



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:10 pm BST

PDB ID : 3ASN
Title : Bovine heart cytochrome C oxidase in the fully oxidized state measured at 1.7470 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 : 3.00 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

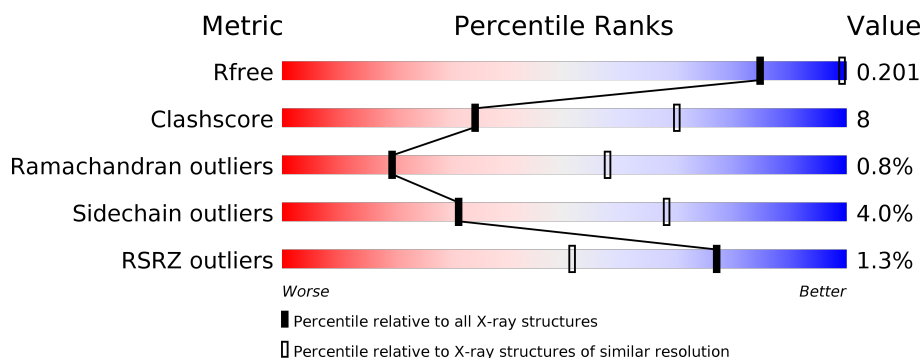
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



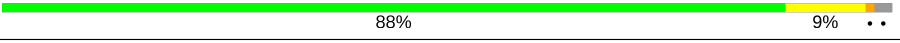










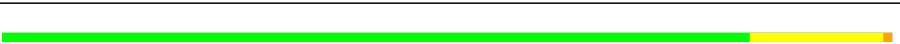




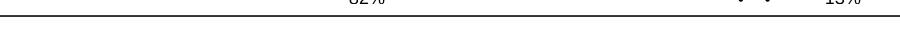
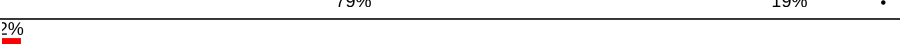
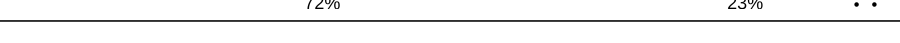
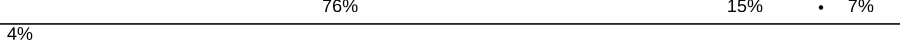
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	515	X	-	-	-
14	HEA	A	516	X	-	-	-
14	HEA	N	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	516	X	-	-	-
18	TGL	N	1523	-	-	-	X
19	PGV	P	1268	-	-	-	X
21	PSC	B	229	-	-	-	X
21	PSC	O	1229	-	-	-	X
22	CHD	J	60	-	-	-	X
22	CHD	W	1059	-	-	-	X
24	PEK	G	1263	-	-	-	X
24	PEK	P	1265	-	-	-	X
24	PEK	T	263	-	-	-	X
25	CDL	G	269	-	-	-	X
25	CDL	T	1269	-	-	X	X
27	DMU	M	526	X	-	-	-
27	DMU	Z	1526	X	-	-	-
7	TPO	T	11	-	-	-	X
9	SAC	I	1	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 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			

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

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

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

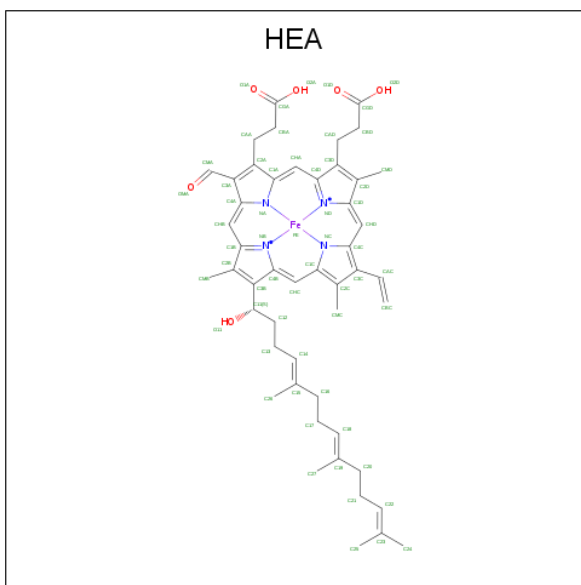
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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		

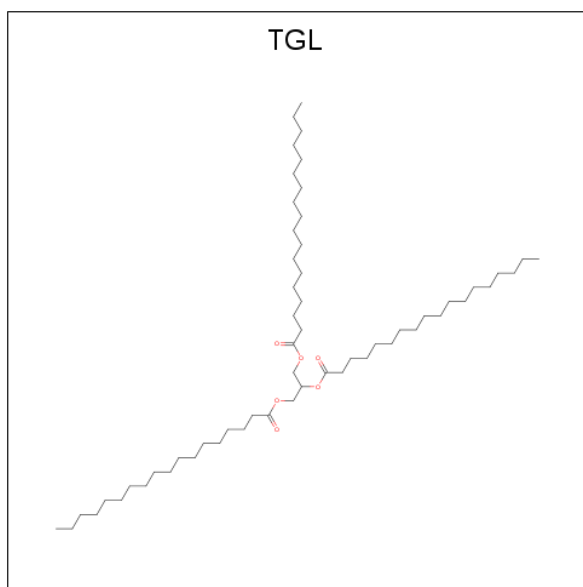
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

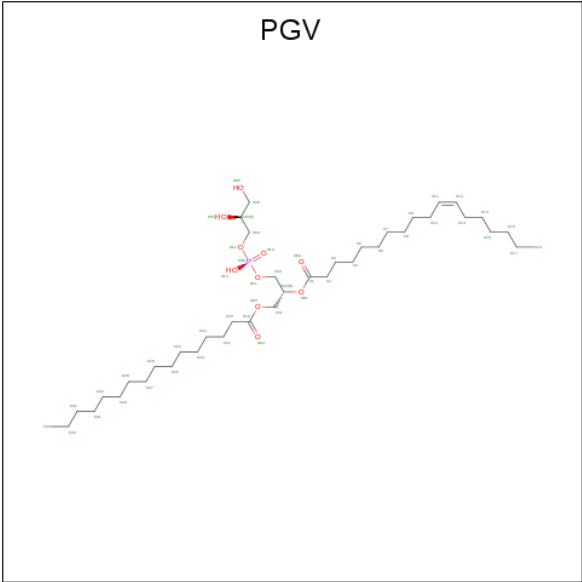
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

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



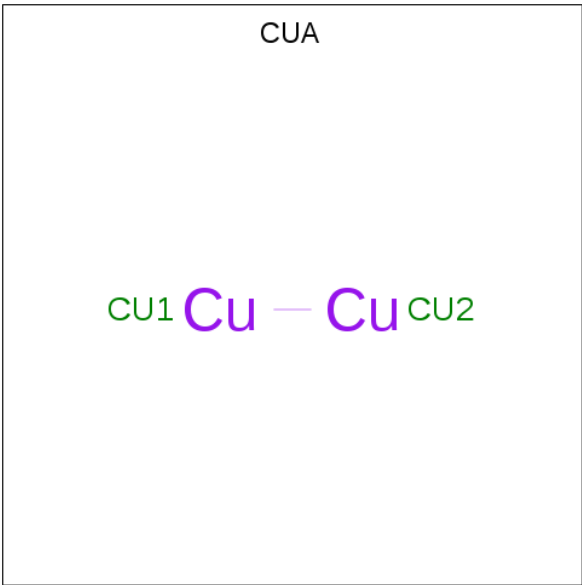
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	D	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		

- 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).



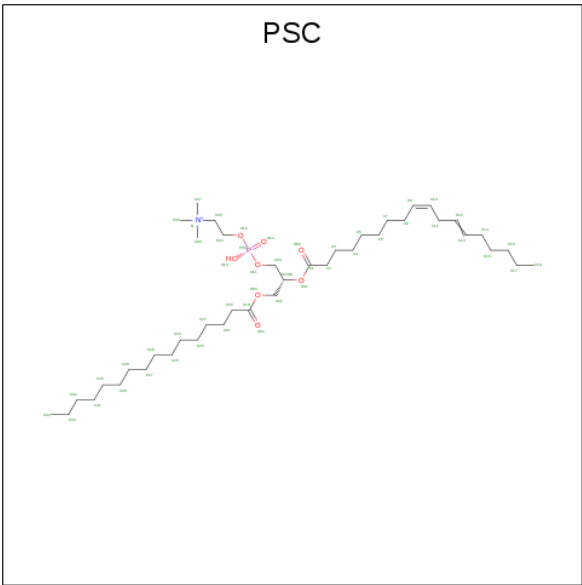
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			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-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



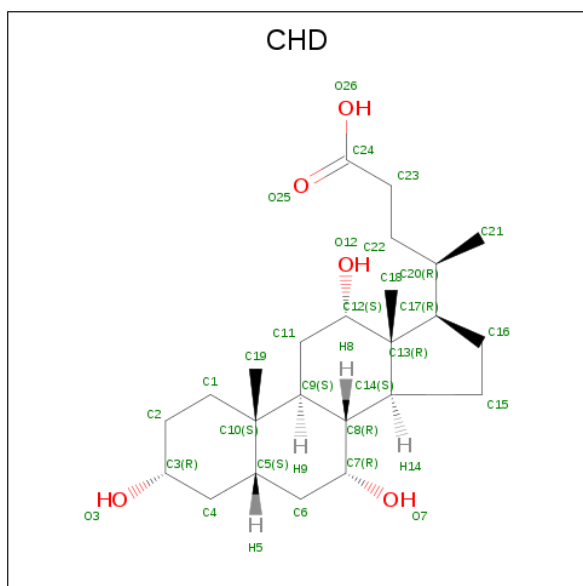
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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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: $C_{24}H_{40}O_5$).

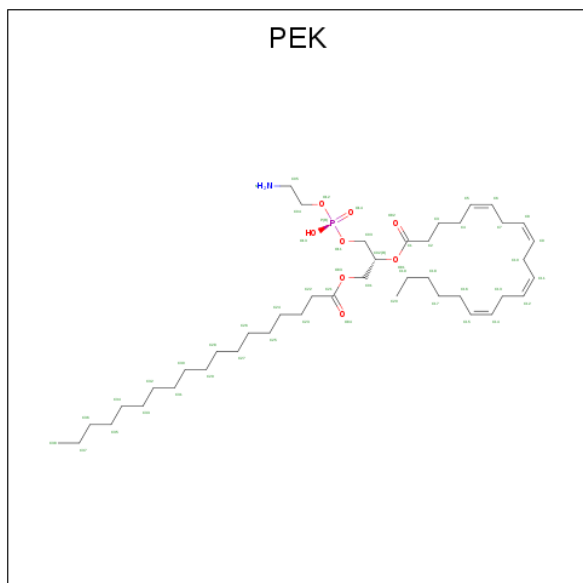


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

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

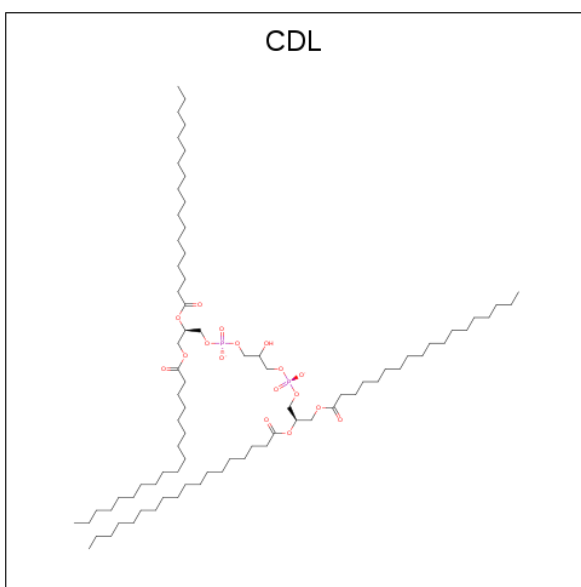
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total X 1 1	0	0
23	C	1	Total X 1 1	0	0

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



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

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

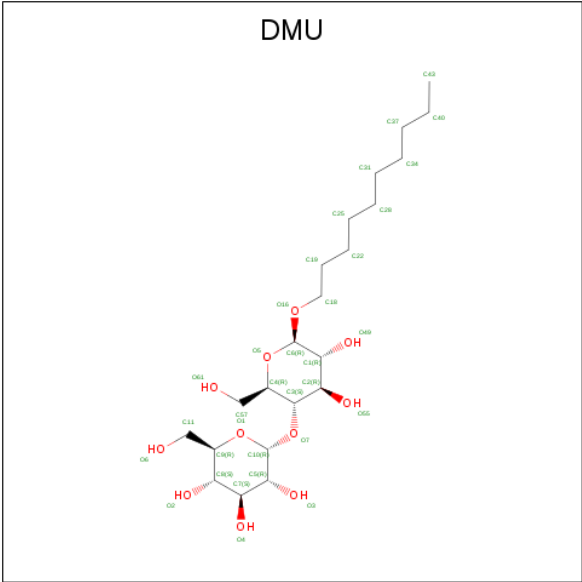


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- 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	C	O	0	0
			33	22	11		
27	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	212	Total	O	0	0
			212	212		
28	B	127	Total	O	0	0
			127	127		
28	C	110	Total	O	0	0
			110	110		
28	D	104	Total	O	0	0
			104	104		
28	E	66	Total	O	0	0
			66	66		
28	F	81	Total	O	0	0
			81	81		
28	G	52	Total	O	0	0
			52	52		
28	H	47	Total	O	0	0
			47	47		
28	I	32	Total	O	0	0
			32	32		
28	J	18	Total	O	0	0
			18	18		

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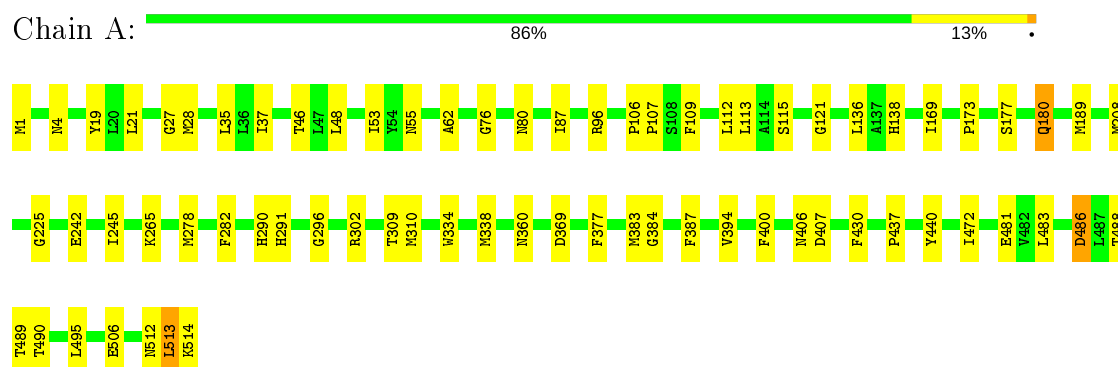
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	20	Total 20	O 20	0	0
28	L	27	Total 27	O 27	0	0
28	M	20	Total 20	O 20	0	0
28	N	210	Total 210	O 210	0	0
28	O	115	Total 115	O 115	0	0
28	P	109	Total 109	O 109	0	0
28	Q	60	Total 60	O 60	0	0
28	R	45	Total 45	O 45	0	0
28	S	79	Total 79	O 79	0	0
28	T	42	Total 42	O 42	0	0
28	U	47	Total 47	O 47	0	0
28	V	24	Total 24	O 24	0	0
28	W	17	Total 17	O 17	0	0
28	X	18	Total 18	O 18	0	0
28	Y	17	Total 17	O 17	0	0
28	Z	12	Total 12	O 12	0	0

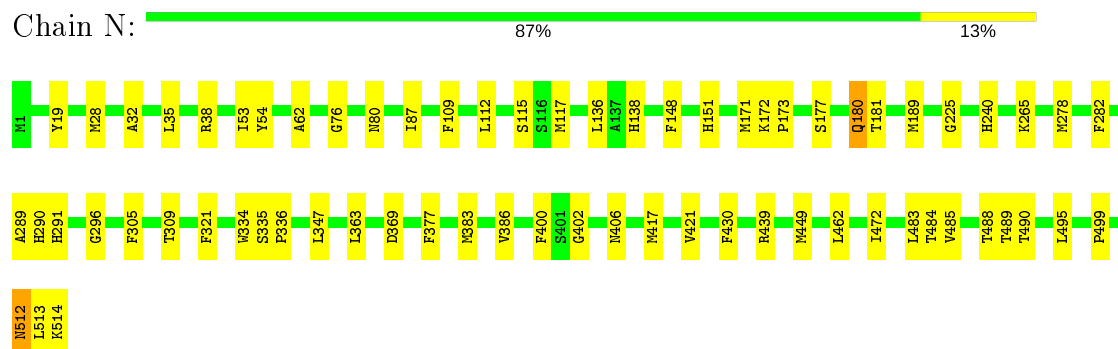
3 Residue-property plots

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.

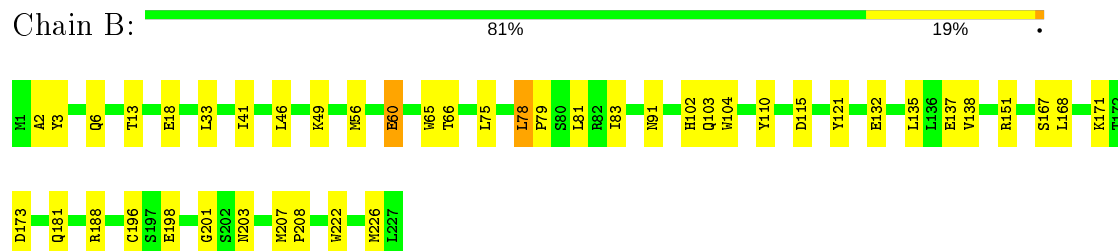
• Molecule 1: Cytochrome c oxidase subunit 1



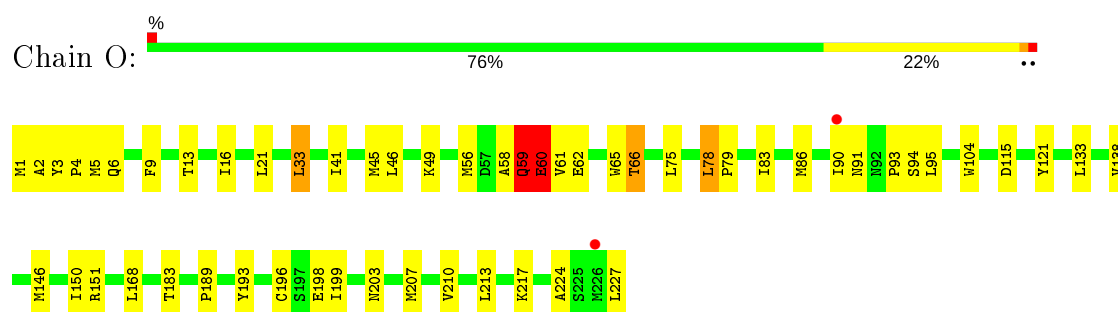
• Molecule 1: Cytochrome c oxidase subunit 1



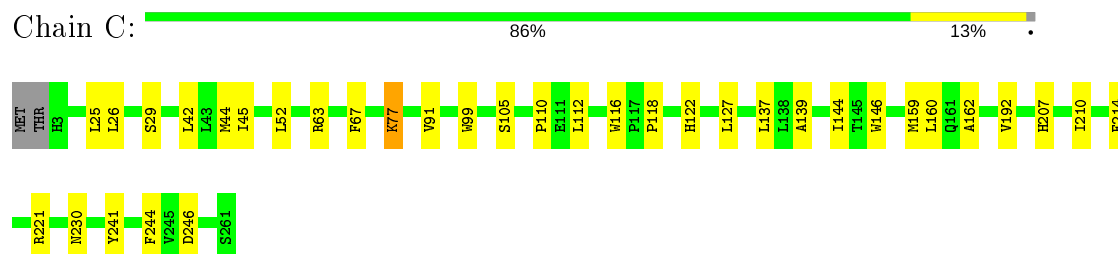
• Molecule 2: Cytochrome c oxidase subunit 2



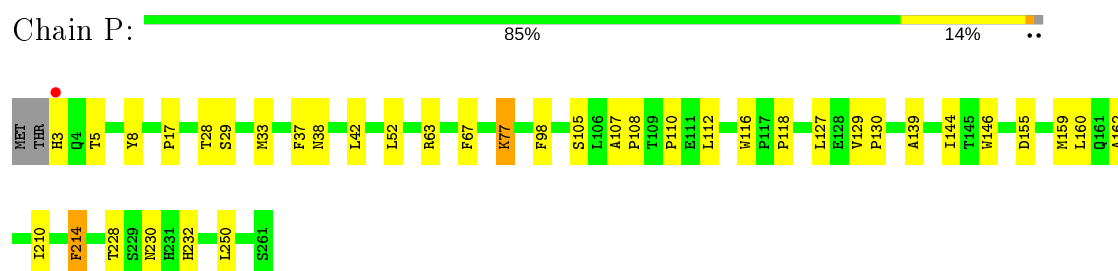
• Molecule 2: Cytochrome c oxidase subunit 2



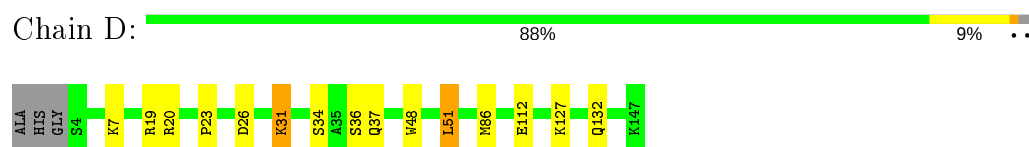
- Molecule 3: Cytochrome c oxidase subunit 3



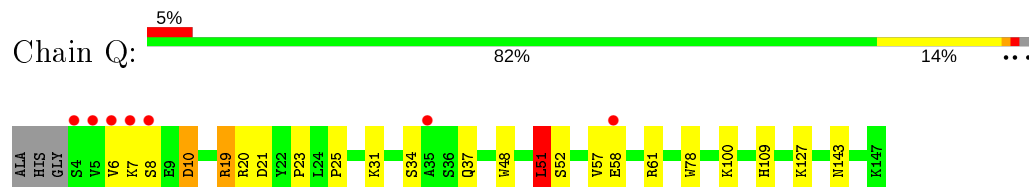
- Molecule 3: Cytochrome c oxidase subunit 3



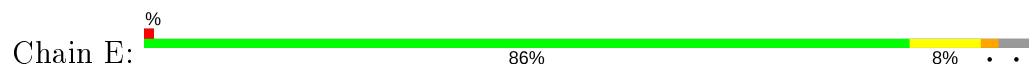
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

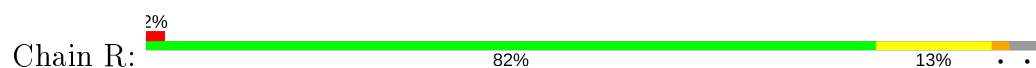


- Molecule 5: Cytochrome c oxidase subunit 5A

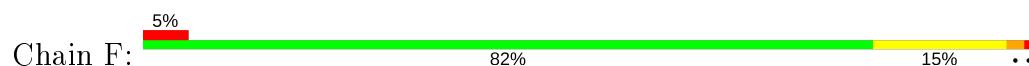




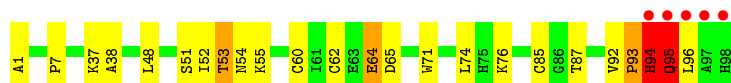
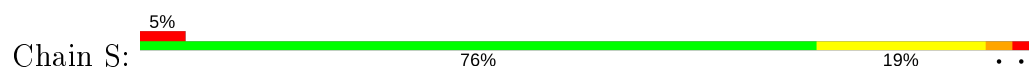
- Molecule 5: Cytochrome c oxidase subunit 5A



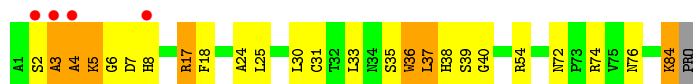
- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B



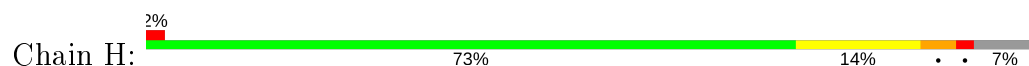
- Molecule 7: Cytochrome c oxidase subunit 6A2



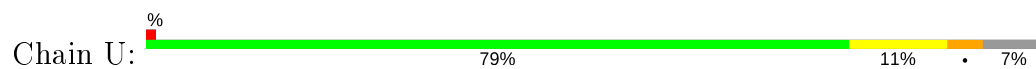
- Molecule 7: Cytochrome c oxidase subunit 6A2



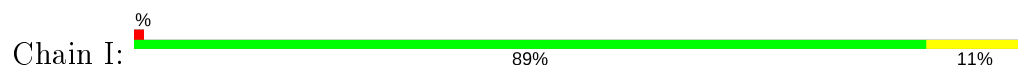
- Molecule 8: Cytochrome c oxidase subunit 6B1



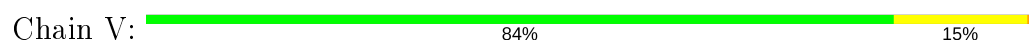
- Molecule 8: Cytochrome c oxidase subunit 6B1



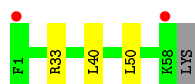
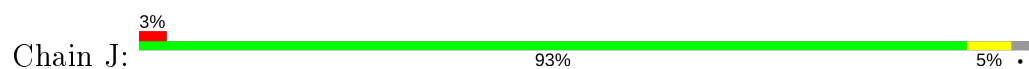
- Molecule 9: Cytochrome c oxidase subunit 6C



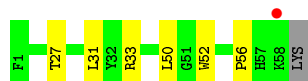
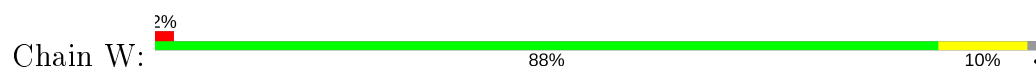
- Molecule 9: Cytochrome c oxidase subunit 6C



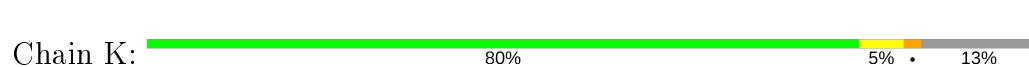
- Molecule 10: Cytochrome c oxidase subunit 7A1



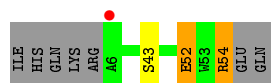
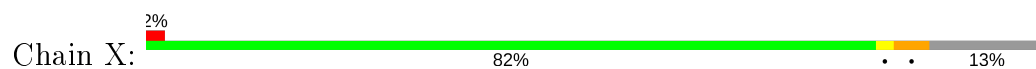
- Molecule 10: Cytochrome c oxidase subunit 7A1




- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B




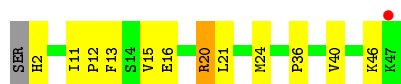
- Molecule 12: Cytochrome c oxidase subunit 7C

Chain L:  79% 19% •




- Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:  2% 72% 23% • •




- Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:  76% 15% • 7%



- Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:  4% 80% 13% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.83Å 204.10Å 177.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 135.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.00) 100.0 (135.76-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	27.93 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.150 , 0.187 0.166 , 0.201	Depositor DCC
R_{free} test set	6633 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32377	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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	0.96	0/4156	0.91	13/5678 (0.2%)
1	N	0.92	0/4156	0.84	3/5678 (0.1%)
2	B	0.98	2/1860 (0.1%)	0.94	2/2534 (0.1%)
2	O	0.98	3/1860 (0.2%)	0.94	0/2534
3	C	0.96	1/2197 (0.0%)	0.81	2/3005 (0.1%)
3	P	0.92	0/2197	0.82	1/3005 (0.0%)
4	D	1.01	1/1229 (0.1%)	0.94	3/1658 (0.2%)
4	Q	0.97	2/1229 (0.2%)	0.85	2/1658 (0.1%)
5	E	0.94	1/871 (0.1%)	0.94	2/1182 (0.2%)
5	R	0.86	1/871 (0.1%)	0.85	3/1182 (0.3%)
6	F	0.91	0/765	0.97	1/1038 (0.1%)
6	S	1.06	2/765 (0.3%)	1.07	3/1038 (0.3%)
7	G	1.07	2/690 (0.3%)	0.92	0/937
7	T	1.00	2/690 (0.3%)	0.91	0/937
8	H	0.94	0/682	0.88	1/921 (0.1%)
8	U	0.86	0/682	0.88	2/921 (0.2%)
9	I	1.07	0/605	0.87	0/802
9	V	1.07	0/605	0.88	0/802
10	J	1.01	0/471	0.86	0/636
10	W	0.92	0/471	0.88	0/636
11	K	0.96	0/398	0.89	1/546 (0.2%)
11	X	1.00	1/398 (0.3%)	0.77	0/546
12	L	0.87	0/393	0.83	0/526
12	Y	1.08	1/393 (0.3%)	0.81	0/526
13	M	0.94	0/345	0.93	1/470 (0.2%)
13	Z	0.81	0/345	0.86	0/470
All	All	0.96	19/29324 (0.1%)	0.89	40/39866 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	8.62	1.65	1.50
7	T	36	TRP	CB-CG	8.62	1.65	1.50
12	Y	16	GLU	CG-CD	8.15	1.64	1.51
2	O	198	GLU	C-O	6.50	1.35	1.23
2	B	198	GLU	C-O	6.47	1.35	1.23
6	S	54	ASN	CB-CG	-6.20	1.36	1.51
2	O	59	GLN	CG-CD	5.88	1.64	1.51
6	S	60	CYS	CB-SG	-5.71	1.72	1.81
4	Q	58	GLU	CG-CD	5.65	1.60	1.51
7	T	5	LYS	CB-CG	5.58	1.67	1.52
4	D	36	SER	CB-OG	-5.44	1.35	1.42
5	R	80	GLU	CG-CD	5.33	1.59	1.51
2	O	60	GLU	CB-CG	5.17	1.61	1.52
2	B	18	GLU	CD-OE1	5.13	1.31	1.25
5	E	9	GLU	CG-CD	5.12	1.59	1.51
7	G	5	LYS	CB-CG	5.11	1.66	1.52
4	Q	10	ASP	CB-CG	5.10	1.62	1.51
3	C	192	VAL	CB-CG2	-5.03	1.42	1.52
11	X	52	GLU	CB-CG	5.02	1.61	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	LEU	CB-CG-CD2	-10.95	92.39	111.00
1	A	136	LEU	CA-CB-CG	8.60	135.08	115.30
1	A	136	LEU	CB-CG-CD1	8.13	124.81	111.00
8	H	27	ARG	NE-CZ-NH1	7.85	124.23	120.30
4	D	20	ARG	NE-CZ-NH2	-7.71	116.44	120.30
5	E	90	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	407	ASP	CB-CG-OD1	-7.32	111.71	118.30
1	A	486	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	486	ASP	CB-CG-OD2	-6.97	112.03	118.30
11	K	54	ARG	NE-CZ-NH1	-6.87	116.86	120.30
5	R	25	ASP	CB-CG-OD1	6.78	124.40	118.30
3	C	44	MET	CG-SD-CE	6.76	111.01	100.20
1	A	96	ARG	NE-CZ-NH2	-6.54	117.03	120.30
6	S	54	ASN	CB-CA-C	-6.46	97.47	110.40
5	E	90	ARG	NE-CZ-NH1	6.46	123.53	120.30
4	D	26	ASP	CB-CG-OD1	6.42	124.08	118.30
2	B	188	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	B	173	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	208	MET	CG-SD-CE	5.89	109.62	100.20
1	A	35	LEU	CA-CB-CG	-5.79	101.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	LEU	CB-CG-CD2	5.79	120.84	111.00
13	M	37	LEU	CB-CG-CD1	-5.76	101.20	111.00
1	N	136	LEU	CB-CG-CD1	5.62	120.55	111.00
4	Q	10	ASP	CB-CG-OD1	5.61	123.35	118.30
6	S	94	HIS	N-CA-C	5.59	126.09	111.00
1	N	117	MET	CA-CB-CG	5.56	122.75	113.30
3	C	221	ARG	NE-CZ-NH1	-5.50	117.55	120.30
8	U	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	96	ARG	NE-CZ-NH1	5.39	122.99	120.30
4	D	20	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	512	ASN	CB-CA-C	-5.31	99.78	110.40
6	F	74	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	A	169	ILE	CG1-CB-CG2	-5.21	99.93	111.40
6	S	93	PRO	C-N-CA	5.19	134.66	121.70
3	P	155	ASP	CB-CG-OD1	5.17	122.95	118.30
4	Q	51	LEU	CA-CB-CG	5.16	127.17	115.30
5	R	14	ARG	NE-CZ-NH1	5.14	122.87	120.30
5	R	30	ARG	NE-CZ-NH2	-5.13	117.73	120.30
8	U	35	ASP	CB-CG-OD2	5.11	122.90	118.30
1	N	512	ASN	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	53	0
1	N	4027	0	4001	61	0
2	B	1824	0	1833	22	0
2	O	1824	0	1833	34	0
3	C	2110	0	2027	28	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	18	0
5	E	852	0	845	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	852	0	845	8	0
6	F	748	0	728	13	0
6	S	748	0	728	27	0
7	G	675	0	644	31	0
7	T	675	0	644	33	0
8	H	662	0	623	11	0
8	U	662	0	623	5	0
9	I	601	0	613	7	0
9	V	601	0	613	10	0
10	J	460	0	459	2	0
10	W	460	0	459	6	0
11	K	384	0	366	2	0
11	X	384	0	366	6	0
12	L	380	0	380	12	0
12	Y	380	0	380	11	1
13	M	335	0	352	3	0
13	Z	335	0	352	1	0
14	A	120	0	108	10	0
14	N	120	0	108	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	63	0	110	6	0
18	D	63	0	110	5	0
18	L	63	0	110	14	0
18	N	189	0	330	22	0
19	A	102	0	152	13	0
19	C	102	0	152	10	0
19	N	102	0	152	9	0
19	P	102	0	152	7	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	52	0	80	11	0
21	O	52	0	80	17	0
22	B	29	0	39	2	0
22	C	58	0	78	2	0
22	G	29	0	39	0	0
22	J	29	0	38	2	0
22	P	58	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	29	0	38	3	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	106	0	154	8	0
24	G	53	0	77	10	0
24	P	106	0	154	13	0
24	T	53	0	77	12	0
25	C	100	0	156	19	0
25	G	100	0	156	20	0
25	P	100	0	156	9	0
25	T	100	0	156	24	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	39	0	0
27	Z	33	0	39	0	0
28	A	212	0	0	13	0
28	B	127	0	0	2	0
28	C	110	0	0	2	0
28	D	104	0	0	4	0
28	E	66	0	0	3	0
28	F	81	0	0	5	0
28	G	52	0	0	3	0
28	H	47	0	0	2	0
28	I	32	0	0	5	0
28	J	18	0	0	0	0
28	K	20	0	0	2	0
28	L	27	0	0	1	0
28	M	20	0	0	0	0
28	N	210	0	0	8	0
28	O	115	0	0	1	0
28	P	109	0	0	5	0
28	Q	60	0	0	4	0
28	R	45	0	0	0	0
28	S	79	0	0	4	0
28	T	42	0	0	4	0
28	U	47	0	0	0	0
28	V	24	0	0	5	1
28	W	17	0	0	1	0
28	X	18	0	0	1	0
28	Y	17	0	0	1	0
28	Z	12	0	0	0	0
All	All	32377	0	31226	521	1

