



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:14 PM UTC

PDB ID : 3ABM / pdb_00003abm
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (200-s X-ray exposure dataset)
Authors : Aoyama, H.; Muramoto, K.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Ogura, T.; Yoshikawa, S.
Deposited on : 2009-12-16
Resolution : 1.95 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

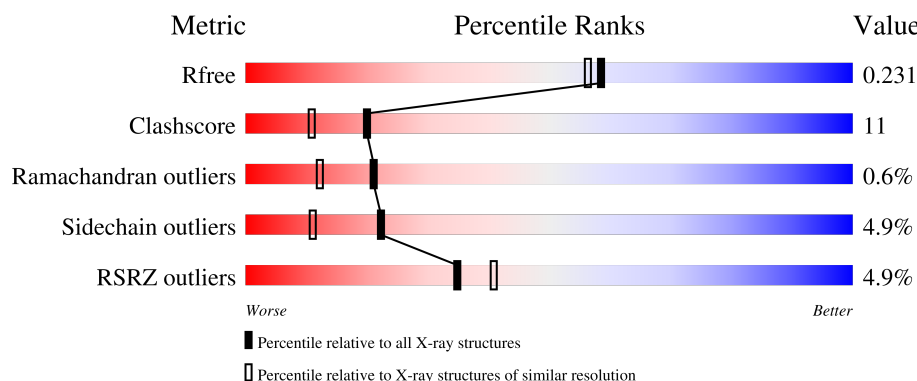
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

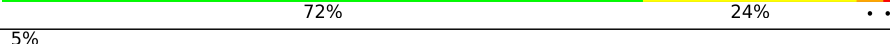
The reported resolution of this entry is 1.95 Å.

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.



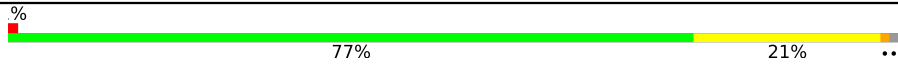
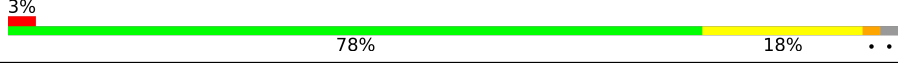
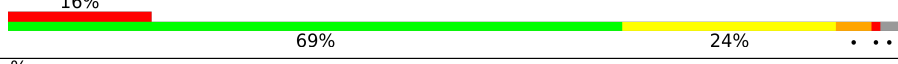
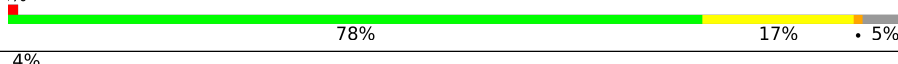
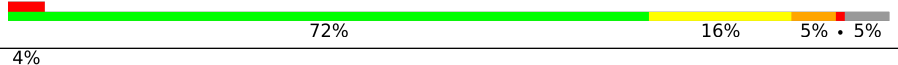
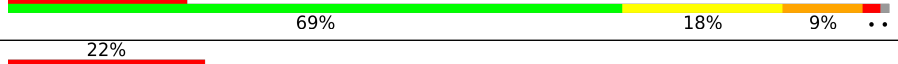
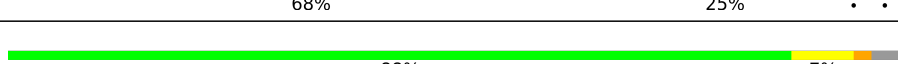
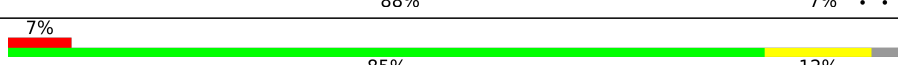
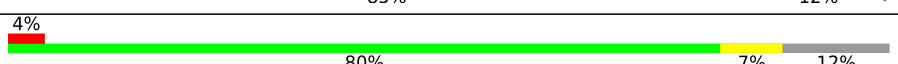
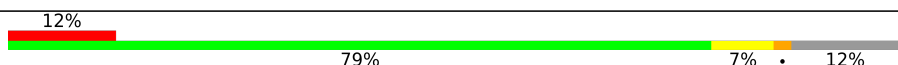
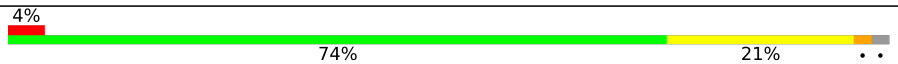
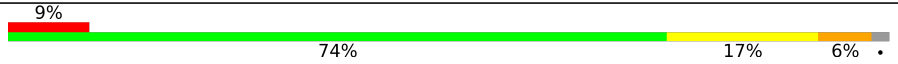
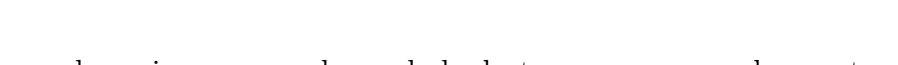
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	 75% 21% .
1	N	514	 70% 26% .
2	B	227	 4% 72% 24% .
2	O	227	 5% 71% 23% 5%

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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
22	CHD	B	1086	X	-	-	-
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	-
24	PEK	T	263	-	-	X	-
25	CDL	G	269	-	-	X	-
25	CDL	P	1270	-	-	X	-
26	PSC	E	230	-	-	X	-
28	DMU	G	272	X	-	-	-
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	-
28	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32113 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	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			
6	S	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			
9	V	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	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			

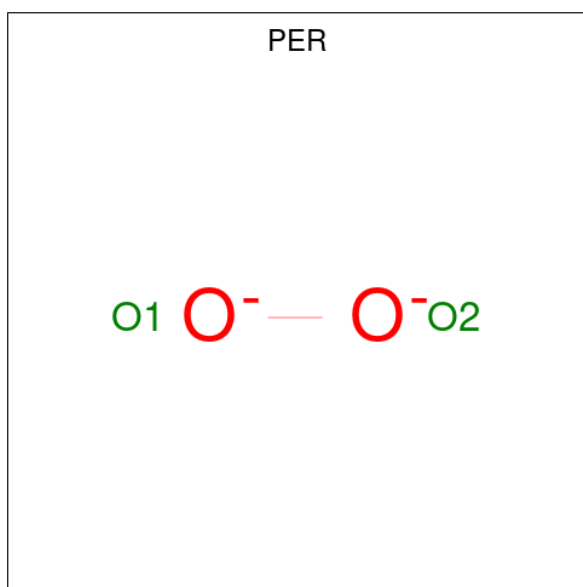
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

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 COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 15 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



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

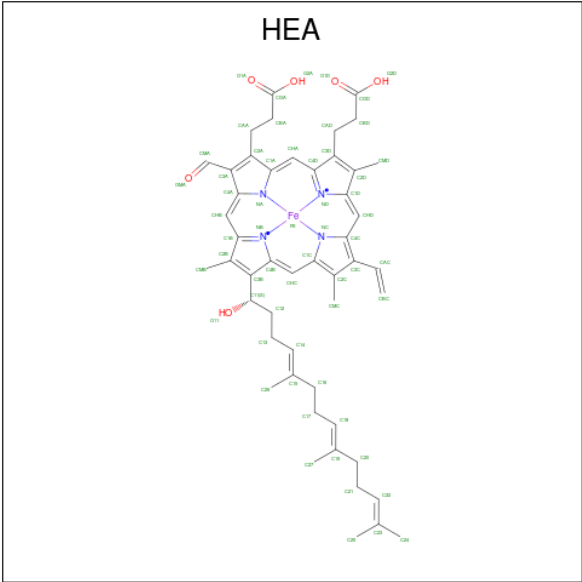
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

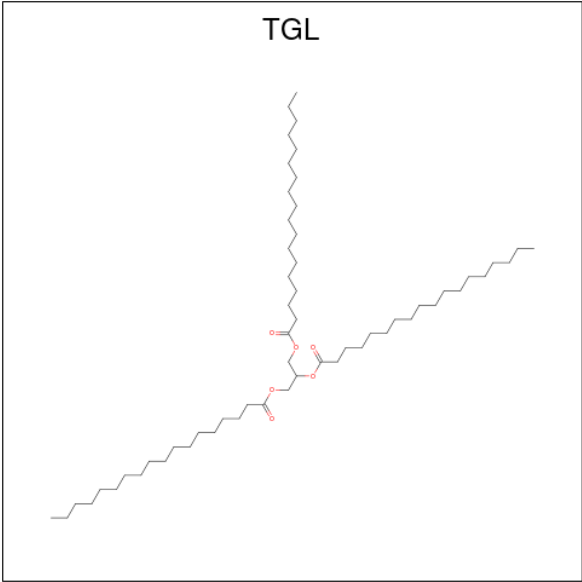
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



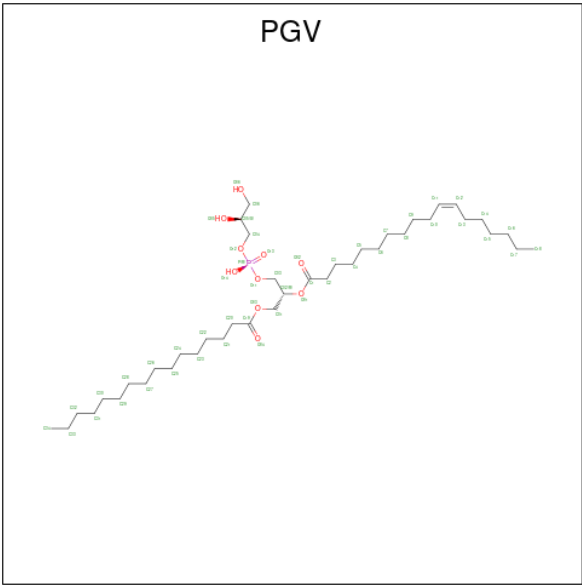
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



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

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



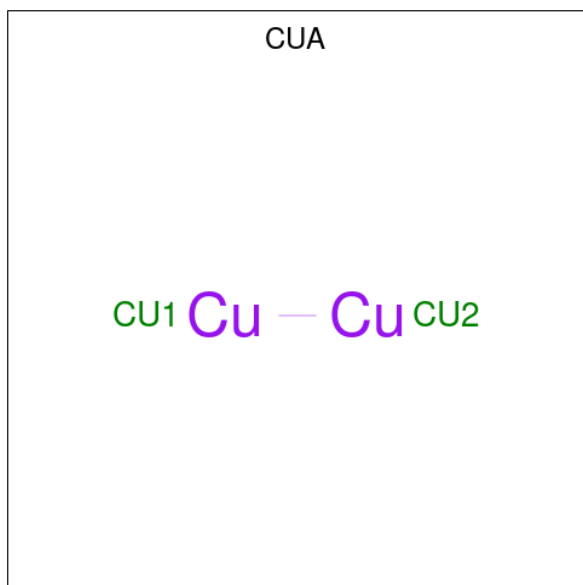
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	H	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		

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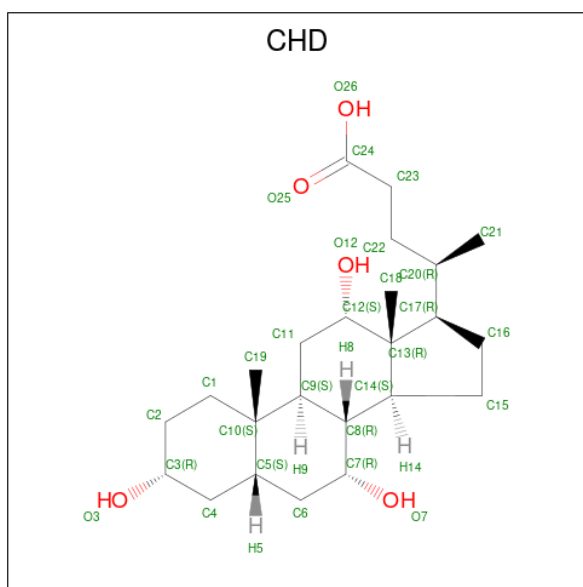
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).

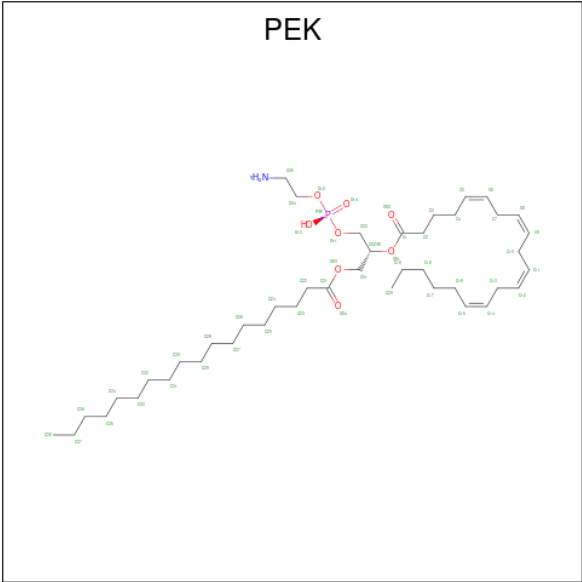


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	O	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

- Molecule 23 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

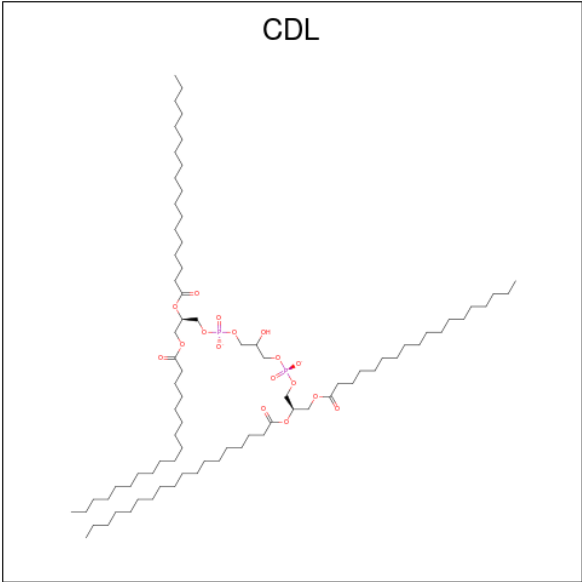
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	C	1	Total	X	0	0
			1	1		
23	P	1	Total	X	0	0
			1	1		

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



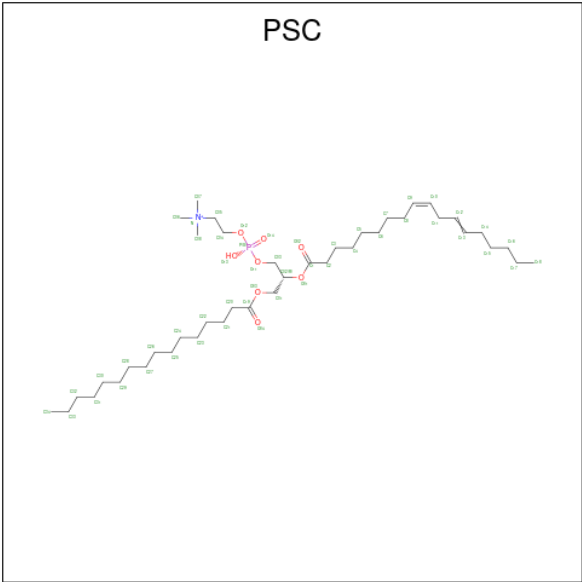
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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

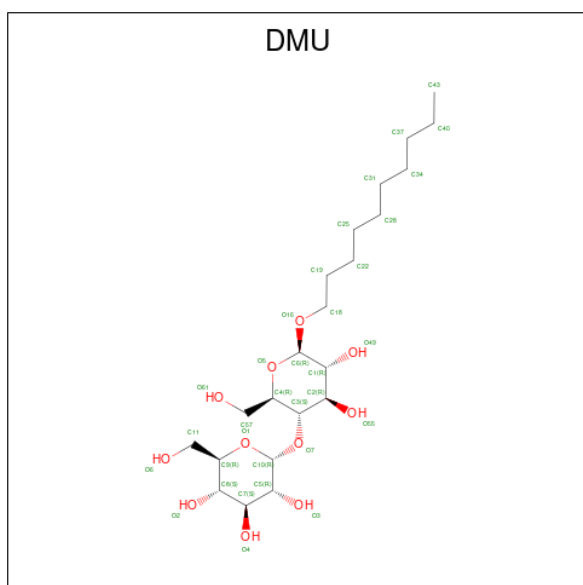


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	203	Total O 203 203	0	0
29	B	131	Total O 131 131	0	0
29	C	90	Total O 90 90	0	0
29	D	96	Total O 96 96	0	0
29	E	62	Total O 62 62	0	0
29	F	70	Total O 70 70	0	0
29	G	41	Total O 41 41	0	0
29	H	46	Total O 46 46	0	0
29	I	44	Total O 44 44	0	0
29	J	17	Total O 17 17	0	0
29	K	22	Total O 22 22	0	0
29	L	23	Total O 23 23	0	0
29	M	19	Total O 19 19	0	0
29	N	196	Total O 196 196	0	0
29	O	106	Total O 106 106	0	0
29	P	89	Total O 89 89	0	0
29	Q	54	Total O 54 54	0	0
29	R	52	Total O 52 52	0	0
29	S	62	Total O 62 62	0	0
29	T	39	Total O 39 39	0	0
29	U	39	Total O 39 39	0	0
29	V	16	Total O 16 16	0	0

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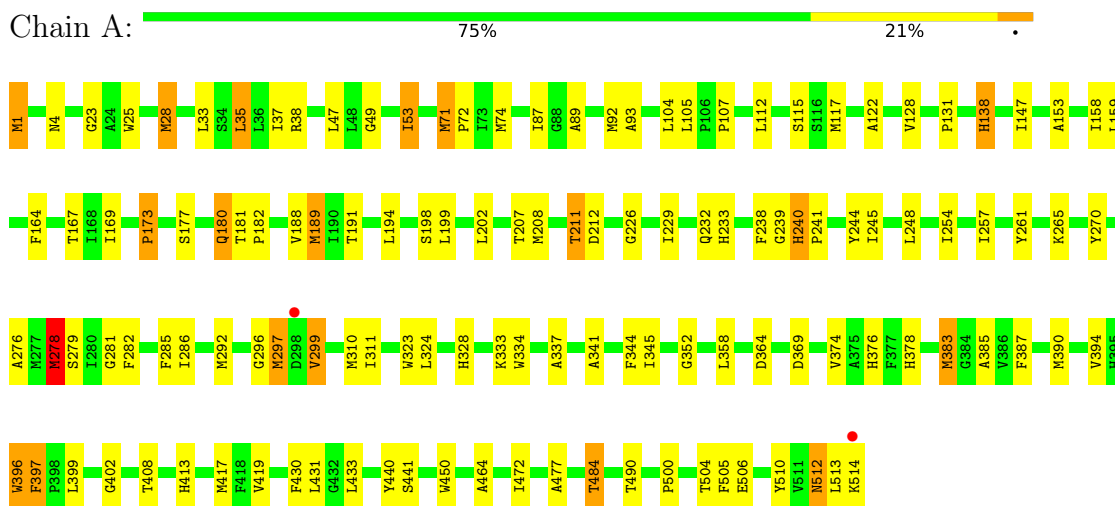
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	W	15	Total 15	O 15	0	0
29	X	16	Total 16	O 16	0	0
29	Y	19	Total 19	O 19	0	0
29	Z	10	Total 10	O 10	0	0

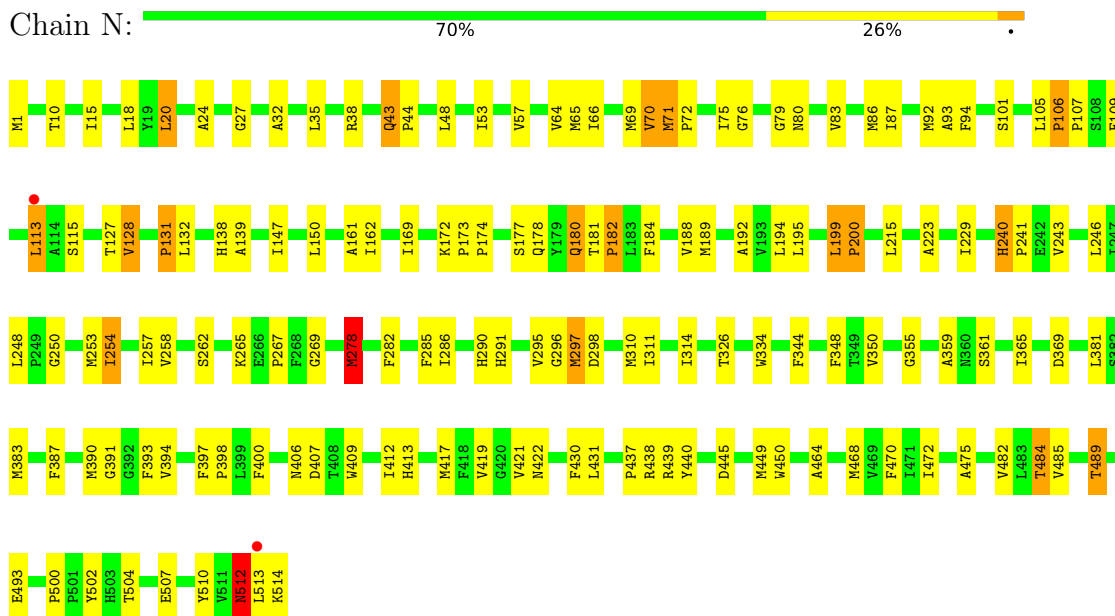
3 Residue-property plots

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.

