	1/1	0.64	0.42	43,43,43,43	0
21	PSC	O	1229	52/52	0.65	0.35	40,85,110,113	0
21	PSC	B	229	52/52	0.67	0.33	48,92,113,115	0
19	PGV	N	1524	51/51	0.70	0.34	43,69,102,102	0
25	CDL	P	1270	100/100	0.73	0.36	45,85,107,109	0
18	TGL	L	522	63/63	0.74	0.30	38,62,80,83	0
19	PGV	A	524	51/51	0.74	0.30	34,69,94,96	0
22	CHD	P	1271	29/29	0.74	0.24	82,90,91,91	0
25	CDL	C	270	100/100	0.75	0.36	42,84,106,108	0
18	TGL	D	523	63/63	0.75	0.26	50,69,91,91	0
22	CHD	C	271	29/29	0.76	0.26	79,89,90,91	0
18	TGL	N	1521	63/63	0.79	0.27	48,73,88,91	0
16	MG	N	518	1/1	0.81	0.13	23,23,23,23	0
18	TGL	A	521	63/63	0.82	0.25	50,70,88,92	0
27	DMU	Z	1526	33/33	0.92	0.18	37,45,57,57	0
16	MG	A	518	1/1	0.93	0.10	21,21,21,21	0
27	DMU	M	526	33/33	0.93	0.13	34,40,51,52	0
24	PEK	T	1264	53/53	0.94	0.16	19,44,71,73	0
14	HEA	N	515	60/60	0.95	0.19	20,33,50,53	0
22	CHD	P	1525	29/29	0.95	0.11	24,28,31,33	0
24	PEK	G	264	53/53	0.95	0.18	17,41,71,72	0
22	CHD	C	525	29/29	0.96	0.13	24,29,32,33	0
19	PGV	C	267	51/51	0.96	0.18	17,29,64,69	0
17	NA	N	519	1/1	0.97	0.07	24,24,24,24	0
19	PGV	P	1267	51/51	0.97	0.18	19,29,65,69	0
19	PGV	N	1266	51/51	0.97	0.17	19,38,57,59	0
19	PGV	A	522	51/51	0.97	0.17	19,32,54,56	0
22	CHD	B	1085	29/29	0.97	0.11	12,15,23,33	0
20	CUA	O	228	2/2	0.97	0.12	22,22,22,22	0
14	HEA	A	515	60/60	0.98	0.16	14,19,41,50	0
14	HEA	N	516	60/60	0.98	0.14	15,19,26,30	0

Continued on next page...

Continued from previous page...

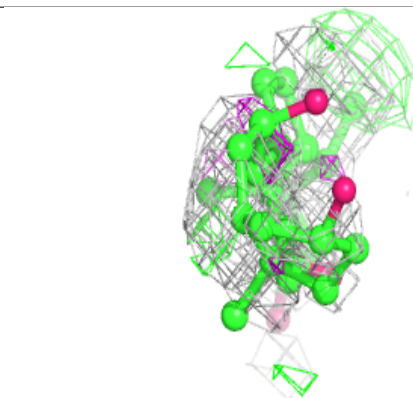
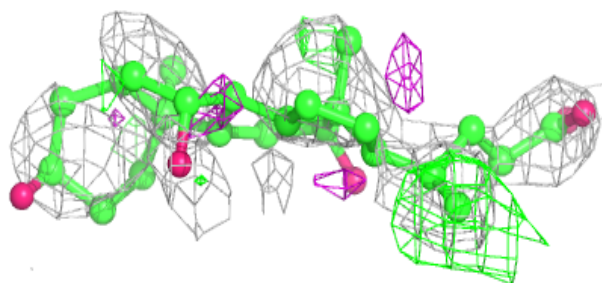
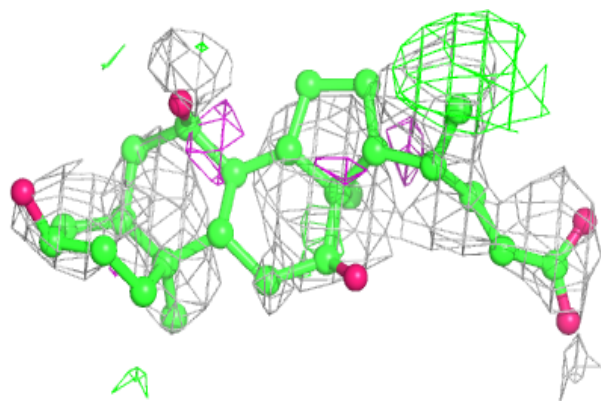
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CHD	G	229	29/29	0.98	0.10	10,16,19,25	0
14	HEA	A	516	60/60	0.98	0.14	11,18,24,26	0
17	NA	A	519	1/1	0.98	0.08	22,22,22,22	0
26	ZN	F	99	1/1	0.99	0.15	23,23,23,23	0
15	CU	A	517	1/1	0.99	0.19	20,20,20,20	0
15	CU	N	517	1/1	0.99	0.20	23,23,23,23	0
20	CUA	B	228	2/2	0.99	0.14	18,18,18,18	0
26	ZN	S	99	1/1	0.99	0.14	23,23,23,23	0

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

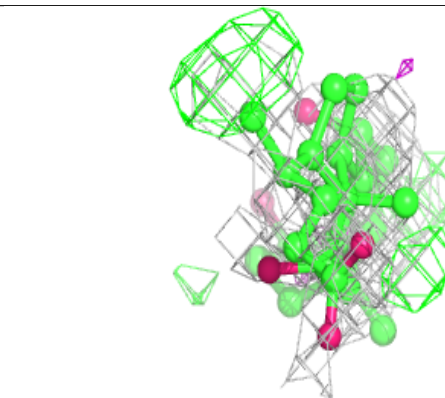
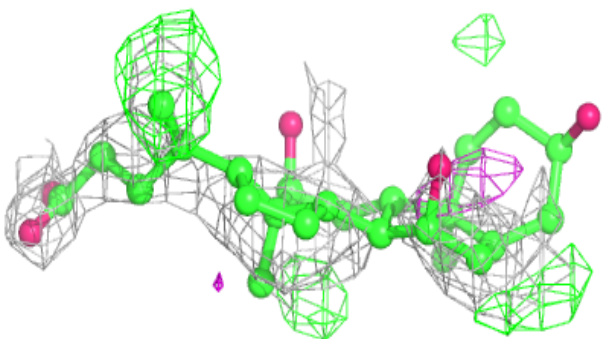
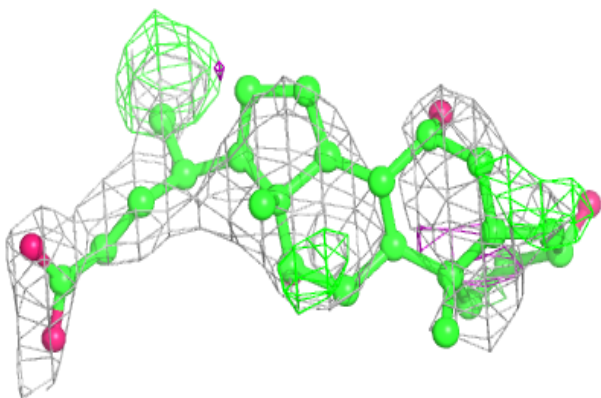


Electron density around CHD W 1059:

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

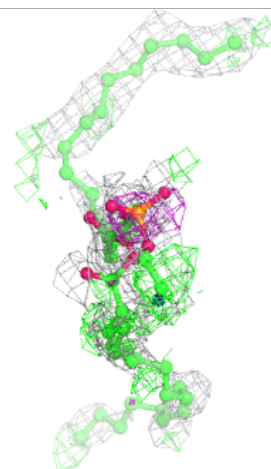
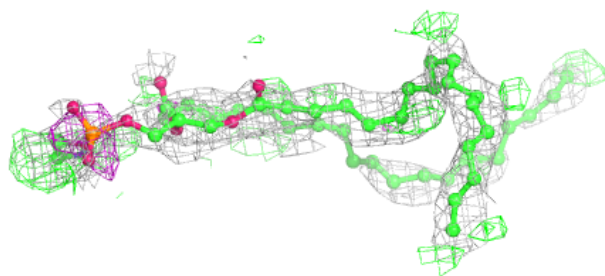
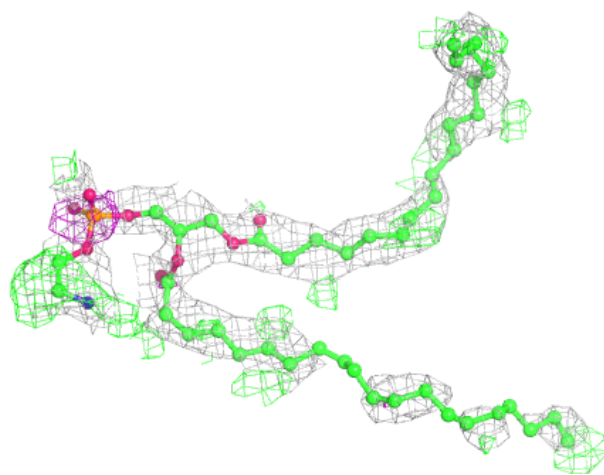
**Electron density around CHD J 60:**