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 (521) 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)
24:P:1265:PEK:H383	25:T:1269:CDL:C27	1.54	1.35
24:P:1265:PEK:C38	25:T:1269:CDL:H273	1.66	1.25
24:C:265:PEK:H383	25:G:269:CDL:H273	1.20	1.19
6:S:52:ILE:O	6:S:94:HIS:CE1	1.96	1.18
28:N:4772:HOH:O	24:P:1264:PEK:H381	1.44	1.14
6:S:52:ILE:O	6:S:94:HIS:NE2	1.80	1.14
7:T:84:LYS:H	7:T:84:LYS:HD2	1.02	1.13
1:A:1:FME:HG3	28:L:4907:HOH:O	1.50	1.11
24:C:265:PEK:H383	25:G:269:CDL:C27	1.83	1.07
21:O:1229:PSC:H142	21:O:1229:PSC:H343	1.07	1.06
25:G:269:CDL:H541	25:G:269:CDL:H231	1.37	1.06
21:O:1229:PSC:C34	21:O:1229:PSC:H142	1.86	1.06
18:D:523:TGL:H361	28:I:4610:HOH:O	1.54	1.04
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.39	1.03
2:O:224:ALA:O	2:O:227:LEU:HG	1.59	1.02
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.22	1.02
24:C:265:PEK:C38	25:G:269:CDL:H273	1.88	1.02
21:B:229:PSC:H142	21:B:229:PSC:H343	1.41	1.01
7:G:84:LYS:HD2	7:G:84:LYS:H	1.19	0.99
7:T:5:LYS:HB2	24:T:263:PEK:H362	1.42	0.98
6:F:54:ASN:HB2	28:F:4662:HOH:O	1.61	0.96
21:O:1229:PSC:H343	21:O:1229:PSC:C14	1.94	0.96
14:A:515:HEA:HMC1	14:A:515:HEA:HBC1	1.49	0.93
6:S:53:THR:HA	6:S:94:HIS:CE1	2.03	0.93
1:N:513:LEU:O	1:N:514:LYS:HB2	1.64	0.92
7:T:84:LYS:H	7:T:84:LYS:CD	1.82	0.92
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.50	0.92
7:T:84:LYS:N	7:T:84:LYS:HD2	1.84	0.90
18:D:523:TGL:HC21	18:D:523:TGL:HG11	1.51	0.90
1:A:55:ASN:HB2	28:A:2299:HOH:O	1.70	0.90
19:P:1268:PGV:H062	28:P:4397:HOH:O	1.68	0.90
7:G:72:ASN:H	7:G:76:ASN:HD22	1.19	0.89
6:S:53:THR:HA	6:S:94:HIS:HE1	1.38	0.89
7:T:72:ASN:H	7:T:76:ASN:HD22	1.18	0.88
7:G:5:LYS:HB2	24:G:1263:PEK:H362	1.56	0.87
1:A:112:LEU:HG	28:A:2701:HOH:O	1.73	0.87
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:13:PHE:HA	18:L:522:TGL:HC31	1.57	0.86
19:A:524:PGV:H311	13:M:19:LEU:HD23	1.57	0.86
3:P:3:HIS:HB3	28:P:4285:HOH:O	1.73	0.86
6:F:85:CYS:SG	6:F:87:THR:HG23	2.16	0.85
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.41	0.85
18:A:521:TGL:HC82	28:A:4504:HOH:O	1.76	0.84
1:A:278:MET:SD	7:T:5:LYS:HB3	2.17	0.84
1:N:112:LEU:HG	28:N:3701:HOH:O	1.77	0.84
6:S:64:GLU:O	6:S:65:ASP:HB2	1.77	0.82
25:T:1269:CDL:H541	25:T:1269:CDL:H231	1.62	0.82
7:T:31:CYS:SG	25:T:1269:CDL:H532	2.20	0.82
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.45	0.82
25:G:269:CDL:C54	25:G:269:CDL:H231	2.11	0.80
25:G:269:CDL:H522	25:G:269:CDL:H202	1.63	0.80
24:P:1265:PEK:H383	25:T:1269:CDL:H273	0.82	0.80
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.64	0.79
1:N:513:LEU:O	1:N:514:LYS:CB	2.30	0.79
25:C:270:CDL:PA1	25:C:270:CDL:HB22	2.22	0.78
3:C:246:ASP:HB2	28:C:4249:HOH:O	1.82	0.78
7:G:5:LYS:HB3	1:N:278:MET:SD	2.23	0.78
19:A:524:PGV:H062	28:A:2126:HOH:O	1.83	0.78
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.66	0.77
7:T:3:ALA:HB1	24:T:263:PEK:H382	1.64	0.77
2:B:56:MET:HG2	21:B:229:PSC:H211	1.67	0.77
18:N:1523:TGL:HC21	18:N:1523:TGL:HG11	1.67	0.77
14:A:516:HEA:HMC1	14:A:516:HEA:HBC1	1.67	0.76
4:D:34:SER:H	4:D:37:GLN:HE21	1.34	0.76
6:S:52:ILE:C	6:S:94:HIS:CE1	2.59	0.76
6:S:85:CYS:SG	6:S:87:THR:HG23	2.25	0.76
2:B:78:LEU:HD12	25:T:1269:CDL:H352	1.68	0.75
18:N:1521:TGL:H201	18:N:1521:TGL:H241	1.69	0.75
24:C:264:PEK:HN2	7:G:76:ASN:HD21	1.34	0.74
1:A:506:GLU:HG3	28:A:4882:HOH:O	1.87	0.74
6:S:52:ILE:O	6:S:94:HIS:CD2	2.40	0.73
21:B:229:PSC:H072	9:I:10:ARG:HH21	1.54	0.73
7:G:5:LYS:HG3	24:G:1263:PEK:H383	1.70	0.72
7:G:84:LYS:H	7:G:84:LYS:CD	2.01	0.72
24:P:1265:PEK:H041	6:S:1:ALA:N	2.05	0.72
2:B:13:THR:HB	2:B:168:LEU:HD23	1.70	0.72
21:B:229:PSC:C07	9:I:10:ARG:HH21	2.02	0.71
7:G:2:SER:O	24:G:1263:PEK:H322	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N:4478:HOH:O	4:Q:100:LYS:HE2	1.90	0.71
9:V:18:ARG:HD3	28:V:4483:HOH:O	1.90	0.71
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.27	0.70
1:A:472:ILE:HG21	18:L:522:TGL:HA92	1.73	0.70
24:P:1264:PEK:H161	24:P:1264:PEK:H101	1.74	0.70
10:W:33:ARG:HG2	22:W:1059:CHD:H151	1.74	0.69
7:G:3:ALA:HB1	24:G:1263:PEK:H382	1.73	0.69
2:B:41:ILE:HD13	21:B:229:PSC:H342	1.74	0.69
1:A:406:ASN:HD21	19:A:524:PGV:H22	1.57	0.69
9:I:73:LYS:HB3	28:I:4200:HOH:O	1.91	0.68
18:D:523:TGL:HB62	18:D:523:TGL:HA52	1.74	0.68
19:A:524:PGV:H82	19:A:524:PGV:H262	1.75	0.68
18:N:1521:TGL:C28	18:N:1521:TGL:H101	2.24	0.68
24:C:264:PEK:H101	24:C:264:PEK:H161	1.76	0.68
24:P:1265:PEK:H383	25:T:1269:CDL:H272	1.72	0.68
7:G:30:LEU:CD2	25:G:269:CDL:H462	2.24	0.67
6:F:95:GLN:OE1	6:F:95:GLN:HA	1.94	0.67
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.58	0.67
28:G:4789:HOH:O	19:P:1268:PGV:H341	1.94	0.67
1:A:513:LEU:O	1:A:514:LYS:HB2	1.94	0.67
28:B:2562:HOH:O	18:D:523:TGL:HC72	1.95	0.67
7:T:5:LYS:HD2	24:T:263:PEK:H371	1.76	0.67
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.77	0.67
7:G:72:ASN:H	7:G:76:ASN:ND2	1.92	0.66
7:T:72:ASN:H	7:T:76:ASN:ND2	1.90	0.66
7:G:30:LEU:HD21	25:G:269:CDL:H462	1.77	0.66
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.76	0.66
28:B:3446:HOH:O	7:T:17:ARG:HD2	1.96	0.66
6:S:95:GLN:HB2	28:S:4523:HOH:O	1.96	0.65
7:T:3:ALA:CB	24:T:263:PEK:H382	2.27	0.64
7:G:3:ALA:O	7:G:4:ALA:HB2	1.97	0.64
24:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.43	0.64
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.12	0.64
21:O:1229:PSC:O01	21:O:1229:PSC:H212	1.98	0.64
3:C:210:ILE:HG12	19:C:267:PGV:H132	1.79	0.63
12:L:11:ILE:CG2	18:L:522:TGL:H271	2.29	0.63
9:V:65:LYS:O	11:X:54:ARG:NH1	2.32	0.63
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.80	0.63
7:T:3:ALA:O	7:T:4:ALA:HB2	1.99	0.63
4:Q:31:LYS:HB3	28:Q:4834:HOH:O	1.97	0.62
25:T:1269:CDL:H172	25:T:1269:CDL:H511	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:3:HIS:HD2	28:P:4343:HOH:O	1.81	0.62
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.82	0.62
2:O:41:ILE:HD13	21:O:1229:PSC:H342	1.82	0.62
1:A:430:PHE:HE1	18:A:521:TGL:HB21	1.65	0.62
19:C:267:PGV:H182	25:C:270:CDL:C67	2.30	0.62
18:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.80	0.62
25:T:1269:CDL:H171	28:T:4708:HOH:O	2.00	0.62
3:C:63:ARG:HE	25:C:270:CDL:CA2	2.11	0.62
10:W:33:ARG:HG2	22:W:1059:CHD:C15	2.30	0.62
1:A:302:ARG:NH1	28:A:4472:HOH:O	2.29	0.61
4:D:7:LYS:HE3	28:D:4308:HOH:O	2.01	0.61
7:T:2:SER:O	24:T:263:PEK:H322	2.00	0.61
6:S:96:LEU:HD12	28:S:4273:HOH:O	1.99	0.61
1:N:321:PHE:CD2	21:O:1229:PSC:H341	2.36	0.61
7:T:7:ASP:HB2	28:T:4216:HOH:O	2.01	0.61
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.66	0.60
19:C:268:PGV:H42	28:P:4823:HOH:O	2.01	0.60
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	2.01	0.60
12:L:20:ARG:HH22	18:L:522:TGL:HC62	1.67	0.59
6:F:64:GLU:O	6:F:65:ASP:HB2	2.02	0.59
3:P:52:LEU:HD21	25:P:1270:CDL:H412	1.83	0.59
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.84	0.59
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.37	0.59
1:A:46:THR:HG23	28:A:2466:HOH:O	2.03	0.59
3:C:52:LEU:HD21	25:C:270:CDL:H412	1.83	0.59
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.68	0.59
1:A:406:ASN:HD21	19:A:524:PGV:C2	2.16	0.59
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.02	0.59
6:F:19:GLU:HG2	28:F:4411:HOH:O	2.00	0.59
7:T:5:LYS:CB	24:T:263:PEK:H362	2.26	0.59
1:N:430:PHE:HE1	18:N:1521:TGL:HB21	1.68	0.58
4:Q:127:LYS:HD2	28:V:3618:HOH:O	2.03	0.58
18:D:523:TGL:H242	18:D:523:TGL:HA91	1.85	0.58
9:V:2:THR:HG22	9:V:3:ALA:H	1.69	0.58
25:G:269:CDL:C52	25:G:269:CDL:H202	2.33	0.58
1:N:400:PHE:HB3	18:N:1522:TGL:H282	1.86	0.58
2:O:41:ILE:CD1	21:O:1229:PSC:H342	2.33	0.58
18:N:1521:TGL:H281	18:N:1521:TGL:H101	1.85	0.58
9:I:32:ALA:O	9:I:36:LYS:HE3	2.04	0.57
18:N:1523:TGL:HB22	4:Q:78:TRP:HA	1.85	0.57
19:A:524:PGV:H02	19:A:524:PGV:O14	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:522:PGV:H183	24:C:264:PEK:H332	1.86	0.57
25:C:270:CDL:H642	25:C:270:CDL:H191	1.85	0.57
1:N:177:SER:H	1:N:180:GLN:NE2	2.02	0.57
21:B:229:PSC:H042	28:E:2664:HOH:O	2.05	0.57
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.85	0.57
1:N:28:MET:CE	14:N:515:HEA:C27	2.83	0.57
21:O:1229:PSC:H222	21:O:1229:PSC:H21	1.87	0.57
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.85	0.57
1:A:383:MET:O	1:A:387:PHE:HB2	2.04	0.56
1:N:112:LEU:HD12	28:N:4714:HOH:O	2.04	0.56
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.86	0.56
18:L:522:TGL:CC6	18:L:522:TGL:HC22	2.35	0.56
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.87	0.56
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.88	0.56
6:S:53:THR:CA	6:S:94:HIS:CE1	2.84	0.56
24:P:1265:PEK:C38	25:T:1269:CDL:C27	2.47	0.56
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.18	0.56
25:G:269:CDL:H1	25:G:269:CDL:OB4	2.06	0.55
25:T:1269:CDL:OB4	25:T:1269:CDL:H1	2.07	0.55
8:H:27:ARG:HD3	28:H:4760:HOH:O	2.07	0.55
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.22	0.55
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.88	0.55
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.95	0.54
1:N:400:PHE:HB3	18:N:1522:TGL:C28	2.37	0.54
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.90	0.54
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.07	0.54
21:O:1229:PSC:C07	9:V:10:ARG:HH21	2.21	0.54
7:T:3:ALA:O	7:T:4:ALA:CB	2.54	0.54
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.88	0.54
4:D:31:LYS:HE2	28:D:4278:HOH:O	2.07	0.54
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.47	0.54
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.73	0.54
1:A:514:LYS:HE2	28:F:2514:HOH:O	2.06	0.54
1:N:151:HIS:CD2	24:P:1264:PEK:H382	2.43	0.54
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.90	0.54
24:P:1265:PEK:H041	6:S:1:ALA:H1	1.72	0.54
6:S:87:THR:HG21	28:S:3514:HOH:O	2.07	0.54
8:H:7:LYS:O	8:H:8:ILE:HB	2.07	0.54
7:G:31:CYS:SG	25:G:269:CDL:H552	2.49	0.53
28:A:2527:HOH:O	12:L:7:PRO:HG3	2.07	0.53
1:A:87:ILE:O	1:A:173:PRO:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:488:THR:HB	1:N:495:LEU:HD13	1.90	0.53
6:F:87:THR:HG21	28:F:4250:HOH:O	2.08	0.53
18:N:1521:TGL:C10	18:N:1521:TGL:H281	2.38	0.53
1:N:449:MET:SD	2:O:5:MET:HG2	2.49	0.53
21:B:229:PSC:C14	21:B:229:PSC:H343	2.27	0.52
2:O:59:GLN:O	2:O:59:GLN:CG	2.57	0.52
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.91	0.52
24:G:1263:PEK:H042	3:P:77:LYS:NZ	2.24	0.52
19:N:1524:PGV:H011	19:N:1524:PGV:H221	1.90	0.52
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.92	0.52
19:N:1524:PGV:H011	19:N:1524:PGV:H22	1.91	0.52
3:P:63:ARG:NE	25:P:1270:CDL:HA22	2.07	0.52
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.91	0.52
21:O:1229:PSC:H322	21:O:1229:PSC:H12	1.92	0.52
25:C:270:CDL:CB3	25:C:270:CDL:HB21	2.40	0.52
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.45	0.52
7:G:2:SER:OG	24:G:1263:PEK:H301	2.10	0.52
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.45	0.52
21:O:1229:PSC:H071	9:V:10:ARG:HE	1.75	0.52
7:G:37:LEU:CD2	25:G:269:CDL:H361	2.40	0.51
3:P:250:LEU:HD22	25:T:1269:CDL:H662	1.91	0.51
19:C:267:PGV:H12	19:C:267:PGV:H161	1.91	0.51
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.92	0.51
14:A:515:HEA:HMC1	14:A:515:HEA:CB3	2.31	0.51
14:N:516:HEA:HBC1	14:N:516:HEA:HMC1	1.92	0.51
7:G:3:ALA:O	7:G:4:ALA:CB	2.58	0.51
1:A:400:PHE:HB3	18:L:522:TGL:H282	1.93	0.51
28:N:4478:HOH:O	4:Q:100:LYS:CE	2.54	0.51
5:R:80:GLU:N	5:R:80:GLU:OE1	2.42	0.51
24:P:1265:PEK:H041	6:S:1:ALA:H2	1.76	0.51
1:A:1:FME:HCN	1:A:4:ASN:H	1.76	0.51
7:T:5:LYS:HD2	24:T:263:PEK:C37	2.39	0.51
7:G:17:ARG:HD2	28:G:2446:HOH:O	2.10	0.51
1:N:400:PHE:O	18:N:1522:TGL:H283	2.11	0.51
1:A:48:LEU:N	28:A:2466:HOH:O	2.44	0.51
19:A:524:PGV:H201	28:A:4726:HOH:O	2.11	0.50
25:T:1269:CDL:H111	25:T:1269:CDL:HA21	1.92	0.50
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.94	0.50
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.93	0.50
19:N:1266:PGV:H182	3:P:28:THR:HG22	1.93	0.50
2:O:58:ALA:O	2:O:62:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.36	0.50
12:L:11:ILE:HG22	18:L:522:TGL:H271	1.92	0.50
25:G:269:CDL:H352	2:O:78:LEU:HD12	1.93	0.50
1:A:21:LEU:HD23	18:L:522:TGL:H211	1.94	0.50
1:A:76:GLY:O	1:A:80:ASN:HB2	2.12	0.49
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.93	0.49
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.00	0.49
9:V:15:ARG:HB2	28:V:4449:HOH:O	2.12	0.49
18:N:1521:TGL:HC22	28:Q:3606:HOH:O	2.12	0.49
21:B:229:PSC:H322	21:B:229:PSC:H12	1.94	0.49
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.11	0.49
2:B:135:LEU:O	2:B:208:PRO:HG3	2.12	0.49
10:J:33:ARG:HG2	22:J:60:CHD:H151	1.95	0.49
2:O:1:FME:CE	2:O:133:LEU:HD13	2.43	0.49
19:A:524:PGV:H011	19:A:524:PGV:H221	1.95	0.49
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.12	0.49
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.95	0.49
3:C:122:HIS:HD2	28:C:4770:HOH:O	1.95	0.49
24:C:265:PEK:C37	25:G:269:CDL:H273	2.42	0.49
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.95	0.49
8:H:27:ARG:NH1	28:H:2431:HOH:O	2.44	0.49
1:N:112:LEU:HD23	1:N:112:LEU:C	2.33	0.49
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.43	0.49
1:N:514:LYS:HE2	28:S:3514:HOH:O	2.13	0.48
25:C:270:CDL:OA5	25:C:270:CDL:HB22	2.11	0.48
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.28	0.48
6:F:76:LYS:HD2	6:F:93:PRO:HG2	1.94	0.48
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.48	0.48
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.49	0.48
2:O:1:FME:HE1	2:O:133:LEU:HD13	1.94	0.48
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.13	0.48
12:L:20:ARG:NH2	18:L:522:TGL:HC42	2.29	0.48
18:N:1522:TGL:H271	12:Y:11:ILE:CG2	2.44	0.48
2:O:56:MET:HA	21:O:1229:PSC:H202	1.96	0.47
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.96	0.47
19:N:1524:PGV:H132	19:N:1524:PGV:H301	1.96	0.47
1:A:488:THR:HB	1:A:495:LEU:HD13	1.95	0.47
1:A:27:GLY:HA3	14:A:515:HEA:H273	1.97	0.47
3:C:52:LEU:HD23	25:C:270:CDL:H382	1.96	0.47
21:B:229:PSC:H21	21:B:229:PSC:H222	1.97	0.47
7:G:4:ALA:CB	1:N:282:PHE:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:334:TRP:CZ3	18:N:1523:TGL:HA51	2.50	0.47
2:O:59:GLN:HG3	2:O:59:GLN:O	2.14	0.47
2:O:62:GLU:O	2:O:66:THR:HB	2.14	0.47
25:T:1269:CDL:H561	25:T:1269:CDL:H592	1.51	0.47
12:Y:15:VAL:HG12	12:Y:21:LEU:HD22	1.95	0.47
5:E:105:GLY:O	5:E:108:LYS:HG2	2.14	0.47
1:N:489:THR:HA	6:S:71:TRP:O	2.15	0.47
25:C:270:CDL:H172	25:C:270:CDL:H741	1.97	0.47
3:C:26:LEU:HD13	3:C:45:ILE:HG22	1.97	0.47
1:N:417:MET:O	1:N:421:VAL:HG22	2.15	0.47
5:R:5:HIS:HB3	5:R:6:GLU:H	1.64	0.47
6:S:64:GLU:O	6:S:65:ASP:CB	2.51	0.47
1:A:486:ASP:OD2	4:D:19:ARG:HD3	2.15	0.46
5:R:82:TYR:N	5:R:83:PRO:HD2	2.29	0.46
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.16	0.46
3:P:214:PHE:CD1	19:P:1267:PGV:H62	2.51	0.46
1:A:377:PHE:HB2	14:A:516:HEA:HMD3	1.96	0.46
2:B:3:TYR:CZ	2:B:6:GLN:HG3	2.51	0.46
2:B:79:PRO:O	2:B:83:ILE:HG13	2.15	0.46
3:P:5:THR:CG2	6:S:96:LEU:HD13	2.43	0.46
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.96	0.46
11:K:52:GLU:HG3	28:K:4808:HOH:O	2.15	0.46
2:O:79:PRO:O	2:O:83:ILE:HG13	2.15	0.46
2:B:78:LEU:CD1	25:T:1269:CDL:H352	2.42	0.46
3:C:77:LYS:NZ	24:T:263:PEK:H042	2.29	0.46
18:A:521:TGL:H281	18:A:521:TGL:C10	2.46	0.46
7:G:5:LYS:CG	24:G:1263:PEK:H383	2.44	0.46
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.40	0.46
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.16	0.46
6:S:94:HIS:HB3	6:S:95:GLN:H	1.02	0.46
1:N:177:SER:H	1:N:180:GLN:HE21	1.64	0.46
4:Q:109:HIS:HD2	28:Q:3122:HOH:O	1.98	0.46
3:C:77:LYS:HZ1	24:T:263:PEK:H042	1.81	0.46
7:G:37:LEU:HD21	25:G:269:CDL:H361	1.97	0.46
5:E:25:ASP:OD1	5:E:28:GLU:HG3	2.16	0.46
18:N:1521:TGL:H252	18:N:1521:TGL:HA91	1.98	0.46
2:O:13:THR:HB	2:O:168:LEU:HD23	1.98	0.46
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.16	0.46
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.97	0.46
2:B:102:HIS:O	2:B:104:TRP:HA	2.16	0.46
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:CG	28:A:2701:HOH:O	2.45	0.45
12:L:20:ARG:HH22	18:L:522:TGL:HC42	1.81	0.45
4:D:86:MET:CE	28:K:4688:HOH:O	2.63	0.45
8:H:17:ASP:OD1	8:H:17:ASP:C	2.54	0.45
19:A:524:PGV:O02	19:A:524:PGV:O13	2.34	0.45
6:S:92:VAL:HG23	6:S:92:VAL:O	2.15	0.45
10:W:56:PRO:HD3	12:Y:46:LYS:HG2	1.98	0.45
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.51	0.45
1:N:309:THR:HG22	14:N:516:HEA:HMB2	1.97	0.45
3:P:108:PRO:HA	28:P:3226:HOH:O	2.16	0.45
19:N:1266:PGV:H183	24:P:1264:PEK:H332	1.98	0.45
2:B:222:TRP:O	2:B:226:MET:HB2	2.17	0.45
19:C:267:PGV:H182	25:C:270:CDL:H671	1.97	0.45
8:H:60:TYR:C	8:H:60:TYR:CD1	2.89	0.45
1:N:402:GLY:HA3	1:N:499:PRO:HD3	1.99	0.45
3:C:112:LEU:HD13	3:C:118:PRO:HG3	1.99	0.45
3:C:139:ALA:CB	7:G:24:ALA:HB1	2.46	0.45
7:G:84:LYS:HD2	7:G:84:LYS:N	2.05	0.45
7:T:5:LYS:HG3	24:T:263:PEK:H383	1.98	0.45
22:B:1085:CHD:H212	22:B:1085:CHD:H12	1.98	0.45
18:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.98	0.45
7:T:12:GLY:HA3	28:T:3372:HOH:O	2.17	0.45
28:O:4335:HOH:O	8:U:61:LYS:HD2	2.17	0.45
1:A:115:SER:O	1:A:121:GLY:HA2	2.17	0.45
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.98	0.45
6:F:25:ARG:HD2	28:F:4164:HOH:O	2.17	0.45
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.98	0.45
4:D:132:GLN:OE1	9:I:43:ARG:HD3	2.17	0.44
11:K:24:PHE:O	11:K:28:VAL:HG12	2.17	0.44
1:N:335:SER:HB2	1:N:336:PRO:HD2	1.98	0.44
19:A:524:PGV:H232	19:A:524:PGV:H42	1.98	0.44
7:G:5:LYS:HD2	24:G:1263:PEK:H371	1.99	0.44
19:N:1524:PGV:O13	19:N:1524:PGV:O02	2.35	0.44
21:O:1229:PSC:H251	21:O:1229:PSC:H221	1.73	0.44
1:A:430:PHE:CE1	18:A:521:TGL:HB21	2.48	0.44
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.62	0.44
1:A:19:TYR:CD1	1:A:76:GLY:HA3	2.52	0.44
24:G:1263:PEK:H182	3:P:98:PHE:CD2	2.53	0.44
1:A:483:LEU:HD21	13:M:4:LYS:HD3	2.00	0.44
1:N:472:ILE:HG21	18:N:1522:TGL:CA9	2.47	0.44
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:MET:HG2	7:T:5:LYS:HA	2.00	0.44
2:B:81:LEU:HD12	25:T:1269:CDL:H351	1.99	0.44
7:G:31:CYS:SG	25:G:269:CDL:H532	2.57	0.44
18:N:1523:TGL:C36	28:V:4391:HOH:O	2.66	0.44
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	2.00	0.44
3:C:105:SER:HA	3:C:116:TRP:CE3	2.53	0.44
7:G:2:SER:OG	24:G:1263:PEK:H291	2.18	0.44
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.52	0.44
2:O:95:LEU:HD23	2:O:150:ILE:HG12	2.00	0.44
1:A:310:MET:CE	1:A:360:ASN:HD21	2.30	0.44
25:C:270:CDL:H652	25:C:270:CDL:H611	1.98	0.44
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.18	0.44
3:P:228:THR:HA	6:S:7:PRO:O	2.18	0.44
6:S:55:LYS:HA	6:S:74:LEU:O	2.18	0.44
12:Y:2:HIS:N	28:Y:4664:HOH:O	2.50	0.44
3:C:99:TRP:CE2	19:C:268:PGV:H232	2.53	0.44
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.98	0.44
2:O:146:MET:HA	2:O:213:LEU:HD12	2.00	0.44
25:C:270:CDL:H202	25:C:270:CDL:H171	1.81	0.43
25:C:270:CDL:HB32	25:C:270:CDL:HB21	2.00	0.43
7:G:30:LEU:HD23	25:G:269:CDL:C46	2.48	0.43
3:P:107:ALA:HB2	19:P:1268:PGV:H031	1.99	0.43
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.18	0.43
22:W:1059:CHD:H193	22:W:1059:CHD:H111	1.77	0.43
6:F:92:VAL:O	6:F:92:VAL:HG23	2.18	0.43
12:L:24:MET:SD	18:L:522:TGL:H161	2.58	0.43
1:A:37:ILE:HG21	14:A:515:HEA:CMA	2.47	0.43
21:B:229:PSC:H251	21:B:229:PSC:H221	1.67	0.43
4:D:112:GLU:HB2	28:D:4721:HOH:O	2.17	0.43
1:N:148:PHE:HB3	3:P:28:THR:HB	2.00	0.43
25:T:1269:CDL:C57	25:T:1269:CDL:H782	2.29	0.43
1:N:87:ILE:O	1:N:173:PRO:HD3	2.18	0.43
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.18	0.43
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.01	0.43
1:A:310:MET:HE1	1:A:360:ASN:HD21	1.84	0.43
11:X:52:GLU:HG2	28:X:4813:HOH:O	2.18	0.43
1:A:309:THR:HG22	14:A:516:HEA:HMB2	2.01	0.43
5:E:14:ARG:HD2	28:E:4284:HOH:O	2.18	0.43
18:N:1523:TGL:H361	28:V:4391:HOH:O	2.17	0.43
2:O:121:TYR:O	2:O:138:VAL:HA	2.18	0.43
1:A:37:ILE:HG21	14:A:515:HEA:HMA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:TYR:CG	1:N:76:GLY:HA3	2.53	0.43
1:N:54:TYR:HB2	28:N:4621:HOH:O	2.19	0.43
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.43
21:O:1229:PSC:C02	21:O:1229:PSC:H212	2.49	0.43
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.19	0.43
1:A:489:THR:HA	6:F:71:TRP:O	2.19	0.43
2:B:121:TYR:O	2:B:138:VAL:HA	2.19	0.43
4:D:34:SER:H	4:D:37:GLN:NE2	2.07	0.43
7:G:38:HIS:CE1	25:G:269:CDL:H111	2.54	0.43
1:N:400:PHE:C	18:N:1522:TGL:H283	2.39	0.43
2:O:93:PRO:HG3	2:O:151:ARG:HB2	2.00	0.43
25:T:1269:CDL:H182	25:T:1269:CDL:H152	1.85	0.43
25:C:270:CDL:H532	25:C:270:CDL:H561	1.81	0.42
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.19	0.42
1:N:347:LEU:HD13	1:N:383:MET:SD	2.59	0.42
1:N:76:GLY:O	1:N:80:ASN:HB2	2.18	0.42
22:C:271:CHD:H12A	22:C:271:CHD:H112	1.87	0.42
24:C:265:PEK:C38	25:G:269:CDL:C27	2.66	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.42
7:T:11:TPO:O	7:T:11:TPO:CG2	2.66	0.42
1:A:437:PRO:HG2	1:A:440:TYR:CZ	2.54	0.42
18:L:522:TGL:HA81	18:L:522:TGL:H211	1.55	0.42
1:N:386:VAL:HG11	14:N:515:HEA:H261	2.01	0.42
1:N:495:LEU:HA	1:N:495:LEU:HD12	1.92	0.42
12:L:12:PRO:HB2	18:L:522:TGL:HG2	2.01	0.42
21:O:1229:PSC:H081	5:R:8:ASP:OD1	2.18	0.42
7:T:38:HIS:NE2	25:T:1269:CDL:H111	2.35	0.42
7:G:25:LEU:HA	7:G:25:LEU:HD23	1.90	0.42
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.19	0.42
1:A:28:MET:CE	14:A:515:HEA:H271	2.49	0.42
3:C:91:VAL:HG22	24:T:263:PEK:H14	2.00	0.42
4:D:23:PRO:HG3	5:E:70:VAL:HG21	2.01	0.42
25:T:1269:CDL:H522	25:T:1269:CDL:H202	2.01	0.42
19:A:524:PGV:H061	19:A:524:PGV:P	2.59	0.42
8:H:37:HIS:NE2	8:H:76:ARG:NH2	2.67	0.42
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.42
28:G:4541:HOH:O	19:P:1268:PGV:H301	2.18	0.42
25:T:1269:CDL:HA62	25:T:1269:CDL:H322	2.00	0.42
1:A:514:LYS:NZ	28:A:2645:HOH:O	2.41	0.42
18:A:521:TGL:H281	18:A:521:TGL:H102	2.02	0.42
19:C:268:PGV:H341	28:T:4364:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.55	0.42
1:N:377:PHE:HB2	14:N:516:HEA:HMD3	2.01	0.42
21:O:1229:PSC:C07	9:V:10:ARG:HE	2.33	0.42
22:P:1525:CHD:H152	19:P:1268:PGV:H11	2.02	0.42
1:N:472:ILE:HG21	18:N:1522:TGL:HA91	2.02	0.42
25:C:270:CDL:C19	25:C:270:CDL:H642	2.49	0.42
4:D:127:LYS:HD2	28:I:2618:HOH:O	2.20	0.42
6:F:55:LYS:HA	6:F:74:LEU:O	2.19	0.42
25:G:269:CDL:H511	25:G:269:CDL:H172	2.02	0.42
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.59	0.42
7:T:84:LYS:N	7:T:84:LYS:CD	2.62	0.42
12:Y:20:ARG:NH2	12:Y:24:MET:CG	2.82	0.42
3:C:210:ILE:HD13	19:C:267:PGV:H301	2.01	0.41
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.71	0.41
1:N:406:ASN:HD21	19:N:1524:PGV:C2	2.33	0.41
22:B:1085:CHD:H212	22:B:1085:CHD:H183	2.01	0.41
25:P:1270:CDL:H242	25:P:1270:CDL:H661	2.01	0.41
4:Q:7:LYS:HA	28:Q:4706:HOH:O	2.19	0.41
10:W:27:THR:HB	28:W:4729:HOH:O	2.20	0.41
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.84	0.41
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	2.02	0.41
2:B:49:LYS:HE2	28:E:4606:HOH:O	2.19	0.41
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.02	0.41
3:C:207:HIS:CE1	19:C:267:PGV:H343	2.56	0.41
28:N:3199:HOH:O	3:P:17:PRO:HG2	2.20	0.41
7:T:2:SER:OG	24:T:263:PEK:H301	2.21	0.41
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.50	0.41
5:R:52:LEU:O	5:R:55:CYS:HB2	2.20	0.41
21:B:229:PSC:H031	21:B:229:PSC:O02	2.20	0.41
4:D:112:GLU:CB	28:D:4721:HOH:O	2.68	0.41
18:N:1523:TGL:HA32	18:N:1523:TGL:HB42	2.02	0.41
2:O:33:LEU:HD12	2:O:33:LEU:HA	1.93	0.41
3:P:37:PHE:CD1	10:W:52:TRP:HZ3	2.38	0.41
19:A:524:PGV:H152	19:A:524:PGV:H321	2.03	0.41
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.02	0.41
3:P:129:VAL:N	3:P:130:PRO:CD	2.82	0.41
1:N:289:ALA:HB3	1:N:305:PHE:CG	2.55	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.21	0.41
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.50	0.41
1:A:177:SER:H	1:A:180:GLN:HE21	1.69	0.41
18:A:521:TGL:HC22	28:I:2606:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:TYR:O	3:C:244:PHE:HB3	2.20	0.41
2:B:103:GLN:HA	2:B:104:TRP:HA	1.90	0.41
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.34	0.41
3:C:137:LEU:HD23	3:C:137:LEU:HA	1.85	0.41
12:L:20:ARG:HH12	18:L:522:TGL:HC62	1.86	0.41
3:P:139:ALA:CB	7:T:24:ALA:HB1	2.51	0.41
9:I:73:LYS:CB	28:I:4200:HOH:O	2.61	0.41
1:N:240:HIS:C	1:N:240:HIS:CD2	2.94	0.41
1:N:62:ALA:HB1	14:N:515:HEA:HMD3	2.03	0.41
19:C:267:PGV:H182	25:C:270:CDL:H673	2.01	0.41
10:J:40:LEU:HD12	22:J:60:CHD:H183	2.03	0.41
2:O:193:TYR:CD1	2:O:210:VAL:HG22	2.56	0.41
8:U:9:LYS:HB3	8:U:10:ASN:H	1.61	0.41
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.92	0.41
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.03	0.40
28:A:2690:HOH:O	2:B:201:GLY:HA2	2.21	0.40
1:N:172:LYS:HD2	1:N:181:THR:HG22	2.02	0.40
2:O:16:ILE:HD11	2:O:86:MET:HG2	2.04	0.40
3:P:105:SER:HA	3:P:116:TRP:CE3	2.55	0.40
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.57	0.40
6:F:53:THR:HB	6:F:54:ASN:H	1.74	0.40
2:O:3:TYR:CZ	2:O:6:GLN:HG3	2.56	0.40
2:O:4:PRO:HB2	11:X:43:SER:HA	2.03	0.40
6:S:51:SER:O	6:S:94:HIS:HA	2.20	0.40
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.56	0.40
8:H:9:LYS:HD3	8:H:9:LYS:HA	1.91	0.40
3:C:67:PHE:CE1	25:C:270:CDL:H1	2.31	0.40
8:H:39:CYS:O	8:H:43:MET:HG2	2.22	0.40
2:O:90:ILE:HG12	8:U:16:PHE:CE2	2.56	0.40
21:O:1229:PSC:H071	9:V:10:ARG:HH21	1.87	0.40
8:H:75:ARG:HG2	8:H:80:THR:OG1	2.21	0.40
1:N:335:SER:HB2	28:N:3257:HOH:O	2.20	0.40
7:T:37:LEU:HD23	25:T:1269:CDL:H361	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:2:HIS:N	28:V:4556:HOH:O[2_685]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	494 (96%)	17 (3%)	1 (0%)	47	82
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	34	72
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	34	72
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	250 (97%)	5 (2%)	2 (1%)	19	57
4	D	142/147 (97%)	136 (96%)	6 (4%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	87 (91%)	8 (8%)	1 (1%)	15	53
6	S	96/98 (98%)	88 (92%)	6 (6%)	2 (2%)	7	33
7	G	81/85 (95%)	65 (80%)	8 (10%)	8 (10%)	0	2
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	1	8
8	H	77/85 (91%)	69 (90%)	5 (6%)	3 (4%)	3	17
8	U	77/85 (91%)	71 (92%)	4 (5%)	2 (3%)	5	27
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	68 (96%)	2 (3%)	1 (1%)	11	43
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3504/3614 (97%)	3351 (96%)	126 (4%)	27 (1%)	19	57

All (27) 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	4	ALA
7	T	7	ASP
7	T	8	HIS
1	A	384	GLY
2	B	60	GLU
7	G	6	GLY
7	T	3	ALA
8	U	8	ILE
7	T	6	GLY
7	G	3	ALA
8	H	45	ALA
8	H	46	LYS
2	O	60	GLU
3	P	38	ASN
3	P	232	HIS
7	G	37	LEU
8	U	10	ASN
7	G	40	GLY
9	V	36	LYS

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	84
1	N	426/426 (100%)	415 (97%)	11 (3%)	46	78
2	B	210/210 (100%)	199 (95%)	11 (5%)	23	59
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	52
3	C	224/226 (99%)	218 (97%)	6 (3%)	44	77
3	P	224/226 (99%)	217 (97%)	7 (3%)	40	75
4	D	128/129 (99%)	126 (98%)	2 (2%)	62	86
4	Q	128/129 (99%)	123 (96%)	5 (4%)	32	69
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	81
5	R	92/95 (97%)	90 (98%)	2 (2%)	52	81
6	F	81/81 (100%)	77 (95%)	4 (5%)	25	61
6	S	81/81 (100%)	76 (94%)	5 (6%)	18	52
7	G	67/68 (98%)	59 (88%)	8 (12%)	5	22
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	35
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	38
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	47
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	58
9	V	57/57 (100%)	54 (95%)	3 (5%)	22	58
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	83
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	83
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	78
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	78
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	78
13	M	37/38 (97%)	31 (84%)	6 (16%)	2	12
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	17
All	All	3040/3082 (99%)	2917 (96%)	123 (4%)	31	68

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	189	MET
1	A	338	MET
1	A	369	ASP
1	A	394	VAL
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
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
3	C	77	LYS
3	C	127	LEU
3	C	144	ILE
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	31	LYS
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	84	SER
6	F	87	THR
6	F	95	GLN
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	35	SER
7	G	36	TRP
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	27	ARG

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Mol	Chain	Res	Type
8	H	51	SER
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
10	J	50	LEU
11	K	54	ARG
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
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	363	LEU
1	N	369	ASP
1	N	484	THR
1	N	485	VAL
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	183	THR
2	O	217	LYS
3	P	33	MET
3	P	77	LYS
3	P	127	LEU
3	P	144	ILE
3	P	159	MET

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Mol	Chain	Res	Type
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	19	ARG
4	Q	51	LEU
4	Q	52	SER
4	Q	143	ASN
5	R	5	HIS
5	R	79	LYS
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	64	GLU
6	S	95	GLN
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	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
8	U	70	SER
9	V	2	THR
9	V	8	GLN
9	V	26	MET
10	W	50	LEU
11	X	54	ARG
12	Y	20	ARG
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 (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	512	ASN
2	B	22	HIS
2	B	52	HIS
2	B	181	GLN
3	C	68	GLN
3	C	122	HIS
4	D	29	HIS
4	D	37	GLN
4	D	109	HIS
4	D	143	ASN
5	E	94	ASN
7	G	8	HIS
7	G	71	HIS
7	G	76	ASN
9	I	8	GLN
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	22	HIS
2	O	181	GLN
3	P	3	HIS
3	P	68	GLN
4	Q	37	GLN
4	Q	109	HIS
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	0.78	0	7,9,11	5.09	3 (42%)
7	TPO	T	11	7	8,10,11	2.26	3 (37%)	10,14,16	1.55	2 (20%)
2	FME	B	1	2	8,9,10	1.09	0	7,9,11	5.95	3 (42%)
9	SAC	I	1	9	7,8,9	2.60	2 (28%)	8,9,11	1.76	3 (37%)
1	FME	N	1	1	8,9,10	0.66	0	7,9,11	5.58	2 (28%)
9	SAC	V	1	9	7,8,9	2.56	2 (28%)	8,9,11	4.91	3 (37%)
1	FME	A	1	1	8,9,10	0.80	0	7,9,11	4.67	3 (42%)
7	TPO	G	11	7	8,10,11	2.63	3 (37%)	10,14,16	1.58	2 (20%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	5.29	1.35	1.23
7	G	11	TPO	P-OG1	5.18	1.69	1.59
9	V	1	SAC	CA-N	4.86	1.53	1.46
9	V	1	SAC	OAC-C1A	4.47	1.33	1.23
9	I	1	SAC	CA-N	3.77	1.51	1.46
7	T	11	TPO	P-OG1	3.67	1.66	1.59
7	T	11	TPO	P-O1P	3.47	1.61	1.50
7	G	11	TPO	P-O1P	3.27	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O2P	2.22	1.63	1.54
7	G	11	TPO	P-O2P	2.22	1.63	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CA-N-CN	-14.36	100.73	122.82
2	B	1	FME	CA-N-CN	-14.25	100.91	122.82
2	O	1	FME	CA-N-CN	-12.59	103.45	122.82
1	A	1	FME	CA-N-CN	-11.19	105.61	122.82
9	V	1	SAC	CB-CA-N	-8.76	90.89	110.55
9	V	1	SAC	C-CA-N	7.89	123.97	109.73
9	V	1	SAC	CA-N-C1A	6.54	135.21	123.15
2	B	1	FME	CG-CB-CA	-4.48	100.52	112.95
2	B	1	FME	C-CA-N	4.10	117.14	109.73
1	A	1	FME	CE-SD-CG	3.71	113.16	100.40
1	A	1	FME	CG-CB-CA	-3.49	103.26	112.95
2	O	1	FME	C-CA-N	3.36	115.79	109.73
9	I	1	SAC	C2A-C1A-N	-2.99	111.03	116.10
7	G	11	TPO	O2P-P-OG1	2.86	118.81	105.99
7	T	11	TPO	CG2-CB-CA	2.75	118.59	113.16
2	O	1	FME	CG-CB-CA	-2.61	105.69	112.95
7	G	11	TPO	P-OG1-CB	2.52	130.81	123.21
1	N	1	FME	CE-SD-CG	2.42	108.72	100.40
9	I	1	SAC	CA-N-C1A	2.23	127.25	123.15
9	I	1	SAC	OG-CB-CA	2.12	116.38	110.97
7	T	11	TPO	O-C-CA	-2.08	119.34	124.78

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

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

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	2	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
14	HEA	N	515	1	44,67,67	1.09	3 (6%)	37,103,103	3.41	17 (45%)
20	CUA	B	228	2	0,1,1	0.00	-	-		
20	CUA	O	228	2	0,1,1	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	PSC	O	1229	-	51,51,51	1.18	3 (5%)	57,59,59	1.09	4 (7%)
24	PEK	G	1263	-	52,52,52	1.32	3 (5%)	55,57,57	1.31	6 (10%)
19	PGV	A	524	-	50,50,50	1.29	2 (4%)	53,56,56	1.25	7 (13%)
22	CHD	C	525	-	29,32,32	0.80	0	48,51,51	1.31	7 (14%)
24	PEK	P	1264	-	52,52,52	0.99	4 (7%)	55,57,57	1.37	10 (18%)
18	TGL	A	521	-	62,62,62	1.28	6 (9%)	65,65,65	1.83	15 (23%)
24	PEK	P	1265	-	52,52,52	1.35	5 (9%)	55,57,57	1.31	6 (10%)
19	PGV	C	268	-	50,50,50	1.27	2 (4%)	53,56,56	1.34	6 (11%)
22	CHD	C	271	-	29,32,32	0.60	0	48,51,51	2.37	22 (45%)
25	CDL	C	270	-	99,99,99	1.37	13 (13%)	105,111,111	1.36	15 (14%)
14	HEA	A	516	1	44,67,67	1.10	2 (4%)	37,103,103	1.87	7 (18%)
14	HEA	N	516	1	44,67,67	1.02	1 (2%)	37,103,103	1.57	11 (29%)
25	CDL	G	269	-	99,99,99	1.43	12 (12%)	105,111,111	1.34	11 (10%)
14	HEA	A	515	1	44,67,67	0.97	1 (2%)	37,103,103	2.91	18 (48%)
19	PGV	N	1524	-	50,50,50	1.00	2 (4%)	53,56,56	1.23	7 (13%)
22	CHD	B	1085	-	29,32,32	0.78	0	48,51,51	1.94	16 (33%)
19	PGV	P	1268	-	50,50,50	1.25	2 (4%)	53,56,56	1.50	6 (11%)
18	TGL	L	522	-	62,62,62	1.40	7 (11%)	65,65,65	1.62	12 (18%)
19	PGV	A	522	-	50,50,50	0.85	2 (4%)	53,56,56	1.16	2 (3%)
21	PSC	B	229	-	51,51,51	1.20	3 (5%)	57,59,59	1.11	2 (3%)
24	PEK	T	263	-	52,52,52	1.32	4 (7%)	55,57,57	1.20	7 (12%)
24	PEK	C	265	-	52,52,52	1.28	3 (5%)	55,57,57	1.24	6 (10%)
22	CHD	G	229	-	29,32,32	0.54	0	48,51,51	1.24	2 (4%)
27	DMU	M	526	-	34,34,34	0.96	2 (5%)	45,45,45	2.59	15 (33%)
25	CDL	T	1269	-	99,99,99	1.38	12 (12%)	105,111,111	1.28	10 (9%)
18	TGL	N	1521	-	62,62,62	1.28	6 (9%)	65,65,65	1.59	12 (18%)
19	PGV	P	1267	-	50,50,50	0.92	3 (6%)	53,56,56	1.08	4 (7%)
27	DMU	Z	1526	-	34,34,34	0.90	2 (5%)	45,45,45	2.55	15 (33%)
22	CHD	P	1271	-	29,32,32	0.60	0	48,51,51	2.34	19 (39%)
25	CDL	P	1270	-	99,99,99	1.41	12 (12%)	105,111,111	1.43	16 (15%)
18	TGL	N	1523	-	62,62,62	1.40	6 (9%)	65,65,65	1.48	12 (18%)
22	CHD	J	60	-	29,32,32	0.96	1 (3%)	48,51,51	3.09	24 (50%)
22	CHD	P	1525	-	29,32,32	0.69	0	48,51,51	1.67	10 (20%)
19	PGV	C	267	-	50,50,50	0.85	3 (6%)	53,56,56	1.08	5 (9%)
19	PGV	N	1266	-	50,50,50	0.85	2 (4%)	53,56,56	1.36	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	TGL	N	1522	-	62,62,62	1.60	7 (11%)	65,65,65	1.59	15 (23%)
24	PEK	C	264	-	52,52,52	0.98	4 (7%)	55,57,57	1.43	8 (14%)
18	TGL	D	523	-	62,62,62	1.38	6 (9%)	65,65,65	1.59	9 (13%)
22	CHD	W	1059	-	29,32,32	0.93	1 (3%)	48,51,51	3.39	23 (47%)

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
14	HEA	N	515	1	3/3/7/16	4/24/76/76	-
14	HEA	A	515	1	3/3/7/16	4/24/76/76	-
24	PEK	G	1263	-	-	31/56/56/56	-
19	PGV	A	524	-	-	35/55/55/55	-
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
24	PEK	P	1264	-	-	23/56/56/56	-
18	TGL	A	521	-	-	35/65/65/65	-
24	PEK	P	1265	-	-	31/56/56/56	-
19	PGV	C	268	-	-	34/55/55/55	-
22	CHD	C	271	-	-	4/7/74/74	0/4/4/4
27	DMU	Z	1526	-	4/4/10/10	10/19/59/59	0/2/2/2
14	HEA	A	516	1	3/3/7/16	2/24/76/76	-
14	HEA	N	516	1	3/3/7/16	2/24/76/76	-
25	CDL	G	269	-	-	64/110/110/110	-
21	PSC	O	1229	-	-	38/55/55/55	-
19	PGV	N	1524	-	-	41/55/55/55	-
22	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
19	PGV	P	1268	-	-	33/55/55/55	-
18	TGL	L	522	-	-	39/65/65/65	-
19	PGV	A	522	-	-	14/55/55/55	-
21	PSC	B	229	-	-	32/55/55/55	-
24	PEK	T	263	-	-	33/56/56/56	-
24	PEK	C	265	-	-	23/56/56/56	-
22	CHD	G	229	-	-	0/7/74/74	0/4/4/4
27	DMU	M	526	-	4/4/10/10	9/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CDL	T	1269	-	-	52/110/110/110	-
18	TGL	N	1521	-	-	33/65/65/65	-
19	PGV	P	1267	-	-	16/55/55/55	-
25	CDL	C	270	-	-	66/110/110/110	-
22	CHD	P	1271	-	-	4/7/74/74	0/4/4/4
25	CDL	P	1270	-	-	67/110/110/110	-
18	TGL	N	1523	-	-	36/65/65/65	-
22	CHD	J	60	-	-	4/7/74/74	0/4/4/4
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
19	PGV	C	267	-	-	16/55/55/55	-
19	PGV	N	1266	-	-	16/55/55/55	-
18	TGL	N	1522	-	-	35/65/65/65	-
24	PEK	C	264	-	-	28/56/56/56	-
18	TGL	D	523	-	-	38/65/65/65	-
22	CHD	W	1059	-	-	6/7/74/74	0/4/4/4

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	1522	TGL	OG1-CA1	6.77	1.53	1.33
18	N	1522	TGL	OG2-CB1	6.23	1.51	1.34
19	A	524	PGV	O03-C19	6.18	1.51	1.33
24	T	263	PEK	O03-C21	6.15	1.51	1.33
24	G	1263	PEK	O03-C21	6.03	1.51	1.33
19	P	1268	PGV	O01-C1	5.98	1.51	1.34
18	L	522	TGL	OG2-CB1	5.96	1.51	1.34
19	C	268	PGV	O01-C1	5.89	1.50	1.34
18	N	1523	TGL	OG2-CB1	5.78	1.50	1.34
24	P	1265	PEK	O01-C1	5.78	1.50	1.34
24	C	265	PEK	O03-C21	5.72	1.50	1.33
25	G	269	CDL	OA6-CA5	5.56	1.50	1.34
18	D	523	TGL	OG2-CB1	5.35	1.49	1.34
18	A	521	TGL	OG1-CA1	5.21	1.48	1.33
24	C	265	PEK	O01-C1	5.19	1.48	1.34
25	P	1270	CDL	OA8-CA7	5.18	1.48	1.33
18	L	522	TGL	OG1-CA1	5.13	1.48	1.33
25	P	1270	CDL	OA6-CA5	5.12	1.48	1.34
24	P	1265	PEK	O03-C21	5.10	1.48	1.33
24	G	1263	PEK	O01-C1	5.09	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	270	CDL	OA8-CA7	5.03	1.48	1.33
24	T	263	PEK	O01-C1	4.99	1.48	1.34
25	G	269	CDL	OB6-CB5	4.95	1.48	1.34
18	D	523	TGL	OG3-CC1	4.92	1.47	1.33
19	C	268	PGV	O03-C19	4.85	1.47	1.33
18	N	1523	TGL	OG3-CC1	4.85	1.47	1.33
18	N	1523	TGL	OG1-CA1	4.80	1.47	1.33
25	T	1269	CDL	OA6-CA5	4.76	1.47	1.34
18	D	523	TGL	OG1-CA1	4.74	1.47	1.33
25	G	269	CDL	OB8-CB7	4.72	1.47	1.33
18	N	1521	TGL	OG1-CA1	4.72	1.47	1.33
19	N	1524	PGV	O03-C19	4.66	1.46	1.33
18	A	521	TGL	OG2-CB1	4.65	1.47	1.34
19	P	1268	PGV	O03-C19	4.64	1.46	1.33
21	B	229	PSC	O01-C1	4.63	1.47	1.34
25	T	1269	CDL	OB8-CB7	4.63	1.46	1.33
21	B	229	PSC	O03-C19	4.59	1.46	1.33
25	G	269	CDL	OA8-CA7	4.57	1.46	1.33
25	T	1269	CDL	OB6-CB5	4.56	1.47	1.34
21	O	1229	PSC	O01-C1	4.55	1.47	1.34
25	C	270	CDL	OA6-CA5	4.55	1.47	1.34
18	N	1521	TGL	OG2-CB1	4.54	1.47	1.34
25	C	270	CDL	OB8-CB7	4.51	1.46	1.33
18	N	1522	TGL	OG3-CC1	4.50	1.46	1.33
18	N	1521	TGL	OG3-CC1	4.35	1.46	1.33
19	A	524	PGV	O01-C1	4.34	1.46	1.34
25	T	1269	CDL	OA8-CA7	4.16	1.45	1.33
25	P	1270	CDL	OB6-CB5	4.11	1.45	1.34
19	P	1267	PGV	O03-C19	4.07	1.45	1.33
21	O	1229	PSC	O03-C19	4.03	1.45	1.33
21	O	1229	PSC	C13-C12	3.95	1.54	1.31
19	N	1266	PGV	O03-C19	3.92	1.44	1.33
21	B	229	PSC	C13-C12	3.83	1.54	1.31
25	P	1270	CDL	OB8-CB7	3.80	1.44	1.33
25	P	1270	CDL	C59-C58	-3.76	1.30	1.51
24	P	1264	PEK	O01-C1	3.69	1.44	1.34
25	C	270	CDL	C59-C58	-3.64	1.31	1.51
24	P	1264	PEK	O03-C21	3.62	1.43	1.33
18	L	522	TGL	C10-CB9	-3.61	1.31	1.51
19	A	522	PGV	O01-C1	3.55	1.44	1.34
18	L	522	TGL	C20-CA9	-3.53	1.31	1.51
24	C	264	PEK	O01-C1	3.51	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	522	PGV	O03-C19	3.50	1.43	1.33
25	P	1270	CDL	C79-C78	-3.48	1.32	1.51
18	N	1521	TGL	C10-CB9	-3.47	1.32	1.51
18	N	1522	TGL	C20-CA9	-3.43	1.32	1.51
25	C	270	CDL	OB6-CB5	3.43	1.44	1.34
19	N	1524	PGV	O01-C1	3.38	1.43	1.34
19	C	267	PGV	O03-C19	3.37	1.43	1.33
18	A	521	TGL	OG3-CC1	3.36	1.43	1.33
25	T	1269	CDL	C59-C58	-3.36	1.32	1.51
25	P	1270	CDL	C62-C61	-3.35	1.32	1.51
18	A	521	TGL	C10-CB9	-3.34	1.32	1.51
25	T	1269	CDL	C42-C41	-3.29	1.33	1.51
25	C	270	CDL	C62-C61	-3.28	1.33	1.51
25	G	269	CDL	C59-C58	-3.28	1.33	1.51
18	N	1522	TGL	C10-CB9	-3.27	1.33	1.51
25	T	1269	CDL	C62-C61	-3.27	1.33	1.51
14	A	516	HEA	C3B-C11	-3.23	1.50	1.52
19	N	1266	PGV	O01-C1	3.21	1.43	1.34
25	G	269	CDL	C42-C41	-3.20	1.33	1.51
24	C	264	PEK	O03-C21	3.16	1.42	1.33
25	P	1270	CDL	C19-C18	-3.14	1.34	1.51
25	C	270	CDL	C19-C18	-3.14	1.34	1.51
27	M	526	DMU	O16-C6	3.13	1.45	1.40
25	C	270	CDL	C79-C78	-3.11	1.34	1.51
14	A	515	HEA	C3B-C11	-3.09	1.50	1.52
18	D	523	TGL	C20-CA9	-3.08	1.34	1.51
25	P	1270	CDL	C82-C81	-3.08	1.34	1.51
18	N	1523	TGL	C20-CA9	-3.06	1.34	1.51
25	C	270	CDL	C82-C81	-3.06	1.34	1.51
27	M	526	DMU	C3-C4	-3.05	1.44	1.52
19	C	267	PGV	O01-C1	3.04	1.42	1.34
27	Z	1526	DMU	C3-C4	-3.04	1.44	1.52
25	T	1269	CDL	C79-C78	-3.02	1.34	1.51
18	N	1523	TGL	C10-CB9	-3.00	1.34	1.51
24	C	264	PEK	O01-C02	-3.00	1.39	1.46
18	A	521	TGL	C20-CA9	-2.98	1.34	1.51
25	C	270	CDL	C22-C21	-2.98	1.34	1.51
14	N	515	HEA	C3A-C2A	-2.98	1.36	1.40
25	G	269	CDL	C62-C61	-2.98	1.34	1.51
18	D	523	TGL	C10-CB9	-2.96	1.35	1.51
25	G	269	CDL	C39-C38	-2.95	1.35	1.51
25	P	1270	CDL	C22-C21	-2.94	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	269	CDL	C22-C21	-2.93	1.35	1.51
18	D	523	TGL	C15-CC9	-2.93	1.35	1.51
25	T	1269	CDL	C39-C38	-2.92	1.35	1.51
18	L	522	TGL	OG3-CC1	2.90	1.41	1.33
25	G	269	CDL	C19-C18	-2.90	1.35	1.51
18	N	1523	TGL	C15-CC9	-2.88	1.35	1.51
25	T	1269	CDL	C19-C18	-2.87	1.35	1.51
25	T	1269	CDL	C22-C21	-2.85	1.35	1.51
25	G	269	CDL	C82-C81	-2.83	1.35	1.51
25	T	1269	CDL	C82-C81	-2.83	1.35	1.51
24	P	1265	PEK	P-O11	2.82	1.70	1.59
14	N	516	HEA	C3B-C11	-2.81	1.50	1.52
25	G	269	CDL	C79-C78	-2.80	1.35	1.51
24	P	1264	PEK	O03-C01	-2.78	1.38	1.45
18	N	1521	TGL	C20-CA9	-2.77	1.36	1.51
19	P	1267	PGV	O01-C1	2.70	1.41	1.34
18	N	1522	TGL	C15-CC9	-2.69	1.36	1.51
25	P	1270	CDL	C39-C38	-2.64	1.36	1.51
18	N	1521	TGL	C15-CC9	-2.61	1.36	1.51
27	Z	1526	DMU	O16-C6	2.60	1.44	1.40
25	C	270	CDL	C42-C41	-2.58	1.37	1.51
25	C	270	CDL	C39-C38	-2.57	1.37	1.51
18	A	521	TGL	C15-CC9	-2.55	1.37	1.51
18	L	522	TGL	C15-CC9	-2.54	1.37	1.51
25	P	1270	CDL	C42-C41	-2.49	1.37	1.51
24	C	264	PEK	O03-C01	-2.49	1.39	1.45
19	P	1267	PGV	O01-C02	-2.46	1.40	1.46
24	P	1264	PEK	O01-C02	-2.46	1.40	1.46
24	T	263	PEK	P-O11	2.45	1.69	1.59
24	P	1265	PEK	P-O12	2.30	1.68	1.59
25	C	270	CDL	OB6-CB4	-2.28	1.40	1.46
19	C	267	PGV	O01-C02	-2.23	1.41	1.46
14	N	515	HEA	C1B-NB	-2.21	1.31	1.36
14	N	515	HEA	C4D-ND	-2.18	1.31	1.36
24	T	263	PEK	C03-C02	2.16	1.57	1.50
18	N	1522	TGL	CG1-CG2	2.16	1.57	1.50
22	W	1059	CHD	C13-C17	2.13	1.59	1.55
24	C	265	PEK	P-O11	2.10	1.67	1.59
14	A	516	HEA	C14-C15	2.09	1.38	1.33
18	L	522	TGL	CG1-CG2	2.08	1.57	1.50
24	P	1265	PEK	C03-C02	2.04	1.57	1.50
22	J	60	CHD	C10-C5	2.02	1.58	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	1263	PEK	C03-C02	2.01	1.56	1.50

