



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:30 PM EDT

PDB ID : 3ASO / pdb_00003aso
Title : Bovine heart cytochrome C oxidase in the fully oxidized state measured at 0.9 angstrom wavelength
Authors : Suga, M.; Yano, N.; Muramoto, K.; Shinzawa-Itoh, K.; Maeda, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-12-17
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

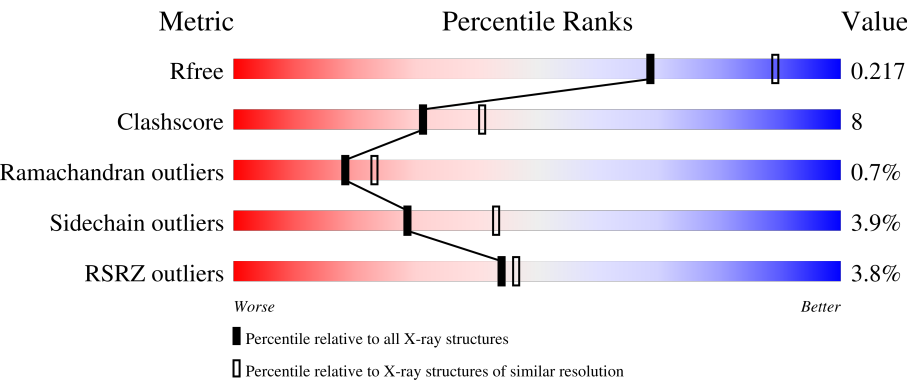
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	514	84%14%•
1	N	514	83%16%•
2	B	227	2% 80%18%•
2	O	227	4% 78%19%•

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Mol	Chain	Length	Quality of chain
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CDL	T	1269	-	-	X	-
27	DMU	M	526	X	-	-	-
27	DMU	Z	1526	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			

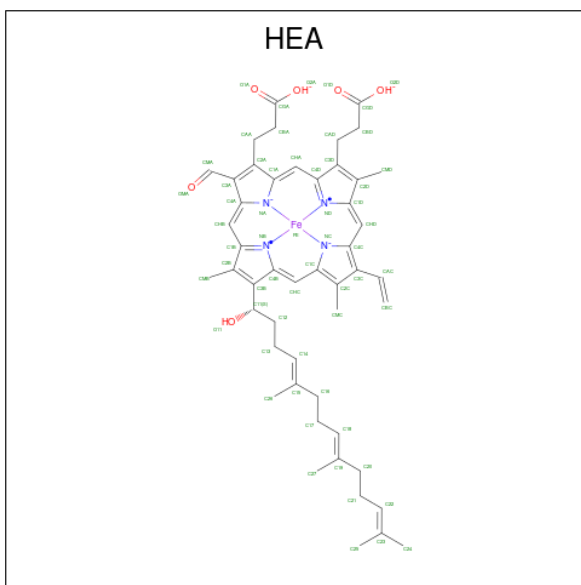
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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 (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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 (CCD ID: 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		

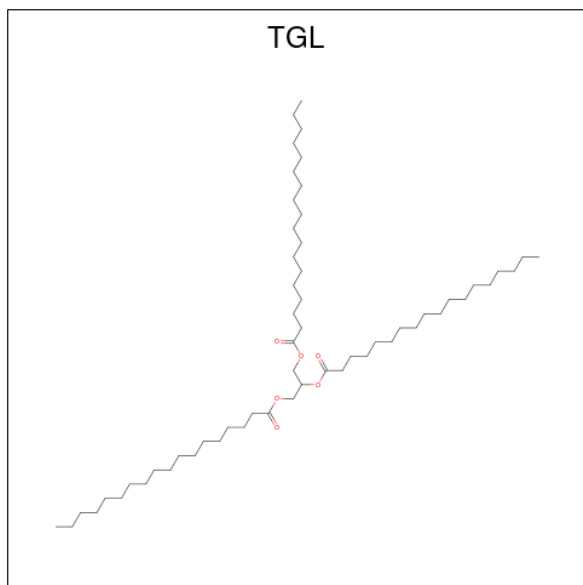
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: NA) (formula: Na).

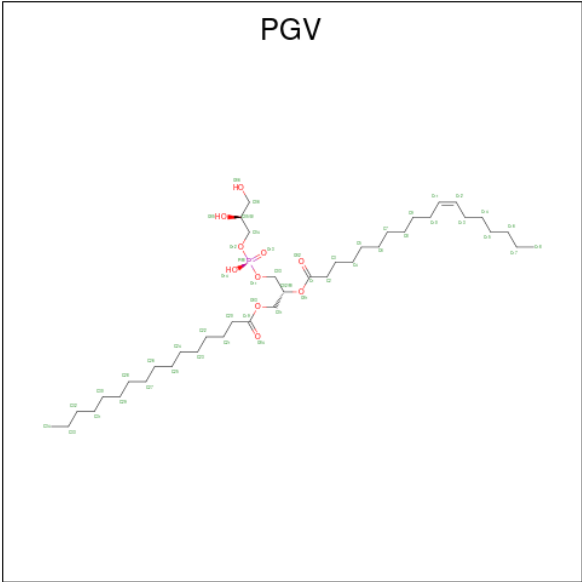
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



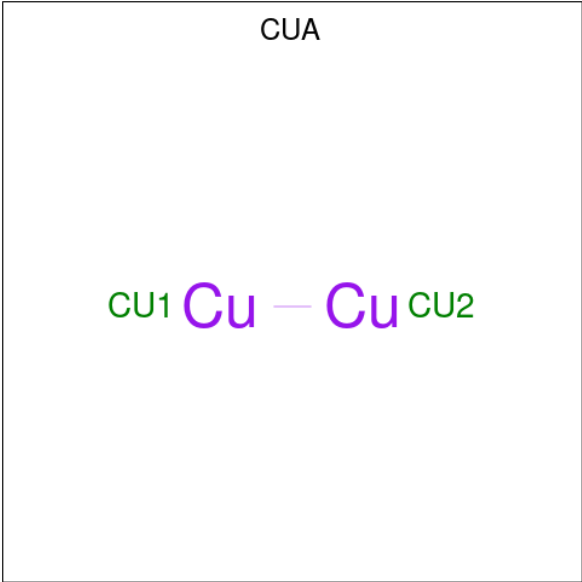
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	D	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



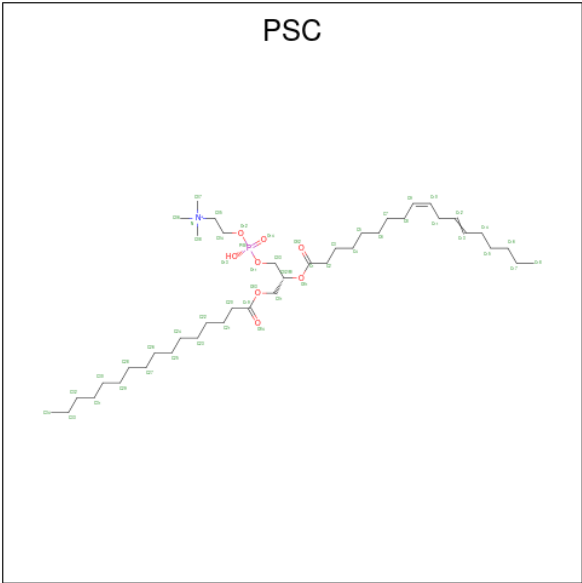
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

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



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

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



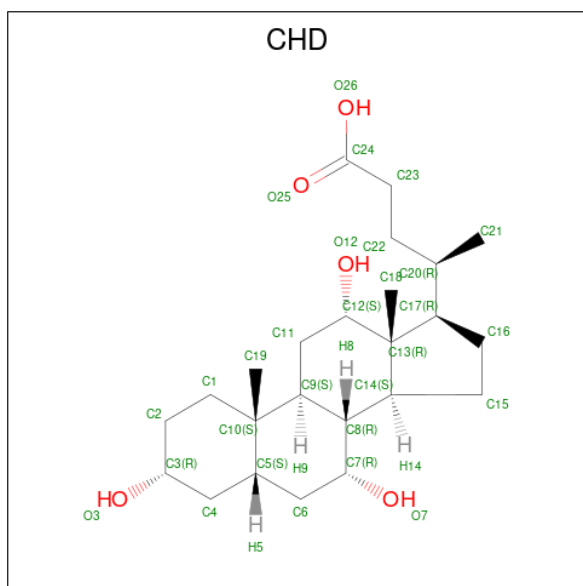
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

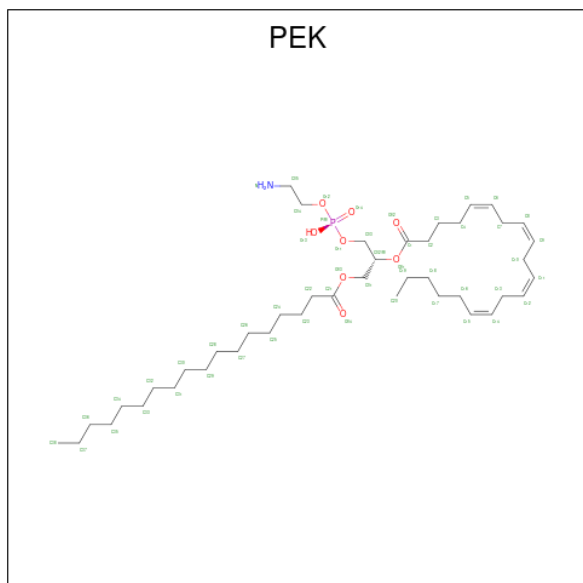


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

- Molecule 23 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

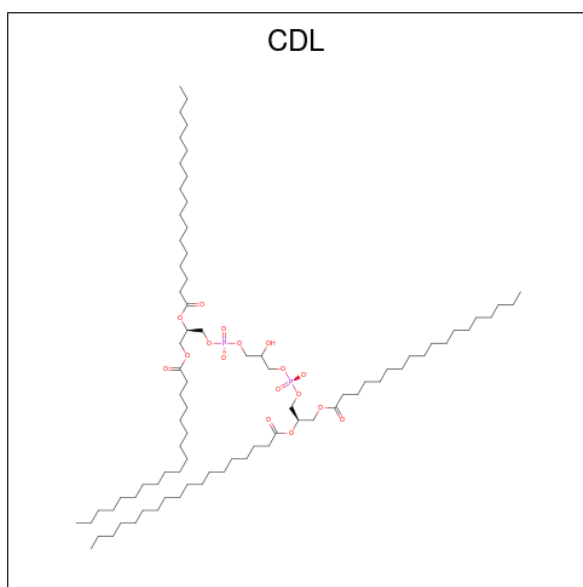
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total X 1 1	0	0
23	P	1	Total X 1 1	0	0

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



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

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).

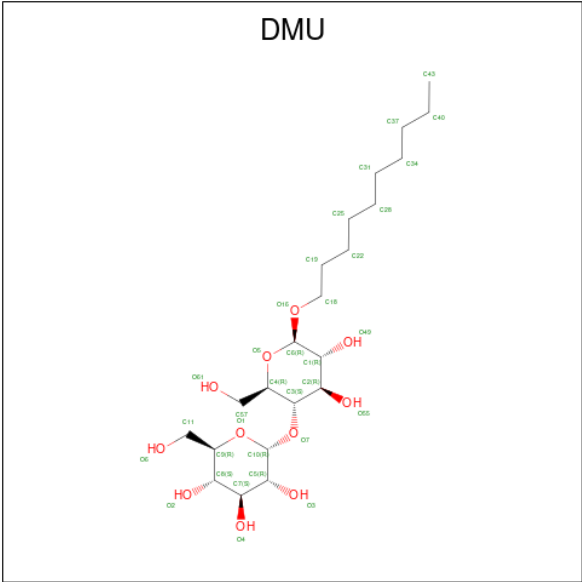


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: 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	215	Total	O	0	0
			215	215		
28	B	124	Total	O	0	0
			124	124		
28	C	109	Total	O	0	0
			109	109		
28	D	102	Total	O	0	0
			102	102		
28	E	67	Total	O	0	0
			67	67		
28	F	81	Total	O	0	0
			81	81		
28	G	48	Total	O	0	0
			48	48		
28	H	48	Total	O	0	0
			48	48		
28	I	31	Total	O	0	0
			31	31		
28	J	16	Total	O	0	0
			16	16		

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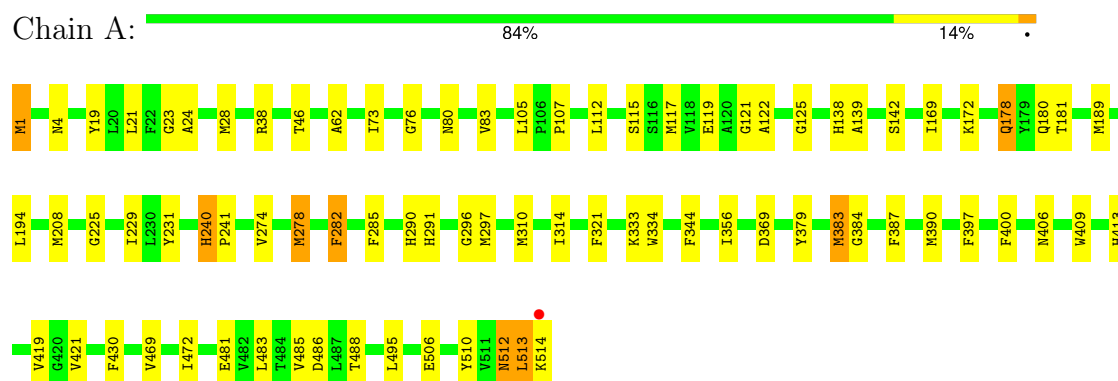
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	26	Total 26	O 26	0	0
28	L	28	Total 28	O 28	0	0
28	M	20	Total 20	O 20	0	0
28	N	220	Total 220	O 220	0	0
28	O	114	Total 114	O 114	0	0
28	P	109	Total 109	O 109	0	0
28	Q	60	Total 60	O 60	0	0
28	R	45	Total 45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

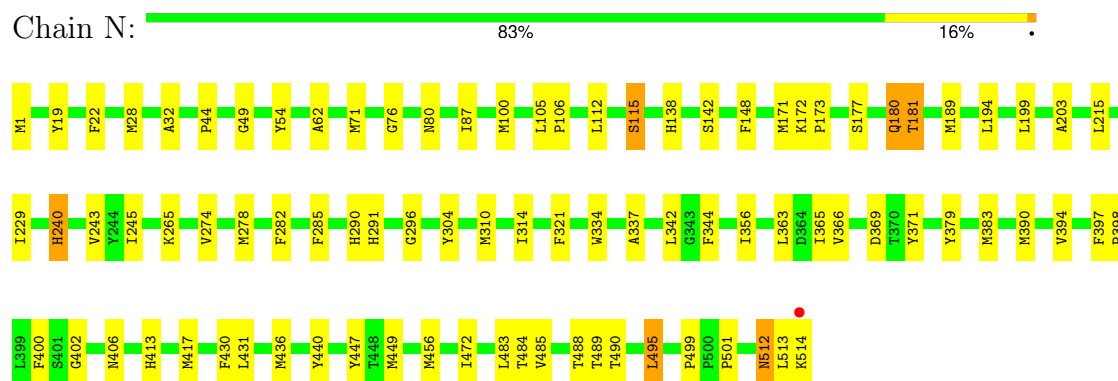
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

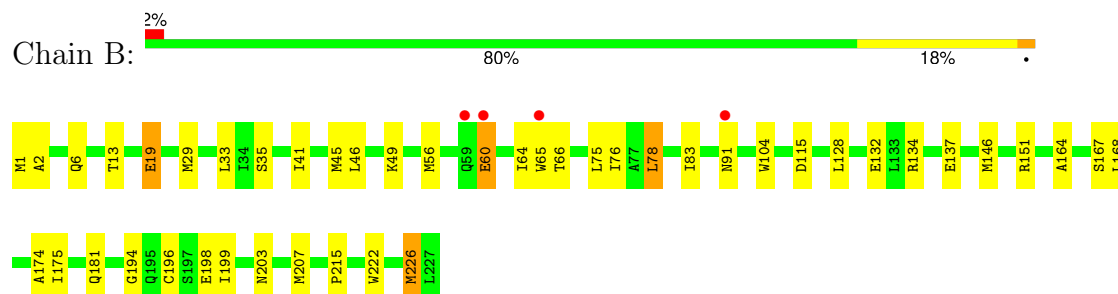
• Molecule 1: Cytochrome c oxidase subunit 1



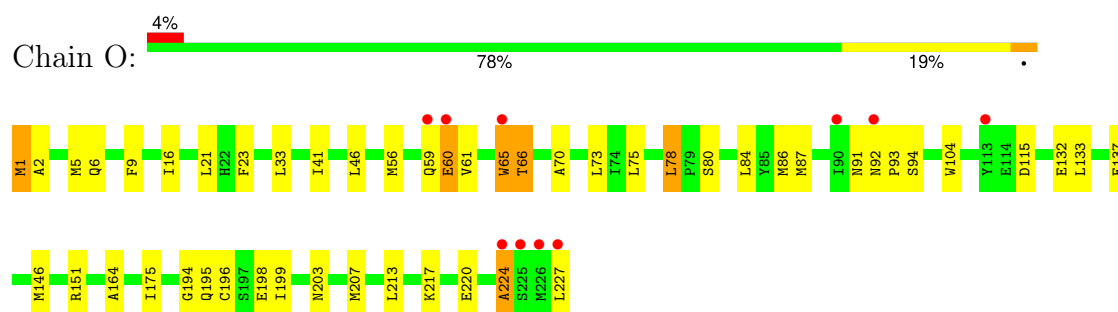
• Molecule 1: Cytochrome c oxidase subunit 1



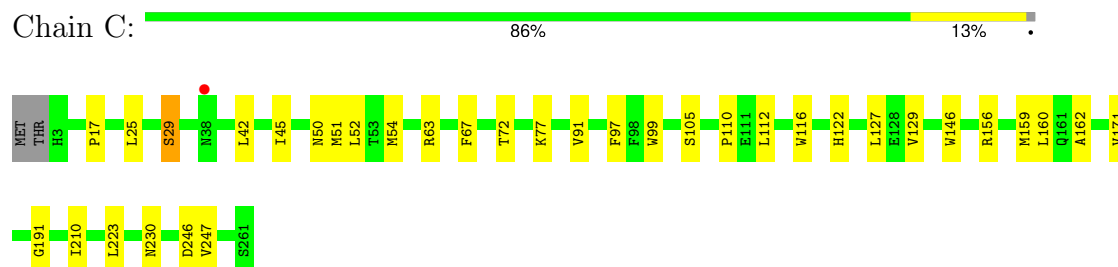
• Molecule 2: Cytochrome c oxidase subunit 2



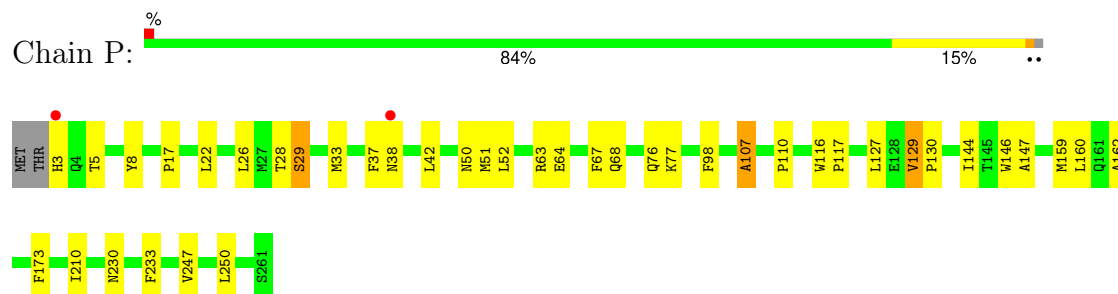
• Molecule 2: Cytochrome c oxidase subunit 2



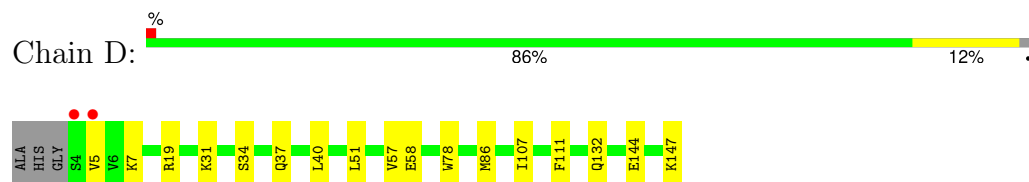
• Molecule 3: Cytochrome c oxidase subunit 3



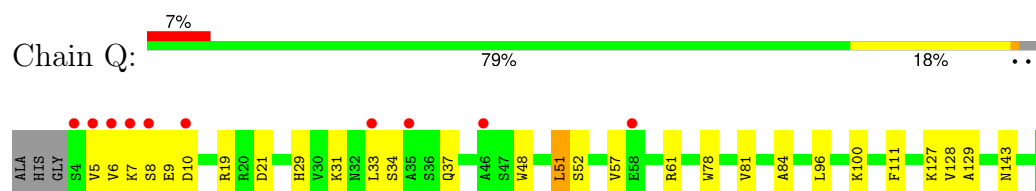
• Molecule 3: Cytochrome c oxidase subunit 3



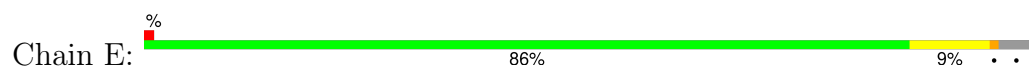
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



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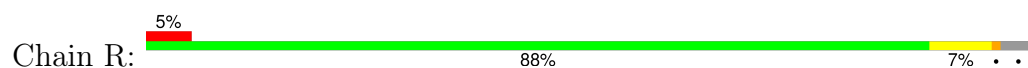


• Molecule 5: Cytochrome c oxidase subunit 5A

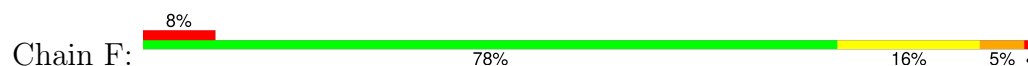




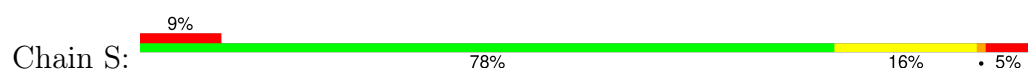
- Molecule 5: Cytochrome c oxidase subunit 5A



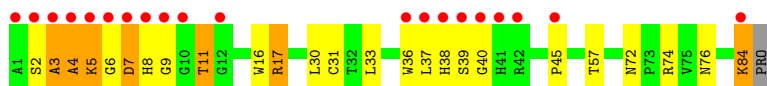
- Molecule 6: Cytochrome c oxidase subunit 5B



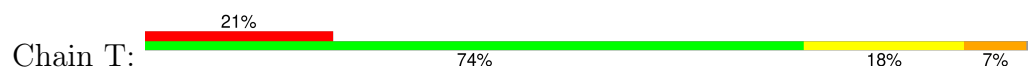
- Molecule 6: Cytochrome c oxidase subunit 5B



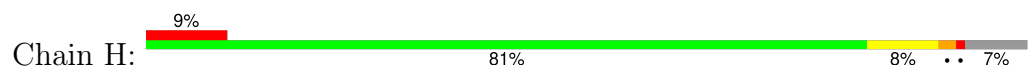
- Molecule 7: Cytochrome c oxidase subunit 6A2



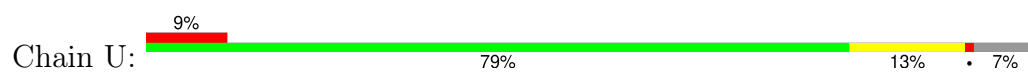
- Molecule 7: Cytochrome c oxidase subunit 6A2



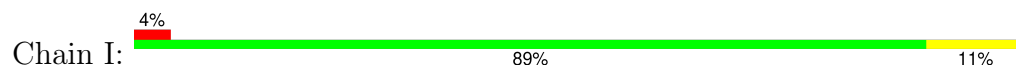
- Molecule 8: Cytochrome c oxidase subunit 6B1



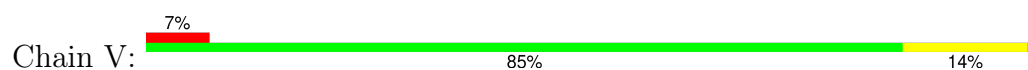
- Molecule 8: Cytochrome c oxidase subunit 6B1



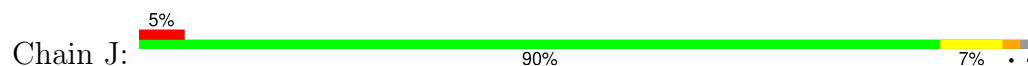
- Molecule 9: Cytochrome c oxidase subunit 6C



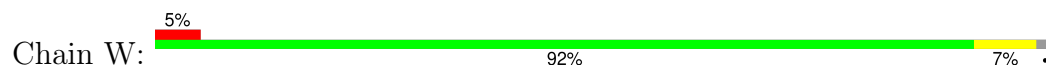
- Molecule 9: Cytochrome c oxidase subunit 6C



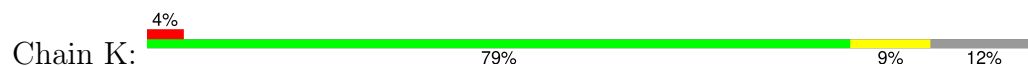
- Molecule 10: Cytochrome c oxidase subunit 7A1



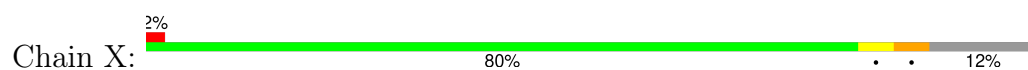
- Molecule 10: Cytochrome c oxidase subunit 7A1



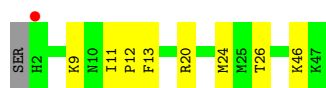
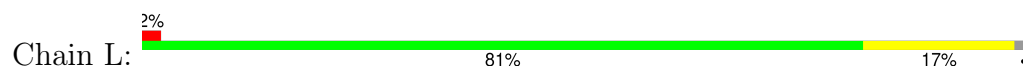
- Molecule 11: Cytochrome c oxidase subunit 7B



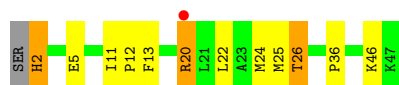
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



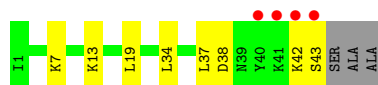
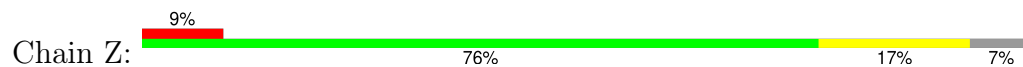
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.87Å 204.11Å 177.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 15.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.30) 99.3 (15.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.169 , 0.205 0.185 , 0.217	Depositor DCC
R_{free} test set	14532 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32377	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.37	13/4156 (0.3%)	1.15	14/5678 (0.2%)
1	N	1.26	3/4156 (0.1%)	1.10	11/5678 (0.2%)
2	B	1.32	2/1860 (0.1%)	1.11	2/2534 (0.1%)
2	O	1.18	2/1860 (0.1%)	1.14	2/2534 (0.1%)
3	C	1.21	2/2197 (0.1%)	1.07	6/3005 (0.2%)
3	P	1.22	2/2197 (0.1%)	1.05	3/3005 (0.1%)
4	D	1.20	1/1229 (0.1%)	1.10	1/1658 (0.1%)
4	Q	1.04	1/1229 (0.1%)	1.08	1/1658 (0.1%)
5	E	1.20	0/871	1.08	2/1182 (0.2%)
5	R	1.10	0/871	1.20	4/1182 (0.3%)
6	F	1.28	4/765 (0.5%)	1.21	8/1038 (0.8%)
6	S	1.30	1/765 (0.1%)	1.37	11/1038 (1.1%)
7	G	1.26	1/690 (0.1%)	1.11	1/937 (0.1%)
7	T	1.17	1/690 (0.1%)	1.15	0/937
8	H	1.15	1/682 (0.1%)	1.10	1/921 (0.1%)
8	U	1.05	1/682 (0.1%)	1.13	2/921 (0.2%)
9	I	1.12	0/605	1.07	0/802
9	V	1.05	0/605	1.19	0/802
10	J	1.14	0/471	1.05	0/636
10	W	1.06	0/471	1.01	0/636
11	K	1.25	1/398 (0.3%)	1.23	2/546 (0.4%)
11	X	1.08	1/398 (0.3%)	1.09	0/546
12	L	1.20	1/393 (0.3%)	1.06	0/526
12	Y	1.17	0/393	1.02	0/526
13	M	1.17	0/345	1.12	0/470
13	Z	1.02	0/345	1.08	0/470
All	All	1.22	38/29324 (0.1%)	1.12	71/39866 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S	0	1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	198	GLU	C-O	10.30	1.35	1.23
2	B	198	GLU	C-O	9.85	1.35	1.23
1	A	139	ALA	CA-CB	9.62	1.69	1.53
3	C	129	VAL	CA-CB	9.40	1.60	1.53
2	B	174	ALA	CA-CB	8.01	1.64	1.53
6	S	54	ASN	CB-CG	-6.86	1.34	1.52
1	A	383	MET	CA-C	6.83	1.58	1.52
1	A	333	LYS	CA-C	6.76	1.61	1.52
2	O	66	THR	CA-C	6.57	1.59	1.52
4	Q	5	VAL	CA-CB	6.54	1.61	1.53
8	H	8	ILE	CA-CB	6.41	1.63	1.54
1	A	282	PHE	CA-C	6.22	1.60	1.52
11	X	41	ASN	C-O	-6.00	1.21	1.23
8	U	8	ILE	CA-CB	5.93	1.62	1.54
1	A	421	VAL	CA-CB	5.92	1.62	1.54
1	A	485	VAL	C-O	-5.89	1.17	1.24
1	A	83	VAL	CA-CB	5.89	1.57	1.54
3	P	107	ALA	CA-CB	5.88	1.59	1.53
6	F	7	PRO	C-O	5.81	1.30	1.23
1	N	203	ALA	CA-C	5.78	1.60	1.52
6	F	92	VAL	CA-CB	5.67	1.61	1.54
1	A	122	ALA	CA-CB	5.60	1.60	1.53
11	K	41	ASN	C-O	-5.59	1.21	1.23
3	C	171	VAL	CA-CB	5.55	1.61	1.54
4	D	57	VAL	CA-CB	5.48	1.61	1.54
1	N	106	PRO	CA-C	5.48	1.57	1.52
1	N	49	GLY	N-CA	5.47	1.50	1.45
7	G	5	LYS	CA-C	5.35	1.56	1.53
6	F	68	THR	CA-CB	5.31	1.60	1.53
1	A	24	ALA	CA-CB	5.20	1.61	1.53
1	A	83	VAL	C-O	-5.19	1.20	1.24
1	A	419	VAL	CA-CB	5.17	1.60	1.54
1	A	278	MET	CA-C	5.14	1.59	1.52
7	T	75	VAL	CA-CB	5.11	1.61	1.54
3	P	147	ALA	CA-CB	5.07	1.61	1.53
6	F	45	ASP	CA-C	5.04	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	9	LYS	C-O	-5.01	1.17	1.24
1	A	469	VAL	CA-C	5.01	1.58	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	53	THR	CA-C-N	9.14	134.21	120.31
6	S	53	THR	C-N-CA	9.14	134.21	120.31
1	N	240	HIS	N-CA-CB	8.41	118.38	110.39
5	R	100	THR	CA-C-N	8.04	128.12	119.28
5	R	100	THR	C-N-CA	8.04	128.12	119.28
2	O	220	GLU	N-CA-C	7.95	119.95	111.28
1	A	169	ILE	CB-CA-C	-7.77	101.49	112.22
1	A	240	HIS	N-CA-CB	7.49	119.25	110.42
1	N	199	LEU	CA-C-N	-7.43	112.06	119.56
1	N	199	LEU	C-N-CA	-7.43	112.06	119.56
6	S	94	HIS	N-CA-C	7.29	126.32	110.80
1	N	105	LEU	CA-C-N	-6.96	113.22	120.38
1	N	105	LEU	C-N-CA	-6.96	113.22	120.38
1	A	314	ILE	CA-C-N	-6.81	111.79	119.28
1	A	314	ILE	C-N-CA	-6.81	111.79	119.28
1	A	119	GLU	CB-CA-C	-6.75	108.77	116.54
1	A	125	GLY	N-CA-C	-6.60	104.50	112.48
6	S	93	PRO	CA-C-N	6.58	134.11	121.54
6	S	93	PRO	C-N-CA	6.58	134.11	121.54
7	G	57	THR	N-CA-C	-6.56	105.43	113.50
6	F	94	HIS	N-CA-C	6.51	124.67	110.80
6	S	54	ASN	N-CA-C	6.40	119.24	111.82
6	S	54	ASN	CB-CA-C	-6.30	98.57	110.67
4	Q	29	HIS	N-CA-C	6.24	119.73	111.75
4	D	5	VAL	N-CA-C	6.20	117.40	107.73
3	P	129	VAL	N-CA-CB	6.17	114.39	110.50
6	F	35	ALA	CA-C-N	-6.14	113.64	119.85
6	F	35	ALA	C-N-CA	-6.14	113.64	119.85
6	F	93	PRO	CA-C-N	6.13	133.25	121.54
6	F	93	PRO	C-N-CA	6.13	133.25	121.54
11	K	6	ALA	CA-C-N	6.12	126.44	119.83
11	K	6	ALA	C-N-CA	6.12	126.44	119.83
1	N	181	THR	CA-C-N	-6.02	114.07	120.03
1	N	181	THR	C-N-CA	-6.02	114.07	120.03
3	C	45	ILE	N-CA-C	-6.01	104.44	111.00
5	R	76	GLY	CA-C-N	6.01	126.53	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	76	GLY	C-N-CA	6.01	126.53	120.04
1	A	117	MET	CG-SD-CE	-5.88	87.96	100.90
6	S	94	HIS	CA-C-N	5.75	132.53	121.54
6	S	94	HIS	C-N-CA	5.75	132.53	121.54
6	F	2	SER	N-CA-C	5.72	117.77	109.07
5	E	84	TYR	N-CA-C	-5.66	105.02	111.14
8	H	54	GLU	N-CA-C	5.65	117.89	111.11
1	A	397	PHE	CA-C-N	-5.61	113.24	119.19
1	A	397	PHE	C-N-CA	-5.61	113.24	119.19
3	C	72	THR	CA-C-N	-5.59	113.13	119.28
3	C	72	THR	C-N-CA	-5.59	113.13	119.28
6	S	64	GLU	CA-C-N	-5.57	116.59	126.45
6	S	64	GLU	C-N-CA	-5.57	116.59	126.45
2	B	65	TRP	N-CA-C	5.50	119.69	113.15
1	N	314	ILE	CA-C-N	-5.48	113.39	119.19
1	N	314	ILE	C-N-CA	-5.48	113.39	119.19
3	C	29	SER	CB-CA-C	-5.44	102.11	110.81
1	A	105	LEU	CA-C-N	-5.38	114.84	120.38
1	A	105	LEU	C-N-CA	-5.38	114.84	120.38
5	E	81	ILE	N-CA-C	5.33	115.54	110.53
3	C	129	VAL	CA-C-N	-5.31	113.44	119.28
3	C	129	VAL	C-N-CA	-5.31	113.44	119.28
1	A	19	TYR	N-CA-C	5.26	116.70	111.07
1	N	240	HIS	CA-CB-CG	-5.26	108.54	113.80
1	N	512	ASN	CB-CA-C	-5.23	99.92	109.54
2	O	65	TRP	N-CA-C	5.18	118.74	112.93
1	A	240	HIS	CA-CB-CG	-5.17	108.63	113.80
8	U	49	ASP	N-CA-C	5.16	117.38	109.07
2	B	64	ILE	N-CA-C	-5.16	105.68	110.53
6	F	64	GLU	CA-C-N	-5.14	117.35	126.45
6	F	64	GLU	C-N-CA	-5.14	117.35	126.45
3	P	29	SER	CB-CA-C	-5.14	101.94	110.68
3	P	233	PHE	N-CA-C	5.10	116.84	111.28
1	A	512	ASN	CB-CA-C	-5.05	100.25	109.54
8	U	9	LYS	N-CA-C	5.04	112.91	108.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	55	0
1	N	4027	0	4001	78	0
2	B	1824	0	1833	29	0
2	O	1824	0	1833	34	0
3	C	2110	0	2027	26	0
3	P	2110	0	2027	35	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	19	0
5	E	852	0	845	3	0
5	R	852	0	845	5	0
6	F	748	0	728	9	0
6	S	748	0	728	28	0
7	G	675	0	644	28	0
7	T	675	0	644	28	0
8	H	662	0	623	9	0
8	U	662	0	623	5	0
9	I	601	0	613	8	0
9	V	601	0	613	9	0
10	J	460	0	459	6	0
10	W	460	0	459	4	0
11	K	384	0	366	1	0
11	X	384	0	366	6	0
12	L	380	0	380	10	0
12	Y	380	0	380	11	0
13	M	335	0	352	7	0
13	Z	335	0	352	3	0
14	A	120	0	108	3	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	6	0
18	L	63	0	110	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	126	0	220	22	0
18	Q	63	0	110	4	0
19	A	102	0	152	10	0
19	C	102	0	152	8	0
19	N	102	0	152	11	0
19	P	102	0	152	6	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	52	0	80	13	0
21	O	52	0	80	17	0
22	B	29	0	39	1	0
22	C	58	0	78	3	0
22	G	29	0	39	0	0
22	J	29	0	38	3	0
22	P	58	0	78	1	0
22	W	29	0	38	3	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	5	0
24	G	106	0	154	12	0
24	T	159	0	231	21	0
25	C	100	0	156	16	0
25	G	100	0	156	18	0
25	P	100	0	156	13	0
25	T	100	0	156	22	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	41	0	0
27	Z	33	0	40	0	0
28	A	215	0	0	7	0
28	B	124	0	0	2	0
28	C	109	0	0	2	0
28	D	102	0	0	3	0
28	E	67	0	0	1	0
28	F	81	0	0	1	0
28	G	48	0	0	6	0
28	H	48	0	0	2	0
28	I	31	0	0	1	0
28	J	16	0	0	0	0
28	K	26	0	0	2	0
28	L	28	0	0	1	0
28	M	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	N	220	0	0	6	0
28	O	114	0	0	0	0
28	P	109	0	0	4	0
28	Q	60	0	0	3	0
28	R	45	0	0	0	0
28	S	77	0	0	4	0
28	T	39	0	0	2	0
28	U	45	0	0	1	0
28	V	21	0	0	2	0
28	W	16	0	0	0	0
28	X	17	0	0	2	0
28	Y	19	0	0	1	0
28	Z	14	0	0	1	0
All	All	32377	0	31229	508	0