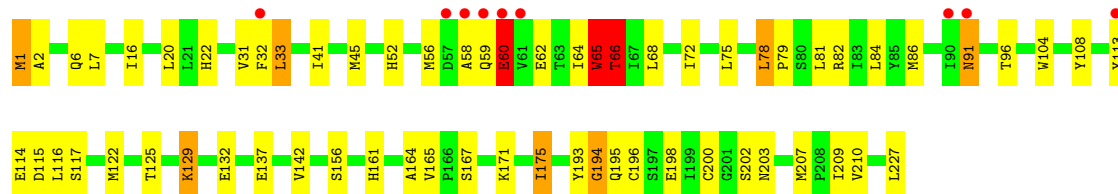
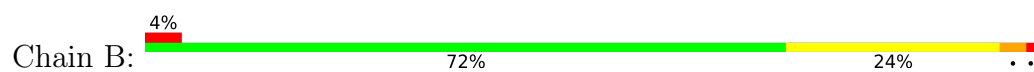
• Molecule 1: Cytochrome c oxidase subunit 1



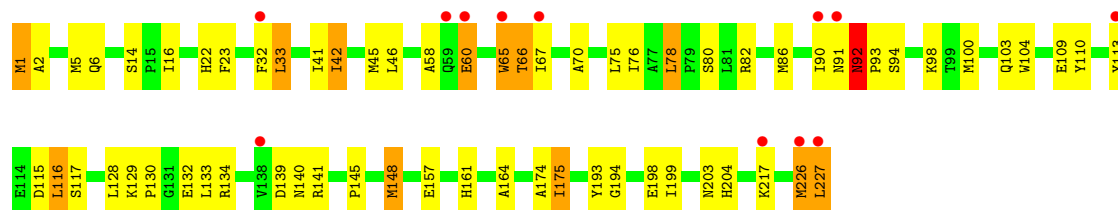
• Molecule 1: Cytochrome c oxidase subunit 1



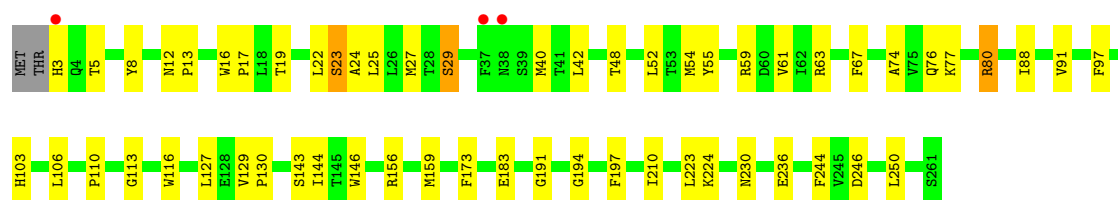
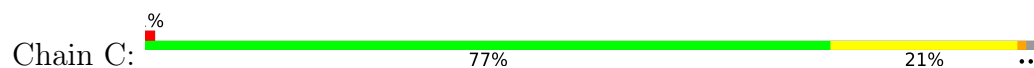
• Molecule 2: Cytochrome c oxidase subunit 2



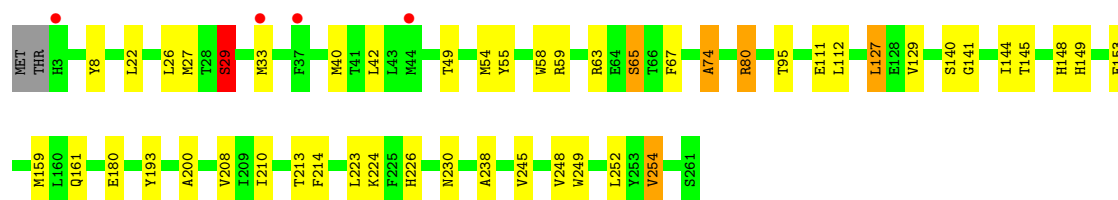
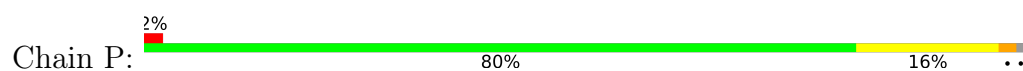
• Molecule 2: Cytochrome c oxidase subunit 2



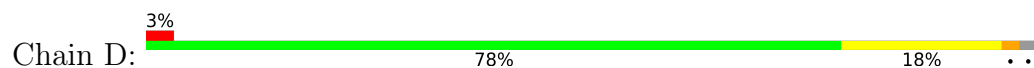
• Molecule 3: Cytochrome c oxidase subunit 3



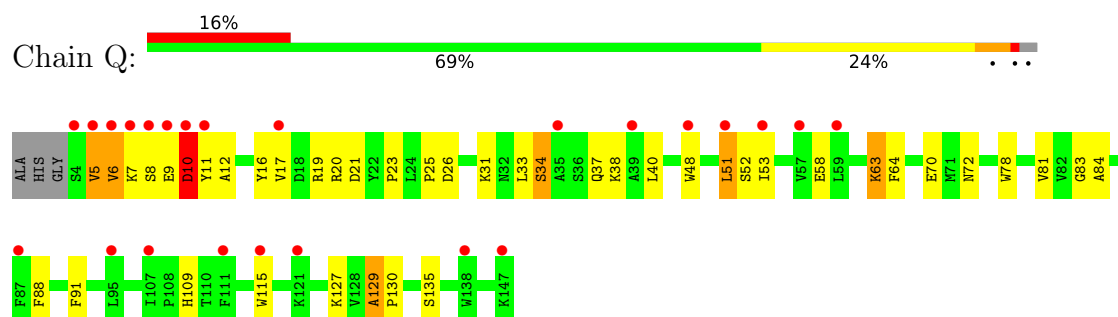
• Molecule 3: Cytochrome c oxidase subunit 3



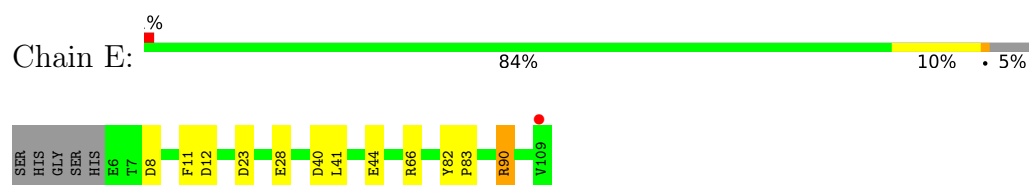
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



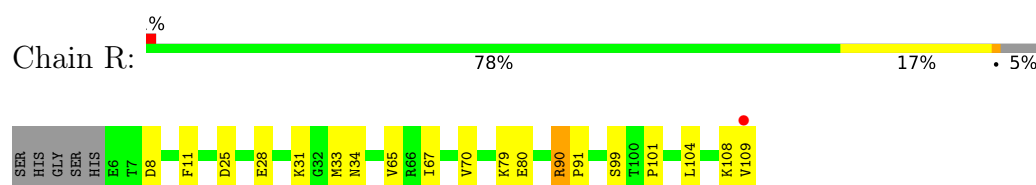
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



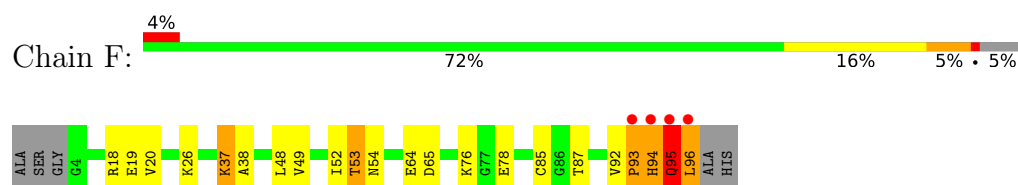
- Molecule 5: Cytochrome c oxidase subunit 5A



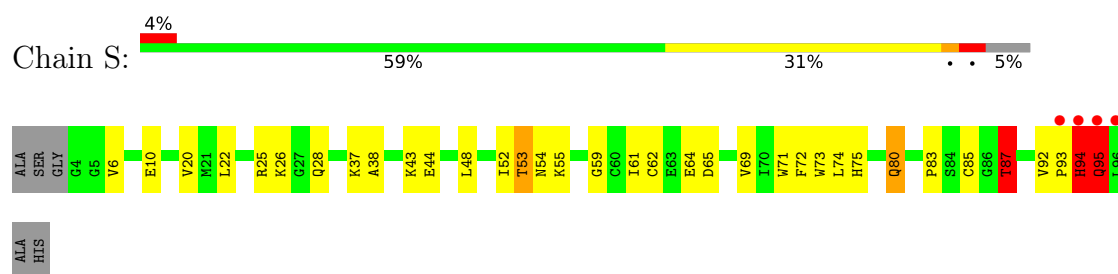
- Molecule 5: Cytochrome c oxidase subunit 5A



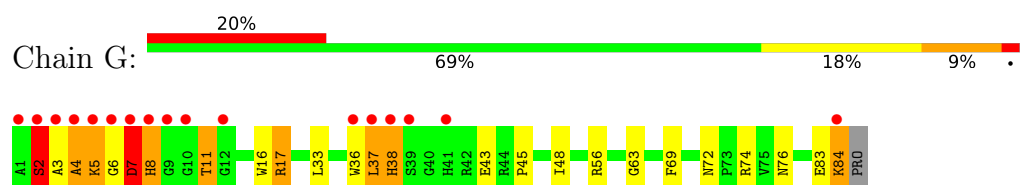
- Molecule 6: Cytochrome c oxidase subunit 5B



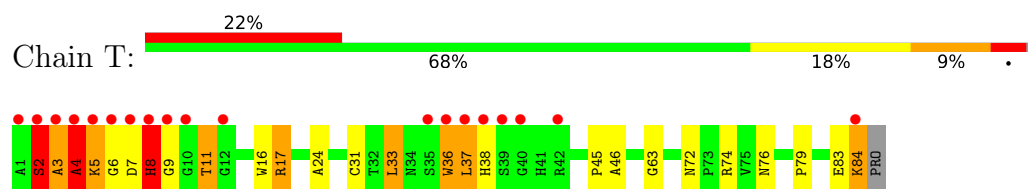
- Molecule 6: Cytochrome c oxidase subunit 5B



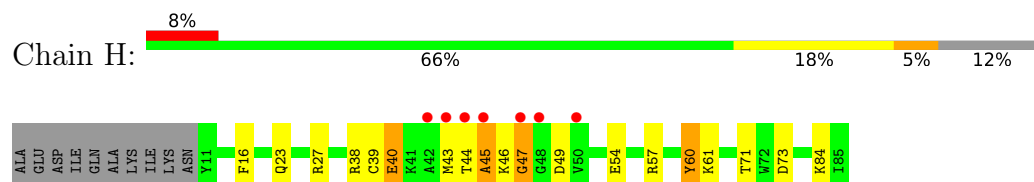
- Molecule 7: Cytochrome c oxidase subunit 6A2



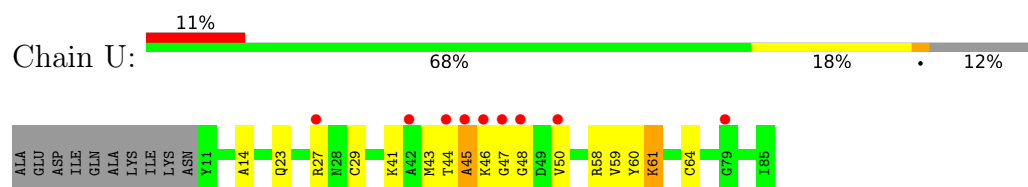
- Molecule 7: Cytochrome c oxidase subunit 6A2



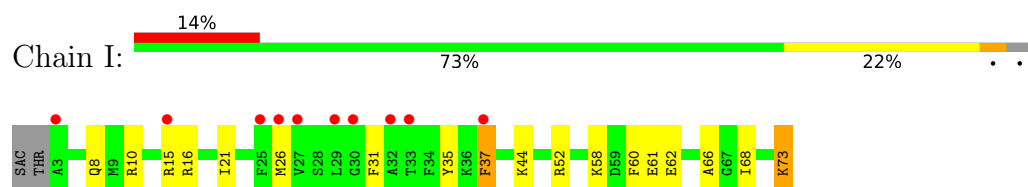
- Molecule 8: Cytochrome c oxidase subunit 6B1



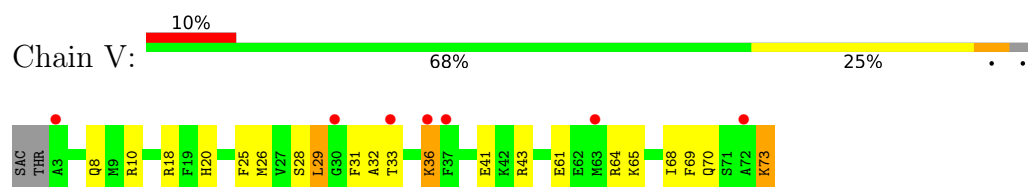
- Molecule 8: Cytochrome c oxidase subunit 6B1



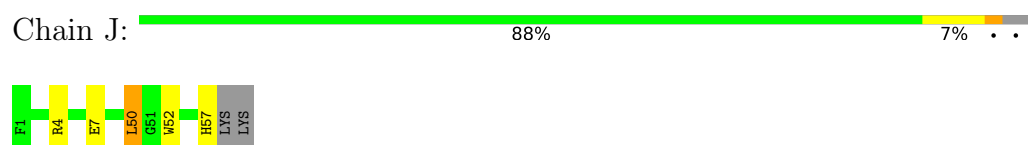
- Molecule 9: Cytochrome c oxidase subunit 6C



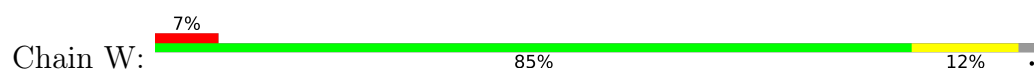
- Molecule 9: Cytochrome c oxidase subunit 6C

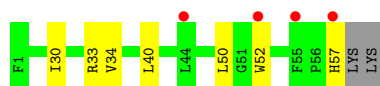


- Molecule 10: Cytochrome c oxidase polypeptide 7A1

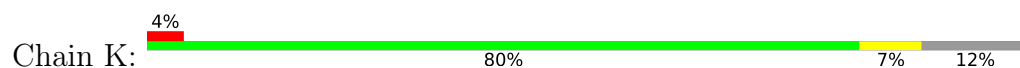


- Molecule 10: Cytochrome c oxidase polypeptide 7A1

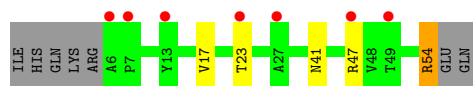
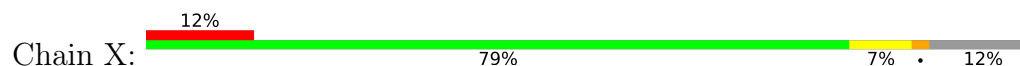




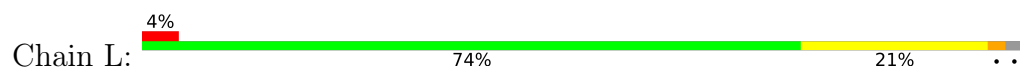
- Molecule 11: Cytochrome c oxidase subunit 7B



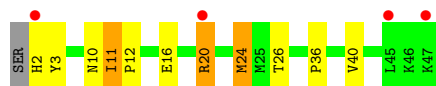
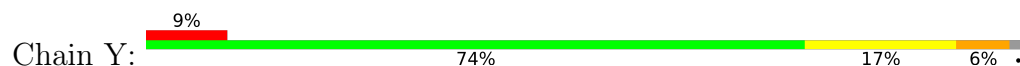
- Molecule 11: Cytochrome c oxidase subunit 7B



- 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	183.70Å 206.99Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 40.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.95) 96.4 (40.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.181 , 0.214 (Not available) , 0.231	Depositor DCC
R_{free} test set	16433 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32113	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: CUA, CU, CHD, PER, TPO, PGV, PEK, CDL, UNX, TGL, NA, HEA, DMU, ZN, PSC, MG, FME

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	1.82	47/4156 (1.1%)	1.57	47/5678 (0.8%)
1	N	1.67	44/4156 (1.1%)	1.53	62/5678 (1.1%)
2	B	1.68	17/1860 (0.9%)	1.50	9/2534 (0.4%)
2	O	1.44	5/1860 (0.3%)	1.40	11/2534 (0.4%)
3	C	1.52	8/2197 (0.4%)	1.39	15/3005 (0.5%)
3	P	1.53	6/2197 (0.3%)	1.39	15/3005 (0.5%)
4	D	1.56	6/1229 (0.5%)	1.48	19/1658 (1.1%)
4	Q	1.27	5/1229 (0.4%)	1.31	11/1658 (0.7%)
5	E	1.46	0/860	1.26	4/1167 (0.3%)
5	R	1.24	0/860	1.19	1/1167 (0.1%)
6	F	1.63	6/733 (0.8%)	1.51	7/996 (0.7%)
6	S	1.65	9/733 (1.2%)	1.59	9/996 (0.9%)
7	G	1.56	4/690 (0.6%)	1.36	2/937 (0.2%)
7	T	1.53	6/690 (0.9%)	1.45	8/937 (0.9%)
8	H	1.47	2/648 (0.3%)	1.41	3/877 (0.3%)
8	U	1.24	1/648 (0.2%)	1.30	4/877 (0.5%)
9	I	1.38	0/598	1.32	4/792 (0.5%)
9	V	1.23	0/598	1.20	1/792 (0.1%)
10	J	1.42	0/462	1.30	0/625
10	W	1.21	0/462	1.18	0/625
11	K	1.53	0/398	1.37	0/546
11	X	1.19	0/398	1.31	2/546 (0.4%)
12	L	1.62	2/393 (0.5%)	1.45	3/526 (0.6%)
12	Y	1.35	1/393 (0.3%)	1.35	4/526 (0.8%)
13	M	1.60	3/345 (0.9%)	1.34	0/470
13	Z	1.17	0/345	1.43	5/470 (1.1%)
All	All	1.56	172/29138 (0.6%)	1.43	246/39622 (0.6%)