All (425) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	515	HEA	C17-C18-C19	-9.17	105.58	127.66
14	N	515	HEA	C17-C18-C19	-8.89	106.25	127.66
22	W	1059	CHD	C13-C17-C20	8.44	129.57	119.50
14	N	515	HEA	C17-C16-C15	8.34	140.40	112.98
14	N	515	HEA	C4B-C3B-C2B	-7.84	101.39	106.87
14	A	515	HEA	C17-C16-C15	7.58	137.93	112.98
22	J	60	CHD	C6-C5-C10	7.40	120.52	112.66
22	W	1059	CHD	C18-C13-C12	-7.33	101.61	109.07
22	W	1059	CHD	C11-C12-C13	7.20	118.64	111.24
22	J	60	CHD	C13-C17-C20	7.12	127.99	119.50
19	P	1268	PGV	O01-C1-C2	6.96	126.50	111.50
22	W	1059	CHD	C17-C13-C14	-6.88	93.16	100.09
18	A	521	TGL	CG2-OG2-CB1	6.84	134.63	117.79
22	W	1059	CHD	C6-C5-C10	6.15	119.18	112.66
22	J	60	CHD	C17-C13-C14	-6.04	94.00	100.09
22	W	1059	CHD	C14-C13-C12	6.04	113.03	107.40
22	W	1059	CHD	C9-C10-C5	6.03	117.05	108.58
22	J	60	CHD	C10-C9-C8	5.93	118.19	111.82
27	M	526	DMU	O5-C4-C57	5.90	121.09	106.44
27	M	526	DMU	O7-C3-C2	5.80	122.72	107.28
27	M	526	DMU	O1-C9-C11	5.77	120.78	106.44
27	Z	1526	DMU	O7-C3-C2	5.73	122.51	107.28
14	A	516	HEA	CAD-CBD-CGD	-5.71	103.09	112.67
27	Z	1526	DMU	O5-C6-C1	5.70	122.42	110.35
18	L	522	TGL	OG3-CC1-OC1	-5.60	109.47	123.59
27	M	526	DMU	C2-C3-C4	5.46	123.44	110.93
25	P	1270	CDL	OA6-CA5-C11	5.43	123.20	111.50
19	C	268	PGV	O01-C1-C2	5.33	123.00	111.50
18	N	1521	TGL	CG2-OG2-CB1	5.29	130.80	117.79
22	P	1271	CHD	C1-C2-C3	5.25	117.21	110.47
22	J	60	CHD	C9-C10-C5	5.22	115.92	108.58
27	Z	1526	DMU	O5-C4-C57	5.17	119.30	106.44
25	C	270	CDL	OA6-CA5-C11	5.06	122.42	111.50
27	Z	1526	DMU	O1-C9-C8	5.06	118.89	109.69
22	J	60	CHD	C1-C10-C5	5.06	115.25	107.77
22	C	271	CHD	C19-C10-C1	-5.02	100.18	108.26
22	B	1085	CHD	C4-C3-C2	4.98	116.50	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1265	PEK	O01-C1-C2	4.97	122.20	111.50
19	N	1266	PGV	O03-C19-C20	4.97	127.49	111.91
25	G	269	CDL	OB6-CB5-C51	4.97	122.20	111.50
14	N	515	HEA	C12-C13-C14	-4.95	99.17	112.23
27	Z	1526	DMU	O5-C4-C3	4.94	120.17	109.75
25	T	1269	CDL	OA6-CA5-C11	4.94	122.14	111.50
18	N	1522	TGL	CG2-OG2-CB1	4.92	129.90	117.79
18	N	1523	TGL	OG2-CB1-CB2	4.91	122.09	111.50
27	M	526	DMU	O1-C10-C5	4.88	120.67	110.35
22	C	271	CHD	C1-C2-C3	4.85	116.69	110.47
22	W	1059	CHD	C9-C11-C12	4.82	120.66	114.30
22	P	1271	CHD	C19-C10-C1	-4.80	100.53	108.26
14	N	515	HEA	C26-C15-C16	-4.73	107.31	115.27
22	W	1059	CHD	C18-C13-C17	4.70	118.57	111.21
25	T	1269	CDL	OB6-CB5-C51	4.69	121.62	111.50
27	Z	1526	DMU	O1-C9-C11	4.64	117.98	106.44
25	G	269	CDL	OA6-CA5-C11	4.62	121.46	111.50
22	C	271	CHD	C18-C13-C12	-4.61	104.37	109.07
22	W	1059	CHD	C17-C13-C12	4.61	121.88	117.67
27	Z	1526	DMU	C8-C7-C5	4.59	118.84	110.82
19	N	1266	PGV	O03-C19-O04	-4.57	112.05	123.59
22	P	1271	CHD	C2-C1-C10	4.56	120.61	112.78
27	M	526	DMU	O1-C9-C8	4.56	117.97	109.69
18	D	523	TGL	OG1-CG1-CG2	4.55	121.68	108.43
22	B	1085	CHD	C6-C7-C8	4.48	116.26	111.48
19	P	1268	PGV	O03-C19-C20	4.47	125.93	111.91
18	D	523	TGL	CG3-CG2-CG1	-4.45	101.26	111.79
27	M	526	DMU	O5-C6-C1	4.43	119.73	110.35
22	J	60	CHD	C5-C4-C3	4.42	119.25	112.76
22	C	271	CHD	C22-C23-C24	-4.40	104.14	113.59
22	P	1271	CHD	C22-C23-C24	-4.38	104.17	113.59
24	G	1263	PEK	O01-C1-C2	4.37	120.93	111.50
14	A	515	HEA	C16-C15-C14	4.37	129.96	121.12
14	N	515	HEA	C20-C19-C18	4.36	129.94	121.12
22	C	271	CHD	C10-C9-C8	4.30	116.43	111.82
27	M	526	DMU	C8-C7-C5	4.29	118.32	110.82
18	N	1523	TGL	CG3-CG2-CG1	-4.29	101.65	111.79
24	G	1263	PEK	O03-C21-C22	4.26	125.28	111.91
24	C	265	PEK	O03-C21-C22	4.24	125.20	111.91
18	A	521	TGL	OG2-CB1-CB2	4.24	120.63	111.50
14	N	515	HEA	C16-C15-C14	4.21	129.63	121.12
22	P	1271	CHD	C10-C9-C8	4.20	116.33	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	515	HEA	CBA-CAA-C2A	4.20	120.22	112.48
14	N	515	HEA	C12-C11-C3B	4.19	123.56	112.56
27	Z	1526	DMU	C2-C3-C4	4.15	120.43	110.93
24	C	264	PEK	O01-C1-O02	-4.14	113.69	123.70
22	J	60	CHD	C6-C5-C4	-4.13	106.43	111.19
19	A	522	PGV	O03-C19-C20	4.12	124.84	111.91
18	N	1521	TGL	OG2-CG2-CG3	4.12	123.31	108.40
22	J	60	CHD	C4-C3-C2	4.06	115.40	110.55
18	N	1521	TGL	OG2-CB1-CB2	4.06	120.25	111.50
18	A	521	TGL	CA3-CA2-CA1	-4.06	98.86	113.62
19	C	268	PGV	O03-C19-C20	4.06	124.64	111.91
19	A	522	PGV	O03-C19-O04	-4.02	113.44	123.59
24	P	1264	PEK	O01-C1-O02	-4.01	114.02	123.70
14	A	516	HEA	CAA-CBA-CGA	-4.00	105.95	112.67
24	P	1265	PEK	O03-C21-C22	3.99	124.43	111.91
22	C	271	CHD	C1-C10-C5	3.97	113.64	107.77
22	P	1525	CHD	C22-C23-C24	-3.97	105.07	113.59
22	P	1271	CHD	C15-C14-C13	3.97	107.44	103.55
21	B	229	PSC	O01-C1-C2	3.96	120.04	111.50
18	D	523	TGL	OG2-CB1-CB2	3.93	119.97	111.50
14	A	515	HEA	C12-C13-C14	-3.92	101.87	112.23
22	P	1271	CHD	C18-C13-C12	-3.92	105.07	109.07
14	N	515	HEA	C27-C19-C18	-3.88	113.72	123.68
18	D	523	TGL	OG3-CC1-CC2	3.88	124.07	111.91
14	N	515	HEA	OMA-CMA-C3A	-3.87	116.47	124.91
22	P	1271	CHD	C1-C10-C5	3.87	113.49	107.77
22	J	60	CHD	C22-C20-C17	3.86	118.26	110.28
18	A	521	TGL	CG3-CG2-CG1	-3.85	102.69	111.79
22	J	60	CHD	C14-C13-C12	3.83	110.97	107.40
18	L	522	TGL	OG3-CC1-CC2	3.82	123.89	111.91
22	C	271	CHD	O7-C7-C8	3.80	117.91	109.43
24	T	263	PEK	O03-C21-C22	3.79	123.81	111.91
22	G	229	CHD	O12-C12-C13	-3.78	104.64	111.03
22	W	1059	CHD	C1-C10-C5	3.77	113.34	107.77
24	G	1263	PEK	C02-O01-C1	3.72	126.95	117.79
24	T	263	PEK	O01-C1-C2	3.71	119.49	111.50
22	C	271	CHD	C2-C1-C10	3.70	119.13	112.78
24	C	265	PEK	O01-C1-C2	3.69	119.45	111.50
19	N	1524	PGV	O01-C1-C2	3.68	119.42	111.50
14	A	515	HEA	C12-C11-C3B	3.66	122.18	112.56
22	J	60	CHD	C4-C5-C10	3.65	116.53	112.66
22	B	1085	CHD	C14-C13-C12	-3.63	104.02	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	526	DMU	O5-C4-C3	3.61	117.37	109.75
22	P	1271	CHD	C18-C13-C14	3.58	116.82	111.21
14	A	515	HEA	C4B-C3B-C2B	-3.57	104.37	106.87
14	A	515	HEA	C25-C23-C24	3.56	122.48	114.60
19	A	524	PGV	C4-C3-C2	-3.51	100.59	113.19
18	N	1521	TGL	CG3-OG3-CC1	3.50	130.10	117.12
25	P	1270	CDL	OB8-CB7-C71	3.50	122.89	111.91
18	L	522	TGL	OG1-CA1-CA2	3.47	122.79	111.91
22	W	1059	CHD	C1-C10-C9	-3.46	105.92	111.35
18	L	522	TGL	CG2-OG2-CB1	3.45	126.28	117.79
25	T	1269	CDL	OA6-CA5-OA7	-3.44	115.39	123.70
25	P	1270	CDL	OB8-CB7-OB9	-3.44	114.91	123.59
22	C	525	CHD	C6-C5-C10	-3.44	109.01	112.66
18	N	1523	TGL	OG3-CC1-CC2	3.43	122.69	111.91
22	J	60	CHD	C19-C10-C5	-3.43	104.55	110.36
24	G	1263	PEK	O03-C01-C02	3.41	118.37	108.43
18	A	521	TGL	OG1-CG1-CG2	3.41	118.37	108.43
22	C	525	CHD	O12-C12-C11	3.41	116.07	109.12
14	A	516	HEA	OMA-CMA-C3A	-3.39	117.52	124.91
21	O	1229	PSC	O01-C1-C2	3.39	118.80	111.50
18	A	521	TGL	OG3-CC1-OC1	-3.38	115.05	123.59
24	P	1265	PEK	O03-C21-O04	-3.37	115.10	123.59
22	W	1059	CHD	C5-C4-C3	3.36	117.69	112.76
18	N	1522	TGL	OG1-CA1-CA2	3.35	122.41	111.91
22	B	1085	CHD	C22-C23-C24	-3.34	106.42	113.59
25	G	269	CDL	C79-C78-C77	3.34	131.36	114.42
25	T	1269	CDL	OA8-CA7-C31	3.34	122.38	111.91
22	P	1525	CHD	C14-C13-C12	3.33	110.50	107.40
22	W	1059	CHD	C22-C20-C17	3.33	117.16	110.28
22	C	271	CHD	C6-C5-C10	3.32	116.19	112.66
22	J	60	CHD	C19-C10-C1	-3.32	102.92	108.26
22	W	1059	CHD	C19-C10-C5	-3.31	104.74	110.36
14	A	515	HEA	C13-C12-C11	3.31	119.32	114.35
25	P	1270	CDL	OA8-CA7-C31	3.30	122.27	111.91
19	N	1524	PGV	O01-C1-O02	-3.30	115.74	123.70
22	C	271	CHD	C6-C7-C8	3.29	115.00	111.48
27	Z	1526	DMU	C11-C9-C8	3.28	120.69	113.00
18	N	1521	TGL	OG1-CA1-CA2	3.27	122.18	111.91
22	C	271	CHD	C15-C14-C8	3.26	122.89	118.33
22	W	1059	CHD	C6-C5-C4	-3.25	107.44	111.19
14	A	516	HEA	C27-C19-C20	3.25	120.75	115.27
18	N	1523	TGL	OG1-CA1-CA2	3.25	122.11	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	523	TGL	CG3-OG3-CC1	3.24	129.13	117.12
22	G	229	CHD	C14-C13-C12	-3.24	104.38	107.40
22	B	1085	CHD	C1-C2-C3	3.24	114.62	110.47
19	A	524	PGV	O03-C19-C20	3.24	122.07	111.91
22	B	1085	CHD	C19-C10-C5	-3.21	104.91	110.36
14	N	515	HEA	C13-C12-C11	3.20	119.16	114.35
19	P	1267	PGV	O14-P-O13	3.20	128.04	112.24
14	A	515	HEA	C21-C20-C19	-3.19	102.47	112.98
14	N	515	HEA	C21-C20-C19	-3.19	102.47	112.98
18	N	1522	TGL	OG2-CB1-CB2	3.18	118.35	111.50
22	B	1085	CHD	C9-C10-C5	3.18	113.04	108.58
19	N	1524	PGV	O03-C19-C20	3.16	121.82	111.91
24	T	263	PEK	C02-O01-C1	3.16	125.57	117.79
25	C	270	CDL	OB8-CB7-C71	3.16	121.82	111.91
22	P	1525	CHD	C6-C5-C4	-3.15	107.56	111.19
22	P	1271	CHD	C15-C14-C8	3.15	122.73	118.33
22	J	60	CHD	C18-C13-C12	-3.13	105.88	109.07
18	A	521	TGL	OG2-CG2-CG3	3.12	119.70	108.40
22	B	1085	CHD	C22-C20-C17	3.12	116.73	110.28
25	C	270	CDL	C52-C51-CB5	-3.11	102.30	113.62
18	D	523	TGL	OG1-CA1-CA2	3.10	121.64	111.91
19	C	267	PGV	O03-C19-O04	-3.09	115.80	123.59
18	A	521	TGL	OG2-CG2-CG1	3.09	119.58	108.40
18	N	1521	TGL	OG1-CG1-CG2	3.08	117.41	108.43
14	A	515	HEA	C25-C23-C22	-3.08	113.75	122.65
22	W	1059	CHD	C10-C9-C8	3.07	115.12	111.82
25	C	270	CDL	OA8-CA7-C31	3.07	121.55	111.91
14	N	516	HEA	OMA-CMA-C3A	-3.04	118.28	124.91
24	C	265	PEK	C24-C23-C22	3.04	124.11	113.19
22	P	1271	CHD	C16-C17-C13	3.03	106.53	103.55
22	P	1525	CHD	O12-C12-C11	3.02	115.27	109.12
18	N	1522	TGL	OG3-CC1-CC2	3.01	121.34	111.91
14	A	516	HEA	C1B-C2B-C3B	-2.98	104.92	107.00
24	C	264	PEK	O03-C01-C02	-2.97	99.79	108.43
14	A	516	HEA	C13-C12-C11	-2.96	109.90	114.35
22	J	60	CHD	C1-C10-C9	-2.95	106.71	111.35
27	M	526	DMU	C7-C8-C9	2.95	115.50	110.24
14	N	516	HEA	C17-C18-C19	2.94	134.74	127.66
27	Z	1526	DMU	O1-C10-C5	2.93	116.56	110.35
24	P	1264	PEK	O03-C01-C02	-2.93	99.90	108.43
25	G	269	CDL	C80-C79-C78	2.92	129.25	114.42
19	A	524	PGV	O01-C02-C01	2.92	118.97	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	60	CHD	C17-C13-C12	2.90	120.32	117.67
22	P	1271	CHD	C6-C5-C10	2.90	115.73	112.66
22	P	1271	CHD	C6-C7-C8	2.90	114.57	111.48
22	W	1059	CHD	C4-C3-C2	2.88	114.00	110.55
22	C	271	CHD	C5-C6-C7	2.88	117.64	114.46
22	C	271	CHD	C15-C14-C13	2.87	106.37	103.55
24	T	263	PEK	O03-C01-C02	2.87	116.78	108.43
22	J	60	CHD	C14-C8-C7	2.86	115.60	111.81
18	A	521	TGL	CB3-CB2-CB1	-2.86	103.23	113.62
19	P	1268	PGV	C03-C02-C01	-2.84	105.06	111.79
18	D	523	TGL	CC3-CC2-CC1	-2.84	103.29	113.62
18	N	1522	TGL	CG3-OG3-CC1	2.83	127.61	117.12
14	N	515	HEA	C25-C23-C22	-2.83	114.47	122.65
22	P	1271	CHD	C5-C4-C3	-2.82	108.61	112.76
18	N	1522	TGL	OG1-CG1-CG2	2.82	116.64	108.43
22	W	1059	CHD	C4-C5-C10	2.82	115.65	112.66
14	A	515	HEA	C26-C15-C16	-2.81	110.55	115.27
22	C	271	CHD	C14-C13-C12	2.81	110.01	107.40
27	M	526	DMU	C11-C9-C8	2.80	119.56	113.00
14	N	516	HEA	C20-C21-C22	2.80	121.08	111.88
22	C	525	CHD	C22-C23-C24	-2.79	107.59	113.59
21	B	229	PSC	O03-C19-C20	2.79	120.67	111.91
22	C	271	CHD	C23-C22-C20	-2.79	110.96	114.72
25	C	270	CDL	C39-C38-C37	2.78	128.51	114.42
18	A	521	TGL	OG1-CA1-CA2	2.77	120.61	111.91
19	N	1266	PGV	O01-C1-C2	2.77	117.47	111.50
27	Z	1526	DMU	O7-C3-C4	2.77	117.03	109.45
22	P	1525	CHD	O12-C12-C13	-2.76	106.36	111.03
18	N	1522	TGL	CC3-CC2-CC1	2.76	123.64	113.62
25	C	270	CDL	OA8-CA6-CA4	2.75	116.45	108.43
18	N	1522	TGL	CG1-OG1-CA1	2.75	127.30	117.12
25	G	269	CDL	OA8-CA7-C31	2.74	120.49	111.91
22	P	1525	CHD	C11-C9-C10	2.73	116.55	113.73
19	N	1524	PGV	O03-C19-O04	-2.73	116.69	123.59
22	P	1525	CHD	C21-C20-C22	-2.73	106.08	110.36
22	J	60	CHD	C5-C6-C7	2.73	117.47	114.46
24	C	265	PEK	O03-C21-O04	-2.73	116.71	123.59
14	A	515	HEA	O11-C11-C3B	-2.72	104.15	112.00
24	C	264	PEK	C03-C02-C01	-2.72	105.35	111.79
22	P	1271	CHD	O7-C7-C8	2.72	115.50	109.43
14	A	515	HEA	C20-C19-C18	2.71	126.61	121.12
18	L	522	TGL	CB6-CB5-CB4	-2.71	100.66	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1264	PEK	C28-C27-C26	-2.71	100.67	114.42
18	N	1523	TGL	CC3-CC2-CC1	-2.70	103.81	113.62
22	J	60	CHD	C16-C17-C20	2.70	116.32	112.15
14	N	516	HEA	CAD-CBD-CGD	-2.69	108.16	112.67
25	P	1270	CDL	C42-C41-C40	2.69	128.07	114.42
18	D	523	TGL	OG1-CA1-OA1	-2.68	116.83	123.59
25	G	269	CDL	OA6-CA5-OA7	-2.68	117.23	123.70
19	C	268	PGV	C03-C02-C01	-2.68	105.46	111.79
14	A	515	HEA	C27-C19-C18	-2.67	116.83	123.68
18	N	1523	TGL	CG3-OG3-CC1	2.67	127.00	117.12
18	N	1523	TGL	OG2-CG2-CG3	2.66	118.05	108.40
14	N	515	HEA	CMB-C2B-C1B	-2.66	124.38	128.46
19	P	1268	PGV	O03-C19-O04	-2.65	116.90	123.59
22	J	60	CHD	O7-C7-C8	2.65	115.35	109.43
25	C	270	CDL	C53-C52-C51	-2.65	103.68	113.19
18	N	1522	TGL	OG3-CC1-OC1	-2.65	116.91	123.59
14	N	516	HEA	CAA-CBA-CGA	-2.64	108.23	112.67
22	W	1059	CHD	C5-C6-C7	2.64	117.38	114.46
22	P	1525	CHD	C15-C14-C13	2.64	106.14	103.55
22	J	60	CHD	C18-C13-C17	2.64	115.35	111.21
18	D	523	TGL	CB3-CB2-CB1	2.63	123.20	113.62
19	N	1266	PGV	O03-C01-C02	2.62	116.06	108.43
25	C	270	CDL	OB8-CB6-CB4	-2.61	100.83	108.43
22	B	1085	CHD	C6-C5-C4	-2.61	108.19	111.19
25	P	1270	CDL	C39-C38-C37	2.59	127.57	114.42
25	P	1270	CDL	OA8-CA7-OA9	-2.59	117.06	123.59
18	N	1522	TGL	C25-C24-C23	-2.59	101.28	114.42
24	P	1264	PEK	C30-C29-C28	-2.58	101.30	114.42
25	P	1270	CDL	OB6-CB5-C51	2.58	117.06	111.50
22	P	1525	CHD	C18-C13-C12	-2.58	106.44	109.07
14	N	516	HEA	C12-C11-C3B	2.56	119.28	112.56
18	A	521	TGL	CB7-CB6-CB5	-2.56	101.43	114.42
19	C	268	PGV	O03-C19-O04	-2.56	117.14	123.59
18	N	1522	TGL	C23-C22-C21	-2.55	101.46	114.42
18	L	522	TGL	OG1-CG1-CG2	2.55	115.86	108.43
27	Z	1526	DMU	C6-C1-C2	2.55	115.30	110.00
27	M	526	DMU	O55-C2-C1	2.54	116.23	110.35
27	M	526	DMU	C6-C1-C2	2.54	115.28	110.00
22	C	525	CHD	O12-C12-C13	-2.54	106.74	111.03
22	P	1271	CHD	C14-C8-C7	2.54	115.17	111.81
24	C	264	PEK	O01-C1-C2	2.54	116.97	111.50
25	G	269	CDL	OB8-CB7-OB9	-2.53	117.20	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	60	CHD	C21-C20-C17	-2.53	109.05	112.92
24	C	265	PEK	C01-O03-C21	2.53	126.48	117.12
18	N	1521	TGL	C21-C20-CA9	2.52	127.21	114.42
27	Z	1526	DMU	C7-C8-C9	2.51	114.72	110.24
22	C	271	CHD	C5-C4-C3	-2.51	109.07	112.76
18	A	521	TGL	CG3-OG3-CC1	2.50	126.38	117.12
18	L	522	TGL	CB4-CB3-CB2	-2.47	104.32	113.19
24	T	263	PEK	C01-O03-C21	2.46	126.24	117.12
24	C	264	PEK	C24-C23-C22	-2.46	104.36	113.19
22	B	1085	CHD	C1-C10-C5	2.45	111.39	107.77
21	O	1229	PSC	O03-C19-C20	2.45	119.58	111.91
24	P	1265	PEK	O03-C01-C02	2.44	115.55	108.43
25	P	1270	CDL	OA4-PA1-OA3	2.44	124.31	112.24
19	P	1268	PGV	O02-C1-C2	-2.42	114.27	123.73
25	C	270	CDL	C42-C41-C40	2.42	126.70	114.42
25	T	1269	CDL	OA8-CA7-OA9	-2.42	117.49	123.59
22	P	1271	CHD	C9-C10-C5	2.41	111.97	108.58
18	L	522	TGL	C15-CC9-CC8	2.41	126.64	114.42
19	P	1268	PGV	O01-C02-C03	2.39	117.07	108.40
24	C	264	PEK	O01-C02-C01	-2.39	99.75	108.40
27	Z	1526	DMU	C10-O1-C9	-2.39	109.00	113.69
24	P	1264	PEK	C01-O03-C21	2.39	125.97	117.12
24	C	265	PEK	O03-C01-C02	2.39	115.38	108.43
21	O	1229	PSC	C32-C31-C30	-2.38	102.33	114.42
14	N	516	HEA	O11-C11-C3B	-2.38	105.13	112.00
14	N	516	HEA	C26-C15-C16	2.38	119.28	115.27
18	N	1521	TGL	CA3-CA2-CA1	-2.38	104.97	113.62
14	A	515	HEA	CBA-CAA-C2A	2.38	116.86	112.48
24	P	1264	PEK	O01-C1-C2	2.37	116.61	111.50
22	B	1085	CHD	C18-C13-C14	2.37	114.92	111.21
14	N	515	HEA	C1B-C2B-C3B	2.35	108.63	107.00
25	C	270	CDL	OB8-CB7-OB9	-2.34	117.68	123.59
25	C	270	CDL	C40-C39-C38	2.34	126.32	114.42
24	P	1264	PEK	O13-P-O14	2.34	123.81	112.24
22	C	271	CHD	C9-C10-C5	2.33	111.85	108.58
25	C	270	CDL	CA6-CA4-CA3	-2.32	106.29	111.79
25	P	1270	CDL	C40-C39-C38	2.32	126.21	114.42
22	B	1085	CHD	C18-C13-C17	-2.31	107.60	111.21
25	P	1270	CDL	C52-C51-CB5	-2.30	105.24	113.62
24	G	1263	PEK	C01-O03-C21	2.30	125.65	117.12
22	W	1059	CHD	C19-C10-C1	-2.30	104.56	108.26
18	N	1522	TGL	OA1-CA1-CA2	-2.29	114.80	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	1269	CDL	CB6-OB8-CB7	2.29	125.59	117.12
19	N	1524	PGV	O01-C02-C03	2.28	116.67	108.40
19	C	268	PGV	O02-C1-C2	-2.28	114.85	123.73
19	P	1267	PGV	C8-C9-C10	-2.28	103.88	113.79
27	M	526	DMU	O16-C6-C1	2.28	111.86	108.30
18	A	521	TGL	OB1-CB1-CB2	-2.27	114.87	123.73
18	N	1521	TGL	CG1-OG1-CA1	-2.27	108.72	117.12
24	P	1264	PEK	C03-C02-C01	-2.27	106.43	111.79
22	C	271	CHD	C16-C17-C13	2.26	105.77	103.55
24	P	1265	PEK	C01-O03-C21	2.25	125.47	117.12
25	T	1269	CDL	OB8-CB6-CB4	2.25	115.00	108.43
14	A	516	HEA	CMC-C2C-C3C	2.25	128.88	124.68
18	A	521	TGL	OG3-CC1-CC2	2.24	118.95	111.91
25	P	1270	CDL	C43-C42-C41	2.24	125.81	114.42
18	A	521	TGL	C15-CC9-CC8	2.24	125.80	114.42
18	L	522	TGL	CC3-CC2-CC1	2.24	121.76	113.62
25	G	269	CDL	C83-C82-C81	2.24	125.78	114.42
19	N	1266	PGV	C01-O03-C19	-2.24	108.84	117.12
22	P	1271	CHD	C14-C8-C9	-2.23	106.65	109.71
22	B	1085	CHD	C14-C8-C7	2.23	114.76	111.81
24	P	1264	PEK	C24-C23-C22	-2.22	105.21	113.19
25	C	270	CDL	C57-C56-C55	-2.22	103.16	114.42
22	B	1085	CHD	C13-C17-C20	-2.21	116.85	119.50
21	O	1229	PSC	C02-O01-C1	2.21	123.23	117.79
25	G	269	CDL	C82-C81-C80	2.21	125.65	114.42
18	L	522	TGL	C22-C21-C20	-2.21	103.21	114.42
14	N	515	HEA	CMD-C2D-C3D	2.21	129.10	124.94
22	C	271	CHD	C14-C8-C7	2.20	114.72	111.81
19	N	1524	PGV	C4-C3-C2	-2.20	105.29	113.19
19	C	267	PGV	O03-C19-C20	2.20	118.80	111.91
27	M	526	DMU	C10-C5-C7	2.19	114.57	110.00
18	L	522	TGL	OG2-CB1-CB2	2.19	116.22	111.50
18	N	1521	TGL	C16-C15-CC9	2.17	125.45	114.42
22	P	1271	CHD	C13-C14-C8	2.17	117.51	114.74
18	L	522	TGL	CB9-CB8-CB7	-2.17	103.43	114.42
24	G	1263	PEK	O03-C21-O04	-2.16	118.14	123.59
25	G	269	CDL	CB6-OB8-CB7	2.16	125.12	117.12
25	T	1269	CDL	C82-C81-C80	2.15	125.36	114.42
24	T	263	PEK	O04-C21-C22	-2.15	115.33	123.73
25	T	1269	CDL	C83-C82-C81	2.14	125.31	114.42
19	N	1524	PGV	C8-C9-C10	-2.14	104.46	113.79
25	P	1270	CDL	OA8-CA6-CA4	2.14	114.65	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1525	CHD	C11-C9-C8	2.13	114.00	110.88
22	B	1085	CHD	O12-C12-C13	-2.13	107.43	111.03
18	N	1523	TGL	C21-C20-CA9	2.13	125.23	114.42
22	W	1059	CHD	C16-C17-C20	2.13	115.44	112.15
18	N	1523	TGL	OG1-CG1-CG2	2.12	114.61	108.43
25	T	1269	CDL	C19-C18-C17	2.12	125.18	114.42
18	N	1523	TGL	OG2-CB1-OB1	-2.12	118.58	123.70
19	A	524	PGV	O03-C01-C02	2.12	114.59	108.43
18	N	1522	TGL	OB1-CB1-CB2	-2.12	115.48	123.73
14	N	516	HEA	C26-C15-C14	-2.11	118.26	123.68
18	N	1523	TGL	C11-C10-CB9	2.11	125.15	114.42
22	B	1085	CHD	O3-C3-C2	-2.11	104.78	110.16
24	P	1265	PEK	P-O11-C03	2.11	134.06	121.68
24	C	264	PEK	C2-C3-C4	2.11	116.99	113.23
25	C	270	CDL	C43-C42-C41	2.11	125.12	114.42
19	A	524	PGV	O03-C19-O04	-2.10	118.28	123.59
19	C	267	PGV	O14-P-O13	2.10	122.63	112.24
19	N	1266	PGV	C15-C14-C13	-2.10	104.65	113.79
19	P	1267	PGV	C9-C8-C7	-2.09	103.81	114.42
22	C	271	CHD	C9-C8-C7	2.09	114.38	111.88
19	C	268	PGV	O03-C01-C02	2.09	114.52	108.43
25	G	269	CDL	CA6-OA8-CA7	2.09	124.85	117.12
14	N	516	HEA	C13-C12-C11	-2.08	111.22	114.35
18	N	1522	TGL	C26-C25-C24	-2.08	103.87	114.42
27	Z	1526	DMU	O16-C6-C1	2.08	111.54	108.30
22	C	525	CHD	C15-C14-C13	2.07	105.59	103.55
14	A	515	HEA	CMD-C2D-C3D	2.07	128.85	124.94
18	N	1523	TGL	OG1-CA1-OA1	-2.07	118.36	123.59
25	P	1270	CDL	CB6-CB4-CB3	-2.06	106.91	111.79
24	T	263	PEK	P-O11-C03	2.06	133.75	121.68
25	P	1270	CDL	C82-C81-C80	2.06	124.86	114.42
22	C	525	CHD	C10-C9-C8	2.05	114.02	111.82
22	C	271	CHD	C4-C5-C10	2.05	114.83	112.66
19	P	1267	PGV	O03-C19-O04	-2.04	118.44	123.59
24	P	1264	PEK	C34-C33-C32	-2.03	104.10	114.42
14	A	515	HEA	C21-C22-C23	-2.03	120.80	127.75
19	A	524	PGV	C01-O03-C19	2.03	124.65	117.12
19	C	267	PGV	O01-C1-O02	-2.03	118.80	123.70
22	C	525	CHD	C5-C6-C7	2.03	116.70	114.46
19	C	267	PGV	O01-C1-C2	2.03	115.87	111.50
18	N	1522	TGL	C11-C10-CB9	2.03	124.71	114.42
22	W	1059	CHD	C14-C8-C7	2.02	114.49	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	524	PGV	C3-C2-C1	-2.02	106.26	113.62
25	C	270	CDL	OA6-CA5-OA7	-2.02	118.81	123.70
22	C	271	CHD	C6-C5-C4	-2.02	108.86	111.19
18	N	1521	TGL	OB1-CB1-CB2	-2.02	115.86	123.73
25	P	1270	CDL	C55-C54-C53	-2.02	104.19	114.42
14	N	516	HEA	C1B-C2B-C3B	-2.02	105.59	107.00
14	A	515	HEA	C3C-C4C-NC	2.01	111.81	109.21
22	J	60	CHD	C11-C9-C10	2.01	115.80	113.73
18	N	1521	TGL	C20-CA9-CA8	2.01	124.62	114.42
24	C	264	PEK	C27-C26-C25	-2.01	104.24	114.42

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
14	A	516	HEA	ND
14	A	516	HEA	NA
14	A	516	HEA	NB
14	N	516	HEA	ND
14	N	516	HEA	NA
14	N	516	HEA	NB
14	A	515	HEA	ND
14	A	515	HEA	NA
14	A	515	HEA	NB
27	M	526	DMU	C2
27	M	526	DMU	C3
27	M	526	DMU	C9
27	M	526	DMU	C5
27	Z	1526	DMU	C2
27	Z	1526	DMU	C3
27	Z	1526	DMU	C5
27	Z	1526	DMU	C4

All (958) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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

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Mol	Chain	Res	Type	Atoms
21	O	1229	PSC	C11-C10-C9-C8
24	G	1263	PEK	C03-O11-P-O14
24	G	1263	PEK	O03-C01-C02-O01
24	G	1263	PEK	O12-C04-C05-N
19	A	524	PGV	C04-O12-P-O11
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	C05-C04-O12-P
19	A	524	PGV	O02-C1-O01-C02
24	P	1264	PEK	C7-C8-C9-C10
18	A	521	TGL	OB1-CB1-OG2-CG2
18	A	521	TGL	OG1-CG1-CG2-OG2
24	P	1265	PEK	C04-O12-P-O13
24	P	1265	PEK	O12-C04-C05-N
24	P	1265	PEK	C4-C5-C6-C7
24	P	1265	PEK	C10-C11-C12-C13
19	C	268	PGV	C04-O12-P-O14
19	C	268	PGV	O12-C04-C05-C06
19	C	268	PGV	C04-C05-C06-O06
19	C	268	PGV	C2-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
14	N	516	HEA	C3B-C11-C12-C13
14	N	516	HEA	O11-C11-C12-C13
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	C04-C05-C06-O06
19	N	1524	PGV	O02-C1-O01-C02
19	P	1268	PGV	C04-C05-C06-O06
19	P	1268	PGV	O05-C05-C06-O06
19	P	1268	PGV	C2-C1-O01-C02
21	B	229	PSC	C04-O12-P-O14
24	T	263	PEK	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
24	T	263	PEK	C03-O11-P-O13
24	T	263	PEK	C03-O11-P-O14
24	T	263	PEK	O12-C04-C05-N
24	T	263	PEK	C7-C8-C9-C10
24	C	265	PEK	O12-C04-C05-N
24	C	265	PEK	C10-C11-C12-C13
25	T	1269	CDL	O1-C1-CA2-OA2
25	T	1269	CDL	C1-CB2-OB2-PB2
25	T	1269	CDL	CB3-OB5-PB2-OB3
25	T	1269	CDL	CB3-OB5-PB2-OB4
25	T	1269	CDL	OB6-CB4-CB6-OB8
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	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
22	W	1059	CHD	C13-C17-C20-C22
22	W	1059	CHD	C16-C17-C20-C22
19	A	524	PGV	O04-C19-O03-C01
19	N	1524	PGV	O04-C19-O03-C01
18	N	1523	TGL	OC1-CC1-OG3-CG3
18	D	523	TGL	OC1-CC1-OG3-CG3
19	A	524	PGV	C20-C19-O03-C01
19	N	1524	PGV	C20-C19-O03-C01
18	N	1523	TGL	CC2-CC1-OG3-CG3
18	D	523	TGL	CC2-CC1-OG3-CG3
25	T	1269	CDL	OA9-CA7-OA8-CA6
22	J	60	CHD	C16-C17-C20-C22
19	C	268	PGV	O02-C1-O01-C02
19	P	1268	PGV	O02-C1-O01-C02
25	G	269	CDL	OA7-CA5-OA6-CA4
25	P	1270	CDL	OA7-CA5-OA6-CA4
18	L	522	TGL	CA2-CA1-OG1-CG1
21	B	229	PSC	C20-C19-O03-C01
19	A	524	PGV	C2-C1-O01-C02
19	N	1524	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
25	G	269	CDL	C11-CA5-OA6-CA4
18	N	1522	TGL	OA1-CA1-OG1-CG1
25	T	1269	CDL	C31-CA7-OA8-CA6
18	N	1521	TGL	CA2-CA1-OG1-CG1
25	G	269	CDL	C31-CA7-OA8-CA6
18	N	1523	TGL	CA2-CA1-OG1-CG1
21	O	1229	PSC	C11-C12-C13-C14
24	G	1263	PEK	C4-C5-C6-C7
24	G	1263	PEK	C7-C8-C9-C10
24	G	1263	PEK	C13-C14-C15-C16
24	P	1265	PEK	C7-C8-C9-C10
24	P	1265	PEK	C13-C14-C15-C16
19	P	1268	PGV	C10-C11-C12-C13
21	B	229	PSC	C11-C10-C9-C8
24	T	263	PEK	C4-C5-C6-C7
24	T	263	PEK	C10-C11-C12-C13
24	C	265	PEK	C7-C8-C9-C10
24	C	265	PEK	C13-C14-C15-C16
24	C	264	PEK	C10-C11-C12-C13
24	C	264	PEK	C13-C14-C15-C16
18	L	522	TGL	CC2-CC3-CC4-CC5
25	C	270	CDL	OA7-CA5-OA6-CA4
18	L	522	TGL	OA1-CA1-OG1-CG1
25	G	269	CDL	OA9-CA7-OA8-CA6
25	G	269	CDL	C40-C41-C42-C43
22	W	1059	CHD	C16-C17-C20-C21
22	J	60	CHD	C13-C17-C20-C22
19	C	268	PGV	O12-C04-C05-O05
25	G	269	CDL	O1-C1-CA2-OA2
18	A	521	TGL	C21-C20-CA9-CA8
21	B	229	PSC	O04-C19-O03-C01
18	A	521	TGL	CB2-CB1-OG2-CG2
25	T	1269	CDL	C11-CA5-OA6-CA4
25	G	269	CDL	C77-C78-C79-C80
25	T	1269	CDL	C22-C23-C24-C25
21	O	1229	PSC	C22-C23-C24-C25
18	N	1523	TGL	C11-C10-CB9-CB8
18	N	1523	TGL	C16-C15-CC9-CC8
18	N	1522	TGL	C21-C20-CA9-CA8
25	C	270	CDL	C17-C18-C19-C20
21	B	229	PSC	C20-C21-C22-C23
25	G	269	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
21	O	1229	PSC	C20-C19-O03-C01
18	N	1522	TGL	CA2-CA1-OG1-CG1
18	D	523	TGL	C16-C15-CC9-CC8
18	N	1523	TGL	OA1-CA1-OG1-CG1
25	T	1269	CDL	C79-C80-C81-C82
22	P	1271	CHD	C21-C20-C22-C23
27	M	526	DMU	O5-C4-C57-O61
18	N	1521	TGL	OA1-CA1-OG1-CG1
27	M	526	DMU	O5-C6-O16-C18
18	N	1521	TGL	C21-C20-CA9-CA8
25	P	1270	CDL	C79-C80-C81-C82
22	P	1271	CHD	C17-C20-C22-C23
18	N	1523	TGL	C21-C20-CA9-CA8
18	D	523	TGL	C21-C22-C23-C24
19	A	524	PGV	O12-C04-C05-C06
25	C	270	CDL	CB2-C1-CA2-OA2
19	N	1524	PGV	O12-C04-C05-C06
25	T	1269	CDL	OA7-CA5-OA6-CA4
18	D	523	TGL	CA2-CA1-OG1-CG1
21	O	1229	PSC	C20-C21-C22-C23
22	J	60	CHD	C13-C17-C20-C21
25	T	1269	CDL	C73-C74-C75-C76
25	G	269	CDL	C57-C58-C59-C60
22	C	271	CHD	C17-C20-C22-C23
22	W	1059	CHD	C17-C20-C22-C23
21	O	1229	PSC	O04-C19-O03-C01
25	G	269	CDL	C15-C16-C17-C18
25	P	1270	CDL	C17-C18-C19-C20
19	A	524	PGV	O12-C04-C05-O05
25	C	270	CDL	O1-C1-CA2-OA2
19	N	1524	PGV	O12-C04-C05-O05
25	G	269	CDL	O1-C1-CB2-OB2
25	P	1270	CDL	O1-C1-CB2-OB2
22	C	271	CHD	C21-C20-C22-C23
24	T	263	PEK	O03-C01-C02-O01
22	J	60	CHD	C16-C17-C20-C21
21	B	229	PSC	C2-C1-O01-C02
27	M	526	DMU	O6-C11-C9-C8
24	C	264	PEK	C1-C2-C3-C4
18	L	522	TGL	C20-C21-C22-C23
27	Z	1526	DMU	O6-C11-C9-C8
25	G	269	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	C	265	PEK	C4-C5-C6-C7
19	P	1267	PGV	C10-C11-C12-C13
21	O	1229	PSC	C1-C2-C3-C4
19	P	1268	PGV	C1-C2-C3-C4
21	B	229	PSC	C1-C2-C3-C4
25	T	1269	CDL	CA5-C11-C12-C13
18	N	1521	TGL	OB1-CB1-OG2-CG2
18	N	1522	TGL	CC3-CC4-CC5-CC6
25	P	1270	CDL	CA5-C11-C12-C13
25	P	1270	CDL	CB7-C71-C72-C73
18	D	523	TGL	CB1-CB2-CB3-CB4
18	N	1521	TGL	CC5-CC6-CC7-CC8
18	N	1521	TGL	C16-C15-CC9-CC8
22	W	1059	CHD	C13-C17-C20-C21
27	M	526	DMU	O16-C18-C19-C22
14	N	515	HEA	C15-C16-C17-C18
14	A	515	HEA	C15-C16-C17-C18
25	T	1269	CDL	C15-C16-C17-C18
18	A	521	TGL	C22-C23-C24-C25
25	T	1269	CDL	C40-C41-C42-C43
25	C	270	CDL	O1-C1-CB2-OB2
19	P	1268	PGV	O12-C04-C05-O05
25	T	1269	CDL	O1-C1-CB2-OB2
21	B	229	PSC	O02-C1-O01-C02
18	D	523	TGL	OA1-CA1-OG1-CG1
19	A	524	PGV	C19-C20-C21-C22
18	N	1521	TGL	CB1-CB2-CB3-CB4
21	B	229	PSC	C11-C12-C13-C14
24	C	264	PEK	C4-C5-C6-C7
24	C	264	PEK	C7-C8-C9-C10
25	T	1269	CDL	C60-C61-C62-C63
18	N	1521	TGL	CB2-CB1-OG2-CG2
21	O	1229	PSC	C03-O11-P-O12
24	G	1263	PEK	C03-O11-P-O12
24	P	1265	PEK	C04-O12-P-O11
19	C	268	PGV	C04-O12-P-O11
25	C	270	CDL	CB2-OB2-PB2-OB5
19	N	1524	PGV	C04-O12-P-O11
19	P	1268	PGV	C04-O12-P-O11
21	B	229	PSC	C04-O12-P-O11
24	C	265	PEK	C04-O12-P-O11
25	T	1269	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
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
18	A	521	TGL	OA1-CA1-OG1-CG1
25	C	270	CDL	CB7-C71-C72-C73
25	C	270	CDL	CA2-C1-CB2-OB2
19	P	1268	PGV	O12-C04-C05-C06
25	T	1269	CDL	CA2-C1-CB2-OB2
21	O	1229	PSC	O02-C1-O01-C02
21	O	1229	PSC	C04-C05-N-C06
18	A	521	TGL	CA2-CA1-OG1-CG1
25	G	269	CDL	C71-CB7-OB8-CB6
25	T	1269	CDL	C56-C57-C58-C59
18	N	1523	TGL	CB1-CB2-CB3-CB4
21	B	229	PSC	C26-C27-C28-C29
25	P	1270	CDL	C51-C52-C53-C54
19	C	267	PGV	C7-C8-C9-C10
21	O	1229	PSC	C2-C1-O01-C02
25	P	1270	CDL	C51-CB5-OB6-CB4
24	P	1264	PEK	C24-C25-C26-C27
25	C	270	CDL	C73-C74-C75-C76
19	N	1524	PGV	C4-C5-C6-C7
19	N	1524	PGV	C24-C25-C26-C27
19	N	1524	PGV	C28-C29-C30-C31
21	B	229	PSC	C2-C3-C4-C5
21	B	229	PSC	C22-C23-C24-C25
25	G	269	CDL	C13-C14-C15-C16
18	N	1523	TGL	CC6-CC7-CC8-CC9
18	N	1523	TGL	C17-C18-C19-C33
19	C	267	PGV	C30-C31-C32-C33
19	P	1268	PGV	C24-C25-C26-C27
24	T	263	PEK	C34-C35-C36-C37
25	T	1269	CDL	C20-C21-C22-C23
18	N	1521	TGL	CA4-CA5-CA6-CA7
25	G	269	CDL	C20-C21-C22-C23
25	P	1270	CDL	C37-C38-C39-C40
18	N	1523	TGL	CA9-C20-C21-C22
19	N	1266	PGV	C23-C24-C25-C26
18	N	1522	TGL	CC6-CC7-CC8-CC9
24	C	264	PEK	C31-C32-C33-C34
19	A	524	PGV	C03-C02-O01-C1