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

All (508) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:84:LYS:HD2	7:T:84:LYS:N	1.80	0.94
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.47	0.94
6:S:52:ILE:O	6:S:94:HIS:CD2	2.22	0.93
7:T:84:LYS:H	7:T:84:LYS:CD	1.82	0.93
19:A:524:PGV:H311	13:M:19:LEU:HD23	1.51	0.92
24:C:265:PEK:C38	25:G:269:CDL:H273	1.99	0.92
6:S:53:THR:HA	6:S:94:HIS:CE1	2.03	0.92
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.32	0.91
28:N:4772:HOH:O	24:T:1264:PEK:H381	1.72	0.89
3:P:3:HIS:HB3	28:P:4285:HOH:O	1.72	0.89
7:G:5:LYS:HB2	24:G:1263:PEK:H362	1.55	0.89
4:D:31:LYS:HD2	28:D:4414:HOH:O	1.73	0.88
18:D:523:TGL:HC21	18:D:523:TGL:HG11	1.56	0.88
21:B:229:PSC:H072	9:I:10:ARG:HH21	1.39	0.87
21:O:1229:PSC:H142	21:O:1229:PSC:C34	2.04	0.87
7:G:84:LYS:HD2	7:G:84:LYS:N	1.90	0.86
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.56	0.86
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.12	0.84
19:C:268:PGV:H42	28:P:4823:HOH:O	1.75	0.84
7:G:72:ASN:H	7:G:76:ASN:HD22	1.23	0.84
6:S:52:ILE:C	6:S:94:HIS:CE1	2.56	0.84
21:B:229:PSC:C07	9:I:10:ARG:HH21	1.89	0.84
1:N:513:LEU:O	1:N:514:LYS:CB	2.21	0.84
25:T:1269:CDL:H541	25:T:1269:CDL:H231	1.59	0.84
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.44	0.83
6:S:53:THR:HA	6:S:94:HIS:HE1	1.42	0.83
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.43	0.83
1:A:1:FME:HG3	28:L:4907:HOH:O	1.78	0.82
18:N:1521:TGL:H241	18:N:1521:TGL:H201	1.62	0.81
1:A:310:MET:HE1	2:B:76:ILE:HG21	1.64	0.79
21:O:1229:PSC:H343	21:O:1229:PSC:C14	2.14	0.77
7:G:76:ASN:HD21	24:G:264:PEK:HN2	1.28	0.77
12:L:13:PHE:HA	18:L:522:TGL:HC31	1.67	0.77
2:O:59:GLN:O	2:O:59:GLN:HG3	1.83	0.77
24:G:264:PEK:H101	24:G:264:PEK:H161	1.68	0.76
19:P:1268:PGV:H062	28:P:4397:HOH:O	1.84	0.76
25:G:269:CDL:H231	25:G:269:CDL:C54	2.15	0.76
7:G:84:LYS:H	7:G:84:LYS:CD	1.89	0.76
7:T:31:CYS:SG	25:T:1269:CDL:H532	2.26	0.75
1:A:112:LEU:HG	28:A:2701:HOH:O	1.87	0.74
7:T:76:ASN:HD21	24:T:1264:PEK:HN2	1.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:LYS:HE2	28:E:4606:HOH:O	1.87	0.74
7:T:3:ALA:HB1	24:T:263:PEK:H382	1.68	0.73
18:Q:1523:TGL:HC21	18:Q:1523:TGL:HG11	1.71	0.72
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.71	0.72
1:A:472:ILE:HG21	18:L:522:TGL:HA92	1.72	0.72
19:C:267:PGV:H12	19:C:267:PGV:H161	1.72	0.72
4:D:34:SER:H	4:D:37:GLN:HE21	1.36	0.72
3:C:246:ASP:HB2	28:C:4249:HOH:O	1.89	0.71
25:C:270:CDL:PA1	25:C:270:CDL:HB22	2.30	0.71
1:N:310:MET:HE3	1:N:356:ILE:HG23	1.73	0.71
7:T:72:ASN:H	7:T:76:ASN:ND2	1.87	0.71
18:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.72	0.70
1:A:513:LEU:O	1:A:514:LYS:HB2	1.91	0.70
6:F:54:ASN:HB2	28:F:4662:HOH:O	1.90	0.69
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.75	0.69
7:T:5:LYS:HD2	24:T:263:PEK:H371	1.74	0.69
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.75	0.69
12:L:11:ILE:CG2	18:L:522:TGL:H271	2.23	0.69
7:G:5:LYS:NZ	28:G:4202:HOH:O	2.25	0.69
4:Q:31:LYS:HB3	28:Q:4834:HOH:O	1.92	0.68
10:W:33:ARG:HG2	22:W:1059:CHD:H151	1.75	0.68
1:N:274:VAL:HG12	1:N:278:MET:HE2	1.75	0.68
1:A:406:ASN:HD21	19:A:524:PGV:H22	1.59	0.68
4:Q:100:LYS:HE2	28:Q:4478:HOH:O	1.94	0.68
9:V:65:LYS:O	11:X:54:ARG:NH1	2.27	0.67
6:S:95:GLN:HB2	28:S:4523:HOH:O	1.93	0.67
7:G:5:LYS:HB3	1:N:278:MET:SD	2.34	0.67
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.75	0.67
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.25	0.67
28:G:4789:HOH:O	19:P:1268:PGV:H341	1.93	0.67
19:N:1266:PGV:H182	3:P:28:THR:HG22	1.75	0.67
18:N:1521:TGL:H101	18:N:1521:TGL:C28	2.25	0.67
2:O:59:GLN:O	2:O:59:GLN:CG	2.42	0.66
1:A:406:ASN:HD21	19:A:524:PGV:C2	2.08	0.66
18:N:1521:TGL:HC22	28:V:3606:HOH:O	1.95	0.66
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.60	0.66
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.78	0.66
1:A:278:MET:SD	7:T:5:LYS:HB3	2.36	0.66
7:G:17:ARG:HD2	28:G:2446:HOH:O	1.95	0.65
8:H:43:MET:HE1	8:U:43:MET:HE1	1.79	0.65
1:A:486:ASP:OD2	4:D:19:ARG:HD3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:1229:PSC:H222	21:O:1229:PSC:H21	1.78	0.65
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.60	0.65
2:B:56:MET:HG2	21:B:229:PSC:H211	1.78	0.65
7:G:2:SER:O	24:G:1263:PEK:H322	1.97	0.64
1:A:310:MET:HE2	1:A:356:ILE:HG23	1.79	0.64
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.79	0.64
2:B:41:ILE:CD1	21:B:229:PSC:H342	2.25	0.63
8:H:27:ARG:HD3	28:H:4760:HOH:O	1.98	0.63
21:O:1229:PSC:C07	9:V:10:ARG:HH21	2.12	0.63
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.63	0.63
6:S:64:GLU:O	6:S:65:ASP:HB2	1.99	0.62
3:C:210:ILE:HG12	19:C:267:PGV:H132	1.81	0.62
7:T:3:ALA:O	7:T:4:ALA:HB2	2.00	0.62
6:S:1:ALA:N	24:T:1265:PEK:H041	2.14	0.61
7:G:3:ALA:O	7:G:4:ALA:HB2	2.00	0.61
5:R:80:GLU:N	5:R:80:GLU:OE1	2.33	0.61
1:A:430:PHE:HE1	18:A:521:TGL:HB21	1.66	0.61
2:O:41:ILE:HD13	21:O:1229:PSC:H342	1.82	0.61
7:T:3:ALA:CB	24:T:263:PEK:H382	2.30	0.61
25:C:270:CDL:H191	25:C:270:CDL:H642	1.82	0.60
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.01	0.60
19:A:524:PGV:H062	28:A:2126:HOH:O	2.00	0.60
6:S:52:ILE:O	6:S:94:HIS:CG	2.54	0.60
18:A:521:TGL:H111	2:B:35:SER:OG	2.02	0.60
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.16	0.60
7:G:45:PRO:HD2	28:G:2099:HOH:O	2.01	0.60
10:W:33:ARG:HG2	22:W:1059:CHD:C15	2.32	0.60
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	2.01	0.60
18:D:523:TGL:HB62	18:D:523:TGL:HA52	1.83	0.60
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.01	0.60
1:A:483:LEU:HD21	13:M:4:LYS:HD3	1.83	0.60
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.84	0.60
2:B:78:LEU:HD12	25:T:1269:CDL:H352	1.85	0.59
19:A:524:PGV:H82	19:A:524:PGV:H262	1.84	0.59
1:N:177:SER:H	1:N:180:GLN:NE2	2.00	0.59
3:C:63:ARG:HE	25:C:270:CDL:CA2	2.14	0.59
1:N:28:MET:CE	14:N:515:HEA:C27	2.80	0.59
10:J:33:ARG:HG2	22:J:60:CHD:H151	1.84	0.59
2:O:56:MET:HG2	21:O:1229:PSC:H211	1.84	0.59
1:N:28:MET:CE	14:N:515:HEA:H271	2.32	0.58
24:C:265:PEK:H383	25:G:269:CDL:H272	1.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:CYS:SG	25:G:269:CDL:H552	2.44	0.58
18:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.85	0.58
7:G:3:ALA:HB1	24:G:1263:PEK:H382	1.85	0.58
4:D:34:SER:H	4:D:37:GLN:NE2	2.01	0.58
6:F:64:GLU:O	6:F:65:ASP:HB2	2.04	0.58
21:O:1229:PSC:O01	21:O:1229:PSC:H212	2.04	0.58
6:S:52:ILE:O	6:S:94:HIS:ND1	2.30	0.58
12:L:11:ILE:HG22	18:L:522:TGL:H271	1.85	0.57
28:B:3446:HOH:O	7:T:17:ARG:HD2	2.03	0.57
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.86	0.57
4:Q:7:LYS:HA	28:Q:4706:HOH:O	2.03	0.57
7:T:5:LYS:CB	24:T:263:PEK:H362	2.27	0.57
13:Z:7:LYS:NZ	28:Z:4640:HOH:O	2.36	0.57
6:S:87:THR:HG22	28:S:4582:HOH:O	2.04	0.57
21:B:229:PSC:H343	21:B:229:PSC:H142	1.86	0.57
1:N:400:PHE:HB3	18:N:1522:TGL:H282	1.87	0.57
12:L:20:ARG:HH22	18:L:522:TGL:HC62	1.70	0.57
1:A:274:VAL:HG12	1:A:278:MET:HE2	1.87	0.57
18:N:1521:TGL:HA91	18:N:1521:TGL:H252	1.86	0.57
4:Q:127:LYS:HD2	28:V:3618:HOH:O	2.05	0.57
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.40	0.56
19:A:522:PGV:H183	24:G:264:PEK:H332	1.87	0.56
6:S:1:ALA:H2	24:T:1265:PEK:H041	1.70	0.56
1:A:488:THR:HB	1:A:495:LEU:HD13	1.87	0.56
24:G:1263:PEK:H132	3:P:247:VAL:CG1	2.36	0.56
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.05	0.56
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.34	0.56
1:N:472:ILE:HG21	18:N:1522:TGL:HA91	1.88	0.55
1:A:21:LEU:HD23	18:L:522:TGL:H211	1.88	0.55
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.89	0.55
3:C:210:ILE:HD13	19:C:267:PGV:H301	1.88	0.55
6:S:53:THR:CA	6:S:94:HIS:CE1	2.86	0.55
2:O:84:LEU:HA	2:O:87:MET:HE2	1.87	0.55
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.19	0.54
18:A:521:TGL:HC22	28:D:2606:HOH:O	2.06	0.54
21:B:229:PSC:H322	21:B:229:PSC:H12	1.89	0.54
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.89	0.54
3:P:52:LEU:HD21	25:P:1270:CDL:H412	1.88	0.54
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.23	0.54
1:N:430:PHE:HE1	18:N:1521:TGL:HB21	1.72	0.54
2:B:19:GLU:HG3	2:B:83:ILE:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:37:LEU:CD2	25:G:269:CDL:H361	2.38	0.54
9:V:2:THR:HG22	9:V:3:ALA:H	1.72	0.54
2:B:13:THR:HB	2:B:168:LEU:HD23	1.90	0.53
18:N:1521:TGL:H101	18:N:1521:TGL:H281	1.90	0.53
4:Q:78:TRP:HA	18:Q:1523:TGL:HB22	1.89	0.53
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.90	0.53
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.42	0.53
1:N:417:MET:CE	28:N:3166:HOH:O	2.56	0.53
21:O:1229:PSC:H071	9:V:10:ARG:HE	1.73	0.53
1:N:112:LEU:HD23	1:N:112:LEU:C	2.34	0.53
14:N:515:HEA:HBC1	14:N:515:HEA:HMC3	1.90	0.53
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.89	0.53
7:G:30:LEU:CD2	25:G:269:CDL:H462	2.39	0.53
3:C:67:PHE:CE1	25:C:270:CDL:H1	2.25	0.53
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.74	0.53
3:C:52:LEU:HD21	25:C:270:CDL:H412	1.91	0.52
1:N:321:PHE:CD2	21:O:1229:PSC:H341	2.44	0.52
7:T:5:LYS:HD2	24:T:263:PEK:C37	2.39	0.52
11:X:52:GLU:HG2	28:X:4813:HOH:O	2.09	0.52
12:Y:2:HIS:N	28:Y:4664:HOH:O	2.43	0.52
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.73	0.52
3:P:5:THR:CG2	6:S:96:LEU:HD13	2.39	0.52
25:T:1269:CDL:OB4	25:T:1269:CDL:H1	2.10	0.52
7:T:3:ALA:O	7:T:4:ALA:CB	2.56	0.52
12:L:12:PRO:HB2	18:L:522:TGL:HG2	1.92	0.52
3:P:50:ASN:HD22	3:P:51:MET:HE2	1.75	0.52
19:A:524:PGV:H02	19:A:524:PGV:O14	2.10	0.52
7:G:72:ASN:H	7:G:76:ASN:ND2	1.99	0.52
12:L:20:ARG:HH12	18:L:522:TGL:HC62	1.75	0.52
18:L:522:TGL:CC6	18:L:522:TGL:HC22	2.40	0.52
18:N:1521:TGL:H281	18:N:1521:TGL:C10	2.40	0.51
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.91	0.51
19:N:1524:PGV:H22	19:N:1524:PGV:H011	1.91	0.51
25:T:1269:CDL:HA21	25:T:1269:CDL:H111	1.92	0.51
1:N:449:MET:SD	2:O:5:MET:HG2	2.50	0.51
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.91	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.45	0.51
12:L:20:ARG:HH12	18:L:522:TGL:CC6	2.23	0.51
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.40	0.51
18:D:523:TGL:H242	18:D:523:TGL:HA91	1.91	0.51
1:N:112:LEU:HG	28:N:3701:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:400:PHE:O	18:N:1522:TGL:H283	2.11	0.51
1:A:76:GLY:O	1:A:80:ASN:HB2	2.11	0.51
1:A:112:LEU:CG	28:A:2701:HOH:O	2.54	0.51
7:G:4:ALA:CB	1:N:282:PHE:HA	2.41	0.51
1:N:406:ASN:HD21	19:N:1524:PGV:C2	2.24	0.51
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.26	0.51
12:L:24:MET:SD	18:L:522:TGL:H161	2.51	0.51
7:G:30:LEU:HD21	25:G:269:CDL:H462	1.92	0.50
1:N:366:VAL:HG11	2:O:9:PHE:CE2	2.46	0.50
1:N:488:THR:HB	1:N:495:LEU:HD13	1.93	0.50
3:P:76:GLN:NE2	28:P:3284:HOH:O	2.37	0.50
1:N:400:PHE:HB3	18:N:1522:TGL:C28	2.40	0.50
1:N:472:ILE:HD13	18:N:1522:TGL:HA91	1.94	0.50
2:O:164:ALA:O	2:O:194:GLY:HA3	2.12	0.50
3:P:5:THR:HG22	6:S:96:LEU:CD1	2.41	0.50
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.94	0.50
7:T:2:SER:O	24:T:263:PEK:H322	2.12	0.50
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.94	0.50
2:O:146:MET:HA	2:O:213:LEU:HD12	1.94	0.50
3:P:210:ILE:HD13	19:P:1267:PGV:H301	1.93	0.50
1:A:430:PHE:CE1	18:A:521:TGL:HB21	2.47	0.50
21:O:1229:PSC:H071	9:V:10:ARG:HH21	1.77	0.50
2:B:45:MET:HE2	2:B:45:MET:HA	1.94	0.50
7:G:37:LEU:HD21	25:G:269:CDL:H361	1.93	0.50
8:H:7:LYS:O	8:H:8:ILE:HB	2.11	0.50
1:N:177:SER:H	1:N:180:GLN:HE21	1.59	0.50
21:B:229:PSC:H222	21:B:229:PSC:H21	1.94	0.49
2:B:146:MET:HE2	2:B:215:PRO:HG3	1.95	0.49
4:D:78:TRP:HA	18:D:523:TGL:HB22	1.94	0.49
1:N:172:LYS:HD2	1:N:181:THR:HG22	1.93	0.49
8:H:60:TYR:CD1	8:H:60:TYR:C	2.89	0.49
18:L:522:TGL:OA1	18:L:522:TGL:OG3	2.30	0.49
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.47	0.49
18:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.95	0.49
7:G:3:ALA:O	7:G:4:ALA:CB	2.60	0.49
24:G:1263:PEK:H182	3:P:98:PHE:CD2	2.48	0.49
25:T:1269:CDL:H172	25:T:1269:CDL:H511	1.94	0.49
8:H:43:MET:CE	8:U:43:MET:HE1	2.41	0.49
8:U:46:LYS:NZ	28:U:4474:HOH:O	2.24	0.49
18:N:1522:TGL:H271	12:Y:11:ILE:CG2	2.43	0.49
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:GLU:HG3	28:A:4882:HOH:O	2.12	0.48
10:J:50:LEU:HD22	10:J:54:SER:OG	2.14	0.48
5:R:80:GLU:H	5:R:80:GLU:CD	2.20	0.48
1:A:172:LYS:HZ2	1:A:178:GLN:HE22	1.59	0.48
4:D:86:MET:CE	28:K:4688:HOH:O	2.61	0.48
24:G:1263:PEK:H132	3:P:247:VAL:HG12	1.94	0.48
2:O:41:ILE:CD1	21:O:1229:PSC:H342	2.43	0.48
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.48
25:T:1269:CDL:H782	25:T:1269:CDL:C57	2.32	0.48
1:N:310:MET:HE2	2:O:73:LEU:HD22	1.95	0.48
21:O:1229:PSC:H081	5:R:8:ASP:OD1	2.14	0.48
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.53	0.48
7:T:38:HIS:NE2	25:T:1269:CDL:H111	2.29	0.48
11:K:24:PHE:O	11:K:28:VAL:HG12	2.14	0.48
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.02	0.48
3:C:91:VAL:HG22	24:T:263:PEK:H14	1.95	0.48
11:X:41:ASN:OD1	28:X:4655:HOH:O	2.20	0.48
5:E:105:GLY:O	5:E:108:LYS:HG2	2.14	0.48
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.49	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
1:A:28:MET:CE	14:A:515:HEA:H271	2.44	0.47
3:C:122:HIS:HD2	28:C:4770:HOH:O	1.97	0.47
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.15	0.47
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.14	0.47
2:B:78:LEU:CD1	25:T:1269:CDL:H352	2.44	0.47
2:B:29:MET:HG3	9:I:35:TYR:CD2	2.49	0.47
28:B:3446:HOH:O	7:T:17:ARG:CD	2.63	0.47
1:N:243:VAL:HB	14:N:516:HEA:CAC	2.45	0.47
18:N:1521:TGL:H201	18:N:1521:TGL:C24	2.41	0.47
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.96	0.47
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.14	0.47
3:C:191:GLY:HA3	28:G:2132:HOH:O	2.14	0.47
25:C:270:CDL:HB21	25:C:270:CDL:CB3	2.45	0.47
28:G:4541:HOH:O	19:P:1268:PGV:H301	2.14	0.47
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	1.97	0.47
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.45	0.47
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.14	0.47
18:N:1522:TGL:H302	28:N:4751:HOH:O	2.15	0.47
19:N:1524:PGV:H011	19:N:1524:PGV:H221	1.96	0.47
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.80	0.47
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.97	0.47
3:P:51:MET:HB3	25:P:1270:CDL:H622	1.96	0.47
25:G:269:CDL:HB32	1:N:304:TYR:HD1	1.80	0.46
1:A:46:THR:HG23	28:A:2466:HOH:O	2.15	0.46
1:A:379:TYR:O	1:A:383:MET:HB2	2.16	0.46
18:A:521:TGL:HC82	28:A:4504:HOH:O	2.14	0.46
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.97	0.46
12:Y:20:ARG:HH11	12:Y:20:ARG:HB3	1.79	0.46
21:B:229:PSC:C07	9:I:10:ARG:NH2	2.68	0.46
1:N:148:PHE:HB3	3:P:28:THR:HB	1.97	0.46
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.15	0.46
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.97	0.46
1:N:240:HIS:C	1:N:240:HIS:CD2	2.94	0.46
2:O:56:MET:HA	21:O:1229:PSC:H202	1.98	0.46
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.16	0.46
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.16	0.46
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.97	0.46
25:G:269:CDL:H1	25:G:269:CDL:OB4	2.16	0.46
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.51	0.45
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.50	0.45
24:T:1264:PEK:C10	24:T:1264:PEK:H161	2.46	0.45
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.97	0.45
2:B:222:TRP:O	2:B:226:MET:HB2	2.16	0.45
25:C:270:CDL:HB22	25:C:270:CDL:OA5	2.15	0.45
4:D:86:MET:HE3	28:K:4688:HOH:O	2.17	0.45
1:N:87:ILE:O	1:N:173:PRO:HD3	2.15	0.45
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.99	0.45
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.56	0.45
6:S:51:SER:O	6:S:94:HIS:HA	2.16	0.45
1:A:321:PHE:CD2	21:B:229:PSC:H341	2.51	0.45
7:G:38:HIS:CE1	25:G:269:CDL:H111	2.52	0.45
14:N:515:HEA:H172	14:N:515:HEA:H273	1.41	0.45
25:C:270:CDL:H741	25:C:270:CDL:H172	1.98	0.45
6:F:70:ILE:HG13	6:F:84:SER:HB3	1.98	0.45
25:T:1269:CDL:H171	28:T:4708:HOH:O	2.17	0.45
1:A:115:SER:O	1:A:121:GLY:HA2	2.17	0.45
6:F:55:LYS:HA	6:F:74:LEU:O	2.16	0.45
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.71	0.45
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.98	0.45
24:T:1264:PEK:H161	24:T:1264:PEK:H102	1.98	0.45
10:W:56:PRO:HD3	12:Y:46:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:22:LEU:O	12:Y:26:THR:HB	2.17	0.45
3:C:105:SER:HA	3:C:116:TRP:CE3	2.52	0.45
3:P:250:LEU:HD22	25:T:1269:CDL:H662	1.98	0.45
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.52	0.44
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.82	0.44
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.52	0.44
25:C:270:CDL:H611	25:C:270:CDL:H652	2.00	0.44
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.05	0.44
18:A:521:TGL:H281	18:A:521:TGL:H101	1.99	0.44
2:O:16:ILE:HD11	2:O:86:MET:HG2	2.00	0.44
1:A:1:FME:HCN	1:A:4:ASN:H	1.82	0.44
21:B:229:PSC:H062	21:B:229:PSC:H042	1.80	0.44
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.82	0.44
18:L:522:TGL:H231	18:L:522:TGL:H202	1.41	0.44
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.99	0.44
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.83	0.44
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.48	0.44
2:B:78:LEU:HD12	25:T:1269:CDL:C35	2.48	0.44
22:B:1085:CHD:H12	22:B:1085:CHD:H212	1.99	0.44
1:N:344:PHE:CD1	1:N:344:PHE:C	2.96	0.44
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.18	0.44
25:P:1270:CDL:H242	25:P:1270:CDL:H661	1.98	0.44
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.82	0.44
10:J:40:LEU:HD12	22:J:60:CHD:H183	2.00	0.44
1:N:501:PRO:HB3	12:Y:5:GLU:OE2	2.17	0.44
1:A:481:GLU:HB2	13:M:4:LYS:HE2	2.00	0.44
25:C:270:CDL:H642	25:C:270:CDL:C19	2.47	0.44
19:A:524:PGV:H312	13:M:16:ALA:HA	1.99	0.43
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.18	0.43
1:N:334:TRP:CZ3	18:Q:1523:TGL:HA51	2.53	0.43
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.75	0.43
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.79	0.43
5:R:86:ILE:HD13	5:R:86:ILE:HA	1.87	0.43
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.32	0.43
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.53	0.43
1:N:71:MET:HE3	1:N:245:ILE:HG21	2.00	0.43
3:P:64:GLU:HA	3:P:68:GLN:HE21	1.83	0.43
24:T:1265:PEK:H383	25:T:1269:CDL:H272	1.90	0.43
6:S:87:THR:HG21	28:S:3514:HOH:O	2.18	0.43
1:A:282:PHE:HA	7:T:4:ALA:CB	2.45	0.43
1:A:406:ASN:HD21	19:A:524:PGV:H21	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.53	0.43
19:C:267:PGV:H182	25:C:270:CDL:C67	2.49	0.43
25:G:269:CDL:H352	2:O:78:LEU:HD12	2.00	0.43
1:N:215:LEU:HD11	24:T:1264:PEK:H271	2.00	0.43
2:O:65:TRP:CZ3	21:O:1229:PSC:H331	2.54	0.43
3:P:63:ARG:NE	25:P:1270:CDL:HA22	2.07	0.43
1:N:472:ILE:HG21	18:N:1522:TGL:CA9	2.49	0.43
19:N:1524:PGV:H132	19:N:1524:PGV:H301	2.01	0.43
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.54	0.43
25:G:269:CDL:H451	2:O:70:ALA:HB1	2.01	0.43
21:O:1229:PSC:C07	9:V:10:ARG:HE	2.32	0.43
22:W:1059:CHD:H193	22:W:1059:CHD:H111	1.73	0.43
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.01	0.43
1:A:383:MET:O	1:A:387:PHE:HB2	2.18	0.43
4:D:132:GLN:OE1	9:I:43:ARG:HD3	2.19	0.43
10:J:33:ARG:HG2	22:J:60:CHD:C15	2.48	0.43
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.96	0.43
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.43
3:C:156:ARG:HE	22:C:271:CHD:C24	2.32	0.43
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.76	0.43
1:N:365:ILE:HD11	28:N:4859:HOH:O	2.18	0.43
1:N:310:MET:HB3	2:O:73:LEU:HD22	2.00	0.43
3:P:37:PHE:CD1	10:W:52:TRP:HZ3	2.36	0.43
3:P:107:ALA:HB2	19:P:1268:PGV:H031	2.01	0.43
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.01	0.43
25:T:1269:CDL:H152	25:T:1269:CDL:H182	1.85	0.43
25:P:1270:CDL:C19	25:P:1270:CDL:H642	2.49	0.42
4:D:7:LYS:HE3	28:D:4308:HOH:O	2.18	0.42
12:L:20:ARG:NH2	18:L:522:TGL:HC42	2.34	0.42
13:M:4:LYS:H	13:M:4:LYS:HG2	1.64	0.42
1:N:54:TYR:HB2	28:N:4621:HOH:O	2.19	0.42
6:S:52:ILE:C	6:S:94:HIS:ND1	2.76	0.42
2:B:199:ILE:O	2:B:199:ILE:HG23	2.19	0.42
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.50	0.42
3:P:29:SER:CB	3:P:42:LEU:HD13	2.48	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.42
1:N:489:THR:HA	6:S:71:TRP:O	2.19	0.42
21:B:229:PSC:H62	21:B:229:PSC:H241	2.02	0.42
1:N:115:SER:HB2	1:N:142:SER:O	2.20	0.42
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.18	0.42
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:247:VAL:CG1	24:T:263:PEK:H132	2.50	0.42
5:E:5:HIS:HB3	5:E:6:GLU:H	1.62	0.42
7:G:31:CYS:SG	25:G:269:CDL:H532	2.59	0.42
10:J:56:PRO:HD3	12:L:46:LYS:HG2	2.01	0.42
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.55	0.42
1:N:397:PHE:HB3	1:N:398:PRO:HD3	2.01	0.42
2:O:9:PHE:HB2	2:O:21:LEU:HD21	2.01	0.42
1:A:344:PHE:CD1	1:A:344:PHE:C	2.97	0.42
3:C:51:MET:HB3	25:C:270:CDL:H622	2.01	0.42
19:C:268:PGV:H341	28:T:4364:HOH:O	2.19	0.42
7:G:5:LYS:HD2	24:G:1263:PEK:H371	2.00	0.42
7:T:31:CYS:SG	25:T:1269:CDL:C55	3.07	0.42
4:D:78:TRP:CA	18:D:523:TGL:HB22	2.50	0.42
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.02	0.42
1:N:342:LEU:HD13	2:O:46:LEU:HD11	2.01	0.42
3:P:116:TRP:HA	3:P:117:PRO:C	2.45	0.42
6:S:95:GLN:CB	28:S:4523:HOH:O	2.61	0.42
1:A:115:SER:HB2	1:A:142:SER:O	2.20	0.41
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.20	0.41
9:V:73:LYS:HB3	9:V:73:LYS:HE3	1.96	0.41
3:C:99:TRP:CE2	19:C:268:PGV:H232	2.55	0.41
1:N:22:PHE:HA	18:N:1522:TGL:HB72	2.02	0.41
1:N:371:TYR:CE2	1:N:436:MET:HE2	2.55	0.41
1:N:379:TYR:O	1:N:383:MET:HB2	2.20	0.41
19:N:1524:PGV:H322	13:Z:19:LEU:HD23	2.02	0.41
2:O:199:ILE:O	2:O:199:ILE:HG23	2.19	0.41
2:B:29:MET:HG3	9:I:35:TYR:CG	2.55	0.41
1:N:100:MET:HE1	19:N:1266:PGV:H81	2.02	0.41
1:N:456:MET:HG2	4:Q:96:LEU:HD13	2.01	0.41
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.56	0.41
1:N:243:VAL:HB	14:N:516:HEA:HAC	2.01	0.41
1:N:431:LEU:HD22	1:N:447:TYR:HB3	2.03	0.41
4:Q:128:VAL:O	4:Q:129:ALA:C	2.62	0.41
1:A:400:PHE:HB3	18:L:522:TGL:H282	2.03	0.41
6:F:46:PRO:O	6:F:48:LEU:HD13	2.21	0.41
19:N:1266:PGV:H183	24:T:1264:PEK:H332	2.03	0.41
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.35	0.41
21:B:229:PSC:H251	21:B:229:PSC:H221	1.79	0.41
5:E:48:ILE:O	5:E:52:LEU:HG	2.20	0.41
7:G:7:ASP:O	7:G:9:GLY:N	2.49	0.41
13:M:10:THR:HG22	13:M:15:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:76:GLY:O	1:N:80:ASN:HB2	2.20	0.41
3:P:173:PHE:CD2	3:P:173:PHE:C	2.98	0.41
6:S:70:ILE:HG13	6:S:84:SER:HB3	2.01	0.41
8:H:39:CYS:O	8:H:43:MET:HG2	2.21	0.41
1:N:430:PHE:CE1	18:N:1521:TGL:HB21	2.55	0.41
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.56	0.41
3:P:129:VAL:N	3:P:130:PRO:CD	2.82	0.41
1:A:240:HIS:O	1:A:241:PRO:C	2.60	0.41
14:A:515:HEA:H273	14:A:515:HEA:H172	1.30	0.41
3:C:223:LEU:HD21	22:C:271:CHD:H183	2.01	0.41
25:C:270:CDL:H171	25:C:270:CDL:H202	1.87	0.41
24:G:264:PEK:H352	24:G:264:PEK:H382	1.72	0.41
1:N:400:PHE:C	18:N:1522:TGL:H283	2.46	0.41
25:P:1270:CDL:H792	25:P:1270:CDL:H821	1.86	0.41
7:T:11:TPO:O	7:T:11:TPO:CG2	2.68	0.41
6:F:51:SER:O	6:F:94:HIS:N	2.47	0.41
24:G:1263:PEK:H132	3:P:247:VAL:HG11	2.03	0.41
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.90	0.41
21:O:1229:PSC:H22	9:V:14:ALA:CB	2.51	0.41
1:A:231:TYR:CD1	1:A:231:TYR:C	2.98	0.40
24:C:265:PEK:C38	25:G:269:CDL:C27	2.70	0.40
8:H:27:ARG:NH1	28:H:2431:HOH:O	2.53	0.40
10:J:50:LEU:HD22	10:J:50:LEU:O	2.21	0.40
19:N:1524:PGV:H92	4:Q:84:ALA:HB2	2.02	0.40
25:T:1269:CDL:H322	25:T:1269:CDL:HA62	2.02	0.40
25:T:1269:CDL:H561	25:T:1269:CDL:H592	1.63	0.40
1:A:409:TRP:CH2	19:A:524:PGV:H81	2.57	0.40
25:P:1270:CDL:H611	25:P:1270:CDL:H652	2.03	0.40
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.03	0.40
1:A:194:LEU:HD13	28:A:4206:HOH:O	2.21	0.40
2:B:196:CYS:CB	2:B:207:MET:HG3	2.52	0.40
19:C:267:PGV:H172	25:C:270:CDL:H662	2.02	0.40
1:N:28:MET:HE2	14:N:515:HEA:C27	2.49	0.40
3:P:22:LEU:O	3:P:26:LEU:HG	2.21	0.40
4:Q:81:VAL:HG11	18:Q:1523:TGL:HB51	2.04	0.40
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.47	0.40
1:N:402:GLY:HA3	1:N:499:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

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%)	496 (97%)	15 (3%)	1 (0%)	43	55
1	N	512/514 (100%)	499 (98%)	13 (2%)	0	100	100
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	30	38
2	O	225/227 (99%)	214 (95%)	8 (4%)	3 (1%)	9	10
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	250 (97%)	6 (2%)	1 (0%)	30	38
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	12	15
6	S	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	3	2
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	0	0
7	T	81/85 (95%)	66 (82%)	9 (11%)	6 (7%)	1	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	9	10
8	U	77/85 (91%)	71 (92%)	4 (5%)	2 (3%)	4	3
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	47 (100%)	0	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3371 (96%)	107 (3%)	26 (1%)	18	23

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
8	H	8	ILE
6	S	94	HIS
6	S	95	GLN
7	T	3	ALA
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
1	A	384	GLY
2	B	60	GLU
8	U	8	ILE
7	G	6	GLY
2	O	224	ALA
7	T	6	GLY
7	G	3	ALA
7	G	40	GLY
2	O	60	GLU
3	P	38	ASN
7	T	39	SER
8	U	10	ASN
6	S	96	LEU
2	O	92	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	418 (98%)	8 (2%)	50	69
1	N	426/426 (100%)	416 (98%)	10 (2%)	44	63
2	B	210/210 (100%)	200 (95%)	10 (5%)	23	35
2	O	210/210 (100%)	200 (95%)	10 (5%)	23	35
3	C	224/226 (99%)	219 (98%)	5 (2%)	45	65
3	P	224/226 (99%)	217 (97%)	7 (3%)	35	52
4	D	128/129 (99%)	127 (99%)	1 (1%)	73	86
4	Q	128/129 (99%)	123 (96%)	5 (4%)	28	43
5	E	92/95 (97%)	88 (96%)	4 (4%)	26	39
5	R	92/95 (97%)	88 (96%)	4 (4%)	26	39
6	F	81/81 (100%)	77 (95%)	4 (5%)	22	34
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	17
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	17
7	T	67/68 (98%)	62 (92%)	5 (8%)	12	17
8	H	71/75 (95%)	67 (94%)	4 (6%)	19	28
8	U	71/75 (95%)	66 (93%)	5 (7%)	14	19
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	30
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	30
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	67
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	67
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	59
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	32
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	59
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	16
13	M	37/38 (97%)	30 (81%)	7 (19%)	1	1
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	4
All	All	3040/3082 (99%)	2920 (96%)	120 (4%)	28	43

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	138	HIS
1	A	178	GLN

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Mol	Chain	Res	Type
1	A	180	GLN
1	A	189	MET
1	A	297	MET
1	A	369	ASP
1	A	513	LEU
2	B	19	GLU
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	167	SER
2	B	226	MET
3	C	17	PRO
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	230	ASN
4	D	51	LEU
5	E	5	HIS
5	E	31	LYS
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	84	SER
6	F	87	THR
6	F	95	GLN
7	G	17	ARG
7	G	33	LEU
7	G	36	TRP
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	44	THR
8	H	60	TYR
9	I	8	GLN
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU

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Mol	Chain	Res	Type
11	K	54	ARG
12	L	26	THR
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
13	M	43	SER
1	N	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	495	LEU
1	N	512	ASN
2	O	33	LEU
2	O	60	GLU
2	O	61	VAL
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	217	LYS
3	P	17	PRO
3	P	33	MET
3	P	77	LYS
3	P	127	LEU
3	P	144	ILE
3	P	159	MET
3	P	230	ASN
4	Q	8	SER
4	Q	9	GLU
4	Q	51	LEU
4	Q	52	SER
4	Q	143	ASN
5	R	5	HIS

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Mol	Chain	Res	Type
5	R	14	ARG
5	R	79	LYS
5	R	80	GLU
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	90	LYS
6	S	95	GLN
6	S	96	LEU
7	T	17	ARG
7	T	33	LEU
7	T	37	LEU
7	T	74	ARG
7	T	84	LYS
8	U	8	ILE
8	U	29	CYS
8	U	60	TYR
8	U	70	SER
8	U	84	LYS
9	V	2	THR
9	V	8	GLN
9	V	29	LEU
10	W	50	LEU
11	X	20	SER
11	X	54	ARG
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	43	GLN
1	A	55	ASN
1	A	178	GLN
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	491	ASN
1	A	512	ASN
2	B	52	HIS
2	B	59	GLN
2	B	140	ASN
2	B	181	GLN
3	C	68	GLN
3	C	161	GLN
4	D	29	HIS
4	D	37	GLN
4	D	143	ASN
5	E	94	ASN
7	G	8	HIS
7	G	34	ASN
7	G	71	HIS
7	G	76	ASN
8	H	31	GLN
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	91	ASN
2	O	181	GLN
3	P	3	HIS
3	P	50	ASN
3	P	68	GLN
3	P	122	HIS
4	Q	37	GLN
4	Q	109	HIS
4	Q	119	GLN
4	Q	143	ASN
5	R	94	ASN
7	T	76	ASN
8	U	31	GLN
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
7	TPO	G	11	7	8,10,11	2.31	2 (25%)	10,14,16	1.40	2 (20%)
9	SAC	V	1	9	7,8,9	2.44	2 (28%)	7,9,11	2.86	1 (14%)
9	SAC	I	1	9	7,8,9	2.55	2 (28%)	7,9,11	1.88	2 (28%)
1	FME	N	1	1	8,9,10	0.68	0	8,9,11	5.48	2 (25%)
7	TPO	T	11	7	8,10,11	2.07	3 (37%)	10,14,16	1.35	2 (20%)
2	FME	B	1	2	8,9,10	1.37	1 (12%)	8,9,11	6.55	5 (62%)
2	FME	O	1	2	8,9,10	0.84	0	8,9,11	5.62	4 (50%)
1	FME	A	1	1	8,9,10	0.68	0	8,9,11	4.68	2 (25%)

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

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	5.53	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	4.56	1.33	1.23
9	V	1	SAC	CA-N	4.34	1.52	1.46
7	G	11	TPO	P-OG1	4.02	1.66	1.59
7	T	11	TPO	P-O1P	3.50	1.61	1.50
9	I	1	SAC	CA-N	3.46	1.51	1.46
7	G	11	TPO	P-O1P	3.42	1.61	1.50
7	T	11	TPO	P-OG1	3.02	1.64	1.59
2	B	1	FME	CA-N	2.78	1.50	1.46
7	T	11	TPO	P-O2P	2.06	1.62	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-17.00	96.68	122.82
2	O	1	FME	CA-N-CN	-14.97	99.80	122.82
1	N	1	FME	CA-N-CN	-14.72	100.18	122.82
1	A	1	FME	CA-N-CN	-12.61	103.43	122.82
9	V	1	SAC	C-CA-N	6.73	122.48	109.50
2	B	1	FME	O1-CN-N	4.46	136.83	125.32
2	B	1	FME	CG-CB-CA	-4.12	100.25	112.87
1	N	1	FME	CB-CA-N	3.80	117.43	110.52
9	I	1	SAC	C2A-C1A-N	-3.52	110.29	116.12
2	O	1	FME	CG-CB-CA	-3.35	102.64	112.87
2	O	1	FME	C-CA-N	3.13	115.53	109.50
2	B	1	FME	C-CA-N	2.80	114.91	109.50
9	I	1	SAC	OAC-C1A-N	2.63	126.62	121.98
2	B	1	FME	O-C-CA	-2.60	118.09	124.77
1	A	1	FME	CG-CB-CA	-2.37	105.62	112.87
7	T	11	TPO	O-C-CA	-2.22	119.05	124.77
7	G	11	TPO	O3P-P-OG1	2.09	114.01	105.85
7	G	11	TPO	O-C-CA	-2.09	119.39	124.77
2	O	1	FME	O-C-CA	-2.04	119.52	124.77
7	T	11	TPO	CG2-CB-CA	2.03	117.22	113.26

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2

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

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - 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
20	CUA	B	228	2	0,1,1	-	-	-		
22	CHD	C	271	-	32,32,32	0.64	0	51,51,51	2.04	17 (33%)
27	DMU	Z	1526	-	34,34,34	0.84	1 (2%)	45,45,45	2.54	16 (35%)
18	TGL	N	1521	-	62,62,62	1.29	6 (9%)	65,65,65	1.52	10 (15%)
18	TGL	L	522	-	62,62,62	1.42	7 (11%)	65,65,65	1.55	12 (18%)
14	HEA	A	516	1	67,67,67	1.92	21 (31%)	81,103,103	1.88	25 (30%)
24	PEK	G	1263	-	52,52,52	1.20	2 (3%)	55,57,57	1.21	6 (10%)
14	HEA	A	515	1	67,67,67	2.08	26 (38%)	81,103,103	2.20	15 (18%)
24	PEK	G	264	-	52,52,52	1.02	4 (7%)	55,57,57	1.48	9 (16%)
19	PGV	N	1266	-	50,50,50	0.86	2 (4%)	53,56,56	1.26	5 (9%)
22	CHD	J	60	-	32,32,32	0.83	0	51,51,51	2.86	22 (43%)
18	TGL	D	523	-	62,62,62	1.35	6 (9%)	65,65,65	1.58	10 (15%)
22	CHD	P	1525	-	32,32,32	0.96	1 (3%)	51,51,51	1.42	7 (13%)
27	DMU	M	526	-	34,34,34	0.85	1 (2%)	45,45,45	2.48	16 (35%)
24	PEK	T	1264	-	52,52,52	1.00	4 (7%)	55,57,57	1.39	9 (16%)
19	PGV	A	522	-	50,50,50	0.82	2 (4%)	53,56,56	1.16	2 (3%)
25	CDL	T	1269	-	99,99,99	1.44	12 (12%)	105,111,111	1.27	10 (9%)
18	TGL	Q	1523	-	62,62,62	1.37	6 (9%)	65,65,65	1.41	12 (18%)
21	PSC	O	1229	-	51,51,51	1.17	3 (5%)	57,59,59	0.98	2 (3%)
22	CHD	C	525	-	32,32,32	0.83	0	51,51,51	0.99	3 (5%)
22	CHD	G	229	-	32,32,32	0.92	0	51,51,51	1.55	9 (17%)
19	PGV	C	268	-	50,50,50	1.21	2 (4%)	53,56,56	1.30	4 (7%)
19	PGV	P	1268	-	50,50,50	1.18	2 (4%)	53,56,56	1.33	5 (9%)
19	PGV	N	1524	-	50,50,50	1.03	2 (4%)	53,56,56	1.16	4 (7%)
22	CHD	B	1085	-	32,32,32	1.15	3 (9%)	51,51,51	1.47	9 (17%)
22	CHD	P	1271	-	32,32,32	0.63	0	51,51,51	2.07	17 (33%)
14	HEA	N	516	1	67,67,67	1.80	19 (28%)	81,103,103	2.01	29 (35%)
19	PGV	C	267	-	50,50,50	0.83	2 (4%)	53,56,56	1.13	5 (9%)
19	PGV	A	524	-	50,50,50	1.18	2 (4%)	53,56,56	1.05	5 (9%)
14	HEA	N	515	1	67,67,67	2.18	20 (29%)	81,103,103	2.87	38 (46%)
19	PGV	P	1267	-	50,50,50	0.78	1 (2%)	53,56,56	1.13	3 (5%)
25	CDL	G	269	-	99,99,99	1.46	12 (12%)	105,111,111	1.32	9 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	TGL	N	1522	-	62,62,62	1.56	7 (11%)	65,65,65	1.59	15 (23%)
25	CDL	P	1270	-	99,99,99	1.46	13 (13%)	105,111,111	1.38	13 (12%)
22	CHD	W	1059	-	32,32,32	0.85	0	51,51,51	3.10	21 (41%)
18	TGL	A	521	-	62,62,62	1.32	6 (9%)	65,65,65	1.77	14 (21%)
24	PEK	T	1265	-	52,52,52	1.27	4 (7%)	55,57,57	1.14	5 (9%)
21	PSC	B	229	-	51,51,51	1.20	3 (5%)	57,59,59	1.06	3 (5%)
20	CUA	O	228	2	0,1,1	-	-	-	-	-
25	CDL	C	270	-	99,99,99	1.46	13 (13%)	105,111,111	1.32	14 (13%)
24	PEK	T	263	-	52,52,52	1.23	3 (5%)	55,57,57	1.14	5 (9%)
24	PEK	C	265	-	52,52,52	1.21	2 (3%)	55,57,57	1.15	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	Z	1526	-	4/4/10/10	9/19/59/59	0/2/2/2
22	CHD	C	271	-	-	6/9/74/74	0/4/4/4
18	TGL	N	1521	-	-	31/65/65/65	-
18	TGL	L	522	-	-	39/65/65/65	-
14	HEA	A	516	1	-	6/36/76/76	-
24	PEK	G	1263	-	-	32/56/56/56	-
14	HEA	A	515	1	-	6/36/76/76	-
19	PGV	N	1266	-	-	15/55/55/55	-
22	CHD	J	60	-	-	6/9/74/74	0/4/4/4
18	TGL	D	523	-	-	36/65/65/65	-
22	CHD	P	1525	-	-	1/9/74/74	0/4/4/4
27	DMU	M	526	-	2/2/10/10	8/19/59/59	0/2/2/2
24	PEK	T	1264	-	-	23/56/56/56	-
19	PGV	A	522	-	-	14/55/55/55	-
25	CDL	T	1269	-	-	50/110/110/110	-
18	TGL	Q	1523	-	-	36/65/65/65	-
21	PSC	O	1229	-	-	36/55/55/55	-
22	CHD	C	525	-	-	2/9/74/74	0/4/4/4
22	CHD	G	229	-	-	2/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	C	268	-	-	35/55/55/55	-
19	PGV	P	1268	-	-	33/55/55/55	-
19	PGV	N	1524	-	-	40/55/55/55	-
22	CHD	B	1085	-	-	2/9/74/74	0/4/4/4
22	CHD	P	1271	-	-	6/9/74/74	0/4/4/4
14	HEA	N	516	1	-	9/36/76/76	-
19	PGV	C	267	-	-	17/55/55/55	-
19	PGV	A	524	-	-	32/55/55/55	-
14	HEA	N	515	1	-	8/36/76/76	-
19	PGV	P	1267	-	-	14/55/55/55	-
25	CDL	G	269	-	-	66/110/110/110	-
18	TGL	N	1522	-	-	34/65/65/65	-
25	CDL	P	1270	-	-	68/110/110/110	-
22	CHD	W	1059	-	-	8/9/74/74	0/4/4/4
18	TGL	A	521	-	-	35/65/65/65	-
24	PEK	T	1265	-	-	30/56/56/56	-
21	PSC	B	229	-	-	34/55/55/55	-
24	PEK	G	264	-	-	25/56/56/56	-
25	CDL	C	270	-	-	69/110/110/110	-
24	PEK	T	263	-	-	33/56/56/56	-
24	PEK	C	265	-	-	21/56/56/56	-

All (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	1522	TGL	OG2-CB1	6.23	1.51	1.34
18	N	1522	TGL	OG1-CA1	6.17	1.51	1.33
14	N	515	HEA	CHC-C4B	5.86	1.50	1.38
18	L	522	TGL	OG2-CB1	5.81	1.50	1.34
24	T	263	PEK	O03-C21	5.79	1.50	1.33
19	A	524	PGV	O03-C19	5.64	1.49	1.33
24	G	1263	PEK	O03-C21	5.62	1.49	1.33
19	P	1268	PGV	O01-C1	5.56	1.50	1.34
19	C	268	PGV	O01-C1	5.50	1.49	1.34
24	C	265	PEK	O03-C21	5.44	1.49	1.33
24	T	1265	PEK	O01-C1	5.42	1.49	1.34
14	A	515	HEA	FE-NA	5.34	2.12	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	1265	PEK	O03-C21	5.27	1.48	1.33
18	Q	1523	TGL	OG2-CB1	5.19	1.48	1.34
25	G	269	CDL	OA6-CA5	5.19	1.48	1.34
25	P	1270	CDL	OA8-CA7	5.05	1.48	1.33
25	C	270	CDL	OA8-CA7	5.02	1.48	1.33
24	C	265	PEK	O01-C1	4.94	1.48	1.34
18	A	521	TGL	OG1-CA1	4.92	1.47	1.33
25	P	1270	CDL	OA6-CA5	4.88	1.48	1.34
18	L	522	TGL	OG1-CA1	4.88	1.47	1.33
19	C	268	PGV	O03-C19	4.83	1.47	1.33
24	T	263	PEK	O01-C1	4.83	1.47	1.34
19	P	1268	PGV	O03-C19	4.82	1.47	1.33
25	G	269	CDL	OB6-CB5	4.81	1.47	1.34
24	G	1263	PEK	O01-C1	4.78	1.47	1.34
25	T	1269	CDL	OA6-CA5	4.75	1.47	1.34
19	N	1524	PGV	O03-C19	4.74	1.47	1.33
18	Q	1523	TGL	OG1-CA1	4.72	1.47	1.33
18	D	523	TGL	OG3-CC1	4.69	1.47	1.33
25	C	270	CDL	OA6-CA5	4.60	1.47	1.34
18	Q	1523	TGL	OG3-CC1	4.60	1.46	1.33
25	G	269	CDL	OB8-CB7	4.60	1.46	1.33
21	B	229	PSC	O01-C1	4.60	1.47	1.34
14	N	516	HEA	FE-NA	4.60	2.10	1.95
14	N	515	HEA	C3A-C4A	-4.60	1.38	1.46
18	D	523	TGL	OG1-CA1	4.56	1.46	1.33
18	D	523	TGL	OG2-CB1	4.56	1.47	1.34
18	A	521	TGL	OG2-CB1	4.54	1.47	1.34
21	B	229	PSC	O03-C19	4.53	1.46	1.33
25	T	1269	CDL	OB6-CB5	4.51	1.47	1.34
14	N	515	HEA	C1A-C2A	-4.50	1.37	1.45
25	C	270	CDL	OB8-CB7	4.47	1.46	1.33
25	T	1269	CDL	OB8-CB7	4.47	1.46	1.33
18	N	1521	TGL	OG2-CB1	4.44	1.46	1.34
21	O	1229	PSC	O01-C1	4.42	1.46	1.34
25	G	269	CDL	OA8-CA7	4.41	1.46	1.33
18	N	1521	TGL	OG3-CC1	4.38	1.46	1.33
21	O	1229	PSC	O03-C19	4.35	1.46	1.33
14	N	515	HEA	C1A-NA	-4.29	1.31	1.39
19	A	524	PGV	O01-C1	4.29	1.46	1.34
25	T	1269	CDL	OA8-CA7	4.27	1.45	1.33
18	N	1522	TGL	OG3-CC1	4.26	1.45	1.33
14	N	515	HEA	FE-NC	4.16	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	515	HEA	CHC-C4B	4.12	1.46	1.38
14	N	515	HEA	CHA-C1A	4.08	1.46	1.38
14	A	515	HEA	FE-ND	4.08	2.07	1.94
25	C	270	CDL	C59-C58	-4.07	1.31	1.51
18	L	522	TGL	C20-CA9	-4.06	1.31	1.51
19	N	1524	PGV	O01-C1	4.06	1.45	1.34
25	P	1270	CDL	OB6-CB5	4.05	1.45	1.34
18	N	1521	TGL	C10-CB9	-4.04	1.31	1.51
14	N	515	HEA	FE-NA	4.03	2.08	1.95
19	N	1266	PGV	O03-C19	4.01	1.45	1.33
14	A	515	HEA	C3A-C4A	-4.00	1.39	1.46
21	O	1229	PSC	C13-C12	3.98	1.54	1.31
18	N	1522	TGL	C20-CA9	-3.95	1.32	1.51
25	P	1270	CDL	OB8-CB7	3.95	1.44	1.33
14	A	515	HEA	FE-NC	3.92	2.08	1.95
14	N	515	HEA	CHD-C4C	3.91	1.48	1.39
14	A	516	HEA	FE-NC	3.90	2.08	1.95
21	B	229	PSC	C13-C12	3.90	1.53	1.31
25	P	1270	CDL	C59-C58	-3.89	1.32	1.51
18	N	1521	TGL	OG1-CA1	3.86	1.44	1.33
14	A	516	HEA	C4B-NB	-3.85	1.33	1.40
25	P	1270	CDL	C79-C78	-3.83	1.32	1.51
25	T	1269	CDL	C59-C58	-3.83	1.32	1.51
18	A	521	TGL	OG3-CC1	3.82	1.44	1.33
14	A	516	HEA	C4C-NC	-3.82	1.32	1.39
14	N	515	HEA	CHD-C1D	3.80	1.46	1.38
25	C	270	CDL	C62-C61	-3.79	1.32	1.51
24	G	264	PEK	O01-C1	3.77	1.44	1.34
25	C	270	CDL	C79-C78	-3.77	1.33	1.51
25	G	269	CDL	C59-C58	-3.72	1.33	1.51
25	T	1269	CDL	C42-C41	-3.71	1.33	1.51
25	C	270	CDL	OB6-CB5	3.70	1.44	1.34
14	N	515	HEA	C1C-NC	-3.69	1.32	1.39
25	P	1270	CDL	C62-C61	-3.68	1.33	1.51
14	N	516	HEA	C3A-C4A	-3.68	1.39	1.46
18	A	521	TGL	C10-CB9	-3.68	1.33	1.51
24	T	1264	PEK	O01-C1	3.66	1.44	1.34
25	T	1269	CDL	C62-C61	-3.65	1.33	1.51
18	L	522	TGL	C10-CB9	-3.64	1.33	1.51
25	G	269	CDL	C42-C41	-3.63	1.33	1.51
14	N	515	HEA	O11-C11	3.63	1.50	1.42
19	P	1267	PGV	O03-C19	3.62	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	515	HEA	CHB-C4A	3.59	1.45	1.38
25	C	270	CDL	C82-C81	-3.58	1.34	1.51
14	N	516	HEA	CHB-C4A	3.57	1.45	1.38
14	A	515	HEA	CHA-C1A	3.56	1.45	1.38
25	P	1270	CDL	C82-C81	-3.55	1.34	1.51
25	C	270	CDL	C19-C18	-3.53	1.34	1.51
25	P	1270	CDL	C19-C18	-3.52	1.34	1.51
18	Q	1523	TGL	C20-CA9	-3.50	1.34	1.51
18	L	522	TGL	OG3-CC1	3.49	1.43	1.33
18	N	1522	TGL	C10-CB9	-3.49	1.34	1.51
18	Q	1523	TGL	C15-CC9	-3.48	1.34	1.51
25	G	269	CDL	C62-C61	-3.47	1.34	1.51
18	D	523	TGL	C20-CA9	-3.46	1.34	1.51
25	G	269	CDL	C22-C21	-3.46	1.34	1.51
14	A	516	HEA	C4D-C3D	-3.45	1.39	1.45
25	C	270	CDL	C22-C21	-3.44	1.34	1.51
14	A	516	HEA	FE-NB	3.42	2.05	1.94
25	P	1270	CDL	C22-C21	-3.41	1.34	1.51
24	T	1264	PEK	O01-C02	-3.40	1.38	1.46
18	D	523	TGL	C15-CC9	-3.39	1.34	1.51
25	G	269	CDL	C39-C38	-3.38	1.35	1.51
25	G	269	CDL	C19-C18	-3.38	1.35	1.51
14	A	516	HEA	CHA-C1A	3.37	1.45	1.38
14	N	516	HEA	C1A-NA	-3.37	1.33	1.39
25	T	1269	CDL	C19-C18	-3.37	1.35	1.51
18	Q	1523	TGL	C10-CB9	-3.35	1.35	1.51
18	A	521	TGL	C20-CA9	-3.34	1.35	1.51
14	A	516	HEA	FE-NA	3.34	2.06	1.95
18	D	523	TGL	C10-CB9	-3.31	1.35	1.51
14	N	515	HEA	C4C-NC	-3.31	1.33	1.39
25	T	1269	CDL	C82-C81	-3.31	1.35	1.51
14	A	516	HEA	CHC-C4B	3.29	1.45	1.38
25	T	1269	CDL	C39-C38	-3.29	1.35	1.51
18	N	1521	TGL	C20-CA9	-3.28	1.35	1.51
14	N	516	HEA	C4D-ND	-3.28	1.32	1.38
14	A	515	HEA	FE-NB	3.26	2.04	1.94
25	T	1269	CDL	C79-C78	-3.26	1.35	1.51
14	N	515	HEA	C4A-NA	-3.25	1.33	1.39
25	G	269	CDL	C82-C81	-3.22	1.35	1.51
25	T	1269	CDL	C22-C21	-3.20	1.35	1.51
14	A	515	HEA	CHB-C1B	3.18	1.46	1.39
27	M	526	DMU	C3-C4	-3.17	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	522	PGV	O03-C19	3.17	1.42	1.33
25	G	269	CDL	C79-C78	-3.15	1.36	1.51
14	A	516	HEA	C1A-NA	-3.15	1.33	1.39
14	A	515	HEA	CHB-C4A	3.15	1.44	1.38
25	P	1270	CDL	C39-C38	-3.14	1.36	1.51
25	C	270	CDL	C42-C41	-3.14	1.36	1.51
18	L	522	TGL	C15-CC9	-3.13	1.36	1.51
14	N	516	HEA	CHA-C1A	3.12	1.44	1.38
14	A	516	HEA	CHB-C4A	3.12	1.44	1.38
25	P	1270	CDL	C42-C41	-3.11	1.36	1.51
18	N	1521	TGL	C15-CC9	-3.09	1.36	1.51
25	C	270	CDL	C39-C38	-3.09	1.36	1.51
18	N	1522	TGL	C15-CC9	-3.07	1.36	1.51
14	N	516	HEA	CHD-C1D	3.02	1.44	1.38
14	A	515	HEA	CHD-C4C	3.02	1.46	1.39
14	A	516	HEA	C4A-NA	-3.02	1.33	1.39
19	A	522	PGV	O01-C1	3.02	1.42	1.34
14	N	516	HEA	CHB-C1B	3.01	1.46	1.39
14	A	515	HEA	CHD-C1D	2.97	1.44	1.38
14	A	515	HEA	CHA-C4D	2.95	1.45	1.39
18	A	521	TGL	C15-CC9	-2.95	1.37	1.51
24	G	264	PEK	O03-C01	-2.92	1.38	1.45
14	A	515	HEA	C4C-NC	-2.92	1.34	1.39
14	A	515	HEA	C4B-C3B	-2.91	1.39	1.44
19	C	267	PGV	O03-C19	2.91	1.41	1.33
24	T	1264	PEK	O03-C21	2.87	1.41	1.33
14	N	515	HEA	C3B-C2B	2.86	1.41	1.34
14	N	516	HEA	CHC-C1C	2.83	1.45	1.39
14	A	515	HEA	C4B-NB	-2.83	1.35	1.40
22	B	1085	CHD	C11-C12	2.81	1.57	1.53
14	N	516	HEA	C4D-C3D	-2.81	1.40	1.45
14	N	516	HEA	C1D-ND	-2.80	1.35	1.40
14	N	515	HEA	C1D-ND	-2.78	1.35	1.40
14	N	516	HEA	CHC-C4B	2.77	1.44	1.38
14	A	515	HEA	C1D-C2D	-2.73	1.39	1.44
14	A	515	HEA	C1B-NB	-2.68	1.33	1.38
14	A	516	HEA	CHC-C1C	2.67	1.45	1.39
14	A	516	HEA	CHD-C1D	2.66	1.43	1.38
19	N	1266	PGV	O01-C1	2.62	1.41	1.34
14	N	516	HEA	FE-NC	2.59	2.03	1.95
27	Z	1526	DMU	C3-C4	-2.54	1.46	1.52
14	A	516	HEA	C1B-NB	-2.49	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	515	HEA	C1A-C2A	-2.44	1.40	1.45
14	A	515	HEA	C12-C13	2.44	1.61	1.53
14	N	515	HEA	CHC-C1C	2.44	1.44	1.39
14	N	516	HEA	C4B-NB	-2.44	1.36	1.40
14	A	516	HEA	C1C-NC	-2.42	1.35	1.39
14	A	516	HEA	C3A-C4A	-2.40	1.41	1.46
25	C	270	CDL	OB6-CB4	-2.38	1.41	1.46
19	C	267	PGV	O01-C1	2.38	1.41	1.34
14	N	516	HEA	C4C-NC	-2.37	1.35	1.39
14	A	515	HEA	C1A-NA	-2.37	1.35	1.39
24	T	1264	PEK	O03-C01	-2.34	1.39	1.45
14	N	516	HEA	C1B-NB	-2.34	1.34	1.38
14	A	515	HEA	C1D-ND	-2.34	1.36	1.40
14	N	516	HEA	C1A-C2A	-2.34	1.41	1.45
14	A	515	HEA	C1B-C2B	-2.33	1.39	1.44
14	A	515	HEA	C4D-C3D	-2.33	1.41	1.45
14	A	516	HEA	C1D-C2D	-2.30	1.39	1.44
14	N	516	HEA	C4A-NA	-2.28	1.35	1.39
22	B	1085	CHD	C4-C3	2.28	1.56	1.52
24	G	264	PEK	O01-C02	-2.27	1.41	1.46
14	A	516	HEA	C1D-ND	-2.26	1.36	1.40
22	P	1525	CHD	C11-C9	2.25	1.57	1.53
14	N	516	HEA	C1D-C2D	-2.25	1.39	1.44
14	A	515	HEA	C4A-NA	-2.21	1.35	1.39
24	G	264	PEK	O03-C21	2.18	1.39	1.33
14	A	515	HEA	C1C-NC	-2.15	1.35	1.39
14	N	515	HEA	C4D-ND	-2.14	1.34	1.38
22	B	1085	CHD	O25-C24	2.11	1.29	1.22
24	T	263	PEK	P-O11	2.10	1.67	1.59
14	N	515	HEA	CHA-C4D	2.09	1.44	1.39
14	N	515	HEA	C4D-C3D	-2.09	1.41	1.45
18	N	1522	TGL	CG1-CG2	2.09	1.57	1.50
14	A	516	HEA	C1B-C2B	-2.08	1.40	1.44
24	T	1265	PEK	P-O11	2.06	1.67	1.59
14	A	515	HEA	O2A-CGA	-2.05	1.24	1.30
25	P	1270	CDL	OB6-CB4	-2.04	1.41	1.46
14	A	516	HEA	C20-C19	2.04	1.55	1.51
14	A	516	HEA	C4D-ND	-2.04	1.34	1.38
18	L	522	TGL	CG1-CG2	2.01	1.57	1.50
24	T	1265	PEK	P-O12	2.01	1.67	1.59