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



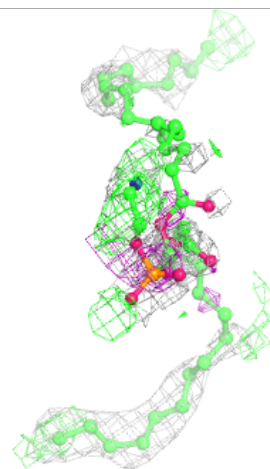
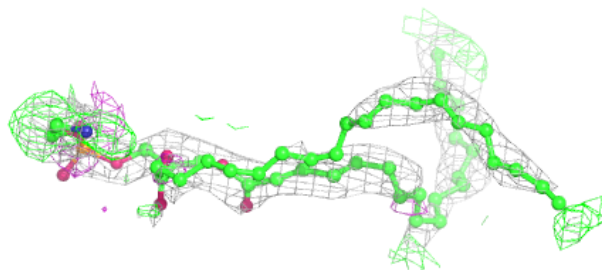
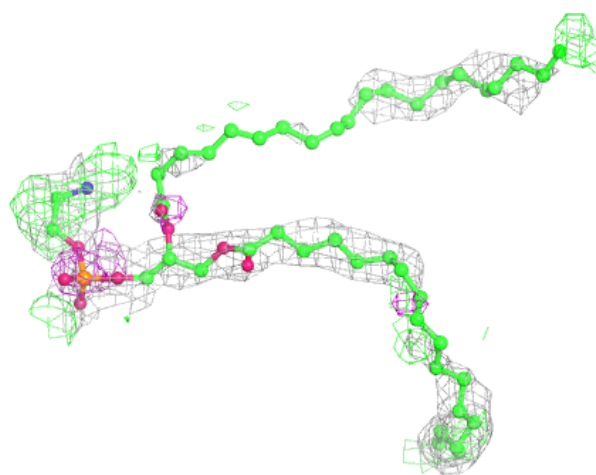
Electron density around PEK C 265:

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



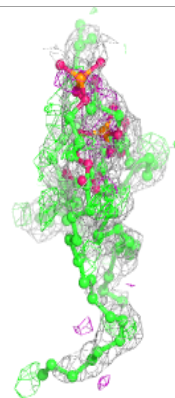
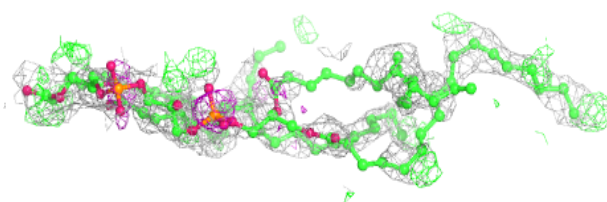
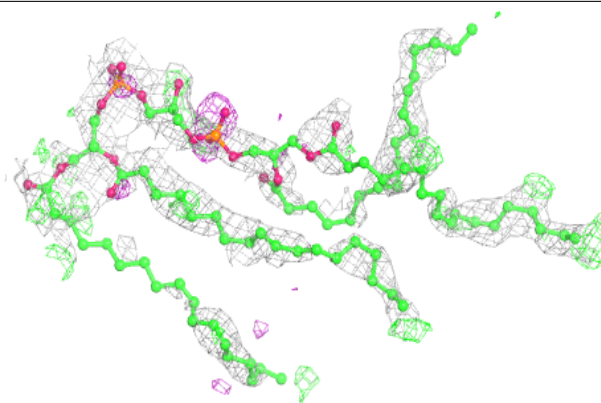
Electron density around PEK T 1265:

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



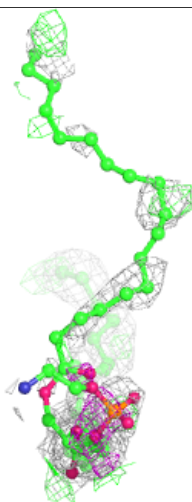
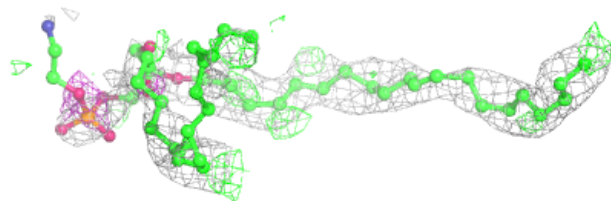
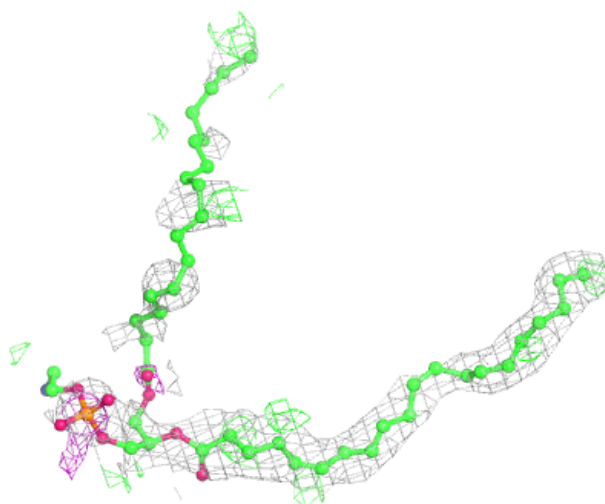
Electron density around CDL T 1269:

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



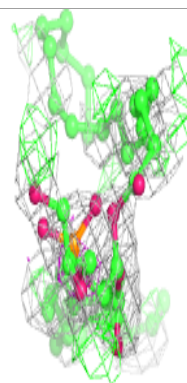
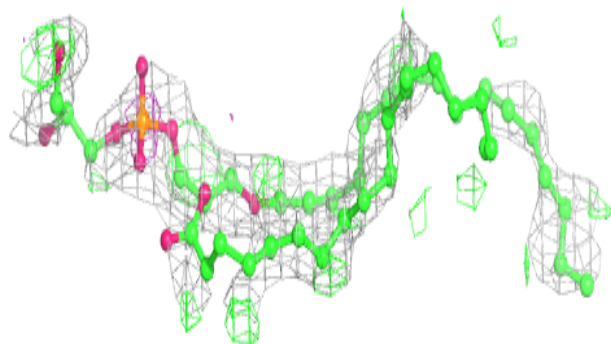
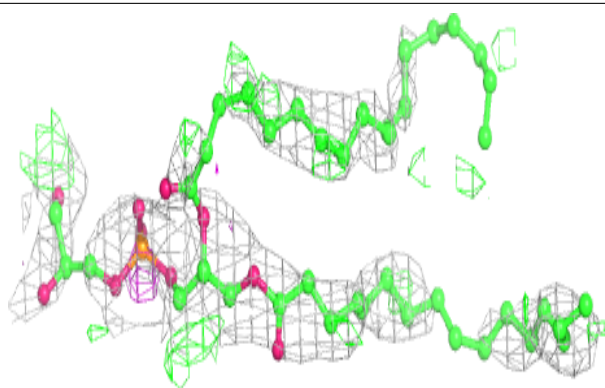
Electron density around PEK G 1263:

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

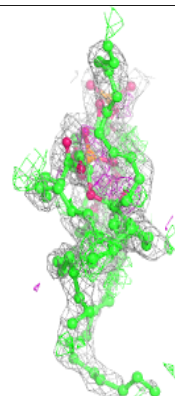
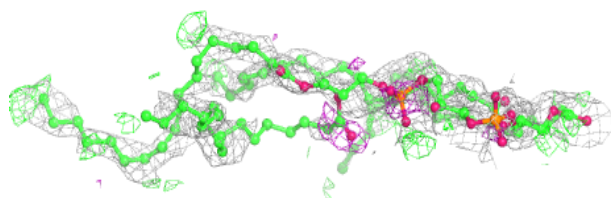
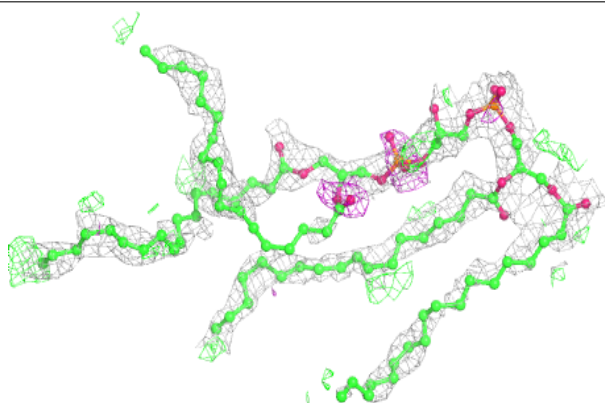


Electron density around PGV P 1268:

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

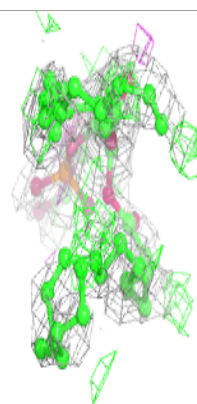
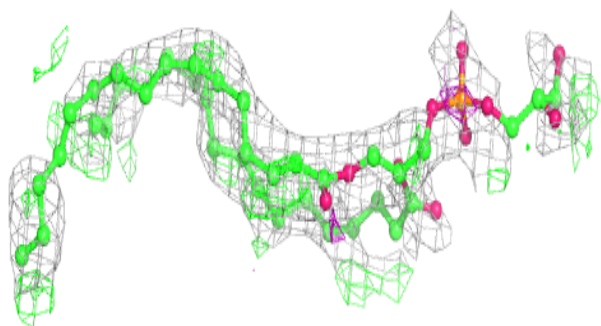
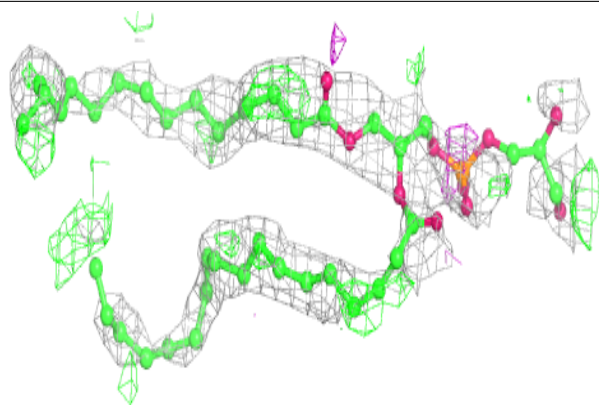
**Electron density around CDL G 269:**

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

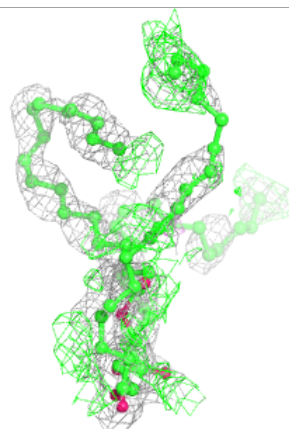
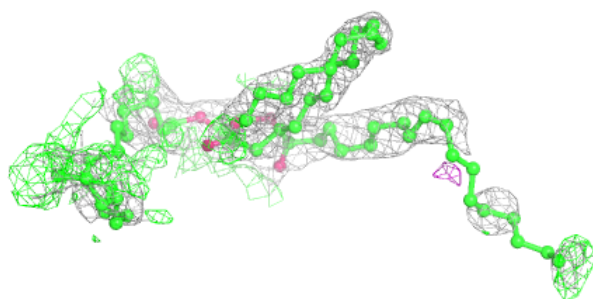
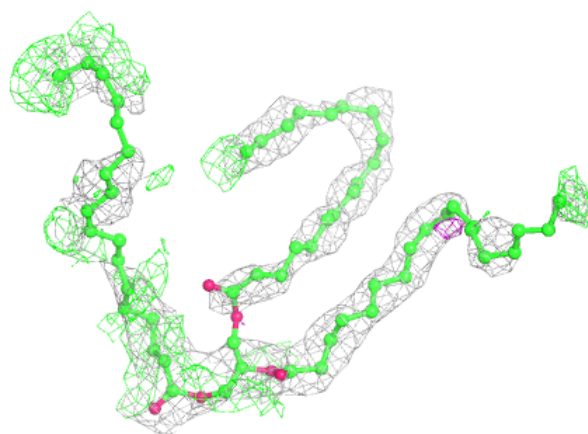


Electron density around PGV C 268:

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

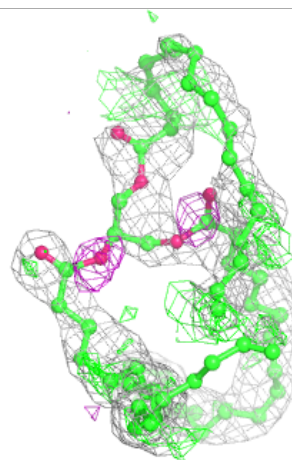
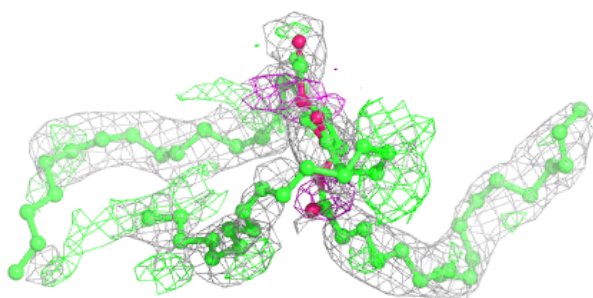
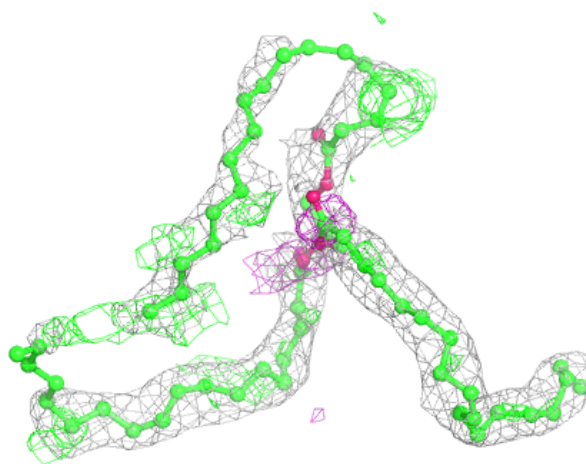
**Electron density around TGL Q 1523:**

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



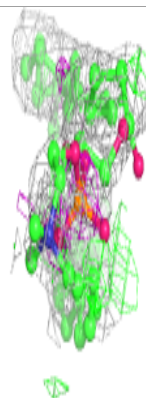
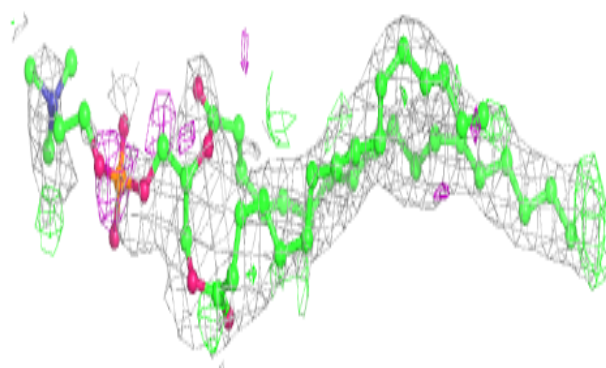
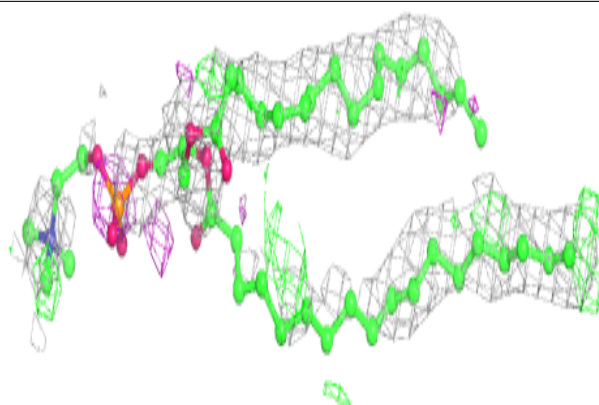
Electron density around TGL N 1522:

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

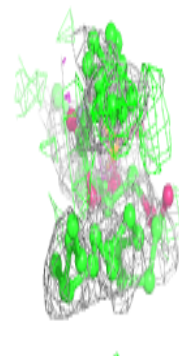
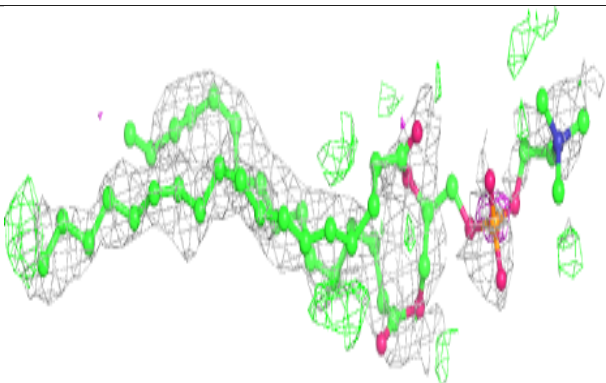
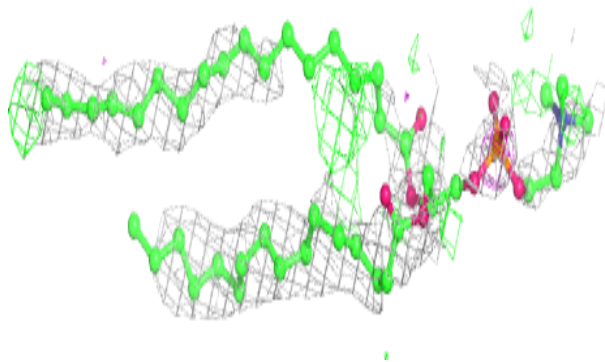


Electron density around PSC O 1229:

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

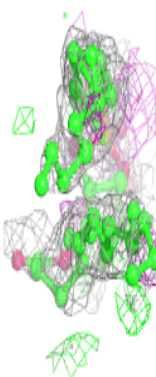
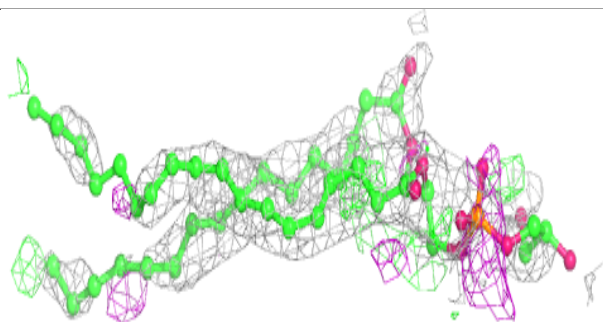
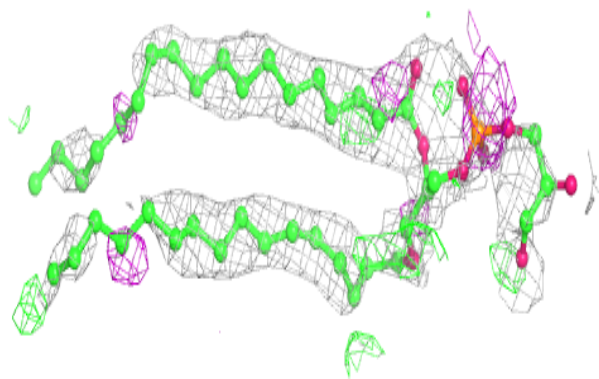
**Electron density around PSC B 229:**

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

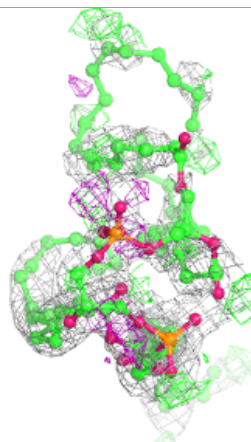
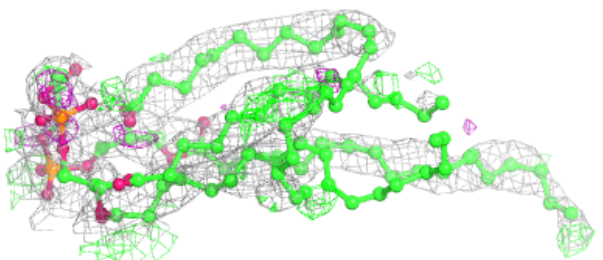
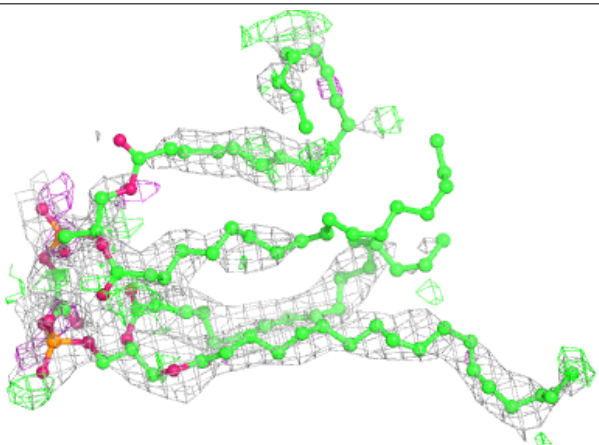


Electron density around PGV N 1524:

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

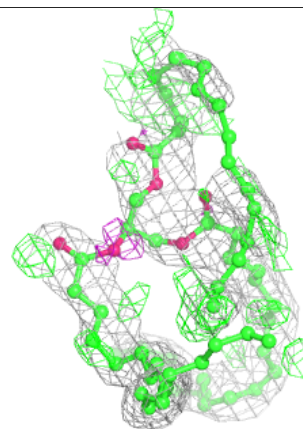
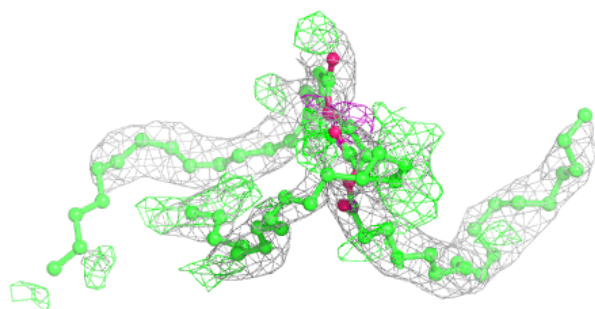
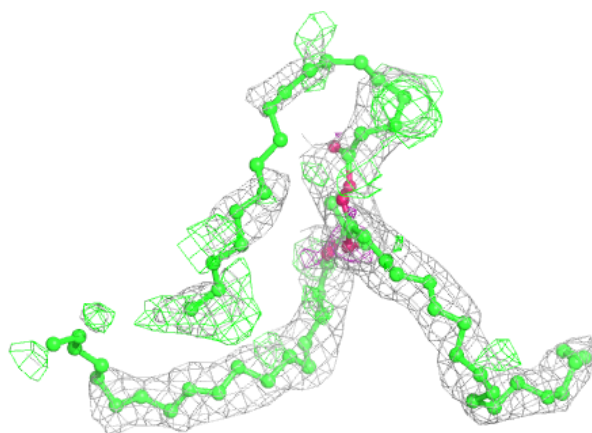
**Electron density around CDL P 1270:**

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

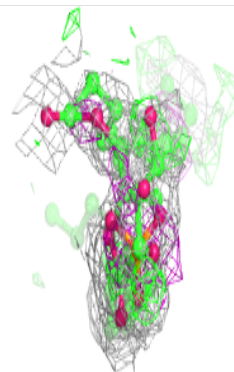
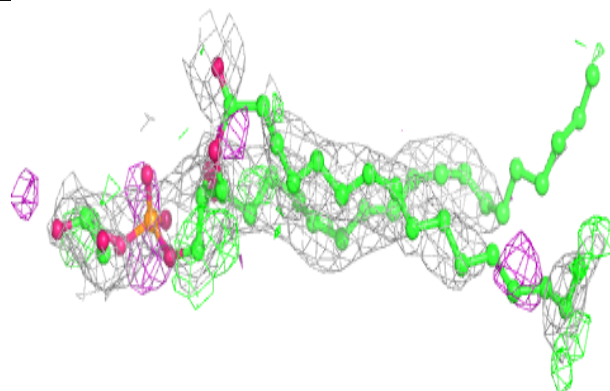
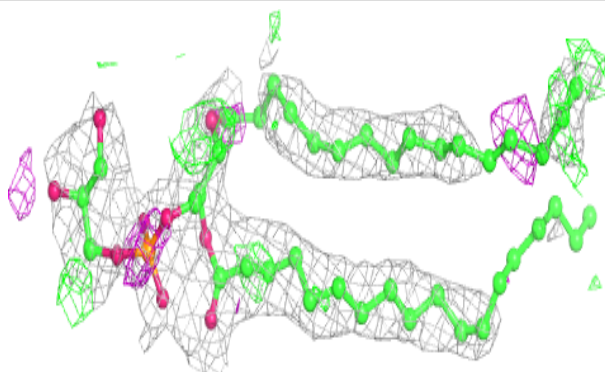


Electron density around TGL L 522:

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

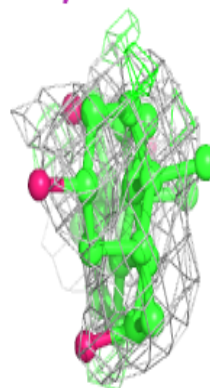
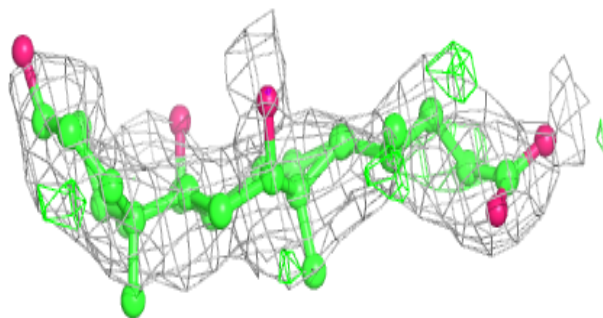
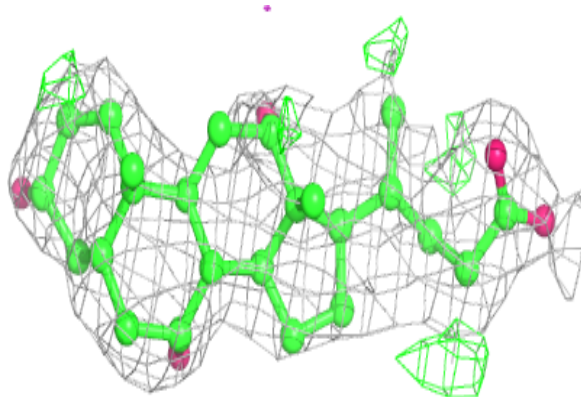
**Electron density around PGV A 524:**