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Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	OB7-CB5-OB6-CB4
18	N	1522	TGL	OB1-CB1-OG2-CG2
18	A	521	TGL	CB1-CB2-CB3-CB4
19	N	1524	PGV	C19-C20-C21-C22
25	T	1269	CDL	C77-C78-C79-C80
18	N	1522	TGL	C17-C18-C19-C33
18	A	521	TGL	C15-C16-C17-C18
18	L	522	TGL	CA5-CA6-CA7-CA8
27	M	526	DMU	C25-C28-C31-C34
25	G	269	CDL	C43-C44-C45-C46
25	P	1270	CDL	C74-C75-C76-C77
19	N	1266	PGV	C6-C7-C8-C9
18	D	523	TGL	CC2-CC3-CC4-CC5
21	O	1229	PSC	C2-C3-C4-C5
25	C	270	CDL	C18-C19-C20-C21
25	C	270	CDL	C76-C77-C78-C79
18	N	1521	TGL	CA5-CA6-CA7-CA8
27	Z	1526	DMU	C25-C28-C31-C34
25	P	1270	CDL	C76-C77-C78-C79
18	N	1523	TGL	CA1-CA2-CA3-CA4
19	C	268	PGV	C20-C19-O03-C01
24	G	1263	PEK	C29-C30-C31-C32
18	A	521	TGL	C16-C17-C18-C19
19	P	1268	PGV	C22-C23-C24-C25
19	A	522	PGV	C23-C24-C25-C26
21	B	229	PSC	C24-C25-C26-C27
25	T	1269	CDL	C54-C55-C56-C57
25	P	1270	CDL	C72-C73-C74-C75
19	N	1266	PGV	C5-C6-C7-C8
25	C	270	CDL	C36-C37-C38-C39
19	P	1268	PGV	C13-C14-C15-C16
18	L	522	TGL	CA7-CA8-CA9-C20
19	A	522	PGV	C7-C8-C9-C10
25	P	1270	CDL	C58-C59-C60-C61
18	N	1523	TGL	CC3-CC4-CC5-CC6
19	N	1266	PGV	C7-C8-C9-C10
18	N	1522	TGL	C23-C24-C25-C26
25	G	269	CDL	CB7-C71-C72-C73
19	C	268	PGV	C27-C28-C29-C30
25	C	270	CDL	C42-C43-C44-C45
25	C	270	CDL	C72-C73-C74-C75
19	A	522	PGV	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	B	229	PSC	C27-C28-C29-C30
25	T	1269	CDL	C13-C14-C15-C16
18	N	1521	TGL	C11-C10-CB9-CB8
25	G	269	CDL	C72-C73-C74-C75
18	N	1523	TGL	CB2-CB3-CB4-CB5
24	C	264	PEK	C22-C23-C24-C25
25	G	269	CDL	OB9-CB7-OB8-CB6
18	A	521	TGL	CA4-CA5-CA6-CA7
18	N	1523	TGL	CC4-CC5-CC6-CC7
19	C	267	PGV	C24-C25-C26-C27
18	N	1522	TGL	C10-C11-C12-C13
18	N	1522	TGL	CB2-CB1-OG2-CG2
25	G	269	CDL	C82-C83-C84-C85
25	P	1270	CDL	C61-C62-C63-C64
18	N	1522	TGL	CB4-CB5-CB6-CB7
18	N	1522	TGL	C21-C22-C23-C24
25	C	270	CDL	CA5-C11-C12-C13
18	L	522	TGL	CC1-CC2-CC3-CC4
24	P	1265	PEK	C16-C17-C18-C19
19	C	268	PGV	C24-C25-C26-C27
25	C	270	CDL	C23-C24-C25-C26
25	C	270	CDL	C74-C75-C76-C77
19	P	1268	PGV	C5-C6-C7-C8
18	L	522	TGL	C21-C20-CA9-CA8
24	T	263	PEK	C27-C28-C29-C30
27	M	526	DMU	C2-C3-O7-C10
25	T	1269	CDL	C39-C40-C41-C42
19	P	1267	PGV	C30-C31-C32-C33
25	G	269	CDL	C39-C40-C41-C42
25	P	1270	CDL	C59-C60-C61-C62
18	N	1523	TGL	CB5-CB6-CB7-CB8
24	C	264	PEK	C23-C24-C25-C26
18	D	523	TGL	CA6-CA7-CA8-CA9
18	D	523	TGL	CB2-CB3-CB4-CB5
18	D	523	TGL	C19-C33-C34-C35
21	O	1229	PSC	C04-C05-N-C08
19	A	524	PGV	C4-C5-C6-C7
18	A	521	TGL	C14-C29-C30-C31
24	P	1265	PEK	C25-C26-C27-C28
25	C	270	CDL	C61-C62-C63-C64
18	L	522	TGL	C12-C13-C14-C29
24	T	263	PEK	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C72-C73-C74-C75
25	P	1270	CDL	C73-C74-C75-C76
25	P	1270	CDL	C82-C83-C84-C85
18	N	1522	TGL	CA7-CA8-CA9-C20
18	D	523	TGL	CB6-CB7-CB8-CB9
18	A	521	TGL	C11-C10-CB9-CB8
19	C	268	PGV	C13-C14-C15-C16
25	C	270	CDL	C77-C78-C79-C80
19	P	1268	PGV	C27-C28-C29-C30
25	T	1269	CDL	C16-C17-C18-C19
18	N	1521	TGL	CB3-CB4-CB5-CB6
18	D	523	TGL	CC4-CC5-CC6-CC7
24	G	1263	PEK	C31-C32-C33-C34
22	C	271	CHD	C20-C22-C23-C24
25	C	270	CDL	C51-C52-C53-C54
18	L	522	TGL	CC9-C15-C16-C17
21	B	229	PSC	C29-C30-C31-C32
24	C	265	PEK	C25-C26-C27-C28
25	T	1269	CDL	C38-C39-C40-C41
18	N	1521	TGL	CB4-CB5-CB6-CB7
25	G	269	CDL	C36-C37-C38-C39
22	P	1271	CHD	C20-C22-C23-C24
21	O	1229	PSC	C24-C25-C26-C27
24	P	1264	PEK	C23-C24-C25-C26
18	A	521	TGL	CA5-CA6-CA7-CA8
18	A	521	TGL	CB3-CB4-CB5-CB6
25	C	270	CDL	C82-C83-C84-C85
19	P	1268	PGV	C4-C5-C6-C7
24	T	263	PEK	C25-C26-C27-C28
18	N	1521	TGL	CB6-CB7-CB8-CB9
18	N	1522	TGL	CC9-C15-C16-C17
24	G	1263	PEK	C27-C28-C29-C30
25	G	269	CDL	C62-C63-C64-C65
18	D	523	TGL	CB5-CB6-CB7-CB8
24	C	265	PEK	C29-C30-C31-C32
24	G	1263	PEK	C10-C11-C12-C13
19	C	268	PGV	C22-C23-C24-C25
18	L	522	TGL	C10-C11-C12-C13
25	T	1269	CDL	C18-C19-C20-C21
27	Z	1526	DMU	C2-C3-O7-C10
25	G	269	CDL	C78-C79-C80-C81
25	P	1270	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
18	N	1522	TGL	C20-C21-C22-C23
24	P	1264	PEK	C1-C2-C3-C4
18	A	521	TGL	CA3-CA4-CA5-CA6
25	C	270	CDL	C71-C72-C73-C74
25	G	269	CDL	C61-C62-C63-C64
18	A	521	TGL	CC2-CC1-OG3-CG3
19	A	522	PGV	C5-C6-C7-C8
18	D	523	TGL	CA9-C20-C21-C22
19	C	268	PGV	O05-C05-C06-O06
19	N	1524	PGV	O05-C05-C06-O06
25	P	1270	CDL	C71-C72-C73-C74
19	C	268	PGV	C11-C10-C9-C8
19	C	268	PGV	C12-C13-C14-C15
19	P	1267	PGV	C12-C13-C14-C15
25	P	1270	CDL	C38-C39-C40-C41
19	N	1524	PGV	C14-C15-C16-C17
25	T	1269	CDL	C59-C60-C61-C62
19	C	268	PGV	C26-C27-C28-C29
24	T	263	PEK	C30-C31-C32-C33
19	C	268	PGV	O04-C19-O03-C01
24	G	1263	PEK	C25-C26-C27-C28
24	G	1263	PEK	C30-C31-C32-C33
24	G	1263	PEK	C34-C35-C36-C37
18	L	522	TGL	C21-C22-C23-C24
18	N	1523	TGL	CB7-CB8-CB9-C10
18	N	1523	TGL	C19-C33-C34-C35
18	N	1522	TGL	CB5-CB6-CB7-CB8
24	P	1264	PEK	C26-C27-C28-C29
25	T	1269	CDL	C43-C44-C45-C46
18	N	1523	TGL	CB6-CB7-CB8-CB9
19	N	1266	PGV	C29-C30-C31-C32
18	A	521	TGL	OC1-CC1-OG3-CG3
25	C	270	CDL	C13-C14-C15-C16
18	N	1521	TGL	C17-C18-C19-C33
25	G	269	CDL	C79-C80-C81-C82
25	P	1270	CDL	C16-C17-C18-C19
21	O	1229	PSC	C04-C05-N-C07
19	A	524	PGV	C2-C3-C4-C5
19	A	524	PGV	C22-C23-C24-C25
27	M	526	DMU	C22-C25-C28-C31
27	Z	1526	DMU	C22-C25-C28-C31
18	N	1522	TGL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
18	L	522	TGL	CB2-CB1-OG2-CG2
18	A	521	TGL	CC6-CC7-CC8-CC9
25	G	269	CDL	C55-C56-C57-C58
25	G	269	CDL	C73-C74-C75-C76
18	L	522	TGL	CC5-CC6-CC7-CC8
18	A	521	TGL	CB6-CB7-CB8-CB9
19	C	268	PGV	C28-C29-C30-C31
25	C	270	CDL	C78-C79-C80-C81
24	P	1265	PEK	C29-C30-C31-C32
25	C	270	CDL	C41-C42-C43-C44
24	P	1265	PEK	C15-C16-C17-C18
24	C	265	PEK	C15-C16-C17-C18
18	L	522	TGL	OB1-CB1-OG2-CG2
19	C	268	PGV	C3-C4-C5-C6
25	C	270	CDL	C80-C81-C82-C83
18	N	1523	TGL	CC2-CC3-CC4-CC5
18	L	522	TGL	C11-C10-CB9-CB8
18	L	522	TGL	C22-C23-C24-C25
18	N	1521	TGL	C14-C29-C30-C31
25	P	1270	CDL	C36-C37-C38-C39
18	N	1523	TGL	CB3-CB4-CB5-CB6
18	D	523	TGL	CB9-C10-C11-C12
25	P	1270	CDL	C18-C19-C20-C21
18	D	523	TGL	CC3-CC4-CC5-CC6
18	L	522	TGL	CC6-CC7-CC8-CC9
18	D	523	TGL	C10-C11-C12-C13
25	C	270	CDL	C58-C59-C60-C61
19	A	522	PGV	C29-C30-C31-C32
18	N	1522	TGL	CC4-CC5-CC6-CC7
24	P	1264	PEK	C2-C1-O01-C02
25	C	270	CDL	C51-CB5-OB6-CB4
19	C	268	PGV	C25-C26-C27-C28
25	P	1270	CDL	C23-C24-C25-C26
19	C	267	PGV	C29-C30-C31-C32
25	G	269	CDL	C80-C81-C82-C83
18	N	1522	TGL	CB1-CB2-CB3-CB4
25	G	269	CDL	OB6-CB4-CB6-OB8
19	A	522	PGV	C26-C27-C28-C29
18	N	1522	TGL	C16-C15-CC9-CC8
18	L	522	TGL	CB4-CB5-CB6-CB7
19	P	1267	PGV	C13-C14-C15-C16
19	A	524	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	P	1268	PGV	C11-C10-C9-C8
19	P	1267	PGV	C11-C10-C9-C8
18	L	522	TGL	CA2-CA3-CA4-CA5
18	L	522	TGL	C24-C25-C26-C27
25	P	1270	CDL	C41-C42-C43-C44
18	N	1521	TGL	CG2-CG3-OG3-CC1
18	D	523	TGL	CB3-CB4-CB5-CB6
25	P	1270	CDL	C13-C14-C15-C16
19	N	1266	PGV	C30-C31-C32-C33
25	C	270	CDL	C16-C17-C18-C19
25	T	1269	CDL	C71-C72-C73-C74
24	C	264	PEK	C25-C26-C27-C28
25	P	1270	CDL	C75-C76-C77-C78
25	G	269	CDL	CA2-OA2-PA1-OA5
21	B	229	PSC	C23-C24-C25-C26
19	P	1267	PGV	C25-C26-C27-C28
25	P	1270	CDL	C77-C78-C79-C80
19	P	1268	PGV	C30-C31-C32-C33
25	G	269	CDL	C52-C53-C54-C55
25	C	270	CDL	OA5-CA3-CA4-CA6
25	C	270	CDL	OB5-CB3-CB4-CB6
25	P	1270	CDL	OA5-CA3-CA4-CA6
25	T	1269	CDL	C31-C32-C33-C34
25	T	1269	CDL	C57-C58-C59-C60
18	N	1522	TGL	C24-C25-C26-C27
24	P	1264	PEK	C31-C32-C33-C34
25	P	1270	CDL	C81-C82-C83-C84
18	N	1523	TGL	C16-C17-C18-C19
18	L	522	TGL	C17-C18-C19-C33
19	N	1266	PGV	C26-C27-C28-C29
19	P	1267	PGV	C7-C8-C9-C10
25	G	269	CDL	C53-C54-C55-C56
24	P	1264	PEK	C2-C3-C4-C5
18	D	523	TGL	C17-C18-C19-C33
19	P	1268	PGV	C20-C21-C22-C23
21	O	1229	PSC	C27-C28-C29-C30
24	P	1265	PEK	C32-C33-C34-C35
18	N	1522	TGL	CB6-CB7-CB8-CB9
19	C	267	PGV	C13-C14-C15-C16
21	O	1229	PSC	C29-C30-C31-C32
24	G	1263	PEK	O03-C01-C02-C03
19	N	1524	PGV	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
24	T	263	PEK	O03-C01-C02-C03
25	T	1269	CDL	CB3-CB4-CB6-OB8
18	N	1521	TGL	C18-C19-C33-C34
25	G	269	CDL	CA3-CA4-CA6-OA8
25	G	269	CDL	CB3-CB4-CB6-OB8
25	P	1270	CDL	CA3-CA4-CA6-OA8
25	P	1270	CDL	C44-C45-C46-C47
25	P	1270	CDL	CB3-CB4-CB6-OB8
24	C	264	PEK	C16-C17-C18-C19
19	C	268	PGV	C10-C11-C12-C13
19	C	267	PGV	C10-C11-C12-C13
19	P	1267	PGV	C29-C30-C31-C32
19	P	1267	PGV	C31-C32-C33-C34
19	C	267	PGV	C23-C24-C25-C26
25	C	270	CDL	C44-C45-C46-C47
18	N	1522	TGL	CB7-CB8-CB9-C10
24	G	1263	PEK	C28-C29-C30-C31
18	A	521	TGL	C13-C14-C29-C30
19	P	1268	PGV	C14-C15-C16-C17
19	C	267	PGV	C15-C16-C17-C18
18	N	1522	TGL	OG1-CA1-CA2-CA3
25	T	1269	CDL	C55-C56-C57-C58
24	T	263	PEK	C33-C34-C35-C36
25	P	1270	CDL	C80-C81-C82-C83
25	C	270	CDL	C55-C56-C57-C58
27	M	526	DMU	C34-C37-C40-C43
24	C	264	PEK	C2-C3-C4-C5
18	A	521	TGL	CC5-CC6-CC7-CC8
25	C	270	CDL	C14-C15-C16-C17
25	T	1269	CDL	C44-C45-C46-C47
19	C	268	PGV	C31-C32-C33-C34
21	B	229	PSC	C3-C4-C5-C6
18	N	1521	TGL	CA3-CA4-CA5-CA6
18	A	521	TGL	CA6-CA7-CA8-CA9
25	P	1270	CDL	C15-C16-C17-C18
24	P	1265	PEK	C21-C22-C23-C24
18	N	1521	TGL	CC2-CC1-OG3-CG3
19	A	524	PGV	C24-C25-C26-C27
18	L	522	TGL	C29-C30-C31-C32
24	T	263	PEK	C26-C27-C28-C29
27	Z	1526	DMU	C34-C37-C40-C43
19	P	1268	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	A	522	PGV	C31-C32-C33-C34
19	P	1267	PGV	C23-C24-C25-C26
25	P	1270	CDL	C24-C25-C26-C27
19	P	1268	PGV	C25-C26-C27-C28
18	N	1521	TGL	C16-C17-C18-C19
24	C	264	PEK	C32-C33-C34-C35
24	P	1264	PEK	C13-C14-C15-C16
19	N	1524	PGV	C10-C11-C12-C13
24	T	263	PEK	C13-C14-C15-C16
18	N	1522	TGL	OG2-CB1-CB2-CB3
18	D	523	TGL	CA5-CA6-CA7-CA8
19	P	1267	PGV	C15-C16-C17-C18
24	C	264	PEK	C17-C18-C19-C20
18	N	1521	TGL	OC1-CC1-OG3-CG3
19	A	524	PGV	C31-C32-C33-C34
19	P	1268	PGV	C23-C24-C25-C26
25	C	270	CDL	C59-C60-C61-C62
19	N	1524	PGV	C26-C27-C28-C29
18	L	522	TGL	CB5-CB6-CB7-CB8
24	C	265	PEK	C34-C35-C36-C37
18	N	1521	TGL	C13-C14-C29-C30
24	P	1264	PEK	O02-C1-O01-C02
25	C	270	CDL	OB7-CB5-OB6-CB4
24	G	1263	PEK	C22-C21-O03-C01
25	C	270	CDL	C38-C39-C40-C41
18	N	1522	TGL	CC5-CC6-CC7-CC8
24	G	1263	PEK	C26-C27-C28-C29
24	P	1264	PEK	C25-C26-C27-C28
18	L	522	TGL	C16-C15-CC9-CC8
25	G	269	CDL	C54-C55-C56-C57
24	P	1265	PEK	C24-C25-C26-C27
19	N	1524	PGV	C21-C22-C23-C24
19	N	1524	PGV	C22-C23-C24-C25
19	C	268	PGV	C5-C6-C7-C8
25	C	270	CDL	C84-C85-C86-C87
25	P	1270	CDL	C62-C63-C64-C65
19	A	524	PGV	C10-C11-C12-C13
24	P	1264	PEK	C10-C11-C12-C13
19	A	522	PGV	C10-C11-C12-C13
18	N	1523	TGL	CB9-C10-C11-C12
18	N	1522	TGL	CC2-CC3-CC4-CC5
19	A	524	PGV	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
24	P	1265	PEK	C01-C02-C03-O11
25	G	269	CDL	OA5-CA3-CA4-CA6
25	P	1270	CDL	OB5-CB3-CB4-CB6
19	C	268	PGV	C14-C15-C16-C17
18	D	523	TGL	C11-C10-CB9-CB8
18	L	522	TGL	C18-C19-C33-C34
21	O	1229	PSC	C21-C22-C23-C24
18	D	523	TGL	CC6-CC7-CC8-CC9
18	D	523	TGL	CC1-CC2-CC3-CC4
25	G	269	CDL	C18-C19-C20-C21
25	P	1270	CDL	CA4-CA3-OA5-PA1
19	C	268	PGV	C7-C8-C9-C10
25	C	270	CDL	C15-C16-C17-C18
19	P	1268	PGV	C31-C32-C33-C34
24	T	263	PEK	C28-C29-C30-C31
18	N	1523	TGL	C24-C25-C26-C27
18	N	1523	TGL	C12-C13-C14-C29
18	D	523	TGL	CA4-CA5-CA6-CA7
25	P	1270	CDL	C57-C58-C59-C60
21	O	1229	PSC	O03-C01-C02-C03
19	A	524	PGV	O03-C01-C02-C03
18	A	521	TGL	OG1-CG1-CG2-CG3
19	N	1524	PGV	O03-C01-C02-C03
25	T	1269	CDL	CA3-CA4-CA6-OA8
18	N	1523	TGL	CG1-CG2-CG3-OG3
24	C	265	PEK	C31-C32-C33-C34
24	C	265	PEK	C32-C33-C34-C35
27	Z	1526	DMU	O16-C18-C19-C22
18	L	522	TGL	CC4-CC5-CC6-CC7
21	O	1229	PSC	C9-C10-C11-C12
24	G	1263	PEK	C11-C10-C9-C8
24	G	1263	PEK	C9-C10-C11-C12
24	P	1264	PEK	C11-C10-C9-C8
24	P	1264	PEK	C9-C10-C11-C12
24	P	1265	PEK	C5-C6-C7-C8
21	B	229	PSC	C9-C10-C11-C12
24	T	263	PEK	C5-C6-C7-C8
24	T	263	PEK	C11-C10-C9-C8
24	T	263	PEK	C9-C10-C11-C12
24	T	263	PEK	C12-C13-C14-C15
24	C	265	PEK	C5-C6-C7-C8
24	C	265	PEK	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	264	PEK	C9-C10-C11-C12
22	W	1059	CHD	C21-C20-C22-C23
25	T	1269	CDL	C64-C65-C66-C67
18	N	1522	TGL	C29-C30-C31-C32
18	D	523	TGL	CB7-CB8-CB9-C10
24	P	1265	PEK	C31-C32-C33-C34
24	G	1263	PEK	O01-C02-C03-O11
19	C	268	PGV	O01-C02-C03-O11
25	C	270	CDL	OA5-CA3-CA4-OA6
25	P	1270	CDL	OA5-CA3-CA4-OA6
18	N	1523	TGL	C21-C22-C23-C24
24	C	264	PEK	C24-C25-C26-C27
18	L	522	TGL	OG1-CA1-CA2-CA3
24	P	1264	PEK	C17-C18-C19-C20
24	P	1265	PEK	O03-C01-C02-O01
25	C	270	CDL	OB6-CB4-CB6-OB8
21	B	229	PSC	O03-C01-C02-O01
25	P	1270	CDL	OB6-CB4-CB6-OB8
18	N	1523	TGL	OG2-CG2-CG3-OG3
24	C	264	PEK	C22-C21-O03-C01
18	L	522	TGL	CA6-CA7-CA8-CA9
14	N	515	HEA	C19-C20-C21-C22
25	T	1269	CDL	CB2-C1-CA2-OA2
27	Z	1526	DMU	O5-C4-C57-O61
14	A	515	HEA	C26-C15-C16-C17
25	P	1270	CDL	C14-C15-C16-C17
19	P	1268	PGV	C05-C04-O12-P
24	G	1263	PEK	O04-C21-O03-C01
18	N	1521	TGL	CB9-C10-C11-C12
18	N	1522	TGL	CA5-CA6-CA7-CA8
19	N	1266	PGV	C31-C32-C33-C34
25	C	270	CDL	C20-C21-C22-C23
27	Z	1526	DMU	C19-C22-C25-C28
18	D	523	TGL	C29-C30-C31-C32
24	G	1263	PEK	C01-C02-C03-O11
19	N	1524	PGV	C01-C02-C03-O11
25	T	1269	CDL	OA5-CA3-CA4-CA6
18	A	521	TGL	C23-C24-C25-C26
18	L	522	TGL	C11-C12-C13-C14
24	P	1264	PEK	C35-C36-C37-C38
19	N	1524	PGV	C31-C32-C33-C34
24	T	263	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C51-CB5-OB6-CB4
19	P	1268	PGV	C26-C27-C28-C29
19	C	267	PGV	C31-C32-C33-C34
21	O	1229	PSC	C03-C02-O01-C1
18	A	521	TGL	CG1-CG2-OG2-CB1
19	N	1524	PGV	C03-C02-O01-C1
18	L	522	TGL	C19-C33-C34-C35
25	G	269	CDL	C16-C17-C18-C19
25	C	270	CDL	C35-C36-C37-C38
18	D	523	TGL	C21-C20-CA9-CA8
19	P	1268	PGV	C20-C19-O03-C01
18	N	1522	TGL	C11-C10-CB9-CB8
24	G	1263	PEK	C2-C3-C4-C5
24	P	1265	PEK	O03-C01-C02-C03
25	C	270	CDL	CB3-CB4-CB6-OB8
21	B	229	PSC	O03-C01-C02-C03
25	G	269	CDL	CB4-CB3-OB5-PB2
18	L	522	TGL	C25-C26-C27-C28
19	P	1268	PGV	O01-C02-C03-O11
18	D	523	TGL	C24-C25-C26-C27
25	T	1269	CDL	OB7-CB5-OB6-CB4
25	P	1270	CDL	C32-C33-C34-C35
18	N	1523	TGL	C33-C34-C35-C36
24	C	265	PEK	O03-C01-C02-O01
25	P	1270	CDL	OA6-CA4-CA6-OA8
18	D	523	TGL	OG2-CG2-CG3-OG3
18	N	1521	TGL	C23-C24-C25-C26
25	C	270	CDL	C11-C12-C13-C14
25	G	269	CDL	C11-C12-C13-C14
21	B	229	PSC	C13-C14-C15-C16
19	A	524	PGV	C21-C22-C23-C24
24	P	1265	PEK	C26-C27-C28-C29
19	N	1524	PGV	C30-C31-C32-C33
19	P	1268	PGV	C28-C29-C30-C31
18	A	521	TGL	CC4-CC5-CC6-CC7
25	T	1269	CDL	C24-C25-C26-C27
19	N	1524	PGV	C15-C16-C17-C18
18	L	522	TGL	C23-C24-C25-C26
14	A	516	HEA	O11-C11-C12-C13
19	P	1267	PGV	C24-C25-C26-C27
25	T	1269	CDL	CB2-OB2-PB2-OB5
25	G	269	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
24	C	265	PEK	C16-C17-C18-C19
27	M	526	DMU	C19-C22-C25-C28
25	C	270	CDL	C1-CA2-OA2-PA1
19	N	1524	PGV	C05-C04-O12-P
19	P	1268	PGV	C02-C03-O11-P
19	C	267	PGV	C02-C03-O11-P
19	C	267	PGV	C05-C04-O12-P
24	C	264	PEK	C30-C31-C32-C33
24	C	264	PEK	O04-C21-O03-C01
21	O	1229	PSC	C03-O11-P-O13
24	G	1263	PEK	C03-O11-P-O13
19	P	1268	PGV	C04-O12-P-O14
21	B	229	PSC	C04-O12-P-O13
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	T	263	PEK	C01-C02-C03-O11
21	O	1229	PSC	C26-C27-C28-C29
24	P	1264	PEK	C29-C30-C31-C32
25	G	269	CDL	C76-C77-C78-C79
19	P	1268	PGV	O04-C19-O03-C01
18	N	1521	TGL	CC6-CC7-CC8-CC9
24	T	263	PEK	C16-C17-C18-C19
25	C	270	CDL	OB5-CB3-CB4-OB6
24	T	263	PEK	O01-C02-C03-O11
25	T	1269	CDL	OA5-CA3-CA4-OA6
25	G	269	CDL	OA5-CA3-CA4-OA6
25	P	1270	CDL	OB5-CB3-CB4-OB6
25	P	1270	CDL	C11-C12-C13-C14
25	P	1270	CDL	C43-C44-C45-C46
18	A	521	TGL	C24-C25-C26-C27
25	G	269	CDL	C31-C32-C33-C34
21	O	1229	PSC	O12-C04-C05-N
21	O	1229	PSC	C5-C6-C7-C8
25	T	1269	CDL	C41-C42-C43-C44
18	D	523	TGL	CG1-CG2-CG3-OG3
21	O	1229	PSC	O03-C01-C02-O01
25	T	1269	CDL	OA6-CA4-CA6-OA8
25	G	269	CDL	OA6-CA4-CA6-OA8
24	C	264	PEK	O03-C01-C02-O01
19	C	268	PGV	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	P	1265	PEK	C34-C35-C36-C37
19	A	524	PGV	C11-C12-C13-C14
19	P	1267	PGV	C22-C23-C24-C25
19	P	1267	PGV	C02-C03-O11-P
14	N	515	HEA	C26-C15-C16-C17
24	P	1265	PEK	C30-C31-C32-C33
19	C	268	PGV	C4-C5-C6-C7
25	G	269	CDL	C24-C25-C26-C27
18	L	522	TGL	OG2-CB1-CB2-CB3
18	A	521	TGL	C20-C21-C22-C23
19	N	1524	PGV	C25-C26-C27-C28
19	C	267	PGV	C1-C2-C3-C4
25	G	269	CDL	C58-C59-C60-C61
18	N	1523	TGL	C10-C11-C12-C13
18	D	523	TGL	CG3-CG2-OG2-CB1
19	C	268	PGV	C01-C02-C03-O11
19	P	1268	PGV	C01-C02-C03-O11
25	C	270	CDL	C62-C63-C64-C65
19	C	267	PGV	C9-C10-C11-C12
24	T	263	PEK	C02-C03-O11-P
24	C	264	PEK	C28-C29-C30-C31
24	G	1263	PEK	C24-C25-C26-C27
19	N	1524	PGV	O03-C01-C02-O01
19	A	524	PGV	C23-C24-C25-C26
19	A	524	PGV	C03-O11-P-O12
19	N	1524	PGV	C03-O11-P-O12
25	C	270	CDL	C32-C33-C34-C35
24	P	1264	PEK	C3-C4-C5-C6
19	N	1524	PGV	C11-C12-C13-C14
19	P	1268	PGV	C3-C4-C5-C6
25	G	269	CDL	C14-C15-C16-C17
18	N	1521	TGL	C15-C16-C17-C18
19	C	268	PGV	C02-C03-O11-P
25	P	1270	CDL	C1-CA2-OA2-PA1
19	N	1266	PGV	C9-C10-C11-C12
19	A	522	PGV	C24-C25-C26-C27
19	N	1266	PGV	C24-C25-C26-C27
24	P	1265	PEK	O04-C21-O03-C01
19	C	268	PGV	C9-C10-C11-C12
18	N	1521	TGL	CB2-CB3-CB4-CB5
19	C	267	PGV	C22-C23-C24-C25
19	C	268	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	A	515	HEA	C19-C20-C21-C22
25	G	269	CDL	C41-C42-C43-C44
25	G	269	CDL	C81-C82-C83-C84
24	C	264	PEK	C26-C27-C28-C29
24	G	1263	PEK	C15-C16-C17-C18
24	C	264	PEK	C15-C16-C17-C18
18	A	521	TGL	C21-C22-C23-C24
19	N	1266	PGV	C4-C5-C6-C7
25	C	270	CDL	C75-C76-C77-C78
24	G	1263	PEK	C02-C03-O11-P
25	T	1269	CDL	CB4-CB3-OB5-PB2
25	T	1269	CDL	C81-C82-C83-C84
21	O	1229	PSC	C12-C13-C14-C15
21	B	229	PSC	C7-C8-C9-C10
19	N	1524	PGV	C11-C10-C9-C8
19	N	1524	PGV	C12-C13-C14-C15
24	C	265	PEK	O03-C01-C02-C03
19	C	268	PGV	C23-C24-C25-C26
19	C	267	PGV	C14-C15-C16-C17
19	A	522	PGV	C22-C23-C24-C25
18	N	1521	TGL	CC4-CC5-CC6-CC7
19	P	1267	PGV	C28-C29-C30-C31
24	T	263	PEK	C21-C22-C23-C24
21	B	229	PSC	C03-C02-O01-C1
18	N	1523	TGL	CG1-CG2-OG2-CB1
18	N	1523	TGL	CG3-CG2-OG2-CB1
19	A	524	PGV	C26-C27-C28-C29
21	B	229	PSC	C04-C05-N-C08
19	A	524	PGV	C25-C26-C27-C28
22	P	1271	CHD	C16-C17-C20-C22
24	G	1263	PEK	C12-C13-C14-C15
24	P	1264	PEK	C6-C7-C8-C9
24	P	1265	PEK	C6-C7-C8-C9
24	P	1265	PEK	C11-C10-C9-C8
24	P	1265	PEK	C9-C10-C11-C12
24	C	265	PEK	C11-C10-C9-C8
25	P	1270	CDL	C35-C36-C37-C38
25	P	1270	CDL	C84-C85-C86-C87
18	N	1522	TGL	OA1-CA1-CA2-CA3
25	C	270	CDL	C52-C53-C54-C55
19	A	522	PGV	O03-C19-C20-C21
18	N	1523	TGL	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
18	L	522	TGL	CB1-CB2-CB3-CB4
18	N	1521	TGL	CA6-CA7-CA8-CA9
27	Z	1526	DMU	C3-C4-C57-O61
24	P	1264	PEK	C30-C31-C32-C33
18	N	1522	TGL	CA6-CA7-CA8-CA9
18	L	522	TGL	CC3-CC4-CC5-CC6
18	D	523	TGL	OG2-CB1-CB2-CB3
24	C	265	PEK	C30-C31-C32-C33
24	T	263	PEK	C2-C3-C4-C5
19	N	1266	PGV	C11-C10-C9-C8
24	C	264	PEK	O03-C01-C02-C03
18	A	521	TGL	CG2-CG3-OG3-CC1
27	Z	1526	DMU	C28-C31-C34-C37
14	A	515	HEA	C14-C15-C16-C17
25	G	269	CDL	C59-C60-C61-C62
19	N	1266	PGV	C11-C12-C13-C14
19	A	524	PGV	O01-C02-C03-O11
25	G	269	CDL	C56-C57-C58-C59
18	D	523	TGL	OB1-CB1-OG2-CG2
21	B	229	PSC	C04-C05-N-C06
19	N	1266	PGV	O03-C19-C20-C21
24	T	263	PEK	C22-C21-O03-C01
24	G	1263	PEK	C21-C22-C23-C24
25	P	1270	CDL	C12-C11-CA5-OA6
24	P	1264	PEK	C16-C17-C18-C19
21	O	1229	PSC	C4-C5-C6-C7
24	P	1265	PEK	C22-C21-O03-C01
21	O	1229	PSC	C7-C8-C9-C10
19	P	1267	PGV	C11-C12-C13-C14
18	A	521	TGL	CC2-CC3-CC4-CC5
24	P	1265	PEK	C1-C2-C3-C4
19	A	522	PGV	C11-C10-C9-C8
25	G	269	CDL	C44-C45-C46-C47
24	T	263	PEK	O04-C21-O03-C01
24	P	1264	PEK	O01-C1-C2-C3
19	A	522	PGV	C9-C10-C11-C12
24	C	264	PEK	C14-C15-C16-C17
24	C	265	PEK	C35-C36-C37-C38
25	T	1269	CDL	C82-C83-C84-C85
18	N	1521	TGL	CG3-CG2-OG2-CB1
24	C	264	PEK	O02-C1-O01-C02
19	N	1524	PGV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C23-C24-C25-C26
19	A	524	PGV	C14-C15-C16-C17
14	N	515	HEA	C14-C15-C16-C17
18	N	1522	TGL	OG3-CC1-CC2-CC3
19	A	522	PGV	C11-C12-C13-C14
19	N	1266	PGV	C12-C13-C14-C15
19	C	267	PGV	C28-C29-C30-C31
19	A	524	PGV	C30-C31-C32-C33
25	C	270	CDL	C43-C44-C45-C46
18	N	1523	TGL	OG3-CC1-CC2-CC3
21	B	229	PSC	C12-C13-C14-C15
24	T	263	PEK	C3-C4-C5-C6
21	O	1229	PSC	O01-C1-C2-C3
21	O	1229	PSC	O03-C19-C20-C21
25	P	1270	CDL	C52-C51-CB5-OB6
24	C	264	PEK	O01-C1-C2-C3
21	B	229	PSC	C04-C05-N-C07
18	A	521	TGL	OG1-CA1-CA2-CA3
18	D	523	TGL	CA3-CA4-CA5-CA6
19	N	1524	PGV	O03-C19-C20-C21
18	N	1523	TGL	OG1-CA1-CA2-CA3
25	G	269	CDL	C33-C34-C35-C36
19	N	1524	PGV	O01-C1-C2-C3
18	L	522	TGL	OA1-CA1-CA2-CA3
24	C	264	PEK	C35-C36-C37-C38
25	C	270	CDL	C32-C31-CA7-OA8
14	A	516	HEA	C26-C15-C16-C17
21	O	1229	PSC	O02-C1-C2-C3
25	C	270	CDL	C24-C25-C26-C27
24	C	265	PEK	C26-C27-C28-C29
25	C	270	CDL	C32-C31-CA7-OA9
18	N	1522	TGL	OC1-CC1-CC2-CC3
18	N	1521	TGL	C29-C30-C31-C32
19	A	524	PGV	C12-C13-C14-C15
19	C	268	PGV	C1-C2-C3-C4
18	A	521	TGL	OA1-CA1-CA2-CA3
18	N	1522	TGL	OB1-CB1-CB2-CB3
21	B	229	PSC	O03-C19-C20-C21
21	O	1229	PSC	O04-C19-C20-C21
25	P	1270	CDL	C12-C11-CA5-OA7
24	C	264	PEK	O02-C1-C2-C3
25	T	1269	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
19	N	1266	PGV	C04-O12-P-O13
25	C	270	CDL	C37-C38-C39-C40
19	A	524	PGV	O01-C1-C2-C3
24	P	1264	PEK	O02-C1-C2-C3
18	L	522	TGL	C16-C17-C18-C19
18	L	522	TGL	CA3-CA4-CA5-CA6
18	N	1521	TGL	CA2-CA3-CA4-CA5
22	C	271	CHD	C16-C17-C20-C22
25	P	1270	CDL	C20-C21-C22-C23
24	P	1265	PEK	O04-C21-C22-C23
24	P	1265	PEK	O03-C21-C22-C23
18	N	1523	TGL	OC1-CC1-CC2-CC3
24	C	265	PEK	O01-C1-C2-C3
19	N	1524	PGV	O02-C1-C2-C3
24	G	1263	PEK	C16-C17-C18-C19
25	C	270	CDL	C12-C11-CA5-OA6
21	B	229	PSC	O01-C1-C2-C3
21	O	1229	PSC	C23-C24-C25-C26
24	T	263	PEK	O01-C1-C2-C3
18	D	523	TGL	OG3-CC1-CC2-CC3
18	A	521	TGL	CC7-CC8-CC9-C15
25	G	269	CDL	C19-C20-C21-C22
19	A	524	PGV	O02-C1-C2-C3
18	D	523	TGL	C16-C17-C18-C19
24	P	1265	PEK	O01-C1-C2-C3
21	B	229	PSC	O04-C19-C20-C21
25	P	1270	CDL	C52-C51-CB5-OB7
19	N	1524	PGV	C5-C6-C7-C8
19	A	524	PGV	O03-C19-C20-C21
18	D	523	TGL	OG1-CA1-CA2-CA3

There are no ring outliers.