All (439) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	515	HEA	C17-C18-C19	-10.92	102.64	127.62
14	A	515	HEA	C17-C18-C19	-10.74	103.05	127.62
14	N	515	HEA	C17-C16-C15	8.65	141.84	113.19
14	N	515	HEA	C3D-C4D-ND	7.88	117.97	110.35
14	A	515	HEA	C17-C16-C15	7.88	139.29	113.19
22	W	1059	CHD	C13-C17-C20	7.57	128.65	119.48
18	A	521	TGL	CG2-OG2-CB1	7.28	135.23	117.80
22	J	60	CHD	C6-C5-C10	7.04	120.15	112.66
22	W	1059	CHD	C11-C12-C13	6.76	118.14	111.26
22	W	1059	CHD	C17-C13-C14	-6.58	93.51	100.11
27	Z	1526	DMU	O7-C3-C2	6.57	123.93	107.23
18	N	1521	TGL	CG2-OG2-CB1	6.26	132.78	117.80
22	J	60	CHD	C13-C17-C20	6.20	127.00	119.48
19	P	1268	PGV	O01-C1-C2	6.17	124.82	111.48
14	N	515	HEA	C12-C11-C3B	6.12	121.69	112.12
22	J	60	CHD	C17-C13-C14	-6.11	93.98	100.11
22	W	1059	CHD	C6-C5-C10	6.07	119.12	112.66
22	W	1059	CHD	C9-C10-C5	5.95	116.78	108.51
22	W	1059	CHD	C14-C13-C12	5.90	112.81	107.42
22	W	1059	CHD	C18-C13-C12	-5.90	103.15	109.06
19	C	268	PGV	O01-C1-C2	5.57	123.54	111.48
22	J	60	CHD	C9-C10-C5	5.56	116.24	108.51
27	Z	1526	DMU	O1-C9-C8	5.55	119.70	109.70
22	P	1271	CHD	C1-C2-C3	5.43	117.68	110.48
27	M	526	DMU	O5-C4-C57	5.37	119.75	106.44
18	D	523	TGL	OG2-CB1-CB2	5.35	123.06	111.48
14	N	515	HEA	CAD-C3D-C4D	5.32	133.96	124.70
25	P	1270	CDL	OA6-CA5-C11	5.31	122.98	111.48
27	M	526	DMU	C2-C3-C4	5.30	122.67	110.93
27	Z	1526	DMU	O5-C6-C1	5.28	121.22	110.37
22	W	1059	CHD	C9-C11-C12	5.24	121.15	114.29
25	G	269	CDL	OA6-CA5-C11	5.24	122.81	111.48
27	Z	1526	DMU	O1-C9-C11	5.10	119.09	106.44
22	J	60	CHD	C10-C9-C8	5.09	117.51	111.84
18	Q	1523	TGL	OG2-CB1-CB2	5.05	122.41	111.48
25	G	269	CDL	OB6-CB5-C51	5.01	122.31	111.48
22	P	1271	CHD	C2-C1-C10	4.99	121.16	112.74
27	M	526	DMU	O1-C9-C8	4.94	118.59	109.70
14	N	516	HEA	C3C-C4C-NC	4.93	113.95	109.80
25	T	1269	CDL	OA6-CA5-C11	4.92	122.13	111.48
18	L	522	TGL	OG3-CC1-OC1	-4.92	111.33	123.63
27	M	526	DMU	O7-C3-C2	4.90	119.68	107.23
25	C	270	CDL	OA6-CA5-C11	4.89	122.06	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	515	HEA	C12-C13-C14	-4.87	99.38	112.16
22	J	60	CHD	C1-C10-C5	4.79	114.62	107.75
27	M	526	DMU	O1-C9-C11	4.79	118.31	106.44
22	C	271	CHD	C1-C2-C3	4.79	116.82	110.48
25	T	1269	CDL	OB6-CB5-C51	4.76	121.79	111.48
14	N	516	HEA	C12-C11-C3B	4.73	119.51	112.12
22	C	271	CHD	C19-C10-C1	-4.72	100.80	108.31
27	M	526	DMU	O1-C10-C5	4.72	120.08	110.37
14	N	516	HEA	C3A-C2A-C1A	-4.70	102.60	107.05
14	A	515	HEA	C12-C13-C14	-4.70	99.81	112.16
27	Z	1526	DMU	O5-C4-C57	4.68	118.03	106.44
27	M	526	DMU	O5-C6-C1	4.68	119.98	110.37
27	Z	1526	DMU	C8-C7-C5	4.62	118.95	110.83
24	G	264	PEK	O01-C1-O02	-4.61	112.94	123.70
14	N	515	HEA	C3B-C4B-NB	4.60	115.12	109.84
19	A	522	PGV	O03-C19-O04	-4.59	112.14	123.63
14	A	515	HEA	C12-C11-C3B	4.50	119.16	112.12
22	G	229	CHD	C18-C13-C12	-4.50	104.55	109.06
18	N	1522	TGL	CG2-OG2-CB1	4.49	128.54	117.80
22	J	60	CHD	C5-C4-C3	4.49	119.48	112.71
19	N	1266	PGV	O03-C19-C20	4.48	125.51	111.83
18	A	521	TGL	OG2-CB1-CB2	4.46	121.12	111.48
19	P	1268	PGV	O03-C19-C20	4.40	125.25	111.83
24	G	1263	PEK	O03-C21-C22	4.36	125.13	111.83
27	Z	1526	DMU	O5-C4-C3	4.32	118.65	109.72
19	C	268	PGV	O03-C19-C20	4.28	124.87	111.83
22	C	271	CHD	C2-C1-C10	4.26	119.93	112.74
22	J	60	CHD	C6-C5-C4	-4.23	106.39	111.23
19	A	522	PGV	O03-C19-C20	4.23	124.72	111.83
14	A	516	HEA	CAD-CBD-CGD	-4.21	102.49	113.67
24	C	265	PEK	O03-C21-C22	4.18	124.57	111.83
19	N	1266	PGV	O03-C19-O04	-4.17	113.19	123.63
18	A	521	TGL	OG1-CG1-CG2	4.10	120.22	108.40
14	A	516	HEA	C13-C12-C11	-4.07	107.89	114.39
22	J	60	CHD	C22-C20-C17	4.05	118.72	110.33
14	A	516	HEA	CMB-C2B-C1B	4.03	131.33	125.03
22	J	60	CHD	C14-C13-C12	4.03	111.10	107.42
14	A	516	HEA	C3A-C2A-C1A	-4.03	103.23	107.05
27	M	526	DMU	C8-C7-C5	4.03	117.90	110.83
18	D	523	TGL	OG1-CG1-CG2	4.02	119.99	108.40
21	B	229	PSC	O01-C1-C2	4.01	120.16	111.48
24	T	263	PEK	O03-C21-C22	4.00	124.04	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	522	TGL	OG3-CC1-CC2	3.94	123.84	111.83
14	N	515	HEA	C4D-C3D-C2D	-3.93	101.16	106.89
18	N	1522	TGL	OG1-CA1-CA2	3.92	123.80	111.83
22	P	1271	CHD	C19-C10-C1	-3.91	102.08	108.31
14	N	516	HEA	C2A-C1A-NA	3.91	114.10	110.32
24	T	1265	PEK	O01-C1-C2	3.87	119.85	111.48
18	N	1522	TGL	OG2-CB1-CB2	3.84	119.79	111.48
18	D	523	TGL	CG3-CG2-CG1	-3.82	102.87	111.78
24	T	1265	PEK	O03-C21-C22	3.82	123.47	111.83
24	T	1264	PEK	O03-C01-C02	-3.82	97.40	108.40
18	N	1521	TGL	OG2-CG2-CG3	3.81	122.03	108.34
22	J	60	CHD	C16-C17-C20	3.79	117.92	112.18
14	A	516	HEA	C2B-C1B-NB	3.79	114.29	109.90
22	W	1059	CHD	C18-C13-C17	3.79	117.14	111.20
14	N	516	HEA	CHB-C1B-NB	3.79	128.50	124.42
22	P	1271	CHD	C18-C13-C12	-3.78	105.27	109.06
27	Z	1526	DMU	O1-C10-C5	3.78	118.14	110.37
27	M	526	DMU	O5-C4-C3	3.77	117.52	109.72
22	J	60	CHD	C19-C10-C5	-3.77	104.14	110.44
22	C	271	CHD	C1-C10-C5	3.76	113.14	107.75
24	T	1264	PEK	O01-C1-O02	-3.74	114.96	123.70
19	N	1524	PGV	O01-C1-C2	3.72	119.54	111.48
14	A	515	HEA	C27-C19-C18	-3.71	114.09	123.63
22	P	1525	CHD	C15-C14-C13	3.71	107.14	103.54
22	W	1059	CHD	C22-C20-C17	3.70	118.01	110.33
18	N	1521	TGL	CG3-OG3-CC1	3.69	130.60	117.12
14	N	515	HEA	C20-C19-C18	3.68	129.43	121.17
22	W	1059	CHD	C5-C4-C3	3.67	118.25	112.71
22	J	60	CHD	C4-C5-C10	3.66	116.55	112.66
14	N	515	HEA	C27-C19-C18	-3.66	114.24	123.63
18	L	522	TGL	CG2-OG2-CB1	3.64	126.52	117.80
22	P	1271	CHD	C10-C9-C8	3.64	115.90	111.84
14	N	515	HEA	C1D-ND-C4D	-3.64	100.90	105.21
22	G	229	CHD	C1-C2-C3	-3.63	105.68	110.48
19	N	1524	PGV	O03-C19-C20	3.59	122.78	111.83
22	W	1059	CHD	C1-C10-C5	3.59	112.90	107.75
22	C	271	CHD	C10-C9-C8	3.58	115.83	111.84
22	P	1271	CHD	C15-C14-C13	3.58	107.02	103.54
14	A	516	HEA	C2A-C1A-NA	3.58	113.78	110.32
25	C	270	CDL	OB8-CB7-C71	3.57	122.73	111.83
22	W	1059	CHD	C17-C13-C12	3.57	120.88	117.67
14	N	515	HEA	CHA-C4D-C3D	-3.57	119.57	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	1270	CDL	OB8-CB7-C71	3.55	122.66	111.83
22	P	1271	CHD	C1-C10-C5	3.54	112.83	107.75
24	T	263	PEK	O01-C1-C2	3.51	119.07	111.48
24	G	1263	PEK	C02-O01-C1	3.45	126.04	117.80
18	Q	1523	TGL	CG3-CG2-CG1	-3.43	103.79	111.78
22	W	1059	CHD	C1-C10-C9	-3.42	106.02	111.34
24	G	264	PEK	C2-C3-C4	3.41	120.79	113.35
24	G	1263	PEK	O01-C1-C2	3.38	118.79	111.48
22	C	271	CHD	C18-C13-C12	-3.37	105.68	109.06
14	A	516	HEA	C17-C18-C19	3.36	135.32	127.62
18	N	1522	TGL	CG1-OG1-CA1	3.35	129.37	117.12
14	A	515	HEA	C3C-C4C-NC	3.35	112.62	109.80
25	P	1270	CDL	OB8-CB7-OB9	-3.33	115.30	123.63
14	N	516	HEA	CHB-C1B-C2B	-3.32	119.78	125.03
25	T	1269	CDL	OA8-CA7-C31	3.32	121.96	111.83
14	N	516	HEA	C4C-C3C-C2C	-3.31	103.18	107.30
14	N	516	HEA	C17-C18-C19	3.30	135.17	127.62
24	G	1263	PEK	O03-C01-C02	3.28	117.85	108.40
22	J	60	CHD	C4-C3-C2	3.28	114.62	110.62
14	N	515	HEA	C3C-C2C-C1C	-3.28	103.31	107.17
14	A	515	HEA	C20-C19-C18	3.27	128.52	121.17
14	N	516	HEA	C3D-C4D-ND	3.26	113.51	110.35
27	Z	1526	DMU	C2-C3-C4	3.26	118.15	110.93
14	A	516	HEA	C3C-C4C-NC	3.25	112.53	109.80
25	P	1270	CDL	OA8-CA7-C31	3.24	121.72	111.83
25	T	1269	CDL	OA6-CA5-OA7	-3.23	116.15	123.70
14	N	516	HEA	O2A-CGA-CBA	3.23	124.21	114.00
24	C	265	PEK	O01-C1-C2	3.23	118.47	111.48
18	D	523	TGL	OG3-CC1-CC2	3.22	121.66	111.83
25	G	269	CDL	C79-C78-C77	3.22	130.64	114.37
22	W	1059	CHD	C19-C10-C5	-3.21	105.06	110.44
18	N	1521	TGL	OG2-CB1-CB2	3.20	118.40	111.48
14	N	515	HEA	O2A-CGA-CBA	3.20	124.11	114.00
18	D	523	TGL	OG2-CB1-OB1	-3.20	116.23	123.70
14	N	516	HEA	O1A-CGA-CBA	-3.19	112.97	123.09
18	Q	1523	TGL	OG1-CA1-CA2	3.19	121.56	111.83
27	Z	1526	DMU	C57-C4-C3	3.19	122.35	113.38
22	G	229	CHD	C4-C3-C2	-3.19	106.73	110.62
14	A	515	HEA	C21-C20-C19	-3.18	102.66	113.19
22	G	229	CHD	C10-C9-C8	3.17	115.37	111.84
18	A	521	TGL	CA3-CA2-CA1	-3.16	102.10	113.69
22	B	1085	CHD	C1-C10-C5	3.16	112.28	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	1059	CHD	C5-C6-C7	3.15	118.15	114.40
22	P	1271	CHD	C16-C17-C13	3.13	106.58	103.54
14	A	516	HEA	C1B-C2B-C3B	-3.13	103.17	106.80
22	P	1271	CHD	C9-C10-C5	3.13	112.86	108.51
22	W	1059	CHD	C6-C5-C4	-3.13	107.66	111.23
18	L	522	TGL	CC3-CC2-CC1	3.12	125.14	113.69
21	O	1229	PSC	O03-C19-C20	3.11	121.33	111.83
14	A	515	HEA	CHB-C1B-NB	3.08	127.73	124.42
14	N	515	HEA	OMA-CMA-C3A	-3.07	118.69	125.62
22	B	1085	CHD	C19-C10-C5	-3.05	105.33	110.44
27	M	526	DMU	C11-C9-C8	3.05	120.50	113.02
19	N	1266	PGV	O01-C1-O02	-3.04	116.59	123.70
14	A	515	HEA	OMA-CMA-C3A	-3.04	118.76	125.62
24	G	264	PEK	C24-C23-C22	-3.02	102.04	113.13
18	N	1522	TGL	OG3-CC1-CC2	3.00	121.00	111.83
22	W	1059	CHD	C10-C9-C8	3.00	115.19	111.84
18	L	522	TGL	OG2-CB1-CB2	3.00	117.97	111.48
27	Z	1526	DMU	O7-C3-C4	3.00	117.33	109.48
18	L	522	TGL	OG1-CA1-CA2	2.99	120.96	111.83
18	A	521	TGL	CG3-OG3-CC1	2.99	128.05	117.12
25	C	270	CDL	OA8-CA7-C31	2.99	120.94	111.83
14	A	516	HEA	CHD-C1D-ND	2.97	128.04	124.37
22	B	1085	CHD	C4-C3-C2	2.96	114.23	110.62
22	C	271	CHD	C15-C14-C8	2.95	122.40	118.36
18	D	523	TGL	CB3-CB2-CB1	2.94	124.46	113.69
18	D	523	TGL	OG1-CA1-CA2	2.94	120.78	111.83
18	A	521	TGL	OG2-CG2-CG3	2.92	118.82	108.34
25	G	269	CDL	OA6-CA5-OA7	-2.90	116.93	123.70
18	N	1521	TGL	OG1-CA1-CA2	2.90	120.66	111.83
14	A	516	HEA	C25-C23-C24	2.89	121.24	114.59
22	J	60	CHD	C1-C10-C9	-2.89	106.86	111.34
18	A	521	TGL	OG2-CG2-CG1	2.89	118.69	108.34
24	C	265	PEK	O03-C21-O04	-2.88	116.42	123.63
22	B	1085	CHD	C15-C14-C13	2.88	106.33	103.54
14	N	515	HEA	C2C-C1C-NC	2.88	114.75	110.14
22	C	271	CHD	C22-C23-C24	-2.87	104.83	112.49
18	A	521	TGL	OG3-CC1-CC2	2.87	120.57	111.83
25	G	269	CDL	OA8-CA7-C31	2.85	120.54	111.83
18	D	523	TGL	CG3-OG3-CC1	2.85	127.52	117.12
25	C	270	CDL	OA8-CA6-CA4	2.84	116.58	108.40
25	C	270	CDL	C52-C51-CB5	-2.84	103.29	113.69
19	P	1267	PGV	O01-C1-O02	-2.83	117.10	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C6-C7-C8	2.82	114.58	111.50
22	C	271	CHD	C6-C7-C8	2.82	114.57	111.50
14	N	515	HEA	CHB-C4A-NA	2.81	127.52	124.45
22	W	1059	CHD	C4-C5-C10	2.81	115.65	112.66
22	G	229	CHD	C6-C5-C4	-2.80	108.02	111.23
18	A	521	TGL	OG3-CC1-OC1	-2.80	116.64	123.63
14	N	516	HEA	O11-C11-C3B	-2.80	106.13	111.26
22	B	1085	CHD	C22-C20-C17	2.79	116.11	110.33
22	J	60	CHD	C18-C13-C12	-2.78	106.28	109.06
18	Q	1523	TGL	OG3-CC1-CC2	2.78	120.31	111.83
21	O	1229	PSC	O01-C1-C2	2.78	117.49	111.48
19	A	524	PGV	O01-C02-C01	2.77	118.28	108.34
14	N	515	HEA	CHD-C1D-ND	2.76	127.79	124.37
14	N	515	HEA	C21-C20-C19	-2.76	104.04	113.19
24	T	1264	PEK	O13-P-O14	2.76	125.28	112.44
25	G	269	CDL	C80-C79-C78	2.76	128.30	114.37
22	J	60	CHD	C5-C6-C7	2.75	117.67	114.40
22	P	1525	CHD	C21-C20-C22	-2.74	106.10	110.34
22	C	271	CHD	C5-C6-C7	2.73	117.65	114.40
19	N	1524	PGV	O03-C19-O04	-2.72	116.83	123.63
18	D	523	TGL	CC3-CC2-CC1	-2.71	103.75	113.69
25	P	1270	CDL	OB6-CB5-C51	2.70	117.33	111.48
14	N	515	HEA	CHB-C1B-C2B	-2.70	120.76	125.03
18	Q	1523	TGL	CG2-OG2-CB1	2.70	124.26	117.80
27	M	526	DMU	C7-C8-C9	2.70	115.12	110.23
14	N	516	HEA	C3B-C4B-NB	2.70	112.94	109.84
24	T	263	PEK	C02-O01-C1	2.70	124.25	117.80
14	N	515	HEA	C13-C14-C15	-2.70	121.45	127.62
14	N	515	HEA	CHD-C1D-C2D	-2.69	119.30	126.95
19	A	524	PGV	O03-C19-C20	2.67	119.99	111.83
18	N	1522	TGL	OB1-CB1-CB2	-2.67	113.32	123.78
24	G	264	PEK	O01-C02-C01	-2.66	98.80	108.34
14	N	516	HEA	CHA-C4D-C3D	-2.66	120.90	124.77
18	N	1522	TGL	OG3-CC1-OC1	-2.65	117.00	123.63
18	Q	1523	TGL	CG3-OG3-CC1	2.64	126.78	117.12
22	J	60	CHD	C19-C10-C1	-2.64	104.11	108.31
24	T	1265	PEK	O03-C21-O04	-2.64	117.03	123.63
24	T	263	PEK	O03-C01-C02	2.62	115.96	108.40
27	M	526	DMU	C1-C2-C3	2.62	115.63	109.68
18	N	1522	TGL	OG1-CG1-CG2	2.62	115.94	108.40
21	B	229	PSC	O03-C19-C20	2.62	119.81	111.83
22	J	60	CHD	C18-C13-C17	2.62	115.30	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	271	CHD	C9-C10-C5	2.61	112.13	108.51
25	C	270	CDL	CA6-CA4-CA3	-2.60	105.73	111.78
14	N	515	HEA	CBA-CAA-C2A	2.60	119.71	112.53
19	P	1267	PGV	C27-C26-C25	-2.59	101.29	114.37
25	T	1269	CDL	OA8-CA7-OA9	-2.58	117.16	123.63
27	M	526	DMU	O16-C6-C1	2.58	112.19	108.27
22	P	1271	CHD	C15-C14-C8	2.56	121.87	118.36
25	C	270	CDL	C39-C38-C37	2.56	127.31	114.37
14	N	516	HEA	CAA-CBA-CGA	-2.56	106.88	113.67
14	N	516	HEA	O1D-CGD-CBD	-2.55	115.00	123.09
14	A	516	HEA	O1A-CGA-CBA	-2.55	115.01	123.09
14	N	516	HEA	C27-C19-C20	2.55	119.65	115.23
27	Z	1526	DMU	C7-C8-C9	2.54	114.83	110.23
22	C	271	CHD	C6-C5-C10	2.53	115.36	112.66
22	P	1525	CHD	C10-C9-C8	-2.53	109.02	111.84
14	A	516	HEA	CMB-C2B-C3B	-2.52	125.39	130.28
27	M	526	DMU	C10-C5-C7	2.52	115.30	110.01
24	T	1264	PEK	O01-C1-C2	2.51	116.92	111.48
14	N	515	HEA	C26-C15-C16	-2.51	110.86	115.23
25	P	1270	CDL	C39-C38-C37	2.51	127.07	114.37
14	A	516	HEA	O11-C11-C3B	-2.51	106.66	111.26
14	N	515	HEA	C3A-C2A-C1A	-2.51	104.67	107.05
14	A	516	HEA	C21-C22-C23	-2.51	119.28	127.64
19	N	1266	PGV	O03-C01-C02	2.51	115.62	108.40
14	N	515	HEA	C2D-C1D-ND	2.50	112.71	109.84
19	C	268	PGV	O03-C19-O04	-2.50	117.38	123.63
14	N	516	HEA	CMB-C2B-C3B	-2.50	125.44	130.28
22	C	271	CHD	C14-C13-C12	2.49	109.69	107.42
22	C	525	CHD	C6-C7-C8	2.49	114.22	111.50
22	C	271	CHD	O7-C7-C8	2.49	115.22	109.52
18	Q	1523	TGL	CC3-CC2-CC1	-2.49	104.58	113.69
24	T	1265	PEK	C01-O03-C21	2.49	126.20	117.12
14	N	516	HEA	C1C-CHC-C4B	-2.48	120.41	126.25
25	P	1270	CDL	OA4-PA1-OA3	2.46	123.91	112.44
24	T	1264	PEK	C24-C23-C22	-2.46	104.08	113.13
25	C	270	CDL	OB8-CB7-OB9	-2.46	117.47	123.63
24	G	264	PEK	O03-C01-C02	-2.46	101.31	108.40
22	W	1059	CHD	C4-C3-C2	2.46	113.61	110.62
25	P	1270	CDL	CB6-CB4-CB3	-2.45	106.07	111.78
14	N	516	HEA	C20-C19-C18	-2.45	115.67	121.17
27	Z	1526	DMU	O3-C5-C7	2.45	116.14	110.38
25	P	1270	CDL	OA8-CA7-OA9	-2.43	117.55	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	524	PGV	C4-C3-C2	-2.43	104.19	113.13
14	A	516	HEA	CHC-C1C-C2C	-2.43	120.37	127.43
14	N	515	HEA	C4C-CHD-C1D	-2.42	120.55	126.25
22	C	271	CHD	C15-C14-C13	2.42	105.89	103.54
14	A	516	HEA	O2D-CGD-CBD	2.42	121.64	114.00
14	N	515	HEA	C4A-CHB-C1B	-2.42	120.88	126.02
24	T	1264	PEK	C30-C29-C28	-2.42	102.15	114.37
18	N	1521	TGL	C21-C20-CA9	2.41	126.57	114.37
19	C	267	PGV	O01-C1-C2	2.41	116.70	111.48
18	A	521	TGL	OB1-CB1-CB2	-2.41	114.36	123.78
14	A	516	HEA	C3D-C4D-ND	2.41	112.68	110.35
14	N	515	HEA	CHC-C4B-C3B	-2.41	119.73	125.80
24	C	265	PEK	C24-C23-C22	2.40	121.95	113.13
25	G	269	CDL	OB8-CB7-OB9	-2.40	117.62	123.63
14	N	515	HEA	C4B-C3B-C2B	-2.40	103.40	107.44
14	N	516	HEA	C12-C13-C14	-2.40	105.86	112.16
22	P	1525	CHD	C22-C23-C24	-2.39	106.11	112.49
22	J	60	CHD	C14-C8-C7	2.39	115.02	111.85
24	G	264	PEK	O01-C1-C2	2.38	116.63	111.48
19	C	267	PGV	C9-C10-C11	-2.38	99.27	112.60
22	G	229	CHD	O3-C3-C4	-2.38	105.11	109.84
18	N	1521	TGL	OG1-CG1-CG2	2.36	115.21	108.40
25	P	1270	CDL	OA6-CA5-OA7	-2.36	118.18	123.70
18	Q	1523	TGL	OG2-CG2-CG3	2.36	116.82	108.34
18	L	522	TGL	CA8-CA7-CA6	-2.36	102.43	114.37
18	Q	1523	TGL	OG1-CA1-OA1	-2.36	117.73	123.63
18	A	521	TGL	OG1-CA1-CA2	2.35	119.01	111.83
22	B	1085	CHD	O25-C24-C23	-2.35	115.64	123.09
25	C	270	CDL	C53-C52-C51	-2.35	104.51	113.13
18	N	1521	TGL	CG1-OG1-CA1	-2.34	108.56	117.12
19	P	1268	PGV	O03-C19-O04	-2.34	117.77	123.63
22	C	271	CHD	C11-C12-C13	2.34	113.64	111.26
24	G	1263	PEK	C01-O03-C21	2.33	125.63	117.12
24	G	264	PEK	C25-C24-C23	-2.32	102.64	114.37
22	P	1271	CHD	C5-C4-C3	-2.32	109.21	112.71
22	C	271	CHD	C16-C17-C13	2.32	105.79	103.54
14	A	516	HEA	CHD-C1D-C2D	-2.31	120.37	126.95
14	N	515	HEA	C25-C23-C22	-2.31	115.72	122.66
22	P	1271	CHD	C18-C13-C14	2.31	114.83	111.20
18	N	1522	TGL	C11-C10-CB9	2.31	126.04	114.37
18	L	522	TGL	OB1-CB1-CB2	-2.31	114.76	123.78
14	A	515	HEA	C3C-C2C-C1C	-2.31	104.45	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1525	CHD	C14-C8-C9	2.30	112.96	109.75
22	J	60	CHD	C17-C13-C12	2.30	119.74	117.67
14	N	515	HEA	C16-C15-C14	2.30	126.32	121.17
22	C	525	CHD	C1-C2-C3	-2.29	107.44	110.48
24	T	263	PEK	C01-O03-C21	2.29	125.49	117.12
24	T	1264	PEK	C34-C33-C32	-2.29	102.79	114.37
22	P	1271	CHD	C14-C8-C9	-2.29	106.55	109.75
22	P	1525	CHD	C6-C5-C4	-2.29	108.61	111.23
21	B	229	PSC	O01-C1-O02	-2.29	118.36	123.70
14	N	516	HEA	CHD-C1D-C2D	-2.28	120.46	126.95
22	P	1271	CHD	C6-C5-C10	2.28	115.08	112.66
19	N	1266	PGV	O01-C1-C2	2.27	116.40	111.48
14	N	516	HEA	CMB-C2B-C1B	2.27	128.59	125.03
22	P	1271	CHD	C22-C23-C24	-2.27	106.43	112.49
14	A	516	HEA	C20-C19-C18	-2.26	116.08	121.17
18	A	521	TGL	CB7-CB6-CB5	-2.26	102.93	114.37
25	T	1269	CDL	C82-C81-C80	2.26	125.80	114.37
18	N	1522	TGL	OA1-CA1-CA2	-2.26	114.94	123.78
24	G	264	PEK	C27-C26-C25	-2.26	102.96	114.37
25	G	269	CDL	C83-C82-C81	2.26	125.77	114.37
14	N	516	HEA	C2D-C1D-ND	2.25	112.43	109.84
18	N	1522	TGL	CG3-OG3-CC1	2.24	125.31	117.12
27	Z	1526	DMU	C11-C9-C8	2.24	118.51	113.02
14	N	515	HEA	C4B-NB-C1B	-2.24	102.56	105.21
22	B	1085	CHD	C14-C8-C7	2.23	114.81	111.85
22	B	1085	CHD	O3-C3-C4	-2.23	105.41	109.84
24	G	1263	PEK	O03-C21-O04	-2.23	118.06	123.63
19	P	1268	PGV	O02-C1-C2	-2.23	115.08	123.78
19	N	1524	PGV	C4-C3-C2	-2.22	104.96	113.13
18	D	523	TGL	OG1-CA1-OA1	-2.22	118.08	123.63
25	G	269	CDL	OA8-CA7-OA9	-2.21	118.09	123.63
14	A	516	HEA	O2A-CGA-CBA	2.21	120.99	114.00
19	C	267	PGV	C4-C3-C2	-2.21	105.01	113.13
18	L	522	TGL	CB4-CB3-CB2	-2.20	105.03	113.13
24	T	1265	PEK	O03-C01-C02	2.20	114.73	108.40
18	L	522	TGL	OG1-CG1-CG2	2.19	114.72	108.40
14	N	515	HEA	CHC-C1C-C2C	-2.19	121.07	127.43
27	Z	1526	DMU	C10-C5-C7	2.19	114.62	110.01
18	N	1522	TGL	OG2-CG2-CG1	2.19	116.20	108.34
19	A	524	PGV	O03-C01-C02	2.19	114.70	108.40
27	M	526	DMU	O3-C5-C7	2.18	115.52	110.38
25	C	270	CDL	OA6-CA5-OA7	-2.18	118.61	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	522	TGL	OG2-CG2-CG1	2.18	116.16	108.34
19	P	1268	PGV	C03-C02-C01	-2.17	106.72	111.78
19	C	268	PGV	O02-C1-C2	-2.17	115.28	123.78
25	C	270	CDL	C40-C39-C38	2.17	125.34	114.37
18	N	1521	TGL	CB7-CB6-CB5	-2.17	103.41	114.37
18	A	521	TGL	CB3-CB2-CB1	-2.16	105.76	113.69
14	N	516	HEA	CHC-C4B-C3B	-2.16	120.34	125.80
18	N	1521	TGL	CA3-CA2-CA1	-2.16	105.77	113.69
14	A	516	HEA	CHB-C4A-NA	-2.16	122.10	124.45
25	T	1269	CDL	C83-C82-C81	2.16	125.29	114.37
14	A	516	HEA	O1D-CGD-CBD	-2.16	116.25	123.09
18	L	522	TGL	C15-CC9-CC8	2.16	125.26	114.37
27	M	526	DMU	C57-C4-C3	2.15	119.44	113.38
18	N	1522	TGL	CC3-CC2-CC1	2.15	121.56	113.69
25	C	270	CDL	C42-C41-C40	2.15	125.21	114.37
14	N	516	HEA	CHA-C1A-NA	-2.14	122.12	124.45
14	A	515	HEA	CAD-C3D-C4D	2.14	128.43	124.70
14	A	515	HEA	C25-C23-C22	-2.14	116.24	122.66
22	W	1059	CHD	C16-C17-C20	2.13	115.41	112.18
25	C	270	CDL	C57-C56-C55	-2.13	103.61	114.37
25	P	1270	CDL	C40-C39-C38	2.12	125.10	114.37
24	G	264	PEK	C32-C31-C30	-2.12	103.65	114.37
14	N	515	HEA	O1D-CGD-CBD	-2.12	116.38	123.09
18	Q	1523	TGL	C11-C10-CB9	2.11	125.06	114.37
14	A	515	HEA	C4B-C3B-C2B	-2.11	103.89	107.44
18	N	1522	TGL	C25-C24-C23	-2.11	103.69	114.37
18	A	521	TGL	C21-C20-CA9	2.11	125.04	114.37
22	G	229	CHD	C18-C13-C14	2.11	114.51	111.20
14	N	515	HEA	CHB-C1B-NB	2.11	126.69	124.42
24	T	1264	PEK	C28-C27-C26	-2.10	103.75	114.37
22	J	60	CHD	C21-C20-C17	-2.10	109.73	112.88
22	P	1525	CHD	C16-C15-C14	-2.10	101.04	105.14
14	A	515	HEA	O11-C11-C3B	-2.10	107.41	111.26
18	Q	1523	TGL	OG1-CG1-CG2	2.09	114.43	108.40
25	P	1270	CDL	C42-C41-C40	2.09	124.93	114.37
19	C	267	PGV	O03-C19-O04	-2.08	118.42	123.63
24	T	1264	PEK	C01-O03-C21	2.08	124.72	117.12
19	A	524	PGV	C02-O01-C1	2.08	122.77	117.80
18	N	1522	TGL	C15-CC9-CC8	2.08	124.87	114.37
27	Z	1526	DMU	C10-O1-C9	-2.07	109.68	113.72
25	T	1269	CDL	OB6-CB5-OB7	-2.06	118.88	123.70
19	P	1267	PGV	C25-C24-C23	-2.05	103.99	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	516	HEA	C13-C12-C11	-2.05	111.11	114.39
18	Q	1523	TGL	C21-C20-CA9	2.05	124.73	114.37
22	G	229	CHD	C11-C9-C8	2.05	113.92	110.89
25	P	1270	CDL	C53-C52-C51	-2.04	105.63	113.13
22	B	1085	CHD	C13-C17-C20	-2.04	117.02	119.48
22	G	229	CHD	C13-C14-C8	-2.03	112.15	114.72
14	N	515	HEA	C2B-C1B-NB	2.03	112.24	109.90
14	A	516	HEA	CAA-C2A-C1A	2.02	128.97	124.85
25	C	270	CDL	OA4-PA1-OA3	2.02	121.86	112.44
14	N	516	HEA	CAD-CBD-CGD	-2.02	108.30	113.67
14	A	516	HEA	C27-C19-C20	2.02	118.74	115.23
22	C	525	CHD	C19-C10-C1	-2.02	105.09	108.31
19	C	267	PGV	C8-C9-C10	-2.02	104.14	113.86
14	N	516	HEA	CHC-C1C-C2C	-2.02	121.57	127.43
25	T	1269	CDL	OB8-CB6-CB4	2.02	114.21	108.40
22	P	1271	CHD	C13-C14-C8	2.01	117.27	114.72
14	N	515	HEA	CAA-CBA-CGA	-2.01	108.33	113.67
25	T	1269	CDL	C39-C38-C37	2.00	124.50	114.37

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	M	526	DMU	C5
27	M	526	DMU	C2
27	Z	1526	DMU	C3
27	Z	1526	DMU	C4
27	Z	1526	DMU	C5
27	Z	1526	DMU	C2