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	2

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	54	ASN	CB-CG	-10.47	1.25	1.52
2	O	198	GLU	C-O	10.33	1.35	1.23
1	N	297	MET	SD-CE	9.78	2.04	1.79
12	L	35	ALA	CA-CB	9.53	1.65	1.53
2	O	175	ILE	CA-CB	9.36	1.61	1.54
1	A	297	MET	SD-CE	9.15	2.02	1.79
1	N	419	VAL	CA-CB	8.89	1.65	1.54
1	N	195	LEU	C-O	8.76	1.34	1.24
1	A	173	PRO	CA-C	8.69	1.56	1.51
1	A	310	MET	SD-CE	-8.68	1.57	1.79
1	A	324	LEU	N-CA	8.47	1.56	1.46
1	N	128	VAL	N-CA	8.35	1.56	1.46
1	N	248	LEU	CA-CB	8.33	1.64	1.53
4	Q	6	VAL	CA-CB	8.20	1.63	1.54
3	P	238	ALA	CA-CB	7.99	1.66	1.53
2	B	194	GLY	N-CA	7.87	1.53	1.45
1	A	128	VAL	N-CA	7.51	1.55	1.46
1	A	93	ALA	C-O	7.32	1.32	1.24
1	A	239	GLY	C-O	7.18	1.33	1.23
3	P	74	ALA	CA-CB	7.12	1.64	1.53
1	N	310	MET	SD-CE	-7.09	1.61	1.79
4	Q	6	VAL	N-CA	6.98	1.55	1.46
6	S	6	VAL	CA-C	6.94	1.58	1.53
1	A	167	THR	N-CA	-6.93	1.38	1.46
1	N	182	PRO	CA-C	6.92	1.60	1.52
1	A	147	ILE	C-O	-6.90	1.16	1.24
1	A	122	ALA	CA-CB	6.85	1.61	1.53
12	L	35	ALA	N-CA	-6.84	1.40	1.46
3	C	113	GLY	C-O	-6.66	1.15	1.24
3	C	8	TYR	N-CA	6.64	1.53	1.45
3	C	27	MET	C-O	-6.58	1.16	1.24
7	T	17	ARG	CD-NE	-6.53	1.37	1.46
4	Q	81	VAL	CA-CB	-6.46	1.46	1.54
1	A	506	GLU	C-O	-6.43	1.16	1.24
1	N	64	VAL	CA-CB	6.41	1.62	1.54
1	A	385	ALA	CA-CB	6.39	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	31	VAL	CA-CB	6.36	1.61	1.54
1	A	89	ALA	CA-CB	6.31	1.62	1.53
1	N	489	THR	N-CA	6.30	1.54	1.46
1	A	188	VAL	CA-CB	-6.29	1.45	1.54
1	N	83	VAL	CA-CB	6.28	1.57	1.54
1	A	341	ALA	C-O	6.22	1.31	1.24
1	A	490	THR	CA-C	-6.20	1.44	1.52
2	B	96	THR	C-O	6.20	1.31	1.24
7	T	5	LYS	CB-CG	6.20	1.71	1.52
13	M	4	LYS	CB-CG	-6.20	1.33	1.52
1	N	162	ILE	CA-CB	6.15	1.62	1.54
1	N	502	TYR	N-CA	-6.15	1.39	1.46
1	A	211	THR	N-CA	-6.14	1.38	1.46
1	A	441	SER	C-O	6.13	1.32	1.24
1	N	258	VAL	C-O	6.11	1.31	1.24
2	B	209	ILE	C-O	-6.10	1.17	1.24
4	Q	5	VAL	CA-C	6.08	1.60	1.52
7	T	4	ALA	CA-CB	-6.06	1.43	1.53
1	N	150	LEU	CA-C	-6.06	1.45	1.52
1	A	191	THR	N-CA	-6.01	1.39	1.46
1	N	106	PRO	CA-C	5.99	1.57	1.52
1	N	200	PRO	N-CA	5.98	1.55	1.47
1	N	295	VAL	CA-CB	5.98	1.61	1.54
1	N	139	ALA	CA-CB	5.97	1.63	1.53
2	B	156	SER	CA-C	-5.97	1.45	1.52
1	N	57	VAL	N-CA	-5.97	1.39	1.46
1	A	376	HIS	CA-C	-5.95	1.45	1.52
1	A	500	PRO	C-O	-5.95	1.17	1.24
1	N	113	LEU	CB-CG	5.95	1.65	1.53
3	C	61	VAL	C-O	5.95	1.31	1.24
2	B	142	VAL	CA-CB	5.92	1.61	1.53
13	M	22	THR	N-CA	5.90	1.53	1.46
7	T	5	LYS	CA-C	5.87	1.57	1.53
4	D	17	VAL	CB-CG1	-5.87	1.33	1.52
1	A	248	LEU	CA-CB	5.86	1.60	1.53
1	N	174	PRO	C-O	-5.84	1.17	1.24
1	A	257	ILE	C-O	-5.83	1.17	1.24
2	B	198	GLU	C-O	5.81	1.30	1.23
7	G	56	ARG	CA-C	-5.79	1.46	1.53
1	A	189	MET	CB-CG	5.76	1.69	1.52
2	O	66	THR	CA-C	5.76	1.58	1.52
6	S	94	HIS	N-CA	5.75	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	VAL	CA-CB	-5.75	1.46	1.54
7	G	5	LYS	CB-CG	5.73	1.69	1.52
2	B	72	ILE	CA-CB	-5.71	1.48	1.54
3	C	116	TRP	CA-C	-5.70	1.46	1.53
7	T	24	ALA	CA-CB	5.69	1.62	1.53
1	A	286	ILE	C-O	5.69	1.30	1.24
2	O	70	ALA	CA-CB	-5.68	1.44	1.53
2	B	113	TYR	C-O	-5.67	1.16	1.24
6	S	61	ILE	CA-CB	5.66	1.60	1.53
1	N	101	SER	N-CA	-5.66	1.39	1.46
1	N	253	MET	C-O	5.64	1.30	1.24
1	A	408	THR	C-O	-5.62	1.17	1.24
1	N	147	ILE	CA-CB	-5.62	1.47	1.54
1	A	104	LEU	N-CA	5.60	1.53	1.46
4	Q	6	VAL	CA-C	5.59	1.59	1.52
1	A	505	PHE	C-O	5.58	1.30	1.23
1	N	326	THR	CA-C	5.57	1.60	1.52
3	C	250	LEU	N-CA	5.56	1.53	1.46
1	A	419	VAL	CA-CB	5.55	1.61	1.54
1	N	188	VAL	CA-CB	-5.54	1.47	1.54
1	A	232	GLN	N-CA	5.53	1.53	1.46
1	A	202	LEU	N-CA	-5.53	1.39	1.46
2	B	66	THR	CA-C	5.53	1.57	1.52
4	D	81	VAL	CA-C	5.52	1.59	1.52
1	N	254	ILE	CG1-CD1	5.52	1.73	1.51
4	D	42	GLU	C-O	-5.49	1.17	1.24
1	N	66	ILE	N-CA	5.48	1.53	1.46
6	F	95	GLN	N-CA	5.47	1.53	1.46
1	N	240	HIS	CA-C	5.47	1.58	1.52
4	D	132	GLN	C-O	-5.45	1.17	1.24
2	B	171	LYS	N-CA	5.43	1.53	1.46
4	D	11	TYR	CA-CB	5.41	1.61	1.53
3	C	61	VAL	CA-CB	5.41	1.61	1.54
3	P	29	SER	CB-OG	-5.38	1.31	1.42
3	P	214	PHE	CD1-CE1	5.38	1.54	1.38
1	A	254	ILE	N-CA	5.38	1.52	1.46
1	N	93	ALA	CA-CB	5.38	1.62	1.53
1	N	246	LEU	N-CA	5.37	1.53	1.46
6	F	20	VAL	CA-CB	5.36	1.61	1.54
1	N	381	LEU	CA-C	-5.36	1.46	1.53
6	S	72	PHE	N-CA	5.35	1.52	1.46
1	A	276	ALA	CA-CB	5.33	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	ASP	C-O	5.33	1.30	1.24
4	D	19	ARG	CZ-NH2	5.31	1.40	1.33
2	O	204	HIS	N-CA	-5.30	1.39	1.46
1	A	173	PRO	C-O	-5.30	1.20	1.25
1	A	345	ILE	CA-CB	5.30	1.60	1.54
1	N	314	ILE	CA-CB	5.29	1.61	1.54
2	B	194	GLY	C-O	5.29	1.30	1.23
1	A	138	HIS	CA-CB	5.29	1.60	1.53
1	A	341	ALA	N-CA	5.29	1.52	1.46
7	T	2	SER	CA-C	5.29	1.59	1.52
6	F	95	GLN	CA-C	5.28	1.59	1.52
7	G	2	SER	CA-C	5.28	1.59	1.52
1	N	92	MET	N-CA	5.27	1.52	1.45
1	N	391	GLY	N-CA	5.27	1.52	1.45
2	B	116	LEU	CA-C	5.25	1.59	1.52
1	A	477	ALA	C-O	-5.25	1.17	1.24
1	A	279	SER	C-O	-5.24	1.18	1.24
3	P	95	THR	CA-CB	5.24	1.61	1.53
12	Y	10	ASN	CA-CB	5.23	1.60	1.53
1	N	298	ASP	CB-CG	5.19	1.65	1.52
3	C	88	ILE	C-O	5.18	1.30	1.24
1	A	261	TYR	CZ-OH	5.18	1.49	1.38
1	N	464	ALA	CA-CB	-5.17	1.45	1.53
8	H	73	ASP	N-CA	5.17	1.52	1.46
1	A	297	MET	CB-CG	5.17	1.68	1.52
2	B	125	THR	CA-CB	5.16	1.61	1.53
1	A	159	LEU	N-CA	5.15	1.52	1.46
6	S	54	ASN	CA-C	-5.15	1.45	1.52
6	S	92	VAL	CA-CB	5.15	1.60	1.54
6	S	62	CYS	C-O	-5.14	1.18	1.24
2	B	122	MET	N-CA	-5.12	1.39	1.46
2	B	165	VAL	CA-CB	5.12	1.60	1.54
6	F	52	ILE	N-CA	-5.12	1.39	1.46
3	P	65	SER	CA-C	5.12	1.57	1.52
1	A	270	TYR	CD1-CE1	5.11	1.53	1.38
1	N	223	ALA	C-O	-5.11	1.17	1.24
13	M	10	THR	CA-CB	5.10	1.60	1.53
1	N	269	GLY	N-CA	5.10	1.52	1.45
7	G	48	ILE	CA-CB	-5.09	1.47	1.54
1	A	396	TRP	CE3-CZ3	5.08	1.53	1.38
2	B	200	CYS	N-CA	5.07	1.50	1.46
1	N	493	GLU	CA-C	5.07	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	267	PRO	CA-C	5.07	1.59	1.52
6	F	19	GLU	N-CA	-5.05	1.40	1.46
6	S	69	VAL	C-O	5.03	1.30	1.24
1	N	127	THR	CA-CB	-5.03	1.45	1.53
6	F	18	ARG	N-CA	5.02	1.52	1.46
8	H	71	THR	CB-CG2	-5.01	1.36	1.52
1	A	323	TRP	CA-CB	-5.01	1.45	1.53
1	N	365	ILE	N-CA	5.01	1.52	1.46
1	N	71	MET	SD-CE	-5.00	1.67	1.79
8	U	59	VAL	C-O	-5.00	1.18	1.24

All (246) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	N-CA-CB	10.68	120.53	110.39
4	Q	10	ASP	N-CA-C	-9.97	101.90	114.56
6	S	20	VAL	N-CA-C	-9.70	100.93	110.72
2	O	226	MET	N-CA-C	-9.09	102.19	113.28
1	N	169	ILE	CB-CA-C	-8.99	100.19	112.24
1	A	310	MET	CG-SD-CE	-8.86	81.42	100.90
1	A	512	ASN	CB-CA-C	-8.49	95.00	109.51
1	N	407	ASP	N-CA-C	8.38	121.47	111.33
1	N	105	LEU	CA-C-N	-8.34	111.79	120.38
1	N	105	LEU	C-N-CA	-8.34	111.79	120.38
4	Q	6	VAL	N-CA-C	8.33	120.62	109.37
3	P	140	SER	N-CA-C	-8.30	102.60	112.89
3	C	80	ARG	NE-CZ-NH2	-8.24	111.78	119.20
8	H	49	ASP	N-CA-C	8.21	122.23	108.20
1	N	20	LEU	N-CA-C	-8.16	101.65	111.69
3	C	29	SER	CB-CA-C	-8.09	96.92	110.68
1	N	79	GLY	N-CA-C	-8.01	103.21	112.50
4	D	19	ARG	NE-CZ-NH1	-7.95	113.55	121.50
4	D	89	ILE	N-CA-C	-7.85	102.79	110.72
4	D	20	ARG	NE-CZ-NH2	-7.84	112.14	119.20
6	S	54	ASN	N-CA-C	7.78	122.54	112.89
1	A	169	ILE	CB-CA-C	-7.70	101.60	112.22
2	O	67	ILE	N-CA-C	7.63	118.40	110.62
7	G	8	HIS	N-CA-C	7.54	126.86	110.80
3	P	80	ARG	CG-CD-NE	-7.50	95.51	112.00
6	S	94	HIS	N-CA-C	7.47	126.71	110.80
1	A	240	HIS	N-CA-CB	7.42	119.18	110.42
3	P	129	VAL	N-CA-CB	7.37	115.14	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	129	ALA	CA-C-N	7.34	127.05	119.64
4	Q	129	ALA	C-N-CA	7.34	127.05	119.64
3	C	236	GLU	CA-CB-CG	-7.24	99.62	114.10
6	S	53	THR	CB-CA-C	-7.23	96.03	110.42
1	A	71	MET	CA-C-N	-7.20	111.06	119.05
1	A	71	MET	C-N-CA	-7.20	111.06	119.05
1	N	470	PHE	N-CA-C	-7.20	103.37	111.14
1	N	71	MET	CG-SD-CE	-7.12	85.24	100.90
1	A	117	MET	CG-SD-CE	-7.07	85.35	100.90
8	H	38	ARG	N-CA-C	-7.07	103.51	111.14
4	D	17	VAL	CB-CA-C	-7.05	100.94	111.80
4	D	102	TYR	CA-C-N	-7.05	115.96	123.08
4	D	102	TYR	C-N-CA	-7.05	115.96	123.08
7	T	5	LYS	N-CA-C	-7.03	103.02	108.78
4	Q	70	GLU	N-CA-C	6.97	118.57	110.97
1	N	70	VAL	N-CA-C	6.97	117.08	110.53
7	T	2	SER	N-CA-C	-6.95	104.46	114.12
2	B	65	TRP	CB-CA-C	6.94	122.82	110.81
13	Z	8	THR	CA-C-N	6.94	126.98	119.90
13	Z	8	THR	C-N-CA	6.94	126.98	119.90
8	U	48	GLY	N-CA-C	-6.91	101.61	111.42
1	N	43	GLN	CA-C-N	6.82	126.85	119.90
1	N	43	GLN	C-N-CA	6.82	126.85	119.90
6	F	93	PRO	CA-C-N	6.80	134.52	121.54
6	F	93	PRO	C-N-CA	6.80	134.52	121.54
1	A	33	LEU	N-CA-C	-6.77	103.90	111.28
1	A	147	ILE	N-CA-C	-6.75	104.19	110.53
3	C	74	ALA	N-CA-C	-6.73	103.41	111.69
7	T	83	GLU	N-CA-C	6.73	119.41	110.53
1	N	359	ALA	N-CA-C	-6.71	104.35	112.54
1	A	131	PRO	CA-C-N	-6.70	110.63	120.28
1	A	131	PRO	C-N-CA	-6.70	110.63	120.28
1	A	397	PHE	CA-C-N	-6.69	112.80	119.56
1	A	397	PHE	C-N-CA	-6.69	112.80	119.56
4	D	24	LEU	CA-C-N	6.68	126.62	120.21
4	D	24	LEU	C-N-CA	6.68	126.62	120.21
4	D	19	ARG	NE-CZ-NH2	6.67	125.20	119.20
4	Q	8	SER	N-CA-C	6.66	119.83	111.24
1	N	75	ILE	N-CA-C	-6.66	105.35	111.67
1	N	27	GLY	N-CA-C	-6.64	106.43	114.66
1	N	240	HIS	CA-C-N	-6.57	111.84	119.32
1	N	240	HIS	C-N-CA	-6.57	111.84	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	184	PHE	N-CA-C	-6.56	104.21	111.82
1	A	35	LEU	CA-CB-CG	-6.54	93.39	116.30
3	P	29	SER	CB-CA-C	-6.53	100.36	110.81
6	F	95	GLN	N-CA-C	6.41	124.46	110.80
3	C	80	ARG	CG-CD-NE	-6.41	97.90	112.00
1	N	500	PRO	CA-C-N	-6.41	114.06	120.21
1	N	500	PRO	C-N-CA	-6.41	114.06	120.21
1	N	355	GLY	N-CA-C	-6.40	104.58	112.77
1	A	402	GLY	N-CA-C	-6.39	106.50	115.32
2	B	64	ILE	N-CA-C	-6.38	104.27	110.72
1	N	94	PHE	CA-C-N	-6.38	113.11	119.56
1	N	94	PHE	C-N-CA	-6.38	113.11	119.56
1	N	472	ILE	N-CA-C	-6.37	104.06	111.00
2	B	202	SER	N-CA-C	6.37	119.90	111.75
1	A	464	ALA	N-CA-C	-6.36	104.42	111.36
1	N	265	LYS	N-CA-C	-6.36	105.35	113.23
1	N	278	MET	CG-SD-CE	-6.34	86.95	100.90
3	P	49	THR	N-CA-C	-6.29	105.09	112.89
13	Z	22	THR	N-CA-C	-6.29	104.35	111.14
1	N	250	GLY	N-CA-C	-6.28	105.21	112.50
2	O	42	ILE	N-CA-C	-6.26	104.41	110.42
1	A	158	ILE	N-CA-C	-6.22	104.44	110.72
4	Q	20	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	N	262	SER	N-CA-C	-6.21	105.71	113.28
6	S	59	GLY	N-CA-C	-6.19	101.24	110.71
4	D	19	ARG	CA-C-N	6.18	128.57	120.28
4	D	19	ARG	C-N-CA	6.18	128.57	120.28
6	S	54	ASN	CB-CA-C	-6.18	97.07	109.99
1	A	72	PRO	N-CA-C	6.17	122.10	113.53
1	N	57	VAL	CB-CA-C	-6.15	103.73	112.22
3	P	248	VAL	CB-CA-C	-6.14	103.85	112.14
4	Q	5	VAL	N-CA-C	6.14	122.11	109.34
3	P	27	MET	N-CA-C	6.14	117.97	111.28
3	C	244	PHE	N-CA-C	-6.13	104.51	111.14
3	C	194	GLY	N-CA-C	-6.13	105.16	113.37
2	B	175	ILE	N-CA-CB	-6.12	105.89	112.37
7	G	7	ASP	N-CA-C	6.11	123.81	110.80
3	P	254	VAL	N-CA-C	6.10	116.85	110.62
1	A	352	GLY	N-CA-C	-6.08	104.99	112.77
2	O	65	TRP	N-CA-C	6.08	119.73	112.93
1	A	105	LEU	CA-C-N	-6.05	114.15	120.38
1	A	105	LEU	C-N-CA	-6.05	114.15	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	475	ALA	N-CA-C	-6.02	104.29	111.69
12	Y	10	ASN	N-CA-C	-6.00	105.78	112.57
12	L	25	MET	CA-C-N	5.99	128.23	120.44
12	L	25	MET	C-N-CA	5.99	128.23	120.44
1	A	49	GLY	N-CA-C	-5.99	102.72	110.38
2	O	14	SER	CA-C-N	5.93	126.08	119.32
2	O	14	SER	C-N-CA	5.93	126.08	119.32
2	O	65	TRP	CB-CA-C	5.93	121.06	110.81
4	D	20	ARG	N-CA-C	-5.89	104.86	111.28
1	A	23	GLY	N-CA-C	-5.89	105.24	112.77
3	C	197	PHE	CB-CA-C	-5.87	101.92	110.96
9	I	66	ALA	N-CA-C	-5.87	106.07	113.18
6	F	93	PRO	N-CA-C	5.86	119.71	111.33
1	A	383	MET	N-CA-C	-5.85	105.23	112.72
1	A	278	MET	CG-SD-CE	-5.84	88.05	100.90
2	B	32	PHE	N-CA-C	-5.83	105.00	111.36
4	Q	20	ARG	NE-CZ-NH1	5.81	127.31	121.50
3	P	193	TYR	N-CA-C	-5.81	104.86	111.14
1	A	153	ALA	N-CA-C	-5.79	105.04	111.36
8	U	64	CYS	N-CA-C	5.79	116.95	109.65
1	N	195	LEU	CA-C-O	5.79	126.69	120.55
2	B	161	HIS	CA-C-N	-5.79	111.76	121.94
2	B	161	HIS	C-N-CA	-5.79	111.76	121.94
4	D	20	ARG	CB-CA-C	-5.78	101.19	110.79
3	P	145	THR	N-CA-C	-5.78	104.58	111.69
1	A	199	LEU	CA-C-N	-5.78	113.07	119.19
1	A	199	LEU	C-N-CA	-5.78	113.07	119.19
3	P	252	LEU	N-CA-C	-5.76	105.08	111.36
1	N	131	PRO	CA-C-N	-5.75	112.50	120.38
1	N	131	PRO	C-N-CA	-5.75	112.50	120.38
1	A	299	VAL	N-CA-C	5.74	116.52	110.72
1	N	512	ASN	CB-CA-C	-5.72	98.38	109.76
1	A	378	HIS	N-CA-C	5.70	118.43	111.82
1	A	226	GLY	N-CA-C	-5.69	104.77	112.57
4	D	133	GLY	N-CA-C	5.69	119.38	112.49
1	A	71	MET	CG-SD-CE	-5.69	88.39	100.90
1	N	278	MET	CA-CB-CG	-5.68	102.75	114.10
1	A	122	ALA	CA-C-O	-5.67	114.71	120.84
2	O	76	ILE	N-CA-C	-5.67	105.57	111.58
1	A	265	LYS	N-CA-C	-5.66	106.37	113.28
3	C	113	GLY	N-CA-C	-5.66	106.84	115.00
3	C	156	ARG	NE-CZ-NH1	-5.63	115.87	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	92	ASN	CA-C-N	5.62	125.59	120.03
2	O	92	ASN	C-N-CA	5.62	125.59	120.03
4	D	20	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	N	15	ILE	CA-C-N	5.59	127.18	120.13
1	N	15	ILE	C-N-CA	5.59	127.18	120.13
1	A	244	TYR	CA-CB-CG	-5.57	103.87	113.90
1	A	278	MET	CA-CB-CG	-5.57	102.95	114.10
3	P	141	GLY	N-CA-C	-5.57	105.91	113.37
7	T	33	LEU	CA-CB-CG	5.55	135.72	116.30
3	C	183	GLU	N-CA-C	5.54	118.25	111.82
1	N	365	ILE	CB-CA-C	-5.53	104.67	112.14
13	Z	4	LYS	CA-C-N	-5.52	114.56	120.03
13	Z	4	LYS	C-N-CA	-5.52	114.56	120.03
11	X	41	ASN	CA-C-N	-5.52	114.91	120.21
11	X	41	ASN	C-N-CA	-5.52	114.91	120.21
4	D	10	ASP	N-CA-C	5.51	119.71	113.15
3	P	200	ALA	N-CA-C	5.51	117.09	111.14
1	A	212	ASP	N-CA-C	-5.48	105.46	111.82
9	V	20	HIS	N-CA-C	5.47	117.33	111.36
4	D	70	GLU	N-CA-C	5.47	116.92	111.07
7	T	17	ARG	CB-CG-CD	-5.45	98.76	111.30
3	P	161	GLN	CB-CA-C	5.45	119.84	110.79
1	N	445	ASP	N-CA-C	5.42	117.89	111.33
3	C	24	ALA	N-CA-C	-5.42	105.38	111.28
1	N	248	LEU	CA-C-N	-5.42	113.32	119.28
1	N	248	LEU	C-N-CA	-5.42	113.32	119.28
1	A	358	LEU	N-CA-C	5.41	117.93	111.71
1	N	199	LEU	CA-C-N	-5.39	113.35	119.28
1	N	199	LEU	C-N-CA	-5.39	113.35	119.28
1	N	257	ILE	N-CA-C	-5.37	105.61	110.82
1	N	10	THR	N-CA-C	-5.37	104.52	111.71
12	Y	24	MET	CB-CA-C	-5.36	102.23	110.81
9	I	68	ILE	CB-CG1-CD1	-5.35	102.56	113.80
1	N	286	ILE	CG1-CB-CG2	-5.34	94.67	110.70
5	E	28	GLU	N-CA-C	5.34	117.10	111.28
6	S	87	THR	N-CA-CB	5.34	117.89	110.04
1	A	74	MET	CB-CG-SD	-5.33	96.70	112.70
8	H	16	PHE	N-CA-C	-5.32	102.74	110.24
1	A	28	MET	N-CA-C	-5.31	105.57	111.36
1	N	507	GLU	CA-C-N	5.31	125.60	119.92
1	N	507	GLU	C-N-CA	5.31	125.60	119.92
1	N	106	PRO	CA-C-N	5.29	124.47	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	106	PRO	C-N-CA	5.29	124.47	118.97
2	O	90	ILE	CB-CA-C	-5.29	102.97	111.59
1	N	65	MET	N-CA-C	-5.25	105.63	111.36
4	Q	26	ASP	N-CA-C	5.25	117.75	111.71
1	N	75	ILE	CA-C-N	-5.25	113.73	120.34
1	N	75	ILE	C-N-CA	-5.25	113.73	120.34
2	B	72	ILE	N-CA-C	5.25	115.87	110.36
4	D	53	ILE	N-CA-C	-5.24	105.39	110.42
5	E	40	ASP	N-CA-C	-5.23	101.78	109.62
1	N	189	MET	CA-CB-CG	-5.23	103.65	114.10
3	C	80	ARG	NE-CZ-NH1	5.21	126.71	121.50
7	T	2	SER	CA-C-N	5.20	131.48	121.54
7	T	2	SER	C-N-CA	5.20	131.48	121.54
1	A	276	ALA	N-CA-C	-5.19	105.70	111.36
1	N	162	ILE	CB-CA-C	-5.18	105.14	112.14
1	N	192	ALA	N-CA-C	-5.18	105.81	111.82
6	F	49	VAL	CA-C-N	-5.17	114.91	120.03
6	F	49	VAL	C-N-CA	-5.17	114.91	120.03
1	N	348	PHE	N-CA-C	-5.17	105.55	111.14
3	C	143	SER	N-CA-C	-5.17	105.82	111.82
1	A	239	GLY	CA-C-N	-5.17	113.38	119.78
1	A	239	GLY	C-N-CA	-5.17	113.38	119.78
1	A	433	LEU	N-CA-C	-5.16	105.65	111.28
5	R	33	MET	N-CA-C	5.16	116.59	111.07
6	S	54	ASN	CA-CB-CG	-5.16	107.44	112.60
5	E	90	ARG	CG-CD-NE	-5.16	100.66	112.00
3	C	144	ILE	N-CA-C	5.15	117.53	111.09
1	N	161	ALA	CA-C-O	5.15	126.01	120.55
12	L	46	LYS	N-CA-C	-5.15	106.08	112.93
9	I	60	PHE	N-CA-C	5.14	117.28	111.11
4	Q	16	TYR	N-CA-C	-5.13	101.35	109.76
2	B	7	LEU	N-CA-C	-5.12	106.72	113.12
6	S	54	ASN	N-CA-CB	-5.12	102.06	110.40
1	A	239	GLY	N-CA-C	5.11	119.93	113.24
1	N	393	PHE	N-CA-C	-5.10	105.80	111.36
9	I	73	LYS	CD-CE-NZ	-5.10	95.58	111.90
1	A	328	HIS	N-CA-C	5.10	117.94	110.30
7	T	8	HIS	N-CA-C	5.08	121.63	110.80
1	N	113	LEU	CB-CA-C	5.08	119.22	110.79
8	U	14	ALA	CA-C-N	-5.07	115.01	120.03
8	U	14	ALA	C-N-CA	-5.07	115.01	120.03
12	Y	11	ILE	CA-C-N	-5.07	113.50	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Y	11	ILE	C-N-CA	-5.07	113.50	119.84
3	P	148	HIS	N-CA-C	5.05	116.48	111.07
1	A	399	LEU	N-CA-C	-5.05	105.86	111.36
4	D	107	ILE	CB-CG1-CD1	-5.05	103.20	113.80
5	E	66	ARG	N-CA-C	-5.02	105.99	111.82
1	N	314	ILE	CA-C-N	-5.00	113.78	119.28
1	N	314	ILE	C-N-CA	-5.00	113.78	119.28
6	F	93	PRO	O-C-N	5.00	128.71	122.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide
6	S	95	GLN	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	57	0
1	N	4027	0	4001	77	0
2	B	1824	0	1833	33	0
2	O	1824	0	1833	49	0
3	C	2110	0	2027	40	0
3	P	2110	0	2027	33	0
4	D	1195	0	1183	24	0
4	Q	1195	0	1183	31	0
5	E	842	0	838	5	0
5	R	842	0	838	11	0
6	F	717	0	700	16	0
6	S	717	0	700	29	0
7	G	675	0	643	38	0
7	T	675	0	644	45	0
8	H	628	0	580	10	0
8	U	628	0	580	9	0
9	I	585	0	597	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	585	0	597	16	0
10	J	451	0	446	5	0
10	W	451	0	446	5	0
11	K	384	0	366	1	0
11	X	384	0	366	5	0
12	L	380	0	380	12	0
12	Y	380	0	380	10	0
13	M	335	0	352	6	0
13	Z	335	0	352	11	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	2	0	0	1	0
15	N	2	0	0	1	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	1	0
17	N	1	0	0	0	0
18	A	120	0	108	8	0
18	N	120	0	108	13	0
19	A	63	0	110	13	0
19	D	63	0	110	9	0
19	L	63	0	110	15	0
19	O	126	0	220	23	0
19	Y	63	0	110	18	0
20	A	102	0	152	8	0
20	C	51	0	76	5	0
20	H	51	0	76	3	0
20	N	153	0	228	12	0
20	P	51	0	76	12	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	2	0
22	C	58	0	70	5	0
22	J	29	0	36	1	0
22	O	29	0	36	0	0
22	P	58	0	71	1	0
22	W	29	0	36	4	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	7	0
24	G	106	0	154	31	0
24	P	53	0	77	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	T	106	0	154	30	0
25	C	100	0	156	19	0
25	G	100	0	156	27	0
25	P	100	0	156	24	0
25	T	100	0	156	19	0
26	E	52	0	80	22	0
26	R	52	0	80	15	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	5	0
28	M	33	0	39	0	0
28	P	33	0	40	1	0
28	Z	33	0	38	3	0
29	A	203	0	0	3	0
29	B	131	0	0	2	0
29	C	90	0	0	4	0
29	D	96	0	0	8	0
29	E	62	0	0	0	0
29	F	70	0	0	1	0
29	G	41	0	0	6	0
29	H	46	0	0	2	0
29	I	44	0	0	3	0
29	J	17	0	0	1	0
29	K	22	0	0	2	0
29	L	23	0	0	1	0
29	M	19	0	0	0	0
29	N	196	0	0	4	0
29	O	106	0	0	2	0
29	P	89	0	0	1	0
29	Q	54	0	0	4	0
29	R	52	0	0	0	0
29	S	62	0	0	6	0
29	T	39	0	0	7	0
29	U	39	0	0	2	0
29	V	16	0	0	3	0
29	W	15	0	0	0	0
29	X	16	0	0	0	0
29	Y	19	0	0	1	0
29	Z	10	0	0	1	0
All	All	32113	0	31063	702	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 11.