36 monomers are involved in 242 short contacts:

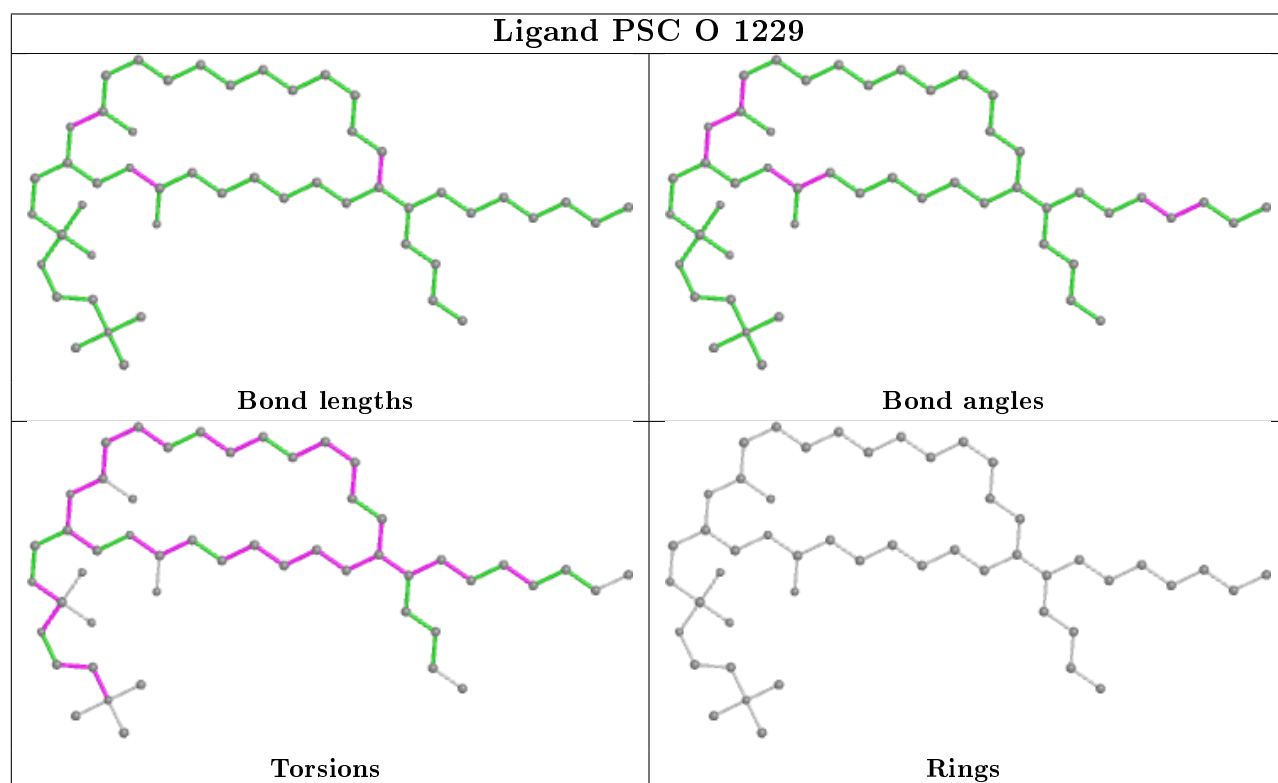
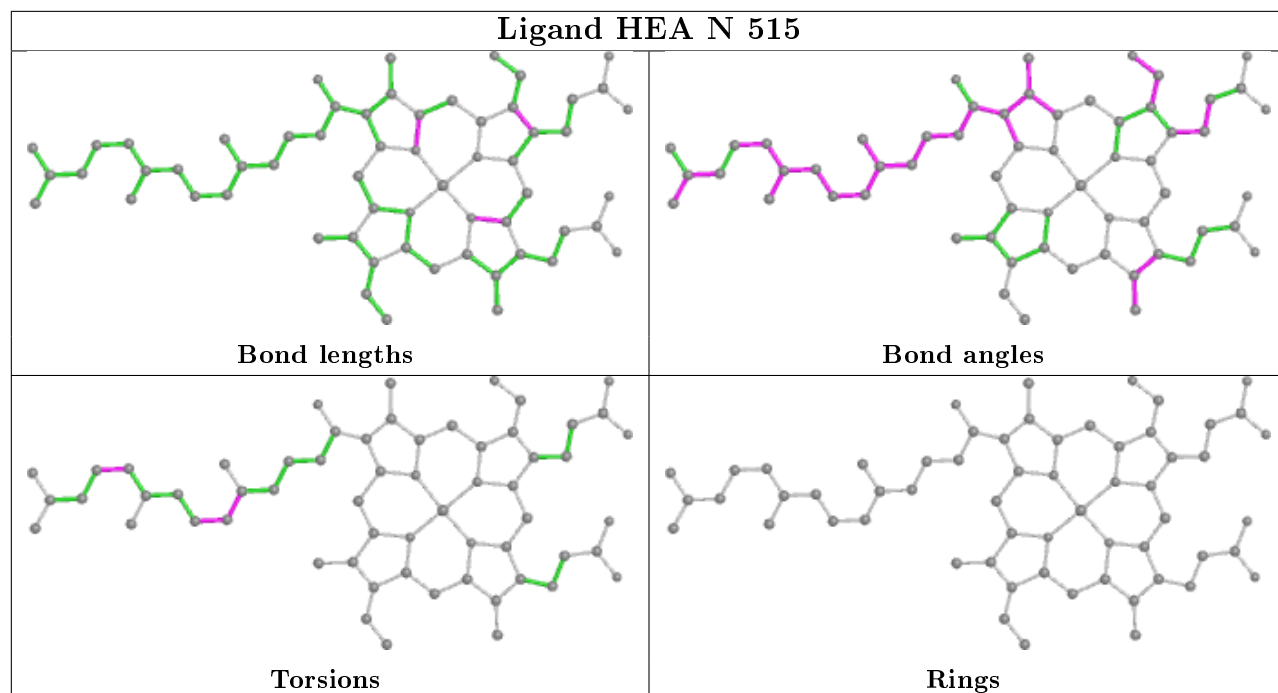
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	515	HEA	5	0
21	O	1229	PSC	17	0
24	G	1263	PEK	10	0
19	A	524	PGV	12	0
24	P	1264	PEK	5	0
18	A	521	TGL	6	0
24	P	1265	PEK	8	0

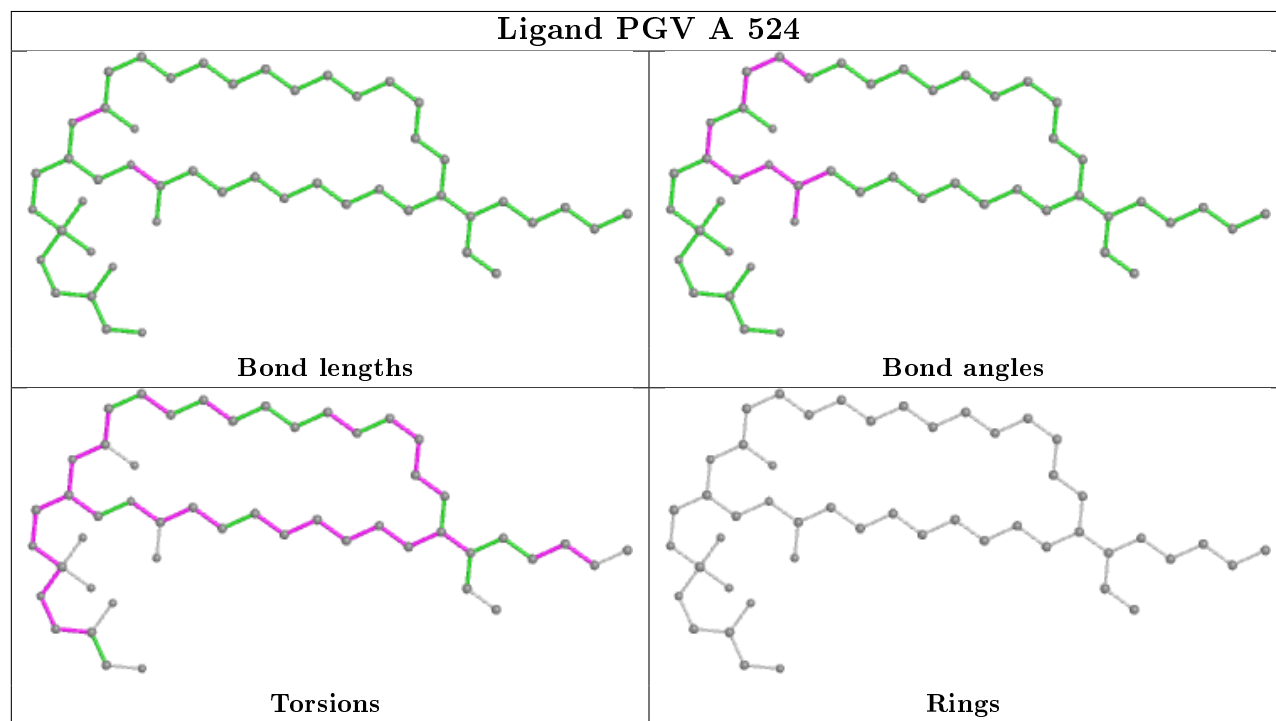
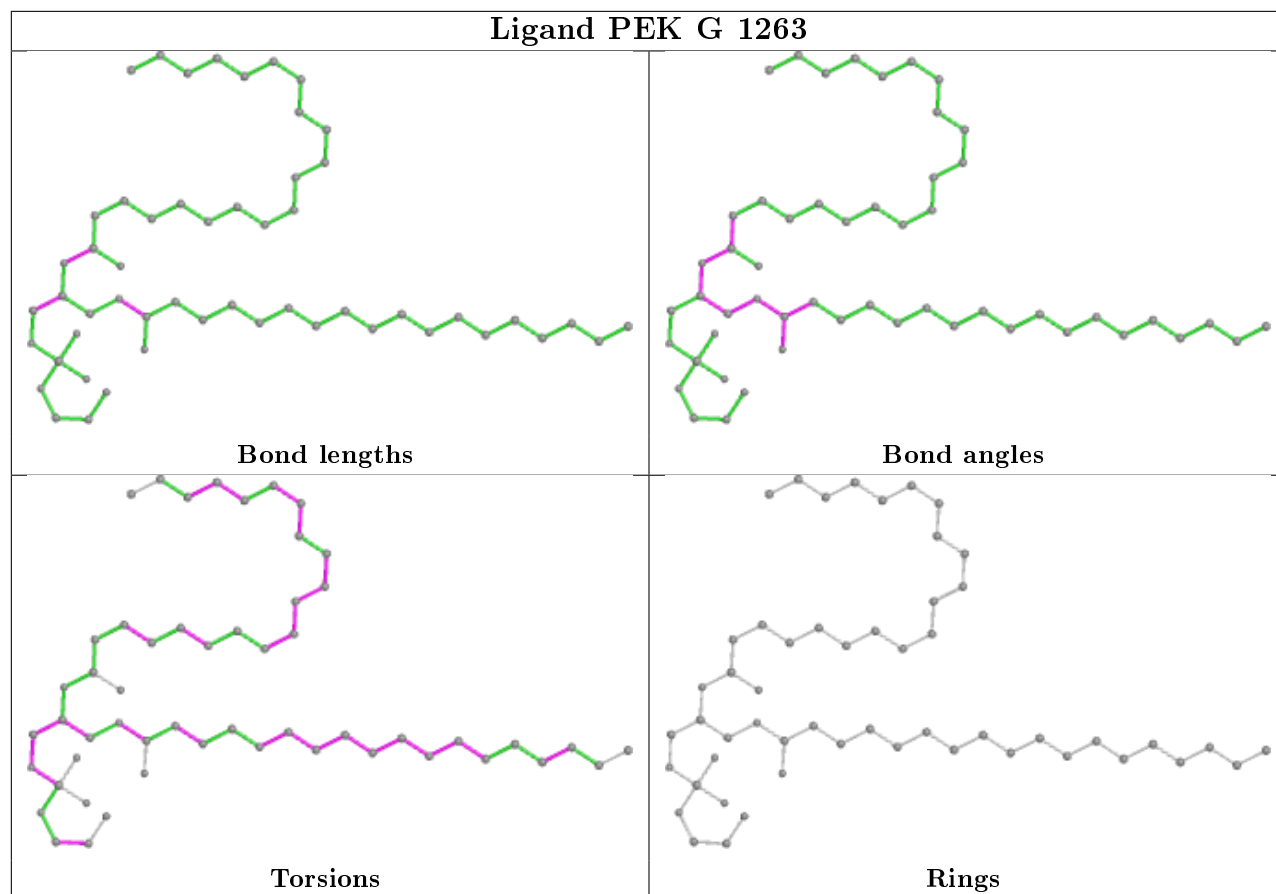
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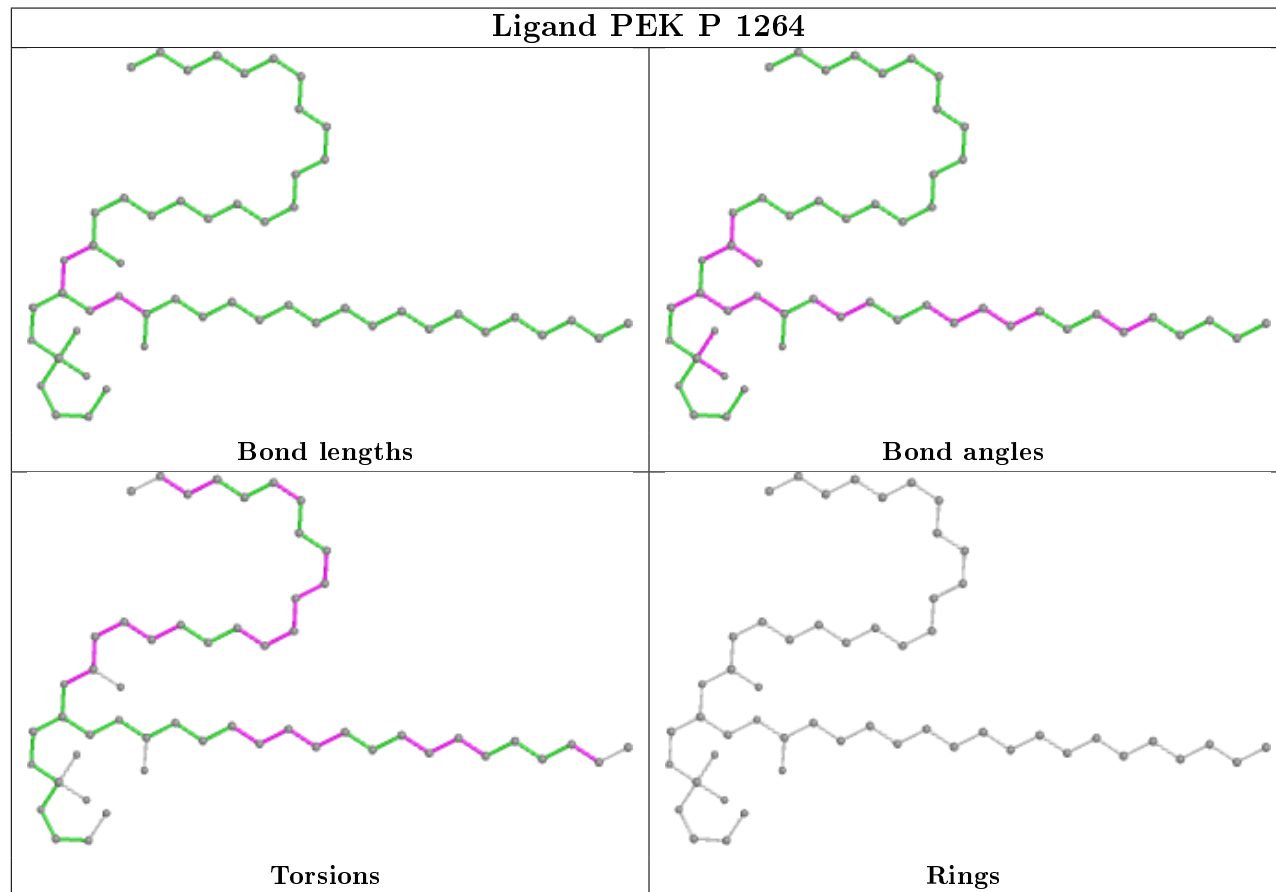
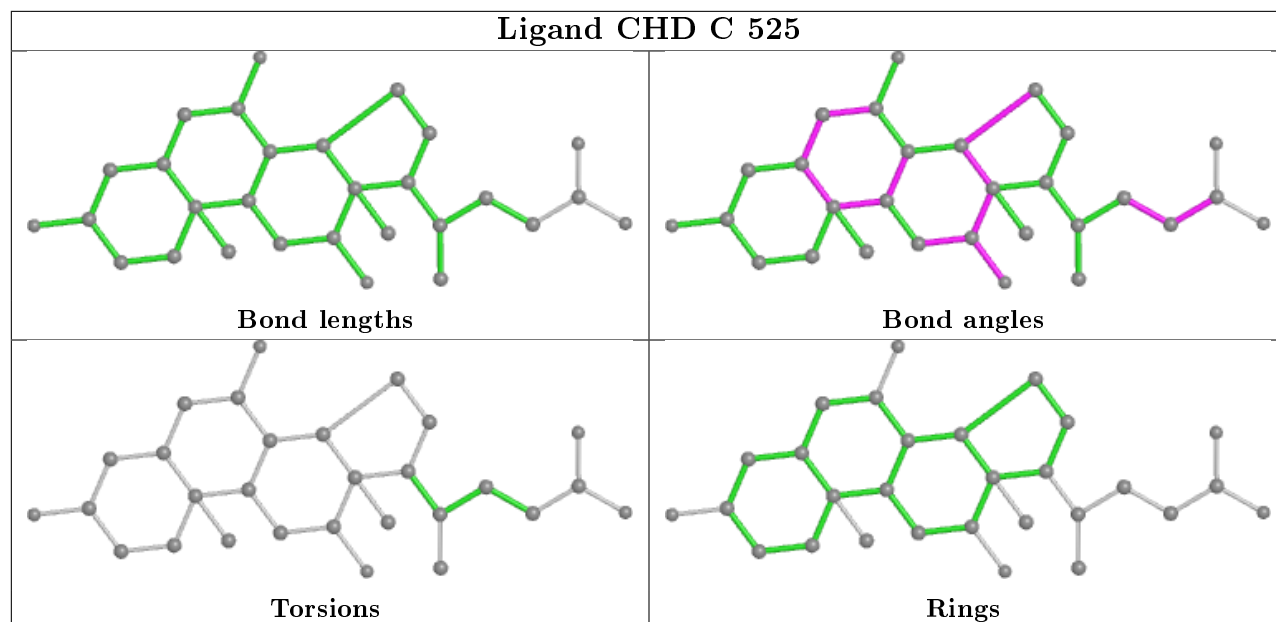
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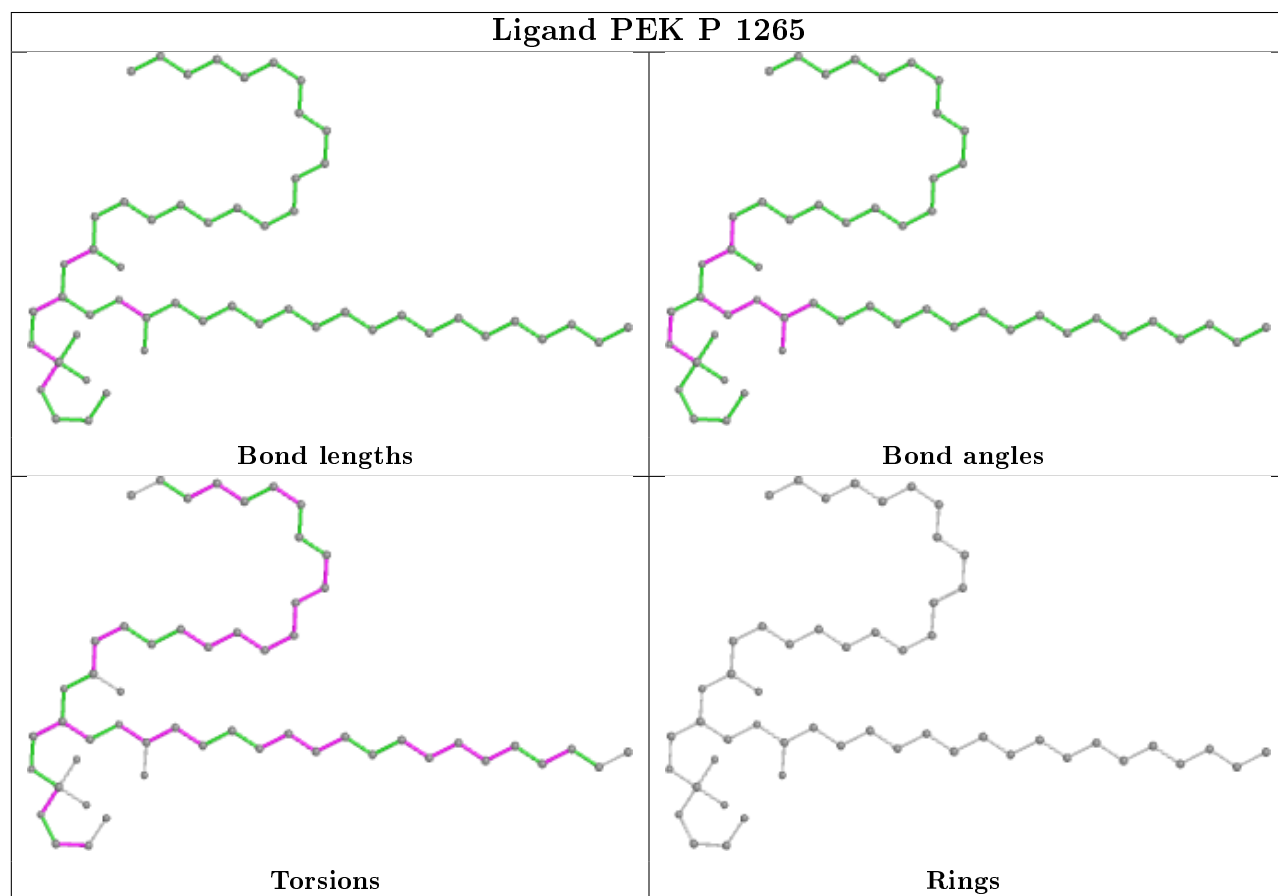
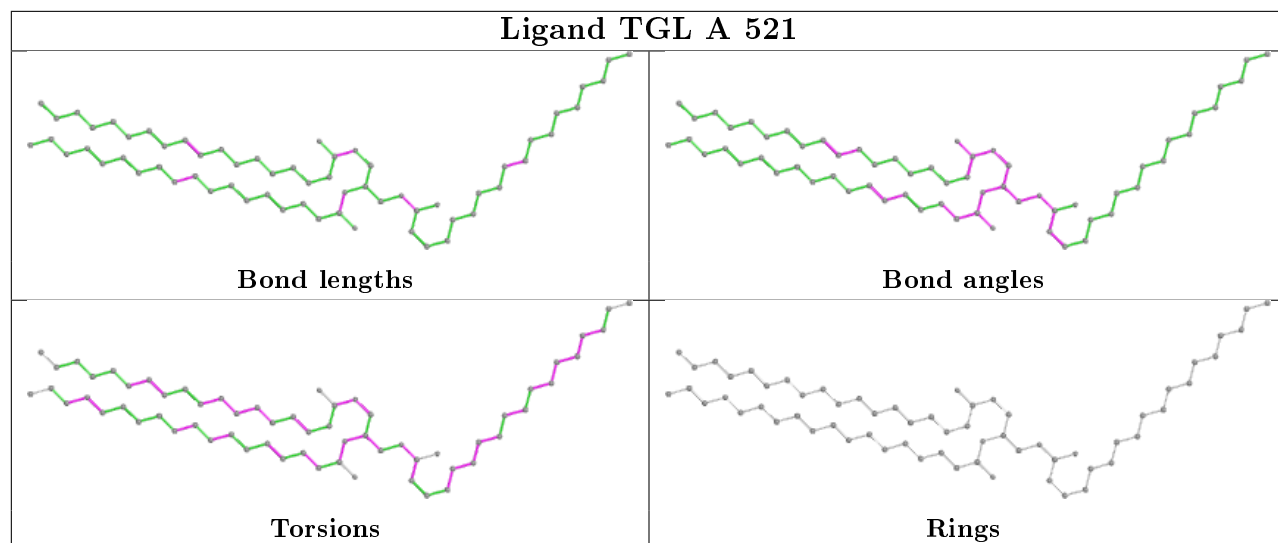
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	268	PGV	3	0
22	C	271	CHD	2	0
25	C	270	CDL	19	0
14	A	516	HEA	3	0
14	N	516	HEA	3	0
25	G	269	CDL	20	0
14	A	515	HEA	7	0
19	N	1524	PGV	7	0
22	B	1085	CHD	2	0
19	P	1268	PGV	5	0
18	L	522	TGL	14	0
19	A	522	PGV	1	0
21	B	229	PSC	11	0
24	T	263	PEK	12	0
24	C	265	PEK	5	0
25	T	1269	CDL	24	0
18	N	1521	TGL	7	0
19	P	1267	PGV	2	0
22	P	1271	CHD	1	0
25	P	1270	CDL	9	0
18	N	1523	TGL	6	0
22	J	60	CHD	2	0
22	P	1525	CHD	1	0
19	C	267	PGV	7	0
19	N	1266	PGV	2	0
18	N	1522	TGL	9	0
24	C	264	PEK	3	0
18	D	523	TGL	5	0
22	W	1059	CHD	3	0

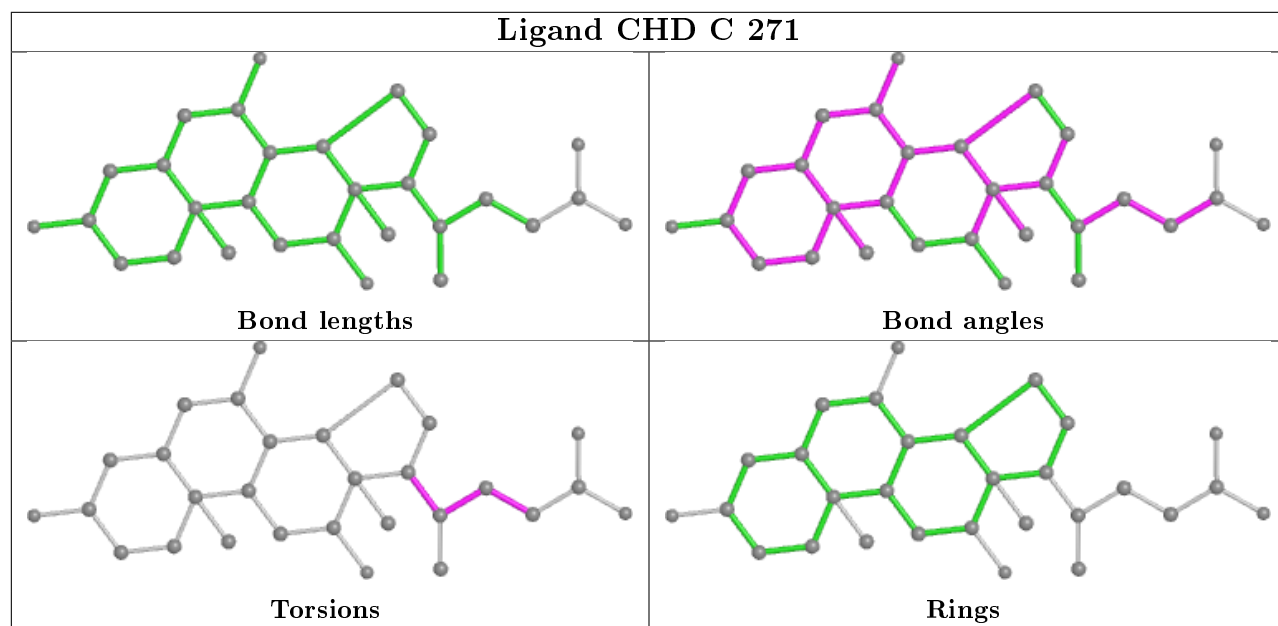
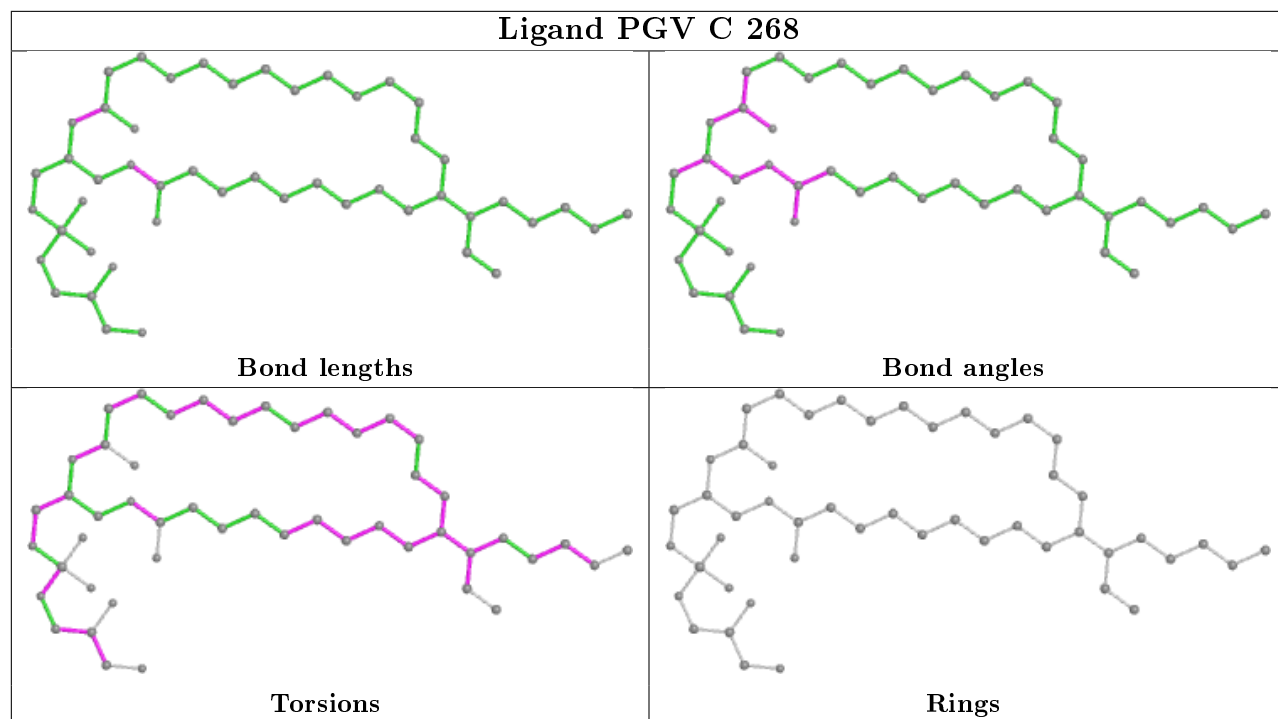
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

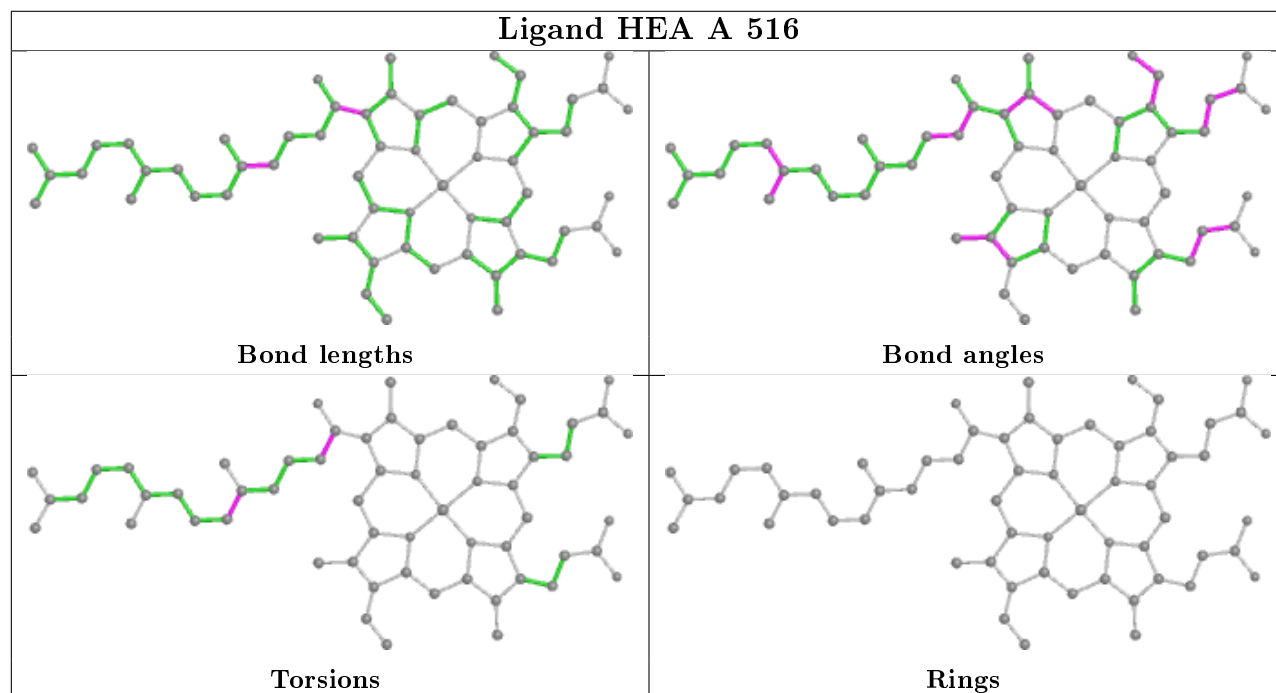
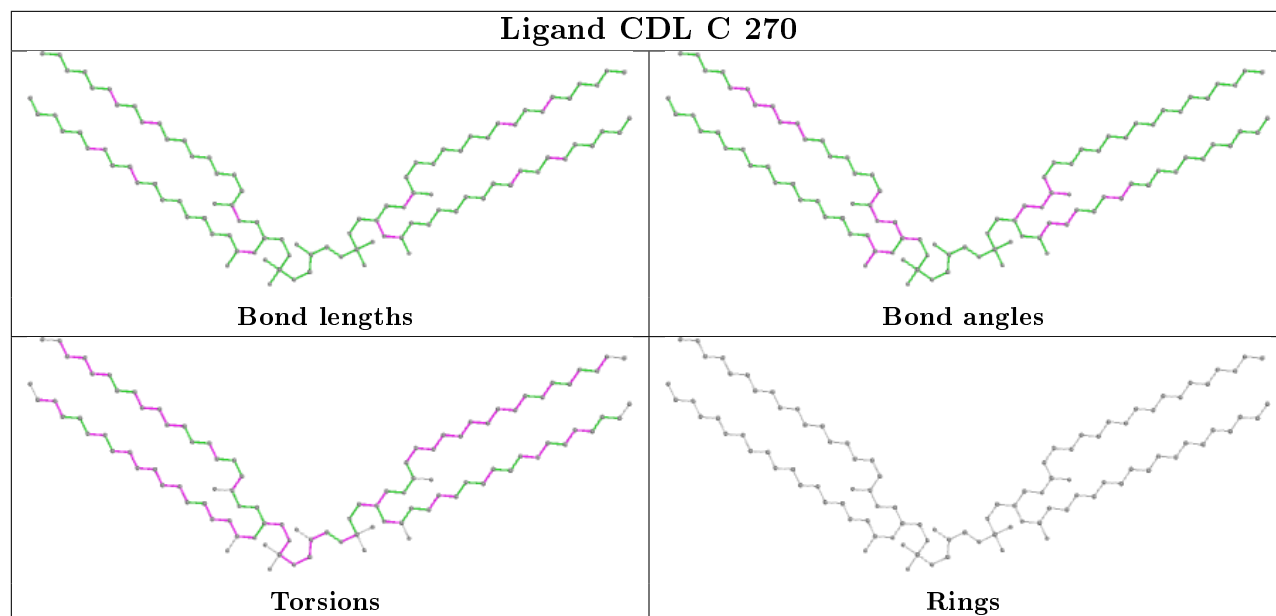


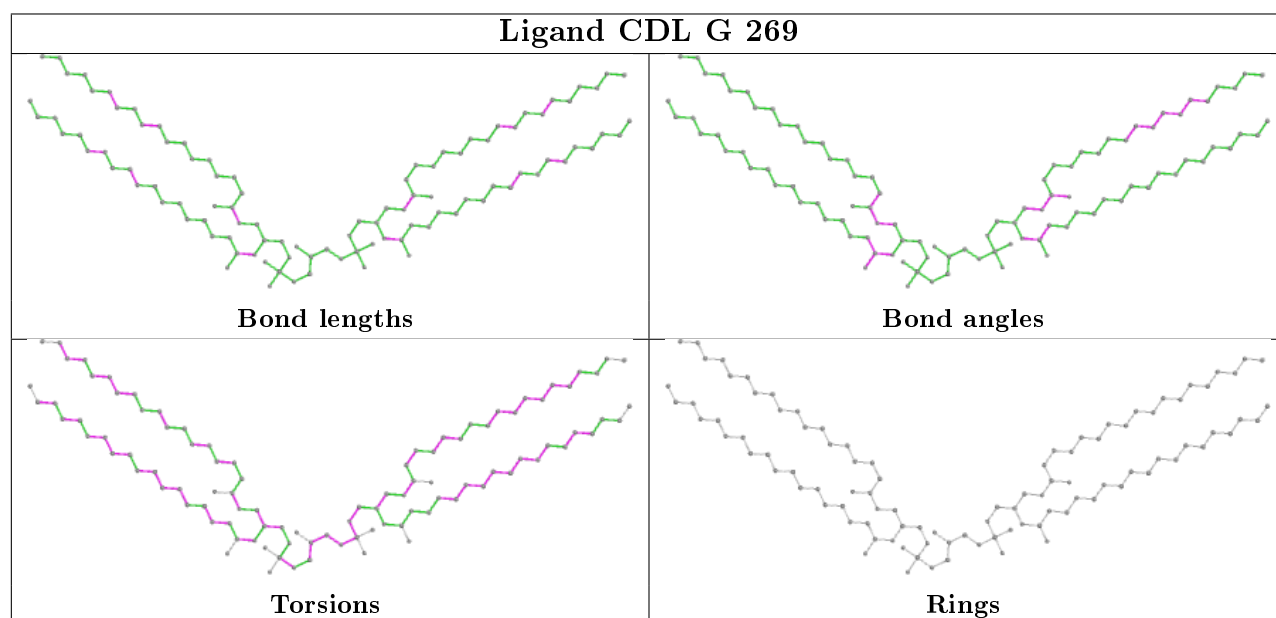
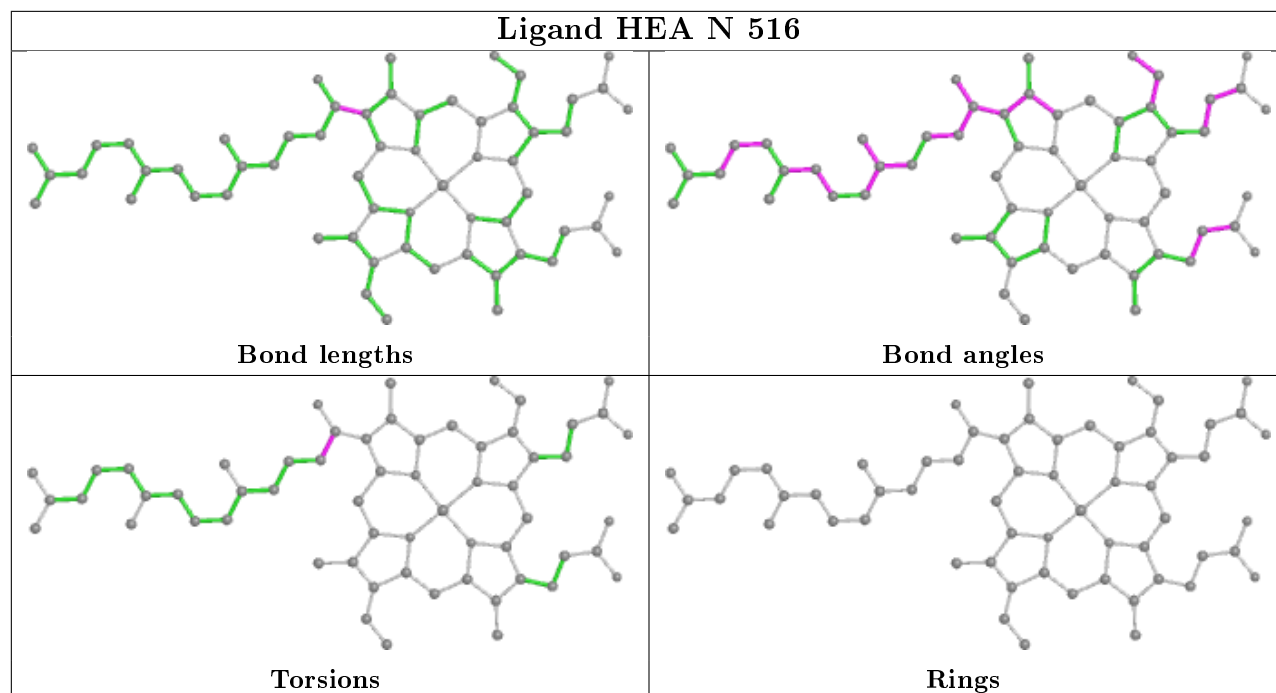


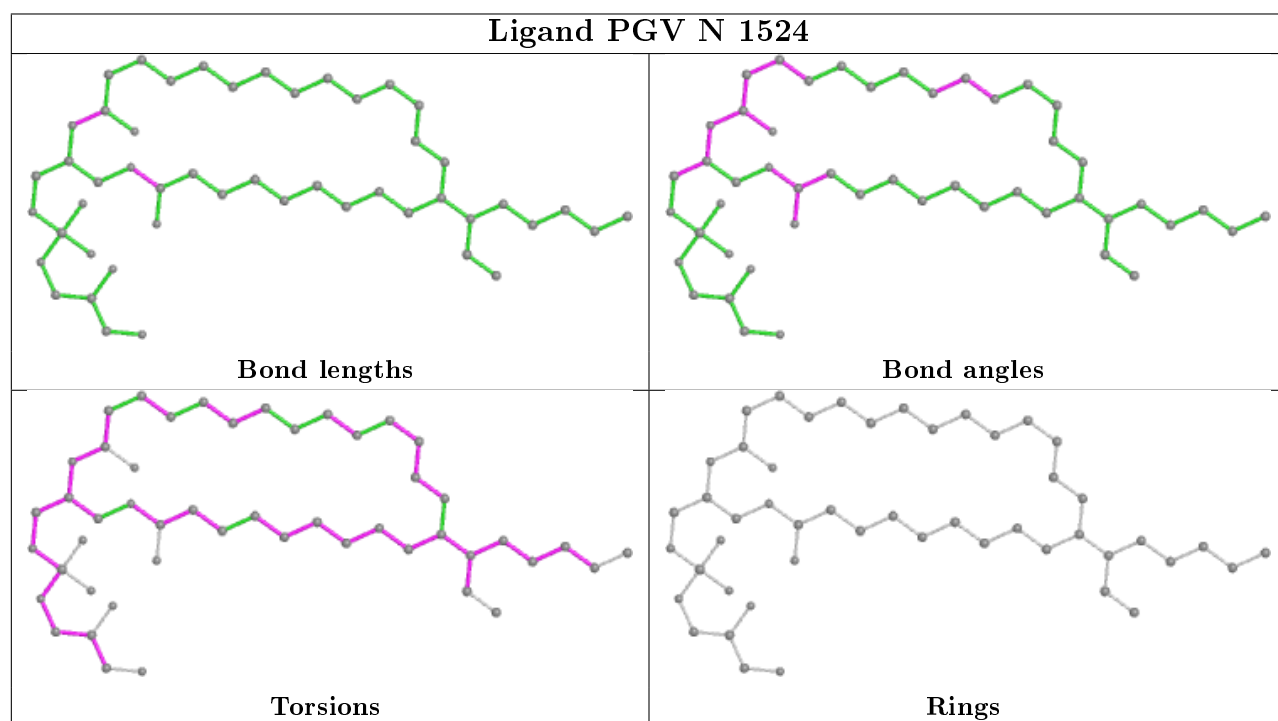
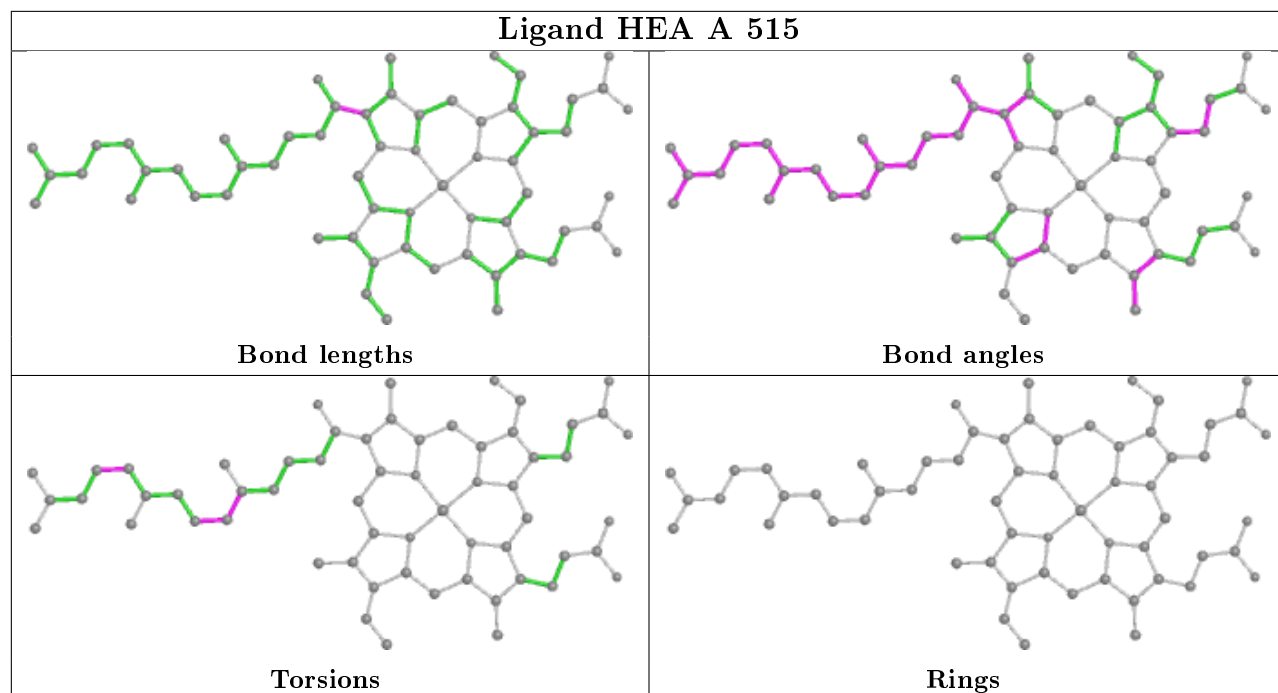