All (977) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	515	HEA	C2A-C3A-CMA-OMA
14	A	515	HEA	C4A-C3A-CMA-OMA
14	N	515	HEA	C2A-C3A-CMA-OMA
14	N	515	HEA	C4A-C3A-CMA-OMA
18	Q	1523	TGL	OC1-CC1-OG3-CG3
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	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C04-O12-P-O11
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	N	1524	PGV	C04-O12-P-O11
19	N	1524	PGV	C04-O12-P-O13
19	N	1524	PGV	C04-O12-P-O14
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	O12-C04-C05-C06
19	N	1524	PGV	C04-C05-C06-O06
19	N	1524	PGV	O05-C05-C06-O06
19	N	1524	PGV	O02-C1-O01-C02
19	P	1268	PGV	C04-O12-P-O11
19	P	1268	PGV	C04-O12-P-O14
19	P	1268	PGV	C04-C05-C06-O06
19	P	1268	PGV	C2-C1-O01-C02
21	B	229	PSC	C03-O11-P-O14
21	B	229	PSC	C04-O12-P-O11
21	B	229	PSC	C04-O12-P-O14
21	O	1229	PSC	C03-O11-P-O12
21	O	1229	PSC	C03-O11-P-O14
21	O	1229	PSC	C04-O12-P-O11
21	O	1229	PSC	C04-O12-P-O13
21	O	1229	PSC	C04-O12-P-O14
21	O	1229	PSC	O12-C04-C05-N
21	O	1229	PSC	C11-C12-C13-C14
22	W	1059	CHD	C13-C17-C20-C22
22	W	1059	CHD	C16-C17-C20-C22
24	C	265	PEK	C04-O12-P-O11
24	C	265	PEK	C04-O12-P-O13
24	C	265	PEK	C5-C6-C7-C8
24	G	1263	PEK	C03-O11-P-O12
24	G	1263	PEK	C03-O11-P-O14
24	G	1263	PEK	O03-C01-C02-O01
24	G	1263	PEK	O12-C04-C05-N
24	T	263	PEK	C03-O11-P-O12
24	T	263	PEK	C03-O11-P-O13
24	T	263	PEK	C03-O11-P-O14
24	T	263	PEK	O03-C01-C02-O01
24	T	263	PEK	O12-C04-C05-N
24	T	263	PEK	C12-C13-C14-C15
24	T	1265	PEK	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
24	T	1265	PEK	C04-O12-P-O13
24	T	1265	PEK	C04-O12-P-O14
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-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
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	CA2-OA2-PA1-OA5
25	G	269	CDL	C11-CA5-OA6-CA4
25	G	269	CDL	C1-CB2-OB2-PB2
25	G	269	CDL	CB3-OB5-PB2-OB2
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	CA2-OA2-PA1-OA5
25	P	1270	CDL	CA3-OA5-PA1-OA2
25	P	1270	CDL	C11-CA5-OA6-CA4
25	P	1270	CDL	CB2-OB2-PB2-OB3
25	P	1270	CDL	CB2-OB2-PB2-OB4
25	T	1269	CDL	C1-CB2-OB2-PB2
25	T	1269	CDL	CB3-OB5-PB2-OB2
25	T	1269	CDL	CB3-OB5-PB2-OB3
25	T	1269	CDL	CB3-OB5-PB2-OB4
25	T	1269	CDL	OB6-CB4-CB6-OB8
27	M	526	DMU	O5-C6-O16-C18
18	D	523	TGL	OC1-CC1-OG3-CG3
19	A	524	PGV	O04-C19-O03-C01
18	D	523	TGL	CC2-CC1-OG3-CG3
19	A	524	PGV	C20-C19-O03-C01
18	N	1522	TGL	OA1-CA1-OG1-CG1
19	N	1524	PGV	O04-C19-O03-C01
25	T	1269	CDL	OA9-CA7-OA8-CA6
18	A	521	TGL	OB1-CB1-OG2-CG2
19	P	1268	PGV	O02-C1-O01-C02
25	G	269	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	OA7-CA5-OA6-CA4
25	T	1269	CDL	OA7-CA5-OA6-CA4
18	Q	1523	TGL	CA2-CA1-OG1-CG1
19	N	1524	PGV	C20-C19-O03-C01
25	G	269	CDL	C31-CA7-OA8-CA6
19	A	524	PGV	C2-C1-O01-C02
19	N	1524	PGV	C2-C1-O01-C02
25	T	1269	CDL	C11-CA5-OA6-CA4
22	J	60	CHD	C16-C17-C20-C22
18	N	1521	TGL	CA2-CA1-OG1-CG1
18	Q	1523	TGL	CC2-CC1-OG3-CG3
21	B	229	PSC	C20-C19-O03-C01
25	T	1269	CDL	C31-CA7-OA8-CA6
19	P	1268	PGV	C10-C11-C12-C13
21	B	229	PSC	C11-C10-C9-C8
24	C	265	PEK	C4-C5-C6-C7
24	C	265	PEK	C7-C8-C9-C10
24	G	264	PEK	C10-C11-C12-C13
24	G	1263	PEK	C7-C8-C9-C10
24	T	263	PEK	C7-C8-C9-C10
24	T	1264	PEK	C7-C8-C9-C10
24	T	1265	PEK	C4-C5-C6-C7
24	T	1265	PEK	C7-C8-C9-C10
24	T	1265	PEK	C10-C11-C12-C13
25	G	269	CDL	OA9-CA7-OA8-CA6
19	C	268	PGV	O02-C1-O01-C02
25	C	270	CDL	OA7-CA5-OA6-CA4
22	W	1059	CHD	C16-C17-C20-C21
21	O	1229	PSC	C22-C23-C24-C25
25	G	269	CDL	O1-C1-CA2-OA2
25	T	1269	CDL	O1-C1-CA2-OA2
18	L	522	TGL	CA2-CA1-OG1-CG1
18	N	1522	TGL	CA2-CA1-OG1-CG1
21	O	1229	PSC	C20-C19-O03-C01
18	Q	1523	TGL	OA1-CA1-OG1-CG1
18	A	521	TGL	CB2-CB1-OG2-CG2
19	C	268	PGV	C2-C1-O01-C02
25	G	269	CDL	C40-C41-C42-C43
18	D	523	TGL	CA2-CA1-OG1-CG1
18	N	1521	TGL	OA1-CA1-OG1-CG1
14	A	515	HEA	C15-C16-C17-C18
14	N	515	HEA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	A	521	TGL	C21-C20-CA9-CA8
22	C	271	CHD	C21-C20-C22-C23
22	P	1271	CHD	C21-C20-C22-C23
25	G	269	CDL	C77-C78-C79-C80
21	B	229	PSC	O04-C19-O03-C01
21	O	1229	PSC	O04-C19-O03-C01
22	C	271	CHD	C17-C20-C22-C23
22	P	1271	CHD	C17-C20-C22-C23
21	O	1229	PSC	C11-C10-C9-C8
24	C	265	PEK	C10-C11-C12-C13
24	C	265	PEK	C13-C14-C15-C16
24	G	264	PEK	C13-C14-C15-C16
24	G	1263	PEK	C4-C5-C6-C7
24	T	263	PEK	C4-C5-C6-C7
24	T	263	PEK	C10-C11-C12-C13
24	T	1265	PEK	C13-C14-C15-C16
18	L	522	TGL	OA1-CA1-OG1-CG1
18	L	522	TGL	CC2-CC3-CC4-CC5
18	Q	1523	TGL	C21-C20-CA9-CA8
18	D	523	TGL	OA1-CA1-OG1-CG1
18	N	1521	TGL	OB1-CB1-OG2-CG2
19	A	524	PGV	O12-C04-C05-C06
19	P	1268	PGV	O12-C04-C05-C06
25	C	270	CDL	CB2-C1-CA2-OA2
18	A	521	TGL	CA2-CA1-OG1-CG1
25	G	269	CDL	C22-C23-C24-C25
18	D	523	TGL	C16-C15-CC9-CC8
18	N	1521	TGL	C21-C20-CA9-CA8
18	Q	1523	TGL	C11-C10-CB9-CB8
18	Q	1523	TGL	C16-C15-CC9-CC8
25	T	1269	CDL	C22-C23-C24-C25
25	P	1270	CDL	C79-C80-C81-C82
25	C	270	CDL	C17-C18-C19-C20
27	Z	1526	DMU	O6-C11-C9-C8
19	A	524	PGV	O12-C04-C05-O05
19	C	268	PGV	O12-C04-C05-O05
25	P	1270	CDL	O1-C1-CB2-OB2
21	B	229	PSC	C20-C21-C22-C23
18	A	521	TGL	OA1-CA1-OG1-CG1
18	L	522	TGL	C21-C20-CA9-CA8
21	O	1229	PSC	C20-C21-C22-C23
21	B	229	PSC	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
18	N	1521	TGL	CB2-CB1-OG2-CG2
21	B	229	PSC	C2-C1-O01-C02
27	M	526	DMU	O5-C4-C57-O61
19	C	268	PGV	C20-C19-O03-C01
19	P	1267	PGV	C10-C11-C12-C13
24	G	264	PEK	C7-C8-C9-C10
19	C	268	PGV	O05-C05-C06-O06
22	J	60	CHD	C13-C17-C20-C22
22	W	1059	CHD	C17-C20-C22-C23
27	M	526	DMU	O6-C11-C9-C8
19	P	1268	PGV	C1-C2-C3-C4
25	G	269	CDL	C57-C58-C59-C60
27	M	526	DMU	O16-C18-C19-C22
25	T	1269	CDL	C60-C61-C62-C63
25	T	1269	CDL	C79-C80-C81-C82
27	Z	1526	DMU	C3-C4-C57-O61
21	O	1229	PSC	C1-C2-C3-C4
24	T	1264	PEK	C1-C2-C3-C4
25	G	269	CDL	CA5-C11-C12-C13
25	P	1270	CDL	CB7-C71-C72-C73
21	B	229	PSC	C1-C2-C3-C4
24	G	264	PEK	C1-C2-C3-C4
25	T	1269	CDL	CA5-C11-C12-C13
25	T	1269	CDL	C73-C74-C75-C76
18	N	1521	TGL	CG2-CG3-OG3-CC1
18	D	523	TGL	C21-C22-C23-C24
18	N	1521	TGL	CC5-CC6-CC7-CC8
18	N	1522	TGL	CC2-CC3-CC4-CC5
25	T	1269	CDL	C15-C16-C17-C18
19	N	1524	PGV	O12-C04-C05-O05
19	P	1268	PGV	O12-C04-C05-O05
25	C	270	CDL	O1-C1-CA2-OA2
25	C	270	CDL	O1-C1-CB2-OB2
25	G	269	CDL	O1-C1-CB2-OB2
25	T	1269	CDL	O1-C1-CB2-OB2
19	A	524	PGV	C19-C20-C21-C22
25	P	1270	CDL	CA5-C11-C12-C13
21	B	229	PSC	C11-C12-C13-C14
24	G	264	PEK	C4-C5-C6-C7
24	T	263	PEK	C13-C14-C15-C16
19	C	268	PGV	O04-C19-O03-C01
25	C	270	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
18	A	521	TGL	CC2-CC1-OG3-CG3
22	J	60	CHD	C16-C17-C20-C21
18	Q	1523	TGL	CA1-CA2-CA3-CA4
25	P	1270	CDL	C17-C18-C19-C20
25	P	1270	CDL	OB7-CB5-OB6-CB4
25	C	270	CDL	CA2-C1-CB2-OB2
25	T	1269	CDL	CA2-C1-CB2-OB2
18	N	1522	TGL	C21-C20-CA9-CA8
27	Z	1526	DMU	O16-C18-C19-C22
27	Z	1526	DMU	C2-C3-O7-C10
21	O	1229	PSC	C04-C05-N-C06
25	P	1270	CDL	C51-CB5-OB6-CB4
18	N	1522	TGL	OB1-CB1-OG2-CG2
21	O	1229	PSC	O02-C1-O01-C02
18	A	521	TGL	C22-C23-C24-C25
25	T	1269	CDL	C40-C41-C42-C43
18	D	523	TGL	C11-C10-CB9-CB8
21	O	1229	PSC	C2-C1-O01-C02
21	O	1229	PSC	C04-C05-N-C07
18	A	521	TGL	CG2-CG3-OG3-CC1
18	N	1522	TGL	C17-C18-C19-C33
19	A	524	PGV	C4-C5-C6-C7
19	A	522	PGV	C6-C7-C8-C9
19	C	267	PGV	C30-C31-C32-C33
19	N	1524	PGV	C4-C5-C6-C7
27	M	526	DMU	C25-C28-C31-C34
18	D	523	TGL	CB1-CB2-CB3-CB4
24	G	1263	PEK	C13-C14-C15-C16
21	B	229	PSC	C26-C27-C28-C29
25	G	269	CDL	C72-C73-C74-C75
25	P	1270	CDL	C51-C52-C53-C54
25	P	1270	CDL	C74-C75-C76-C77
18	A	521	TGL	OC1-CC1-OG3-CG3
18	L	522	TGL	C12-C13-C14-C29
18	L	522	TGL	C22-C23-C24-C25
18	N	1521	TGL	CA5-CA6-CA7-CA8
18	N	1522	TGL	C20-C21-C22-C23
18	Q	1523	TGL	CC6-CC7-CC8-CC9
25	C	270	CDL	C76-C77-C78-C79
19	P	1268	PGV	O05-C05-C06-O06
18	N	1522	TGL	CC6-CC7-CC8-CC9
24	T	1265	PEK	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
21	O	1229	PSC	C2-C3-C4-C5
24	T	263	PEK	C34-C35-C36-C37
25	C	270	CDL	C73-C74-C75-C76
25	G	269	CDL	C82-C83-C84-C85
25	P	1270	CDL	C37-C38-C39-C40
18	N	1522	TGL	CB2-CB1-OG2-CG2
18	Q	1523	TGL	CC4-CC5-CC6-CC7
24	T	1264	PEK	C23-C24-C25-C26
25	G	269	CDL	C20-C21-C22-C23
18	D	523	TGL	CC4-CC5-CC6-CC7
18	Q	1523	TGL	C17-C18-C19-C33
19	N	1266	PGV	C23-C24-C25-C26
19	P	1268	PGV	C24-C25-C26-C27
25	C	270	CDL	C18-C19-C20-C21
25	T	1269	CDL	C20-C21-C22-C23
25	T	1269	CDL	C39-C40-C41-C42
24	G	1263	PEK	C29-C30-C31-C32
25	P	1270	CDL	C82-C83-C84-C85
18	Q	1523	TGL	CA9-C20-C21-C22
19	N	1266	PGV	C6-C7-C8-C9
22	J	60	CHD	C13-C17-C20-C21
25	P	1270	CDL	C72-C73-C74-C75
18	A	521	TGL	CA5-CA6-CA7-CA8
18	A	521	TGL	CB3-CB4-CB5-CB6
21	B	229	PSC	C2-C3-C4-C5
25	C	270	CDL	C61-C62-C63-C64
19	A	522	PGV	C26-C27-C28-C29
25	C	270	CDL	C82-C83-C84-C85
25	G	269	CDL	C71-CB7-OB8-CB6
19	A	522	PGV	C7-C8-C9-C10
19	C	267	PGV	C7-C8-C9-C10
19	P	1268	PGV	C22-C23-C24-C25
21	B	229	PSC	C24-C25-C26-C27
24	T	1264	PEK	C24-C25-C26-C27
25	C	270	CDL	C72-C73-C74-C75
25	G	269	CDL	C39-C40-C41-C42
25	P	1270	CDL	C61-C62-C63-C64
25	P	1270	CDL	C76-C77-C78-C79
25	T	1269	CDL	C54-C55-C56-C57
18	Q	1523	TGL	CB1-CB2-CB3-CB4
19	N	1524	PGV	C19-C20-C21-C22
25	C	270	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	N	1521	TGL	CA4-CA5-CA6-CA7
18	N	1521	TGL	C11-C10-CB9-CB8
18	N	1522	TGL	C23-C24-C25-C26
18	Q	1523	TGL	CB5-CB6-CB7-CB8
19	C	267	PGV	C24-C25-C26-C27
19	N	1524	PGV	C24-C25-C26-C27
19	N	1524	PGV	C28-C29-C30-C31
19	N	1266	PGV	C7-C8-C9-C10
21	B	229	PSC	C27-C28-C29-C30
24	G	264	PEK	C22-C23-C24-C25
25	C	270	CDL	C36-C37-C38-C39
25	T	1269	CDL	C43-C44-C45-C46
27	Z	1526	DMU	C25-C28-C31-C34
18	A	521	TGL	C16-C17-C18-C19
19	N	1266	PGV	C5-C6-C7-C8
19	C	268	PGV	C26-C27-C28-C29
21	O	1229	PSC	C04-C05-N-C08
18	D	523	TGL	CC2-CC3-CC4-CC5
18	D	523	TGL	CA9-C20-C21-C22
19	C	268	PGV	C27-C28-C29-C30
25	C	270	CDL	C38-C39-C40-C41
18	A	521	TGL	CB1-CB2-CB3-CB4
18	D	523	TGL	CB9-C10-C11-C12
18	Q	1523	TGL	CB2-CB3-CB4-CB5
25	C	270	CDL	C13-C14-C15-C16
25	P	1270	CDL	C38-C39-C40-C41
25	P	1270	CDL	C41-C42-C43-C44
25	P	1270	CDL	C73-C74-C75-C76
18	L	522	TGL	CB2-CB1-OG2-CG2
25	C	270	CDL	C51-CB5-OB6-CB4
19	P	1267	PGV	C11-C10-C9-C8
18	L	522	TGL	CA7-CA8-CA9-C20
19	C	268	PGV	C24-C25-C26-C27
19	P	1267	PGV	C13-C14-C15-C16
25	G	269	CDL	C13-C14-C15-C16
25	T	1269	CDL	C13-C14-C15-C16
24	T	263	PEK	C25-C26-C27-C28
25	C	270	CDL	C42-C43-C44-C45
25	C	270	CDL	C74-C75-C76-C77
25	G	269	CDL	OB9-CB7-OB8-CB6
18	N	1522	TGL	CB4-CB5-CB6-CB7
18	N	1522	TGL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	O	1229	PSC	C24-C25-C26-C27
18	A	521	TGL	C15-C16-C17-C18
18	N	1522	TGL	C16-C15-CC9-CC8
24	T	263	PEK	C29-C30-C31-C32
19	P	1267	PGV	C30-C31-C32-C33
25	C	270	CDL	C71-C72-C73-C74
25	T	1269	CDL	C77-C78-C79-C80
19	P	1268	PGV	C13-C14-C15-C16
25	C	270	CDL	C41-C42-C43-C44
25	P	1270	CDL	C58-C59-C60-C61
18	Q	1523	TGL	CC3-CC4-CC5-CC6
19	A	524	PGV	C22-C23-C24-C25
19	P	1268	PGV	C27-C28-C29-C30
25	P	1270	CDL	C59-C60-C61-C62
25	T	1269	CDL	C59-C60-C61-C62
18	D	523	TGL	CB5-CB6-CB7-CB8
18	L	522	TGL	CB4-CB5-CB6-CB7
25	G	269	CDL	C62-C63-C64-C65
18	L	522	TGL	C11-C10-CB9-CB8
19	A	522	PGV	C23-C24-C25-C26
24	G	264	PEK	C31-C32-C33-C34
24	T	1264	PEK	C26-C27-C28-C29
25	C	270	CDL	C51-C52-C53-C54
25	G	269	CDL	C43-C44-C45-C46
25	T	1269	CDL	C72-C73-C74-C75
18	A	521	TGL	C11-C10-CB9-CB8
24	G	1263	PEK	C34-C35-C36-C37
24	T	263	PEK	C27-C28-C29-C30
24	T	1265	PEK	C16-C17-C18-C19
18	L	522	TGL	C21-C22-C23-C24
19	P	1267	PGV	C28-C29-C30-C31
18	N	1521	TGL	CB6-CB7-CB8-CB9
18	N	1522	TGL	CB5-CB6-CB7-CB8
19	C	268	PGV	C22-C23-C24-C25
19	C	268	PGV	C11-C10-C9-C8
19	C	268	PGV	C12-C13-C14-C15
19	P	1267	PGV	C12-C13-C14-C15
24	G	264	PEK	C2-C3-C4-C5
18	A	521	TGL	C14-C29-C30-C31
18	N	1521	TGL	CB3-CB4-CB5-CB6
19	C	268	PGV	C3-C4-C5-C6
25	C	270	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	N	1521	TGL	CB1-CB2-CB3-CB4
18	N	1522	TGL	CA5-CA6-CA7-CA8
18	A	521	TGL	CA3-CA4-CA5-CA6
18	D	523	TGL	CB6-CB7-CB8-CB9
19	P	1268	PGV	C5-C6-C7-C8
25	P	1270	CDL	C71-C72-C73-C74
22	W	1059	CHD	C13-C17-C20-C21
18	N	1522	TGL	C21-C22-C23-C24
18	A	521	TGL	CA4-CA5-CA6-CA7
25	T	1269	CDL	C38-C39-C40-C41
19	A	524	PGV	C24-C25-C26-C27
24	G	1263	PEK	C25-C26-C27-C28
18	L	522	TGL	OB1-CB1-OG2-CG2
18	A	521	TGL	CB6-CB7-CB8-CB9
18	L	522	TGL	CC9-C15-C16-C17
18	N	1521	TGL	OC1-CC1-OG3-CG3
18	N	1522	TGL	CA7-CA8-CA9-C20
18	N	1522	TGL	C24-C25-C26-C27
25	P	1270	CDL	C13-C14-C15-C16
18	N	1521	TGL	C17-C18-C19-C33
18	N	1522	TGL	CC9-C15-C16-C17
25	P	1270	CDL	C36-C37-C38-C39
19	P	1268	PGV	C11-C10-C9-C8
25	G	269	CDL	OB6-CB4-CB6-OB8
18	L	522	TGL	CA5-CA6-CA7-CA8
24	G	1263	PEK	C27-C28-C29-C30
27	Z	1526	DMU	C22-C25-C28-C31
18	N	1521	TGL	CC2-CC1-OG3-CG3
18	L	522	TGL	C17-C18-C19-C33
18	L	522	TGL	C24-C25-C26-C27
18	D	523	TGL	CA6-CA7-CA8-CA9
18	L	522	TGL	C10-C11-C12-C13
25	P	1270	CDL	C42-C43-C44-C45
21	B	229	PSC	C29-C30-C31-C32
19	A	524	PGV	C05-C04-O12-P
18	N	1521	TGL	CA3-CA4-CA5-CA6
25	C	270	CDL	C77-C78-C79-C80
27	M	526	DMU	C22-C25-C28-C31
19	C	267	PGV	C29-C30-C31-C32
18	N	1521	TGL	C18-C19-C33-C34
25	P	1270	CDL	C81-C82-C83-C84
24	G	1263	PEK	C22-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
19	C	267	PGV	C13-C14-C15-C16
19	P	1267	PGV	C7-C8-C9-C10
25	P	1270	CDL	C16-C17-C18-C19
25	T	1269	CDL	C16-C17-C18-C19
18	N	1521	TGL	C14-C29-C30-C31
18	L	522	TGL	CC5-CC6-CC7-CC8
25	G	269	CDL	C79-C80-C81-C82
18	D	523	TGL	CB3-CB4-CB5-CB6
19	N	1266	PGV	C12-C13-C14-C15
24	T	1265	PEK	C15-C16-C17-C18
19	C	268	PGV	C13-C14-C15-C16
21	O	1229	PSC	C27-C28-C29-C30
25	C	270	CDL	OA5-CA3-CA4-CA6
25	C	270	CDL	OB5-CB3-CB4-CB6
25	G	269	CDL	OA5-CA3-CA4-CA6
25	P	1270	CDL	OA5-CA3-CA4-CA6
25	C	270	CDL	OB7-CB5-OB6-CB4
19	N	1266	PGV	C29-C30-C31-C32
21	B	229	PSC	C23-C24-C25-C26
24	G	264	PEK	C16-C17-C18-C19
18	L	522	TGL	CC6-CC7-CC8-CC9
18	Q	1523	TGL	CC2-CC3-CC4-CC5
25	P	1270	CDL	C18-C19-C20-C21
18	Q	1523	TGL	CB6-CB7-CB8-CB9
25	G	269	CDL	C36-C37-C38-C39
25	P	1270	CDL	C75-C76-C77-C78
24	T	263	PEK	C33-C34-C35-C36
24	G	1263	PEK	O04-C21-O03-C01
18	N	1521	TGL	C13-C14-C29-C30
18	Q	1523	TGL	CB9-C10-C11-C12
24	C	265	PEK	C34-C35-C36-C37
25	G	269	CDL	C78-C79-C80-C81
24	T	263	PEK	C30-C31-C32-C33
25	P	1270	CDL	C23-C24-C25-C26
19	C	267	PGV	C10-C11-C12-C13
19	C	268	PGV	C10-C11-C12-C13
24	G	1263	PEK	C10-C11-C12-C13
24	T	1264	PEK	C13-C14-C15-C16
19	N	1524	PGV	O03-C01-C02-C03
24	G	1263	PEK	O03-C01-C02-C03
24	T	263	PEK	O03-C01-C02-C03
25	P	1270	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	CB3-CB4-CB6-OB8
25	T	1269	CDL	CB3-CB4-CB6-OB8
18	D	523	TGL	C10-C11-C12-C13
18	N	1521	TGL	CB4-CB5-CB6-CB7
19	P	1268	PGV	C20-C21-C22-C23
24	C	265	PEK	C15-C16-C17-C18
24	G	1263	PEK	C2-C3-C4-C5
24	T	1264	PEK	C2-C3-C4-C5
25	C	270	CDL	C16-C17-C18-C19
18	D	523	TGL	CB2-CB3-CB4-CB5
19	C	267	PGV	C28-C29-C30-C31
25	G	269	CDL	C55-C56-C57-C58
24	G	264	PEK	C22-C21-O03-C01
18	A	521	TGL	C13-C14-C29-C30
19	N	1524	PGV	C14-C15-C16-C17
24	C	265	PEK	C25-C26-C27-C28
24	T	1264	PEK	C31-C32-C33-C34
25	G	269	CDL	C73-C74-C75-C76
19	P	1268	PGV	C4-C5-C6-C7
25	G	269	CDL	C61-C62-C63-C64
18	Q	1523	TGL	CB7-CB8-CB9-C10
25	G	269	CDL	C53-C54-C55-C56
25	C	270	CDL	C58-C59-C60-C61
18	Q	1523	TGL	C12-C13-C14-C29
19	A	524	PGV	C2-C3-C4-C5
19	A	522	PGV	C25-C26-C27-C28
25	T	1269	CDL	C41-C42-C43-C44
19	A	524	PGV	C03-C02-O01-C1
18	D	523	TGL	C19-C33-C34-C35
18	N	1522	TGL	CC4-CC5-CC6-CC7
24	C	265	PEK	C29-C30-C31-C32
24	G	1263	PEK	C30-C31-C32-C33
24	G	264	PEK	C23-C24-C25-C26
14	N	516	HEA	C2A-C3A-CMA-OMA
19	N	1524	PGV	C22-C23-C24-C25
19	A	524	PGV	C10-C11-C12-C13
19	A	522	PGV	C10-C11-C12-C13
19	P	1268	PGV	C15-C16-C17-C18
27	Z	1526	DMU	O5-C6-O16-C18
19	C	268	PGV	C25-C26-C27-C28
19	N	1524	PGV	C2-C3-C4-C5
19	P	1267	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	N	1521	TGL	C16-C17-C18-C19
19	C	268	PGV	C28-C29-C30-C31
25	C	270	CDL	C37-C38-C39-C40
19	P	1268	PGV	C14-C15-C16-C17
25	G	269	CDL	C80-C81-C82-C83
25	P	1270	CDL	C15-C16-C17-C18
18	L	522	TGL	CB5-CB6-CB7-CB8
19	P	1268	PGV	C30-C31-C32-C33
21	O	1229	PSC	C21-C22-C23-C24
25	C	270	CDL	C59-C60-C61-C62
25	P	1270	CDL	C80-C81-C82-C83
19	P	1268	PGV	C31-C32-C33-C34
18	Q	1523	TGL	C16-C17-C18-C19
18	A	521	TGL	OG1-CG1-CG2-OG2
21	B	229	PSC	O03-C01-C02-O01
19	P	1267	PGV	C31-C32-C33-C34
18	L	522	TGL	C11-C12-C13-C14
19	P	1268	PGV	C25-C26-C27-C28
21	O	1229	PSC	C29-C30-C31-C32
25	T	1269	CDL	C56-C57-C58-C59
22	W	1059	CHD	C21-C20-C22-C23
24	T	1264	PEK	C3-C4-C5-C6
19	A	522	PGV	C5-C6-C7-C8
19	A	524	PGV	C11-C10-C9-C8
19	C	267	PGV	C15-C16-C17-C18
19	P	1268	PGV	C20-C19-O03-C01
19	C	268	PGV	C31-C32-C33-C34
25	P	1270	CDL	C44-C45-C46-C47
18	D	523	TGL	CC3-CC4-CC5-CC6
25	C	270	CDL	C44-C45-C46-C47
25	T	1269	CDL	C44-C45-C46-C47
24	T	263	PEK	C26-C27-C28-C29
18	N	1522	TGL	C11-C10-CB9-CB8
24	G	1263	PEK	C28-C29-C30-C31
19	N	1524	PGV	C10-C11-C12-C13
25	G	269	CDL	C15-C16-C17-C18
18	L	522	TGL	CC1-CC2-CC3-CC4
18	N	1522	TGL	CB7-CB8-CB9-C10
25	C	270	CDL	C11-C12-C13-C14
27	M	526	DMU	C2-C3-O7-C10
18	A	521	TGL	CC6-CC7-CC8-CC9
18	N	1522	TGL	CB6-CB7-CB8-CB9

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C5-C6-C7-C8
18	N	1521	TGL	CB9-C10-C11-C12
18	Q	1523	TGL	CB3-CB4-CB5-CB6
19	N	1266	PGV	C26-C27-C28-C29
18	L	522	TGL	C16-C15-CC9-CC8
21	B	229	PSC	C13-C14-C15-C16
25	T	1269	CDL	C18-C19-C20-C21
18	A	521	TGL	CA6-CA7-CA8-CA9
18	D	523	TGL	CA5-CA6-CA7-CA8
18	Q	1523	TGL	C24-C25-C26-C27
25	T	1269	CDL	C71-C72-C73-C74
19	A	522	PGV	C31-C32-C33-C34
19	N	1524	PGV	C01-C02-C03-O11
25	P	1270	CDL	OB5-CB3-CB4-CB6
25	T	1269	CDL	OA5-CA3-CA4-CA6
25	C	270	CDL	C84-C85-C86-C87
18	Q	1523	TGL	C21-C22-C23-C24
19	A	524	PGV	C31-C32-C33-C34
24	T	1265	PEK	C29-C30-C31-C32
25	P	1270	CDL	C24-C25-C26-C27
18	N	1521	TGL	CC6-CC7-CC8-CC9
25	T	1269	CDL	C31-C32-C33-C34
19	C	268	PGV	C14-C15-C16-C17
19	C	267	PGV	C31-C32-C33-C34
25	C	270	CDL	C15-C16-C17-C18
18	L	522	TGL	CC4-CC5-CC6-CC7
18	Q	1523	TGL	C19-C33-C34-C35
18	A	521	TGL	OG1-CG1-CG2-CG3
18	D	523	TGL	CG1-CG2-CG3-OG3
18	Q	1523	TGL	CG1-CG2-CG3-OG3
19	A	524	PGV	O03-C01-C02-C03
21	O	1229	PSC	O03-C01-C02-C03
25	G	269	CDL	CA3-CA4-CA6-OA8
25	G	269	CDL	CB3-CB4-CB6-OB8
24	G	1263	PEK	C24-C25-C26-C27
19	P	1268	PGV	C3-C4-C5-C6
18	N	1522	TGL	C29-C30-C31-C32
18	L	522	TGL	C29-C30-C31-C32
24	G	1263	PEK	C26-C27-C28-C29
25	T	1269	CDL	C55-C56-C57-C58
24	T	263	PEK	O01-C02-C03-O11
25	C	270	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	OA5-CA3-CA4-OA6
18	L	522	TGL	C20-C21-C22-C23
19	P	1267	PGV	C02-C03-O11-P
25	P	1270	CDL	CA4-CA3-OA5-PA1
19	P	1268	PGV	C26-C27-C28-C29
24	G	264	PEK	O04-C21-O03-C01
18	A	521	TGL	C17-C18-C19-C33
25	G	269	CDL	C16-C17-C18-C19
18	Q	1523	TGL	OG2-CG2-CG3-OG3
24	T	1265	PEK	O03-C01-C02-O01
25	C	270	CDL	OB6-CB4-CB6-OB8
25	P	1270	CDL	OB6-CB4-CB6-OB8
21	B	229	PSC	C9-C10-C11-C12
21	O	1229	PSC	C9-C10-C11-C12
24	C	265	PEK	C9-C10-C11-C12
24	G	264	PEK	C9-C10-C11-C12
24	G	1263	PEK	C11-C10-C9-C8
24	G	1263	PEK	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	1264	PEK	C11-C10-C9-C8
24	T	1264	PEK	C9-C10-C11-C12
24	T	1265	PEK	C5-C6-C7-C8
19	P	1268	PGV	C23-C24-C25-C26
18	A	521	TGL	CC5-CC6-CC7-CC8
18	N	1522	TGL	CC3-CC4-CC5-CC6
25	G	269	CDL	C18-C19-C20-C21
19	C	267	PGV	C1-C2-C3-C4
25	C	270	CDL	C78-C79-C80-C81
25	C	270	CDL	C14-C15-C16-C17
25	P	1270	CDL	C62-C63-C64-C65
18	L	522	TGL	CA2-CA3-CA4-CA5
18	N	1522	TGL	C22-C23-C24-C25
24	G	1263	PEK	C31-C32-C33-C34
19	C	268	PGV	C7-C8-C9-C10
25	C	270	CDL	C20-C21-C22-C23
24	T	1264	PEK	C17-C18-C19-C20
19	N	1266	PGV	C31-C32-C33-C34
25	G	269	CDL	C54-C55-C56-C57
25	T	1269	CDL	C64-C65-C66-C67
18	N	1522	TGL	CC5-CC6-CC7-CC8

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C30-C31-C32-C33
18	L	522	TGL	C25-C26-C27-C28
19	A	524	PGV	C11-C12-C13-C14
24	C	265	PEK	C32-C33-C34-C35
25	G	269	CDL	C58-C59-C60-C61
27	Z	1526	DMU	C34-C37-C40-C43
25	T	1269	CDL	CB2-C1-CA2-OA2
25	C	270	CDL	C55-C56-C57-C58
19	A	524	PGV	C01-C02-C03-O11
24	T	1264	PEK	C25-C26-C27-C28
24	C	265	PEK	C31-C32-C33-C34
19	P	1268	PGV	O04-C19-O03-C01
25	P	1270	CDL	C11-C12-C13-C14
19	N	1524	PGV	C21-C22-C23-C24
25	P	1270	CDL	C32-C33-C34-C35
19	N	1524	PGV	C03-C02-O01-C1
19	N	1524	PGV	C11-C10-C9-C8
19	P	1267	PGV	C29-C30-C31-C32
19	N	1524	PGV	C31-C32-C33-C34
25	P	1270	CDL	C43-C44-C45-C46
24	G	1263	PEK	O01-C02-C03-O11
25	C	270	CDL	OA5-CA3-CA4-OA6
24	C	265	PEK	C16-C17-C18-C19
24	G	264	PEK	O03-C01-C02-C03
25	C	270	CDL	CB3-CB4-CB6-OB8
25	T	1269	CDL	CA3-CA4-CA6-OA8
18	D	523	TGL	CC6-CC7-CC8-CC9
18	D	523	TGL	OG2-CG2-CG3-OG3
19	N	1524	PGV	O03-C01-C02-O01
25	P	1270	CDL	OA6-CA4-CA6-OA8
19	C	268	PGV	C1-C2-C3-C4
18	D	523	TGL	CA4-CA5-CA6-CA7
21	O	1229	PSC	C4-C5-C6-C7
24	T	1265	PEK	C26-C27-C28-C29
19	A	522	PGV	C29-C30-C31-C32
24	T	263	PEK	C31-C32-C33-C34
24	T	1265	PEK	C31-C32-C33-C34
18	L	522	TGL	CA6-CA7-CA8-CA9
25	T	1269	CDL	C51-CB5-OB6-CB4
18	N	1521	TGL	C16-C15-CC9-CC8
19	A	524	PGV	C25-C26-C27-C28
18	N	1521	TGL	CC4-CC5-CC6-CC7

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Mol	Chain	Res	Type	Atoms
24	G	264	PEK	C25-C26-C27-C28
24	G	1263	PEK	C16-C17-C18-C19
25	G	269	CDL	C24-C25-C26-C27
19	N	1524	PGV	C26-C27-C28-C29
19	A	522	PGV	C24-C25-C26-C27
18	N	1521	TGL	C15-C16-C17-C18
21	B	229	PSC	C3-C4-C5-C6
24	T	263	PEK	C16-C17-C18-C19
19	P	1268	PGV	C28-C29-C30-C31
25	G	269	CDL	CB7-C71-C72-C73
24	G	1263	PEK	C01-C02-C03-O11
24	T	263	PEK	C01-C02-C03-O11
24	T	1265	PEK	C01-C02-C03-O11
25	T	1269	CDL	C57-C58-C59-C60
18	D	523	TGL	C29-C30-C31-C32
19	C	268	PGV	C15-C16-C17-C18
24	G	264	PEK	C32-C33-C34-C35
18	A	521	TGL	CC4-CC5-CC6-CC7
25	T	1269	CDL	OB7-CB5-OB6-CB4
25	G	269	CDL	OA5-CA3-CA4-OA6
25	P	1270	CDL	OB5-CB3-CB4-OB6
25	T	1269	CDL	OA5-CA3-CA4-OA6
24	G	264	PEK	C15-C16-C17-C18
14	N	516	HEA	C4A-C3A-CMA-OMA
25	G	269	CDL	C41-C42-C43-C44
21	O	1229	PSC	O03-C01-C02-O01
24	G	264	PEK	O03-C01-C02-O01
25	G	269	CDL	OA6-CA4-CA6-OA8
25	T	1269	CDL	OA6-CA4-CA6-OA8
19	C	268	PGV	C4-C5-C6-C7
18	A	521	TGL	C24-C25-C26-C27
18	D	523	TGL	C11-C12-C13-C14
21	B	229	PSC	O03-C01-C02-C03
18	N	1522	TGL	OG2-CB1-CB2-CB3
19	C	267	PGV	C22-C23-C24-C25
18	A	521	TGL	C20-C21-C22-C23
24	T	263	PEK	C28-C29-C30-C31
25	G	269	CDL	C56-C57-C58-C59
18	N	1521	TGL	C23-C24-C25-C26
24	T	1265	PEK	C24-C25-C26-C27
19	A	522	PGV	C22-C23-C24-C25
19	A	524	PGV	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
21	B	229	PSC	C03-O11-P-O12
21	B	229	PSC	C04-O12-P-O13
21	O	1229	PSC	C03-O11-P-O13
24	C	265	PEK	O12-C04-C05-N
24	G	1263	PEK	C03-O11-P-O13
25	C	270	CDL	CA3-OA5-PA1-OA2
25	C	270	CDL	CB2-OB2-PB2-OB5
25	G	269	CDL	CA2-OA2-PA1-OA4
25	P	1270	CDL	CA2-OA2-PA1-OA4
25	P	1270	CDL	CA3-OA5-PA1-OA3
25	P	1270	CDL	CB2-OB2-PB2-OB5
25	T	1269	CDL	CA2-OA2-PA1-OA3
18	L	522	TGL	CA3-CA4-CA5-CA6
19	N	1266	PGV	C24-C25-C26-C27
25	P	1270	CDL	C14-C15-C16-C17
19	C	267	PGV	C02-C03-O11-P
19	N	1524	PGV	C05-C04-O12-P
25	G	269	CDL	CB4-CB3-OB5-PB2
21	B	229	PSC	C22-C23-C24-C25
18	N	1521	TGL	CA6-CA7-CA8-CA9
21	B	229	PSC	C31-C32-C33-C34
18	A	521	TGL	CG1-CG2-OG2-CB1
18	D	523	TGL	CG3-CG2-OG2-CB1
18	Q	1523	TGL	CG1-CG2-OG2-CB1
21	O	1229	PSC	C03-C02-O01-C1
25	G	269	CDL	C81-C82-C83-C84
25	T	1269	CDL	C84-C85-C86-C87
24	T	263	PEK	O04-C21-O03-C01
18	D	523	TGL	C17-C18-C19-C33
19	N	1266	PGV	C9-C10-C11-C12
24	G	264	PEK	C14-C15-C16-C17
25	G	269	CDL	C31-C32-C33-C34
25	G	269	CDL	C76-C77-C78-C79
19	C	268	PGV	O01-C02-C03-O11
19	P	1268	PGV	O01-C02-C03-O11
24	T	263	PEK	C22-C21-O03-C01
19	A	524	PGV	C23-C24-C25-C26
24	C	265	PEK	O03-C01-C02-O01
24	T	1264	PEK	C4-C5-C6-C7
19	C	267	PGV	C23-C24-C25-C26
24	G	264	PEK	C24-C25-C26-C27
24	T	1265	PEK	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	G	1263	PEK	C15-C16-C17-C18
24	G	264	PEK	C17-C18-C19-C20
24	T	1265	PEK	C30-C31-C32-C33
25	T	1269	CDL	C24-C25-C26-C27
19	N	1524	PGV	C12-C13-C14-C15
18	Q	1523	TGL	C33-C34-C35-C36
25	C	270	CDL	C1-CA2-OA2-PA1
19	P	1267	PGV	C1-C2-C3-C4
24	C	265	PEK	C30-C31-C32-C33
24	T	1265	PEK	O04-C21-O03-C01
22	C	271	CHD	C20-C22-C23-C24
18	L	522	TGL	C19-C33-C34-C35
18	Q	1523	TGL	C29-C30-C31-C32
21	B	229	PSC	C7-C8-C9-C10
18	N	1522	TGL	OG1-CA1-CA2-CA3
24	T	1265	PEK	C33-C34-C35-C36
24	T	1264	PEK	C10-C11-C12-C13
25	C	270	CDL	C35-C36-C37-C38
19	C	267	PGV	C27-C28-C29-C30
19	C	267	PGV	C05-C04-O12-P
24	T	263	PEK	C02-C03-O11-P
25	P	1270	CDL	C1-CA2-OA2-PA1
22	P	1271	CHD	C16-C17-C20-C22
21	B	229	PSC	C04-C05-N-C08
14	N	515	HEA	C26-C15-C16-C17
24	T	1264	PEK	C16-C17-C18-C19
19	C	268	PGV	C9-C10-C11-C12
19	N	1524	PGV	C11-C12-C13-C14
24	T	1265	PEK	C32-C33-C34-C35
18	N	1521	TGL	CG3-CG2-OG2-CB1
21	B	229	PSC	C03-C02-O01-C1
22	B	1085	CHD	C22-C23-C24-O25
14	A	515	HEA	C26-C15-C16-C17
14	N	515	HEA	CAD-CBD-CGD-O1D
22	P	1271	CHD	C22-C23-C24-O26
18	D	523	TGL	CB7-CB8-CB9-C10
21	B	229	PSC	C04-C05-N-C06
22	P	1271	CHD	C22-C23-C24-O25
25	C	270	CDL	C80-C81-C82-C83
25	T	1269	CDL	CB4-CB3-OB5-PB2
14	N	516	HEA	CAD-CBD-CGD-O1D
22	G	229	CHD	C22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
18	N	1521	TGL	CB2-CB3-CB4-CB5
19	N	1524	PGV	C25-C26-C27-C28
24	T	1264	PEK	O03-C01-C02-O01
24	C	265	PEK	C6-C7-C8-C9
24	C	265	PEK	C11-C10-C9-C8
24	G	1263	PEK	C5-C6-C7-C8
24	G	1263	PEK	C12-C13-C14-C15
24	T	1264	PEK	C6-C7-C8-C9
24	T	1265	PEK	C6-C7-C8-C9
24	T	1265	PEK	C11-C10-C9-C8
24	T	1265	PEK	C9-C10-C11-C12
24	T	263	PEK	C21-C22-C23-C24
14	A	516	HEA	CAA-CBA-CGA-O1A
14	N	516	HEA	CAD-CBD-CGD-O2D
18	L	522	TGL	CA9-C20-C21-C22
19	A	522	PGV	O03-C19-C20-C21
18	N	1522	TGL	CA9-C20-C21-C22
25	C	270	CDL	C32-C33-C34-C35
18	L	522	TGL	C18-C19-C33-C34
21	O	1229	PSC	C3-C4-C5-C6
24	C	265	PEK	C22-C23-C24-C25
25	P	1270	CDL	C20-C21-C22-C23
24	G	264	PEK	C26-C27-C28-C29
18	A	521	TGL	C21-C22-C23-C24
14	N	516	HEA	C26-C15-C16-C17
22	B	1085	CHD	C22-C23-C24-O26
19	P	1268	PGV	C05-C04-O12-P
27	M	526	DMU	C34-C37-C40-C43
18	A	521	TGL	C23-C24-C25-C26
22	C	271	CHD	C22-C23-C24-O25
22	G	229	CHD	C22-C23-C24-O26
25	G	269	CDL	C33-C34-C35-C36
18	L	522	TGL	OG2-CB1-CB2-CB3
19	A	524	PGV	C30-C31-C32-C33
18	Q	1523	TGL	OG1-CG1-CG2-CG3
24	T	1264	PEK	O03-C01-C02-C03
24	T	1265	PEK	O03-C01-C02-C03
14	A	516	HEA	CAA-CBA-CGA-O2A
14	N	515	HEA	CAD-CBD-CGD-O2D
22	J	60	CHD	C22-C23-C24-O26
18	Q	1523	TGL	C10-C11-C12-C13
19	A	524	PGV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	L	522	TGL	C13-C14-C29-C30
25	G	269	CDL	C14-C15-C16-C17
22	C	271	CHD	C22-C23-C24-O26
25	C	270	CDL	C75-C76-C77-C78
19	N	1266	PGV	O03-C19-C20-C21
19	C	268	PGV	C01-C02-C03-O11
19	P	1268	PGV	C01-C02-C03-O11
19	A	524	PGV	O03-C01-C02-O01
19	C	267	PGV	C9-C10-C11-C12
19	P	1268	PGV	C02-C03-O11-P
18	D	523	TGL	C16-C17-C18-C19
19	N	1524	PGV	C30-C31-C32-C33
25	P	1270	CDL	C63-C64-C65-C66
18	A	521	TGL	C18-C19-C33-C34
25	G	269	CDL	C11-C12-C13-C14
14	N	516	HEA	C2D-C3D-CAD-CBD
22	C	271	CHD	C16-C17-C20-C22
14	A	516	HEA	CAD-CBD-CGD-O2D
25	C	270	CDL	C24-C25-C26-C27
18	N	1522	TGL	CB1-CB2-CB3-CB4
19	A	522	PGV	C11-C12-C13-C14
19	N	1266	PGV	C11-C12-C13-C14
19	P	1267	PGV	C11-C12-C13-C14
25	C	270	CDL	C52-C53-C54-C55
14	A	516	HEA	C2A-C3A-CMA-OMA
24	T	1265	PEK	C22-C21-O03-C01
18	N	1522	TGL	OB1-CB1-CB2-CB3
25	P	1270	CDL	C77-C78-C79-C80
18	D	523	TGL	C24-C25-C26-C27
19	N	1266	PGV	C4-C5-C6-C7
19	C	268	PGV	C2-C3-C4-C5
18	D	523	TGL	OB1-CB1-OG2-CG2
25	C	270	CDL	C43-C44-C45-C46
25	P	1270	CDL	C52-C53-C54-C55
24	G	264	PEK	C29-C30-C31-C32
25	P	1270	CDL	C35-C36-C37-C38
19	A	522	PGV	C9-C10-C11-C12
19	N	1524	PGV	C5-C6-C7-C8
22	P	1525	CHD	C22-C23-C24-O25
14	A	516	HEA	CAD-CBD-CGD-O1D
25	P	1270	CDL	C84-C85-C86-C87
24	T	263	PEK	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C23-C24-C25-C26
21	O	1229	PSC	C7-C8-C9-C10
18	L	522	TGL	C23-C24-C25-C26
14	A	515	HEA	CAD-CBD-CGD-O1D
21	B	229	PSC	C04-C05-N-C07
25	C	270	CDL	C81-C82-C83-C84
18	D	523	TGL	OG2-CB1-CB2-CB3
19	N	1524	PGV	O03-C19-C20-C21
25	P	1270	CDL	C12-C11-CA5-OA6
24	G	1263	PEK	C21-C22-C23-C24
19	N	1266	PGV	C30-C31-C32-C33
19	C	267	PGV	C11-C12-C13-C14
21	O	1229	PSC	C12-C13-C14-C15
25	G	269	CDL	OB7-CB5-OB6-CB4
25	G	269	CDL	C52-C53-C54-C55
18	D	523	TGL	C21-C20-CA9-CA8
24	T	1265	PEK	C34-C35-C36-C37
14	N	516	HEA	C3B-C11-C12-C13
19	A	524	PGV	O01-C1-C2-C3
25	P	1270	CDL	C52-C51-CB5-OB6
18	L	522	TGL	OG1-CA1-CA2-CA3
25	G	269	CDL	C19-C20-C21-C22
27	Z	1526	DMU	C19-C22-C25-C28
22	C	525	CHD	C22-C23-C24-O25
22	J	60	CHD	C22-C23-C24-O25
18	N	1522	TGL	OG3-CC1-CC2-CC3
24	G	264	PEK	O01-C1-C2-C3
24	T	1264	PEK	O01-C1-C2-C3
24	T	263	PEK	C35-C36-C37-C38
14	N	516	HEA	CAA-CBA-CGA-O1A
22	W	1059	CHD	C22-C23-C24-O26
14	A	516	HEA	C26-C15-C16-C17
25	G	269	CDL	CA7-C31-C32-C33
18	Q	1523	TGL	OG3-CC1-CC2-CC3
22	C	525	CHD	C22-C23-C24-O26
18	L	522	TGL	CB9-C10-C11-C12
14	N	516	HEA	CAA-CBA-CGA-O2A
22	W	1059	CHD	C22-C23-C24-O25
25	C	270	CDL	C62-C63-C64-C65
19	N	1524	PGV	C15-C16-C17-C18
19	N	1524	PGV	O01-C1-C2-C3
21	O	1229	PSC	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	G	269	CDL	C71-C72-C73-C74
19	A	524	PGV	C14-C15-C16-C17
25	G	269	CDL	C51-CB5-OB6-CB4
24	T	1264	PEK	C29-C30-C31-C32
25	C	270	CDL	C63-C64-C65-C66
25	C	270	CDL	C32-C31-CA7-OA8
19	P	1267	PGV	C2-C3-C4-C5
21	B	229	PSC	O03-C19-C20-C21
25	C	270	CDL	C12-C11-CA5-OA6
22	P	1271	CHD	C20-C22-C23-C24
19	C	268	PGV	C02-C03-O11-P
24	G	1263	PEK	C02-C03-O11-P
14	A	515	HEA	CAD-CBD-CGD-O2D
19	N	1266	PGV	C19-C20-C21-C22
24	T	1265	PEK	C1-C2-C3-C4
19	N	1524	PGV	C23-C24-C25-C26
18	D	523	TGL	OG3-CC1-CC2-CC3
24	T	1264	PEK	O02-C1-C2-C3
25	G	269	CDL	C44-C45-C46-C47
14	N	515	HEA	CAA-CBA-CGA-O1A
19	N	1524	PGV	C29-C30-C31-C32
21	O	1229	PSC	O03-C19-C20-C21
18	N	1522	TGL	OC1-CC1-CC2-CC3
18	Q	1523	TGL	OC1-CC1-CC2-CC3
19	A	524	PGV	O02-C1-C2-C3
24	G	264	PEK	O02-C1-C2-C3
25	C	270	CDL	C32-C31-CA7-OA9
24	T	1264	PEK	C30-C31-C32-C33
21	B	229	PSC	O01-C1-C2-C3
24	T	263	PEK	C3-C4-C5-C6
25	C	270	CDL	C60-C61-C62-C63
25	P	1270	CDL	C12-C11-CA5-OA7
18	A	521	TGL	CB5-CB6-CB7-CB8
21	B	229	PSC	O02-C1-C2-C3
25	P	1270	CDL	C52-C51-CB5-OB7
18	A	521	TGL	OG1-CA1-CA2-CA3
18	Q	1523	TGL	OG1-CA1-CA2-CA3
21	O	1229	PSC	O02-C1-C2-C3
18	L	522	TGL	OG3-CC1-CC2-CC3
24	T	1265	PEK	O03-C21-C22-C23
19	N	1524	PGV	O02-C1-C2-C3
14	N	515	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	O	1229	PSC	C19-C20-C21-C22

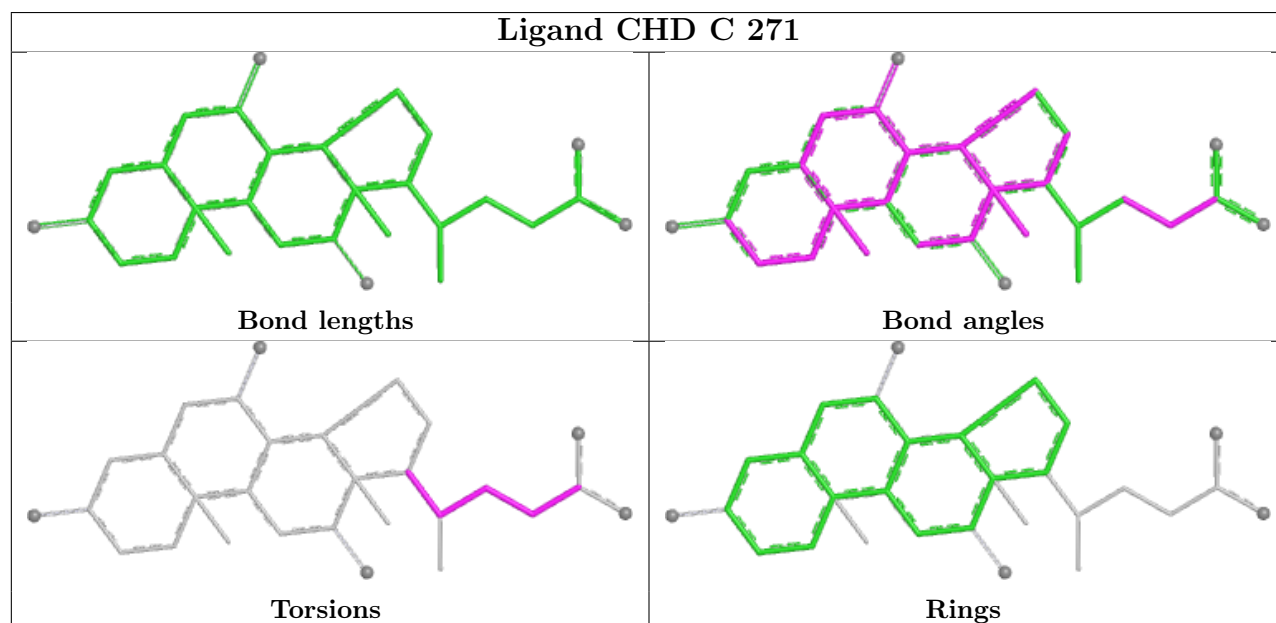
There are no ring outliers.