All (702) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:G:265:PEK:C8	24:G:265:PEK:C7	1.75	1.56
24:G:265:PEK:C8	24:G:265:PEK:C9	1.77	1.55
24:G:265:PEK:C9	24:G:265:PEK:C10	1.81	1.50
1:A:297:MET:SD	1:A:297:MET:CE	2.02	1.48
24:G:265:PEK:H383	25:G:269:CDL:C27	1.46	1.44
1:N:297:MET:SD	1:N:297:MET:CE	2.04	1.44
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.35	1.37
7:G:5:LYS:HD2	24:G:1263:PEK:C37	1.59	1.33
24:T:1265:PEK:H383	25:T:1269:CDL:C27	1.60	1.28
7:G:5:LYS:CD	24:G:1263:PEK:H371	1.65	1.25
24:G:265:PEK:C38	25:G:269:CDL:C27	2.19	1.21
12:L:20:ARG:HH22	19:L:522:TGL:CC3	1.59	1.15
24:G:265:PEK:H383	25:G:269:CDL:H273	1.26	1.14
7:G:5:LYS:CG	24:G:1263:PEK:H371	1.82	1.10
15:A:520:PER:O2	15:A:520:PER:O1	1.70	1.09
7:T:5:LYS:HD2	24:T:263:PEK:H381	1.28	1.09
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.13	1.09
2:O:41:ILE:HD13	26:R:1230:PSC:H342	1.35	1.08
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.12	1.08
26:E:230:PSC:H072	9:I:10:ARG:HH21	1.19	1.08
24:P:1264:PEK:H71	24:P:1264:PEK:H32	1.30	1.08
29:N:4407:HOH:O	19:O:1523:TGL:HC32	1.52	1.06
7:T:84:LYS:HD2	7:T:84:LYS:N	1.70	1.06
15:N:520:PER:O1	15:N:520:PER:O2	1.70	1.06
24:T:1265:PEK:C38	25:T:1269:CDL:C27	2.35	1.03
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.19	1.03
25:G:269:CDL:H242	25:G:269:CDL:H542	1.40	1.02
26:R:1230:PSC:O01	26:R:1230:PSC:H212	1.58	1.01
12:L:20:ARG:NH2	19:L:522:TGL:CC3	2.19	1.01
7:T:84:LYS:HD2	7:T:84:LYS:H	1.20	1.01
7:G:5:LYS:HD2	24:G:1263:PEK:H371	1.14	1.01
2:O:116:LEU:HD12	2:O:117:SER:N	1.75	1.01
7:T:2:SER:OG	24:T:263:PEK:H302	1.60	1.01
25:G:269:CDL:H242	25:G:269:CDL:C54	1.91	1.00
20:N:1524:PGV:H221	20:N:1524:PGV:H31	1.40	0.99
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	1.78	0.99
24:T:1265:PEK:C38	25:T:1269:CDL:H272	1.91	0.99
1:N:113:LEU:HD12	19:Y:1522:TGL:H292	1.43	0.99
24:T:1265:PEK:H383	25:T:1269:CDL:H272	1.01	0.99
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:1267:PGV:H182	25:P:1270:CDL:H662	1.42	0.98
18:N:515:HEA:C27	18:N:515:HEA:C16	2.41	0.98
24:G:265:PEK:C38	25:G:269:CDL:H272	1.93	0.98
19:Y:1522:TGL:HC62	19:Y:1522:TGL:HC22	1.45	0.98
6:S:95:GLN:HA	6:S:95:GLN:HE21	1.27	0.97
7:T:5:LYS:CD	24:T:263:PEK:H381	1.95	0.97
18:N:515:HEA:H161	18:N:515:HEA:H272	1.47	0.97
7:G:5:LYS:HB3	1:N:278:MET:SD	2.07	0.95
6:S:95:GLN:HG2	29:S:4406:HOH:O	1.63	0.94
24:G:265:PEK:H383	25:G:269:CDL:H271	1.47	0.94
26:E:230:PSC:C07	9:I:10:ARG:HH21	1.80	0.93
25:G:269:CDL:H112	25:G:269:CDL:HA21	1.50	0.91
19:A:521:TGL:H281	19:A:521:TGL:H101	1.51	0.91
7:G:5:LYS:HD2	24:G:1263:PEK:H372	1.54	0.90
18:N:515:HEA:C16	18:N:515:HEA:H272	1.99	0.88
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	1.73	0.88
7:T:84:LYS:H	7:T:84:LYS:CD	1.85	0.88
20:P:1267:PGV:C18	25:P:1270:CDL:H662	2.04	0.88
6:S:85:CYS:SG	6:S:87:THR:HG23	2.14	0.88
7:T:5:LYS:HD2	24:T:263:PEK:C38	2.03	0.87
26:R:1230:PSC:C07	9:V:10:ARG:HH21	1.87	0.87
7:G:5:LYS:HB2	24:G:1263:PEK:H351	1.54	0.86
24:G:265:PEK:H382	25:G:269:CDL:H272	1.55	0.86
24:G:265:PEK:C8	24:G:265:PEK:C6	2.53	0.86
24:T:1265:PEK:C38	25:T:1269:CDL:H273	2.03	0.86
24:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.24	0.85
26:E:230:PSC:H343	26:E:230:PSC:H142	1.57	0.85
1:A:296:GLY:HA2	8:H:23:GLN:OE1	1.77	0.84
7:T:5:LYS:CD	24:T:263:PEK:C38	2.55	0.84
10:W:33:ARG:HG2	22:W:1060:CHD:H151	1.59	0.84
7:T:5:LYS:HB2	24:T:263:PEK:H371	1.60	0.83
19:O:1521:TGL:HB92	19:O:1521:TGL:H281	1.59	0.83
7:T:5:LYS:HB2	24:T:263:PEK:C37	2.09	0.82
13:M:39:ASN:O	13:M:43:SER:HB2	1.80	0.82
19:Y:1522:TGL:HA92	19:Y:1522:TGL:H231	1.62	0.81
7:G:38:HIS:CE1	25:G:269:CDL:H111	2.15	0.81
25:T:1269:CDL:HA21	25:T:1269:CDL:H111	1.62	0.81
18:N:515:HEA:H273	18:N:515:HEA:H162	1.60	0.81
20:A:524:PGV:H02	20:A:524:PGV:O14	1.81	0.81
7:G:5:LYS:HG3	24:G:1263:PEK:H371	1.63	0.80
19:O:1521:TGL:H281	19:O:1521:TGL:H101	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:95:GLN:HA	6:S:95:GLN:NE2	1.96	0.80
3:C:3:HIS:HE1	6:F:96:LEU:CD2	1.93	0.80
1:A:430:PHE:HE1	19:A:521:TGL:HB21	1.46	0.80
19:L:522:TGL:CC2	19:L:522:TGL:HC62	2.10	0.80
19:O:1521:TGL:H101	19:O:1521:TGL:C28	2.12	0.79
24:C:264:PEK:C10	24:C:264:PEK:H161	2.11	0.79
8:H:45:ALA:O	8:H:47:GLY:N	2.14	0.79
7:T:2:SER:OG	24:T:263:PEK:C30	2.29	0.79
7:G:72:ASN:H	7:G:76:ASN:HD22	1.26	0.79
10:J:7:GLU:HG3	29:J:4441:HOH:O	1.83	0.79
9:V:73:LYS:HB2	29:V:4544:HOH:O	1.81	0.79
3:P:224:LYS:CD	25:P:1270:CDL:HB31	2.13	0.78
11:X:54:ARG:HH21	11:X:54:ARG:CG	1.96	0.78
9:I:73:LYS:HB3	29:I:4590:HOH:O	1.84	0.78
7:G:5:LYS:CD	24:G:1263:PEK:C37	2.40	0.78
1:N:400:PHE:HB3	19:Y:1522:TGL:H283	1.66	0.78
6:S:52:ILE:O	6:S:94:HIS:CE1	2.36	0.78
1:A:472:ILE:HG21	19:L:522:TGL:HA92	1.66	0.78
6:F:85:CYS:SG	6:F:87:THR:HG23	2.23	0.78
7:G:84:LYS:H	7:G:84:LYS:CD	1.97	0.78
29:O:4115:HOH:O	8:U:61:LYS:HD2	1.83	0.78
4:Q:72:ASN:HB3	29:Q:3133:HOH:O	1.83	0.78
2:O:226:MET:O	2:O:227:LEU:C	2.28	0.77
4:D:34:SER:H	4:D:37:GLN:HE21	1.32	0.77
19:O:1523:TGL:H231	19:O:1523:TGL:HA91	1.67	0.76
3:C:3:HIS:HE1	6:F:96:LEU:HD22	1.47	0.76
2:O:226:MET:O	2:O:227:LEU:O	2.03	0.76
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.68	0.76
20:P:1267:PGV:H182	25:P:1270:CDL:C66	2.15	0.75
1:A:484:THR:HB	13:M:2:THR:OG1	1.86	0.75
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.69	0.75
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.27	0.75
19:A:521:TGL:H322	19:A:521:TGL:HA92	1.68	0.75
24:C:264:PEK:H32	24:C:264:PEK:H71	1.68	0.74
1:N:484:THR:HG22	13:Z:2:THR:OG1	1.87	0.74
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.51	0.74
24:P:1264:PEK:C10	24:P:1264:PEK:H161	2.16	0.74
3:C:3:HIS:CE1	6:F:96:LEU:HD22	2.22	0.74
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.21	0.74
24:T:1265:PEK:H381	25:T:1269:CDL:H273	1.69	0.74
7:G:84:LYS:H	7:G:84:LYS:HD2	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:1524:PGV:H311	13:Z:19:LEU:HD23	1.67	0.74
3:C:63:ARG:HE	25:C:270:CDL:CA2	2.00	0.73
20:C:267:PGV:H172	25:C:270:CDL:H652	1.69	0.73
4:D:31:LYS:HE2	29:D:4577:HOH:O	1.87	0.73
3:C:80:ARG:NH1	24:T:263:PEK:H032	2.04	0.73
7:T:17:ARG:HD3	29:T:3302:HOH:O	1.88	0.73
19:L:522:TGL:HC62	19:L:522:TGL:HC22	1.69	0.73
2:B:56:MET:HA	26:E:230:PSC:H202	1.71	0.72
4:D:31:LYS:CE	29:D:4577:HOH:O	2.37	0.72
29:N:4424:HOH:O	26:R:1230:PSC:H21	1.90	0.72
19:A:521:TGL:HA82	19:A:521:TGL:H282	1.69	0.72
19:L:522:TGL:HC81	29:L:4545:HOH:O	1.89	0.72
18:N:515:HEA:C27	18:N:515:HEA:H162	2.17	0.72
7:G:38:HIS:HE1	25:G:269:CDL:H111	1.53	0.71
25:G:269:CDL:H332	2:O:78:LEU:HD12	1.73	0.71
10:J:52:TRP:O	10:J:57:HIS:HE1	1.74	0.71
4:D:86:MET:HE3	29:K:4663:HOH:O	1.90	0.71
1:N:113:LEU:CD1	19:Y:1522:TGL:H292	2.19	0.71
24:C:264:PEK:H161	24:C:264:PEK:H102	1.70	0.71
2:B:1:FME:HE3	4:D:123:MET:HE3	1.73	0.71
19:A:521:TGL:H281	19:A:521:TGL:C10	2.21	0.71
26:E:230:PSC:H02	26:E:230:PSC:H212	1.73	0.70
25:G:269:CDL:H201	1:N:311:ILE:CD1	2.22	0.70
6:S:75:HIS:H	6:S:80:GLN:HE22	1.39	0.70
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.73	0.70
19:O:1521:TGL:H281	19:O:1521:TGL:CB9	2.21	0.70
24:C:264:PEK:H161	24:C:264:PEK:H101	1.74	0.70
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.72	0.70
19:O:1523:TGL:HC21	19:O:1523:TGL:HG11	1.74	0.70
24:P:1264:PEK:H161	24:P:1264:PEK:H101	1.73	0.70
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.73	0.69
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.22	0.69
10:J:4:ARG:HD2	10:J:7:GLU:OE2	1.92	0.69
2:B:81:LEU:HD12	25:T:1269:CDL:H351	1.74	0.69
18:N:515:HEA:C16	18:N:515:HEA:H273	2.17	0.69
3:C:63:ARG:NE	25:C:270:CDL:HA22	2.01	0.69
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.55	0.69
3:P:224:LYS:HD2	25:P:1270:CDL:HB31	1.74	0.69
4:Q:34:SER:O	4:Q:38:LYS:HG3	1.93	0.69
7:T:8:HIS:CE1	24:T:263:PEK:H321	2.28	0.69
11:X:54:ARG:HG3	11:X:54:ARG:NH2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:521:TGL:HB42	19:A:521:TGL:OB1	1.91	0.69
26:R:1230:PSC:H071	9:V:10:ARG:HH21	1.58	0.69
10:W:33:ARG:HG2	22:W:1060:CHD:C15	2.22	0.68
24:G:265:PEK:C38	25:G:269:CDL:H273	2.06	0.68
29:G:4754:HOH:O	20:N:1268:PGV:H341	1.91	0.68
7:T:5:LYS:CB	24:T:263:PEK:H371	2.23	0.68
3:C:55:TYR:CE1	25:C:270:CDL:H521	2.28	0.68
20:N:1524:PGV:H31	20:N:1524:PGV:C22	2.19	0.68
24:G:1263:PEK:H222	29:G:4660:HOH:O	1.93	0.68
20:A:522:PGV:H183	24:C:264:PEK:H332	1.74	0.68
7:T:72:ASN:H	7:T:76:ASN:HD22	1.40	0.67
26:R:1230:PSC:H032	26:R:1230:PSC:O02	1.94	0.67
20:N:1524:PGV:H221	20:N:1524:PGV:C3	2.20	0.67
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.76	0.67
2:O:116:LEU:HD12	2:O:116:LEU:C	2.20	0.67
25:G:269:CDL:H112	25:G:269:CDL:CA2	2.23	0.66
25:G:269:CDL:H201	1:N:311:ILE:HD11	1.76	0.66
1:A:278:MET:SD	7:T:5:LYS:HB3	2.35	0.66
24:G:265:PEK:C8	24:G:265:PEK:C10	2.73	0.66
7:T:5:LYS:HB2	24:T:263:PEK:H362	1.77	0.66
26:E:230:PSC:H212	26:E:230:PSC:C02	2.26	0.66
3:P:226:HIS:CE1	25:P:1270:CDL:HB32	2.31	0.66
7:T:5:LYS:CG	24:T:263:PEK:H383	2.26	0.66
26:R:1230:PSC:H072	9:V:10:ARG:HH21	1.61	0.65
4:D:31:LYS:NZ	29:D:4577:HOH:O	2.22	0.65
3:P:63:ARG:HE	25:P:1270:CDL:CA2	2.00	0.65
1:A:430:PHE:CE1	19:A:521:TGL:HB21	2.29	0.65
4:Q:109:HIS:HD2	29:Q:3152:HOH:O	1.79	0.65
19:Y:1522:TGL:HC62	19:Y:1522:TGL:CC2	2.06	0.65
20:N:1524:PGV:H032	20:N:1524:PGV:H22	1.78	0.65
24:C:264:PEK:HN2	7:G:76:ASN:HD21	1.43	0.65
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.78	0.65
25:C:270:CDL:H241	25:C:270:CDL:H661	1.79	0.65
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.77	0.65
1:N:113:LEU:HD12	19:Y:1522:TGL:C29	2.24	0.65
2:B:129:LYS:HE3	29:B:4594:HOH:O	1.97	0.64
4:D:78:TRP:CA	19:D:523:TGL:HB22	2.27	0.64
7:G:83:GLU:HA	7:G:84:LYS:HZ2	1.62	0.64
25:G:269:CDL:H511	25:G:269:CDL:H181	1.78	0.64
3:P:213:THR:HG21	20:P:1267:PGV:H11	1.78	0.64
1:A:311:ILE:HD12	25:T:1269:CDL:H201	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:3:ALA:O	7:G:4:ALA:HB2	1.98	0.64
7:G:84:LYS:HD2	7:G:84:LYS:N	2.13	0.64
25:C:270:CDL:H522	25:C:270:CDL:OB9	1.98	0.63
10:J:50:LEU:HD22	10:J:50:LEU:O	1.99	0.63
12:L:20:ARG:HH22	19:L:522:TGL:HC32	0.66	0.63
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.96	0.63
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.34	0.63
25:T:1269:CDL:H571	25:T:1269:CDL:C78	2.25	0.63
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.31	0.63
1:N:177:SER:H	1:N:180:GLN:NE2	1.95	0.63
6:S:94:HIS:CD2	6:S:95:GLN:H	2.16	0.63
20:C:267:PGV:H182	25:C:270:CDL:H671	1.79	0.62
8:H:45:ALA:C	8:H:47:GLY:H	2.05	0.62
1:N:513:LEU:O	1:N:514:LYS:HB2	1.98	0.62
24:G:265:PEK:C9	24:G:265:PEK:C11	2.75	0.62
3:P:111:GLU:HG3	29:U:4773:HOH:O	1.98	0.62
1:A:281:GLY:C	7:T:4:ALA:HB1	2.25	0.62
3:P:55:TYR:CE1	25:P:1270:CDL:H521	2.34	0.62
7:T:5:LYS:HB2	24:T:263:PEK:C36	2.29	0.62
1:A:1:FME:HE2	1:A:4:ASN:HD22	1.64	0.62
6:S:94:HIS:CD2	6:S:95:GLN:N	2.68	0.62
3:C:210:ILE:HG12	20:C:267:PGV:H12	1.81	0.62
1:N:87:ILE:O	1:N:173:PRO:HD3	1.99	0.62
2:O:32:PHE:HE2	19:O:1521:TGL:HA52	1.64	0.62
19:O:1521:TGL:H281	19:O:1521:TGL:C10	2.28	0.61
2:B:62:GLU:O	2:B:66:THR:HB	1.99	0.61
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.18	0.61
2:O:116:LEU:HD12	2:O:117:SER:H	1.62	0.61
25:P:1270:CDL:H222	25:P:1270:CDL:H632	1.83	0.61
19:O:1523:TGL:HG31	29:Q:4568:HOH:O	2.00	0.61
1:A:513:LEU:O	1:A:514:LYS:HB2	1.99	0.61
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.65	0.61
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.81	0.61
3:P:210:ILE:HD13	20:P:1267:PGV:H301	1.83	0.61
25:T:1269:CDL:HA21	25:T:1269:CDL:C11	2.28	0.61
4:D:34:SER:H	4:D:37:GLN:NE2	1.98	0.61
20:A:524:PGV:H311	13:M:19:LEU:HD23	1.81	0.61
1:N:482:VAL:HG22	13:Z:1:ILE:HD11	1.83	0.60
1:A:177:SER:H	1:A:180:GLN:HE21	1.49	0.60
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.37	0.60
26:E:230:PSC:H072	9:I:10:ARG:NH2	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:E:230:PSC:H212	26:E:230:PSC:O01	2.01	0.60
17:A:519:NA:NA	29:A:2026:HOH:O	1.73	0.60
7:G:72:ASN:H	7:G:76:ASN:ND2	1.98	0.60
24:P:1264:PEK:H161	24:P:1264:PEK:H102	1.83	0.60
3:P:63:ARG:NE	25:P:1270:CDL:HA22	1.99	0.59
25:G:269:CDL:H592	25:G:269:CDL:C63	2.31	0.59
6:S:26:LYS:HB3	6:S:28:GLN:NE2	2.17	0.59
7:T:5:LYS:HG3	24:T:263:PEK:H383	1.83	0.59
3:C:52:LEU:HD23	25:C:270:CDL:H362	1.84	0.59
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.03	0.59
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.31	0.59
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.38	0.59
2:O:41:ILE:HD13	26:R:1230:PSC:C34	2.22	0.59
3:C:3:HIS:N	29:C:4573:HOH:O	2.36	0.59
20:N:1524:PGV:H062	29:Z:3153:HOH:O	2.01	0.59
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.38	0.59
24:G:265:PEK:C7	24:G:265:PEK:C9	2.81	0.59
4:D:107:ILE:HB	4:D:108:PRO:CD	2.32	0.59
26:E:230:PSC:H231	26:E:230:PSC:H42	1.84	0.59
19:L:522:TGL:OC1	19:L:522:TGL:HC41	2.02	0.59
1:N:43:GLN:HB2	1:N:44:PRO:HD2	1.85	0.59
2:O:82:ARG:HH11	2:O:86:MET:HE1	1.68	0.59
12:Y:12:PRO:HG2	19:Y:1522:TGL:HG11	1.84	0.59
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.68	0.58
7:T:5:LYS:CG	24:T:263:PEK:C38	2.81	0.58
2:O:42:ILE:HG21	19:O:1523:TGL:H232	1.84	0.58
3:C:80:ARG:HH11	24:T:263:PEK:H032	1.67	0.58
12:L:20:ARG:HH12	19:L:522:TGL:HC61	1.68	0.58
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.69	0.58
7:G:3:ALA:O	7:G:4:ALA:CB	2.51	0.58
7:G:45:PRO:HD2	29:G:2145:HOH:O	2.03	0.58
3:P:54:MET:HE1	20:P:1267:PGV:H141	1.85	0.58
1:A:282:PHE:HA	7:T:4:ALA:CB	2.35	0.57
3:C:3:HIS:N	29:C:4600:HOH:O	2.37	0.57
6:F:64:GLU:O	6:F:65:ASP:HB2	2.05	0.57
12:L:14:SER:H	19:L:522:TGL:HC31	1.69	0.57
3:P:210:ILE:HG21	20:P:1267:PGV:H282	1.86	0.57
2:B:41:ILE:HD13	26:E:230:PSC:H342	1.87	0.57
19:D:523:TGL:HA32	19:D:523:TGL:HB42	1.87	0.57
4:Q:109:HIS:CD2	29:Q:3152:HOH:O	2.54	0.57
3:C:5:THR:HG22	6:F:96:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:5:LYS:HG3	24:G:1263:PEK:C37	2.32	0.56
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.40	0.56
8:H:43:MET:HE1	8:U:43:MET:HE1	1.88	0.56
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.40	0.56
3:C:224:LYS:CD	25:C:270:CDL:HB31	2.36	0.56
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.93	0.56
7:T:36:TRP:HE1	24:T:1265:PEK:C20	2.19	0.56
9:V:36:LYS:O	9:V:41:GLU:HG2	2.06	0.56
1:N:69:MET:HE3	1:N:70:VAL:HG23	1.88	0.56
3:C:48:THR:HG23	25:C:270:CDL:H402	1.88	0.55
24:G:1263:PEK:H382	29:G:4355:HOH:O	2.06	0.55
2:B:45:MET:HE2	2:B:45:MET:HA	1.88	0.55
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.46	0.55
7:T:72:ASN:H	7:T:76:ASN:ND2	2.04	0.55
7:T:45:PRO:HD2	29:T:3145:HOH:O	2.05	0.55
2:B:164:ALA:O	2:B:194:GLY:HA3	2.06	0.55
25:G:269:CDL:H761	25:G:269:CDL:H601	1.89	0.55
26:E:230:PSC:C07	9:I:10:ARG:NH2	2.61	0.55
1:N:240:HIS:O	1:N:243:VAL:HG22	2.07	0.55
19:Y:1522:TGL:HC22	19:Y:1522:TGL:CC6	2.28	0.55
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.88	0.55
6:S:64:GLU:O	6:S:65:ASP:HB2	2.06	0.55
7:T:37:LEU:HD23	7:T:38:HIS:HD1	1.72	0.55
2:B:78:LEU:HD12	25:T:1269:CDL:H352	1.89	0.54
1:A:311:ILE:CD1	25:T:1269:CDL:H201	2.38	0.54
29:A:4231:HOH:O	26:E:230:PSC:H21	2.08	0.54
1:N:430:PHE:CE1	19:O:1521:TGL:HB21	2.43	0.54
19:D:523:TGL:H352	9:I:16:ARG:HH21	1.72	0.54
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.89	0.54
12:Y:20:ARG:NH2	12:Y:24:MET:CG	2.64	0.54
1:N:412:ILE:HD13	4:Q:84:ALA:CB	2.38	0.54
26:R:1230:PSC:H221	26:R:1230:PSC:H42	1.89	0.54
3:P:254:VAL:HG23	25:T:1269:CDL:H672	1.90	0.54
6:S:25:ARG:HD3	29:S:4659:HOH:O	2.07	0.54
2:B:59:GLN:C	2:B:60:GLU:HG3	2.33	0.54
1:N:417:MET:O	1:N:421:VAL:HG22	2.07	0.54
7:G:69:PHE:HZ	28:G:272:DMU:H1	1.72	0.54
1:A:233:HIS:CE1	1:A:292:MET:HE1	2.43	0.53
1:A:297:MET:CE	1:A:297:MET:CB	2.86	0.53
25:P:1270:CDL:H222	25:P:1270:CDL:C63	2.39	0.53
6:S:22:LEU:HD23	6:S:25:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:438:ARG:O	1:N:439:ARG:HB2	2.07	0.53
8:U:45:ALA:O	8:U:47:GLY:N	2.41	0.53
19:A:521:TGL:HC22	29:D:2376:HOH:O	2.08	0.53
25:C:270:CDL:H661	25:C:270:CDL:C24	2.38	0.53
1:A:112:LEU:HG	29:A:2073:HOH:O	2.08	0.53
4:D:68:PHE:HA	4:D:71:MET:HE3	1.90	0.53
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.91	0.53
19:A:521:TGL:H322	19:A:521:TGL:CA9	2.37	0.53
18:A:515:HEA:HHC	18:A:515:HEA:H122	1.89	0.53
4:D:78:TRP:HA	19:D:523:TGL:HB22	1.90	0.53
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.08	0.53
9:I:35:TYR:C	9:I:37:PHE:H	2.17	0.53
20:A:524:PGV:C32	20:A:524:PGV:H152	2.39	0.52
4:D:86:MET:CE	29:K:4663:HOH:O	2.51	0.52
7:G:5:LYS:HD2	24:G:1263:PEK:C38	2.36	0.52
28:G:272:DMU:O1	28:G:272:DMU:H29	2.09	0.52
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.52
26:E:230:PSC:C06	9:I:10:ARG:HE	2.22	0.52
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.92	0.52
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.90	0.52
2:O:129:LYS:O	2:O:132:GLU:HB2	2.09	0.52
3:P:112:LEU:CD2	29:T:3156:HOH:O	2.57	0.52
1:A:514:LYS:OXT	6:F:37:LYS:HE2	2.09	0.52
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.07	0.52
19:O:1523:TGL:HC21	19:O:1523:TGL:CG1	2.40	0.52
9:V:18:ARG:HG3	29:V:3367:HOH:O	2.08	0.52
19:Y:1522:TGL:H171	19:Y:1522:TGL:OA1	2.10	0.52
26:E:230:PSC:H343	26:E:230:PSC:C14	2.36	0.52
1:N:430:PHE:HE1	19:O:1521:TGL:HB21	1.75	0.52
3:P:213:THR:CG2	20:P:1267:PGV:H11	2.39	0.52
3:C:59:ARG:HG3	25:C:270:CDL:H512	1.92	0.52
9:I:58:LYS:O	9:I:62:GLU:HG3	2.10	0.52
2:O:139:ASP:OD2	2:O:140:ASN:N	2.41	0.52
2:O:128:LEU:HD22	2:O:132:GLU:HB3	1.92	0.51
19:O:1523:TGL:HB81	19:O:1523:TGL:H121	1.92	0.51
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.92	0.51
8:H:27:ARG:NH1	29:H:2296:HOH:O	2.43	0.51
24:P:1264:PEK:H32	24:P:1264:PEK:C7	2.19	0.51
2:O:41:ILE:CD1	26:R:1230:PSC:H342	2.23	0.51
7:T:37:LEU:HD23	7:T:38:HIS:ND1	2.25	0.51
20:A:524:PGV:H152	20:A:524:PGV:H322	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:199:LEU:N	1:N:200:PRO:CD	2.74	0.51
4:D:58:GLU:O	4:D:58:GLU:HG3	2.10	0.51
8:H:60:TYR:CD1	8:H:60:TYR:C	2.89	0.51
25:G:269:CDL:H752	1:N:282:PHE:HZ	1.76	0.51
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.93	0.51
13:Z:31:GLY:C	28:Z:1526:DMU:H1	2.36	0.51