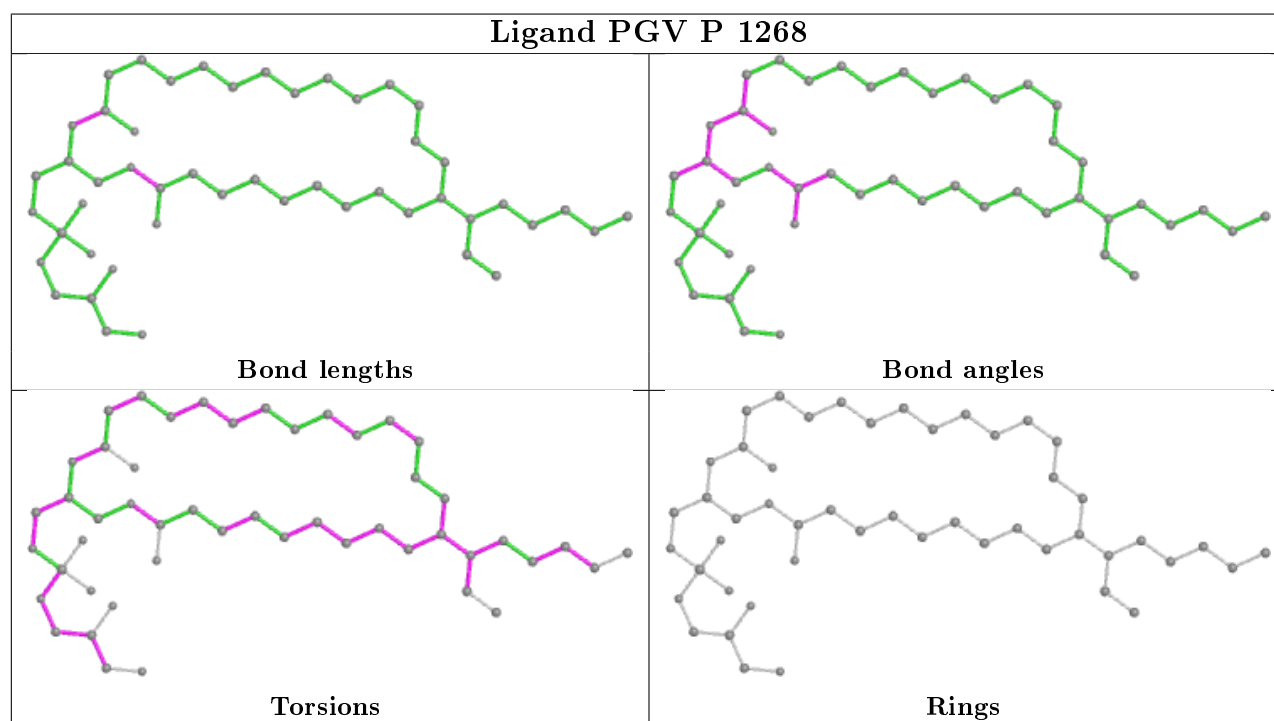
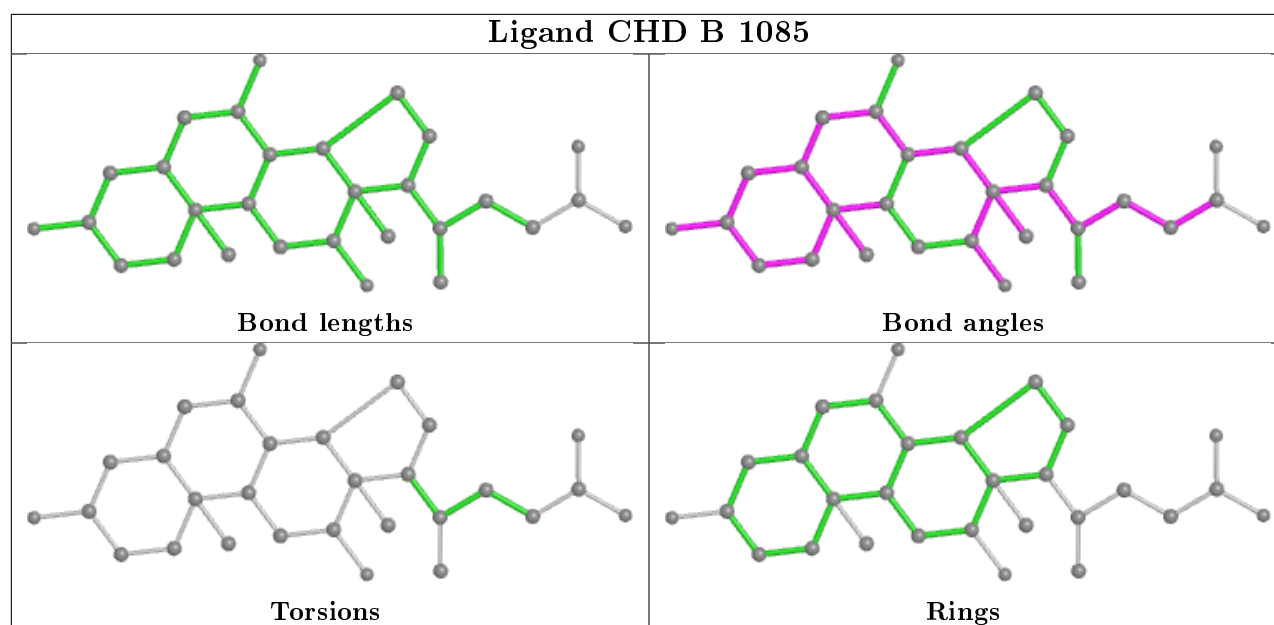


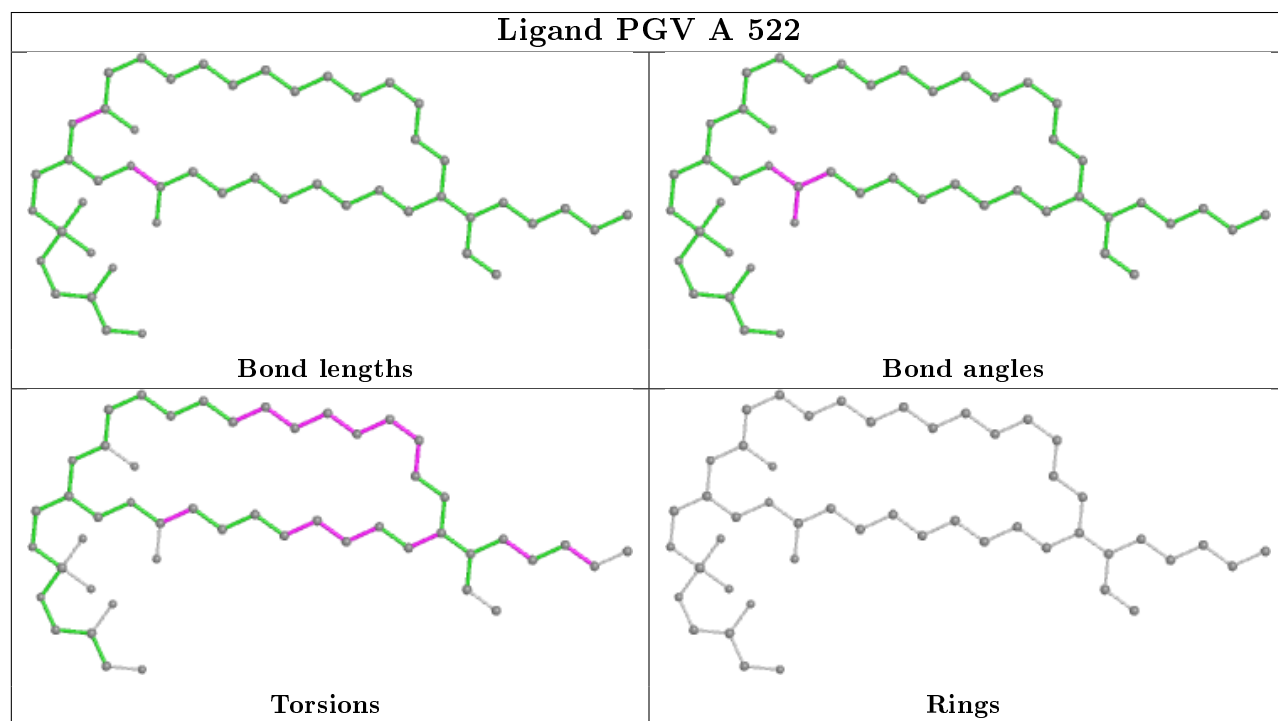
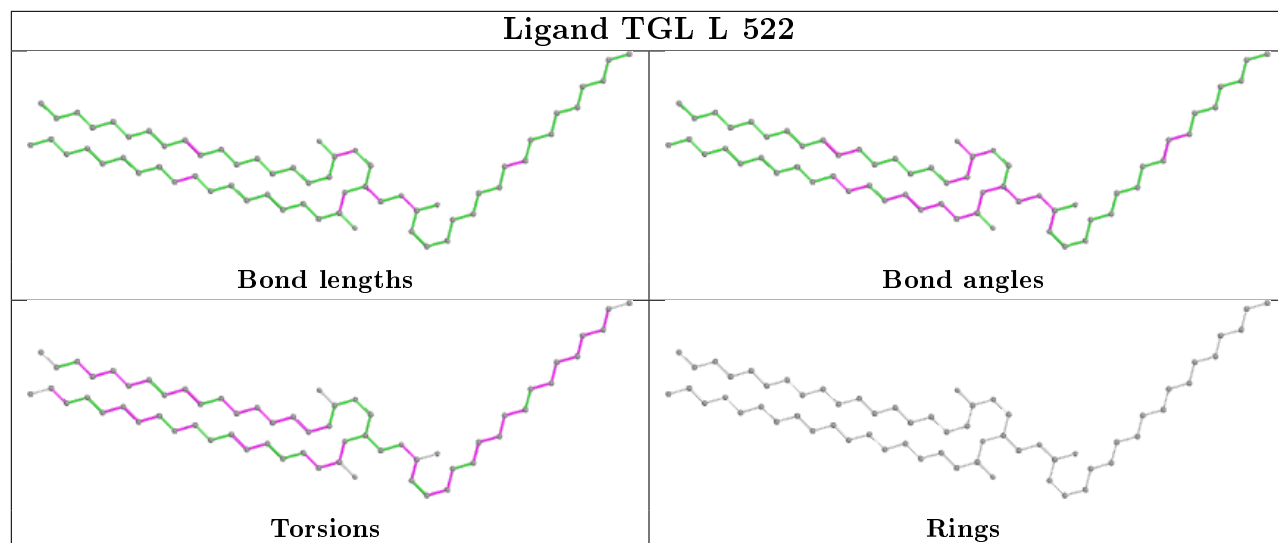


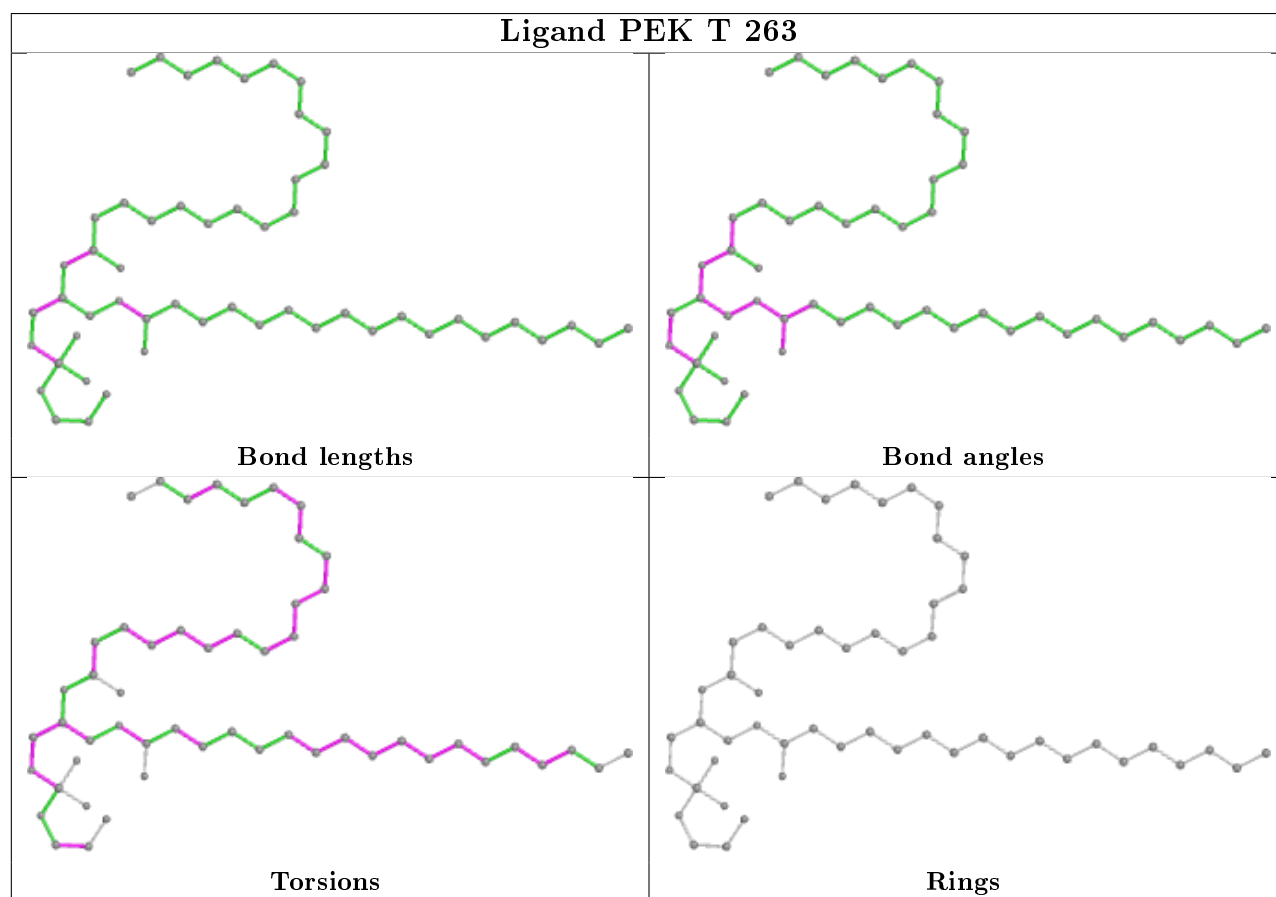
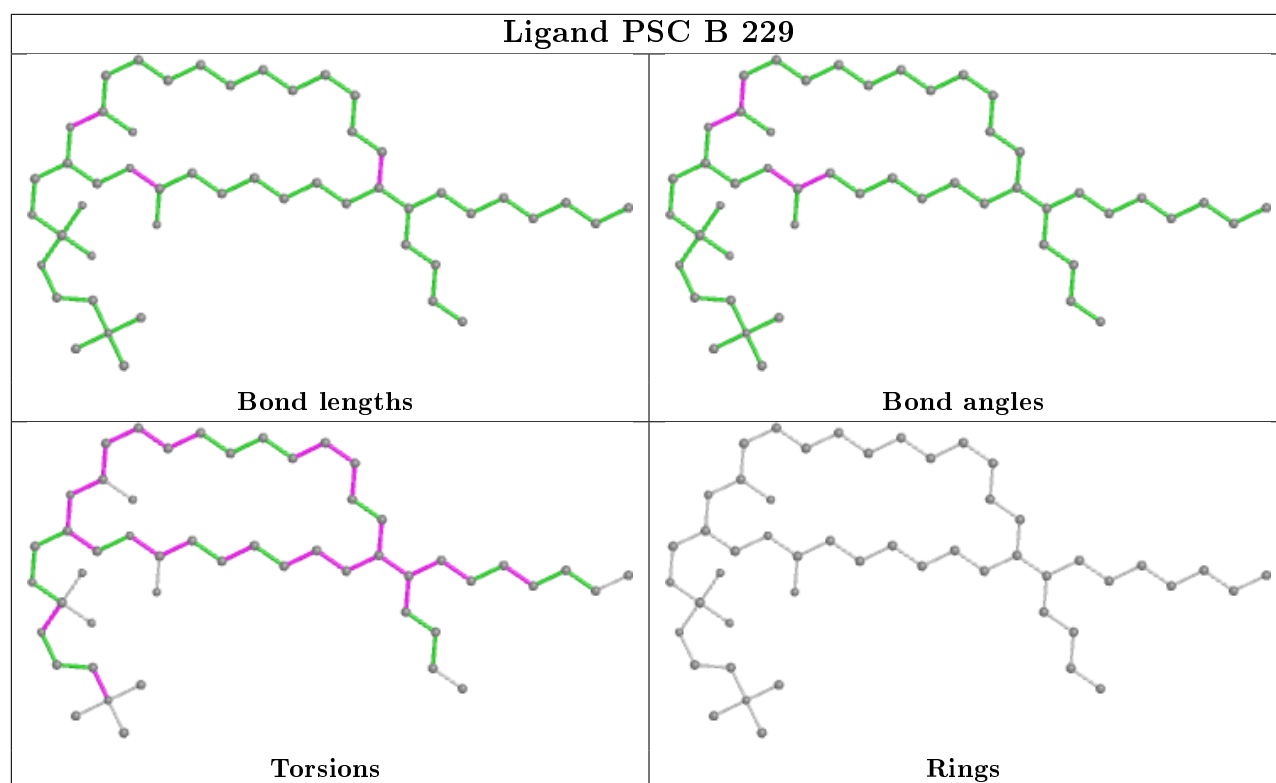




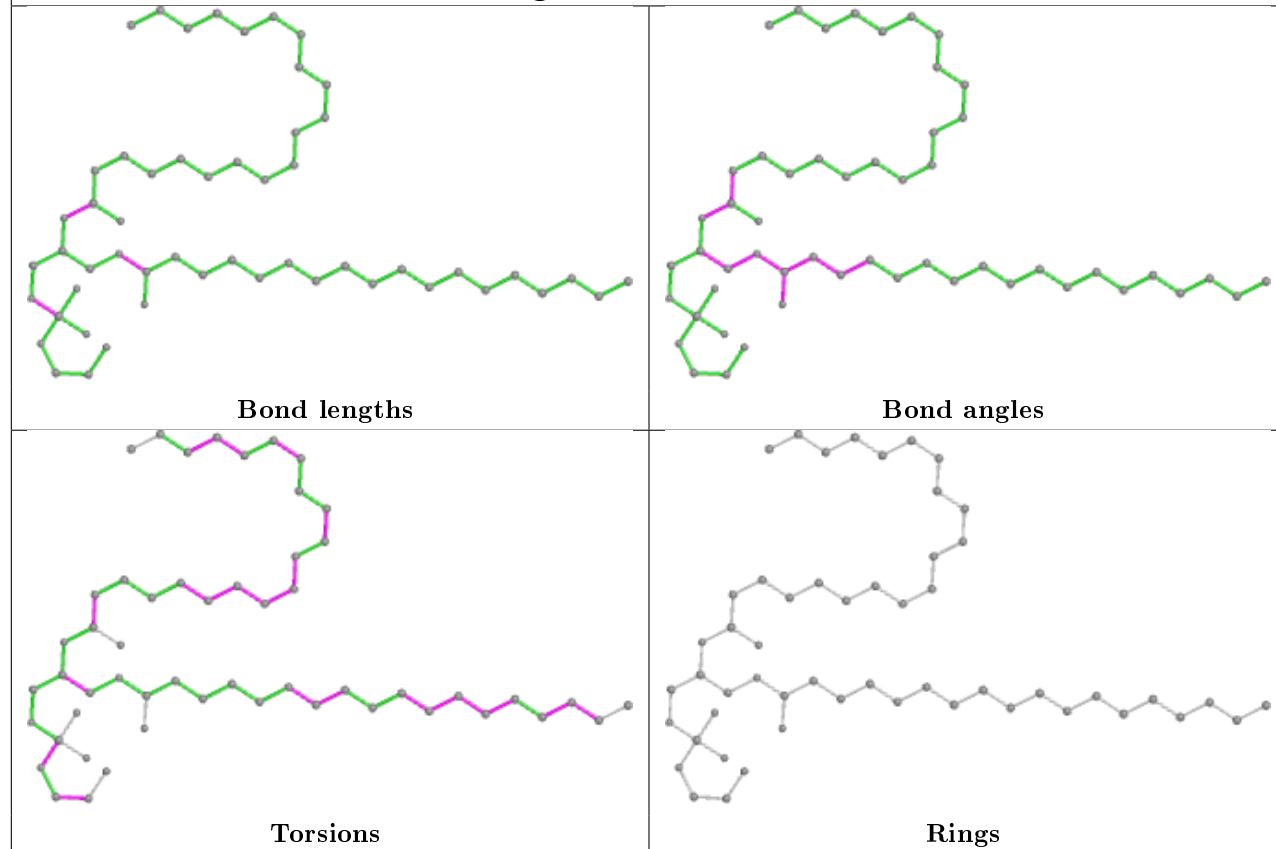




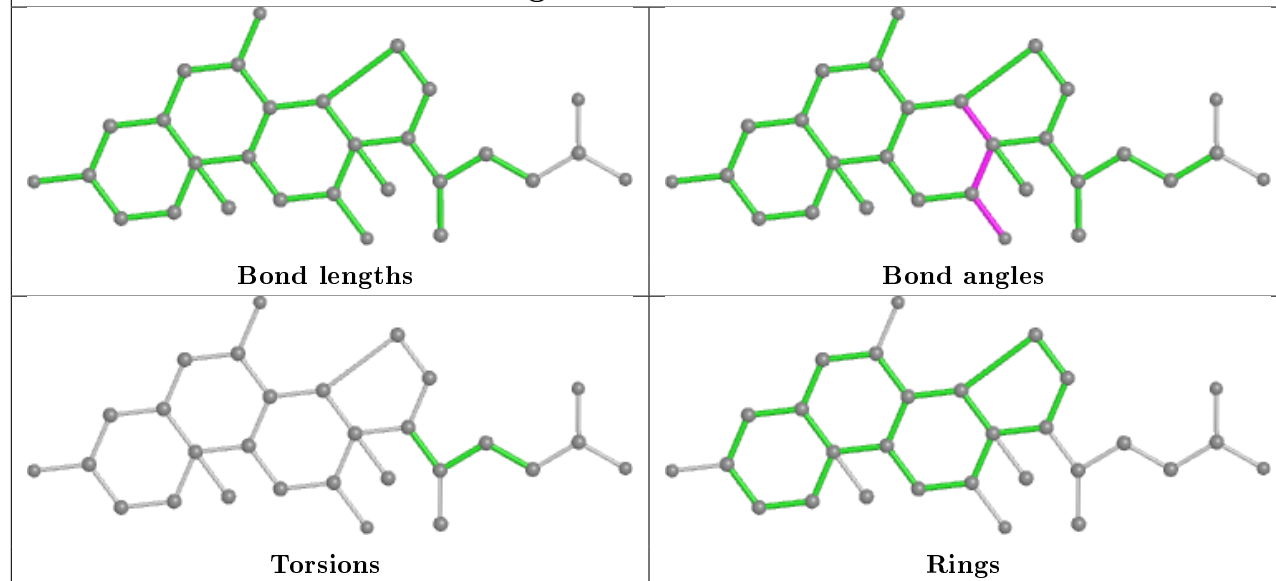


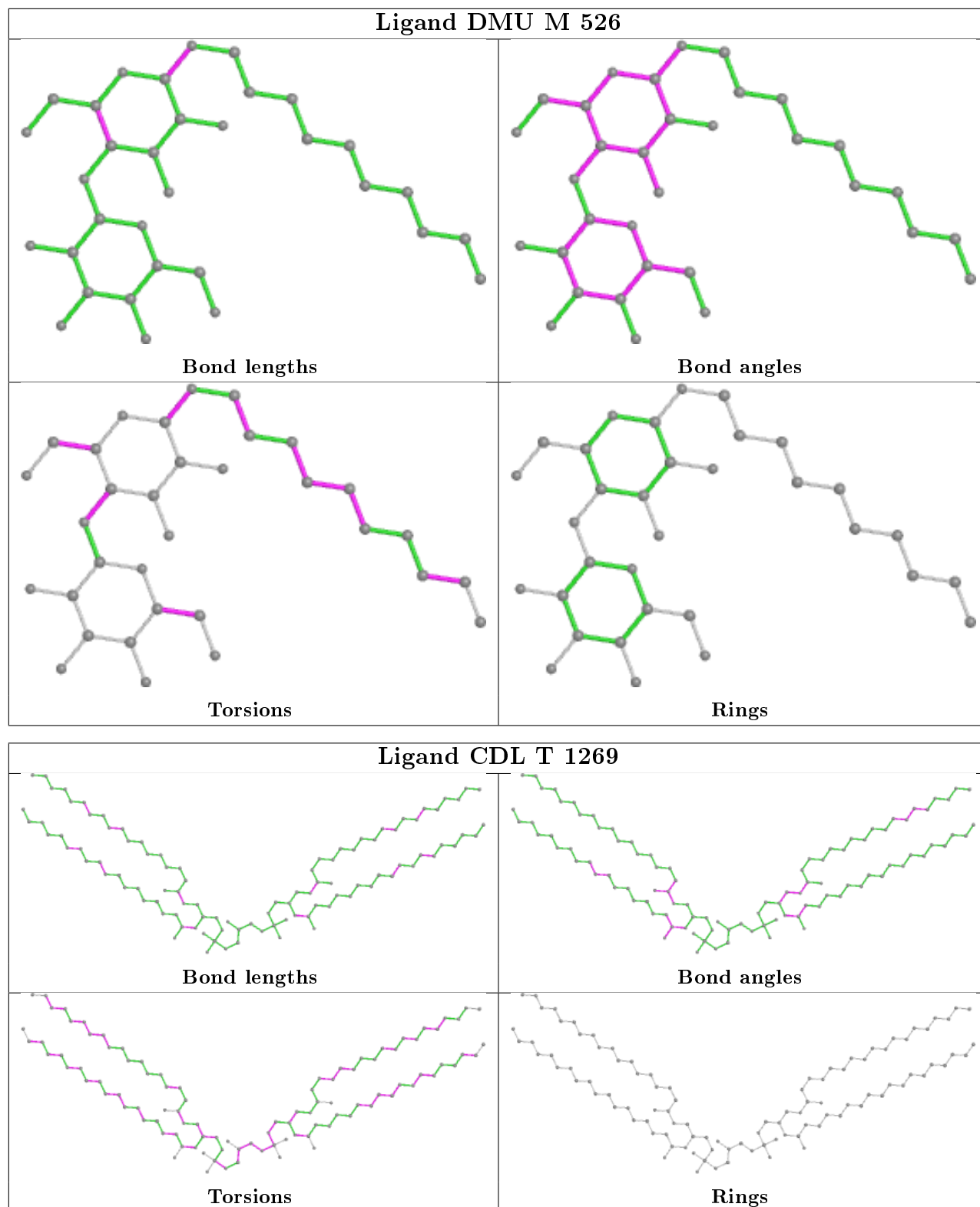


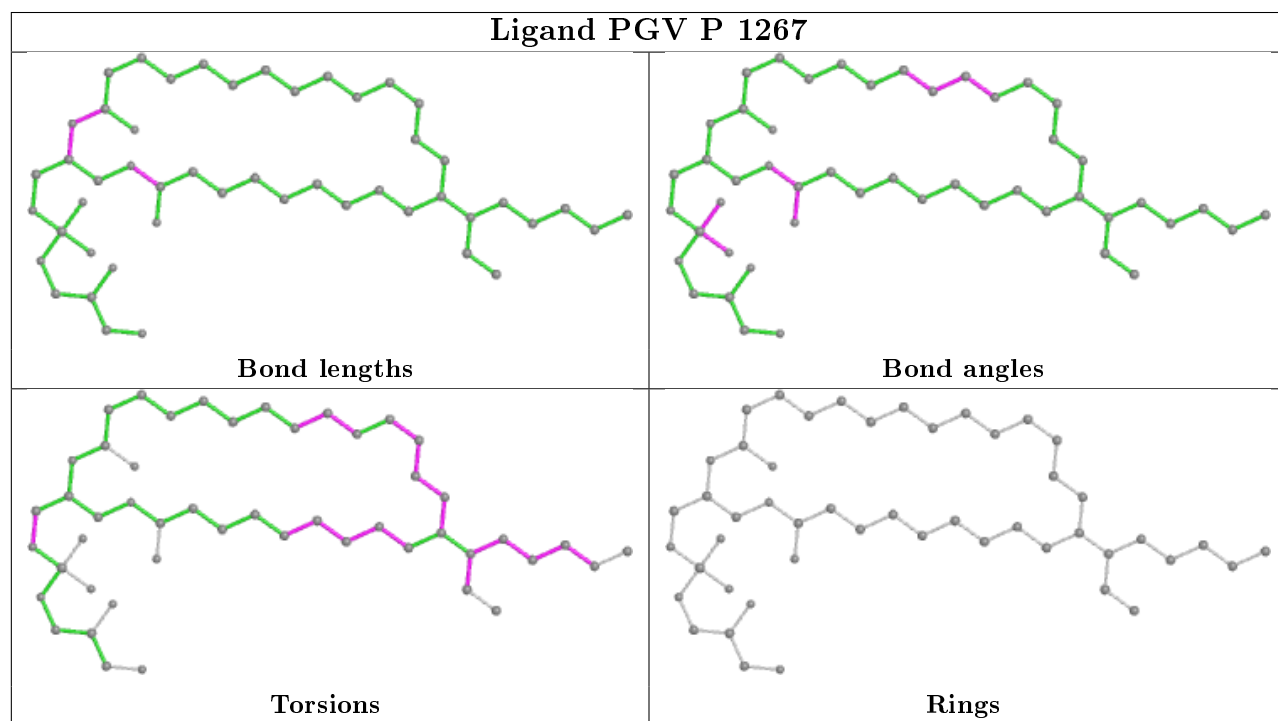
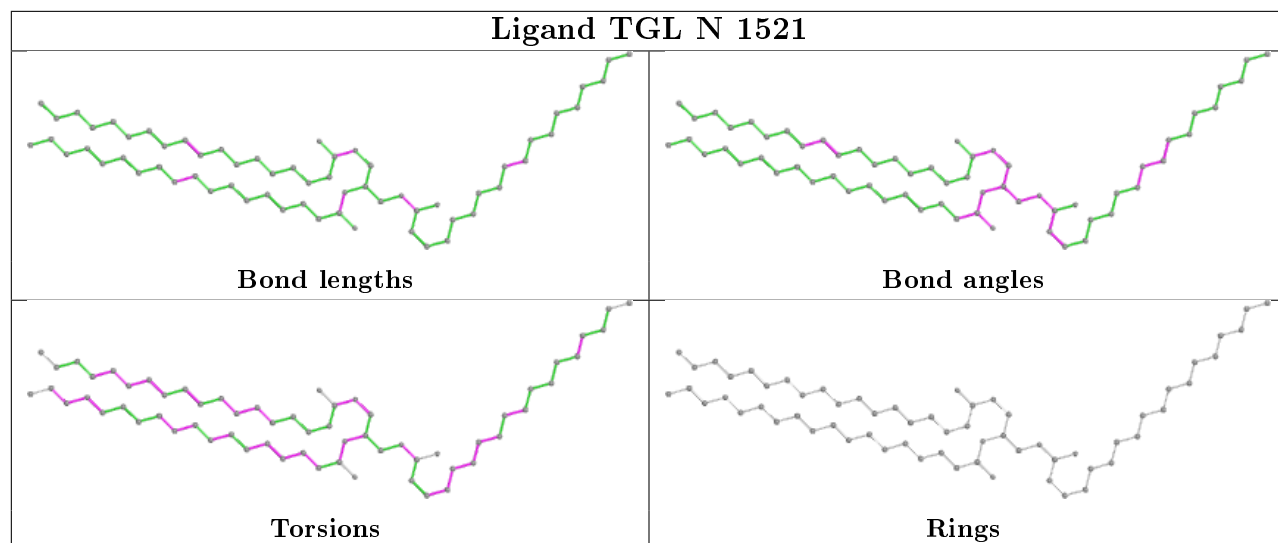
Ligand PEK C 265



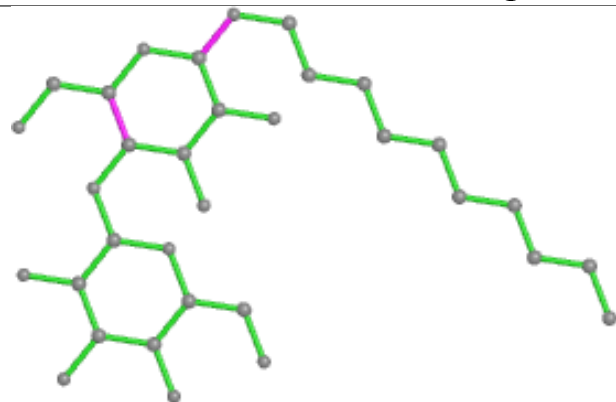
Ligand CHD G 229



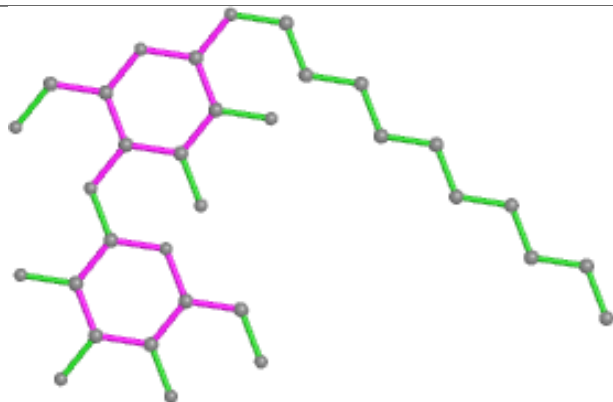




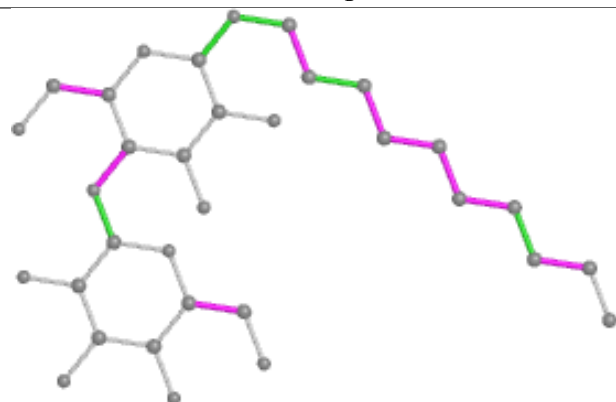
Ligand DMU Z 1526



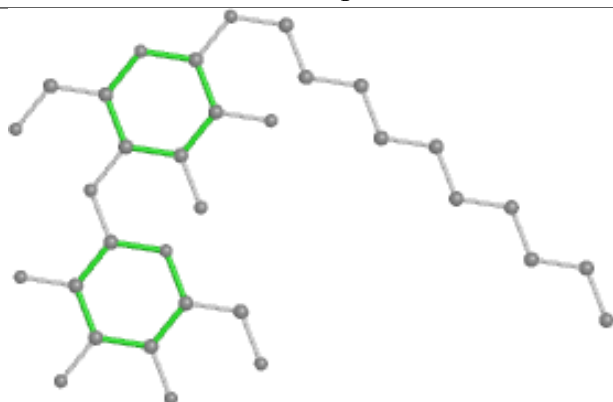
Bond lengths



Bond angles

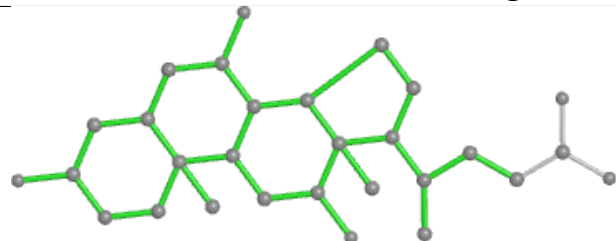


Torsions

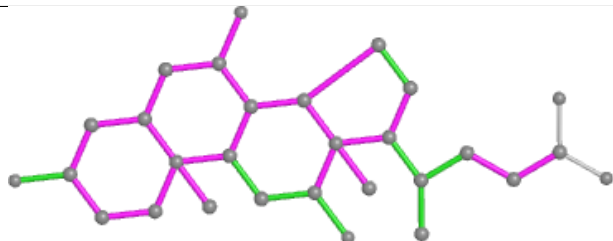


Rings

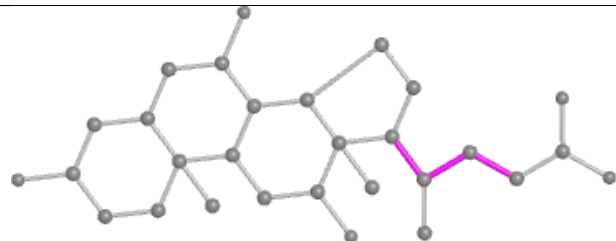
Ligand CHD P 1271



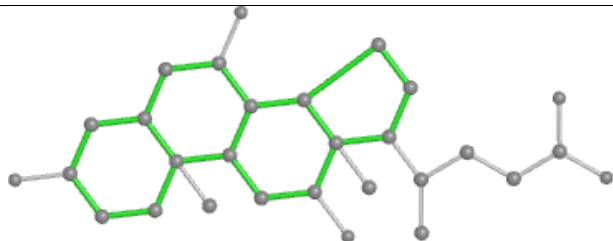
Bond lengths



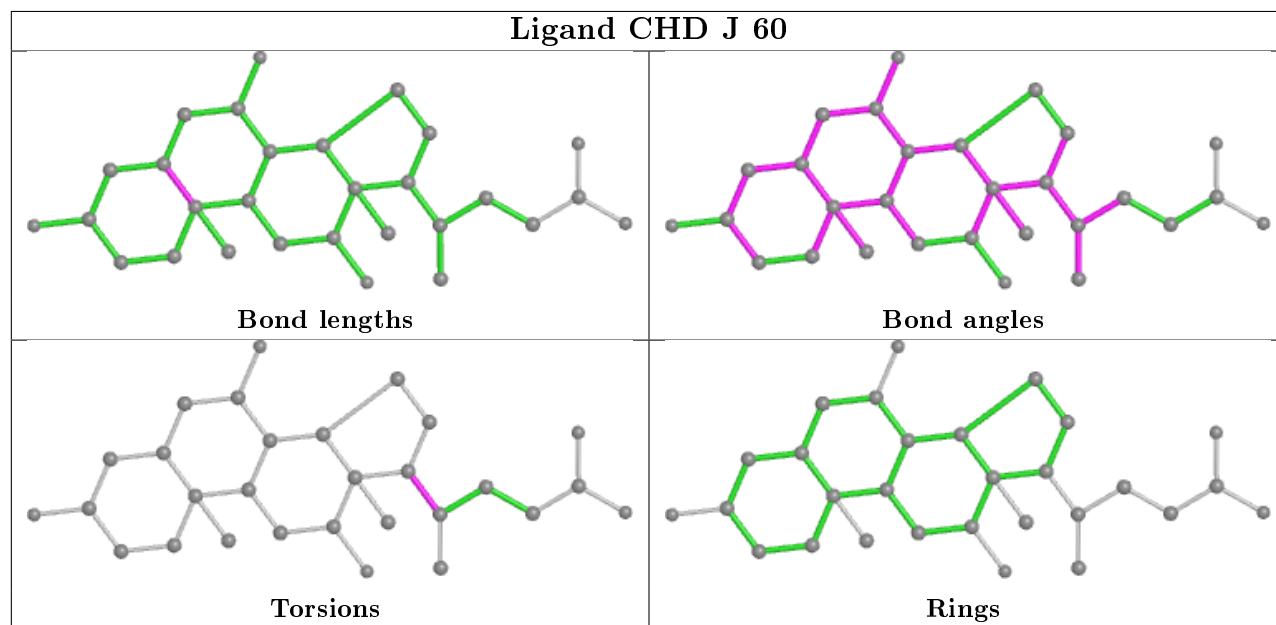
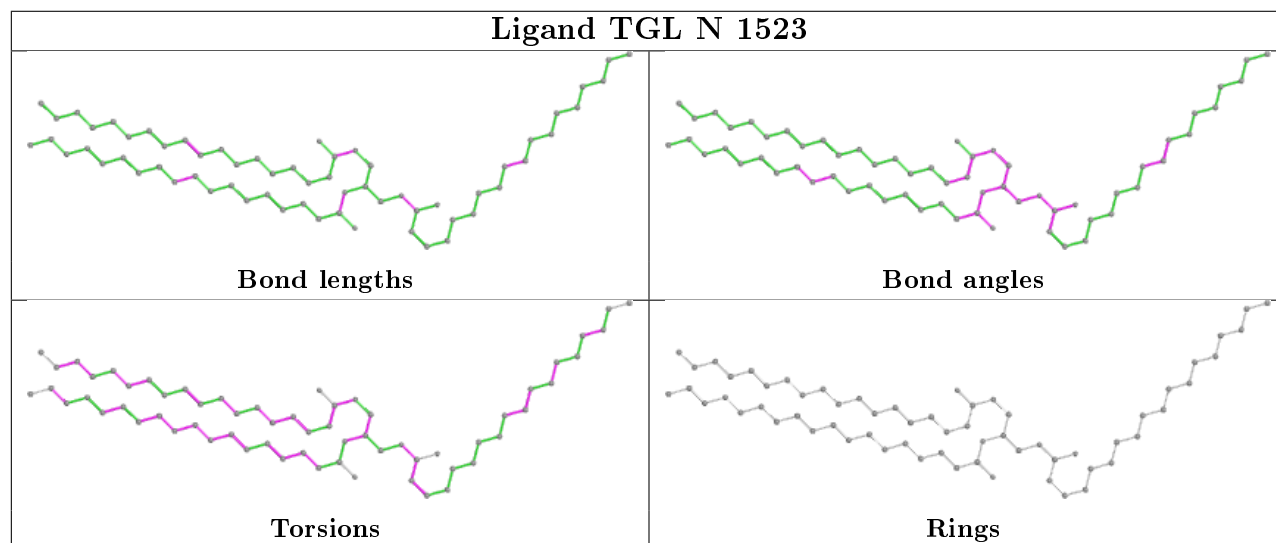
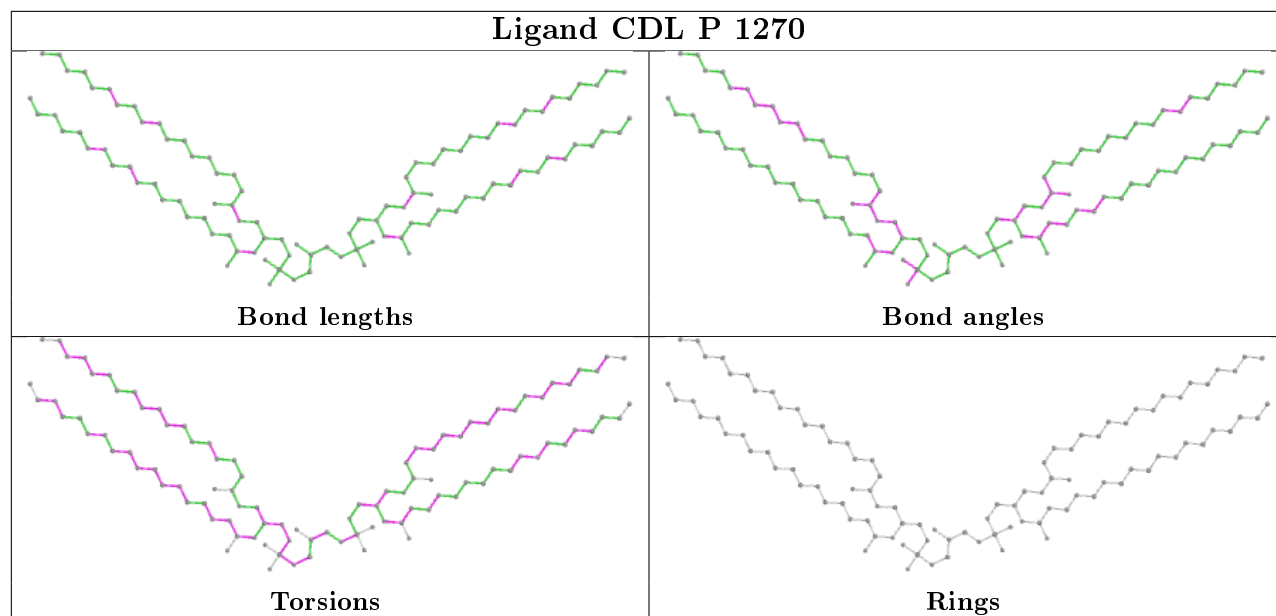
Bond angles