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



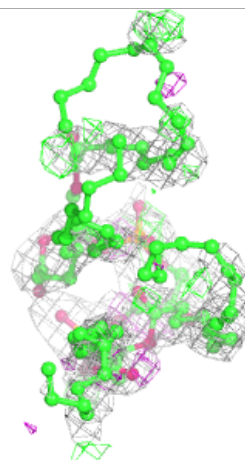
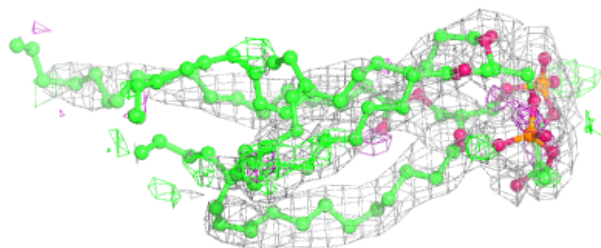
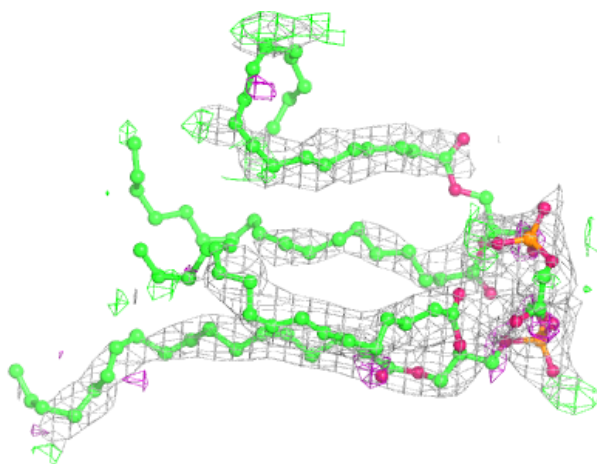
Electron density around CHD P 1271:

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



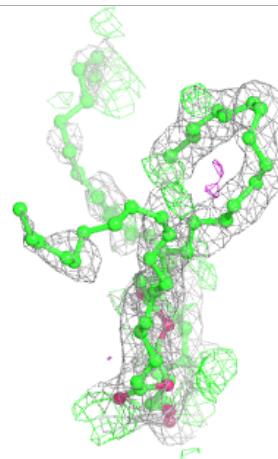
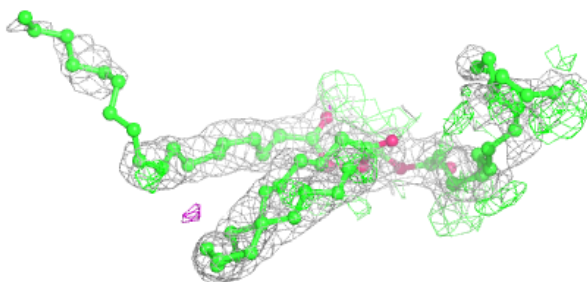
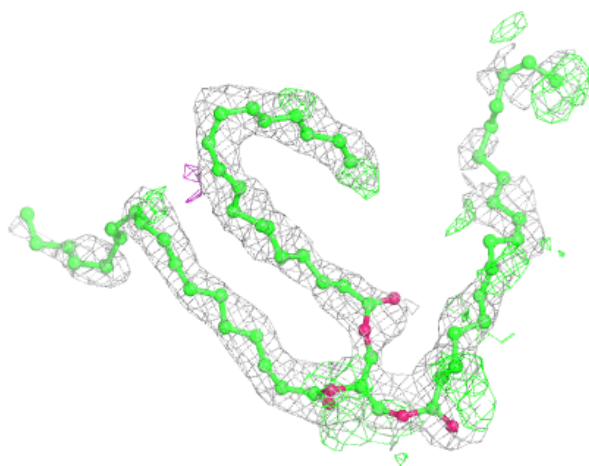
Electron density around CDL C 270:

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



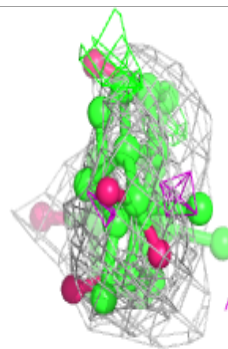
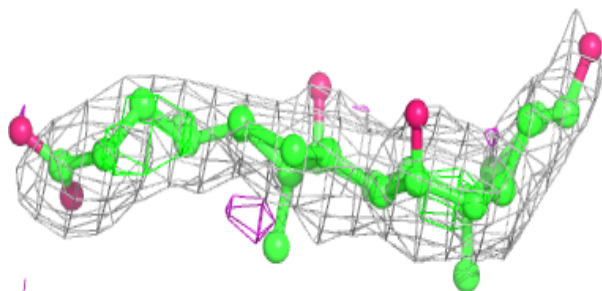
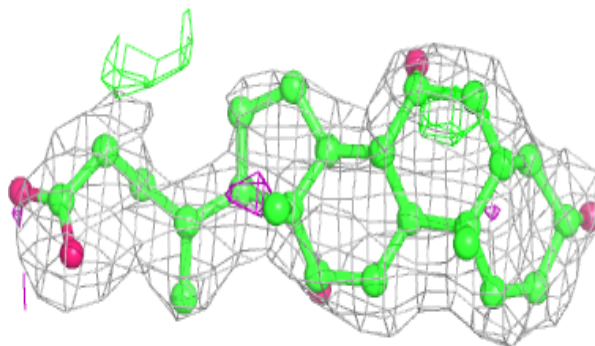
Electron density around TGL D 523:

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

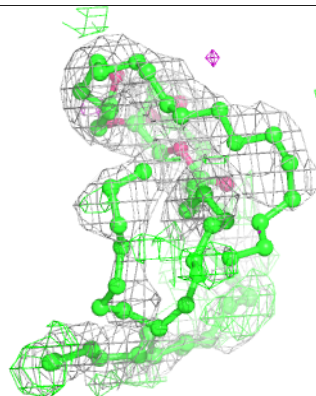
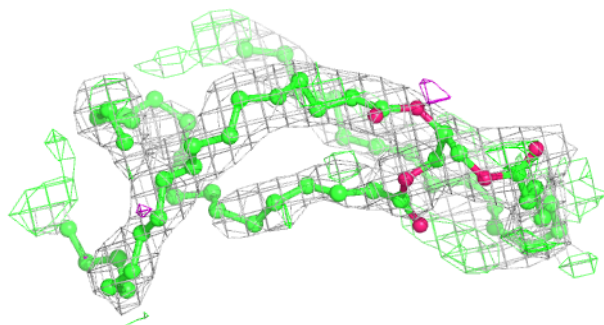
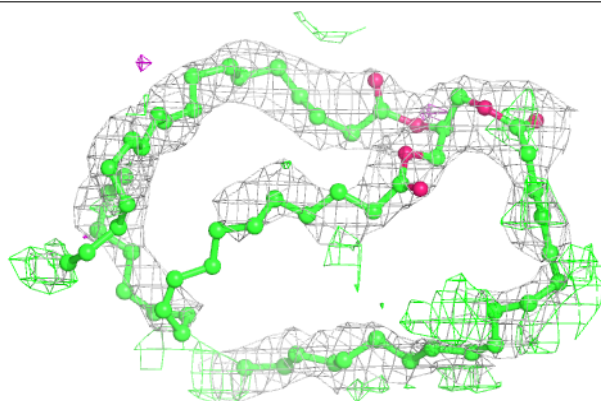


Electron density around CHD C 271:

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

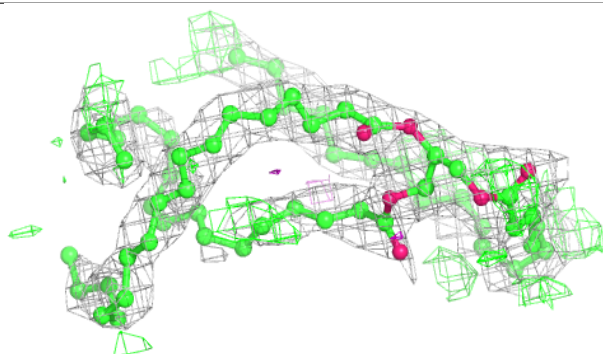
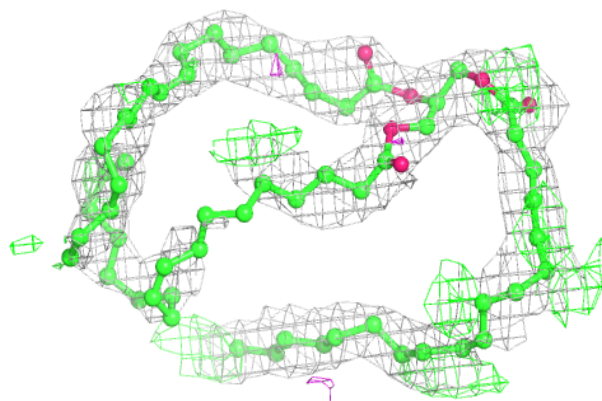
**Electron density around TGL N 1521:**

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

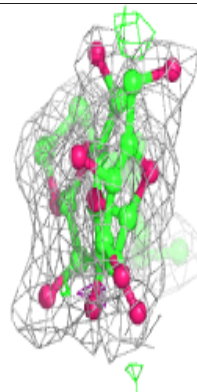
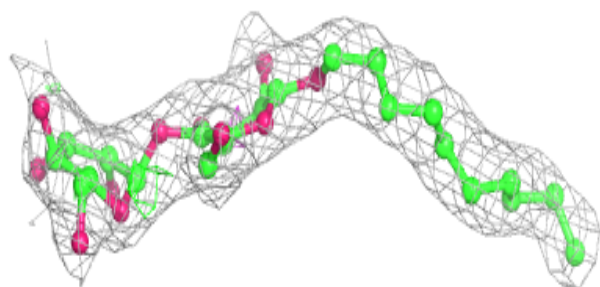
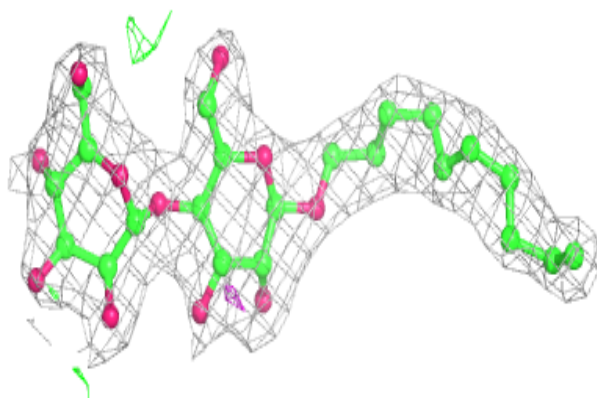