24:C:264:PEK:H102	24:C:264:PEK:C16	2.40	0.50
25:G:269:CDL:H592	25:G:269:CDL:H632	1.92	0.50
6:S:94:HIS:CG	6:S:95:GLN:H	2.24	0.50
12:Y:24:MET:SD	19:Y:1522:TGL:H162	2.51	0.50
19:Y:1522:TGL:H311	29:Y:4350:HOH:O	2.10	0.50
2:O:32:PHE:CE2	19:O:1521:TGL:HA52	2.46	0.50
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.08	0.50
6:S:22:LEU:CD2	6:S:25:ARG:NH1	2.75	0.50
1:N:514:LYS:NZ	29:N:3388:HOH:O	2.39	0.50
8:U:27:ARG:NH1	29:U:3296:HOH:O	2.43	0.50
1:N:20:LEU:HB3	19:Y:1522:TGL:H221	1.93	0.50
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.47	0.50
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.94	0.50
11:X:54:ARG:CG	11:X:54:ARG:NH2	2.65	0.50
1:N:131:PRO:O	1:N:132:LEU:C	2.52	0.50
9:V:25:PHE:O	9:V:28:SER:HB2	2.11	0.49
19:O:1521:TGL:H101	19:O:1521:TGL:H283	1.90	0.49
4:Q:33:LEU:HD22	4:Q:37:GLN:HB3	1.94	0.49
1:A:28:MET:CE	18:A:515:HEA:H271	2.41	0.49
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.25	0.49
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.48	0.49
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.94	0.49
1:A:37:ILE:HG21	18:A:515:HEA:CMA	2.43	0.49
7:G:2:SER:O	24:G:1263:PEK:H322	2.13	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.95	0.49
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.76	0.49
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.78	0.49
2:B:82:ARG:HH11	2:B:86:MET:HE1	1.78	0.48
1:N:383:MET:O	1:N:387:PHE:HB2	2.12	0.48
3:C:54:MET:HE1	20:C:267:PGV:H131	1.96	0.48
2:O:113:TYR:HD1	8:U:58:ARG:HH22	1.61	0.48
28:G:272:DMU:H29	28:G:272:DMU:C10	2.43	0.48
18:N:515:HEA:HBC1	18:N:515:HEA:HMC3	1.95	0.48
2:O:116:LEU:CD2	2:O:226:MET:HG2	2.43	0.48
1:A:47:LEU:O	13:M:41:LYS:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:43:LYS:HE3	29:S:3347:HOH:O	2.13	0.48
6:S:52:ILE:O	6:S:94:HIS:HE1	1.91	0.48
7:T:36:TRP:HD1	29:T:4758:HOH:O	1.96	0.48
20:A:524:PGV:O02	20:A:524:PGV:P	2.72	0.48
2:B:66:THR:HG21	22:B:1086:CHD:H3	1.96	0.48
7:G:84:LYS:CD	7:G:84:LYS:N	2.72	0.48
1:N:48:LEU:HB2	29:N:3109:HOH:O	2.14	0.48
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.59	0.48
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.96	0.48
6:S:26:LYS:HB3	6:S:28:GLN:HE22	1.79	0.48
6:S:95:GLN:HE21	6:S:95:GLN:CA	2.14	0.48
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.40	0.48
7:T:36:TRP:HE1	24:T:1265:PEK:H201	1.79	0.48
1:A:87:ILE:O	1:A:173:PRO:HD3	2.13	0.48
26:E:230:PSC:H201	26:E:230:PSC:H232	1.51	0.48
1:N:422:ASN:OD1	19:O:1521:TGL:H262	2.14	0.48
3:C:246:ASP:HB2	29:C:4215:HOH:O	2.13	0.48
25:G:269:CDL:H782	25:G:269:CDL:H571	1.96	0.48
3:C:106:LEU:HD13	20:H:268:PGV:H22	1.95	0.47
5:E:11:PHE:CB	26:E:230:PSC:H073	2.44	0.47
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.47	0.47
1:A:198:SER:HB2	1:A:238:PHE:HA	1.96	0.47
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.41	0.47
2:B:59:GLN:O	2:B:60:GLU:HG3	2.14	0.47
2:O:1:FME:HCN	2:O:193:TYR:HB2	1.96	0.47
26:R:1230:PSC:H071	9:V:10:ARG:NH2	2.28	0.47
1:A:281:GLY:O	7:T:4:ALA:HB1	2.15	0.47
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.96	0.47
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.14	0.47
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.96	0.47
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.29	0.47
3:C:210:ILE:HD13	20:C:267:PGV:H301	1.97	0.47
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.96	0.47
7:G:2:SER:OG	24:G:1263:PEK:H291	2.14	0.47
2:B:82:ARG:NH1	2:B:86:MET:HE1	2.30	0.47
22:C:271:CHD:H212	22:C:271:CHD:H12	1.97	0.47
7:G:45:PRO:CD	29:G:2145:HOH:O	2.62	0.47
18:N:515:HEA:H172	18:N:515:HEA:H261	1.36	0.47
3:P:254:VAL:CG2	25:T:1269:CDL:H672	2.45	0.47
1:A:25:TRP:CE3	19:L:522:TGL:HB91	2.49	0.47
2:B:52:HIS:CE1	26:E:230:PSC:H211	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:8:ASP:HA	26:E:230:PSC:H071	1.95	0.47
6:F:94:HIS:HB3	6:F:95:GLN:NE2	2.30	0.47
1:N:24:ALA:HA	18:N:515:HEA:H22	1.96	0.47
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.15	0.47
10:W:30:ILE:O	10:W:34:VAL:HG23	2.15	0.47
20:P:1267:PGV:H182	25:P:1270:CDL:C67	2.45	0.46
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.80	0.46
1:N:240:HIS:O	1:N:241:PRO:C	2.55	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.46
2:B:65:TRP:HZ3	26:E:230:PSC:H322	1.79	0.46
4:D:127:LYS:HD2	29:I:2384:HOH:O	2.14	0.46
7:G:69:PHE:CZ	28:G:272:DMU:H1	2.50	0.46
4:Q:63:LYS:HG2	4:Q:64:PHE:CE1	2.51	0.46
25:P:1270:CDL:H411	25:P:1270:CDL:H362	1.97	0.46
10:W:52:TRP:O	10:W:57:HIS:HE1	1.98	0.46
19:A:521:TGL:H241	19:A:521:TGL:HA91	1.96	0.46
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.16	0.46
2:B:91:ASN:C	2:B:91:ASN:HD22	2.24	0.46
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.46	0.46
7:G:37:LEU:HD21	25:G:269:CDL:H341	1.98	0.46
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.46	0.46
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.46
28:P:1272:DMU:H40	7:T:63:GLY:H	1.80	0.46
4:Q:83:GLY:HA3	11:X:17:VAL:HG12	1.97	0.46
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.61	0.46
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.51	0.46
6:F:26:LYS:HE3	29:F:4627:HOH:O	2.16	0.46
25:G:269:CDL:H201	1:N:311:ILE:HD12	1.96	0.46
19:O:1521:TGL:H241	19:O:1521:TGL:H322	1.98	0.46
7:T:79:PRO:HD2	29:T:3129:HOH:O	2.16	0.46
7:G:84:LYS:H	7:G:84:LYS:CE	2.28	0.46
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.97	0.46
1:N:412:ILE:HD13	4:Q:84:ALA:HB3	1.96	0.46
1:N:514:LYS:HE2	29:S:3332:HOH:O	2.15	0.46
3:C:3:HIS:CE1	6:F:96:LEU:CD2	2.83	0.46
1:N:113:LEU:CD1	19:Y:1522:TGL:C29	2.92	0.46
1:N:350:VAL:HG13	19:O:1521:TGL:HB81	1.98	0.46
4:Q:88:PHE:HZ	13:Z:19:LEU:HD21	1.80	0.46
6:S:94:HIS:CG	6:S:95:GLN:N	2.82	0.46
4:D:109:HIS:HD2	29:D:2152:HOH:O	1.99	0.45
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:33:LEU:HD13	9:V:31:PHE:CD1	2.52	0.45
6:S:94:HIS:HD2	6:S:95:GLN:N	2.13	0.45
1:A:430:PHE:CE1	19:A:521:TGL:CB2	2.97	0.45
5:R:11:PHE:HB3	26:R:1230:PSC:H073	1.98	0.45
5:R:67:ILE:O	5:R:70:VAL:HG12	2.16	0.45
1:N:254:ILE:HD12	1:N:254:ILE:HG23	1.60	0.45
20:N:1524:PGV:H152	20:N:1524:PGV:H321	1.97	0.45
2:B:78:LEU:CB	2:B:79:PRO:CD	2.95	0.45
22:J:60:CHD:H112	22:J:60:CHD:H12A	1.44	0.45
1:N:344:PHE:CD1	1:N:344:PHE:C	2.95	0.45
7:T:8:HIS:O	7:T:9:GLY:C	2.60	0.45
3:C:173:PHE:CD2	3:C:173:PHE:C	2.94	0.45
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.82	0.45
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.52	0.45
22:P:1271:CHD:H112	22:P:1271:CHD:H12A	1.51	0.45
25:T:1269:CDL:H562	25:T:1269:CDL:H762	1.98	0.45
9:V:73:LYS:HD2	9:V:73:LYS:HA	1.64	0.45
12:L:6:GLY:O	12:L:7:PRO:C	2.59	0.45
26:R:1230:PSC:H212	26:R:1230:PSC:C1	2.45	0.45
7:T:2:SER:CB	24:T:263:PEK:H302	2.43	0.45
1:N:215:LEU:HD11	24:P:1264:PEK:H271	1.98	0.45
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.16	0.45
22:C:525:CHD:H112	22:C:525:CHD:H12A	1.56	0.45
18:N:515:HEA:HHC	18:N:515:HEA:H122	1.99	0.45
3:P:22:LEU:O	3:P:26:LEU:HG	2.17	0.45
1:A:297:MET:CE	1:A:297:MET:HB2	2.47	0.45
1:A:396:TRP:O	1:A:397:PHE:C	2.57	0.45
22:B:1086:CHD:H112	22:B:1086:CHD:H12A	1.68	0.45
26:E:230:PSC:H061	9:I:10:ARG:HE	1.80	0.45
4:D:107:ILE:HG21	4:D:107:ILE:HD13	1.75	0.44
3:P:226:HIS:HE1	25:P:1270:CDL:HB32	1.81	0.44
24:T:263:PEK:H21	24:T:263:PEK:H5	1.83	0.44
1:A:417:MET:HE1	18:A:515:HEA:H263	1.98	0.44
12:L:13:PHE:HB3	19:L:522:TGL:HG12	2.00	0.44
2:O:22:HIS:CE1	9:V:43:ARG:HG2	2.53	0.44
1:N:172:LYS:NZ	1:N:178:GLN:NE2	2.65	0.44
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.44
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.99	0.44
9:V:68:ILE:HD11	9:V:69:PHE:CZ	2.53	0.44
1:A:92:MET:HE1	1:A:164:PHE:CD2	2.51	0.44
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:LEU:HD23	3:C:22:LEU:HA	1.83	0.44
25:C:270:CDL:HB21	25:C:270:CDL:PA1	2.57	0.44
8:H:44:THR:O	8:H:45:ALA:O	2.36	0.44
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.00	0.44
4:Q:40:LEU:HD22	4:Q:58:GLU:CD	2.43	0.44
3:P:58:TRP:CG	20:P:1267:PGV:H41	2.52	0.44
4:Q:17:VAL:O	4:Q:25:PRO:HG3	2.18	0.44
20:A:524:PGV:O14	20:A:524:PGV:C02	2.61	0.44
3:C:224:LYS:HD2	25:C:270:CDL:HB31	1.98	0.44
6:S:55:LYS:HA	6:S:74:LEU:O	2.18	0.44
6:F:76:LYS:HD2	6:F:93:PRO:HG3	2.00	0.44
24:G:1263:PEK:O13	3:P:80:ARG:HD2	2.17	0.44
25:T:1269:CDL:H561	25:T:1269:CDL:H592	1.26	0.44
4:Q:88:PHE:CZ	13:Z:19:LEU:HD21	2.53	0.44
4:D:31:LYS:HG2	29:D:4601:HOH:O	2.18	0.43
9:I:52:ARG:NH1	29:I:4726:HOH:O	2.51	0.43
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.00	0.43
1:N:449:MET:SD	2:O:5:MET:HG2	2.58	0.43
19:O:1521:TGL:H222	19:O:1521:TGL:H251	1.44	0.43
2:B:22:HIS:CE1	9:I:44:LYS:HG3	2.53	0.43
29:B:2353:HOH:O	19:D:523:TGL:HC61	2.18	0.43
25:C:270:CDL:H642	25:C:270:CDL:H242	2.00	0.43
6:F:92:VAL:HG23	6:F:92:VAL:O	2.17	0.43
8:H:39:CYS:O	8:H:40:GLU:C	2.58	0.43
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.19	0.43
5:R:11:PHE:CB	26:R:1230:PSC:H073	2.48	0.43
4:D:31:LYS:NZ	29:D:4344:HOH:O	2.40	0.43
1:A:299:VAL:CG2	2:B:84:LEU:HG	2.48	0.43
24:G:265:PEK:H361	25:G:269:CDL:H273	2.00	0.43
19:O:1523:TGL:HB22	4:Q:78:TRP:HA	2.01	0.43
4:Q:52:SER:O	4:Q:53:ILE:C	2.60	0.43
5:R:80:GLU:H	5:R:80:GLU:CD	2.26	0.43
6:S:44:GLU:H	6:S:44:GLU:CD	2.26	0.43
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.59	0.43
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.00	0.43
7:T:17:ARG:CD	29:T:3302:HOH:O	2.58	0.43
19:A:521:TGL:H121	19:A:521:TGL:H292	1.79	0.43
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.60	0.43
3:P:55:TYR:HE1	25:P:1270:CDL:H521	1.81	0.43
12:Y:20:ARG:HH21	19:Y:1522:TGL:HC32	1.84	0.43
1:A:383:MET:O	1:A:387:PHE:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.19	0.43
3:C:91:VAL:HG22	24:T:263:PEK:H132	2.01	0.43
10:J:50:LEU:HD22	10:J:50:LEU:C	2.43	0.43
2:O:98:LYS:HB2	2:O:109:GLU:HB2	2.01	0.43
3:P:249:TRP:HD1	29:P:3171:HOH:O	2.00	0.43
10:W:40:LEU:HD12	22:W:1060:CHD:H183	2.01	0.43
22:W:1060:CHD:H232	22:W:1060:CHD:H211	1.69	0.43
13:Z:11:SER:OG	13:Z:14:GLU:HG3	2.19	0.43
24:G:265:PEK:H361	25:G:269:CDL:C27	2.49	0.43
20:H:268:PGV:H231	20:H:268:PGV:H202	1.88	0.43
5:R:31:LYS:HE3	6:S:83:PRO:O	2.18	0.43
13:Z:32:TRP:N	28:Z:1526:DMU:H1	2.34	0.43
1:N:406:ASN:HD21	20:N:1524:PGV:C2	2.32	0.43
18:N:515:HEA:HHA	18:N:515:HEA:HAD1	1.79	0.43
2:O:161:HIS:HB2	2:O:174:ALA:HB3	2.00	0.43
20:P:1267:PGV:C16	20:P:1267:PGV:H12	2.45	0.43
6:S:87:THR:HG21	29:S:4604:HOH:O	2.19	0.43
7:T:3:ALA:O	7:T:4:ALA:HB2	2.17	0.43
18:A:515:HEA:C16	18:A:515:HEA:H272	2.48	0.43
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.54	0.43
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.01	0.43
3:C:19:THR:O	3:C:23:SER:HB3	2.19	0.42
18:N:515:HEA:HBC1	18:N:515:HEA:CMC	2.49	0.42
29:O:3250:HOH:O	4:Q:129:ALA:HB2	2.18	0.42
7:G:63:GLY:HA2	28:G:272:DMU:H34	2.01	0.42
12:L:34:ALA:O	12:L:35:ALA:C	2.61	0.42
1:N:468:MET:HE1	18:N:515:HEA:H212	2.02	0.42
2:O:113:TYR:HD1	8:U:58:ARG:NH2	2.17	0.42
2:O:116:LEU:HD21	2:O:226:MET:HG2	2.01	0.42
2:B:108:TYR:O	2:B:117:SER:HA	2.18	0.42
1:N:290:HIS:HD2	1:N:291:HIS:CD2	2.35	0.42
8:U:50:VAL:O	8:U:50:VAL:CG1	2.68	0.42
26:E:230:PSC:H251	26:E:230:PSC:H221	1.70	0.42
1:N:18:LEU:CD2	19:Y:1522:TGL:HB21	2.49	0.42
2:O:82:ARG:HH11	2:O:86:MET:CE	2.32	0.42
3:P:8:TYR:CE1	3:P:74:ALA:HB1	2.54	0.42
25:P:1270:CDL:H641	25:P:1270:CDL:H612	1.75	0.42
24:T:263:PEK:H361	24:T:263:PEK:H332	1.61	0.42
19:A:521:TGL:OB1	19:A:521:TGL:CB4	2.53	0.42
2:B:1:FME:HE3	4:D:123:MET:CE	2.47	0.42
13:Z:17:ILE:HD13	13:Z:17:ILE:HG21	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:MET:HB3	1:A:189:MET:HE2	1.74	0.42
1:N:86:MET:HB3	1:N:182:PRO:HG2	2.02	0.42
20:N:1524:PGV:H92	4:Q:84:ALA:HB2	2.01	0.42
2:O:100:MET:HE3	2:O:157:GLU:HG3	2.01	0.42
8:U:50:VAL:O	8:U:50:VAL:HG12	2.20	0.42
4:D:20:ARG:HG3	29:D:4139:HOH:O	2.19	0.42
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.94	0.42
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.42
18:A:515:HEA:HA	18:A:515:HEA:HAD1	1.73	0.42
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.93	0.42
4:Q:91:PHE:CD2	4:Q:91:PHE:C	2.97	0.42
5:R:8:ASP:HA	26:R:1230:PSC:H071	2.02	0.42
3:C:76:GLN:O	3:C:80:ARG:HG3	2.20	0.42
5:E:23:ASP:OD2	5:E:23:ASP:N	2.48	0.42
3:C:12:ASN:O	3:C:13:PRO:C	2.62	0.42
1:A:334:TRP:HB2	19:D:523:TGL:HG11	2.01	0.41
3:C:191:GLY:HA3	29:G:2156:HOH:O	2.18	0.41
22:C:525:CHD:H42	3:P:127:LEU:HD21	2.02	0.41
2:O:1:FME:HE1	2:O:133:LEU:HD22	2.02	0.41
3:P:208:VAL:HG22	3:P:245:VAL:CG1	2.51	0.41
1:A:240:HIS:HB3	1:A:241:PRO:HD3	2.02	0.41
2:B:20:LEU:HA	2:B:20:LEU:HD23	1.85	0.41
22:C:271:CHD:H112	22:C:271:CHD:H12A	1.52	0.41
1:N:69:MET:CE	1:N:70:VAL:CG2	2.98	0.41
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.20	0.41
6:S:95:GLN:CG	29:S:4406:HOH:O	2.41	0.41
7:T:37:LEU:HD23	7:T:38:HIS:CE1	2.56	0.41
25:C:270:CDL:H861	25:C:270:CDL:H831	1.92	0.41
1:N:409:TRP:CE2	20:N:1524:PGV:H61	2.55	0.41
1:A:207:THR:O	1:A:211:THR:HG23	2.19	0.41
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.85	0.41
3:C:246:ASP:HB2	29:C:4076:HOH:O	2.20	0.41
11:K:24:PHE:O	11:K:28:VAL:HG12	2.21	0.41
3:P:144:ILE:HG21	3:P:144:ILE:HD13	1.80	0.41
1:A:71:MET:HE3	1:A:245:ILE:HG21	2.02	0.41
3:C:103:HIS:ND1	22:C:525:CHD:O26	2.54	0.41
6:F:53:THR:HB	6:F:54:ASN:H	1.66	0.41
20:H:268:PGV:H52	20:H:268:PGV:H21	1.94	0.41
1:N:35:LEU:HB3	28:Z:1526:DMU:H24	2.03	0.41
25:C:270:CDL:PA1	25:C:270:CDL:CB2	3.09	0.41
26:E:230:PSC:H042	26:E:230:PSC:H062	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:16:ILE:HD12	2:O:16:ILE:HG23	1.82	0.41
3:P:65:SER:HB2	20:P:1267:PGV:H041	2.03	0.41
4:Q:33:LEU:HA	4:Q:37:GLN:HE21	1.84	0.41
4:Q:130:PRO:HA	4:Q:135:SER:HB2	2.02	0.41
1:A:344:PHE:CD1	1:A:344:PHE:C	2.99	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.41
1:N:437:PRO:HG2	1:N:440:TYR:CE1	2.55	0.41
19:O:1523:TGL:OB1	19:O:1523:TGL:CG3	2.68	0.41
9:V:29:LEU:HA	9:V:29:LEU:HD12	1.79	0.41
6:F:64:GLU:O	6:F:65:ASP:CB	2.69	0.41
1:N:109:PHE:HB3	19:Y:1522:TGL:H122	2.03	0.41
3:P:224:LYS:CE	25:P:1270:CDL:HB31	2.49	0.41
1:A:37:ILE:HG21	18:A:515:HEA:HMA	2.02	0.41
20:A:522:PGV:H42	20:A:522:PGV:H251	2.02	0.41
3:C:16:TRP:N	3:C:17:PRO:CD	2.84	0.41
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.21	0.41
2:O:103:GLN:HB3	2:O:104:TRP:CE2	2.55	0.41
4:Q:11:TYR:CD1	4:Q:11:TYR:C	2.98	0.41
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.19	0.41
4:Q:127:LYS:HD2	29:V:3384:HOH:O	2.20	0.41
7:T:5:LYS:CB	24:T:263:PEK:C37	2.89	0.41
1:N:106:PRO:N	1:N:107:PRO:CD	2.84	0.41
2:O:141:ARG:HG3	9:V:70:GLN:NE2	2.36	0.41
7:T:46:ALA:HB1	29:T:4681:HOH:O	2.21	0.41
1:N:69:MET:CE	1:N:70:VAL:HG23	2.51	0.40
1:N:76:GLY:O	1:N:80:ASN:HB2	2.21	0.40
1:N:431:LEU:HD21	1:N:450:TRP:HB2	2.03	0.40
5:R:65:VAL:HG13	5:R:101:PRO:HG3	2.03	0.40
9:V:31:PHE:O	9:V:32:ALA:C	2.64	0.40
1:A:181:THR:HA	1:A:182:PRO:HD3	1.94	0.40
1:A:311:ILE:HD13	1:A:311:ILE:HG21	1.85	0.40
7:G:7:ASP:HA	1:N:178:GLN:HG2	2.03	0.40
25:G:269:CDL:H242	25:G:269:CDL:C53	2.47	0.40
2:O:139:ASP:OD2	2:O:139:ASP:N	2.52	0.40
1:A:1:FME:HE2	1:A:1:FME:HA	2.04	0.40
2:O:58:ALA:C	2:O:60:GLU:H	2.29	0.40
3:P:59:ARG:HG3	25:P:1270:CDL:H512	2.03	0.40
2:B:58:ALA:O	2:B:62:GLU:HG3	2.21	0.40
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.57	0.40
19:D:523:TGL:HB92	19:D:523:TGL:H121	1.47	0.40
8:H:23:GLN:HG3	29:H:4130:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:4:LYS:HB2	13:M:5:PRO:HD2	2.03	0.40
3:P:149:HIS:O	3:P:153:GLU:HG3	2.22	0.40
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.56	0.40
19:Y:1522:TGL:CC2	19:Y:1522:TGL:CC6	2.82	0.40
18:A:515:HEA:HHC	18:A:515:HEA:C12	2.51	0.40
20:N:1524:PGV:H02	20:N:1524:PGV:O14	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	490 (96%)	22 (4%)	0	100	100
2	B	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	30	21
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	30	21
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	129 (91%)	12 (8%)	1 (1%)	18	10
5	E	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
5	R	102/109 (94%)	102 (100%)	0	0	100	100
6	F	91/98 (93%)	87 (96%)	2 (2%)	2 (2%)	5	1
6	S	91/98 (93%)	85 (93%)	5 (6%)	1 (1%)	11	4
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	1	0
8	H	73/85 (86%)	69 (94%)	1 (1%)	3 (4%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	U	73/85 (86%)	66 (90%)	5 (7%)	2 (3%)	4	1
9	I	69/73 (94%)	66 (96%)	3 (4%)	0	100	100
9	V	69/73 (94%)	67 (97%)	2 (3%)	0	100	100
10	J	55/59 (93%)	55 (100%)	0	0	100	100
10	W	55/59 (93%)	55 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	4	1
All	All	3478/3614 (96%)	3328 (96%)	128 (4%)	22 (1%)	21	12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
8	H	45	ALA
8	H	46	LYS
6	S	94	HIS
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	U	45	ALA
6	F	94	HIS
8	H	47	GLY
8	U	46	LYS
13	Z	41	LYS
7	G	6	GLY
7	G	37	LEU
4	Q	34	SER
7	T	3	ALA
7	T	6	GLY
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%)	415 (97%)	11 (3%)	40	33
1	N	426/426 (100%)	413 (97%)	13 (3%)	35	26
2	B	210/210 (100%)	198 (94%)	12 (6%)	18	8
2	O	210/210 (100%)	196 (93%)	14 (7%)	15	5
3	C	224/226 (99%)	216 (96%)	8 (4%)	31	21
3	P	224/226 (99%)	216 (96%)	8 (4%)	31	21
4	D	128/129 (99%)	126 (98%)	2 (2%)	55	52
4	Q	128/129 (99%)	121 (94%)	7 (6%)	19	8
5	E	91/95 (96%)	89 (98%)	2 (2%)	45	40
5	R	91/95 (96%)	87 (96%)	4 (4%)	25	15
6	F	79/81 (98%)	73 (92%)	6 (8%)	12	4
6	S	79/81 (98%)	73 (92%)	6 (8%)	12	4
7	G	67/68 (98%)	59 (88%)	8 (12%)	5	1
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	2
8	H	67/75 (89%)	63 (94%)	4 (6%)	17	7
8	U	67/75 (89%)	62 (92%)	5 (8%)	12	4
9	I	56/57 (98%)	50 (89%)	6 (11%)	6	1
9	V	56/57 (98%)	49 (88%)	7 (12%)	4	1
10	J	48/50 (96%)	47 (98%)	1 (2%)	47	41
10	W	48/50 (96%)	47 (98%)	1 (2%)	47	41
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	10
11	X	39/46 (85%)	36 (92%)	3 (8%)	12	3
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	33
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	3
13	M	37/38 (97%)	31 (84%)	6 (16%)	2	0
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3022/3082 (98%)	2873 (95%)	149 (5%)	22	11