34 monomers are involved in 234 short contacts:

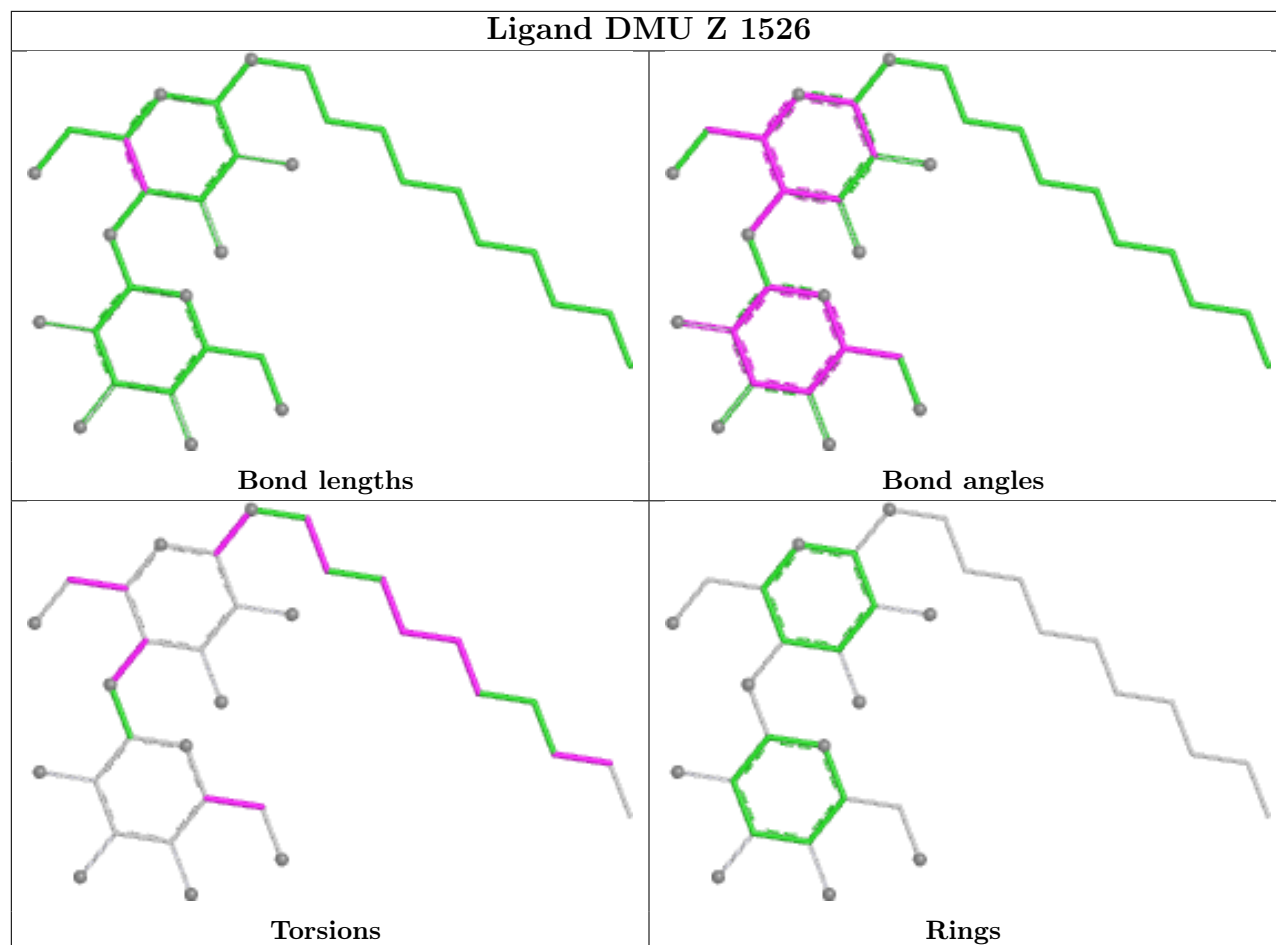
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	271	CHD	3	0
18	N	1521	TGL	9	0
18	L	522	TGL	15	0
24	G	1263	PEK	8	0
14	A	515	HEA	3	0
24	G	264	PEK	4	0
19	N	1266	PGV	3	0
22	J	60	CHD	3	0
18	D	523	TGL	6	0
24	T	1264	PEK	6	0
19	A	522	PGV	1	0
25	T	1269	CDL	22	0
18	Q	1523	TGL	4	0
21	O	1229	PSC	17	0
19	C	268	PGV	3	0
19	P	1268	PGV	4	0
19	N	1524	PGV	8	0
22	B	1085	CHD	1	0
22	P	1271	CHD	1	0
14	N	516	HEA	2	0
19	C	267	PGV	5	0
19	A	524	PGV	9	0
14	N	515	HEA	6	0
19	P	1267	PGV	2	0
25	G	269	CDL	18	0
18	N	1522	TGL	13	0
25	P	1270	CDL	13	0
22	W	1059	CHD	3	0
18	A	521	TGL	6	0
24	T	1265	PEK	6	0
21	B	229	PSC	13	0
25	C	270	CDL	16	0
24	T	263	PEK	9	0
24	C	265	PEK	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

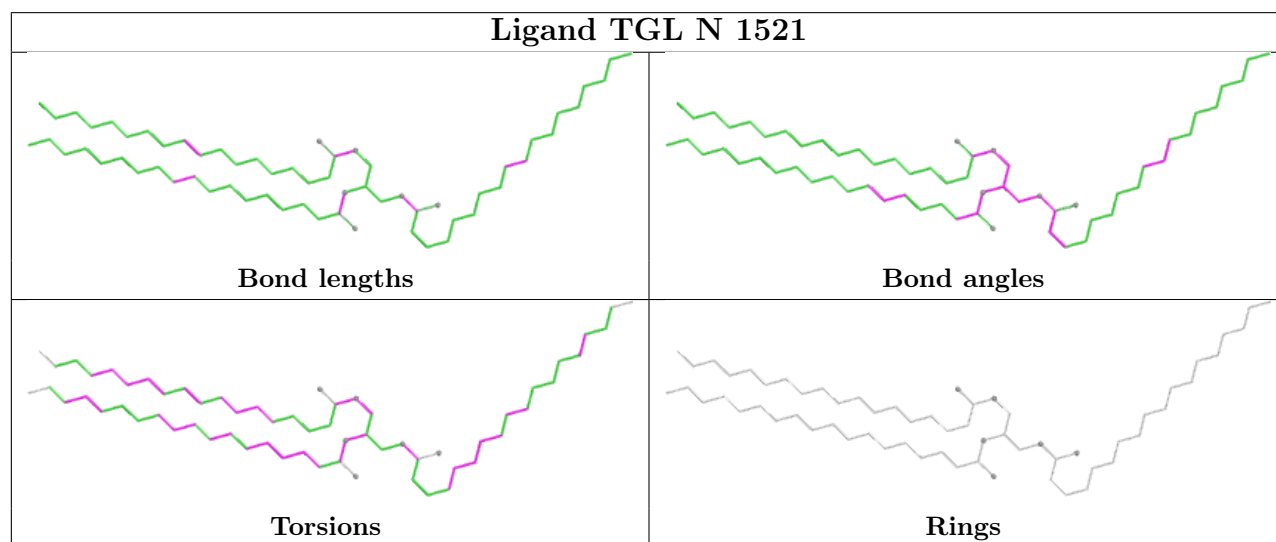
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

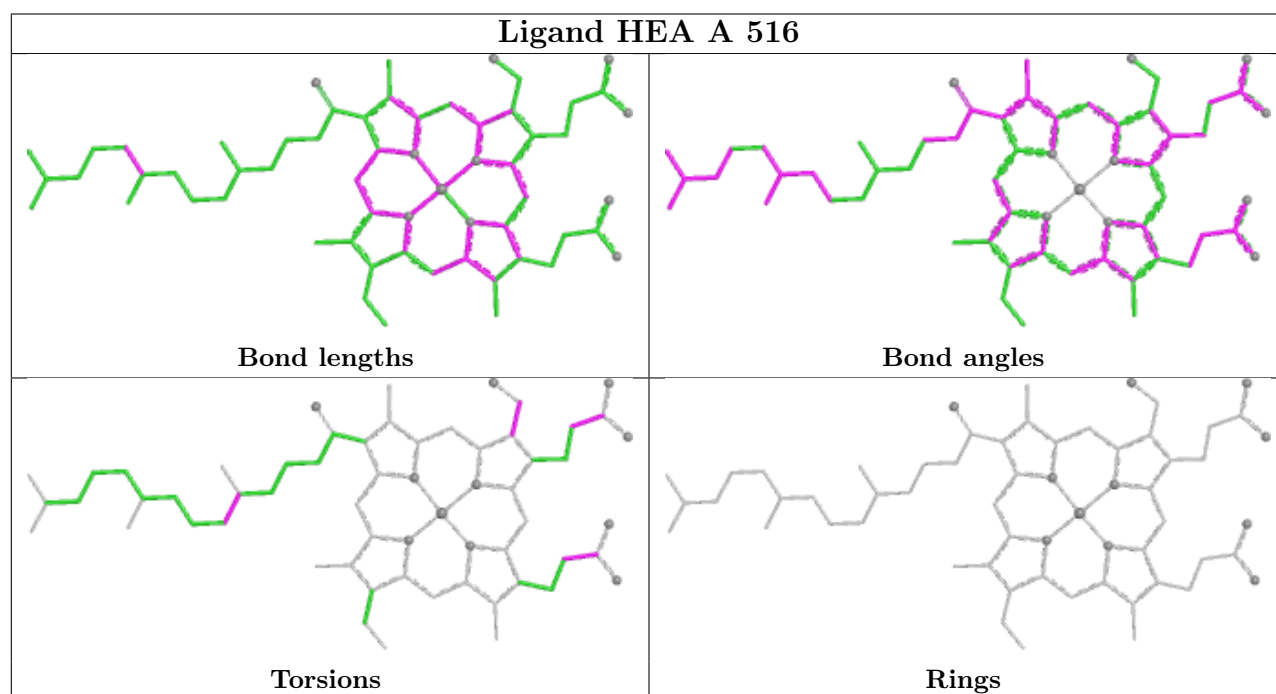
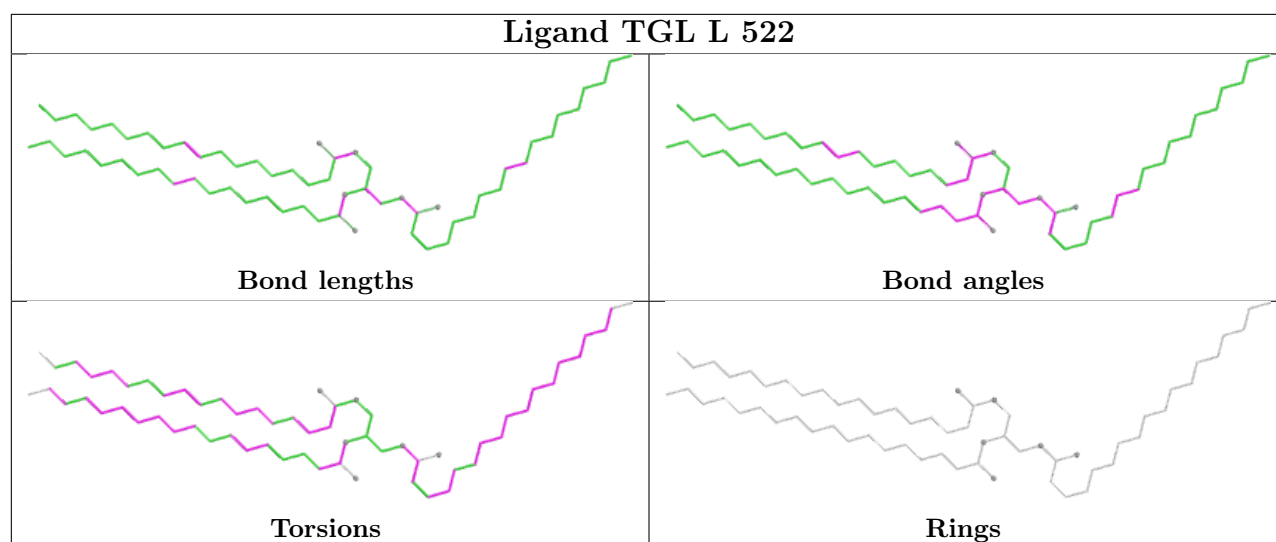


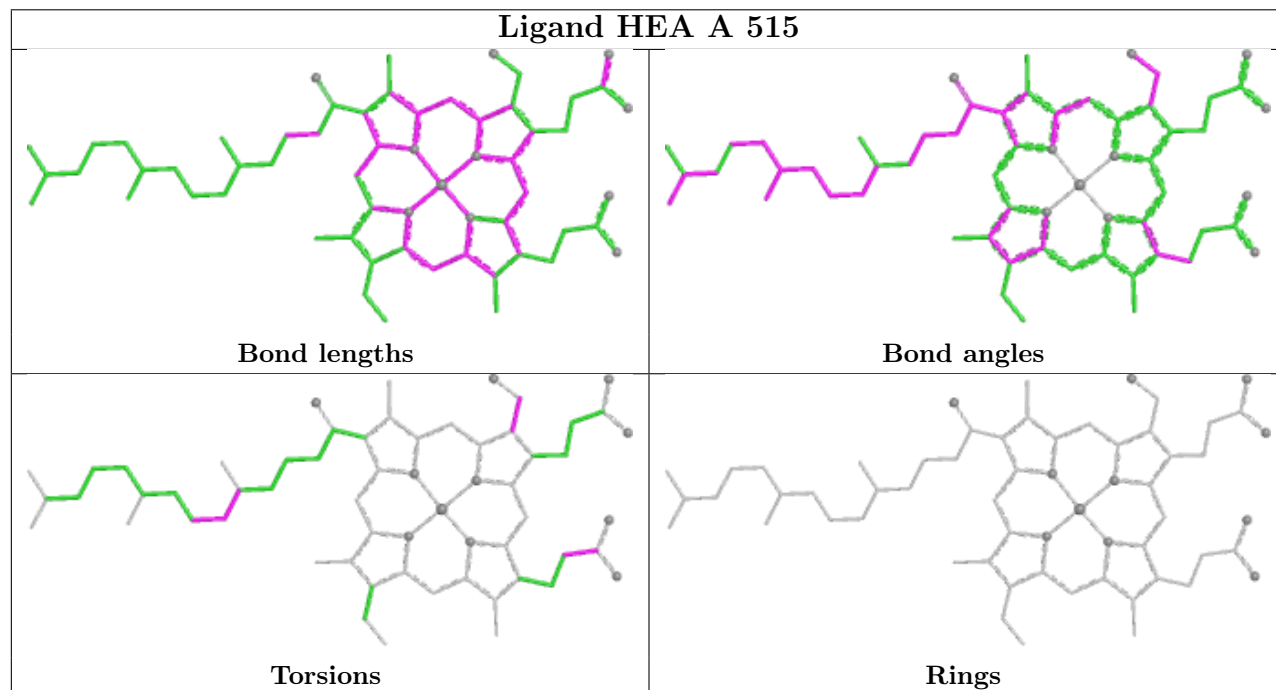
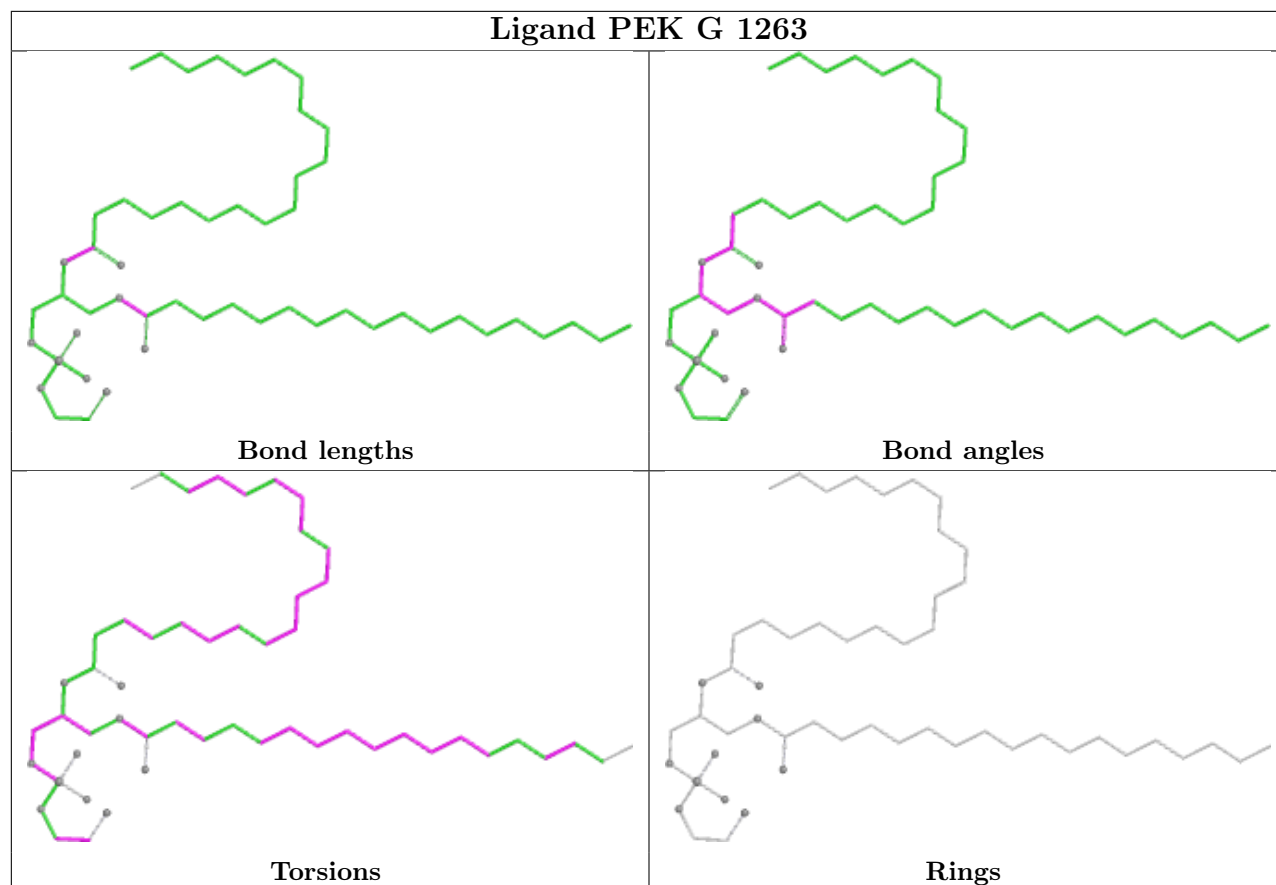
Ligand DMU Z 1526

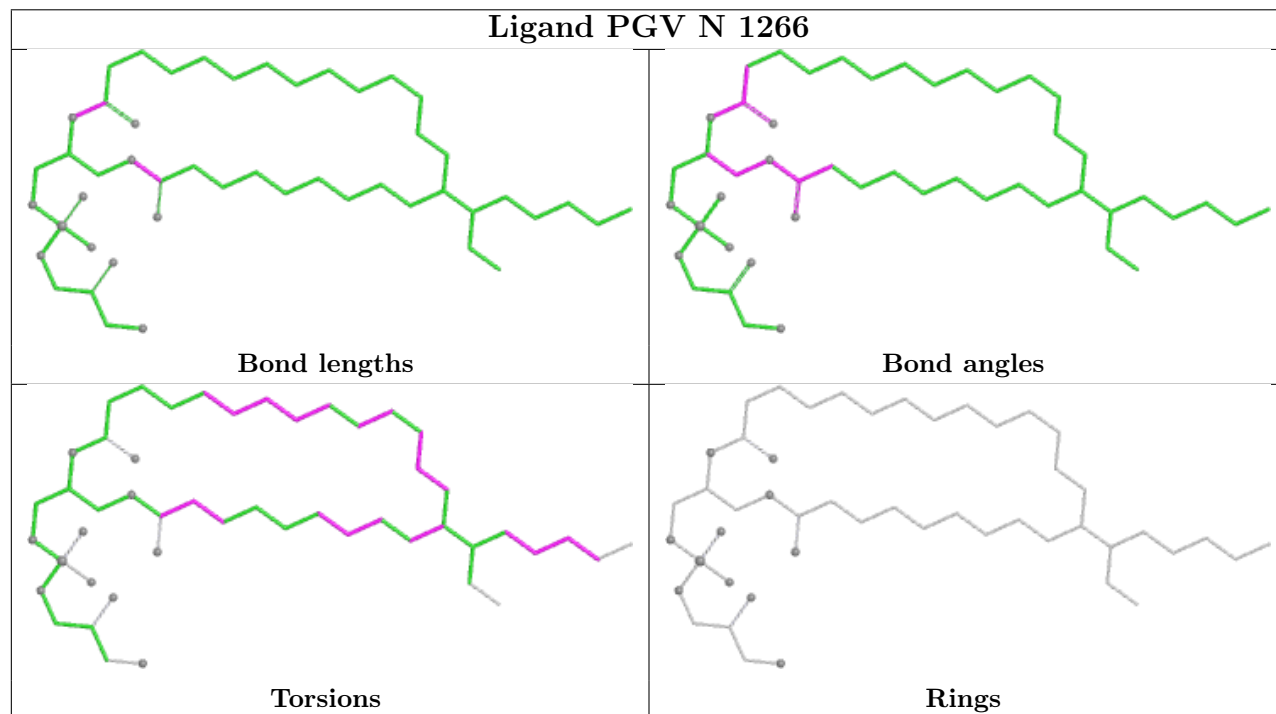
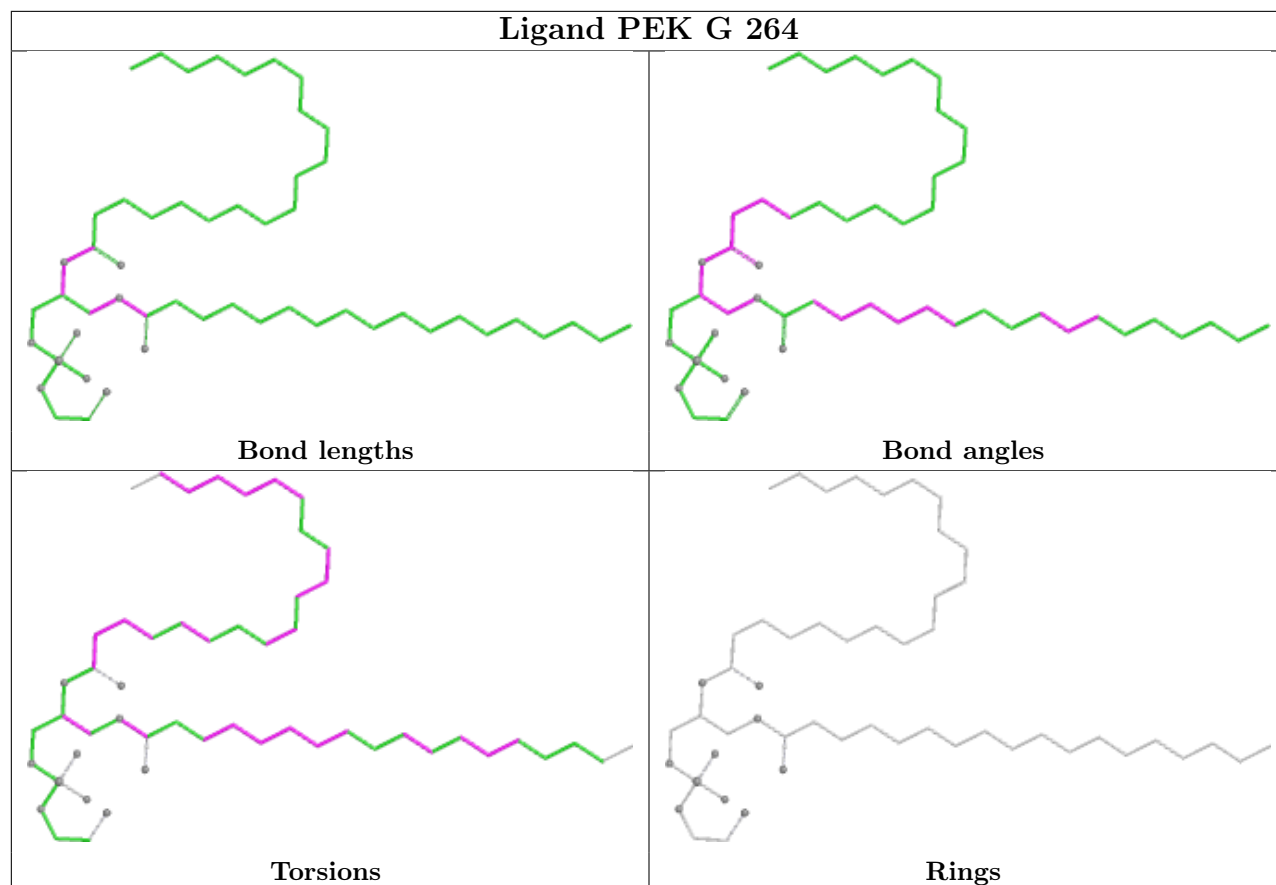


Ligand TGL N 1521

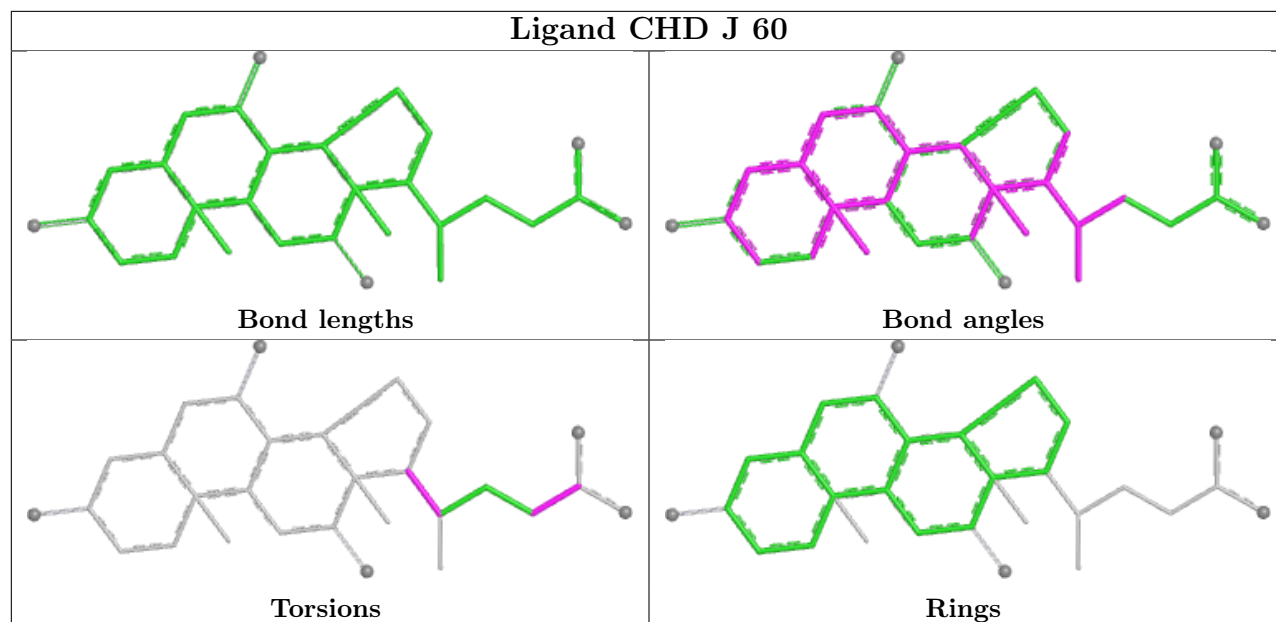




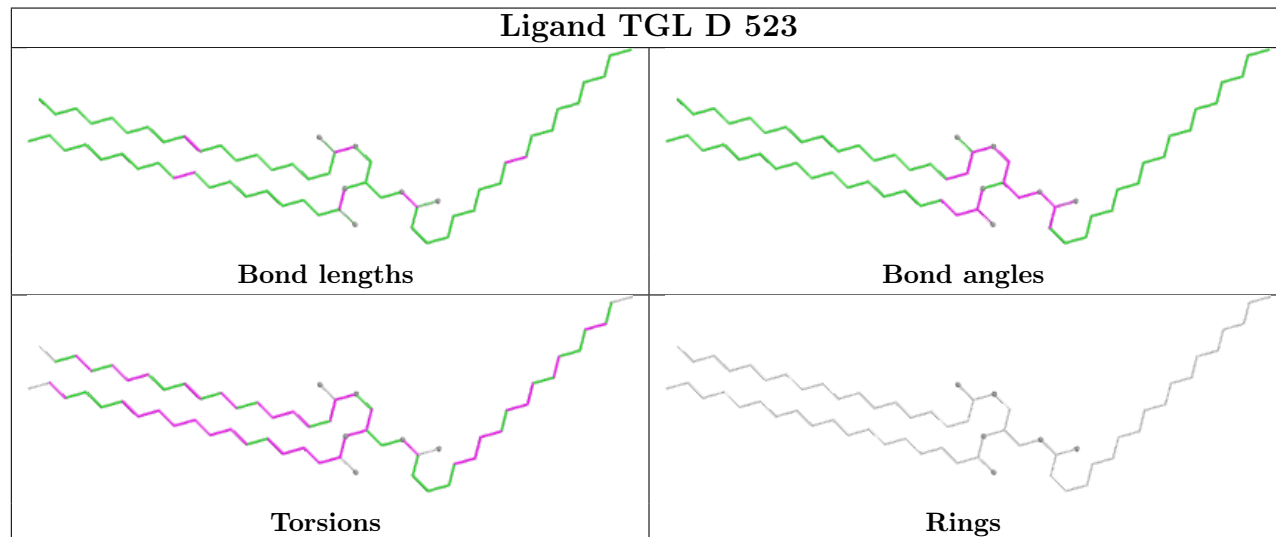




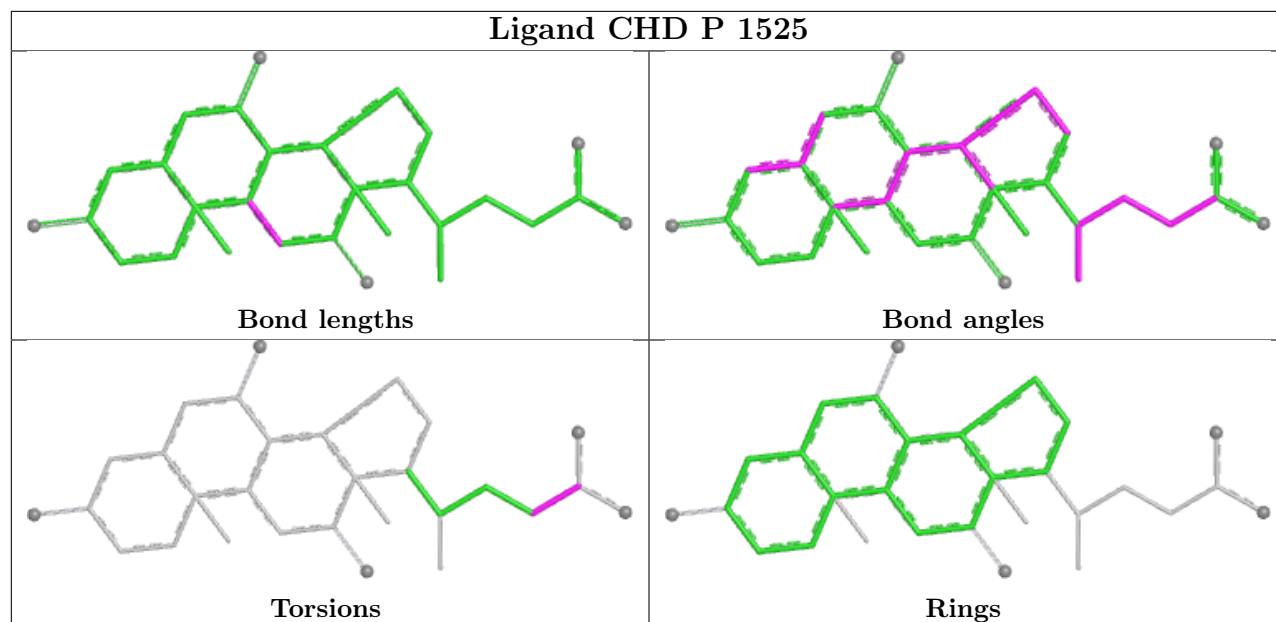
Ligand CHD J 60



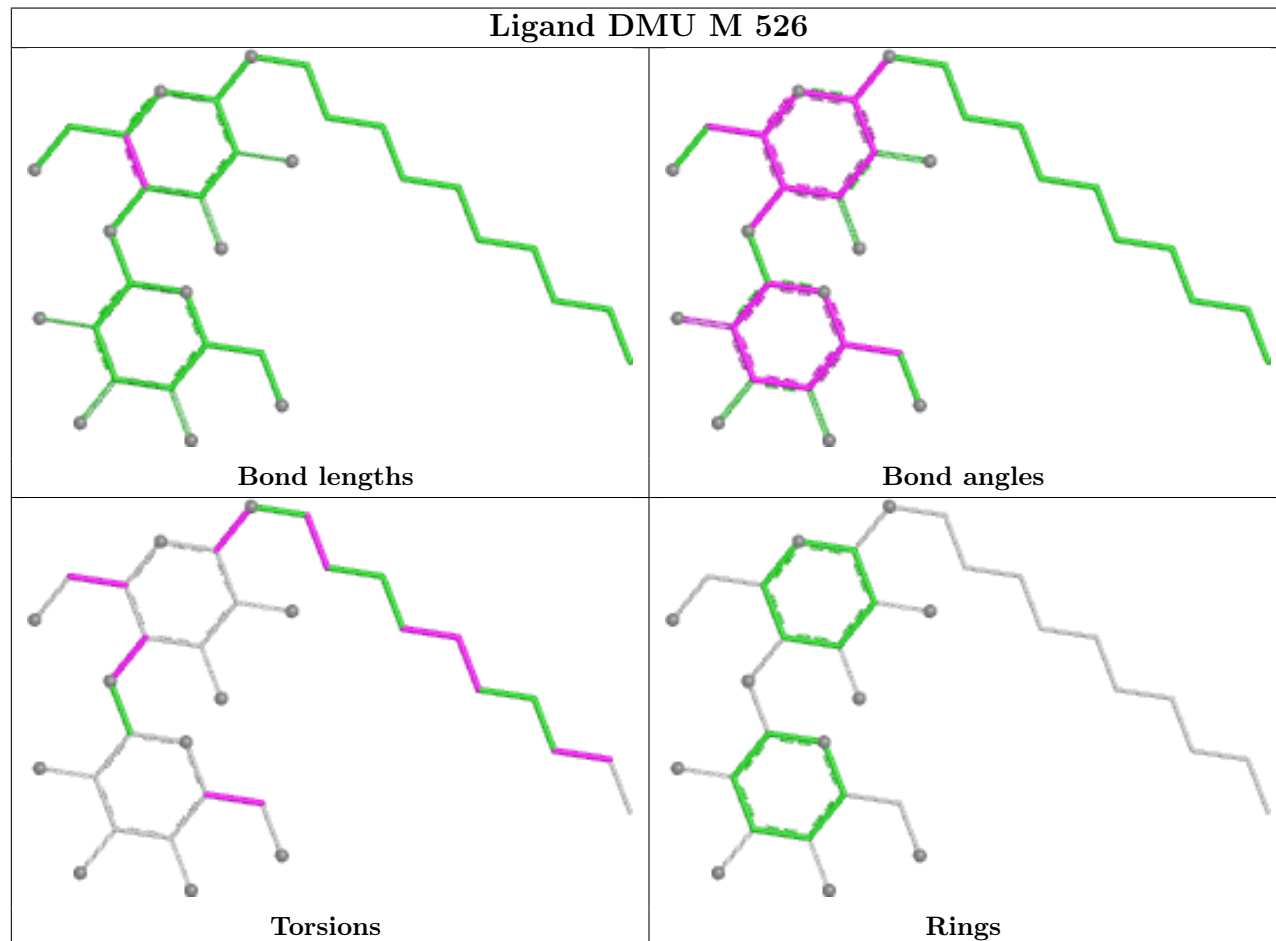
Ligand TGL D 523



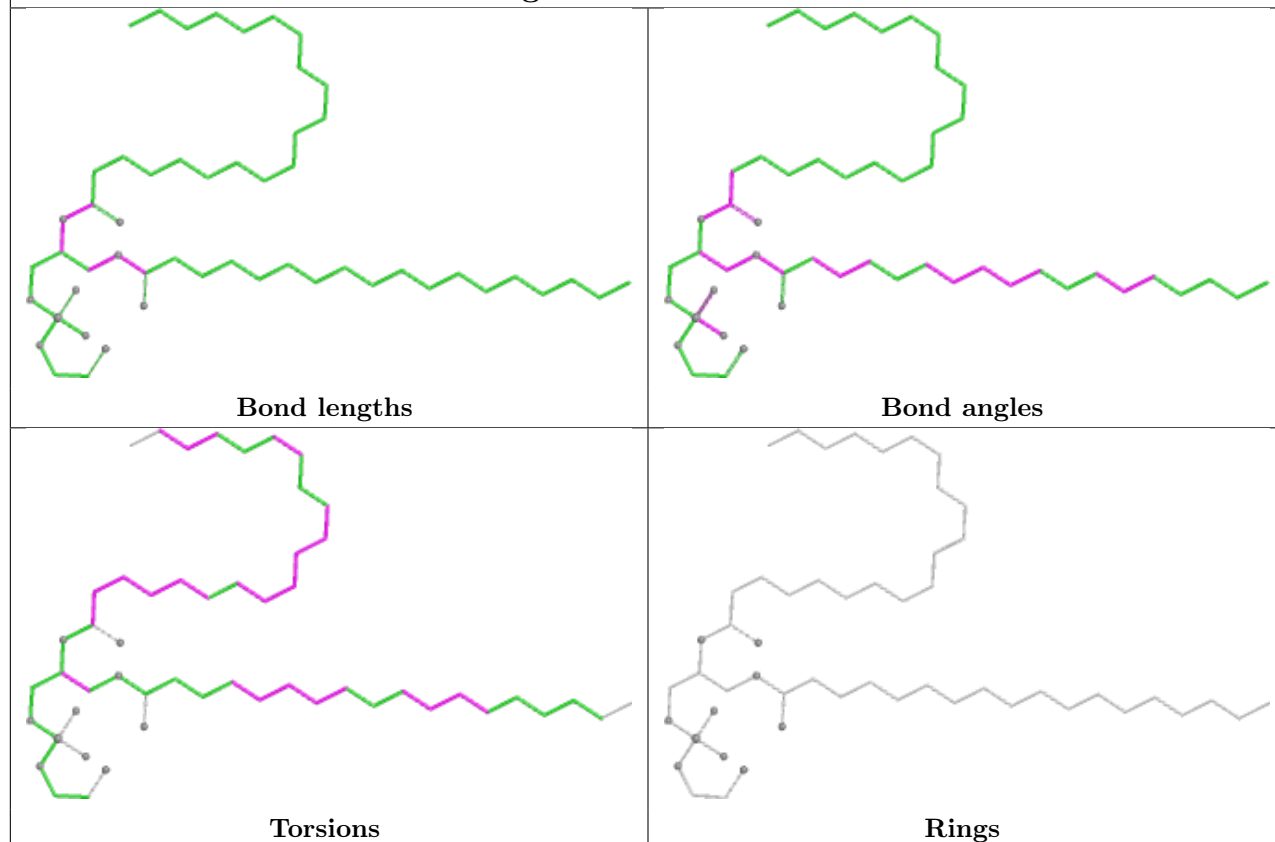
Ligand CHD P 1525



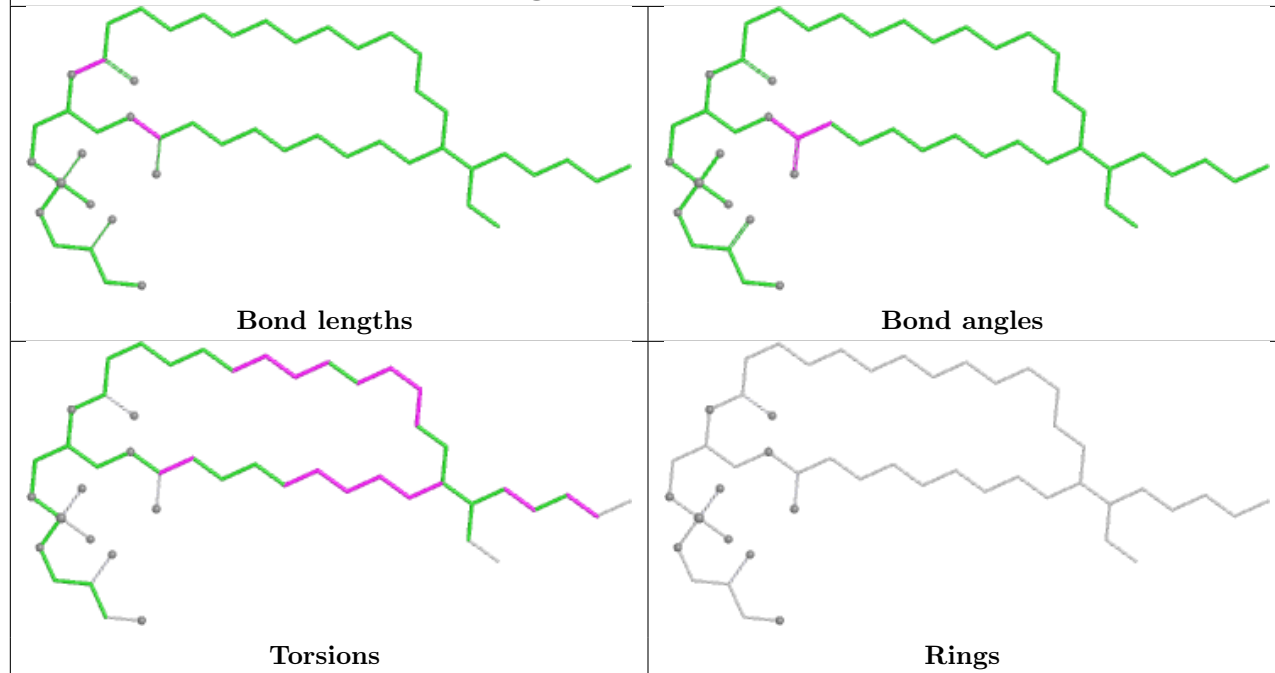
Ligand DMU M 526

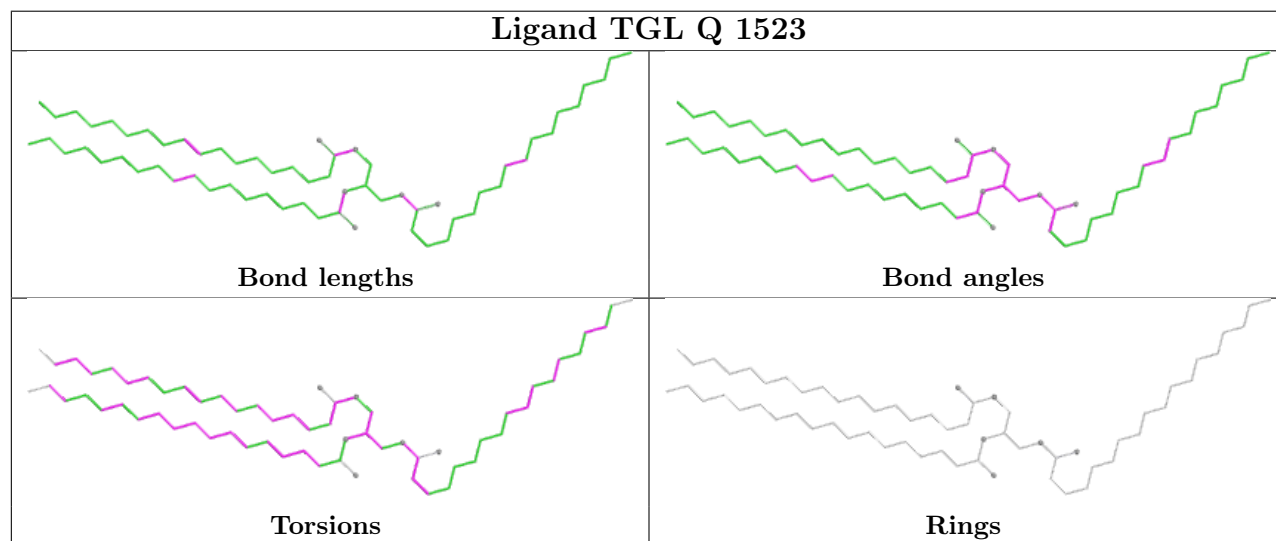
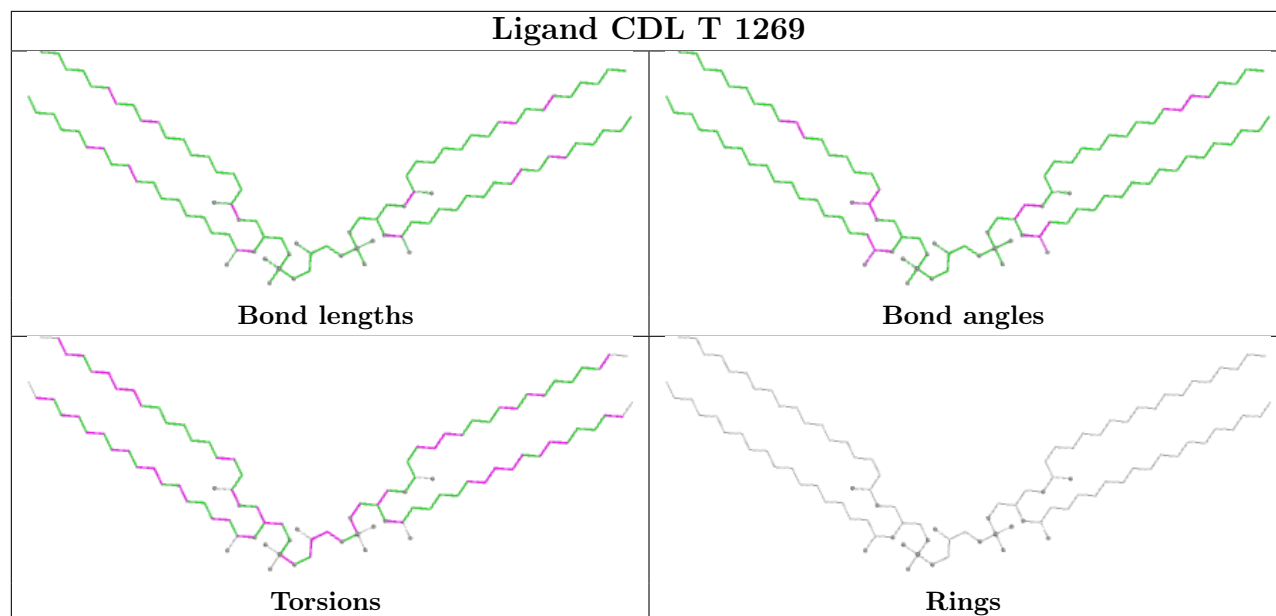