Electron density around TGL A 521:

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

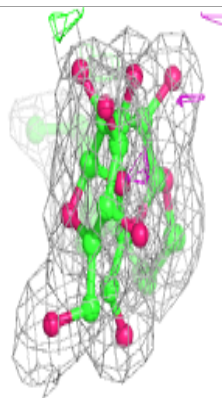
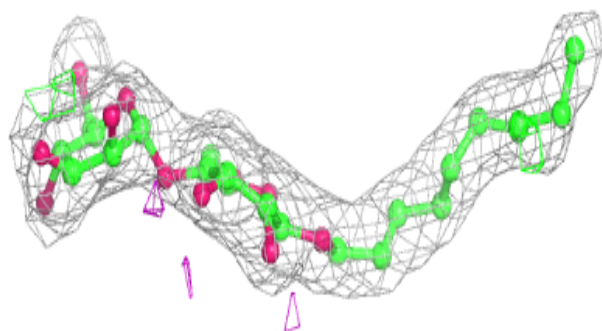
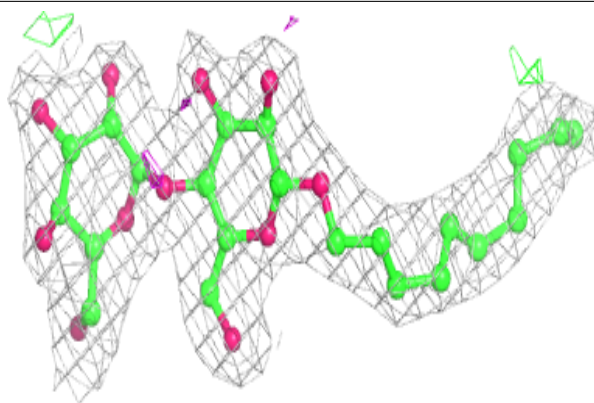
**Electron density around DMU Z 1526:**

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

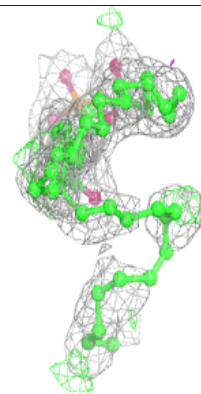
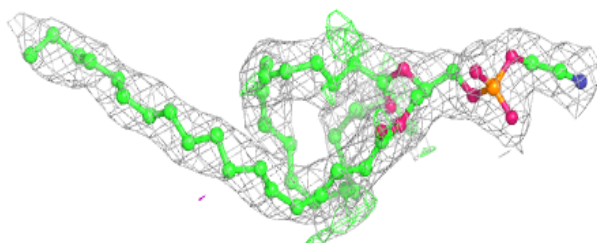
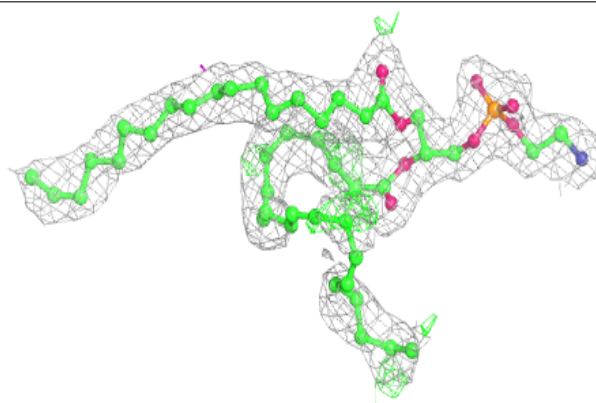


Electron density around DMU M 526:

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

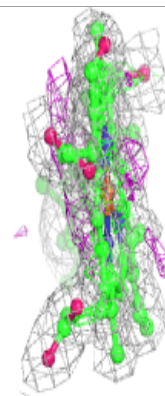
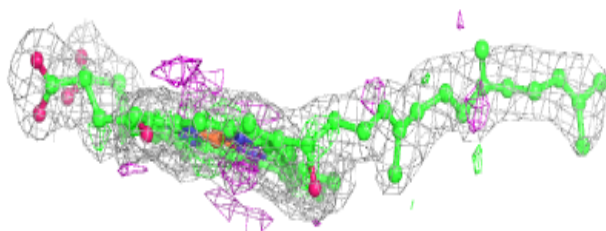
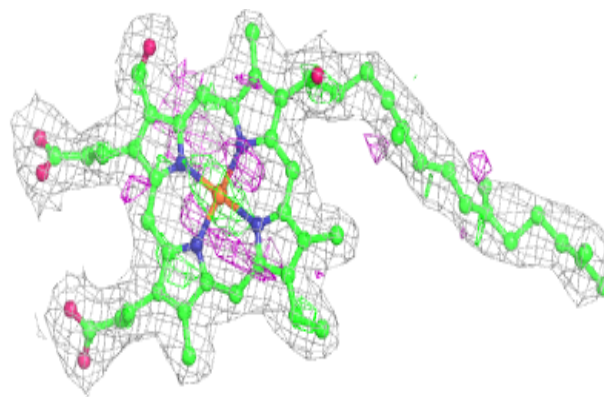
**Electron density around PEK T 1264:**

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

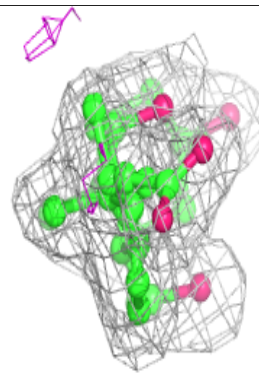
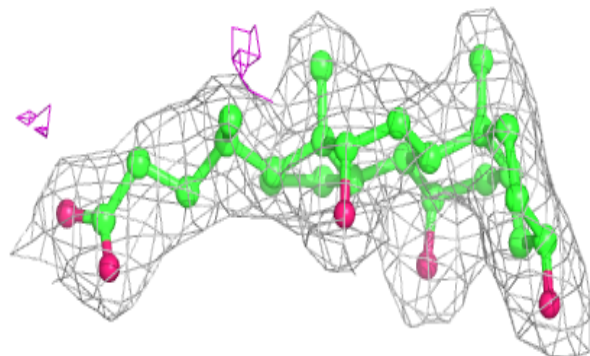
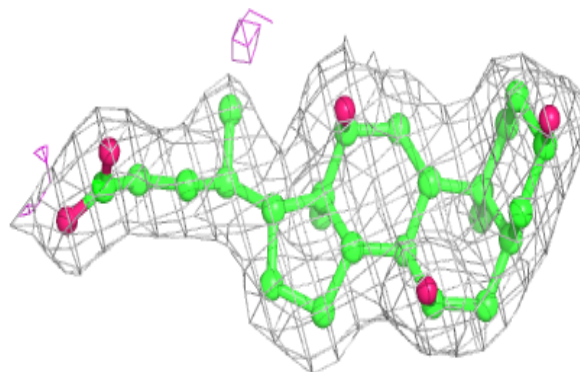


Electron density around HEA N 515:

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

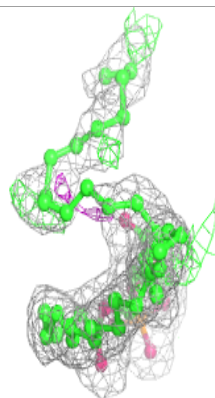
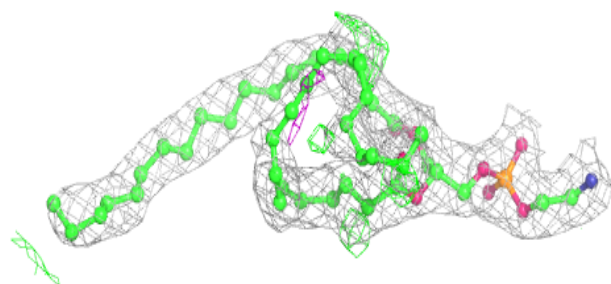
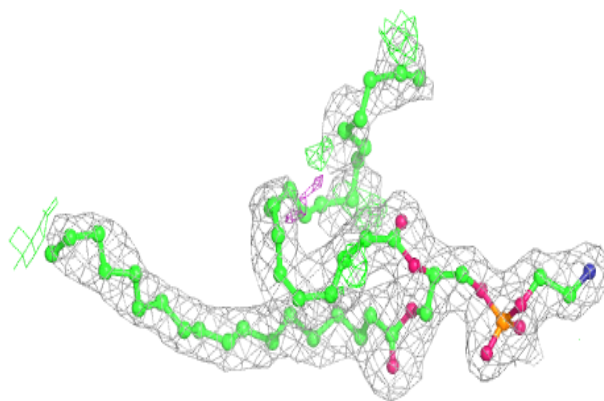
**Electron density around CHD P 1525:**