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	ARG
1	A	53	ILE
1	A	115	SER
1	A	138	HIS
1	A	180	GLN
1	A	278	MET
1	A	333	LYS
1	A	369	ASP
1	A	484	THR
1	A	504	THR
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	129	LYS
2	B	167	SER
3	C	23	SER
3	C	40	MET
3	C	77	LYS
3	C	110	PRO
3	C	127	LEU
3	C	159	MET
3	C	223	LEU
3	C	230	ASN
4	D	51	LEU
4	D	127	LYS
5	E	41	LEU
5	E	90	ARG
6	F	37	LYS
6	F	48	LEU

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Mol	Chain	Res	Type
6	F	53	THR
6	F	78	GLU
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	17	ARG
7	G	33	LEU
7	G	36	TRP
7	G	38	HIS
7	G	43	GLU
7	G	74	ARG
7	G	84	LYS
8	H	40	GLU
8	H	60	TYR
8	H	61	LYS
8	H	84	LYS
9	I	8	GLN
9	I	15	ARG
9	I	21	ILE
9	I	26	MET
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU
11	K	47	ARG
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
1	N	38	ARG
1	N	115	SER
1	N	128	VAL
1	N	138	HIS
1	N	180	GLN
1	N	278	MET
1	N	361	SER
1	N	369	ASP
1	N	394	VAL
1	N	484	THR

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Mol	Chain	Res	Type
1	N	485	VAL
1	N	504	THR
1	N	512	ASN
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	115	ASP
2	O	116	LEU
2	O	148	MET
2	O	217	LYS
2	O	227	LEU
3	P	29	SER
3	P	33	MET
3	P	40	MET
3	P	127	LEU
3	P	159	MET
3	P	180	GLU
3	P	223	LEU
3	P	230	ASN
4	Q	5	VAL
4	Q	6	VAL
4	Q	9	GLU
4	Q	10	ASP
4	Q	31	LYS
4	Q	51	LEU
4	Q	63	LYS
5	R	79	LYS
5	R	90	ARG
5	R	108	LYS
5	R	109	VAL
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	80	GLN
6	S	87	THR
6	S	95	GLN

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Mol	Chain	Res	Type
7	T	2	SER
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
7	T	74	ARG
7	T	84	LYS
8	U	29	CYS
8	U	41	LYS
8	U	44	THR
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	26	MET
9	V	29	LEU
9	V	33	THR
9	V	36	LYS
9	V	65	LYS
9	V	73	LYS
10	W	50	LEU
11	X	23	THR
11	X	47	ARG
11	X	54	ARG
12	Y	11	ILE
12	Y	16	GLU
12	Y	20	ARG
13	Z	13	LYS
13	Z	34	LEU
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	55	ASN
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	22	HIS
2	B	91	ASN

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Mol	Chain	Res	Type
2	B	181	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	149	HIS
3	C	161	GLN
3	C	230	ASN
4	D	37	GLN
4	D	76	ASN
4	D	101	HIS
4	D	109	HIS
5	E	94	ASN
7	G	76	ASN
8	H	12	GLN
9	I	8	GLN
9	I	53	ASN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	55	ASN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	406	ASN
1	N	413	HIS
1	N	491	ASN
1	N	503	HIS
1	N	512	ASN
2	O	10	GLN
2	O	59	GLN
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
3	P	161	GLN
4	Q	32	ASN
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	28	GLN

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Mol	Chain	Res	Type
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
8	U	31	GLN
8	U	32	ASN
10	W	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	O	1	2	8,9,10	0.80	0	8,9,11	5.26	3 (37%)
7	TPO	T	11	7	8,10,11	2.08	6 (75%)	10,14,16	1.98	2 (20%)
2	FME	B	1	2	8,9,10	1.65	3 (37%)	8,9,11	6.37	4 (50%)
1	FME	A	1	1	8,9,10	0.80	0	8,9,11	4.56	3 (37%)
1	FME	N	1	1	8,9,10	0.74	0	8,9,11	5.91	5 (62%)
7	TPO	G	11	7	8,10,11	2.23	4 (50%)	10,14,16	2.37	4 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	T	11	7	-	5/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	4.18	1.63	1.50
7	T	11	TPO	P-O1P	3.48	1.61	1.50
2	B	1	FME	O1-CN	-2.65	1.11	1.22
7	G	11	TPO	P-O2P	2.44	1.63	1.54
2	B	1	FME	CG-SD	-2.38	1.69	1.81
7	G	11	TPO	P-OG1	2.28	1.63	1.59
7	T	11	TPO	P-O3P	2.27	1.63	1.54
2	B	1	FME	CB-CG	2.26	1.60	1.51
7	T	11	TPO	P-O2P	2.12	1.62	1.54
7	T	11	TPO	P-OG1	2.10	1.63	1.59
7	T	11	TPO	CG2-CB	2.06	1.56	1.51
7	T	11	TPO	O-C	2.01	1.27	1.20
7	G	11	TPO	O-C	2.01	1.27	1.20

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.38	97.64	122.82
1	N	1	FME	CA-N-CN	-15.33	99.25	122.82
2	O	1	FME	CA-N-CN	-13.71	101.73	122.82
1	A	1	FME	CA-N-CN	-12.21	104.05	122.82
2	B	1	FME	O1-CN-N	5.35	139.14	125.32
7	T	11	TPO	CG2-CB-CA	4.93	122.86	113.26
1	N	1	FME	CB-CA-N	4.90	119.44	110.52
7	G	11	TPO	CG2-CB-CA	4.68	122.37	113.26
7	G	11	TPO	O2P-P-OG1	4.04	121.61	105.85
2	O	1	FME	CG-CB-CA	-3.86	101.06	112.87
2	B	1	FME	CB-CA-N	-3.30	104.50	110.52
1	N	1	FME	CE-SD-CG	3.21	116.95	100.32
2	O	1	FME	C-CA-N	3.19	115.66	109.50
2	B	1	FME	CB-CG-SD	-3.08	93.50	113.82
1	A	1	FME	CE-SD-CG	2.83	114.99	100.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	11	TPO	O-C-CA	-2.54	118.25	124.77
1	A	1	FME	O-C-CA	-2.34	118.75	124.77
7	G	11	TPO	OG1-P-O1P	-2.29	101.19	109.33
1	N	1	FME	O1-CN-N	2.26	131.15	125.32
7	G	11	TPO	O-C-CA	-2.12	119.31	124.77
1	N	1	FME	O-C-CA	-2.05	119.49	124.77

There are no chirality outliers.