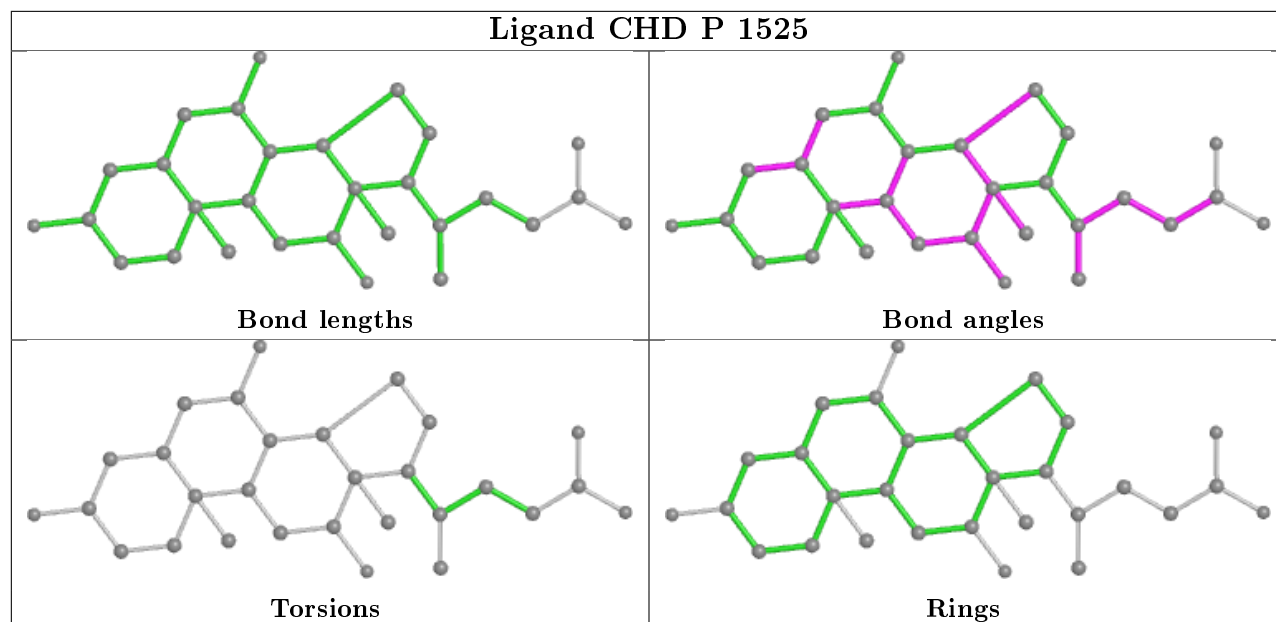
Torsions



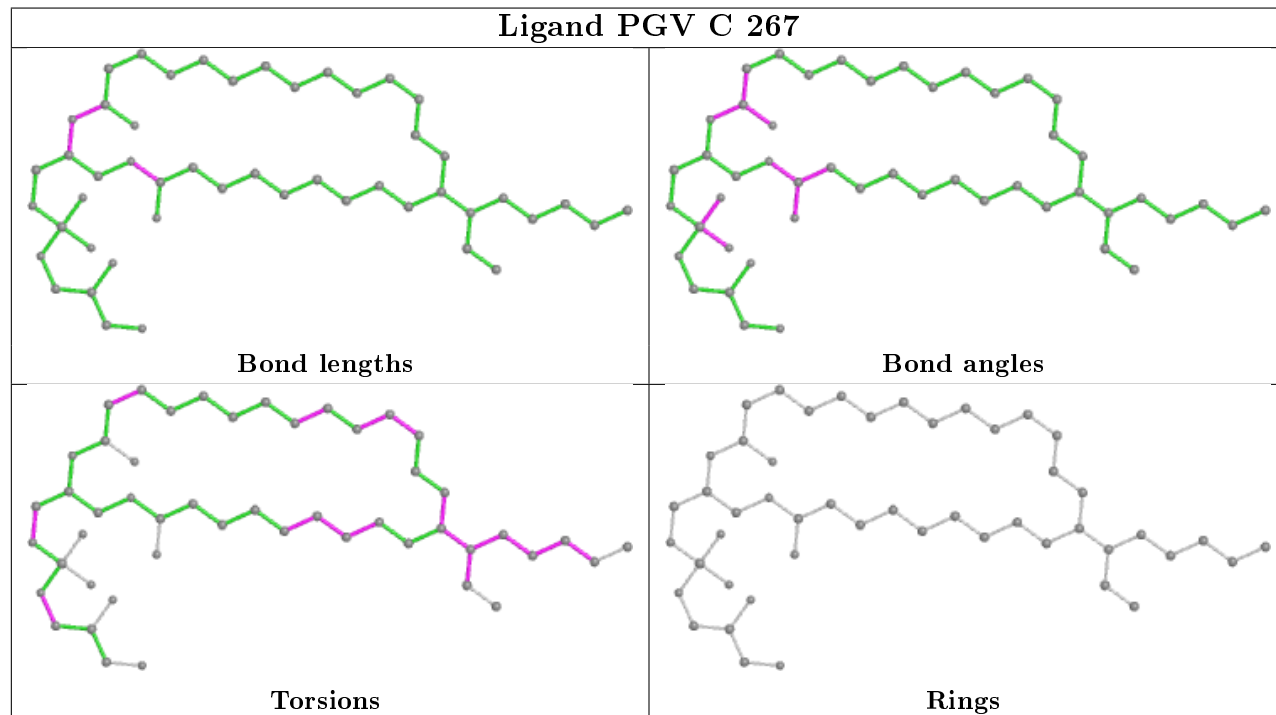
Rings

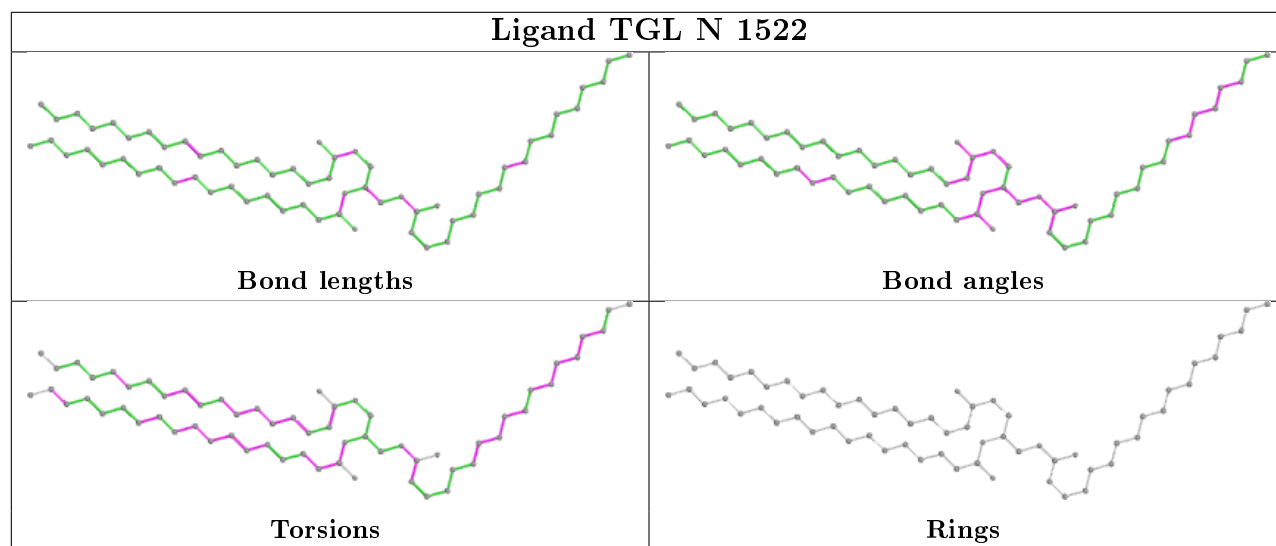
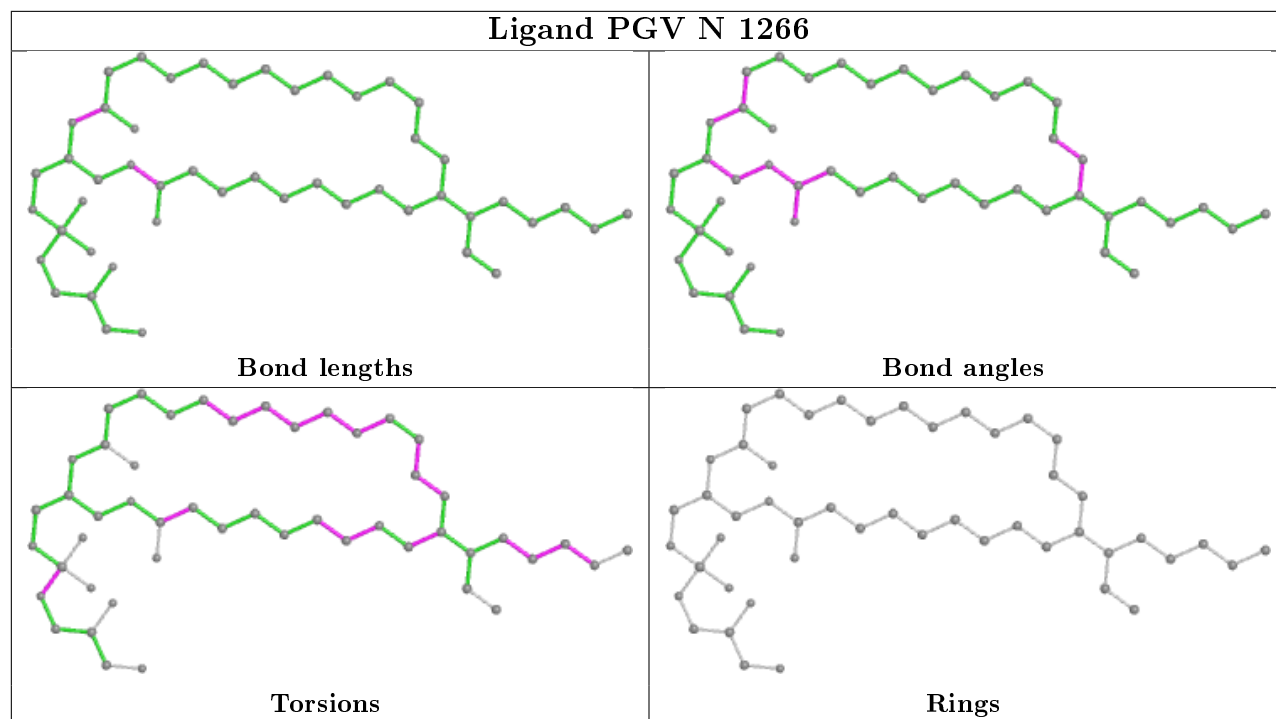


Ligand CHD P 1525

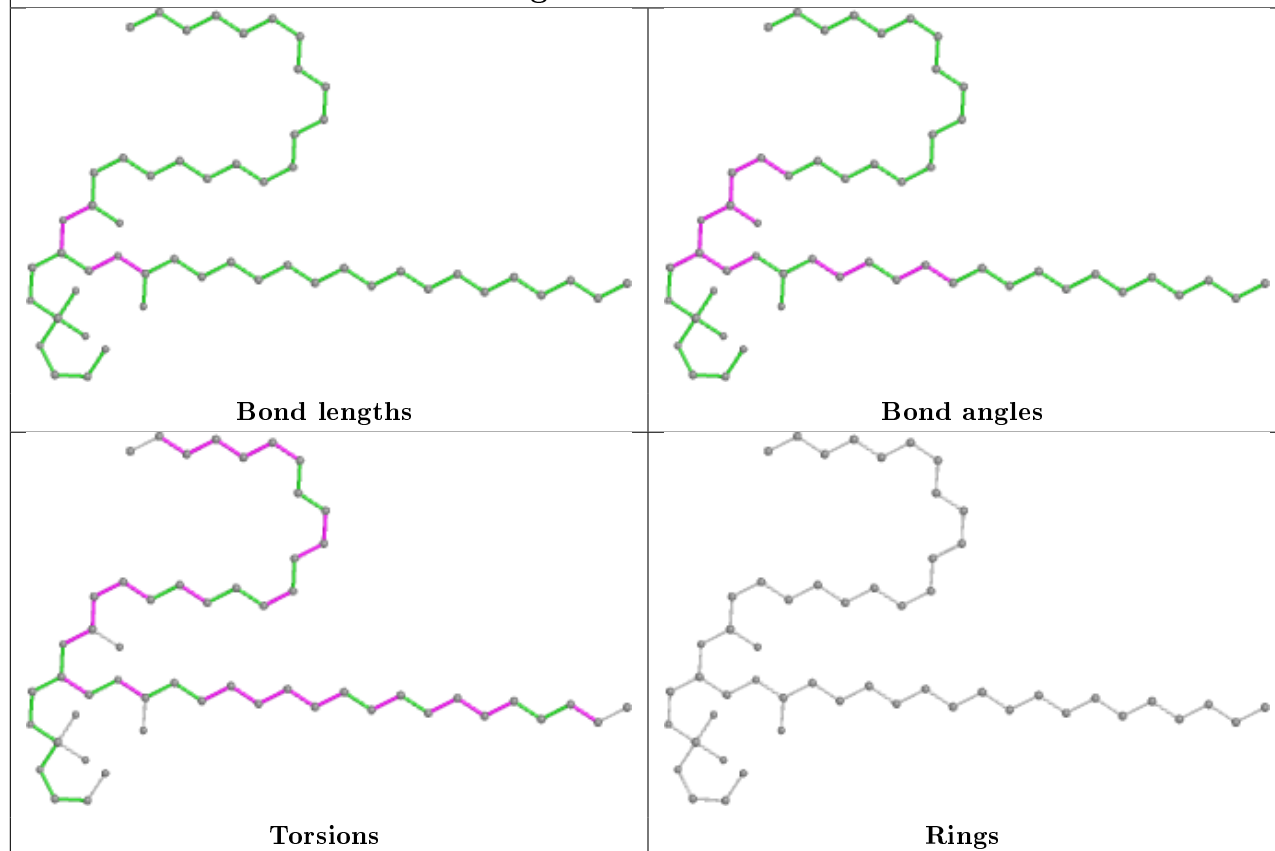


Ligand PGV C 267

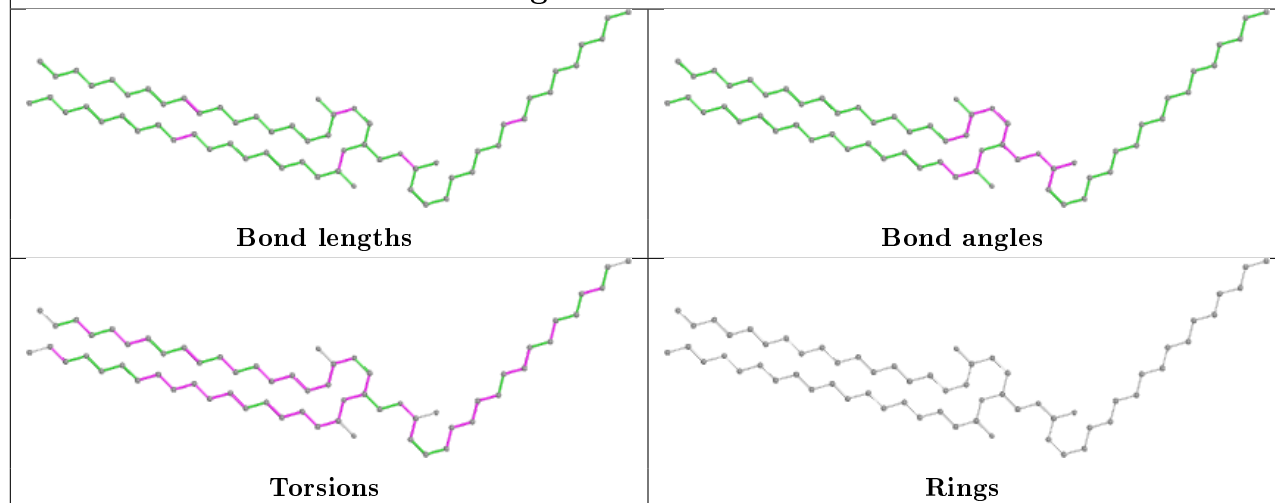


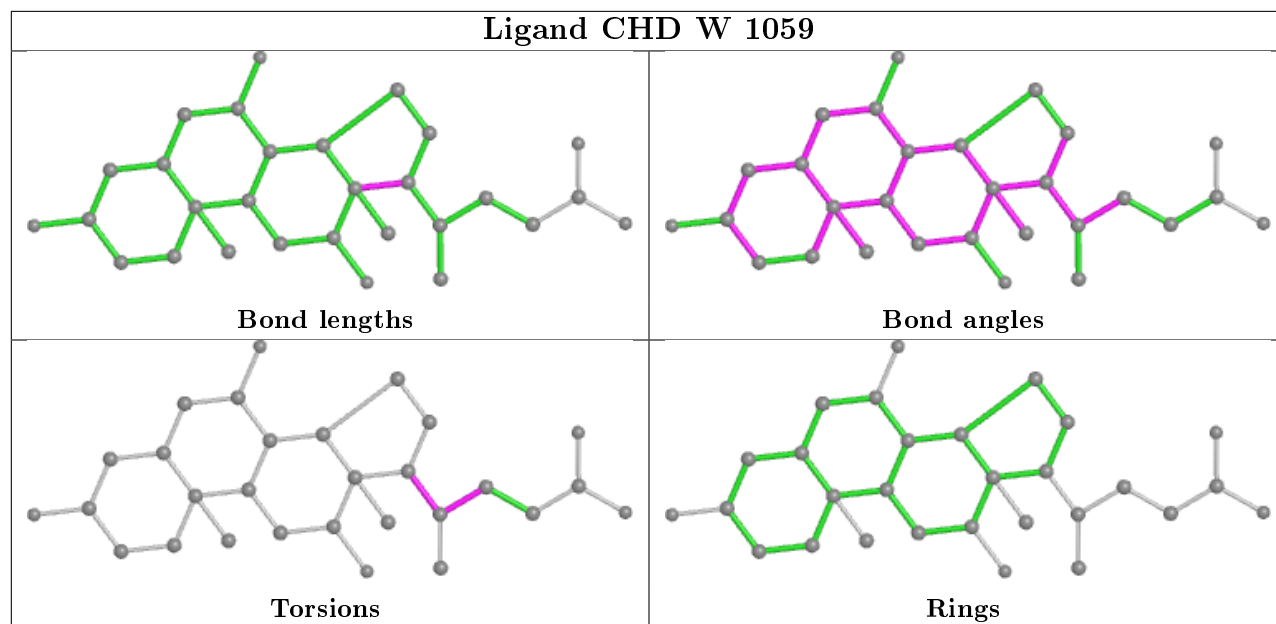


Ligand PEK C 264



Ligand TGL D 523





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.33	0 100 100	13, 17, 24, 50	0
1	N	513/514 (99%)	-0.35	0 100 100	13, 19, 26, 49	0
2	B	226/227 (99%)	-0.27	0 100 100	12, 21, 49, 70	0
2	O	226/227 (99%)	-0.15	2 (0%) 84 63	16, 24, 50, 68	0
3	C	259/261 (99%)	-0.45	0 100 100	13, 18, 30, 48	0
3	P	259/261 (99%)	-0.43	1 (0%) 92 79	14, 20, 33, 52	0
4	D	144/147 (97%)	-0.38	0 100 100	14, 20, 41, 64	0
4	Q	144/147 (97%)	0.14	7 (4%) 29 11	19, 31, 56, 99	0
5	E	105/109 (96%)	-0.49	1 (0%) 82 59	13, 20, 48, 85	0
5	R	105/109 (96%)	-0.36	2 (1%) 66 37	17, 24, 56, 88	0
6	F	98/98 (100%)	-0.06	5 (5%) 28 10	15, 24, 72, 108	0
6	S	98/98 (100%)	0.03	5 (5%) 28 10	14, 23, 74, 106	0
7	G	83/85 (97%)	0.07	4 (4%) 30 11	13, 24, 92, 96	0
7	T	83/85 (97%)	0.20	7 (8%) 11 3	16, 26, 92, 97	0
8	H	79/85 (92%)	-0.07	2 (2%) 57 29	16, 27, 76, 99	0
8	U	79/85 (92%)	-0.05	1 (1%) 77 51	19, 29, 76, 100	0
9	I	72/73 (98%)	-0.17	1 (1%) 75 49	16, 29, 54, 62	0
9	V	72/73 (98%)	-0.02	0 100 100	16, 35, 55, 79	0
10	J	58/59 (98%)	-0.16	2 (3%) 45 19	19, 28, 55, 89	0
10	W	58/59 (98%)	-0.15	1 (1%) 70 41	18, 27, 61, 95	0
11	K	49/56 (87%)	-0.34	0 100 100	19, 26, 37, 49	0
11	X	49/56 (87%)	-0.08	1 (2%) 65 36	24, 32, 47, 61	0
12	L	46/47 (97%)	-0.30	0 100 100	17, 23, 46, 70	0
12	Y	46/47 (97%)	-0.24	1 (2%) 62 33	18, 24, 51, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.14	0 100 100	15, 21, 66, 91	0
13	Z	43/46 (93%)	-0.15	2 (4%) 31 11	22, 26, 75, 94	0
All	All	3550/3614 (98%)	-0.25	45 (1%) 77 51	12, 21, 52, 108	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	12.5
4	Q	4	SER	12.2
6	S	97	ALA	9.2
4	Q	6	VAL	7.5
4	Q	8	SER	6.7
6	F	98	HIS	5.9
7	T	3	ALA	5.8
7	T	1	ALA	5.6
6	F	97	ALA	5.2
7	T	2	SER	5.2
7	T	8	HIS	5.1
6	S	98	HIS	5.0
5	R	5	HIS	4.1
10	J	58	LYS	3.7
8	U	7	LYS	3.7
3	P	3	HIS	3.6
7	G	2	SER	3.4
6	F	96	LEU	3.4
7	G	4	ALA	3.4
6	S	94	HIS	3.4
7	G	8	HIS	3.3
11	X	6	ALA	3.3
7	G	3	ALA	3.2
4	Q	7	LYS	3.2
5	E	5	HIS	3.1
2	O	226	MET	3.0
10	W	58	LYS	3.0
13	Z	42	LYS	3.0
8	H	46	LYS	2.9
13	Z	43	SER	2.9
6	F	95	GLN	2.9
6	S	96	LEU	2.7
7	T	4	ALA	2.6
5	R	109	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
10	J	1	PHE	2.5
6	F	1	ALA	2.4
9	I	37	PHE	2.4
6	S	95	GLN	2.4
7	T	5	LYS	2.4
7	T	7	ASP	2.4
12	Y	47	LYS	2.4
4	Q	35	ALA	2.3
4	Q	58	GLU	2.2
8	H	47	GLY	2.2
2	O	90	ILE	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	I	1	9/10	0.59	0.44	71,74,76,78	0
7	TPO	G	11	11/12	0.60	0.35	61,67,86,87	0
7	TPO	T	11	11/12	0.72	0.41	64,70,88,88	0
9	SAC	V	1	9/10	0.73	0.52	84,85,86,86	0
1	FME	N	1	10/11	0.94	0.31	35,35,51,53	0
1	FME	A	1	10/11	0.96	0.30	34,36,49,58	0
2	FME	B	1	10/11	0.97	0.22	20,21,29,35	0
2	FME	O	1	10/11	0.97	0.26	23,24,32,39	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(\AA^2)	Q<0.9
23	UNX	P	262	1/1	0.56	0.26	42,42,42,42	0
22	CHD	W	1059	29/29	0.65	0.47	91,103,105,105	0
24	PEK	T	263	53/53	0.70	0.52	38,90,112,114	0
22	CHD	J	60	29/29	0.71	0.52	98,105,109,109	0
24	PEK	P	1265	53/53	0.74	0.45	34,86,99,100	0
24	PEK	C	265	53/53	0.74	0.39	36,87,96,98	0
18	TGL	N	1523	63/63	0.75	0.40	45,70,89,91	0
25	CDL	T	1269	100/100	0.76	0.50	51,83,107,108	0
19	PGV	P	1268	51/51	0.76	0.46	74,86,100,101	0
25	CDL	G	269	100/100	0.77	0.57	56,82,107,111	0
24	PEK	G	1263	53/53	0.78	0.41	42,92,110,110	0
21	PSC	B	229	52/52	0.78	0.47	44,89,112,114	0
21	PSC	O	1229	52/52	0.79	0.45	34,82,109,112	0
19	PGV	C	268	51/51	0.80	0.45	57,84,99,100	0
19	PGV	N	1524	51/51	0.80	0.40	36,64,98,101	0
23	UNX	C	262	1/1	0.81	0.29	42,42,42,42	0
18	TGL	N	1522	63/63	0.83	0.39	41,65,81,83	0
18	TGL	D	523	63/63	0.83	0.33	44,64,89,90	0
25	CDL	P	1270	100/100	0.83	0.48	39,83,105,108	0
18	TGL	N	1521	63/63	0.85	0.40	40,68,88,92	0
19	PGV	A	524	51/51	0.85	0.40	29,64,91,94	0
22	CHD	P	1271	29/29	0.85	0.37	78,87,88,88	0
18	TGL	L	522	63/63	0.86	0.36	32,55,78,82	0
25	CDL	C	270	100/100	0.86	0.52	38,80,104,106	0
22	CHD	C	271	29/29	0.86	0.38	76,85,87,88	0
18	TGL	A	521	63/63	0.88	0.35	40,64,86,90	0
27	DMU	Z	1526	33/33	0.94	0.27	29,41,54,57	0
27	DMU	M	526	33/33	0.96	0.19	26,34,43,43	0
22	CHD	P	1525	29/29	0.96	0.20	19,26,29,33	0
14	HEA	N	515	60/60	0.96	0.25	22,41,66,70	0
24	PEK	C	264	53/53	0.96	0.25	14,34,69,70	0
16	MG	N	518	1/1	0.96	0.12	18,18,18,18	0
24	PEK	P	1264	53/53	0.96	0.24	14,35,68,70	0
17	NA	N	519	1/1	0.97	0.10	21,21,21,21	0
22	CHD	B	1085	29/29	0.97	0.17	7,13,15,22	0
15	CU	A	517	1/1	0.97	0.17	22,22,22,22	0
17	NA	A	519	1/1	0.97	0.13	18,18,18,18	0
22	CHD	C	525	29/29	0.97	0.21	18,26,28,28	0
14	HEA	A	515	60/60	0.98	0.21	6,18,35,40	0
19	PGV	P	1267	51/51	0.98	0.27	17,25,63,65	0
19	PGV	C	267	51/51	0.98	0.25	15,23,61,65	0
14	HEA	N	516	60/60	0.98	0.21	5,17,25,27	0
19	PGV	N	1266	51/51	0.98	0.29	20,34,52,53	0

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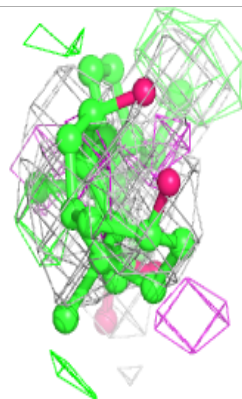
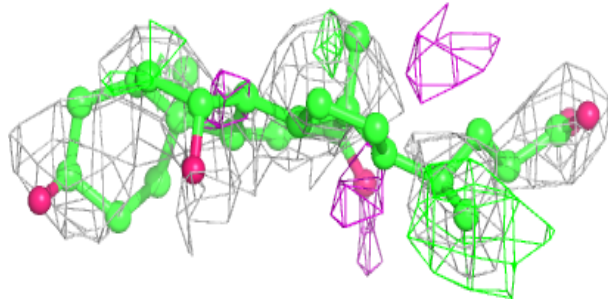
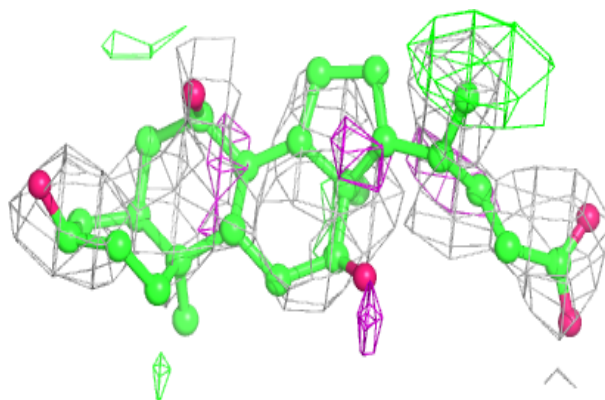
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CHD	G	229	29/29	0.98	0.17	6,12,14,15	0
14	HEA	A	516	60/60	0.98	0.22	10,15,23,26	0
15	CU	N	517	1/1	0.98	0.16	24,24,24,24	0
19	PGV	A	522	51/51	0.98	0.27	14,25,49,51	0
20	CUA	O	228	2/2	0.99	0.10	20,20,20,22	0
20	CUA	B	228	2/2	0.99	0.10	17,17,17,18	0
16	MG	A	518	1/1	0.99	0.10	15,15,15,15	0
26	ZN	S	99	1/1	0.99	0.11	22,22,22,22	0
26	ZN	F	99	1/1	1.00	0.12	22,22,22,22	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.

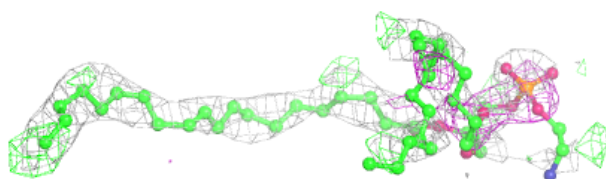
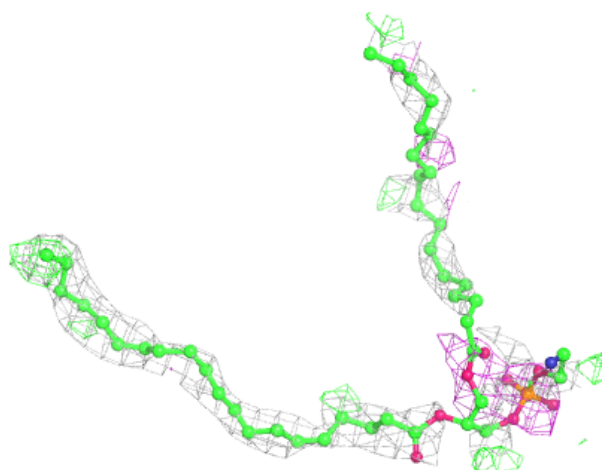
Electron density around CHD W 1059:

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



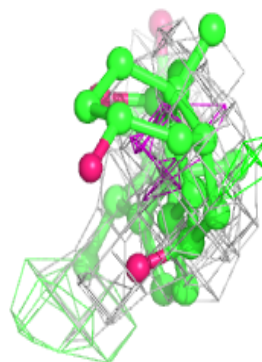
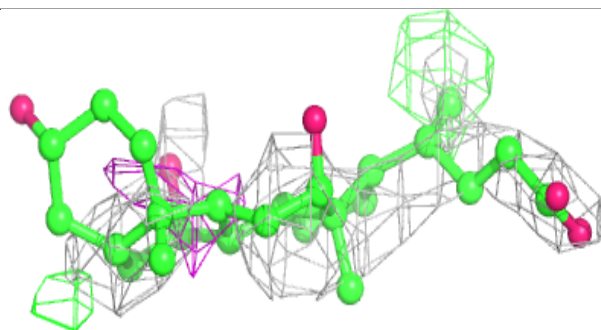
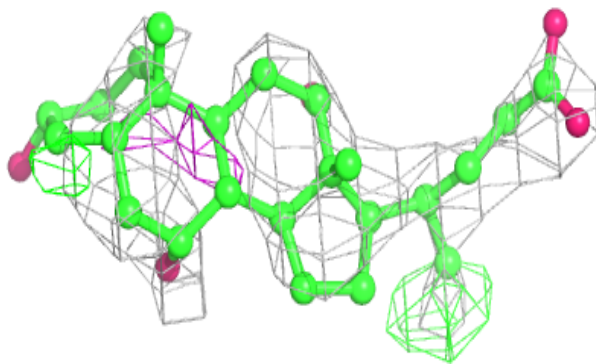
Electron density around PEK T 263:

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



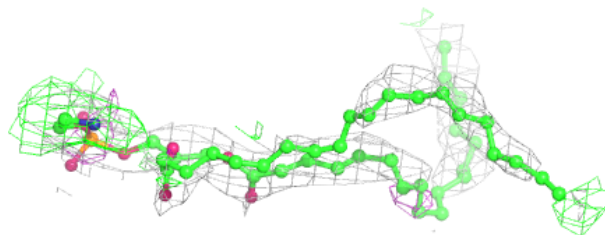
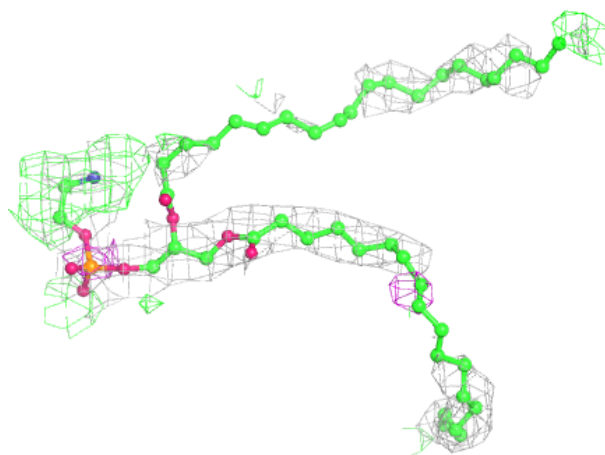
Electron density around CHD J 60:

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



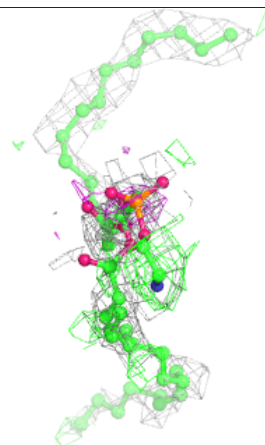
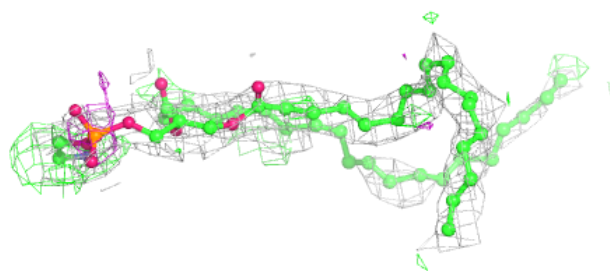
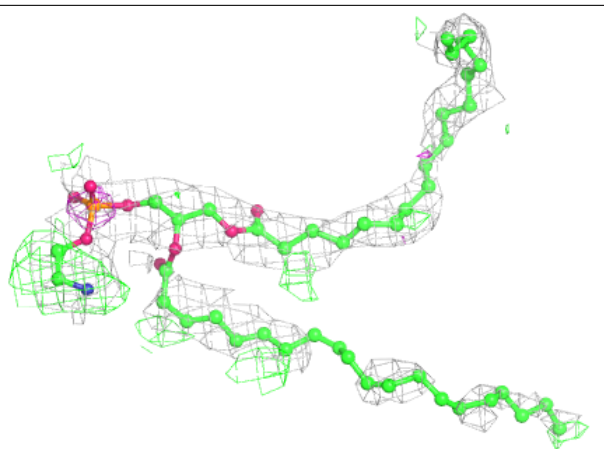
Electron density around PEK P 1265:

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



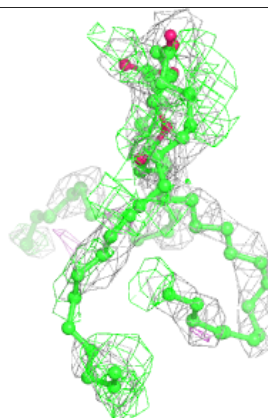
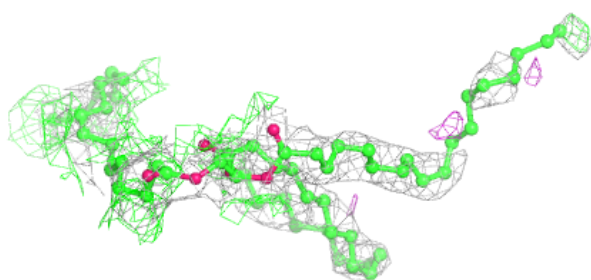
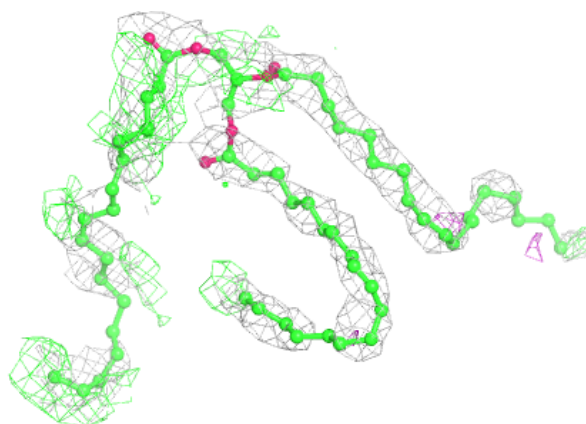
Electron density around PEK C 265:

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

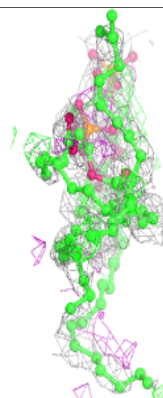
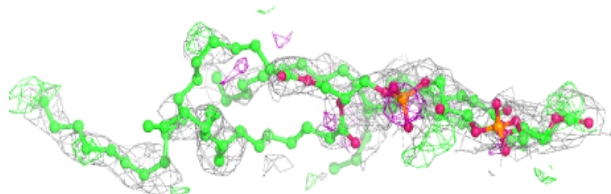
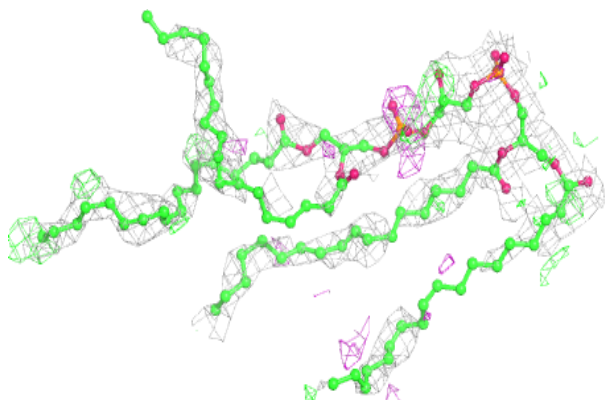


Electron density around TGL N 1523:

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

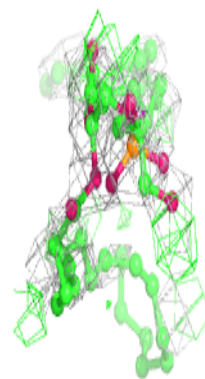
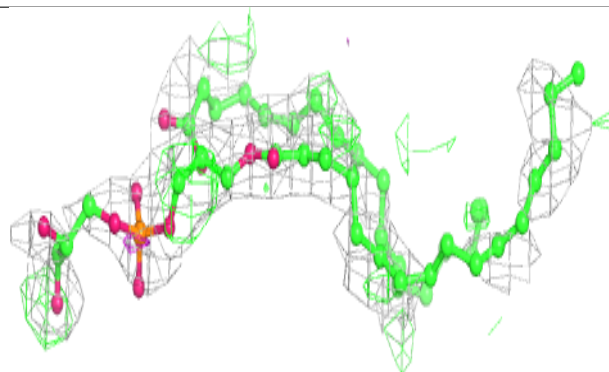
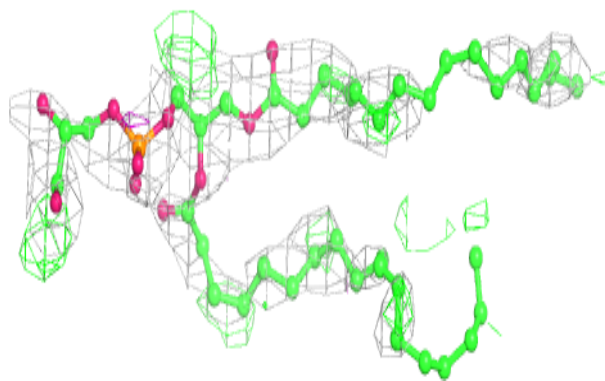
**Electron density around CDL T 1269:**

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

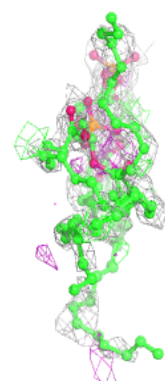
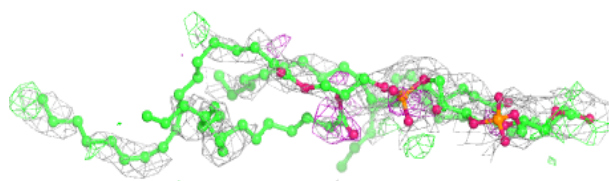
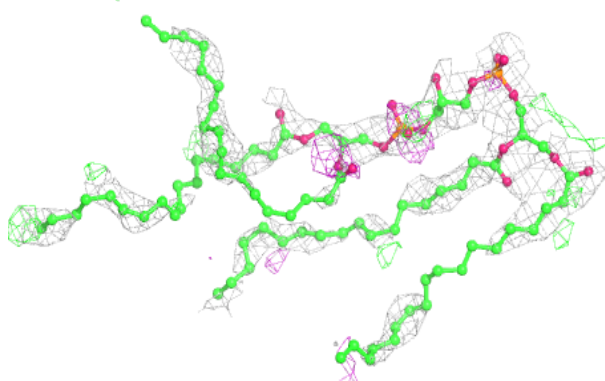


Electron density around PGV P 1268:

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

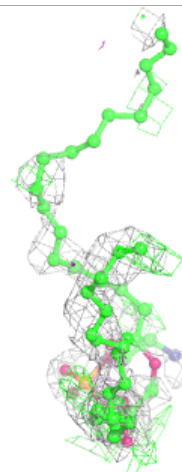
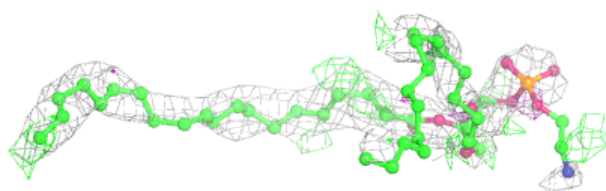
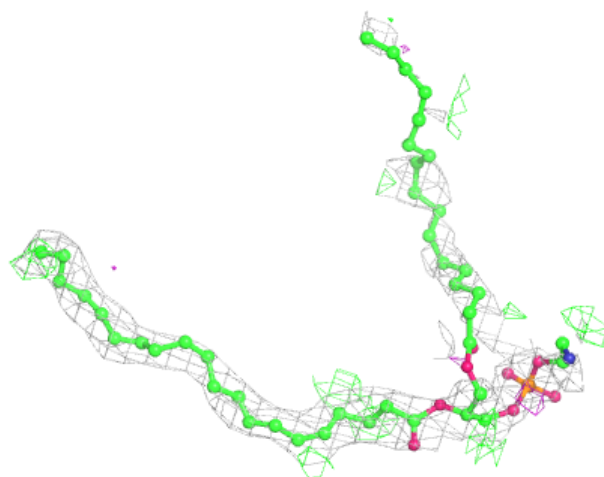
**Electron density around CDL G 269:**

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



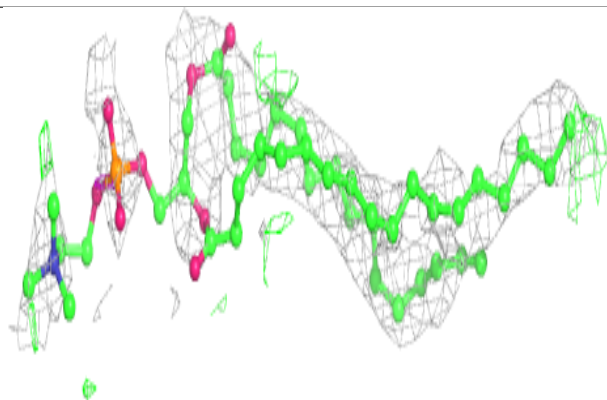
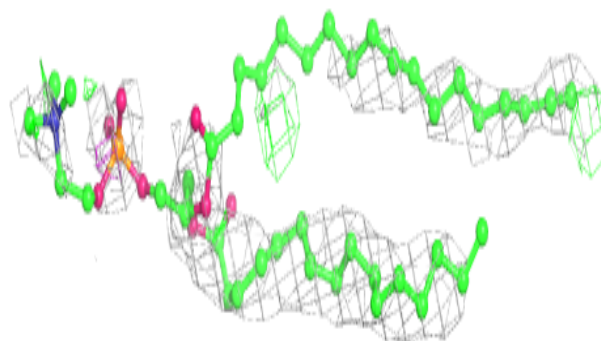
Electron density around PEK G 1263:

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and green (positive)

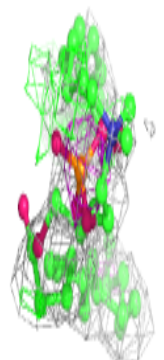
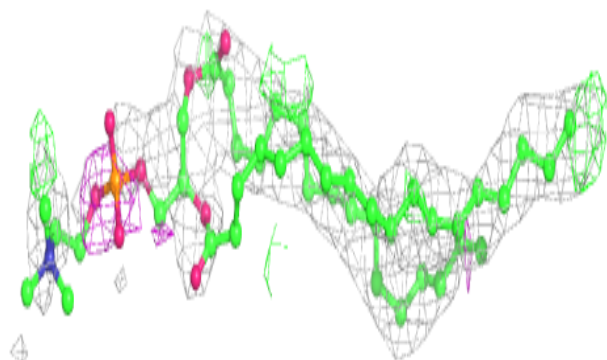
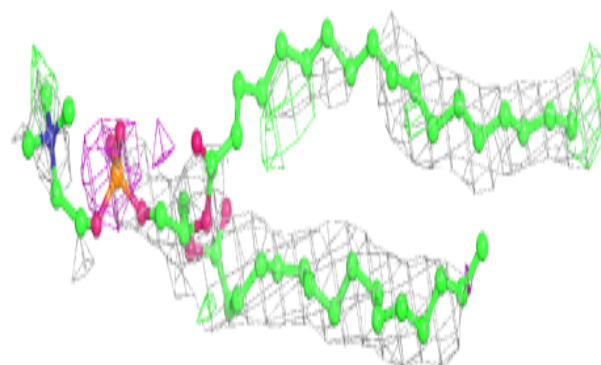


Electron density around PSC B 229:

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

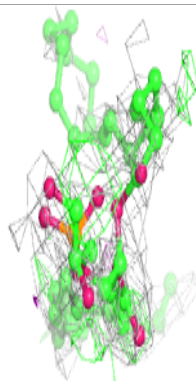
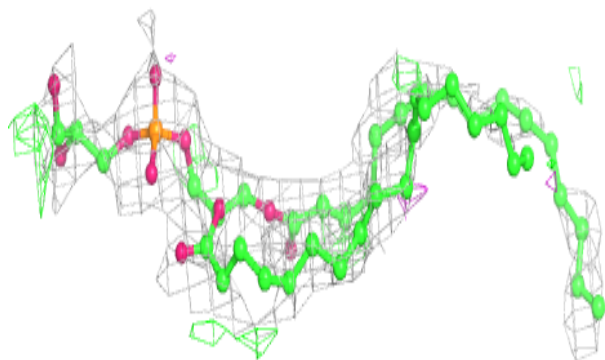
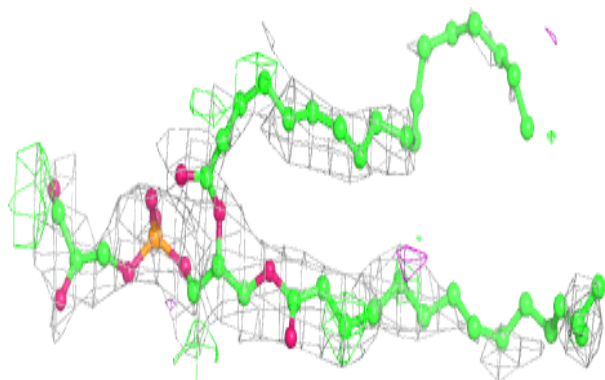
**Electron density around PSC O 1229:**