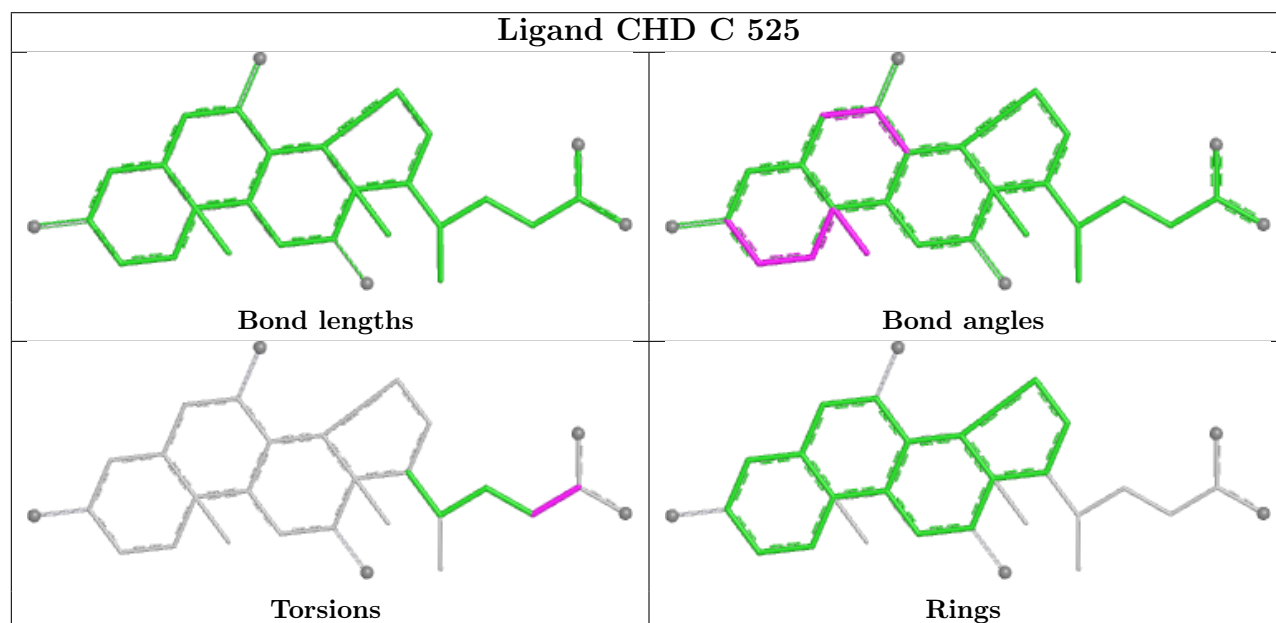
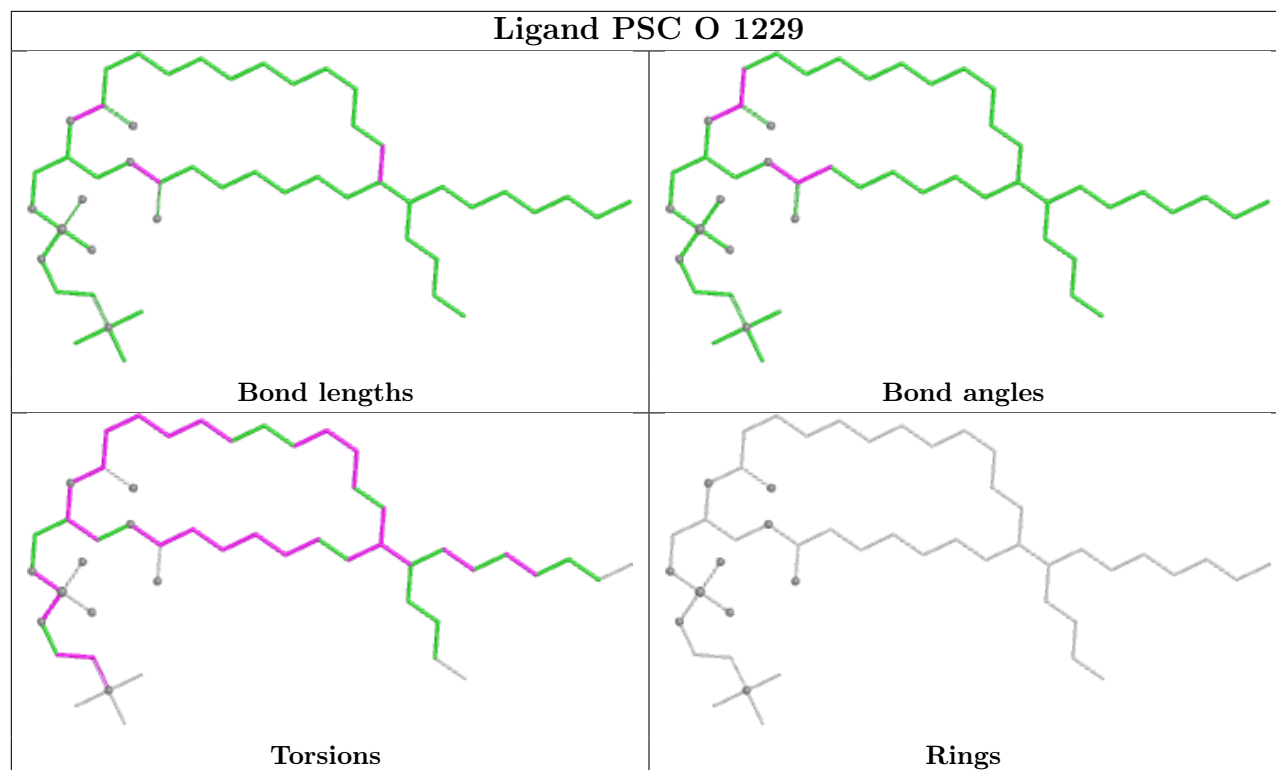
Ligand PEK T 1264

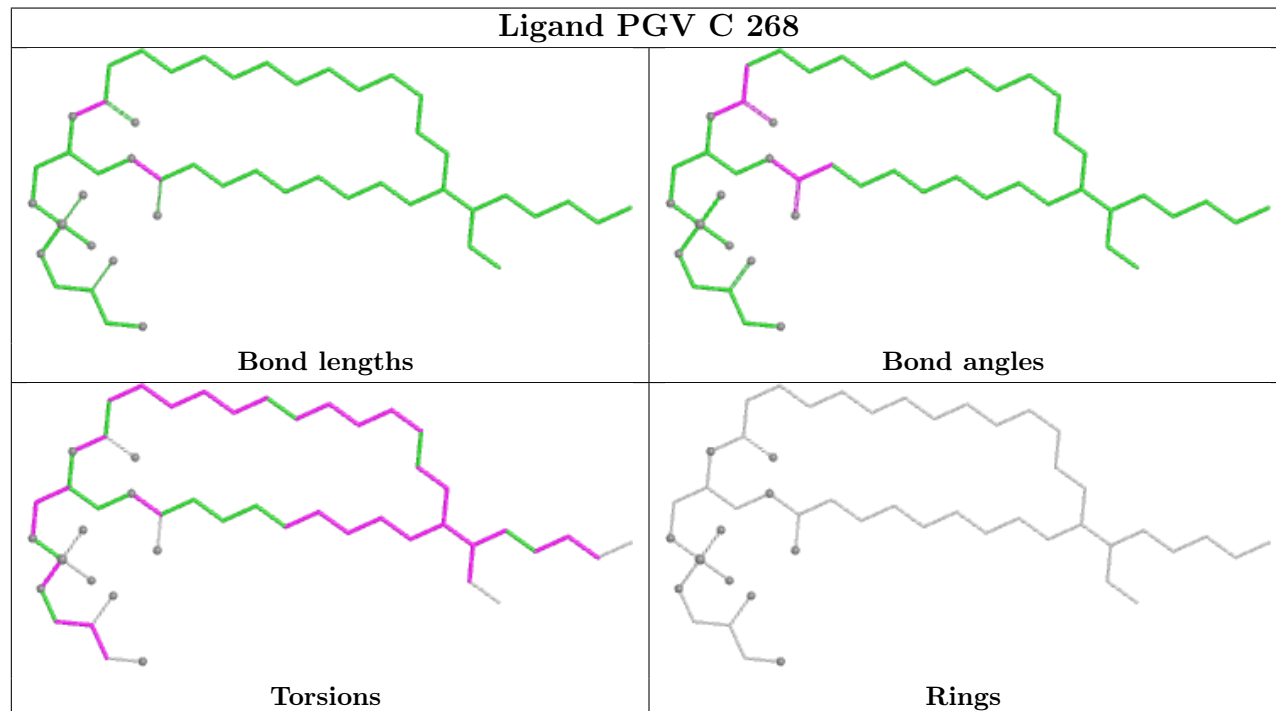
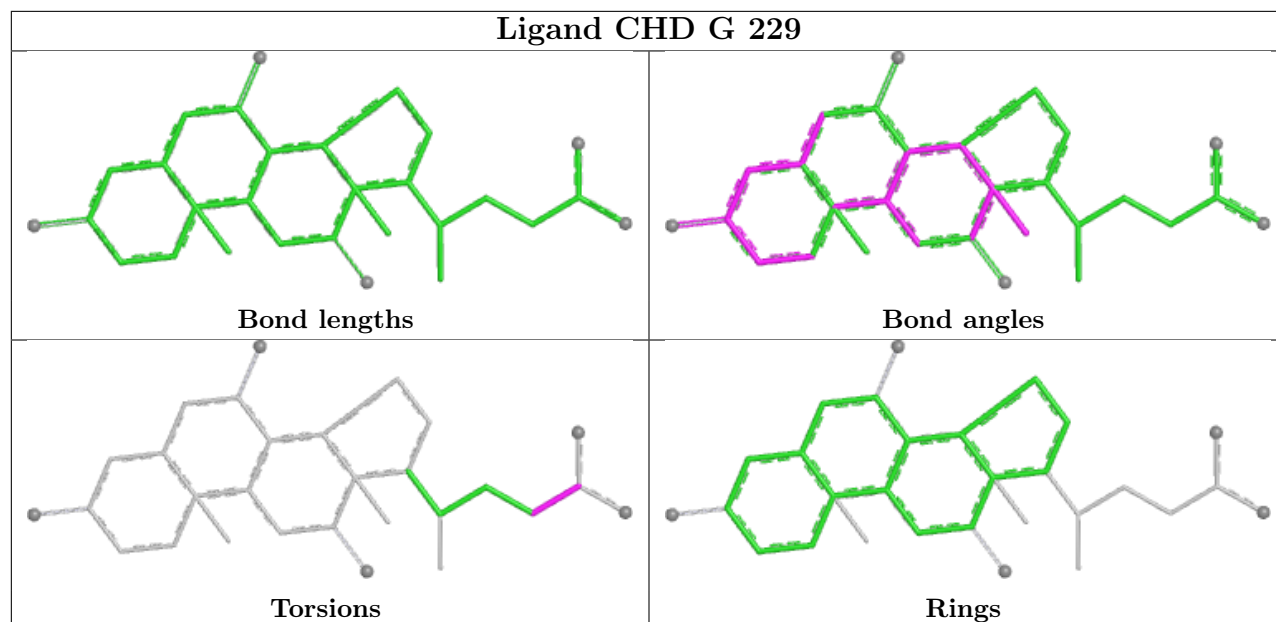


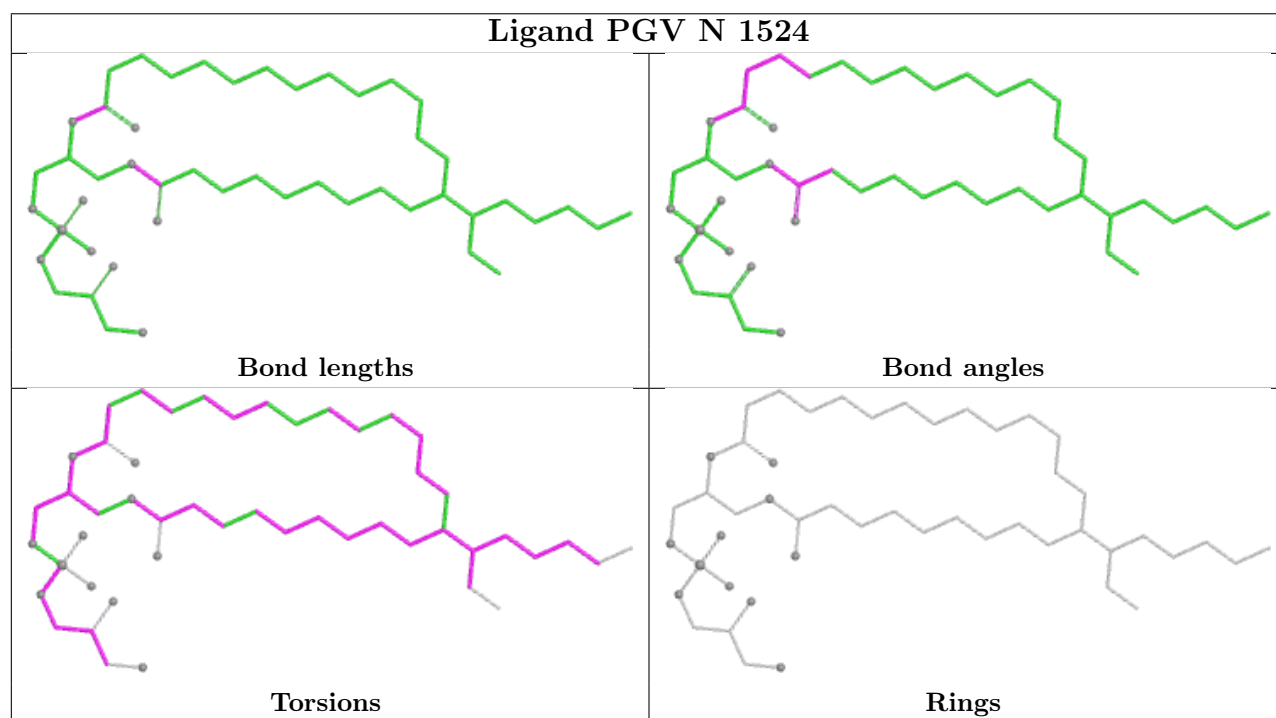
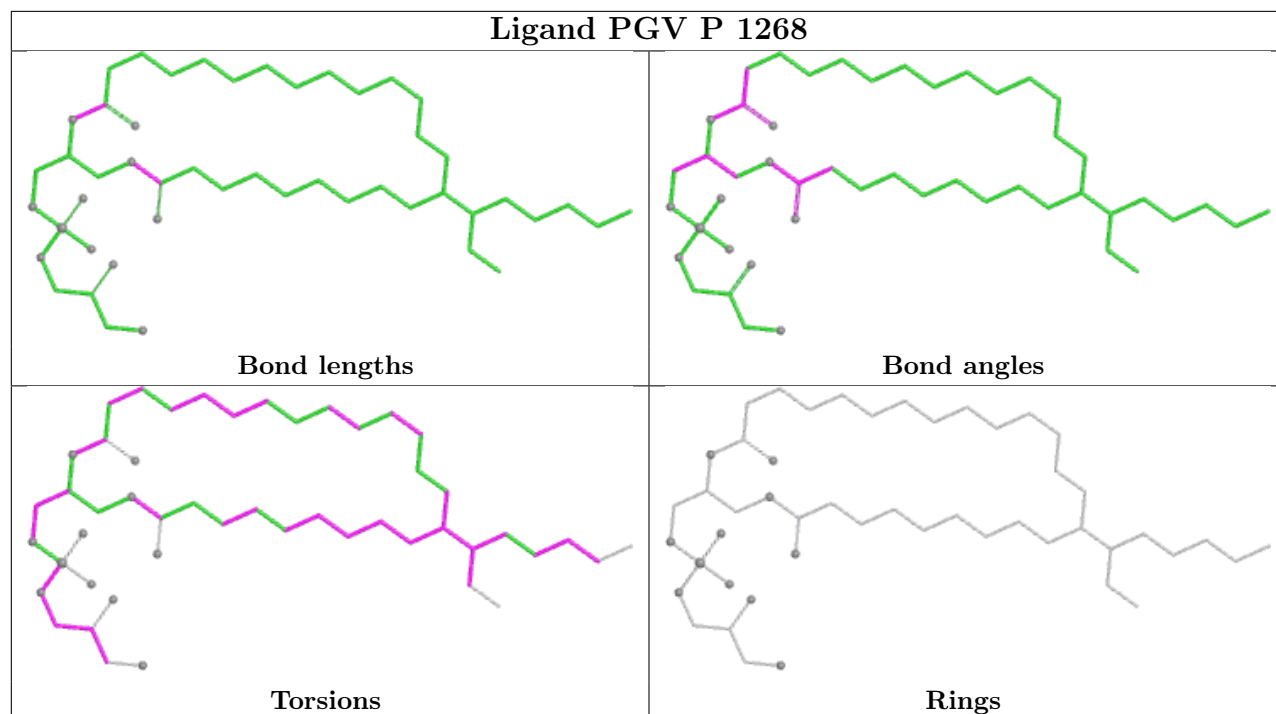
Ligand PGV A 522



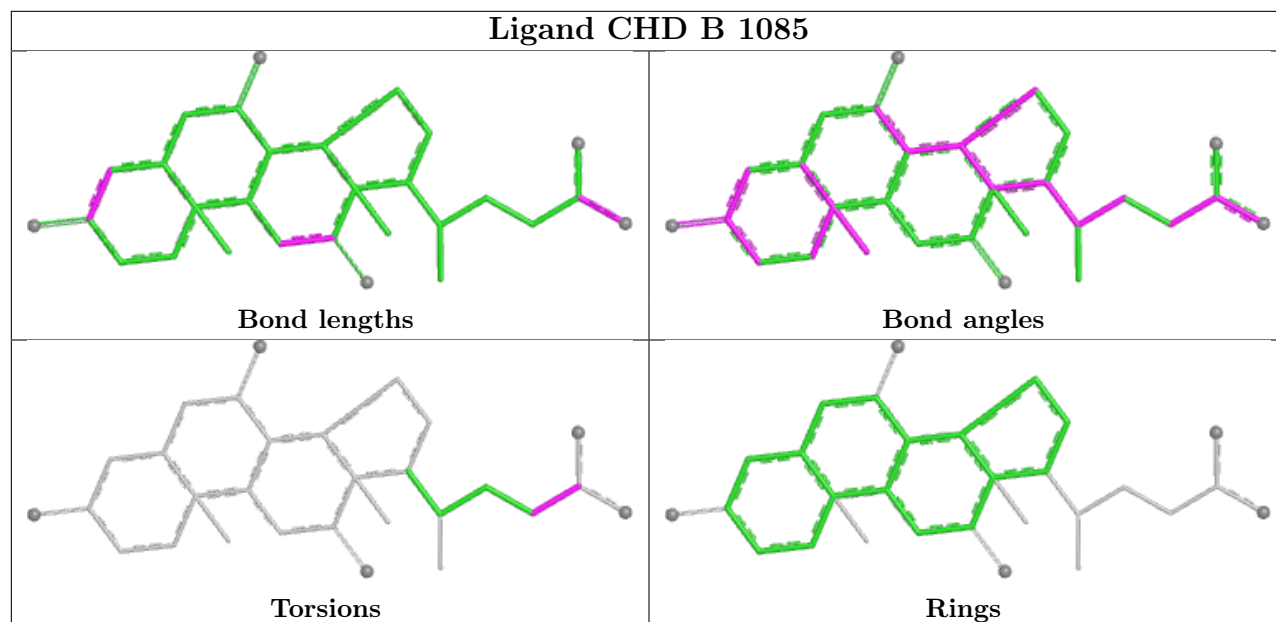




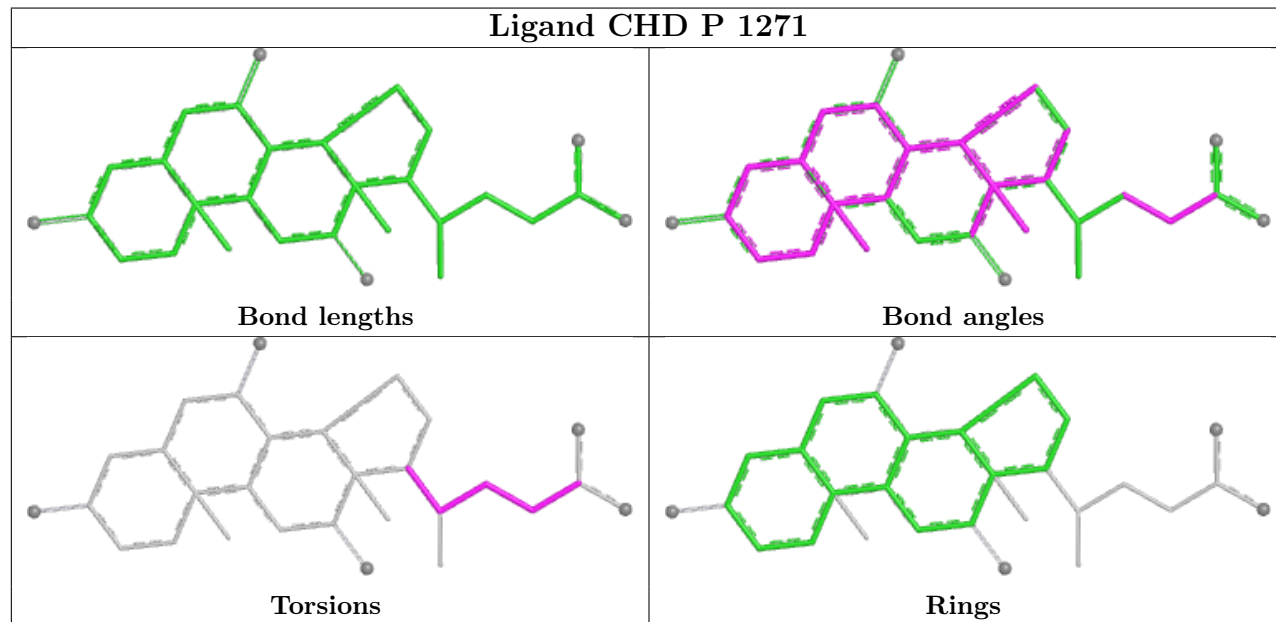


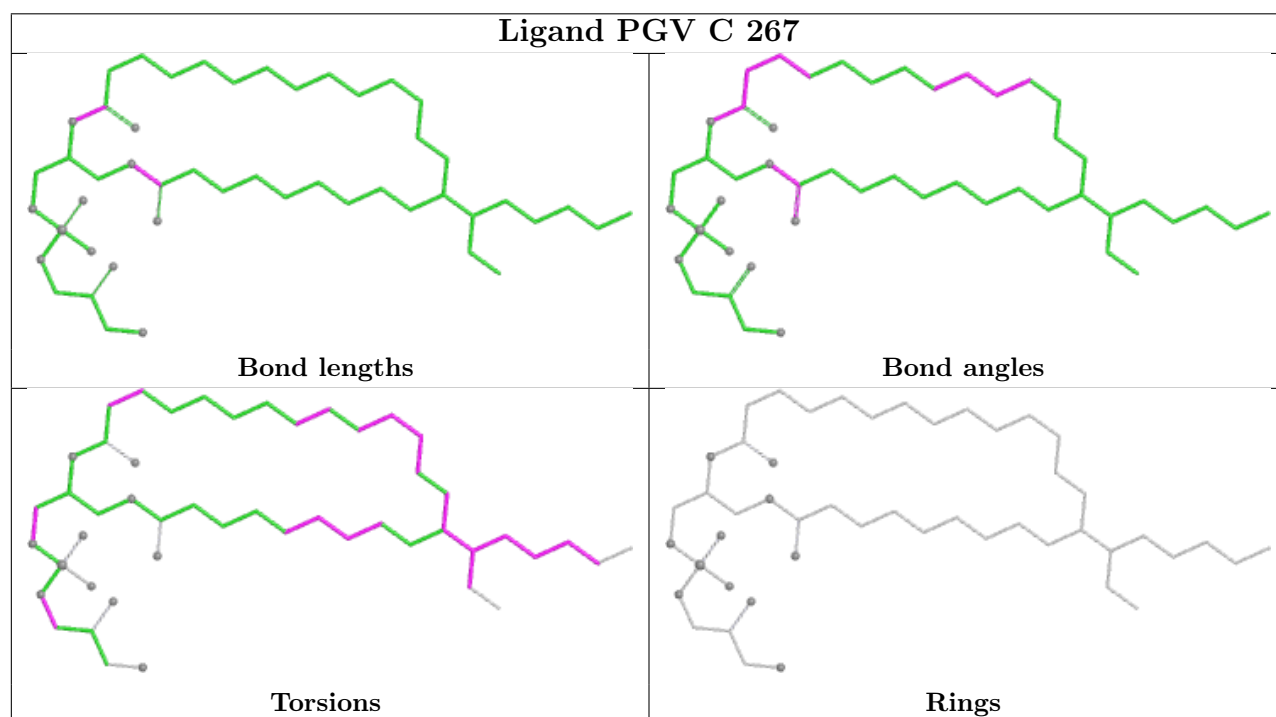
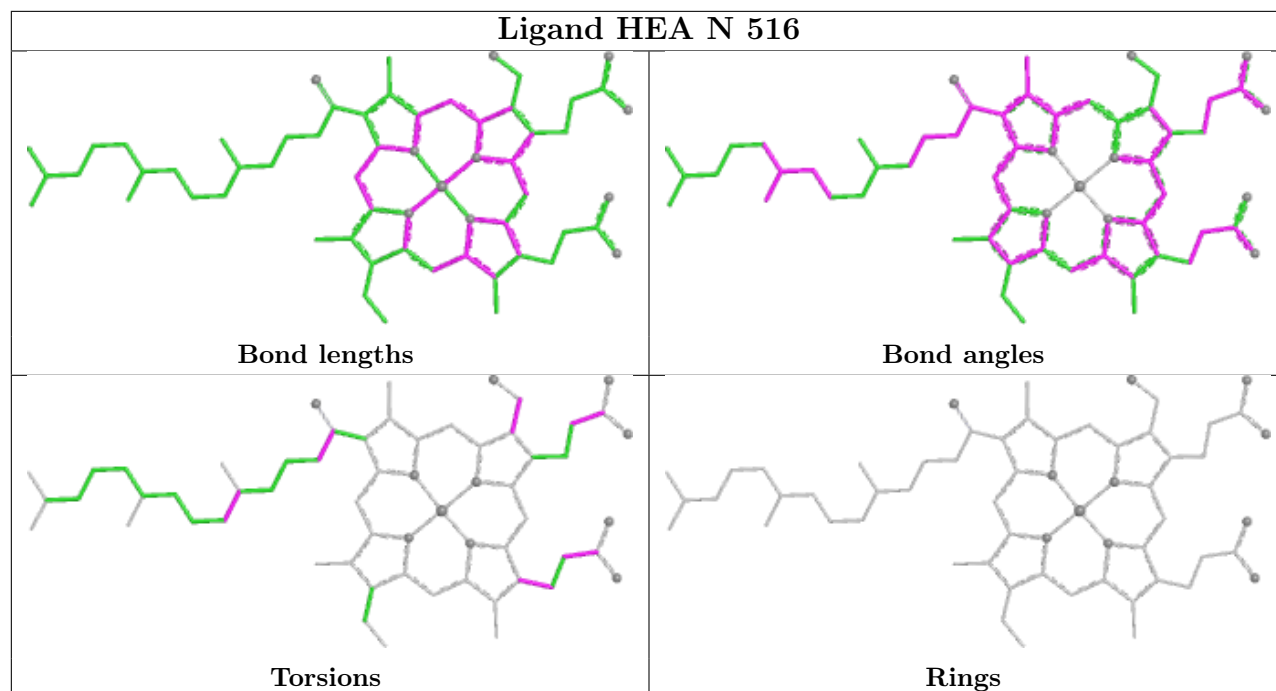


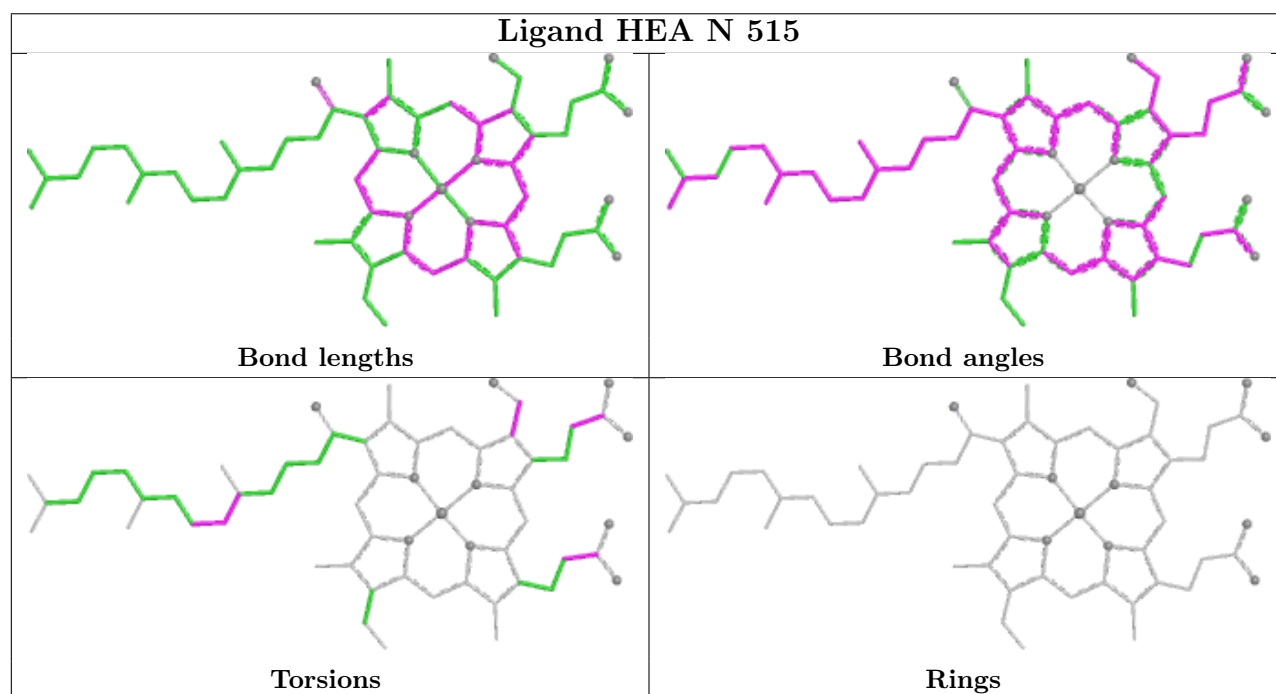
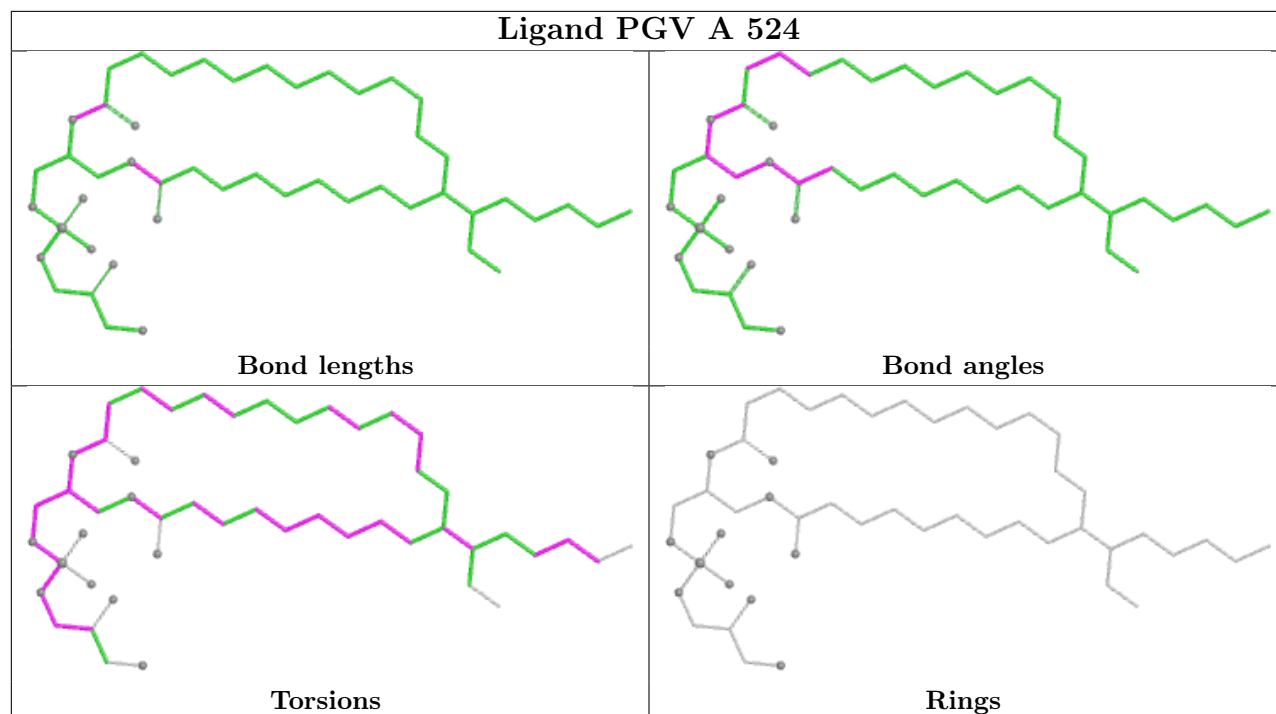
Ligand CHD B 1085

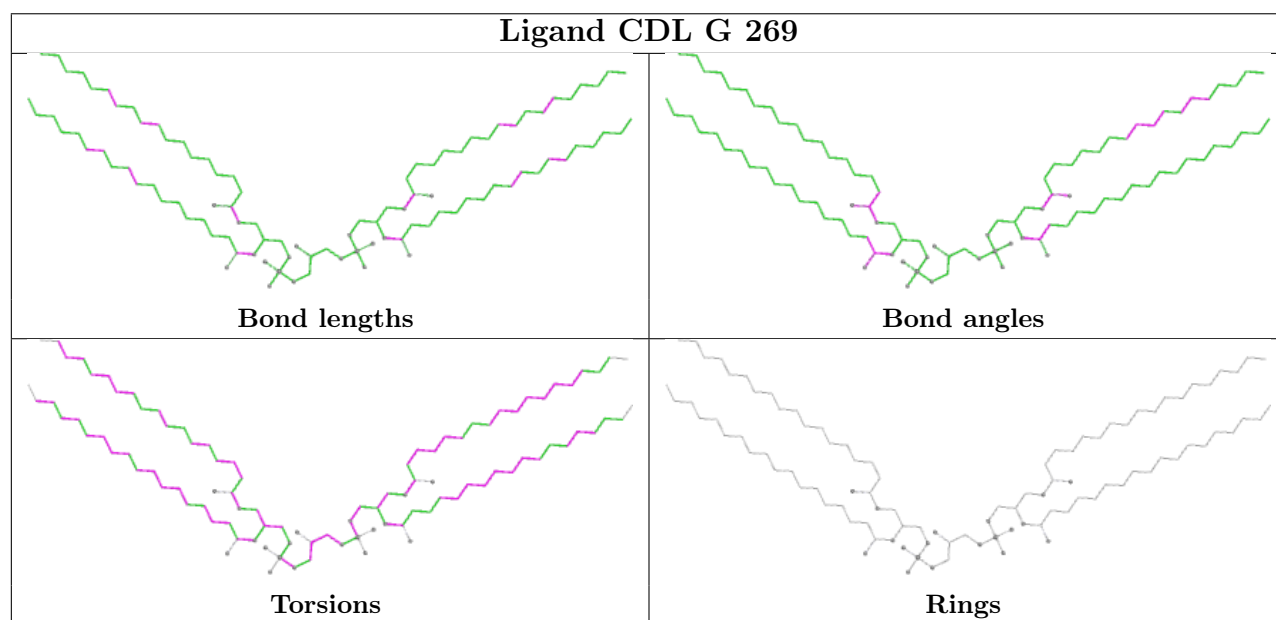
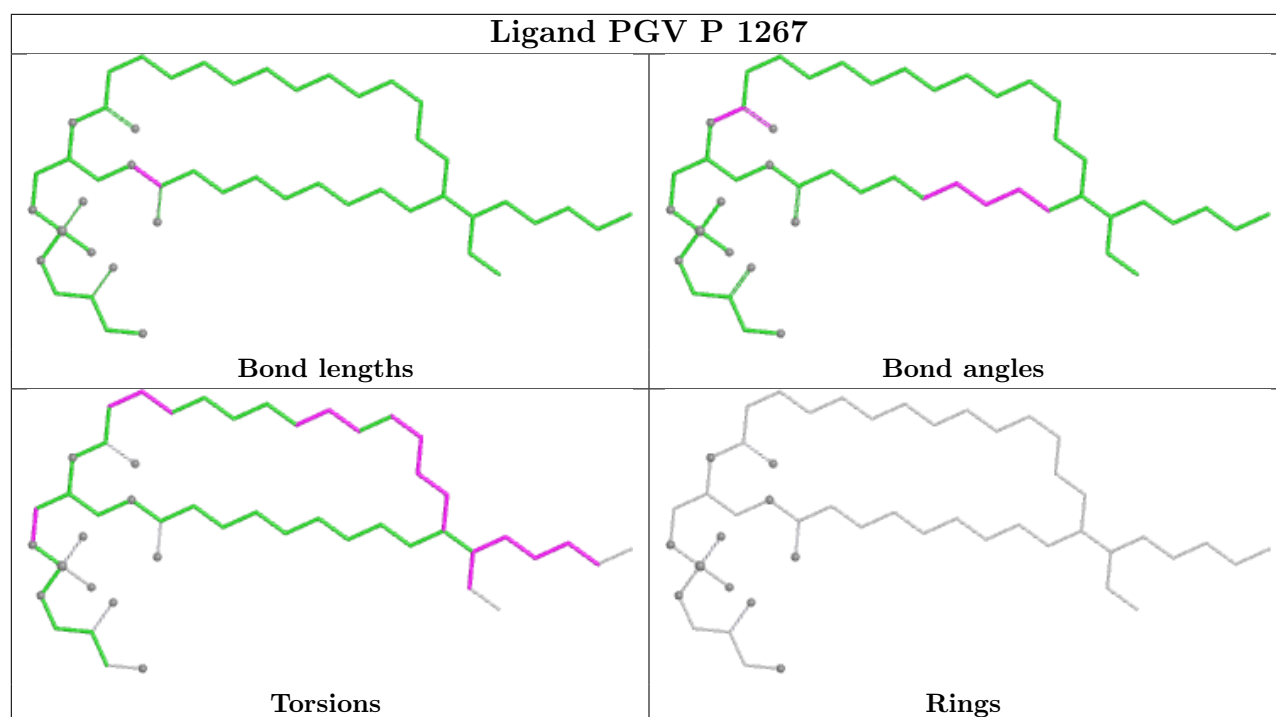


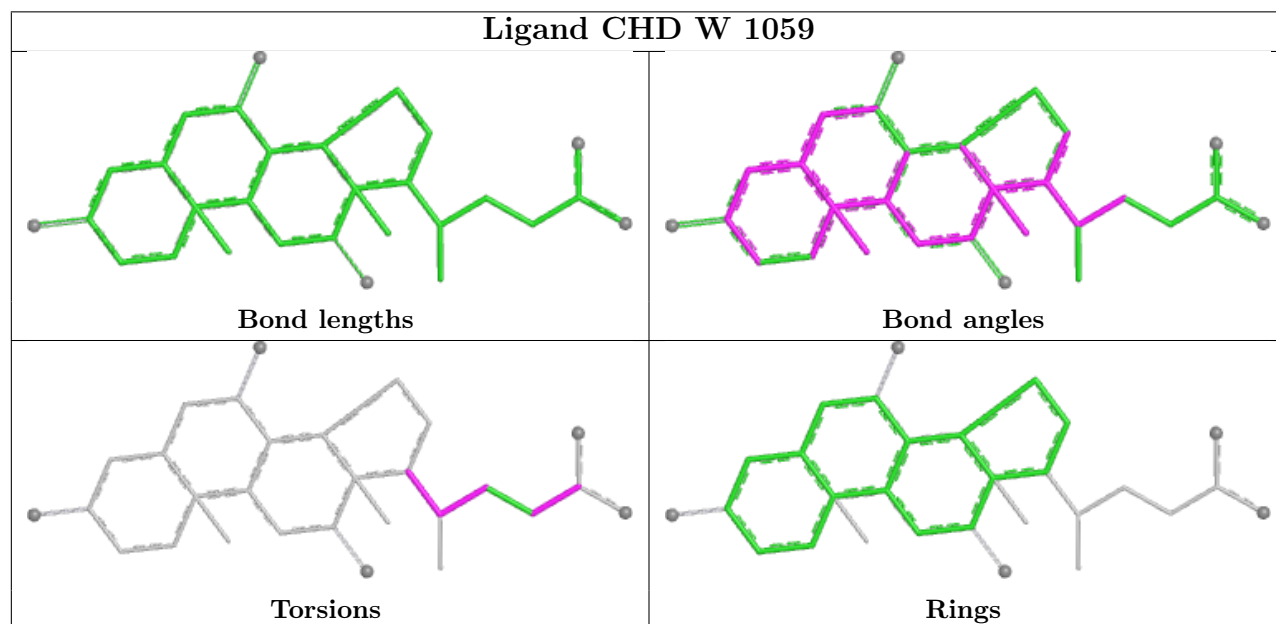
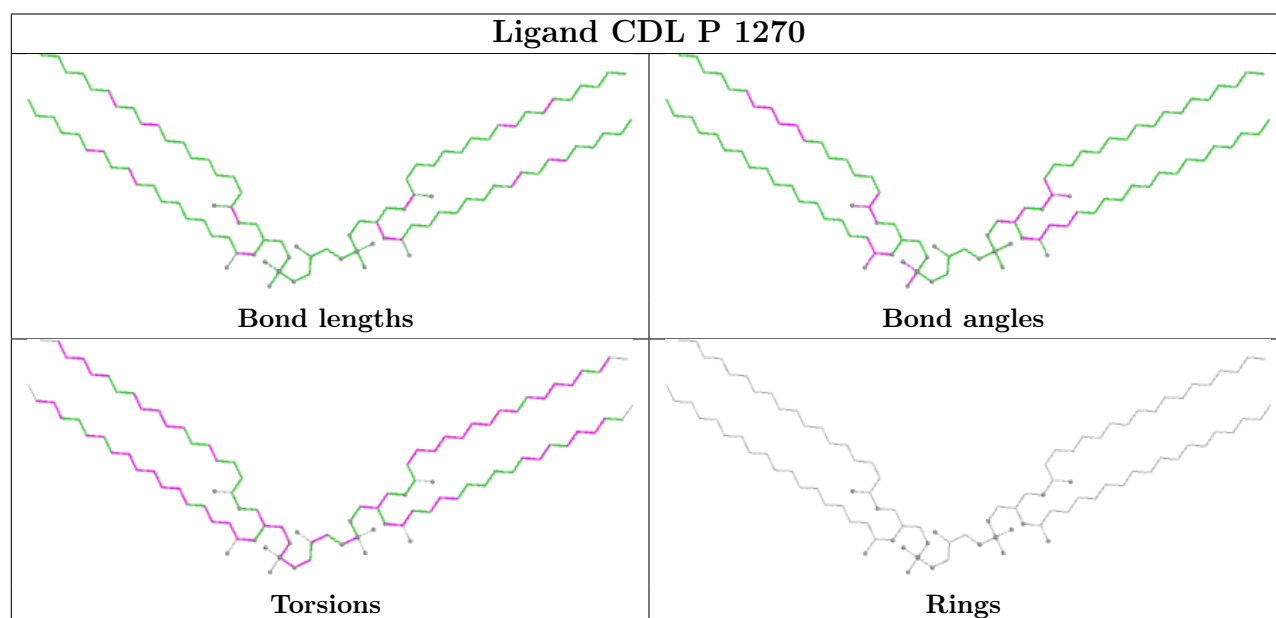
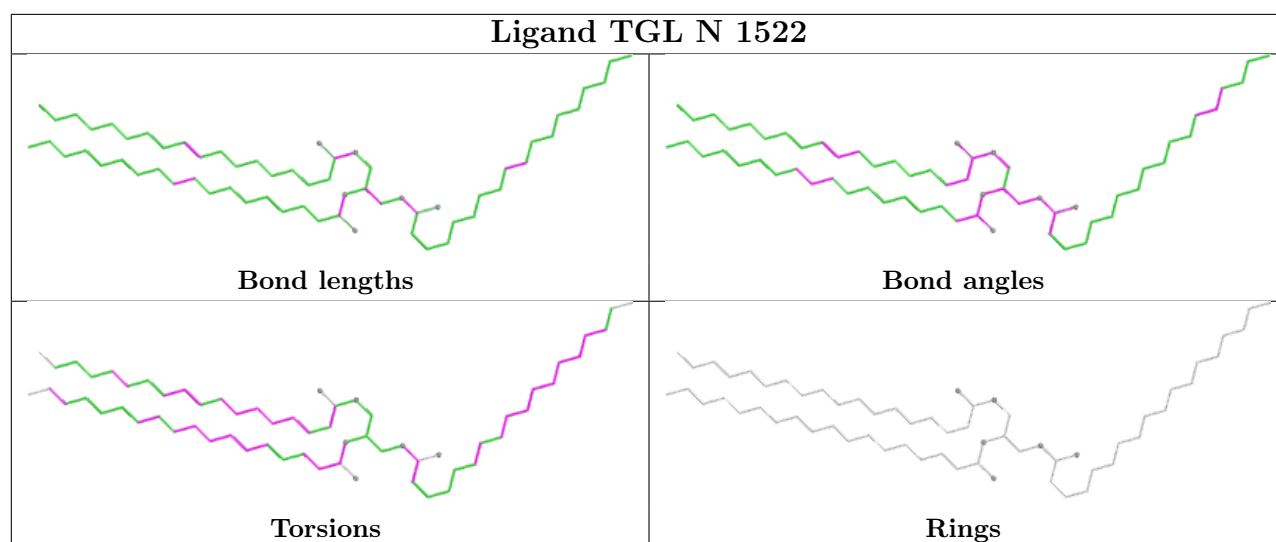
Ligand CHD P 1271