All (19) 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
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
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
7	T	11	TPO	O-C-CA-CB
2	O	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
1	N	1	FME	CB-CG-SD-CE
7	T	11	TPO	CB-OG1-P-O3P
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 46 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
18	HEA	N	515	1	67,67,67	1.96	17 (25%)	81,103,103	2.43	28 (34%)
24	PEK	T	1265	-	52,52,52	1.24	2 (3%)	55,57,57	1.39	7 (12%)
24	PEK	G	1263	-	52,52,52	1.18	2 (3%)	55,57,57	1.35	5 (9%)
15	PER	N	520	18,14	1,1,1	1.97	0	-		
20	PGV	H	268	-	50,50,50	1.35	2 (4%)	53,56,56	1.52	8 (15%)
26	PSC	E	230	-	51,51,51	1.33	3 (5%)	57,59,59	1.17	5 (8%)
22	CHD	W	1060	-	32,32,32	0.86	0	51,51,51	5.01	35 (68%)
26	PSC	R	1230	-	51,51,51	1.22	3 (5%)	57,59,59	1.20	5 (8%)
28	DMU	P	1272	-	34,34,34	1.33	3 (8%)	45,45,45	3.12	22 (48%)
22	CHD	O	229	-	32,32,32	1.41	5 (15%)	51,51,51	5.54	36 (70%)
24	PEK	G	265	-	52,52,52	1.81	5 (9%)	55,57,57	1.39	6 (10%)
19	TGL	O	1521	-	62,62,62	1.39	6 (9%)	65,65,65	1.59	12 (18%)
18	HEA	N	516	1,15	67,67,67	1.91	17 (25%)	81,103,103	2.43	32 (39%)
20	PGV	A	522	-	50,50,50	1.10	3 (6%)	53,56,56	1.52	7 (13%)
24	PEK	C	264	-	52,52,52	0.99	3 (5%)	55,57,57	1.50	11 (20%)
19	TGL	L	522	-	62,62,62	1.66	7 (11%)	65,65,65	1.97	18 (27%)
21	CUA	B	228	2	0,1,1	-	-	-		
22	CHD	B	1086	-	32,32,32	1.33	4 (12%)	51,51,51	5.69	35 (68%)
28	DMU	Z	1526	-	34,34,34	1.10	3 (8%)	45,45,45	3.38	23 (51%)
24	PEK	P	1264	-	52,52,52	1.04	4 (7%)	55,57,57	1.70	10 (18%)
25	CDL	T	1269	-	99,99,99	1.47	12 (12%)	105,111,111	1.43	18 (17%)
18	HEA	A	516	1,15	67,67,67	2.07	23 (34%)	81,103,103	2.59	36 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CHD	J	60	-	32,32,32	0.94	1 (3%)	51,51,51	4.88	37 (72%)
28	DMU	G	272	-	34,34,34	1.33	3 (8%)	45,45,45	3.51	24 (53%)
24	PEK	T	263	-	52,52,52	1.21	2 (3%)	55,57,57	1.39	6 (10%)
20	PGV	N	1266	-	50,50,50	0.90	2 (4%)	53,56,56	1.62	7 (13%)
22	CHD	C	271	-	32,32,32	1.31	3 (9%)	51,51,51	5.28	36 (70%)
28	DMU	M	526	-	34,34,34	0.94	1 (2%)	45,45,45	3.24	23 (51%)
20	PGV	N	1268	-	50,50,50	1.24	3 (6%)	53,56,56	1.48	6 (11%)
25	CDL	P	1270	-	99,99,99	1.50	14 (14%)	105,111,111	1.49	14 (13%)
25	CDL	C	270	-	99,99,99	1.48	15 (15%)	105,111,111	1.60	16 (15%)
22	CHD	P	1271	-	32,32,32	0.92	2 (6%)	51,51,51	5.25	30 (58%)
18	HEA	A	515	1	67,67,67	1.96	20 (29%)	81,103,103	2.70	38 (46%)
22	CHD	C	525	-	32,32,32	1.67	8 (25%)	51,51,51	5.48	38 (74%)
15	PER	A	520	18,14	1,1,1	1.97	0	-	-	-
20	PGV	P	1267	-	50,50,50	0.91	2 (4%)	53,56,56	1.46	10 (18%)
19	TGL	A	521	-	62,62,62	1.28	7 (11%)	65,65,65	2.04	12 (18%)
19	TGL	Y	1522	-	62,62,62	1.60	6 (9%)	65,65,65	1.63	16 (24%)
21	CUA	O	228	2	0,1,1	-	-	-	-	-
19	TGL	D	523	-	62,62,62	1.65	7 (11%)	65,65,65	1.63	16 (24%)
20	PGV	N	1524	-	50,50,50	1.07	2 (4%)	53,56,56	1.55	6 (11%)
20	PGV	C	267	-	50,50,50	0.98	2 (4%)	53,56,56	1.31	5 (9%)
19	TGL	O	1523	-	62,62,62	1.47	6 (9%)	65,65,65	1.46	10 (15%)
22	CHD	P	1525	-	32,32,32	1.47	4 (12%)	51,51,51	5.58	37 (72%)
25	CDL	G	269	-	99,99,99	1.57	13 (13%)	105,111,111	1.53	17 (16%)
20	PGV	A	524	-	50,50,50	1.24	3 (6%)	53,56,56	1.61	10 (18%)

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
18	HEA	N	515	1	-	7/36/76/76	-
24	PEK	T	1265	-	-	32/56/56/56	-
24	PEK	G	1263	-	-	31/56/56/56	-
20	PGV	H	268	-	-	34/55/55/55	-
26	PSC	E	230	-	-	39/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	W	1060	-	2/2/12/12	6/9/74/74	0/4/4/4
28	DMU	P	1272	-	4/4/10/10	10/19/59/59	0/2/2/2
26	PSC	R	1230	-	-	29/55/55/55	-
22	CHD	O	229	-	-	2/9/74/74	0/4/4/4
24	PEK	G	265	-	-	29/56/56/56	-
19	TGL	O	1521	-	-	32/65/65/65	-
18	HEA	N	516	1,15	-	7/36/76/76	-
20	PGV	A	522	-	-	16/55/55/55	-
28	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
22	CHD	B	1086	-	1/1/12/12	2/9/74/74	0/4/4/4
19	TGL	L	522	-	-	34/65/65/65	-
24	PEK	C	264	-	-	21/56/56/56	-
24	PEK	P	1264	-	-	19/56/56/56	-
28	DMU	G	272	-	5/5/10/10	10/19/59/59	0/2/2/2
18	HEA	A	516	1,15	-	7/36/76/76	-
22	CHD	J	60	-	2/2/12/12	6/9/74/74	0/4/4/4
25	CDL	T	1269	-	-	58/110/110/110	-
24	PEK	T	263	-	-	28/56/56/56	-
20	PGV	N	1266	-	-	15/55/55/55	-
22	CHD	C	271	-	1/1/12/12	6/9/74/74	0/4/4/4
28	DMU	M	526	-	4/4/10/10	10/19/59/59	0/2/2/2
20	PGV	N	1268	-	-	26/55/55/55	-
25	CDL	P	1270	-	-	61/110/110/110	-
25	CDL	C	270	-	-	65/110/110/110	-
22	CHD	P	1271	-	1/1/12/12	4/9/74/74	0/4/4/4
18	HEA	A	515	1	-	10/36/76/76	-
22	CHD	C	525	-	-	2/9/74/74	0/4/4/4
20	PGV	P	1267	-	-	15/55/55/55	-
19	TGL	A	521	-	-	31/65/65/65	-
19	TGL	Y	1522	-	-	40/65/65/65	-
19	TGL	D	523	-	-	34/65/65/65	-
20	PGV	N	1524	-	-	32/55/55/55	-
20	PGV	C	267	-	-	13/55/55/55	-
19	TGL	O	1523	-	-	31/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	P	1525	-	-	4/9/74/74	0/4/4/4
25	CDL	G	269	-	-	66/110/110/110	-
20	PGV	A	524	-	-	27/55/55/55	-

All (250) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	265	PEK	C9-C8	7.99	1.77	1.31
19	L	522	TGL	OG2-CB1	6.61	1.52	1.34
19	Y	1522	TGL	OG2-CB1	6.56	1.52	1.34
19	D	523	TGL	OG1-CA1	6.47	1.52	1.33
20	H	268	PGV	O01-C1	6.43	1.52	1.34
18	N	515	HEA	FE-NA	6.31	2.16	1.95
25	G	269	CDL	OB6-CB5	6.05	1.51	1.34
18	A	516	HEA	FE-NC	5.98	2.14	1.95
24	T	1265	PEK	O01-C1	5.92	1.51	1.34
24	G	1263	PEK	O03-C21	5.59	1.49	1.33
25	C	270	CDL	OA8-CA7	5.56	1.49	1.33
25	G	269	CDL	OA6-CA5	5.52	1.49	1.34
20	N	1268	PGV	O01-C1	5.48	1.49	1.34
25	P	1270	CDL	OA8-CA7	5.44	1.49	1.33
19	O	1523	TGL	OG2-CB1	5.38	1.49	1.34
24	T	263	PEK	O03-C21	5.35	1.48	1.33
28	P	1272	DMU	O16-C6	5.35	1.49	1.40
18	A	516	HEA	CMD-C2D	5.28	1.61	1.50
26	E	230	PSC	O01-C1	5.24	1.49	1.34
19	O	1523	TGL	OG1-CA1	5.23	1.48	1.33
19	L	522	TGL	OG1-CA1	5.21	1.48	1.33
24	G	265	PEK	O01-C1	5.16	1.48	1.34
19	L	522	TGL	OG3-CC1	5.16	1.48	1.33
20	A	524	PGV	O03-C19	5.06	1.48	1.33
18	N	515	HEA	FE-NC	5.05	2.11	1.95
19	Y	1522	TGL	OG3-CC1	5.03	1.48	1.33
19	Y	1522	TGL	OG1-CA1	5.03	1.48	1.33
19	O	1521	TGL	OG2-CB1	5.01	1.48	1.34
20	H	268	PGV	O03-C19	4.98	1.47	1.33
18	A	515	HEA	CHD-C1D	4.97	1.48	1.38
26	E	230	PSC	O03-C19	4.96	1.47	1.33
28	G	272	DMU	O16-C6	4.94	1.48	1.40
25	T	1269	CDL	OB6-CB5	4.93	1.48	1.34
18	N	516	HEA	CHD-C1D	4.92	1.48	1.38
25	T	1269	CDL	OA6-CA5	4.89	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	265	PEK	O03-C21	4.87	1.47	1.33
19	D	523	TGL	OB1-CB1	4.87	1.37	1.22
24	T	1265	PEK	O03-C21	4.86	1.47	1.33
19	O	1521	TGL	OG1-CA1	4.81	1.47	1.33
24	T	263	PEK	O01-C1	4.81	1.47	1.34
25	G	269	CDL	OB8-CB7	4.78	1.47	1.33
25	P	1270	CDL	OB8-CB7	4.77	1.47	1.33
19	O	1523	TGL	OG3-CC1	4.74	1.47	1.33
25	T	1269	CDL	OB8-CB7	4.63	1.46	1.33
18	A	515	HEA	FE-NC	4.57	2.10	1.95
19	D	523	TGL	OG3-CC1	4.57	1.46	1.33
25	G	269	CDL	OA8-CA7	4.54	1.46	1.33
18	N	516	HEA	FE-NA	4.54	2.10	1.95
20	N	1524	PGV	O03-C19	4.53	1.46	1.33
25	P	1270	CDL	OA6-CA5	4.53	1.47	1.34
25	C	270	CDL	OA6-CA5	4.51	1.47	1.34
26	R	1230	PSC	O01-C1	4.50	1.47	1.34
18	A	515	HEA	CHA-C1A	4.49	1.47	1.38
22	P	1525	CHD	C13-C14	-4.46	1.48	1.55
19	D	523	TGL	OG2-CB1	4.45	1.46	1.34
20	A	524	PGV	O01-C1	4.40	1.46	1.34
18	N	515	HEA	CHA-C1A	4.40	1.47	1.38
19	L	522	TGL	C20-CA9	-4.38	1.30	1.51
18	N	515	HEA	CHC-C4B	4.36	1.47	1.38
18	A	515	HEA	O11-C11	4.31	1.52	1.42
19	A	521	TGL	OG1-CA1	4.31	1.45	1.33
24	G	265	PEK	C10-C9	4.30	1.81	1.51
22	C	525	CHD	C13-C12	-4.26	1.48	1.54
18	N	516	HEA	CHC-C4B	4.25	1.47	1.38
20	N	1268	PGV	O03-C19	4.24	1.45	1.33
18	A	515	HEA	CHC-C1C	4.24	1.48	1.39
19	A	521	TGL	OG2-CB1	4.21	1.46	1.34
25	P	1270	CDL	OB6-CB5	4.17	1.46	1.34
20	N	1524	PGV	O01-C1	4.15	1.46	1.34
24	P	1264	PEK	O03-C01	-4.14	1.35	1.45
25	T	1269	CDL	C59-C58	-4.10	1.31	1.51
18	N	515	HEA	CMD-C2D	4.10	1.59	1.50
25	G	269	CDL	C59-C58	-4.06	1.31	1.51
26	R	1230	PSC	O03-C19	4.04	1.45	1.33
25	T	1269	CDL	OA8-CA7	4.03	1.45	1.33
18	A	515	HEA	C3A-C4A	-4.02	1.39	1.46
18	A	515	HEA	FE-NA	4.02	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	E	230	PSC	C13-C12	4.01	1.54	1.31
24	G	1263	PEK	O01-C1	4.00	1.45	1.34
19	O	1521	TGL	OG3-CC1	3.99	1.45	1.33
19	O	1521	TGL	C10-CB9	-3.98	1.32	1.51
24	C	264	PEK	O01-C1	3.98	1.45	1.34
28	Z	1526	DMU	C3-C4	-3.89	1.42	1.52
25	T	1269	CDL	C62-C61	-3.88	1.32	1.51
20	A	522	PGV	O01-C1	3.88	1.45	1.34
18	N	516	HEA	FE-NB	3.88	2.06	1.94
19	Y	1522	TGL	C20-CA9	-3.88	1.32	1.51
20	A	522	PGV	O03-C19	3.87	1.44	1.33
26	R	1230	PSC	C13-C12	3.87	1.53	1.31
18	N	515	HEA	C1A-C2A	-3.86	1.38	1.45
18	N	516	HEA	CHD-C4C	3.86	1.48	1.39
25	C	270	CDL	C79-C78	-3.80	1.32	1.51
20	N	1266	PGV	O01-C1	3.80	1.45	1.34
25	C	270	CDL	C59-C58	-3.80	1.32	1.51
19	Y	1522	TGL	C10-CB9	-3.79	1.32	1.51
19	L	522	TGL	C10-CB9	-3.79	1.32	1.51
25	C	270	CDL	OB8-CB7	3.75	1.44	1.33
25	P	1270	CDL	C59-C58	-3.74	1.33	1.51
18	A	516	HEA	CHC-C1C	3.74	1.47	1.39
18	A	516	HEA	CHB-C4A	3.68	1.45	1.38
18	A	516	HEA	C1C-NC	-3.65	1.32	1.39
25	G	269	CDL	C19-C18	-3.64	1.33	1.51
18	A	516	HEA	CHC-C4B	3.63	1.45	1.38
25	T	1269	CDL	C42-C41	-3.63	1.33	1.51
25	C	270	CDL	C39-C38	-3.63	1.33	1.51
25	C	270	CDL	C62-C61	-3.61	1.33	1.51
25	C	270	CDL	C82-C81	-3.51	1.34	1.51
18	N	516	HEA	C1B-NB	-3.50	1.32	1.38
18	N	516	HEA	FE-NC	3.47	2.06	1.95
24	P	1264	PEK	O01-C1	3.47	1.44	1.34
25	P	1270	CDL	C22-C21	-3.47	1.34	1.51
19	A	521	TGL	OG3-CC1	3.47	1.43	1.33
18	N	515	HEA	C1A-NA	-3.46	1.33	1.39
25	G	269	CDL	C22-C21	-3.46	1.34	1.51
19	O	1523	TGL	C10-CB9	-3.44	1.34	1.51
19	A	521	TGL	C10-CB9	-3.44	1.34	1.51
20	C	267	PGV	O01-C1	3.43	1.44	1.34
25	P	1270	CDL	C19-C18	-3.43	1.34	1.51
25	P	1270	CDL	C79-C78	-3.41	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	269	CDL	C42-C41	-3.40	1.34	1.51
24	G	265	PEK	C7-C8	3.40	1.75	1.51
22	C	271	CHD	O26-C24	-3.39	1.19	1.30
18	N	515	HEA	C3A-C2A	3.39	1.44	1.37
19	O	1521	TGL	C20-CA9	-3.38	1.35	1.51
25	G	269	CDL	C62-C61	-3.34	1.35	1.51
19	O	1523	TGL	C20-CA9	-3.34	1.35	1.51
18	N	516	HEA	C3A-C4A	-3.33	1.40	1.46
19	O	1523	TGL	C15-CC9	-3.33	1.35	1.51
25	C	270	CDL	C22-C21	-3.32	1.35	1.51
18	A	516	HEA	C4A-NA	-3.31	1.33	1.39
25	C	270	CDL	C19-C18	-3.30	1.35	1.51
18	A	516	HEA	CHD-C1D	3.29	1.45	1.38
25	P	1270	CDL	C39-C38	-3.27	1.35	1.51
19	A	521	TGL	C20-CA9	-3.27	1.35	1.51
18	A	516	HEA	C18-C19	3.27	1.40	1.33
25	T	1269	CDL	C19-C18	-3.25	1.35	1.51
25	P	1270	CDL	C62-C61	-3.25	1.35	1.51
18	A	516	HEA	C1A-C2A	-3.23	1.39	1.45
18	N	516	HEA	O11-C11	3.21	1.49	1.42
25	T	1269	CDL	C82-C81	-3.19	1.35	1.51
25	P	1270	CDL	C82-C81	-3.19	1.35	1.51
20	P	1267	PGV	O03-C19	3.18	1.42	1.33
19	Y	1522	TGL	C15-CC9	-3.17	1.36	1.51
25	C	270	CDL	C42-C41	-3.11	1.36	1.51
19	D	523	TGL	C10-CB9	-3.10	1.36	1.51
19	O	1521	TGL	C15-CC9	-3.08	1.36	1.51
25	G	269	CDL	C79-C78	-3.08	1.36	1.51
25	T	1269	CDL	C39-C38	-3.08	1.36	1.51
25	G	269	CDL	C39-C38	-3.07	1.36	1.51
25	T	1269	CDL	C79-C78	-3.07	1.36	1.51
19	D	523	TGL	C15-CC9	-3.06	1.36	1.51
18	N	516	HEA	CHA-C4D	3.06	1.46	1.39
19	D	523	TGL	C20-CA9	-3.05	1.36	1.51
24	C	264	PEK	O03-C21	3.05	1.42	1.33
22	C	525	CHD	C13-C14	-3.04	1.50	1.55
25	G	269	CDL	C82-C81	-3.02	1.36	1.51
19	L	522	TGL	C15-CC9	-2.98	1.36	1.51
25	T	1269	CDL	C22-C21	-2.95	1.37	1.51
20	N	1266	PGV	O03-C19	2.93	1.41	1.33
22	C	271	CHD	C10-C5	-2.93	1.50	1.55
19	A	521	TGL	C15-CC9	-2.91	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C1D-C2D	-2.90	1.38	1.44
18	A	515	HEA	CHB-C1B	2.90	1.45	1.39
18	A	516	HEA	O11-C11	2.86	1.49	1.42
18	N	516	HEA	C18-C19	2.86	1.39	1.33
18	A	515	HEA	C1D-ND	-2.84	1.35	1.40
20	C	267	PGV	O03-C19	2.82	1.41	1.33
25	P	1270	CDL	C42-C41	-2.82	1.37	1.51
18	A	516	HEA	FE-NB	2.80	2.03	1.94
25	C	270	CDL	OB6-CB5	2.80	1.42	1.34
22	B	1086	CHD	C11-C12	2.80	1.57	1.53
20	P	1267	PGV	O01-C1	2.79	1.42	1.34
22	O	229	CHD	C1-C10	-2.76	1.49	1.54
18	A	515	HEA	FE-ND	2.72	2.03	1.94
22	B	1086	CHD	C10-C5	-2.70	1.51	1.55
22	C	525	CHD	C1-C10	-2.67	1.49	1.54
22	O	229	CHD	C13-C12	-2.67	1.50	1.54
18	A	515	HEA	CHB-C4A	2.65	1.43	1.38
22	C	525	CHD	C6-C7	-2.64	1.47	1.52
18	N	516	HEA	CHC-C1C	2.64	1.45	1.39
18	N	515	HEA	C3A-C4A	-2.63	1.41	1.46
18	N	515	HEA	CHD-C1D	2.63	1.43	1.38
18	N	515	HEA	C4D-ND	-2.63	1.33	1.38
22	P	1525	CHD	C10-C5	-2.61	1.51	1.55
25	C	270	CDL	OB6-CB4	-2.61	1.40	1.46
22	C	525	CHD	C10-C5	-2.61	1.51	1.55
20	A	524	PGV	C2-C1	-2.61	1.43	1.50
18	A	515	HEA	C1A-C2A	-2.60	1.40	1.45
22	C	525	CHD	C18-C13	2.60	1.58	1.54
22	O	229	CHD	C18-C13	-2.59	1.50	1.54
18	N	515	HEA	C3B-C2B	2.59	1.40	1.34
18	A	516	HEA	C3D-C2D	2.59	1.42	1.36
18	A	515	HEA	C1C-NC	-2.56	1.34	1.39
22	P	1525	CHD	O26-C24	-2.55	1.22	1.30
18	A	515	HEA	CMB-C2B	2.54	1.56	1.50
22	O	229	CHD	C1-C2	-2.54	1.48	1.53
28	M	526	DMU	C3-C4	-2.51	1.46	1.52
22	B	1086	CHD	C11-C9	-2.51	1.49	1.53
25	P	1270	CDL	PB2-OB2	2.46	1.69	1.59
22	O	229	CHD	C10-C5	-2.45	1.51	1.55
18	A	516	HEA	O1A-CGA	2.42	1.30	1.22
28	Z	1526	DMU	O1-C10	2.41	1.48	1.41
24	P	1264	PEK	O03-C21	2.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C4D-C3D	-2.39	1.41	1.45
18	A	515	HEA	C1B-C2B	-2.38	1.39	1.44
18	A	515	HEA	CBD-CGD	2.35	1.56	1.50
18	N	515	HEA	CHD-C4C	2.33	1.44	1.39
20	A	522	PGV	P-O14	-2.32	1.44	1.55
18	N	515	HEA	O11-C11	2.31	1.48	1.42
18	N	516	HEA	C4D-C3D	-2.30	1.41	1.45
18	N	515	HEA	O1A-CGA	2.30	1.29	1.22
22	C	271	CHD	C20-C17	2.30	1.58	1.54
22	J	60	CHD	C23-C24	2.29	1.55	1.50
24	P	1264	PEK	C2-C1	2.29	1.57	1.50
18	N	516	HEA	CHA-C1A	2.29	1.42	1.38
18	N	516	HEA	C4B-C3B	-2.28	1.40	1.44
24	C	264	PEK	O03-C01	-2.27	1.40	1.45
28	G	272	DMU	O1-C10	2.27	1.47	1.41
18	N	516	HEA	C1D-C2D	-2.27	1.39	1.44
18	N	516	HEA	C17-C18	2.27	1.57	1.50
28	Z	1526	DMU	O16-C6	2.25	1.44	1.40
19	L	522	TGL	CG3-CG2	2.25	1.57	1.50
28	G	272	DMU	C3-C4	-2.25	1.46	1.52
28	P	1272	DMU	C3-C4	-2.25	1.46	1.52
19	A	521	TGL	OC1-CC1	-2.25	1.15	1.22
22	B	1086	CHD	C13-C12	-2.18	1.51	1.54
18	A	516	HEA	CMB-C2B	2.15	1.55	1.50
25	C	270	CDL	PA1-OA5	2.15	1.67	1.59
18	A	516	HEA	CHD-C4C	2.15	1.44	1.39
18	A	516	HEA	C1A-NA	-2.13	1.35	1.39
18	A	516	HEA	CMC-C2C	2.13	1.55	1.50
18	N	515	HEA	CHB-C4A	2.11	1.42	1.38
18	A	515	HEA	C13-C14	2.10	1.56	1.50
25	G	269	CDL	C71-CB7	2.09	1.56	1.50
22	P	1271	CHD	O26-C24	-2.07	1.24	1.30
22	P	1271	CHD	C20-C17	2.07	1.57	1.54
28	P	1272	DMU	O1-C10	2.06	1.47	1.41
18	A	515	HEA	C17-C18	2.05	1.56	1.50
22	P	1525	CHD	C19-C10	2.05	1.57	1.54
25	C	270	CDL	CB2-C1	2.05	1.58	1.51
20	N	1268	PGV	P-O11	2.05	1.67	1.59
22	C	525	CHD	C19-C10	2.05	1.57	1.54
18	A	516	HEA	CAC-C3C	2.04	1.52	1.47
18	A	516	HEA	OMA-CMA	2.02	1.26	1.22
25	P	1270	CDL	PA1-OA5	2.02	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	515	HEA	C1C-C2C	-2.02	1.38	1.43
18	N	515	HEA	CHC-C1C	2.01	1.43	1.39
22	C	525	CHD	O12-C12	2.01	1.46	1.43
18	A	515	HEA	C1A-NA	-2.01	1.35	1.39
18	A	516	HEA	CAD-C3D	2.00	1.56	1.51