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and green (positive)

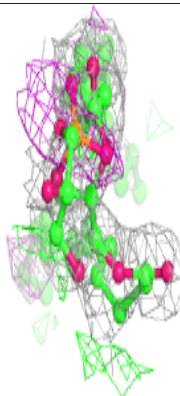
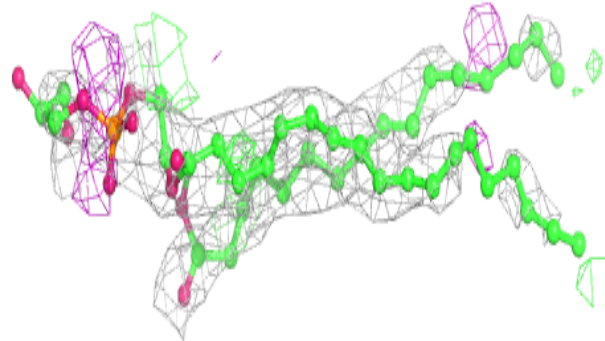
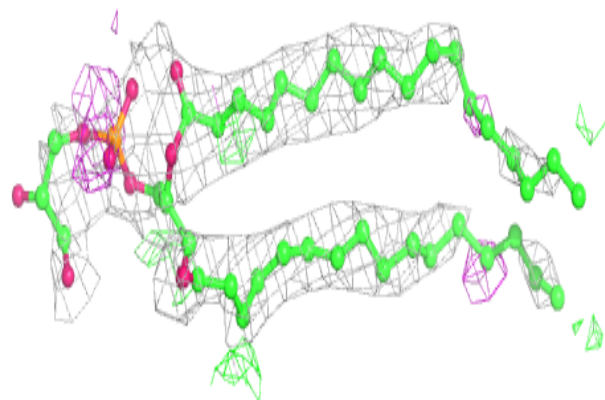


Electron density around PGV C 268:

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

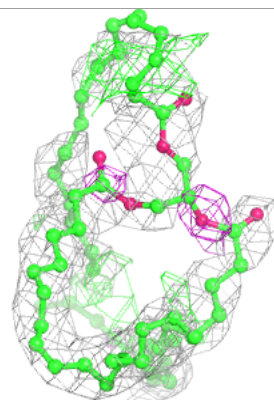
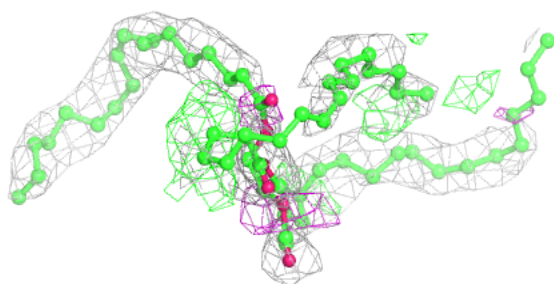
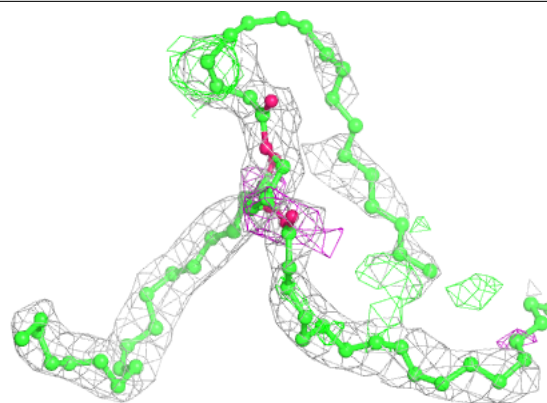
**Electron density around PGV N 1524:**

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

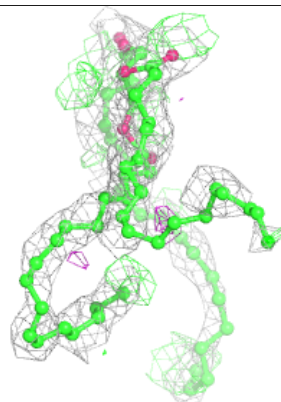
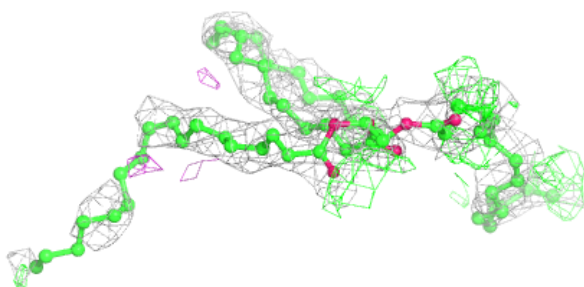
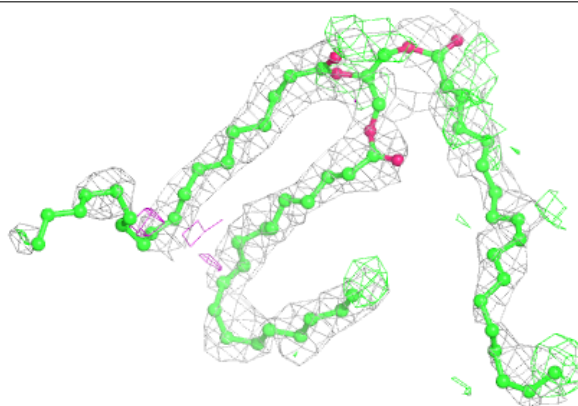


Electron density around TGL N 1522:

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

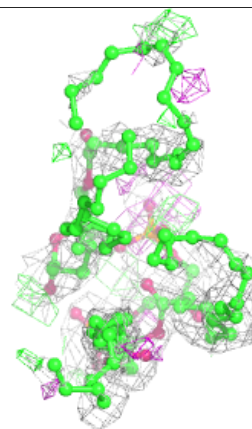
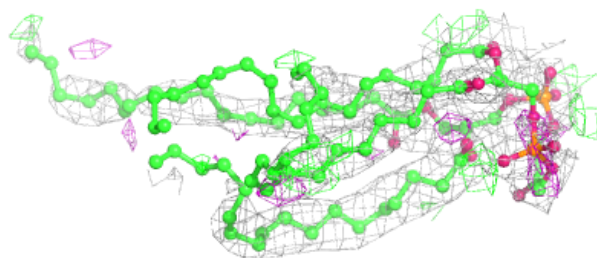
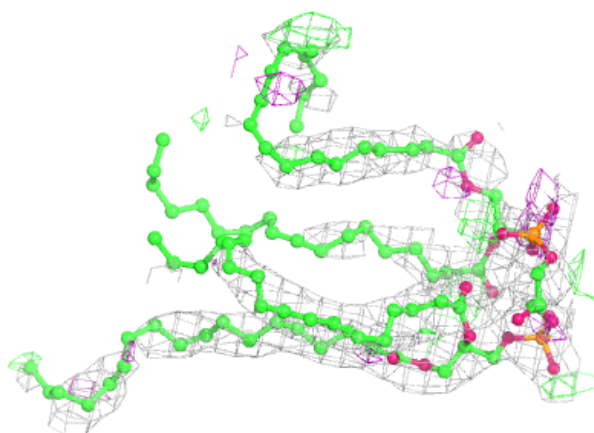
**Electron density around TGL D 523:**

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

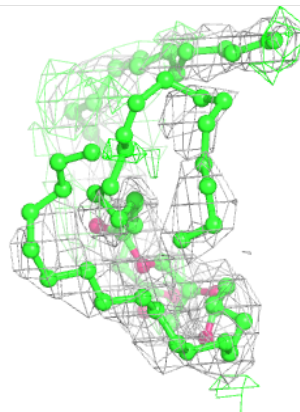
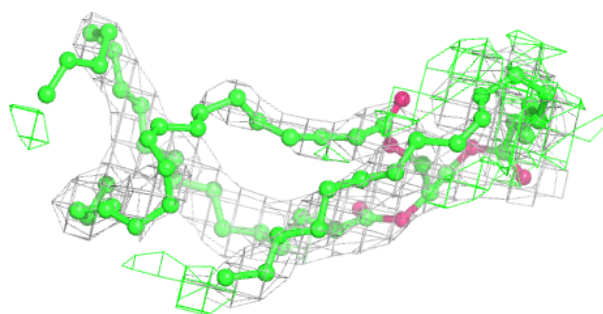
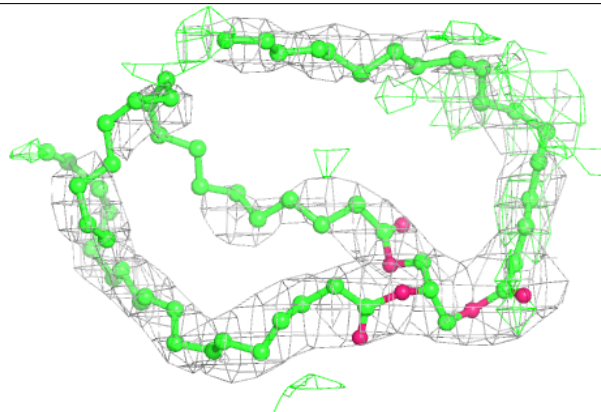


Electron density around CDL P 1270:

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and green (positive)

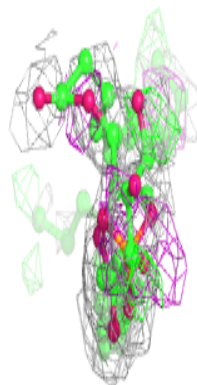
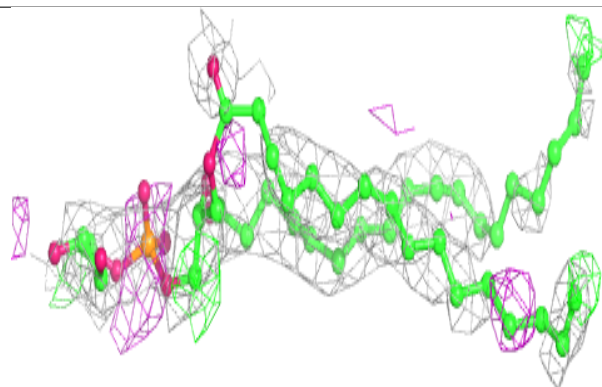
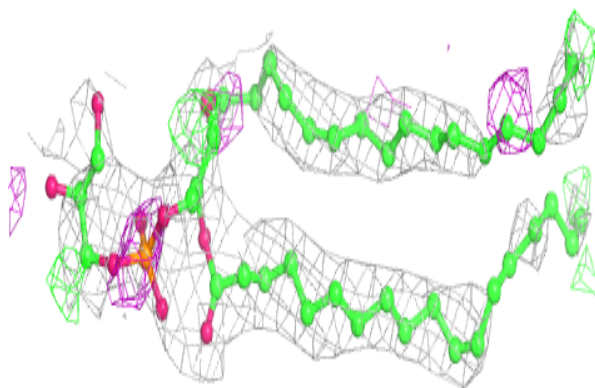
**Electron density around TGL N 1521:**

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

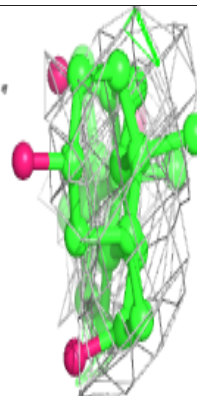
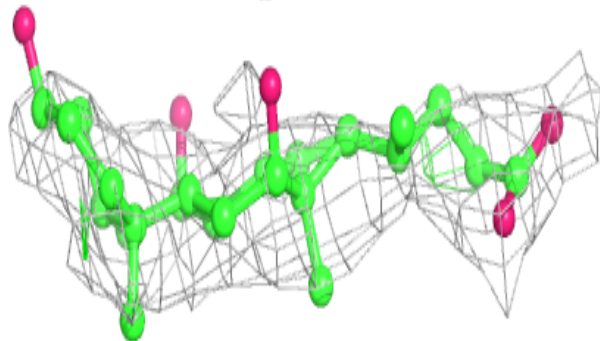
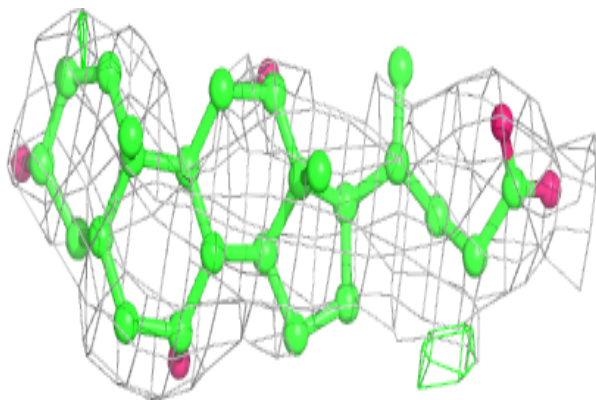


Electron density around PGV A 524:

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

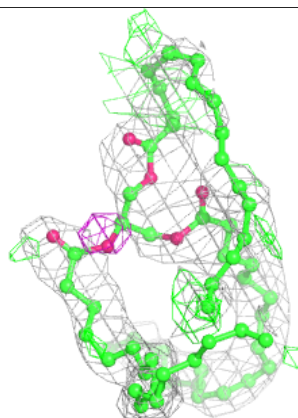
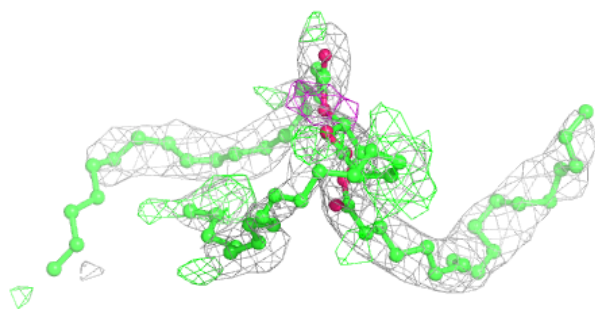
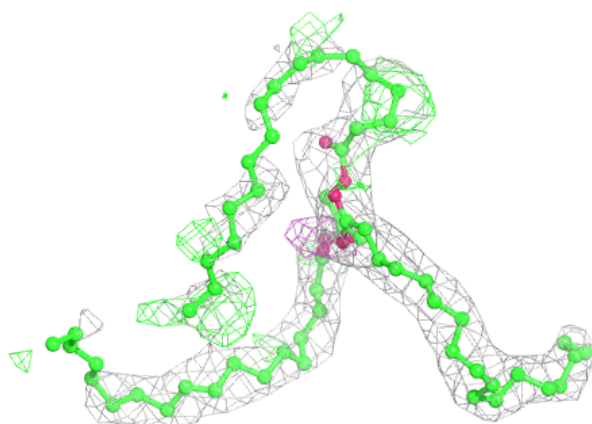
**Electron density around CHD P 1271:**

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



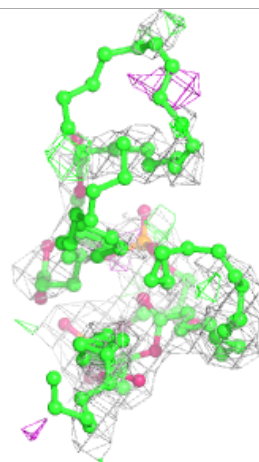
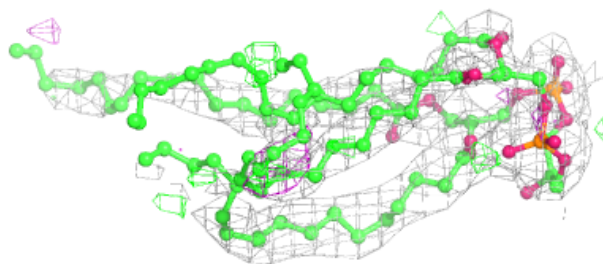
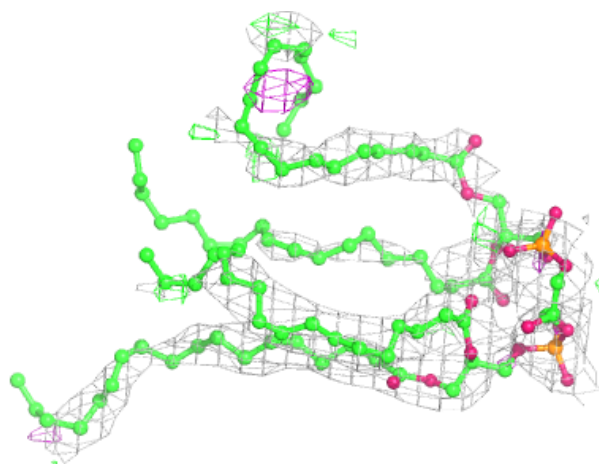
Electron density around TGL L 522:

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



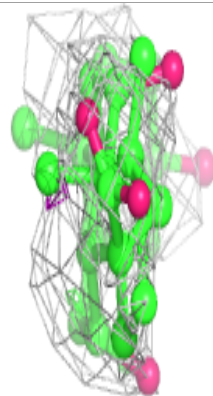
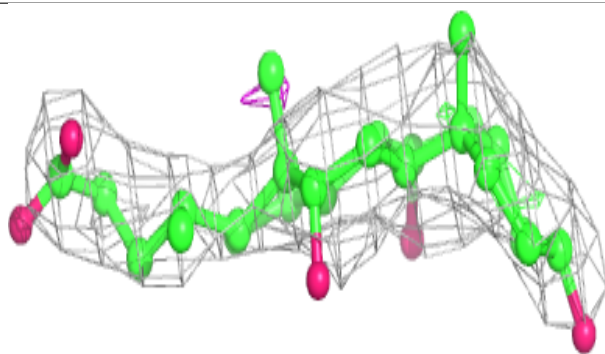
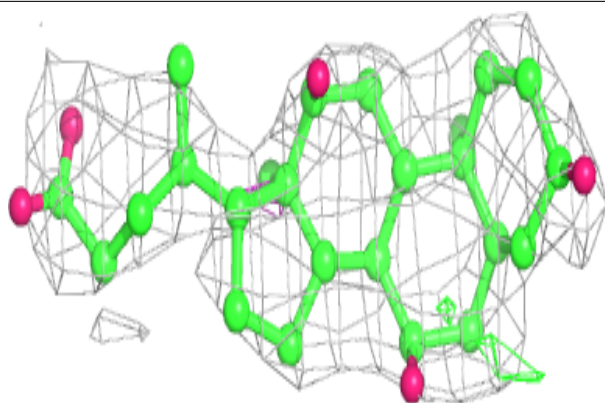
Electron density around CDL C 270:

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

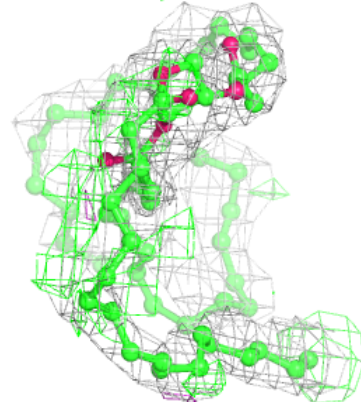
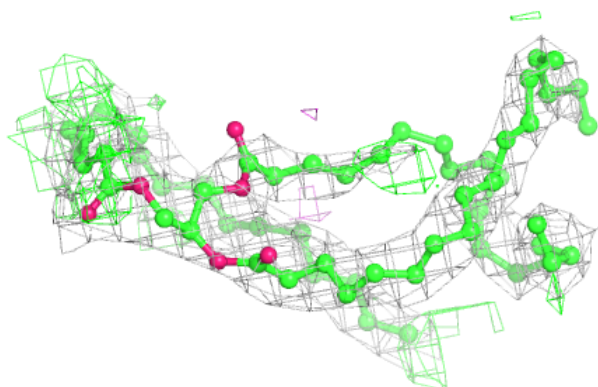
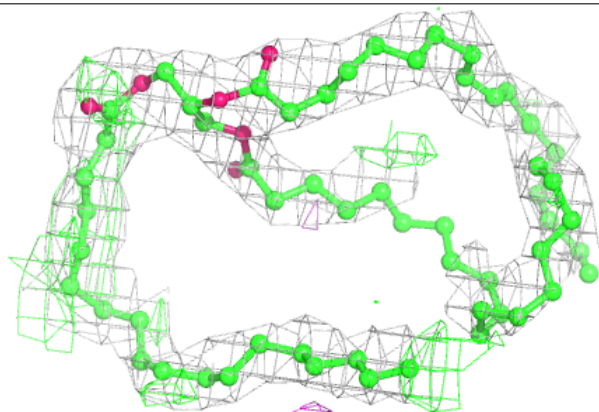


Electron density around CHD C 271:

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

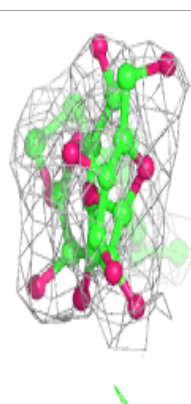
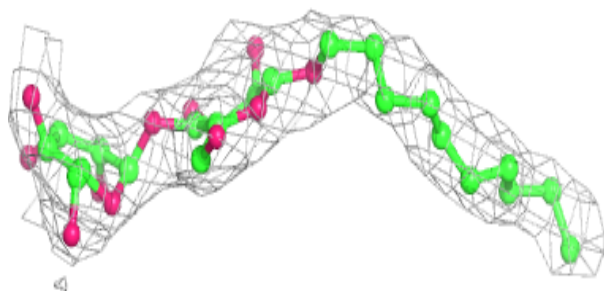
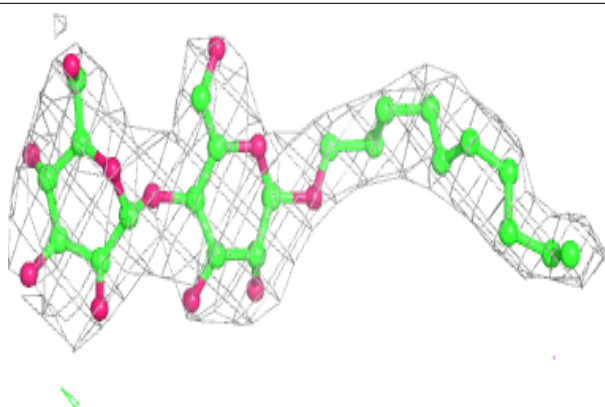
**Electron density around TGL A 521:**

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

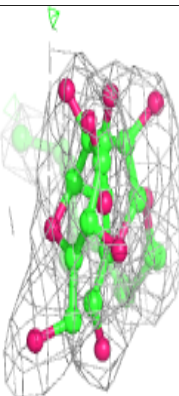
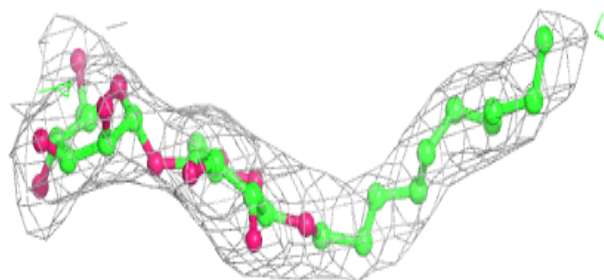
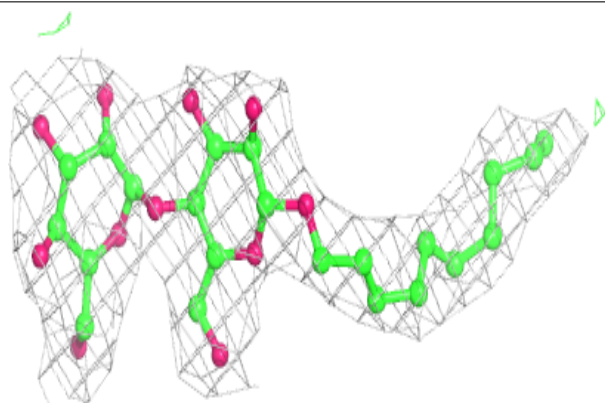


Electron density around DMU Z 1526:

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

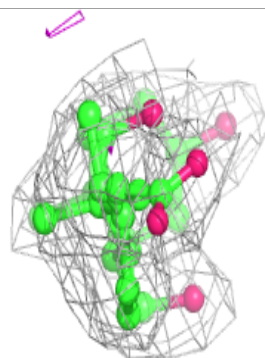
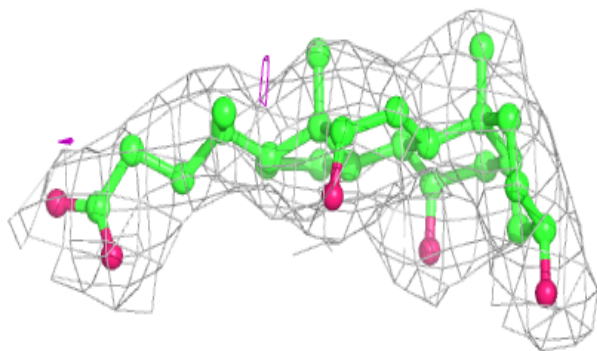
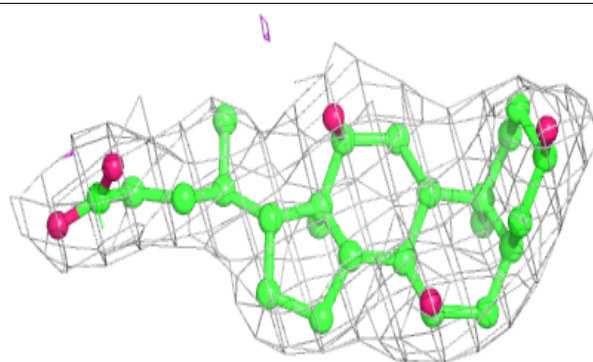
**Electron density around DMU M 526:**

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

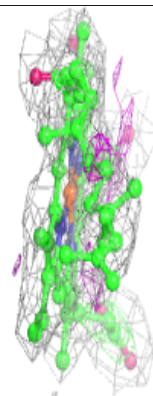
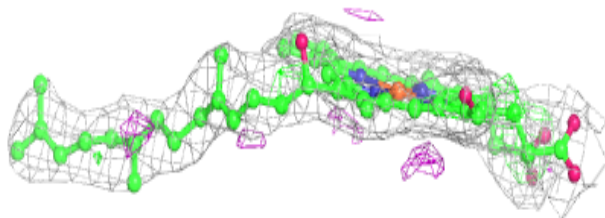
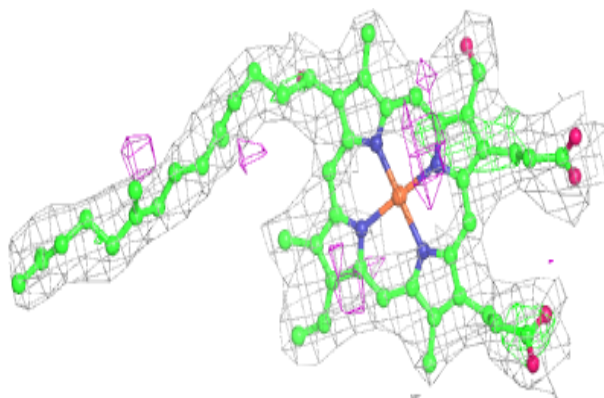


Electron density around CHD P 1525:

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

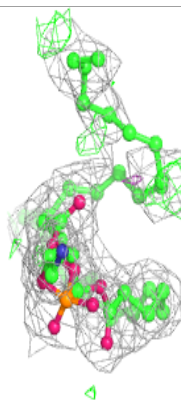
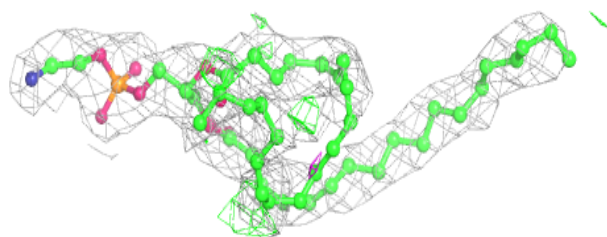
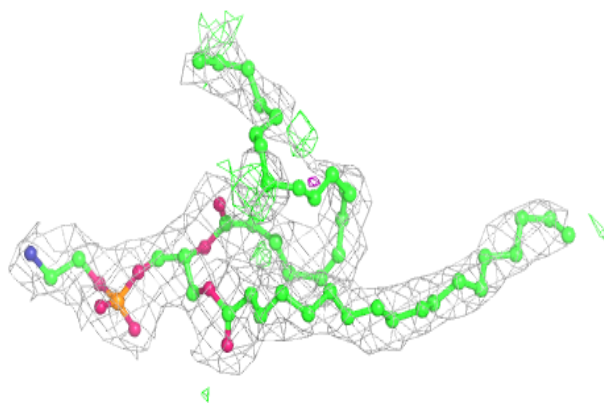
**Electron density around HEA N 515:**

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

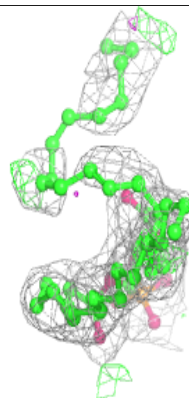
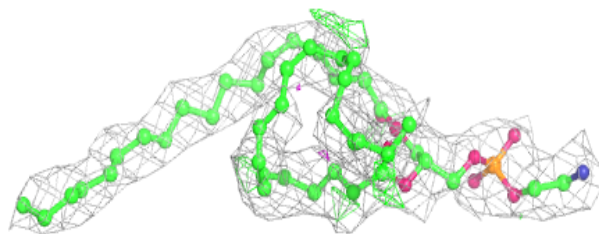
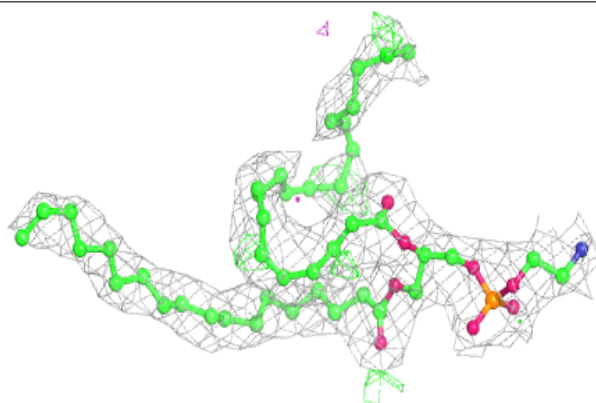


Electron density around PEK C 264:

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

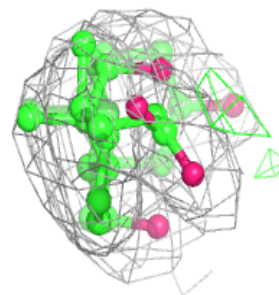
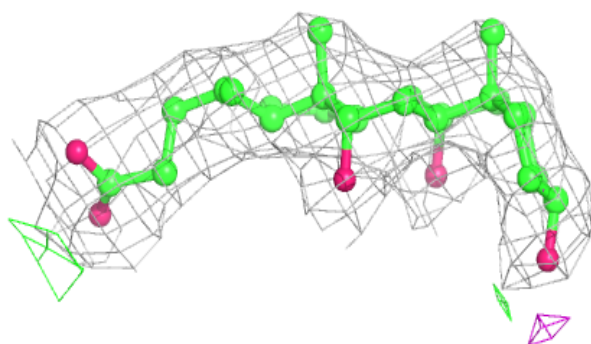
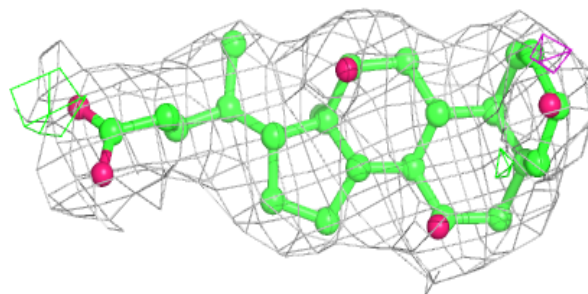
**Electron density around PEK P 1264:**

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

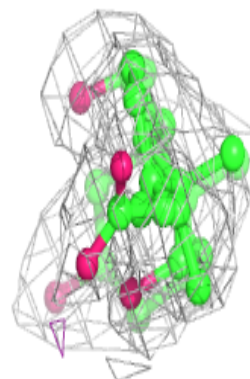
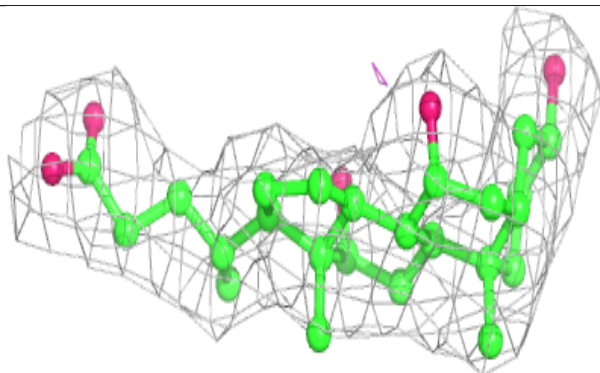
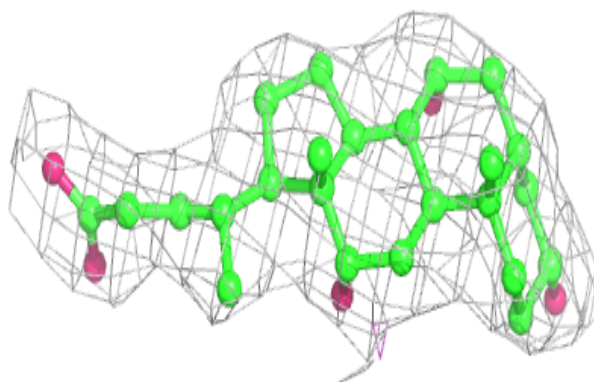


Electron density around CHD B 1085:

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

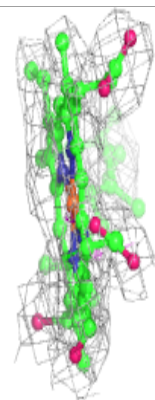
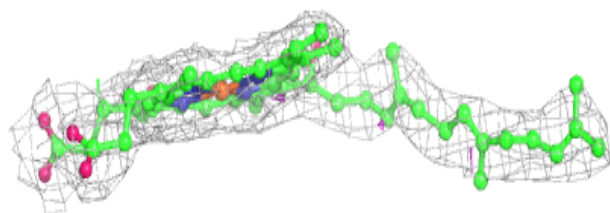
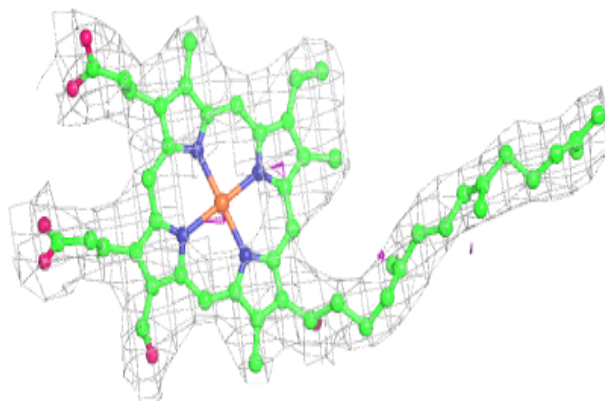
**Electron density around CHD C 525:**

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

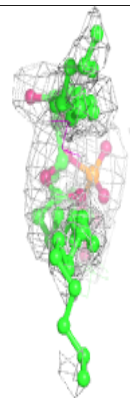
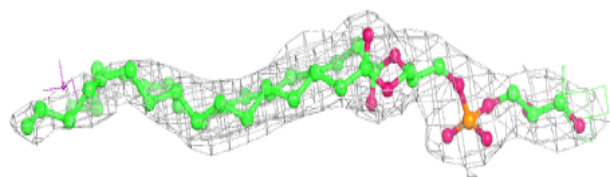
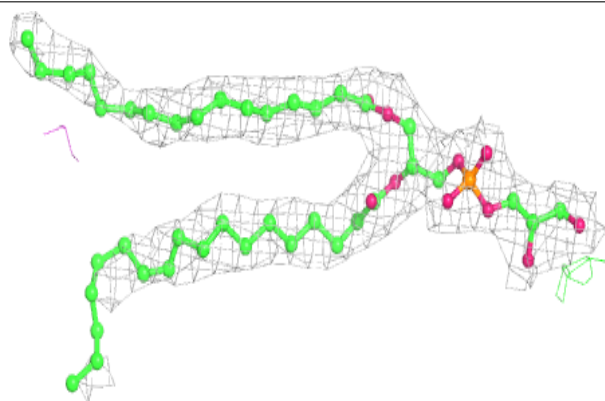


Electron density around HEA A 515:

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

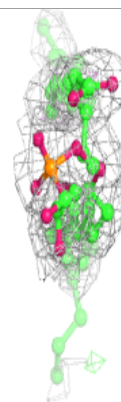
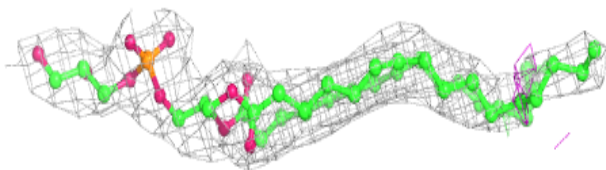
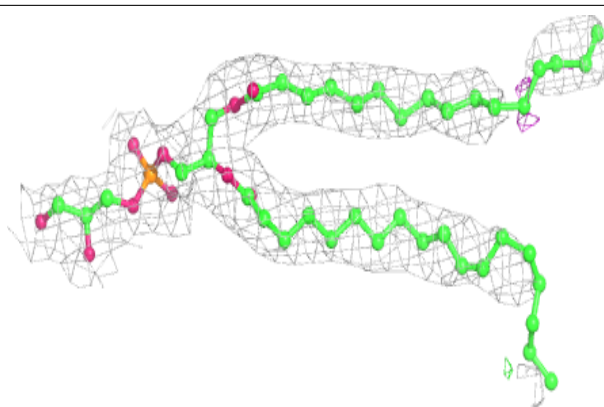
**Electron density around PGV P 1267:**

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

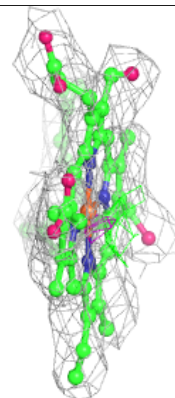
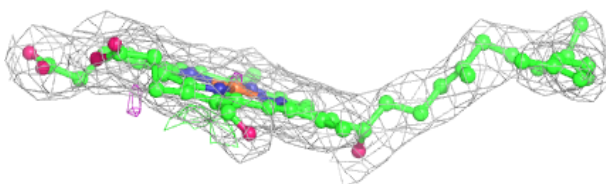
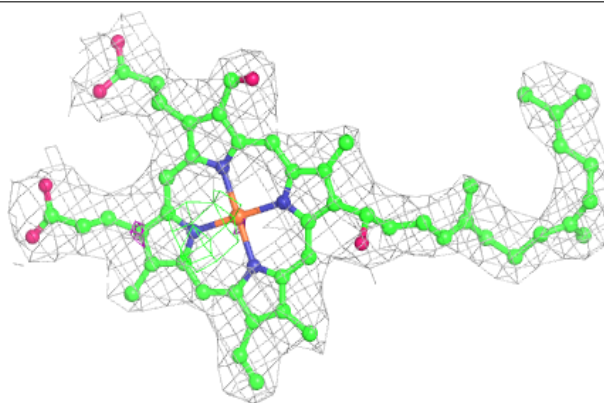


Electron density around PGV C 267:

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

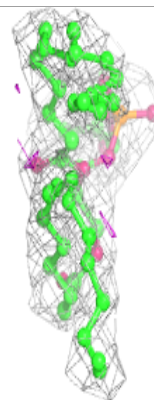
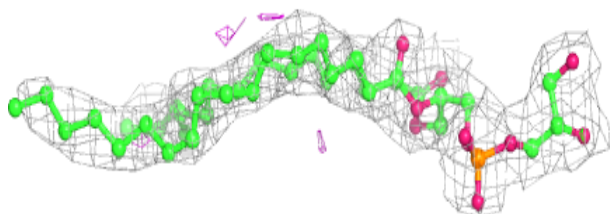
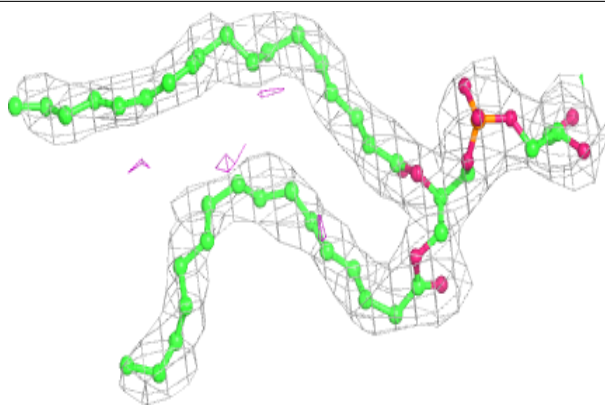
**Electron density around HEA N 516:**

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

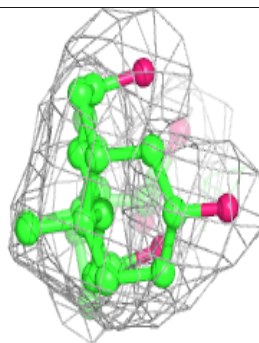
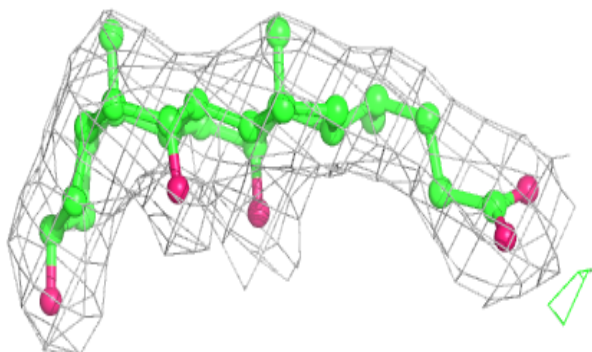
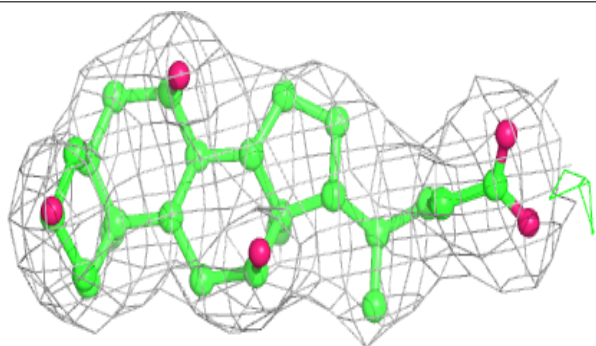


Electron density around PGV N 1266:

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

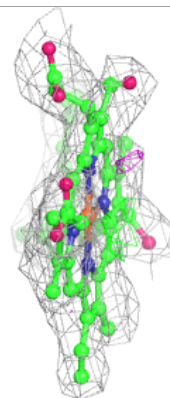
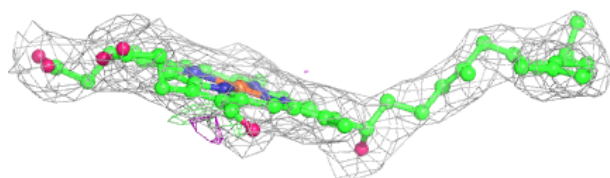
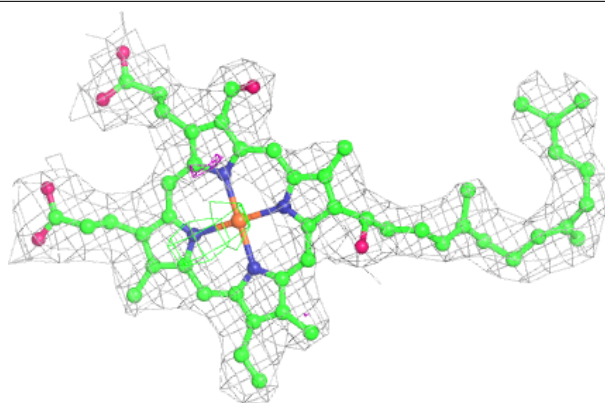
**Electron density around CHD G 229:**

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

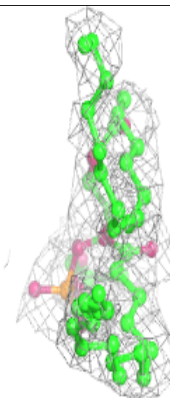
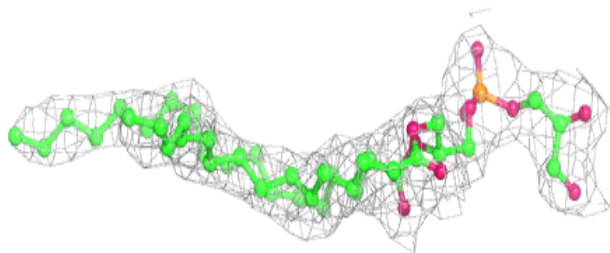
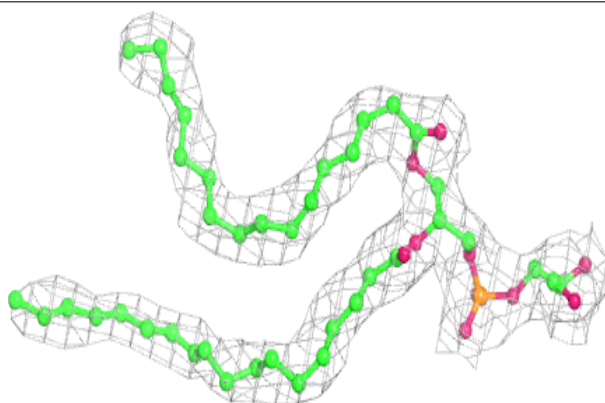


Electron density around HEA A 516:

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

**Electron density around 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)



6.5 Other polymers

There are no such residues in this entry.