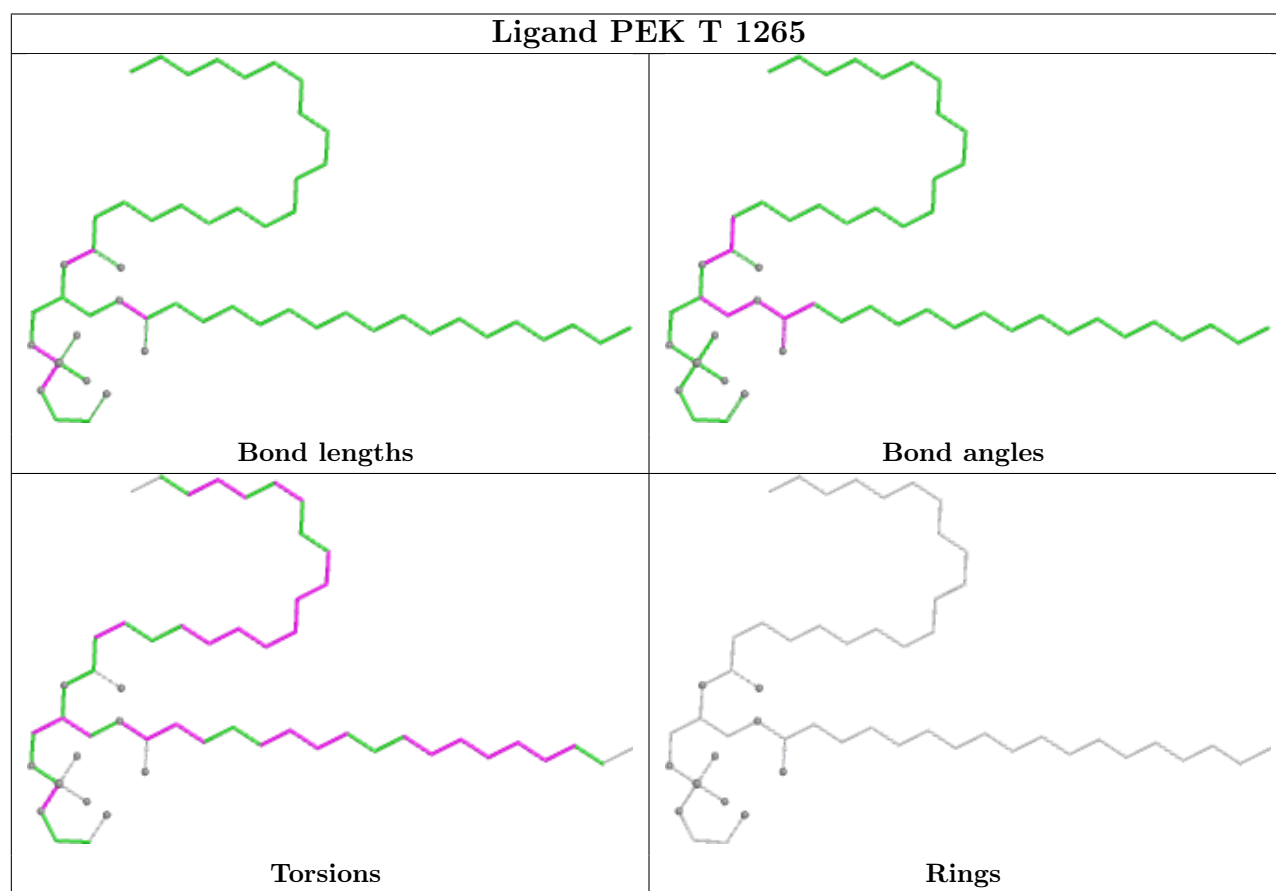
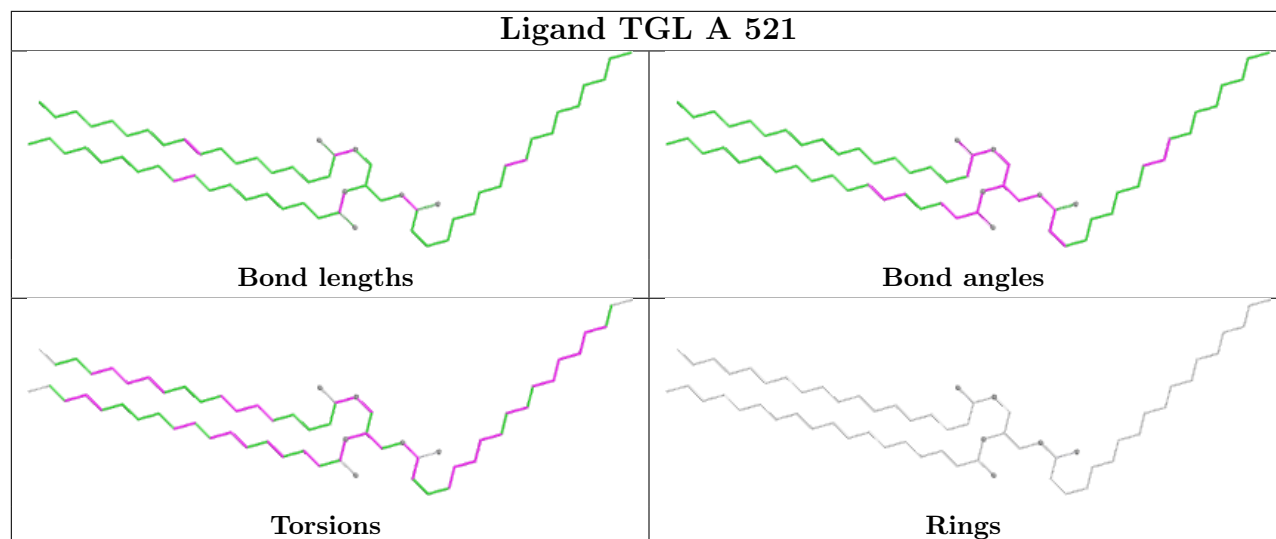


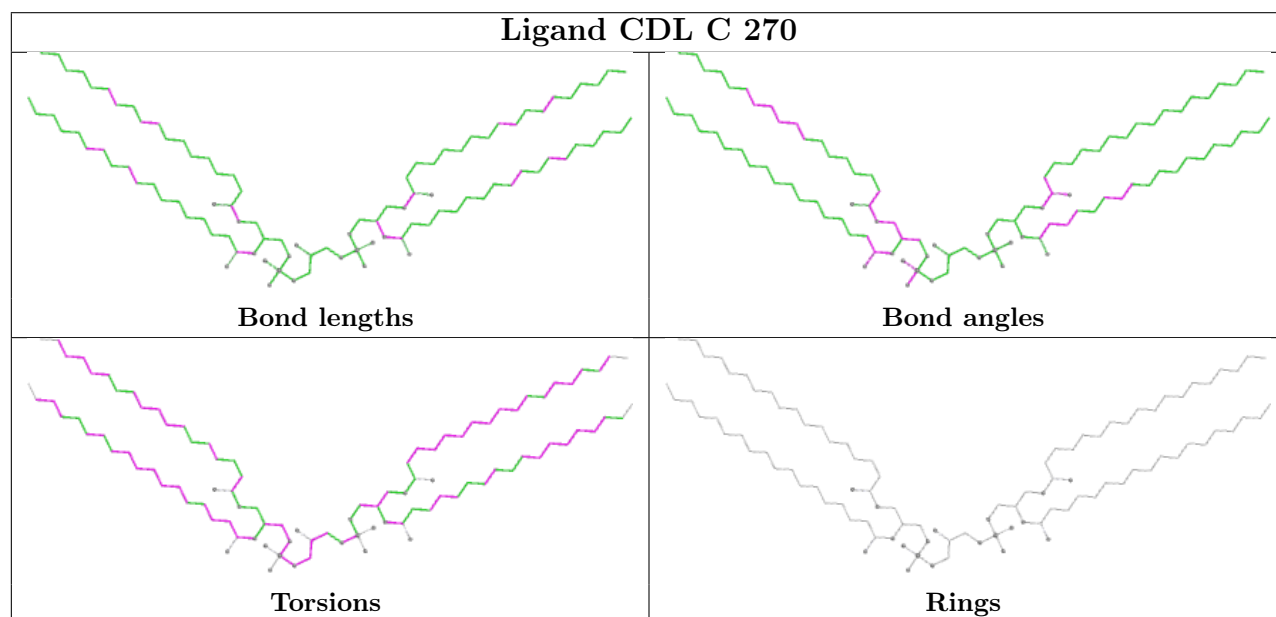
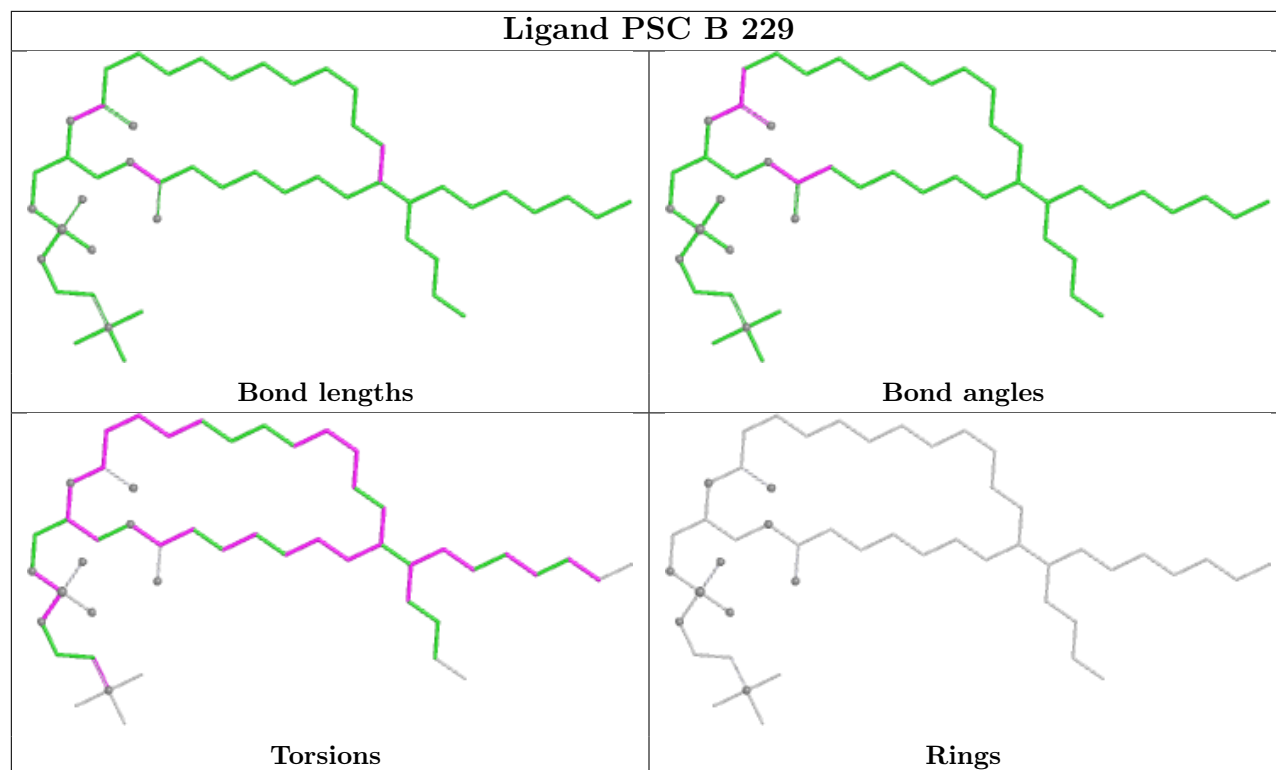




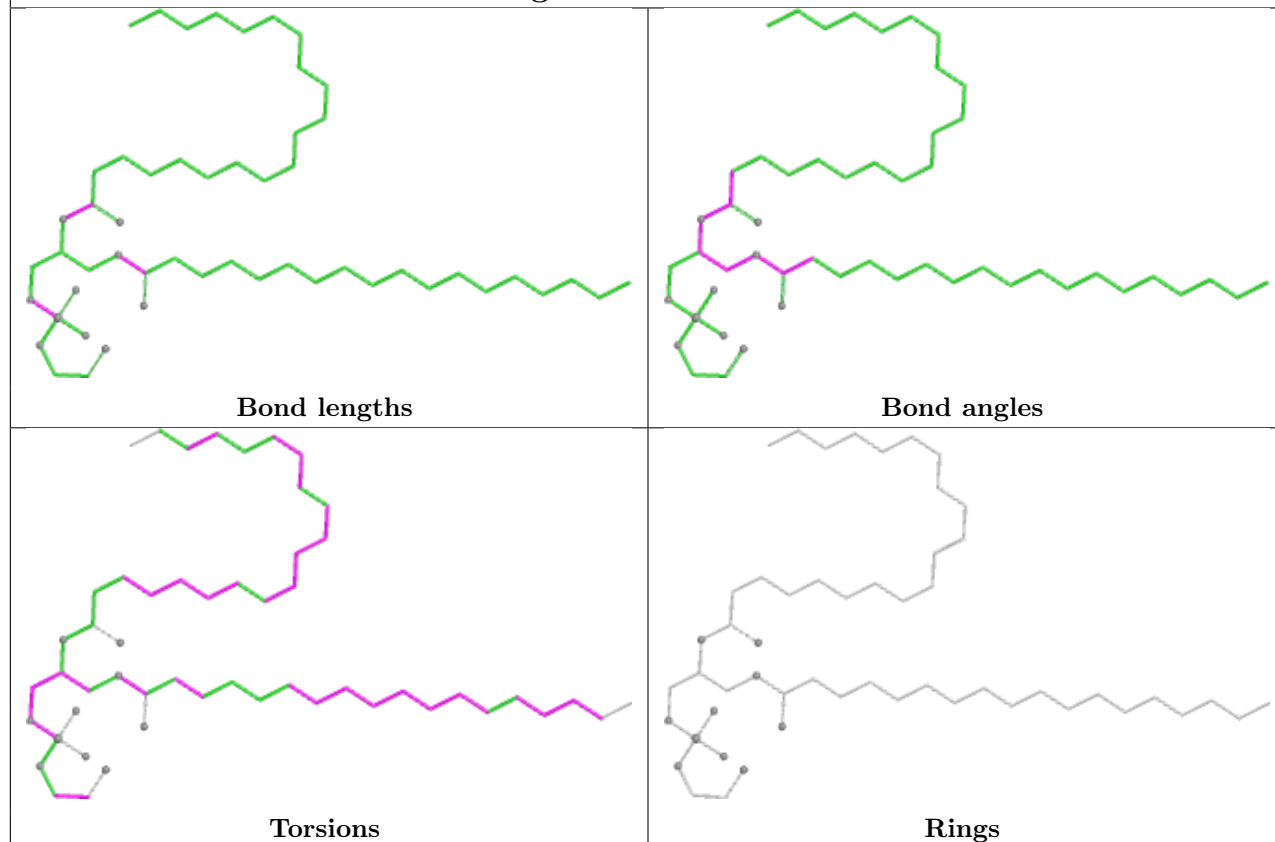




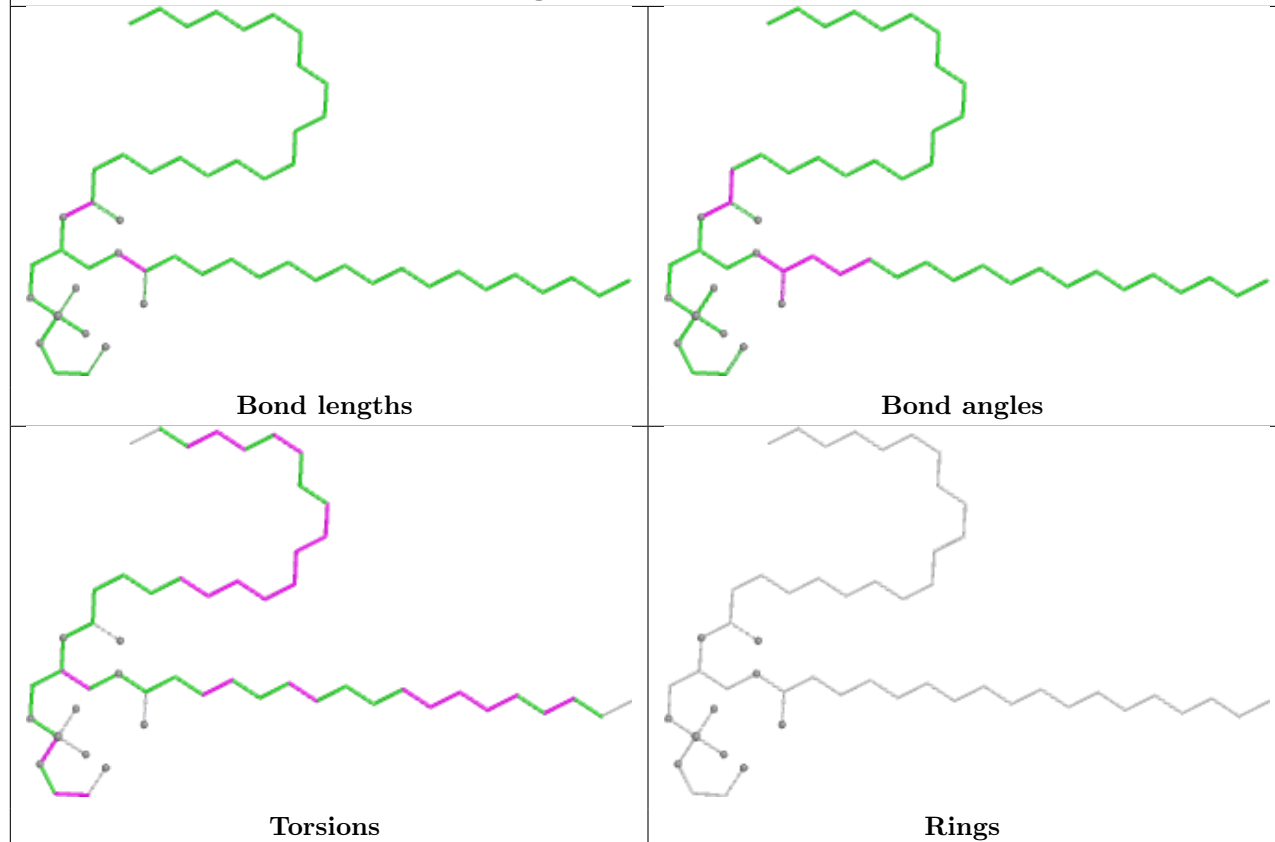




Ligand PEK T 263



Ligand PEK C 265



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.84	1 (0%) 91 91	15, 20, 27, 56	0
1	N	513/514 (99%)	-0.73	1 (0%) 91 91	17, 22, 29, 55	0
2	B	226/227 (99%)	-0.50	4 (1%) 67 69	14, 24, 51, 74	0
2	O	226/227 (99%)	-0.15	10 (4%) 39 41	19, 27, 54, 72	0
3	C	259/261 (99%)	-0.70	1 (0%) 88 89	16, 22, 33, 52	0
3	P	259/261 (99%)	-0.57	2 (0%) 82 83	17, 23, 36, 55	0
4	D	144/147 (97%)	-0.51	2 (1%) 73 75	17, 25, 44, 70	0
4	Q	144/147 (97%)	0.49	10 (6%) 23 25	24, 35, 59, 101	0
5	E	105/109 (96%)	-0.49	1 (0%) 79 80	16, 23, 51, 89	0
5	R	105/109 (96%)	0.08	5 (4%) 35 37	20, 27, 60, 91	0
6	F	98/98 (100%)	-0.08	8 (8%) 17 19	18, 28, 75, 110	0
6	S	98/98 (100%)	0.17	9 (9%) 14 16	16, 26, 79, 108	0
7	G	83/85 (97%)	0.59	20 (24%) 2 2	16, 28, 95, 99	0
7	T	83/85 (97%)	0.61	18 (21%) 2 2	18, 29, 96, 100	0
8	H	79/85 (92%)	0.06	8 (10%) 12 14	20, 31, 79, 104	0
8	U	79/85 (92%)	0.20	8 (10%) 12 14	22, 32, 80, 105	0
9	I	72/73 (98%)	0.11	3 (4%) 40 42	19, 34, 58, 67	0
9	V	72/73 (98%)	0.51	5 (6%) 23 25	20, 39, 59, 83	0
10	J	58/59 (98%)	-0.02	3 (5%) 33 34	22, 31, 60, 94	0
10	W	58/59 (98%)	0.09	3 (5%) 33 34	21, 32, 65, 99	0
11	K	49/56 (87%)	-0.16	2 (4%) 41 43	23, 30, 40, 54	0
11	X	49/56 (87%)	0.36	1 (2%) 65 66	28, 36, 51, 66	0
12	L	46/47 (97%)	-0.38	1 (2%) 62 64	19, 26, 50, 74	0
12	Y	46/47 (97%)	-0.08	1 (2%) 62 64	21, 28, 54, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.20	4 (9%) 14 16	18, 24, 67, 94	0
13	Z	43/46 (93%)	0.30	4 (9%) 14 16	25, 31, 77, 98	0
All	All	3550/3614 (98%)	-0.33	135 (3%) 44 46	14, 24, 55, 110	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	11.1
6	F	1	ALA	10.7
6	S	97	ALA	10.7
4	Q	6	VAL	10.2
4	Q	5	VAL	9.4
6	S	94	HIS	8.4
8	U	8	ILE	7.2
6	F	96	LEU	7.0
4	Q	8	SER	6.7
2	O	226	MET	6.7
9	V	3	ALA	6.5
6	F	97	ALA	6.2
4	Q	4	SER	6.2
6	S	98	HIS	6.1
7	T	5	LYS	6.0
13	Z	43	SER	5.7
7	G	36	TRP	5.7
7	T	36	TRP	5.7
13	Z	42	LYS	5.7
6	S	96	LEU	5.6
8	H	8	ILE	5.6
8	H	47	GLY	5.6
6	S	93	PRO	5.5
2	O	227	LEU	5.5
7	G	5	LYS	5.5
7	G	4	ALA	5.4
7	G	39	SER	5.1
9	V	37	PHE	5.0
2	O	224	ALA	5.0
7	T	4	ALA	4.9
7	G	9	GLY	4.9
9	V	2	THR	4.7
6	S	95	GLN	4.7
7	T	9	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
7	G	1	ALA	4.6
6	F	94	HIS	4.6
7	T	39	SER	4.5
11	X	6	ALA	4.5
7	G	3	ALA	4.4
9	I	37	PHE	4.3
3	P	3	HIS	4.3
10	J	58	LYS	4.2
8	H	10	ASN	4.2
9	V	5	ALA	4.2
7	T	10	GLY	4.1
4	Q	7	LYS	4.1
2	B	59	GLN	4.1
7	G	7	ASP	4.0
2	O	59	GLN	4.0
10	J	57	HIS	3.9
10	W	57	HIS	3.9
5	E	5	HIS	3.9
7	T	3	ALA	3.9
7	T	2	SER	3.8
10	W	58	LYS	3.8
7	G	10	GLY	3.8
7	T	8	HIS	3.7
6	F	95	GLN	3.7
7	T	42	ARG	3.7
6	F	98	HIS	3.7
6	S	2	SER	3.7
6	F	3	GLY	3.6
3	P	38	ASN	3.6
7	T	7	ASP	3.5
6	F	2	SER	3.5
7	T	12	GLY	3.5
8	H	7	LYS	3.5
2	O	113	TYR	3.4
6	S	3	GLY	3.4
13	M	41	LYS	3.4
4	Q	10	ASP	3.4
5	R	109	VAL	3.4
7	G	38	HIS	3.3
7	T	1	ALA	3.3
13	M	43	SER	3.3
9	I	2	THR	3.2

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Mol	Chain	Res	Type	RSRZ
8	U	7	LYS	3.2
7	G	37	LEU	3.2
13	M	40	TYR	3.1
7	T	84	LYS	3.1
7	G	2	SER	3.1
7	T	38	HIS	3.1
7	G	40	GLY	3.1
7	T	37	LEU	3.0
2	O	90	ILE	3.0
10	J	1	PHE	3.0
7	G	8	HIS	3.0
5	R	5	HIS	2.9
13	Z	40	TYR	2.9
8	H	9	LYS	2.9
5	R	7	THR	2.9
7	T	6	GLY	2.9
12	L	2	HIS	2.9
8	U	50	VAL	2.9
2	O	225	SER	2.8
2	O	60	GLU	2.8
11	K	6	ALA	2.8
8	U	47	GLY	2.8
8	U	10	ASN	2.7
2	B	60	GLU	2.7
7	G	41	HIS	2.7
7	T	40	GLY	2.7
4	D	4	SER	2.7
8	H	45	ALA	2.7
4	D	5	VAL	2.7
1	N	514	LYS	2.6
7	G	12	GLY	2.6
7	G	42	ARG	2.6
8	H	46	LYS	2.6
8	U	45	ALA	2.6
2	B	65	TRP	2.6
4	Q	35	ALA	2.6
3	C	38	ASN	2.6
10	W	1	PHE	2.6
7	G	6	GLY	2.6
12	Y	20	ARG	2.5
4	Q	33	LEU	2.5
9	V	4	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
9	I	32	ALA	2.4
4	Q	58	GLU	2.4
4	Q	46	ALA	2.3
1	A	514	LYS	2.3
5	R	108	LYS	2.3
8	U	48	GLY	2.2
5	R	9	GLU	2.2
13	M	42	LYS	2.2
2	O	65	TRP	2.2
2	O	92	ASN	2.2
8	H	48	GLY	2.1
11	K	47	ARG	2.1
7	G	84	LYS	2.1
13	Z	41	LYS	2.1
7	G	45	PRO	2.1
8	U	9	LYS	2.0
2	B	91	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.28	0.26	88,90,91,91	0
9	SAC	I	1	9/10	0.39	0.30	76,79,82,83	0
7	TPO	G	11	11/12	0.46	0.23	63,71,87,88	0
7	TPO	T	11	11/12	0.53	0.23	66,73,89,89	0
1	FME	A	1	10/11	0.83	0.14	36,39,58,66	0
1	FME	N	1	10/11	0.89	0.13	37,41,58,60	0
2	FME	O	1	10/11	0.94	0.09	25,26,33,38	0
2	FME	B	1	10/11	0.95	0.08	23,24,33,45	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CHD	W	1059	29/29	0.48	0.28	95,105,107,107	0
22	CHD	J	60	29/29	0.51	0.28	99,107,110,111	0
24	PEK	T	263	53/53	0.56	0.27	51,91,109,111	0
24	PEK	C	265	53/53	0.60	0.25	43,91,99,100	0
24	PEK	G	1263	53/53	0.61	0.26	55,94,110,110	0
19	PGV	P	1268	51/51	0.64	0.23	77,90,102,103	0
18	TGL	Q	1523	63/63	0.64	0.21	49,74,91,92	0
24	PEK	T	1265	53/53	0.64	0.23	42,90,101,102	0
23	UNX	C	262	1/1	0.66	0.26	43,43,43,43	0
18	TGL	N	1522	63/63	0.67	0.23	47,71,84,86	0
19	PGV	C	268	51/51	0.67	0.22	63,88,101,102	0
25	CDL	G	269	100/100	0.67	0.21	65,85,106,111	0
25	CDL	T	1269	100/100	0.67	0.22	56,86,108,109	0
25	CDL	P	1270	100/100	0.69	0.22	45,85,107,109	0
19	PGV	N	1524	51/51	0.69	0.19	43,69,102,102	0
18	TGL	N	1521	63/63	0.70	0.20	48,73,88,91	0
25	CDL	C	270	100/100	0.71	0.21	42,84,106,108	0
22	CHD	C	271	29/29	0.72	0.20	79,89,90,91	0
19	PGV	A	524	51/51	0.72	0.21	34,69,94,96	0
18	TGL	D	523	63/63	0.72	0.20	50,69,91,91	0
23	UNX	P	262	1/1	0.73	0.30	44,44,44,44	0
21	PSC	B	229	52/52	0.73	0.21	48,92,113,115	0
22	CHD	P	1271	29/29	0.73	0.20	82,90,91,91	0
18	TGL	L	522	63/63	0.75	0.22	38,62,80,83	0
21	PSC	O	1229	52/52	0.75	0.23	40,85,110,113	0
18	TGL	A	521	63/63	0.77	0.18	50,70,88,92	0
16	MG	N	518	1/1	0.87	0.08	23,23,23,23	0
27	DMU	Z	1526	33/33	0.88	0.10	37,45,57,57	0
27	DMU	M	526	33/33	0.90	0.10	34,40,51,52	0
16	MG	A	518	1/1	0.93	0.07	21,21,21,21	0
24	PEK	T	1264	53/53	0.94	0.10	19,44,71,73	0
14	HEA	N	515	60/60	0.95	0.12	20,33,50,53	0
22	CHD	B	1085	29/29	0.95	0.06	12,15,23,33	0
22	CHD	P	1525	29/29	0.95	0.06	24,28,31,33	0
22	CHD	C	525	29/29	0.95	0.06	24,29,32,33	0
24	PEK	G	264	53/53	0.95	0.10	17,41,71,72	0
20	CUA	O	228	2/2	0.96	0.03	22,22,22,22	0

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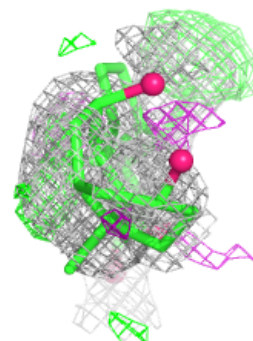
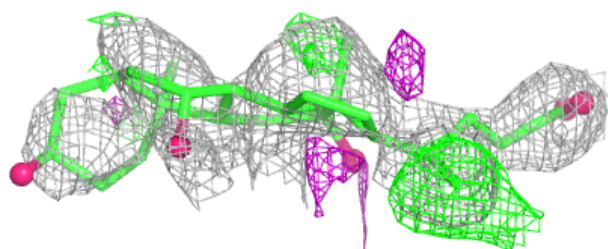
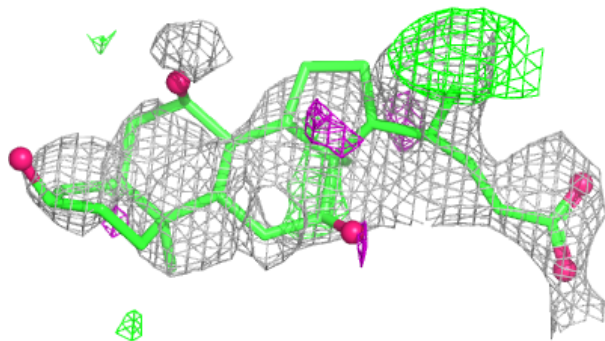
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	NA	N	519	1/1	0.96	0.05	24,24,24,24	0
19	PGV	A	522	51/51	0.96	0.07	19,32,54,56	0
19	PGV	N	1266	51/51	0.96	0.09	19,38,57,59	0
19	PGV	P	1267	51/51	0.96	0.08	19,29,65,69	0
19	PGV	C	267	51/51	0.96	0.08	17,29,64,69	0
22	CHD	G	229	29/29	0.97	0.05	10,16,19,25	0
26	ZN	S	99	1/1	0.98	0.02	23,23,23,23	0
14	HEA	A	515	60/60	0.98	0.07	14,19,41,50	0
14	HEA	N	516	60/60	0.98	0.06	15,19,26,30	0
15	CU	N	517	1/1	0.99	0.05	23,23,23,23	0
14	HEA	A	516	60/60	0.99	0.05	11,18,24,26	0
26	ZN	F	99	1/1	0.99	0.01	23,23,23,23	0
15	CU	A	517	1/1	0.99	0.04	20,20,20,20	0
20	CUA	B	228	2/2	0.99	0.02	18,18,18,18	0
17	NA	A	519	1/1	0.99	0.08	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.

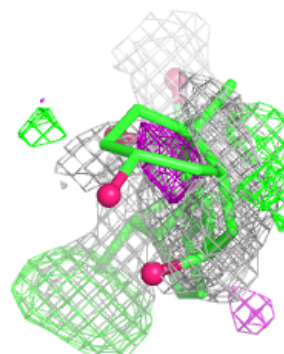
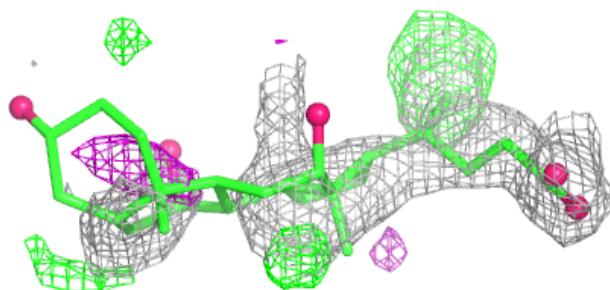
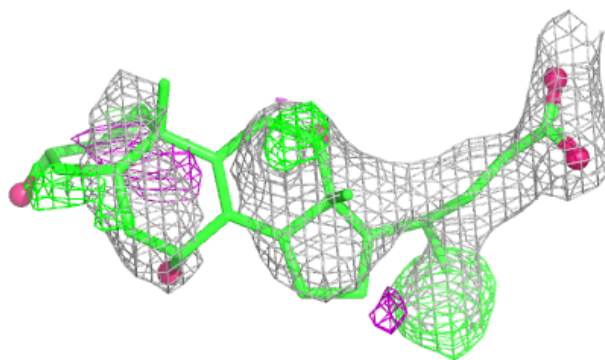
Electron density around CHD W 1059:

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



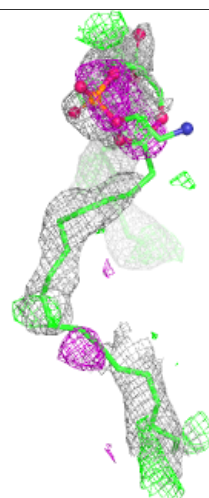
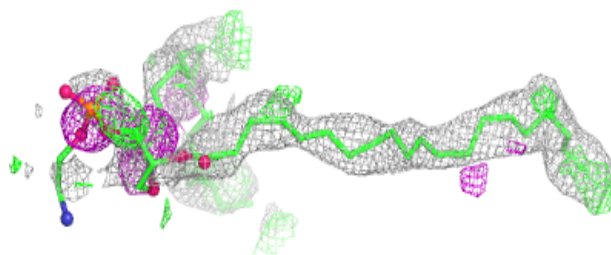
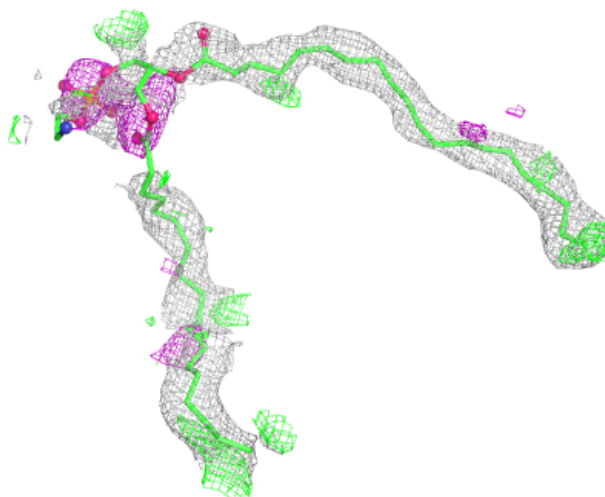
Electron density around CHD J 60:

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



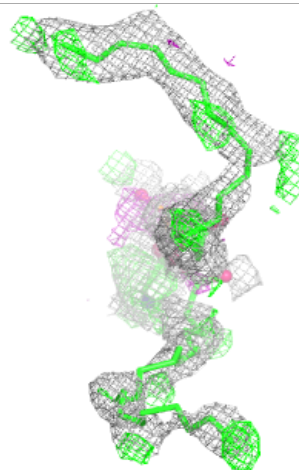
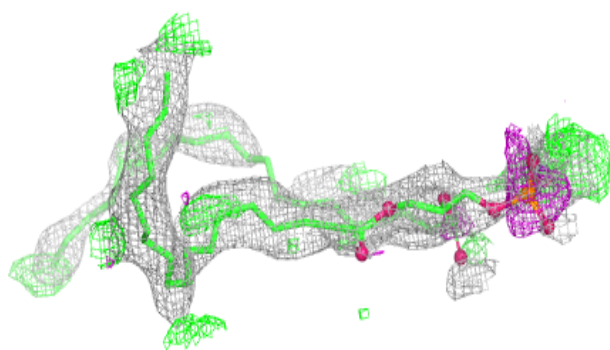
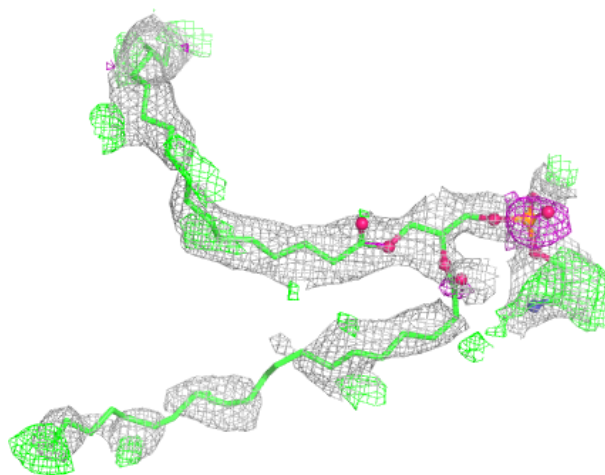
Electron density around PEK T 263:

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



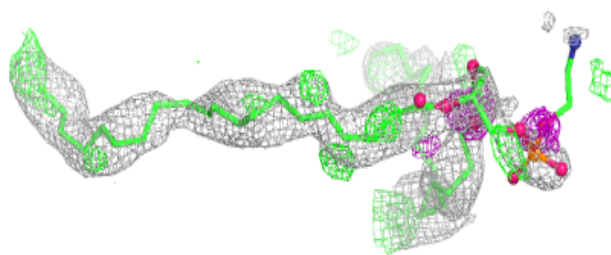
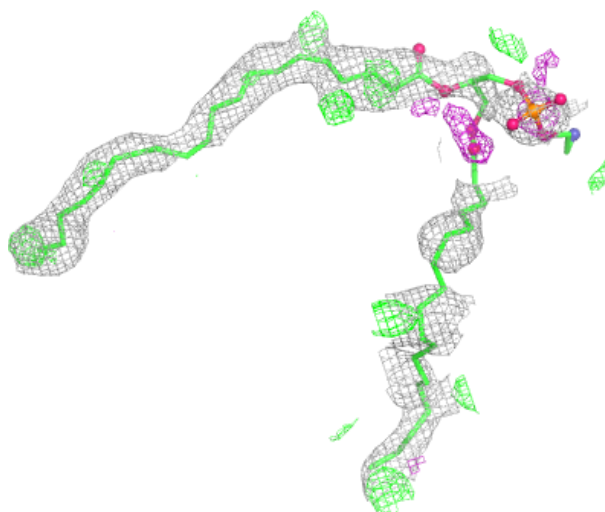
Electron density around PEK C 265:

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



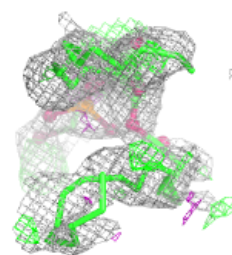
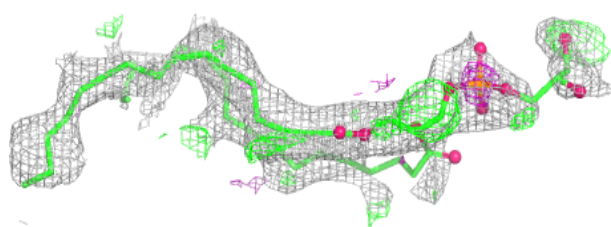
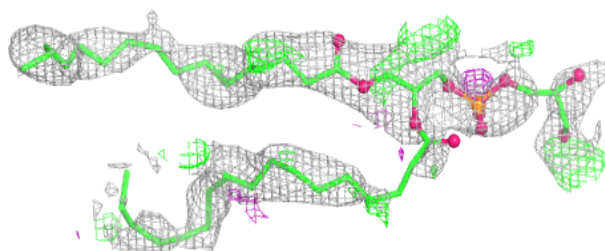
Electron density around PEK G 1263:

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

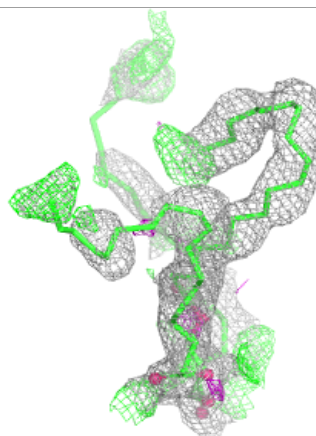
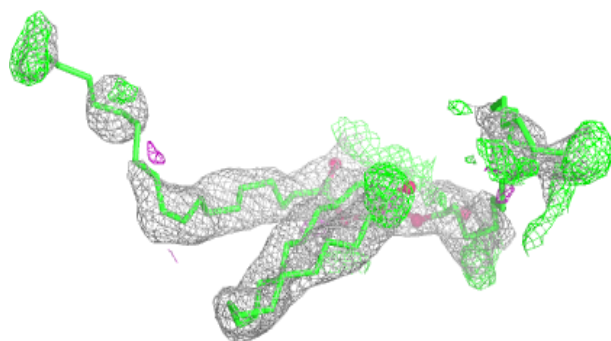
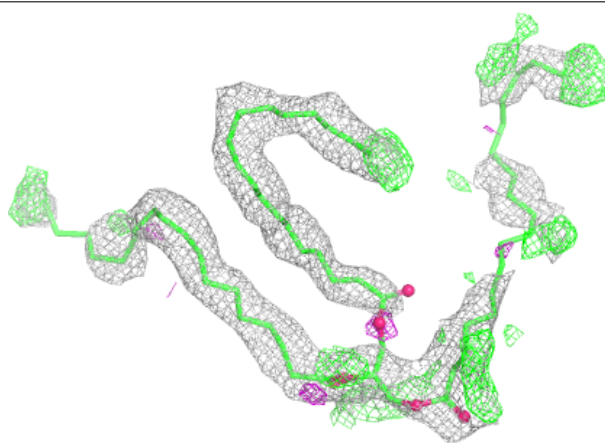


Electron density around PGV P 1268:

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

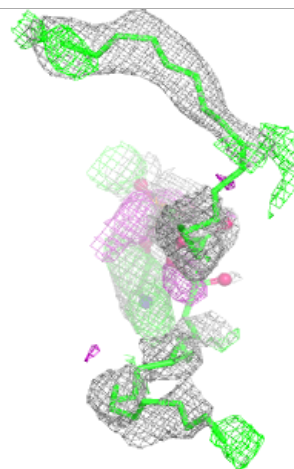
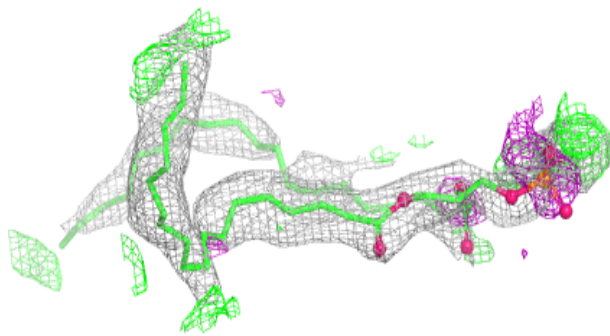
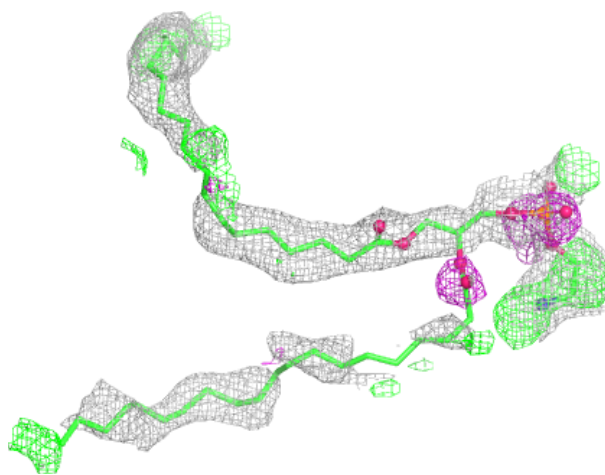
**Electron density around TGL Q 1523:**

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



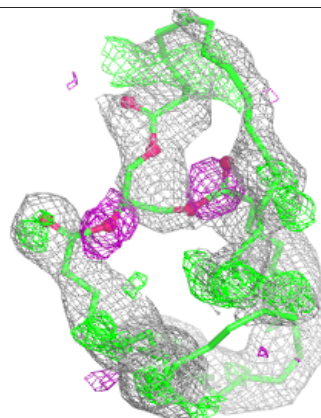
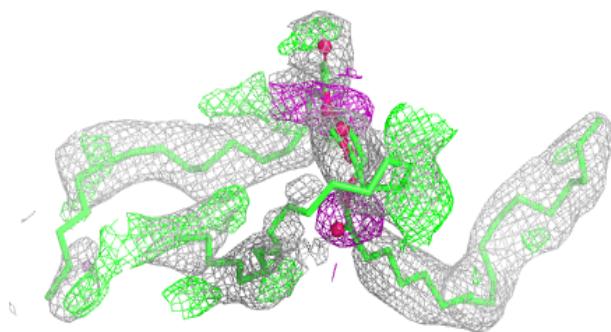
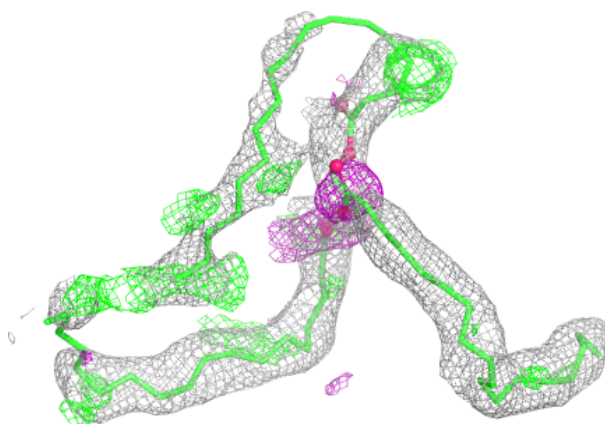
Electron density around PEK T 1265:

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

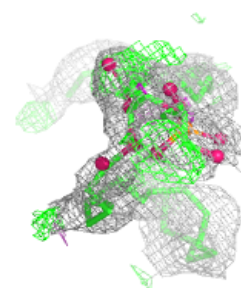
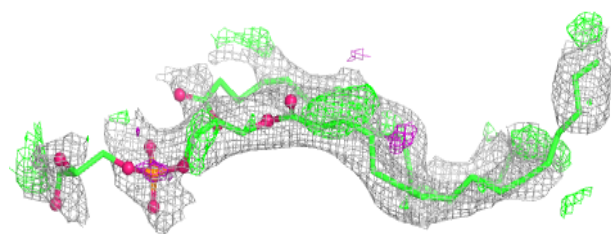
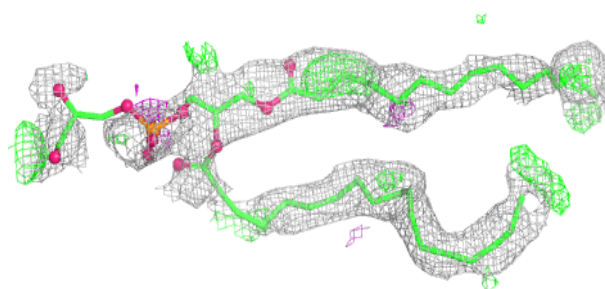


Electron density around TGL N 1522:

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

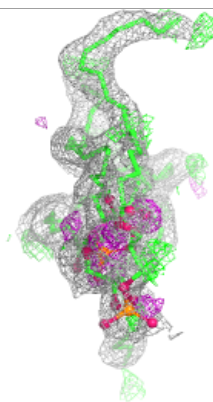
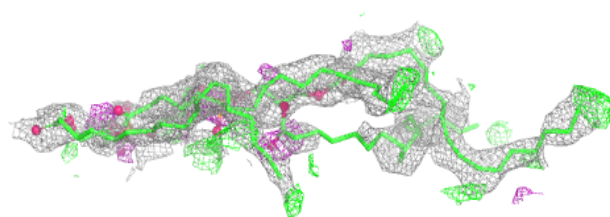
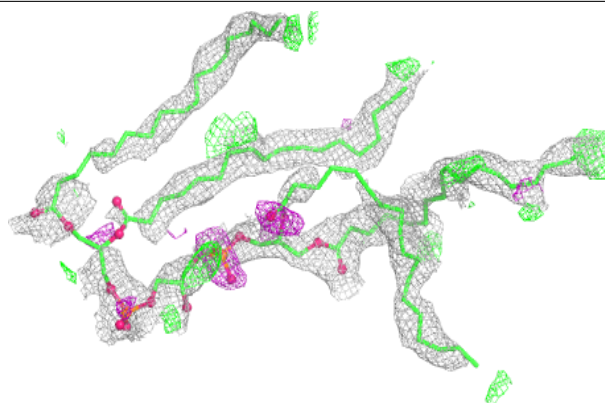
**Electron density around PGV C 268:**

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

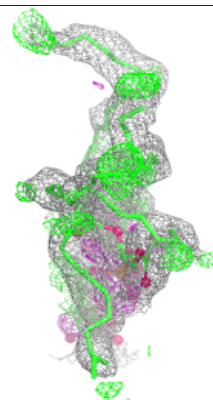
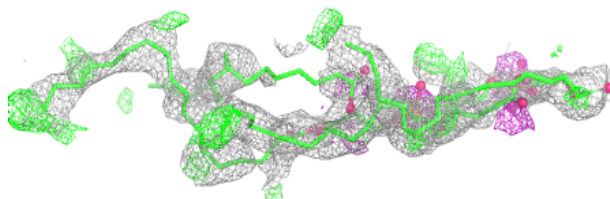
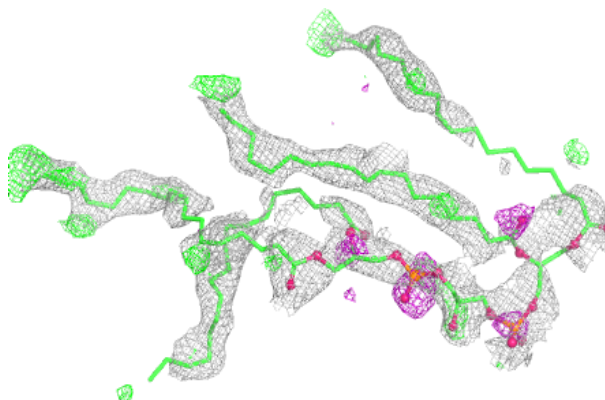


Electron density around CDL G 269:

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

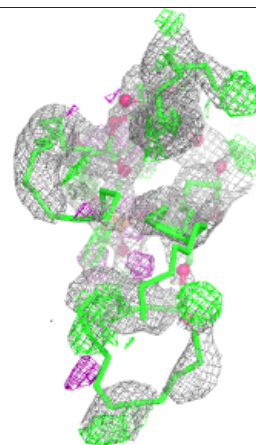
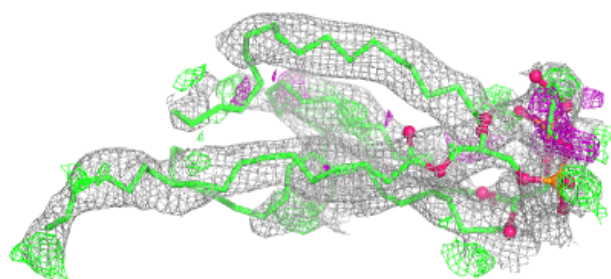
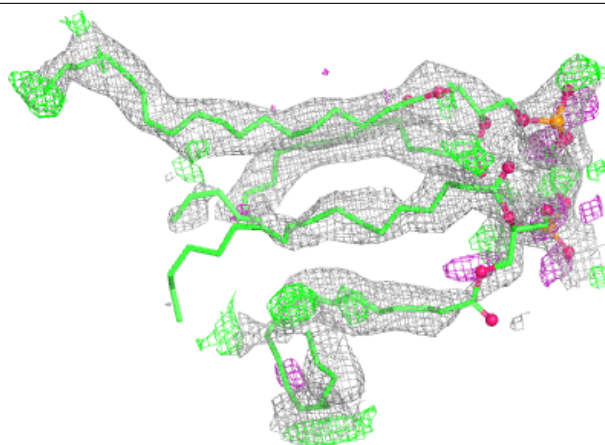
**Electron density around CDL T 1269:**

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

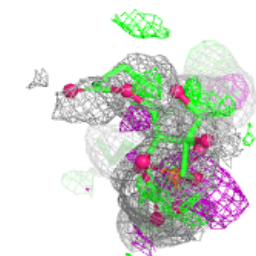
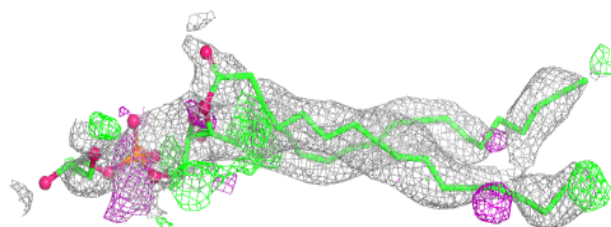
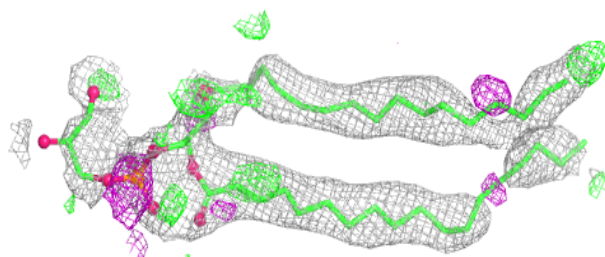


Electron density around CDL P 1270:

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

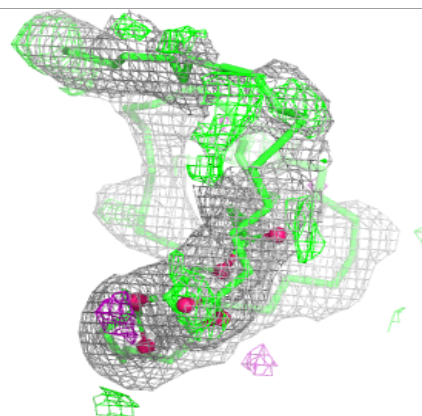
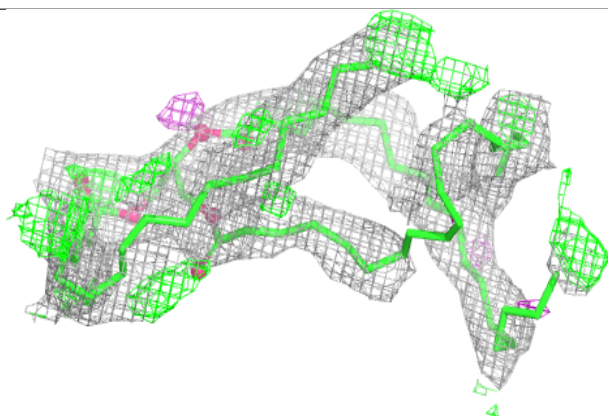
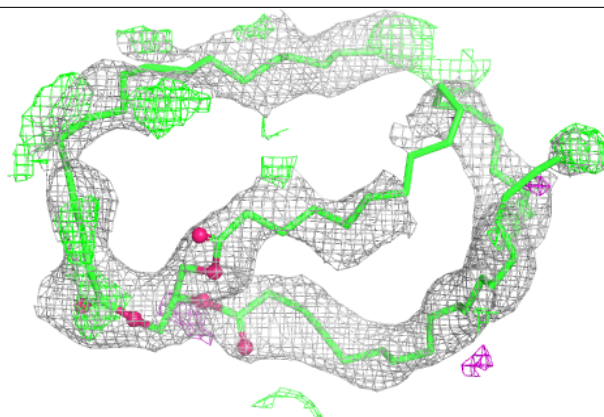
**Electron density around PGV N 1524:**

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



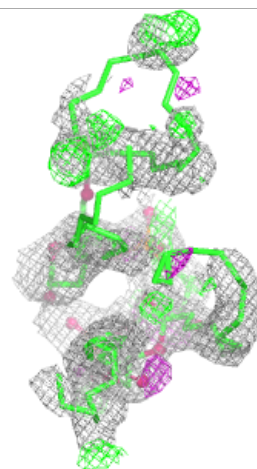
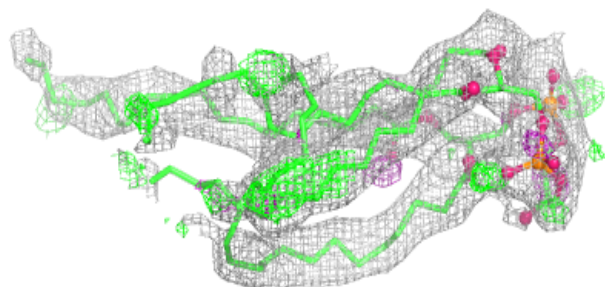
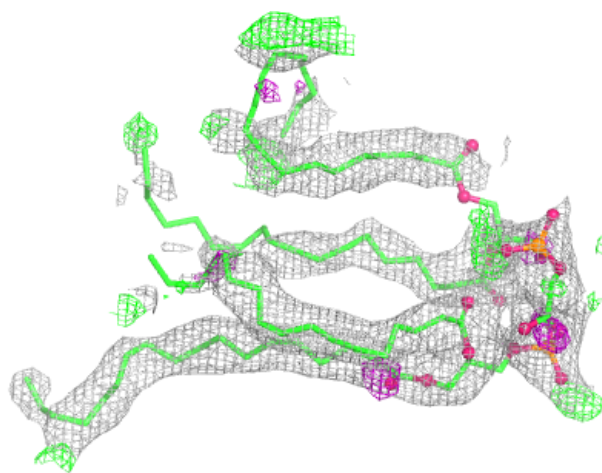
Electron density around TGL N 1521:

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



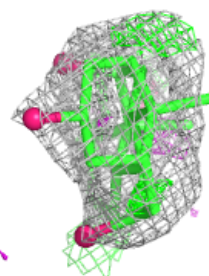
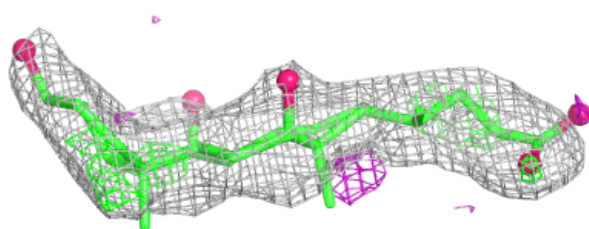
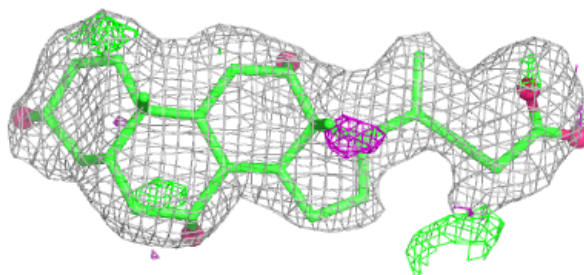
Electron density around CDL C 270:

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

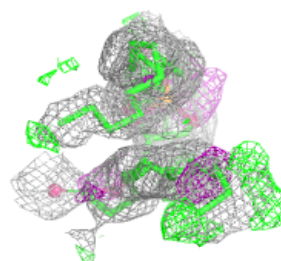
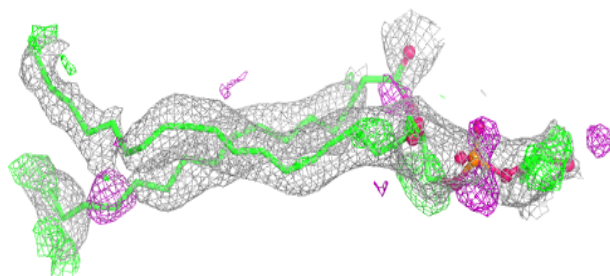
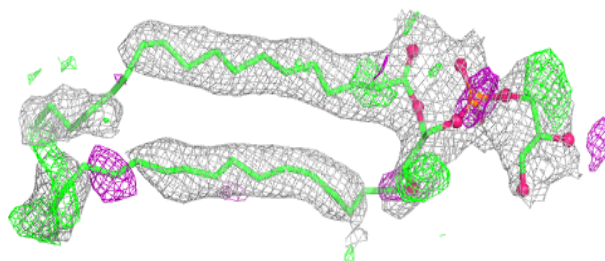


Electron density around CHD C 271:

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

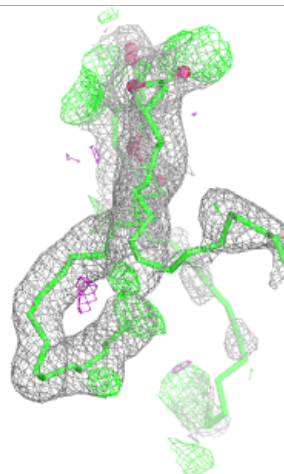
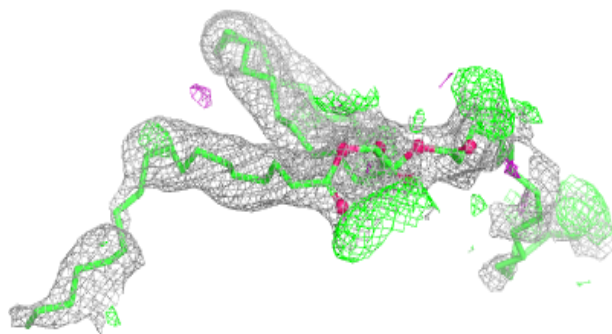
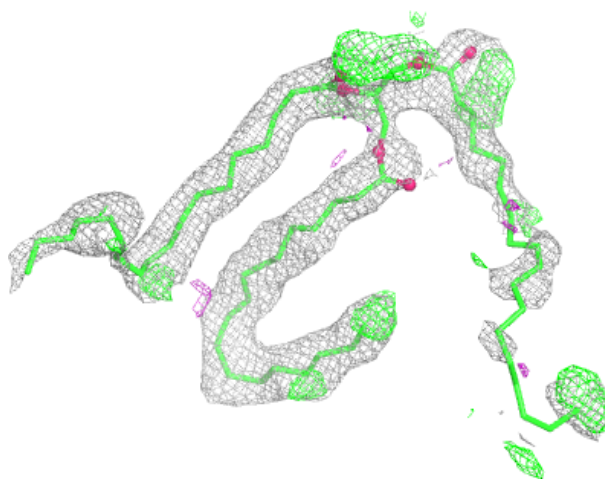
**Electron density around PGV A 524:**

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



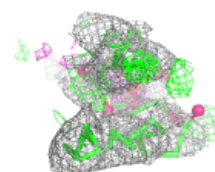
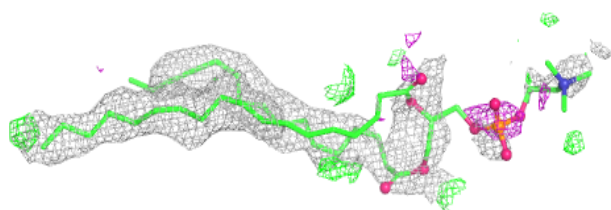
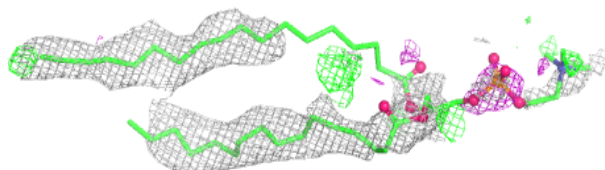
Electron density around TGL D 523:

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

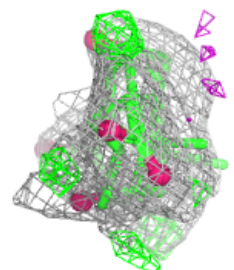
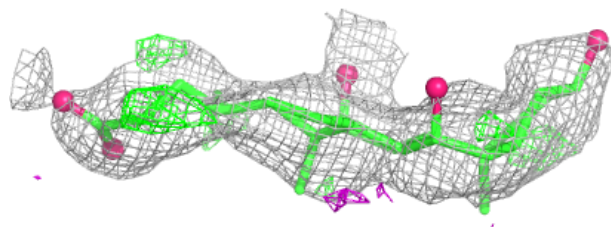
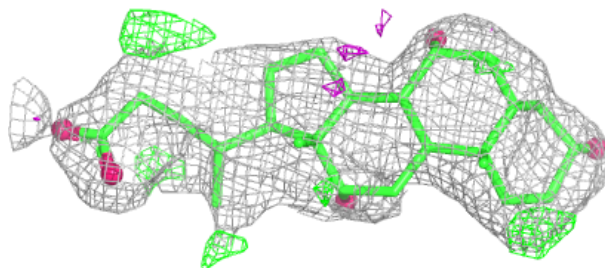


Electron density around PSC B 229:

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

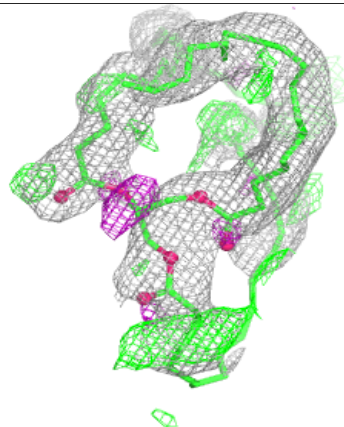
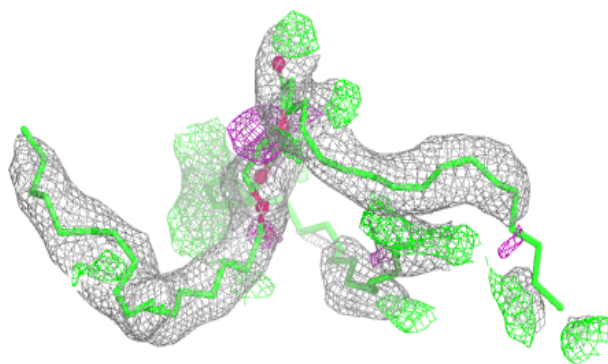
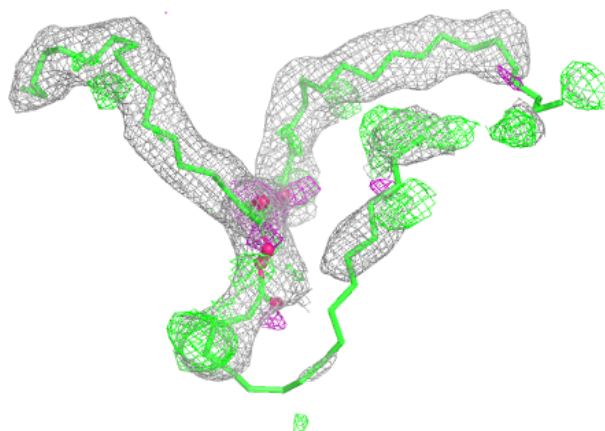
**Electron density around CHD P 1271:**

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

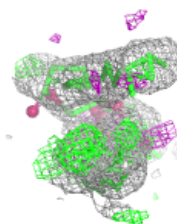
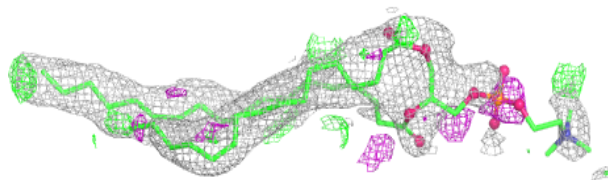
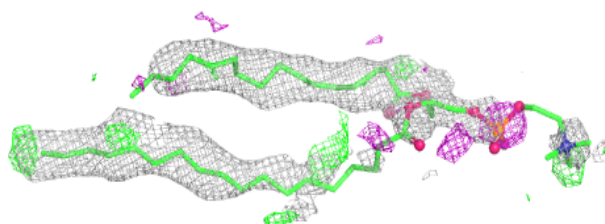


Electron density around TGL L 522:

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

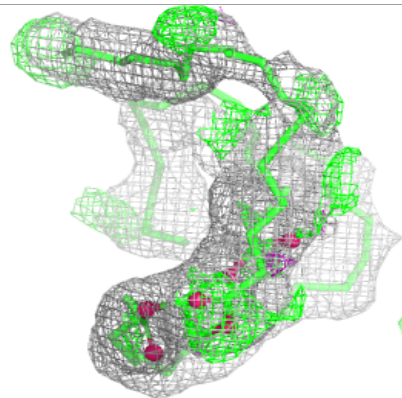
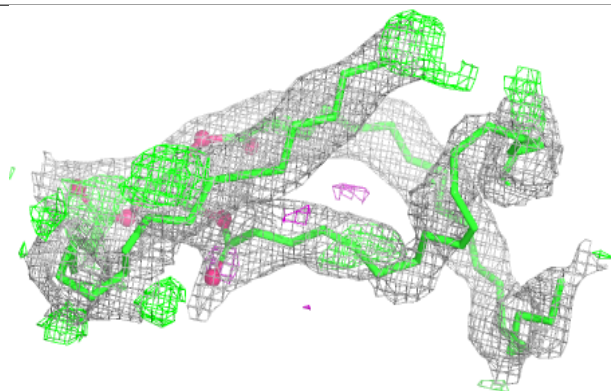
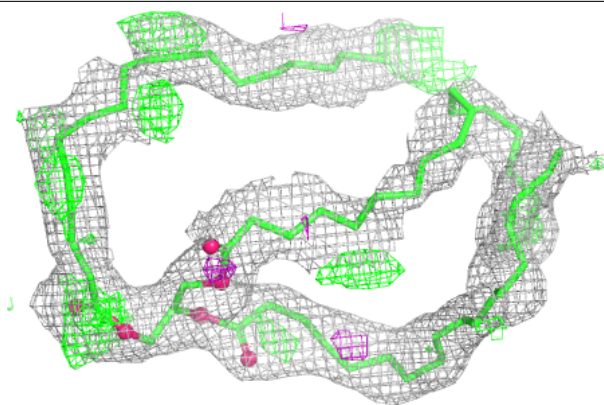
**Electron density around PSC O 1229:**

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

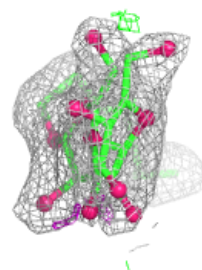
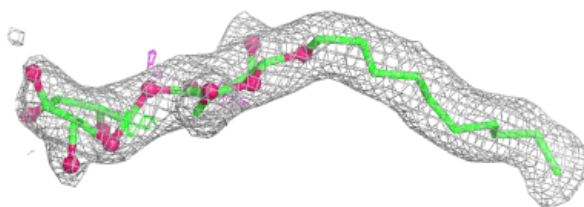
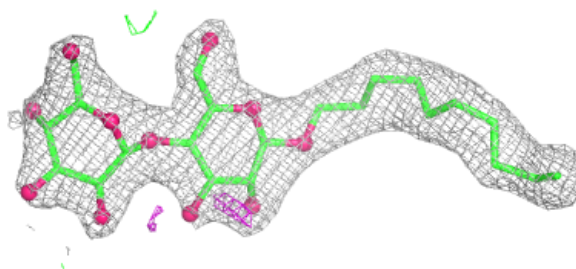


Electron density around TGL A 521:

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

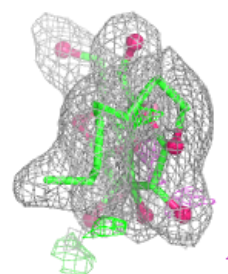
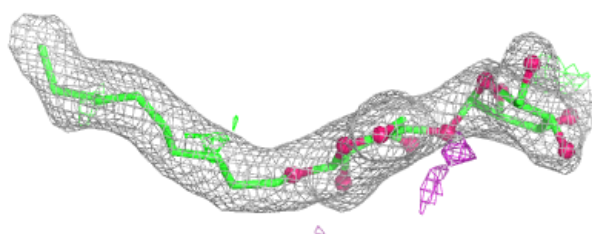
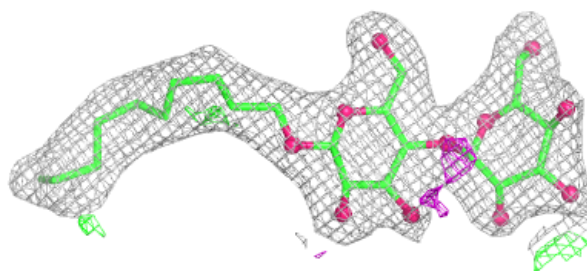
**Electron density around DMU Z 1526:**

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

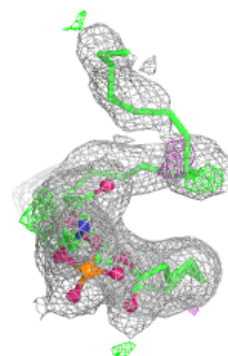
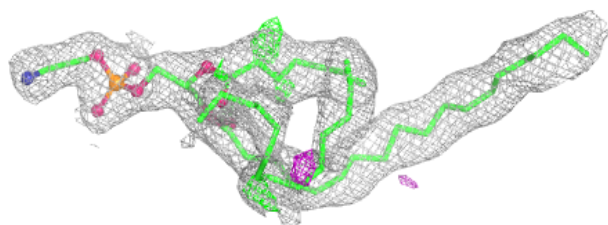
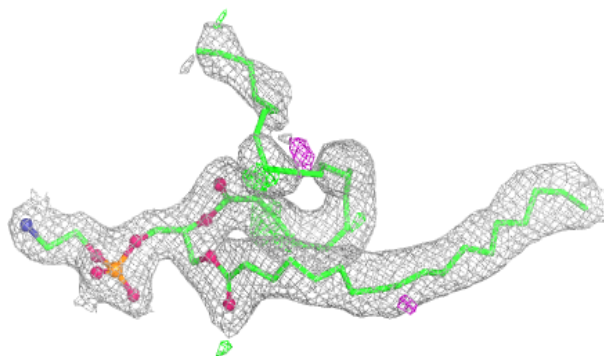


Electron density around DMU M 526:

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

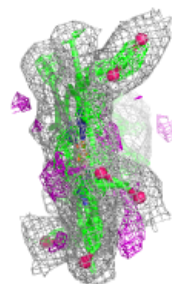
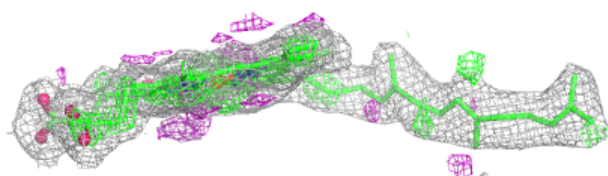
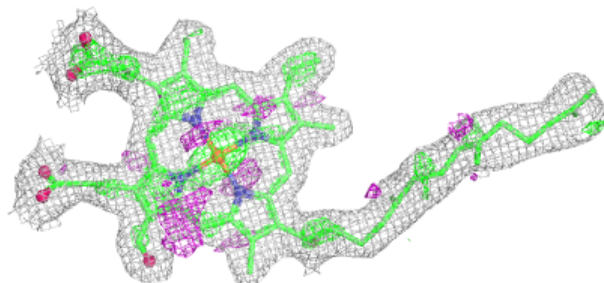
**Electron density around PEK T 1264:**

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

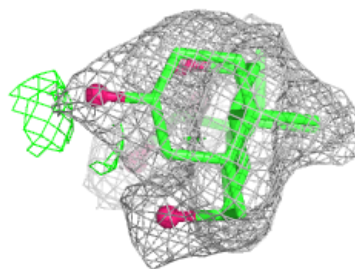
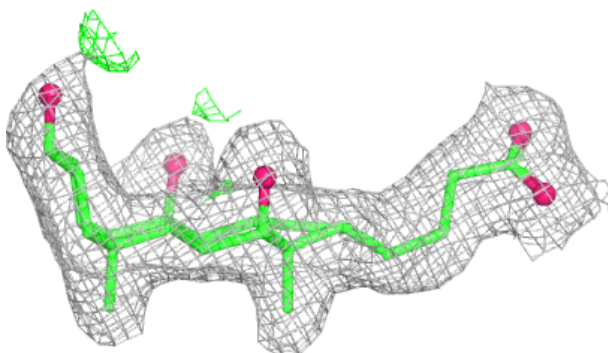
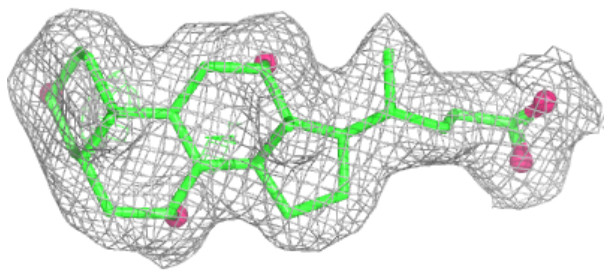


Electron density around HEA N 515:

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

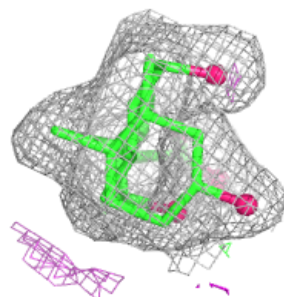
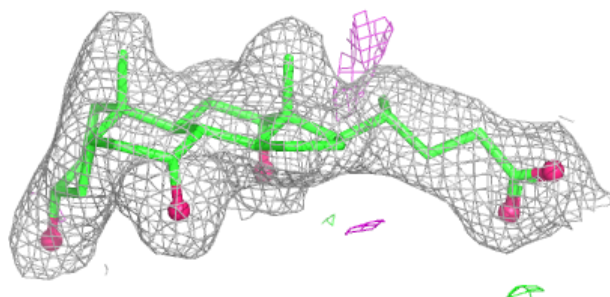
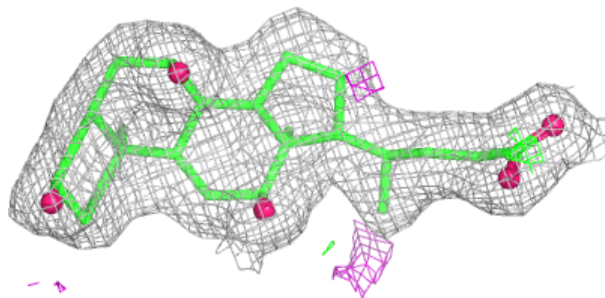
**Electron density around CHD B 1085:**

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

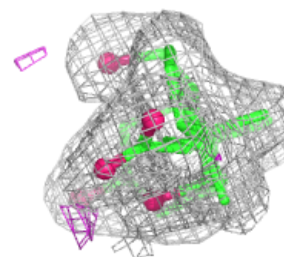
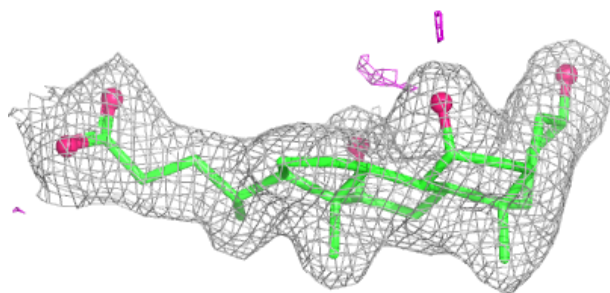
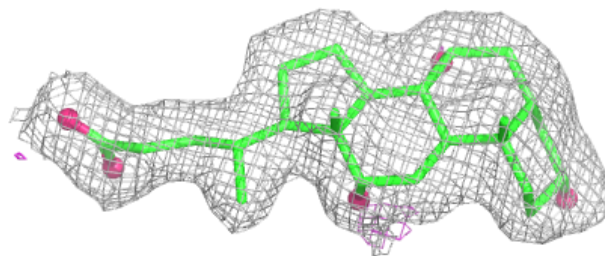


Electron density around CHD P 1525:

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

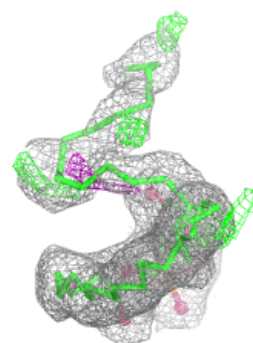
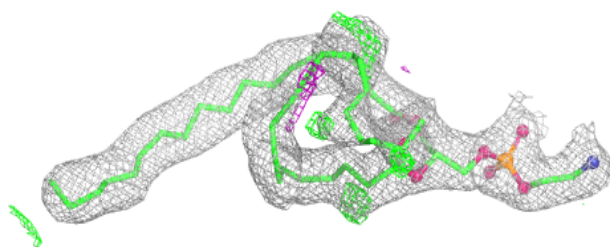
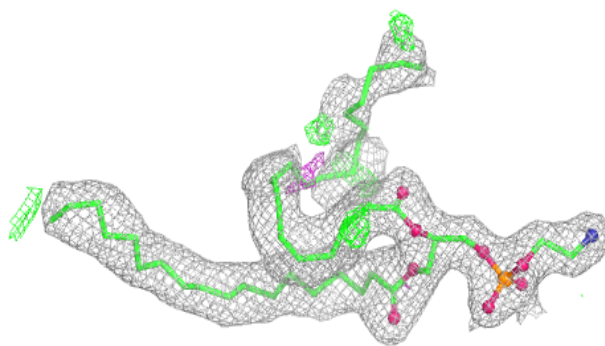
**Electron density around CHD C 525:**

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

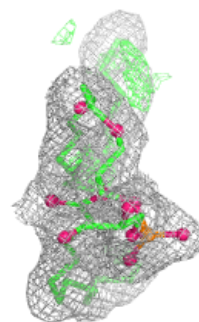
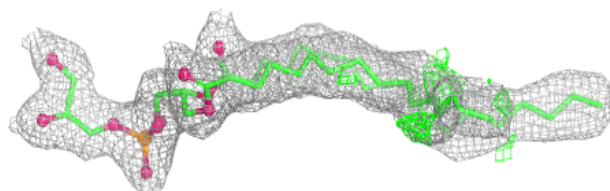
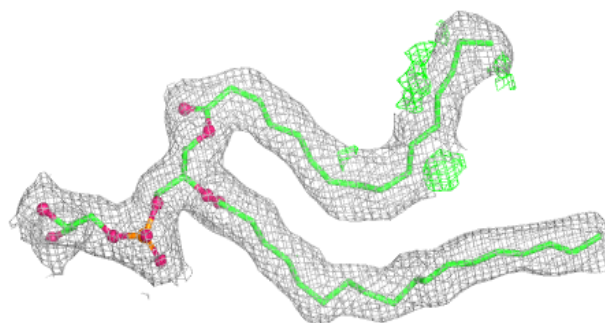


Electron density around PEK G 264:

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

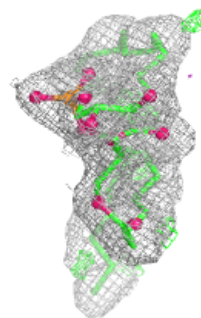
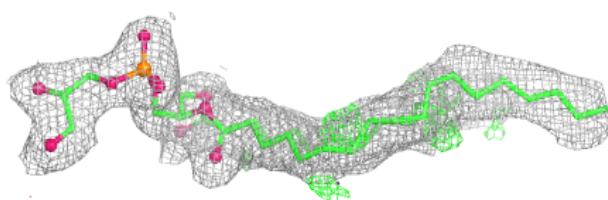
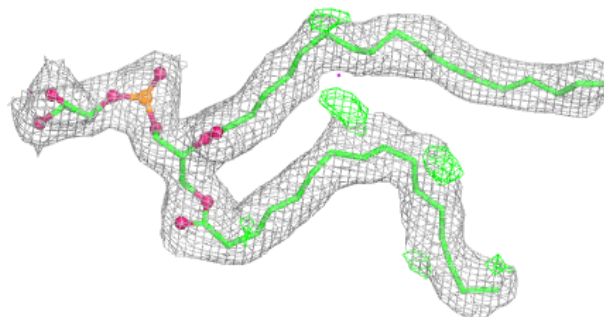
**Electron density around PGV A 522:**

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

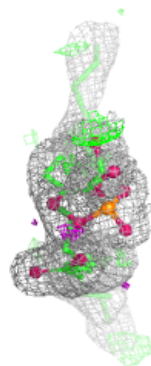
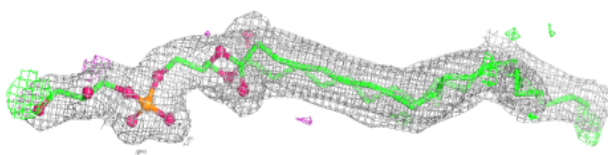
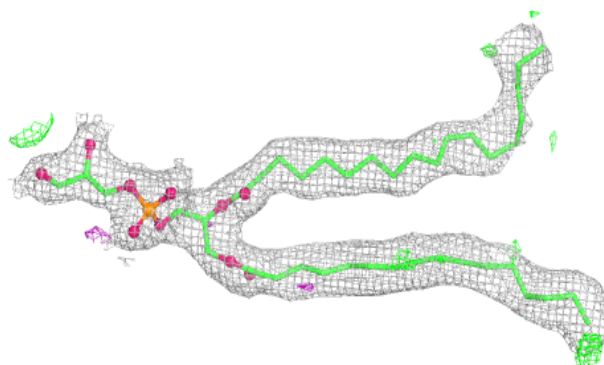


Electron density around PGV N 1266:

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

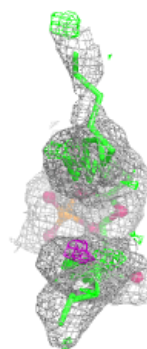
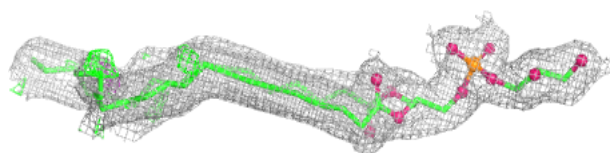
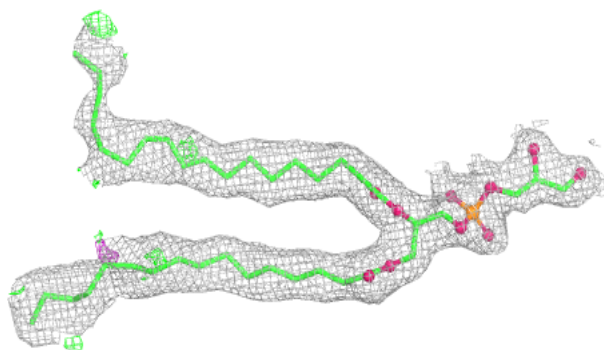
**Electron density around PGV P 1267:**

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

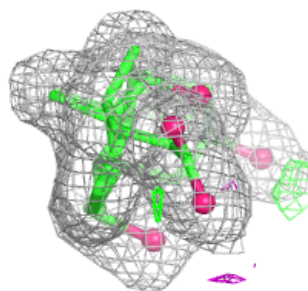
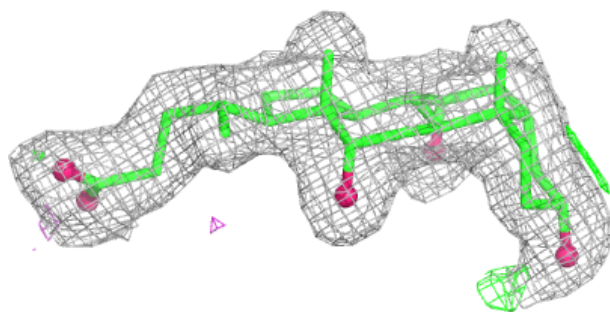
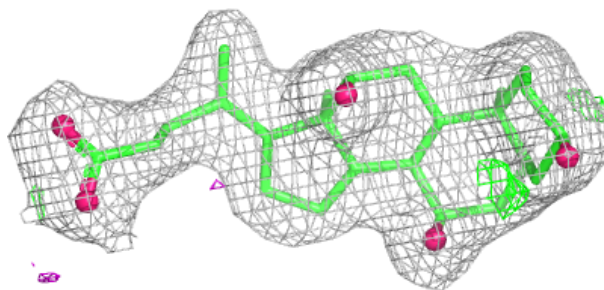


Electron density around PGV C 267:

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

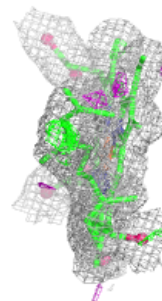
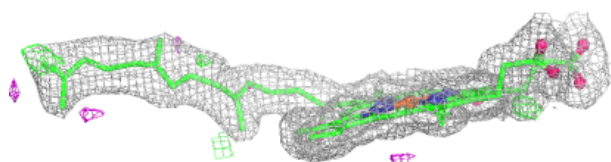
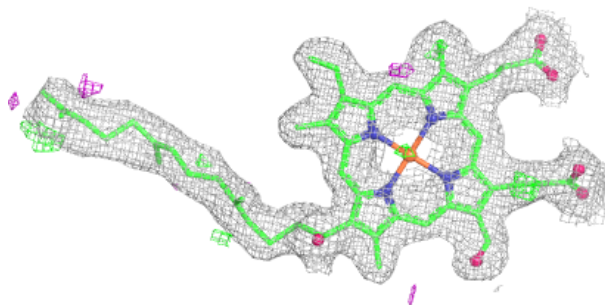
**Electron density around CHD G 229:**

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

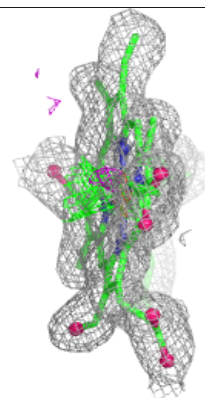
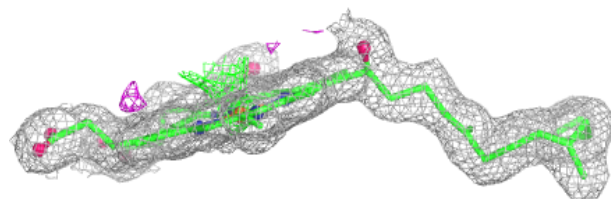
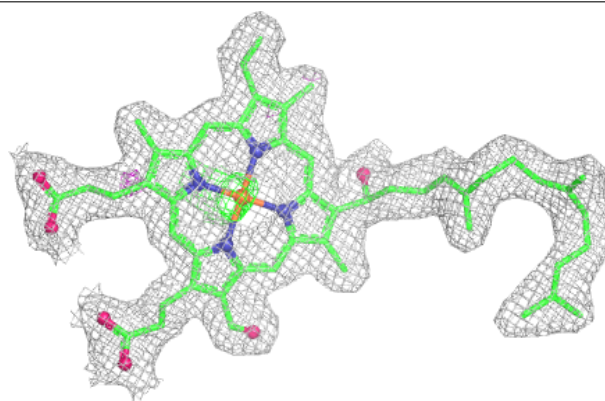


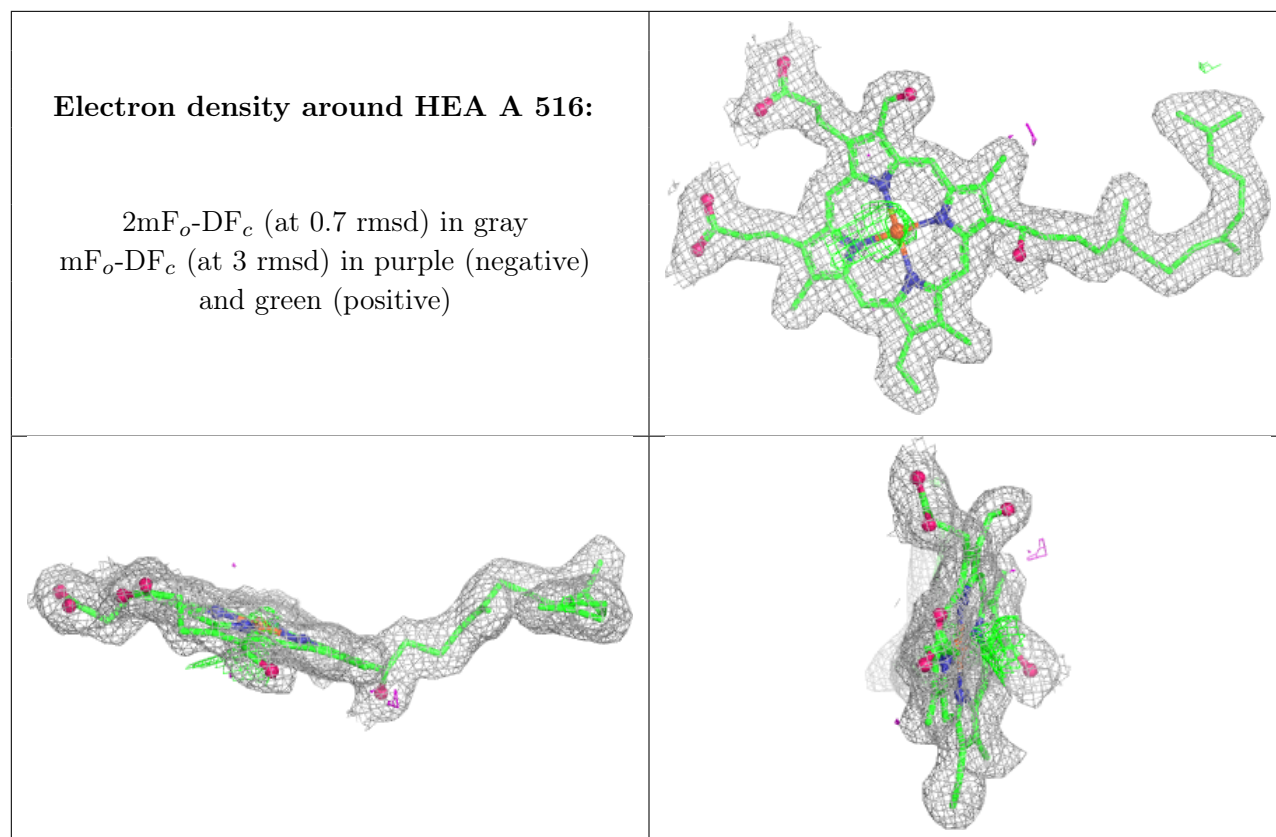
Electron density around HEA A 515:

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

**Electron density around HEA N 516:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.