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

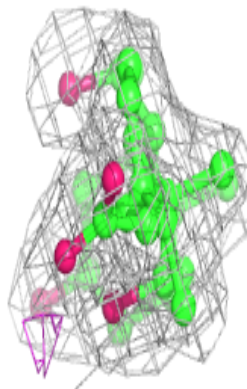
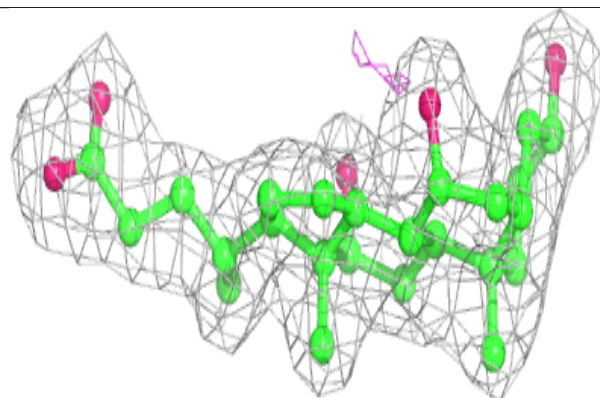
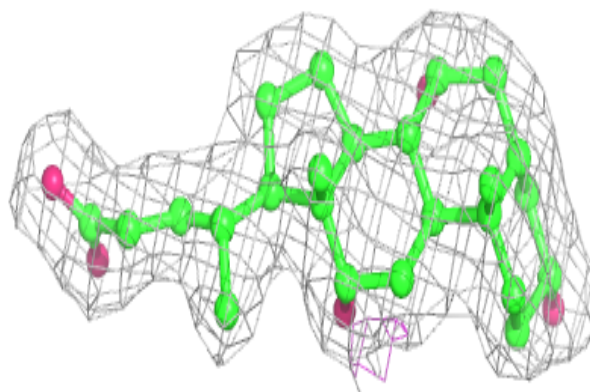


Electron density around PEK G 264:

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

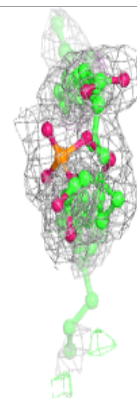
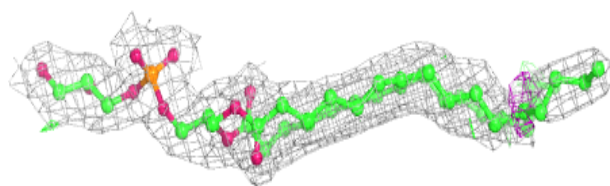
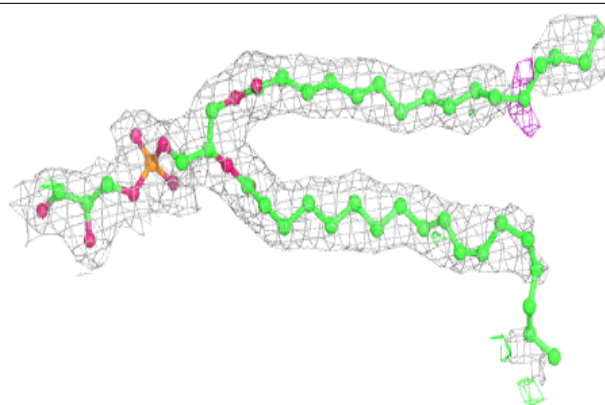
**Electron density around CHD C 525:**

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

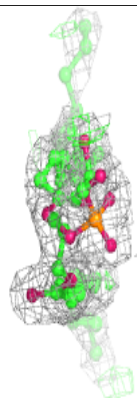
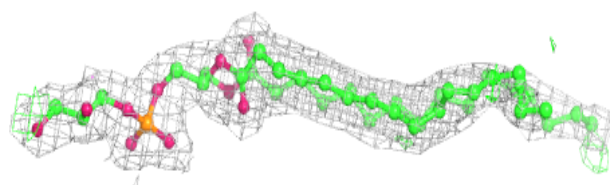
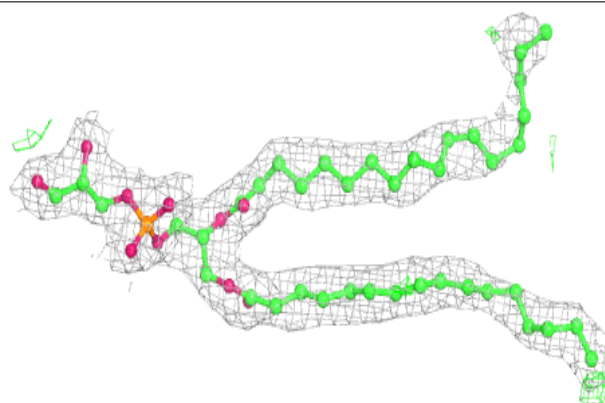


Electron density around PGV C 267:

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

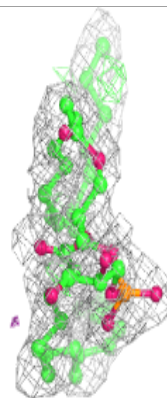
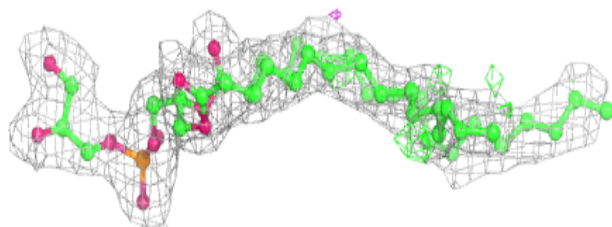
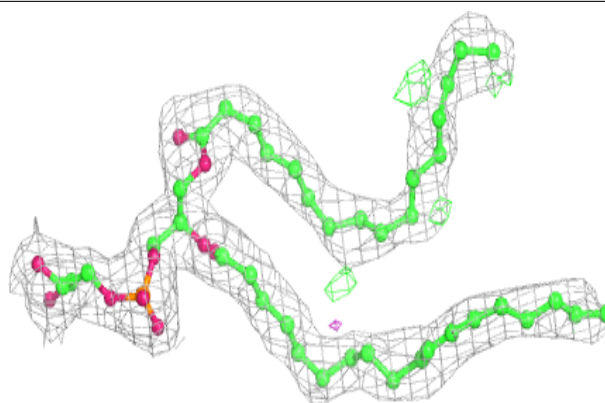
**Electron density around PGV P 1267:**

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

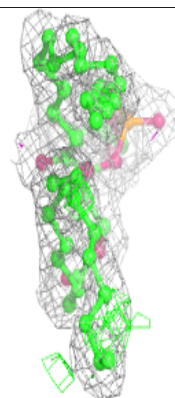
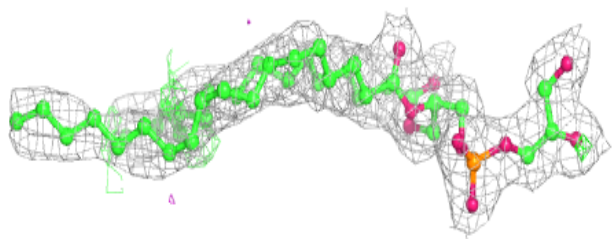
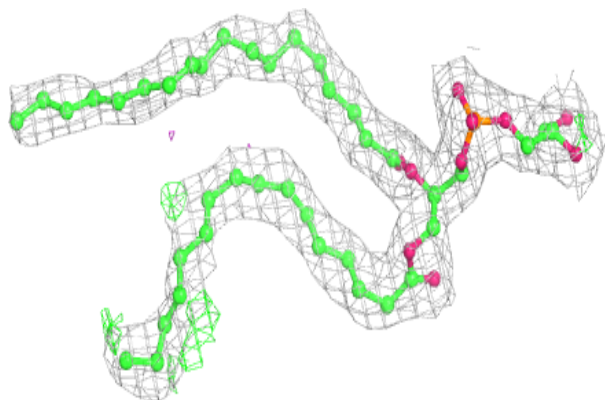


Electron density around PGV N 1266:

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

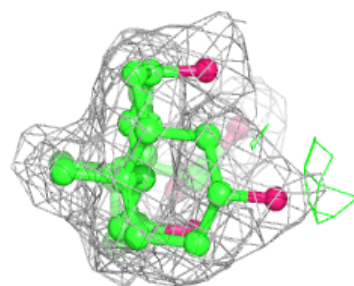
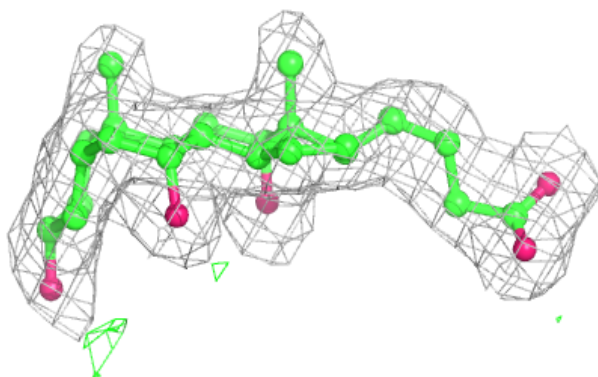
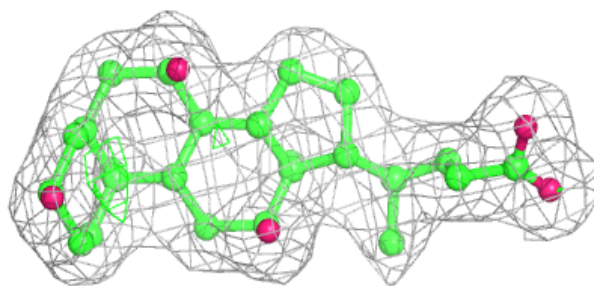
**Electron density around PGV A 522:**

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

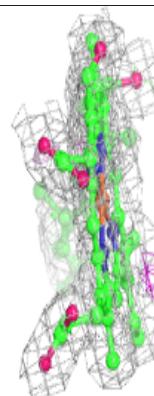
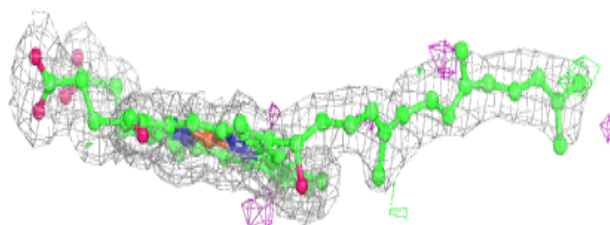
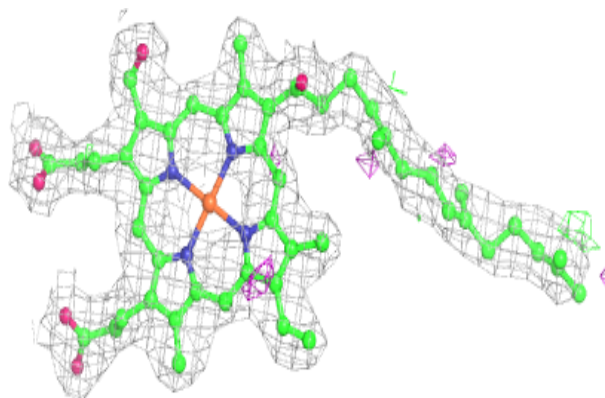


Electron density around CHD B 1085:

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

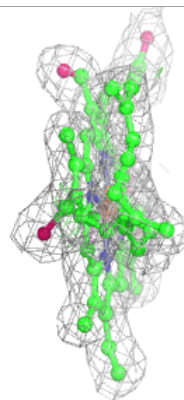
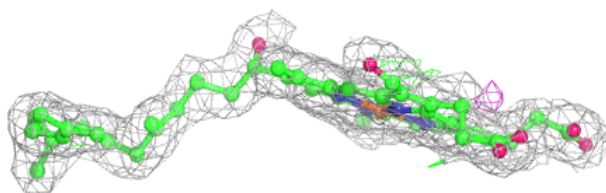
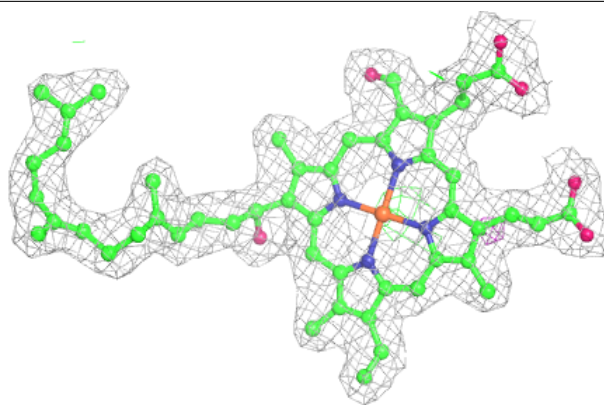
**Electron density around HEA A 515:**

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

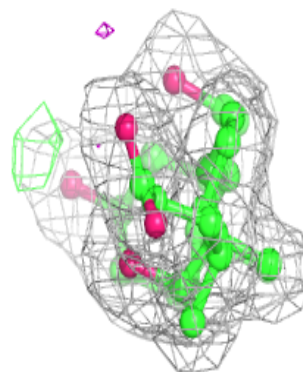
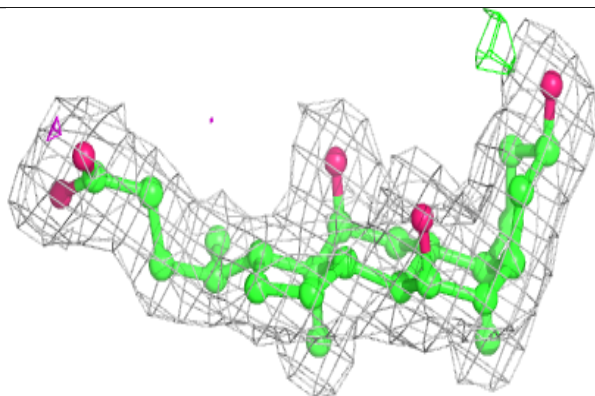
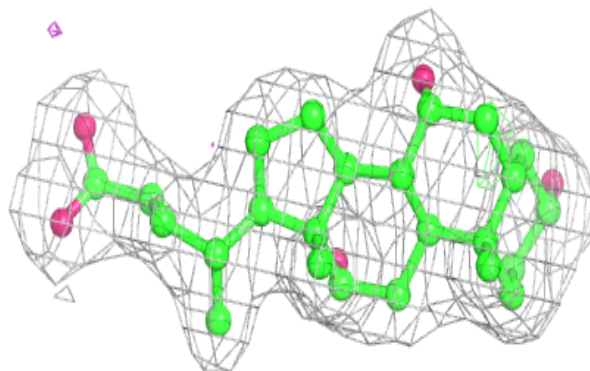


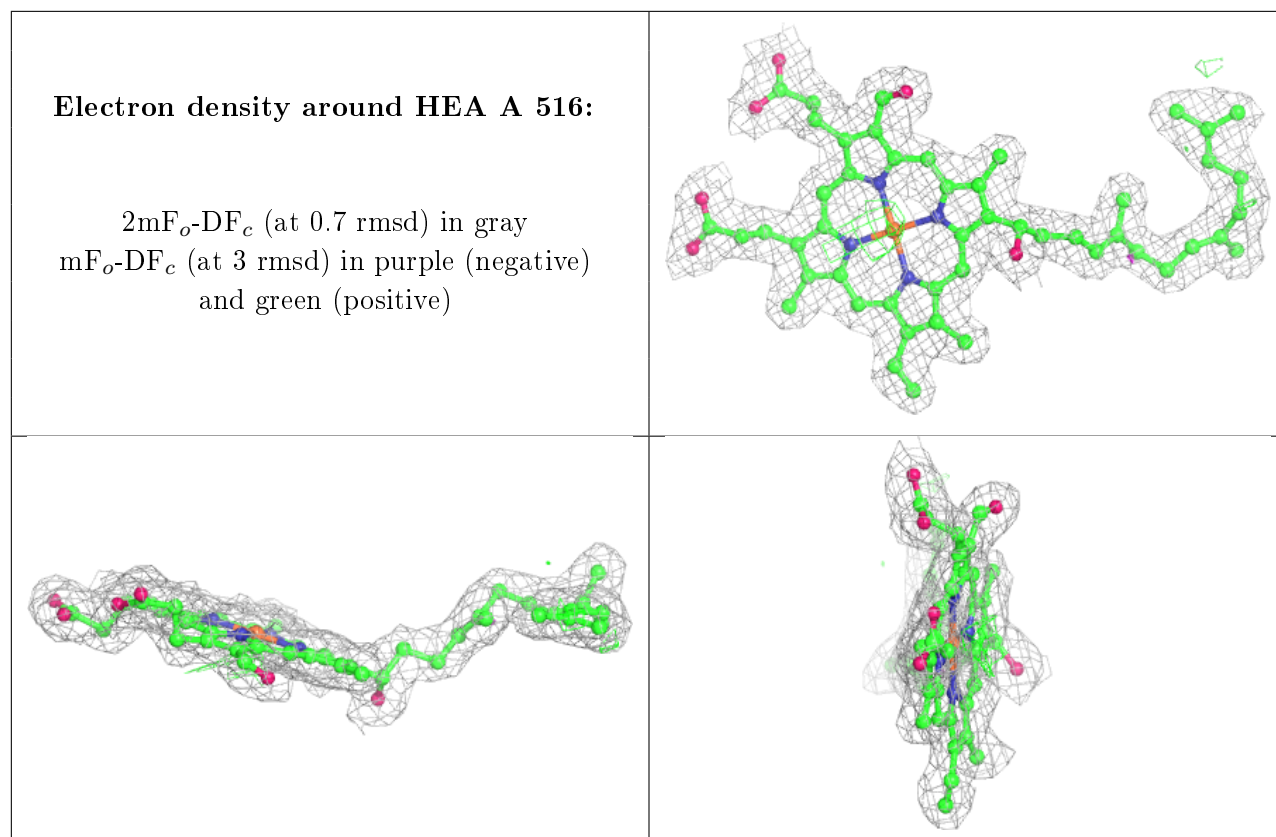
Electron density around HEA N 516:

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

**Electron density around CHD G 229:**

$2mF_o-DF_c$ (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.