All (773) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C18-C13-C12	-15.39	93.65	109.06
22	O	229	CHD	C6-C5-C10	14.15	127.72	112.66
22	B	1086	CHD	C6-C5-C10	13.87	127.42	112.66
22	C	525	CHD	C1-C10-C5	13.84	127.62	107.75
22	P	1271	CHD	C10-C9-C8	13.66	127.07	111.84
22	W	1060	CHD	C10-C9-C8	13.57	126.96	111.84
22	P	1525	CHD	C1-C10-C5	13.21	126.71	107.75
22	P	1525	CHD	C6-C5-C10	12.99	126.48	112.66
22	C	525	CHD	C6-C5-C10	12.42	125.87	112.66
22	P	1271	CHD	C18-C13-C12	-12.11	96.93	109.06
22	J	60	CHD	C10-C9-C8	12.02	125.24	111.84
22	P	1525	CHD	C18-C13-C12	-11.95	97.09	109.06
22	C	271	CHD	C10-C9-C8	11.87	125.07	111.84
22	O	229	CHD	C1-C10-C5	11.78	124.66	107.75
22	B	1086	CHD	C17-C13-C12	11.65	128.15	117.67
22	C	525	CHD	C18-C13-C12	-11.54	97.51	109.06
22	P	1525	CHD	C14-C13-C12	11.10	117.56	107.42
22	B	1086	CHD	C1-C10-C5	10.93	123.44	107.75
22	O	229	CHD	C19-C10-C9	-10.67	96.84	111.18
22	C	525	CHD	C4-C3-C2	10.61	123.56	110.62
22	C	525	CHD	C19-C10-C9	-10.50	97.06	111.18
22	B	1086	CHD	C19-C10-C9	-10.45	97.13	111.18
22	C	525	CHD	C17-C13-C12	10.39	127.02	117.67
22	O	229	CHD	C10-C9-C8	10.19	123.20	111.84
22	P	1525	CHD	C17-C13-C12	10.18	126.82	117.67
22	C	525	CHD	C10-C9-C8	10.14	123.14	111.84
22	B	1086	CHD	C10-C9-C8	9.65	122.59	111.84
22	C	271	CHD	C18-C13-C12	-9.59	99.46	109.06
22	P	1525	CHD	C10-C9-C8	9.53	122.46	111.84
22	P	1525	CHD	C4-C3-C2	9.47	122.17	110.62
22	B	1086	CHD	C6-C7-C8	9.44	121.81	111.50
22	O	229	CHD	C14-C13-C12	9.34	115.95	107.42
22	O	229	CHD	C17-C13-C14	9.26	109.40	100.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1525	CHD	C15-C14-C13	9.24	112.50	103.54
22	C	271	CHD	C21-C20-C22	-9.03	96.37	110.34
22	P	1271	CHD	C6-C5-C10	8.93	122.17	112.66
22	O	229	CHD	C17-C13-C12	8.92	125.69	117.67
22	C	271	CHD	C14-C13-C12	8.91	115.56	107.42
22	B	1086	CHD	C14-C13-C12	8.89	115.54	107.42
22	P	1271	CHD	C19-C10-C9	-8.82	99.32	111.18
22	P	1271	CHD	C17-C13-C12	8.82	125.60	117.67
22	J	60	CHD	C1-C10-C5	8.74	120.30	107.75
22	O	229	CHD	C18-C13-C12	-8.73	100.31	109.06
22	O	229	CHD	C6-C5-C4	-8.64	101.35	111.23
22	C	271	CHD	C17-C13-C12	8.49	125.30	117.67
22	W	1060	CHD	C1-C10-C5	8.45	119.87	107.75
19	A	521	TGL	CG2-OG2-CB1	8.44	137.99	117.80
22	B	1086	CHD	C9-C11-C12	8.43	125.33	114.29
22	C	271	CHD	C16-C17-C20	8.34	124.79	112.18
22	W	1060	CHD	C17-C13-C12	8.31	125.15	117.67
22	W	1060	CHD	C13-C17-C20	8.22	129.44	119.48
22	P	1271	CHD	C1-C2-C3	8.22	121.37	110.48
22	P	1271	CHD	C1-C10-C5	8.18	119.49	107.75
22	C	271	CHD	C6-C5-C10	8.12	121.30	112.66
22	C	271	CHD	C19-C10-C9	-8.10	100.29	111.18
28	G	272	DMU	O16-C6-C1	8.08	120.55	108.27
22	C	271	CHD	C18-C13-C17	-8.07	98.56	111.20
22	O	229	CHD	C18-C13-C17	-8.06	98.58	111.20
22	C	271	CHD	C1-C10-C5	8.03	119.28	107.75
28	P	1272	DMU	O1-C9-C8	7.84	123.83	109.70
22	B	1086	CHD	C1-C2-C3	7.80	120.81	110.48
22	W	1060	CHD	C6-C7-C8	7.69	119.89	111.50
22	J	60	CHD	C4-C3-C2	7.60	119.89	110.62
18	A	516	HEA	C13-C12-C11	-7.54	102.35	114.39
28	M	526	DMU	O1-C9-C8	7.53	123.27	109.70
22	O	229	CHD	O12-C12-C13	-7.51	98.34	111.02
28	G	272	DMU	C18-O16-C6	7.49	126.48	113.68
20	N	1524	PGV	O01-C1-C2	7.49	127.69	111.48
28	M	526	DMU	O1-C10-C5	7.45	125.69	110.37
28	M	526	DMU	O5-C6-C1	7.31	125.38	110.37
22	J	60	CHD	C14-C13-C12	7.29	114.08	107.42
22	P	1525	CHD	C19-C10-C9	-7.27	101.40	111.18
22	J	60	CHD	C6-C7-C8	7.16	119.32	111.50
22	C	271	CHD	C4-C3-C2	7.15	119.34	110.62
22	P	1271	CHD	C6-C7-C8	7.13	119.28	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	271	CHD	C6-C7-C8	7.13	119.28	111.50
22	C	271	CHD	C15-C14-C8	7.09	128.08	118.36
18	N	515	HEA	C27-C19-C20	7.04	127.44	115.23
22	P	1525	CHD	C5-C4-C3	6.99	123.25	112.71
22	J	60	CHD	C17-C13-C12	6.99	123.95	117.67
22	J	60	CHD	C13-C17-C20	6.95	127.91	119.48
28	G	272	DMU	O1-C9-C8	6.95	122.22	109.70
22	P	1271	CHD	C16-C17-C13	6.93	110.26	103.54
22	C	525	CHD	O12-C12-C13	-6.91	99.34	111.02
18	N	516	HEA	O11-C11-C3B	-6.88	98.65	111.26
22	W	1060	CHD	C4-C3-C2	6.85	118.97	110.62
28	Z	1526	DMU	O5-C6-C1	6.82	124.38	110.37
22	C	525	CHD	C15-C14-C13	6.79	110.13	103.54
28	G	272	DMU	O5-C4-C57	6.73	123.11	106.44
19	A	521	TGL	OG2-CB1-CB2	6.72	126.02	111.48
20	N	1268	PGV	O03-C19-C20	6.72	132.32	111.83
22	C	271	CHD	C15-C14-C13	6.72	110.06	103.54
22	C	525	CHD	C13-C17-C20	6.71	127.61	119.48
22	P	1271	CHD	C15-C14-C8	6.69	127.53	118.36
22	C	525	CHD	C14-C13-C12	6.67	113.51	107.42
18	N	516	HEA	CAD-C3D-C4D	6.66	136.30	124.70
22	W	1060	CHD	C14-C13-C12	6.63	113.47	107.42
28	Z	1526	DMU	O1-C10-C5	6.62	123.98	110.37
22	W	1060	CHD	C5-C6-C7	6.62	122.28	114.40
22	W	1060	CHD	C11-C12-C13	6.59	117.96	111.26
22	W	1060	CHD	C1-C2-C3	6.56	119.18	110.48
28	G	272	DMU	O1-C10-C5	6.54	123.81	110.37
22	C	525	CHD	C6-C5-C4	-6.54	103.75	111.23
28	Z	1526	DMU	O1-C9-C8	6.54	121.48	109.70
22	B	1086	CHD	C17-C13-C14	6.53	106.67	100.11
22	P	1271	CHD	O12-C12-C13	-6.53	99.99	111.02
22	B	1086	CHD	C11-C9-C10	6.53	120.33	113.70
28	P	1272	DMU	O16-C6-C1	6.52	118.18	108.27
22	P	1271	CHD	C4-C3-C2	6.52	118.57	110.62
28	Z	1526	DMU	C8-C7-C5	6.49	122.22	110.83
28	Z	1526	DMU	O5-C4-C57	6.48	122.50	106.44
22	C	271	CHD	O7-C7-C6	-6.43	93.87	109.86
22	J	60	CHD	C5-C6-C7	6.43	122.04	114.40
22	W	1060	CHD	C5-C4-C3	6.42	122.40	112.71
22	J	60	CHD	C6-C5-C10	6.40	119.47	112.66
22	P	1271	CHD	C16-C17-C20	6.40	121.86	112.18
22	O	229	CHD	C5-C4-C3	6.39	122.34	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	229	CHD	C18-C13-C14	-6.38	101.20	111.20
22	O	229	CHD	C9-C8-C7	6.32	119.81	111.86
22	J	60	CHD	C16-C17-C13	6.30	109.65	103.54
22	P	1271	CHD	C4-C5-C10	6.30	119.36	112.66
22	W	1060	CHD	C6-C5-C10	6.30	119.36	112.66
22	W	1060	CHD	C9-C11-C12	6.30	122.53	114.29
22	J	60	CHD	C16-C17-C20	6.24	121.62	112.18
22	B	1086	CHD	C5-C4-C3	6.23	122.10	112.71
28	Z	1526	DMU	O16-C6-C1	6.18	117.66	108.27
22	J	60	CHD	C18-C13-C12	-6.17	102.88	109.06
22	P	1271	CHD	C11-C9-C8	6.16	120.01	110.89
22	O	229	CHD	C4-C3-C2	6.15	118.12	110.62
22	P	1525	CHD	C18-C13-C17	-6.13	101.59	111.20
22	P	1271	CHD	C11-C12-C13	6.12	117.49	111.26
22	P	1525	CHD	C11-C9-C8	6.12	119.95	110.89
18	A	515	HEA	CHA-C4D-ND	6.12	131.00	124.42
24	T	263	PEK	O01-C1-C2	6.11	124.70	111.48
22	J	60	CHD	C5-C4-C3	6.11	121.92	112.71
18	N	515	HEA	C12-C11-C3B	6.10	121.65	112.12
22	W	1060	CHD	C16-C17-C13	6.08	109.44	103.54
20	N	1266	PGV	O03-C19-C20	6.08	130.37	111.83
28	Z	1526	DMU	O1-C9-C11	6.05	121.44	106.44
22	J	60	CHD	C1-C2-C3	6.04	118.49	110.48
22	C	271	CHD	C11-C9-C8	6.04	119.83	110.89
22	C	525	CHD	C11-C12-C13	6.03	117.39	111.26
18	N	515	HEA	CMD-C2D-C1D	6.03	134.45	125.03
22	C	525	CHD	C9-C8-C7	6.02	119.43	111.86
22	O	229	CHD	C1-C2-C3	5.99	118.42	110.48
28	P	1272	DMU	O5-C4-C3	5.96	122.05	109.72
18	N	516	HEA	OMA-CMA-C3A	-5.95	112.19	125.62
22	J	60	CHD	C11-C9-C8	5.93	119.67	110.89
22	P	1271	CHD	C5-C6-C7	5.89	121.40	114.40
28	Z	1526	DMU	O7-C10-C5	-5.88	93.61	108.09
19	L	522	TGL	CG2-OG2-CB1	5.88	131.86	117.80
18	A	515	HEA	C2B-C1B-NB	5.87	116.69	109.90
22	B	1086	CHD	C6-C5-C4	-5.83	104.57	111.23
22	C	271	CHD	C11-C12-C13	5.80	117.16	111.26
18	A	516	HEA	C3A-C2A-C1A	-5.70	101.66	107.05
22	P	1525	CHD	C9-C8-C7	5.68	119.00	111.86
18	A	516	HEA	C2D-C1D-ND	5.68	116.36	109.84
22	P	1271	CHD	C6-C5-C4	-5.66	104.76	111.23
25	G	269	CDL	OB6-CB5-C51	5.65	123.70	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	C1D-C2D-C3D	-5.64	101.05	106.98
22	J	60	CHD	C15-C14-C13	5.62	109.00	103.54
18	A	515	HEA	CHB-C4A-NA	5.62	130.57	124.45
25	P	1270	CDL	OA6-CA5-C11	5.62	123.64	111.48
28	P	1272	DMU	O1-C10-C5	5.62	121.91	110.37
22	O	229	CHD	C9-C11-C12	5.60	121.63	114.29
22	C	271	CHD	C5-C4-C3	5.60	121.16	112.71
19	L	522	TGL	OG3-CC1-CC2	5.60	128.90	111.83
25	T	1269	CDL	OB6-CB5-C51	5.58	123.56	111.48
22	P	1271	CHD	O7-C7-C6	-5.58	95.98	109.86
22	P	1271	CHD	C14-C13-C12	5.57	112.51	107.42
22	C	271	CHD	C5-C6-C7	5.56	121.02	114.40
22	C	271	CHD	C2-C1-C10	5.55	122.11	112.74
22	J	60	CHD	C2-C1-C10	5.55	122.10	112.74
22	J	60	CHD	C14-C8-C7	5.53	119.19	111.85
28	G	272	DMU	O5-C4-C3	5.52	121.13	109.72
22	W	1060	CHD	C18-C13-C12	-5.51	103.54	109.06
20	N	1266	PGV	O03-C19-O04	-5.51	109.85	123.63
28	M	526	DMU	C2-C3-C4	5.51	123.14	110.93
25	C	270	CDL	CB4-OB6-CB5	-5.50	104.64	117.80
22	W	1060	CHD	C1-C10-C9	-5.49	102.82	111.34
18	N	515	HEA	C2D-C1D-ND	5.48	116.14	109.84
22	J	60	CHD	O12-C12-C11	-5.48	97.97	109.12
22	P	1525	CHD	C17-C13-C14	5.48	105.61	100.11
25	G	269	CDL	OA6-CA5-C11	5.48	123.33	111.48
22	W	1060	CHD	C15-C14-C13	5.47	108.85	103.54
22	P	1271	CHD	C15-C14-C13	5.46	108.84	103.54
22	W	1060	CHD	C15-C14-C8	5.44	125.82	118.36
18	N	516	HEA	CHB-C4A-NA	-5.40	118.57	124.45
28	P	1272	DMU	C8-C7-C5	5.39	120.30	110.83
22	C	271	CHD	C1-C2-C3	5.39	117.61	110.48
18	N	515	HEA	OMA-CMA-C3A	-5.38	113.48	125.62
22	W	1060	CHD	C2-C1-C10	5.35	121.77	112.74
22	O	229	CHD	C15-C14-C8	5.35	125.70	118.36
22	J	60	CHD	C15-C14-C8	5.35	125.69	118.36
28	P	1272	DMU	O5-C4-C57	5.35	119.69	106.44
22	J	60	CHD	C1-C10-C9	-5.34	103.04	111.34
22	B	1086	CHD	C4-C3-C2	5.34	117.13	110.62
28	M	526	DMU	O7-C10-C5	-5.33	94.97	108.09
24	T	1265	PEK	O01-C1-C2	5.32	122.99	111.48
22	B	1086	CHD	O12-C12-C11	-5.31	98.31	109.12
22	C	525	CHD	C17-C13-C14	5.31	105.44	100.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C18-C13-C17	-5.28	102.94	111.20
24	P	1264	PEK	C2-C3-C4	5.27	124.87	113.35
22	P	1271	CHD	C5-C4-C3	5.27	120.66	112.71
22	O	229	CHD	C11-C9-C8	5.26	118.67	110.89
24	G	1263	PEK	O01-C1-C2	5.23	122.78	111.48
28	G	272	DMU	O1-C9-C11	5.22	119.38	106.44
28	Z	1526	DMU	O5-C4-C3	5.22	120.52	109.72
22	W	1060	CHD	C14-C8-C7	5.19	118.74	111.85
22	C	271	CHD	C16-C17-C13	5.18	108.56	103.54
28	M	526	DMU	O5-C4-C3	5.18	120.42	109.72
19	O	1521	TGL	CG2-OG2-CB1	5.16	130.15	117.80
22	O	229	CHD	C11-C12-C13	5.15	116.50	111.26
19	Y	1522	TGL	OG2-CB1-CB2	5.14	122.59	111.48
28	Z	1526	DMU	C2-C3-C4	5.13	122.30	110.93
22	P	1525	CHD	C13-C17-C20	5.11	125.68	119.48
18	A	515	HEA	C4B-NB-C1B	-5.10	99.17	105.21
22	W	1060	CHD	C13-C14-C8	5.08	121.15	114.72
28	G	272	DMU	C8-C7-C5	5.08	119.74	110.83
20	H	268	PGV	O01-C1-C2	5.06	122.44	111.48
20	H	268	PGV	O03-C19-C20	5.06	127.25	111.83
22	W	1060	CHD	C16-C17-C20	5.03	119.79	112.18
18	A	516	HEA	C2B-C1B-NB	5.02	115.70	109.90
22	P	1525	CHD	C6-C5-C4	-5.01	105.50	111.23
18	A	515	HEA	CMB-C2B-C1B	5.00	132.84	125.03
18	A	515	HEA	C12-C11-C3B	4.98	119.90	112.12
18	A	515	HEA	CMB-C2B-C3B	-4.95	120.71	130.28
28	G	272	DMU	C2-C3-C4	4.94	121.88	110.93
22	W	1060	CHD	O12-C12-C11	-4.93	99.09	109.12
22	C	271	CHD	O12-C12-C13	-4.88	102.78	111.02
22	P	1525	CHD	C18-C13-C14	-4.85	103.60	111.20
19	L	522	TGL	OG3-CC1-OC1	-4.82	111.58	123.63
22	J	60	CHD	C11-C12-C13	4.81	116.16	111.26
22	W	1060	CHD	C19-C10-C5	-4.81	102.40	110.44
22	J	60	CHD	C9-C11-C12	4.79	120.56	114.29
22	P	1525	CHD	O12-C12-C13	-4.78	102.94	111.02
18	A	516	HEA	CHA-C1A-C2A	-4.78	117.32	124.86
25	C	270	CDL	OA6-CA5-C11	4.78	121.81	111.48
22	W	1060	CHD	C4-C5-C10	4.76	117.73	112.66
18	N	515	HEA	C2B-C1B-NB	4.76	115.41	109.90
28	G	272	DMU	O5-C6-C1	4.74	120.11	110.37
18	A	516	HEA	C1D-C2D-C3D	-4.73	102.01	106.98
18	N	515	HEA	C27-C19-C18	-4.72	111.51	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	525	CHD	C5-C4-C3	4.70	119.79	112.71
18	A	515	HEA	CHA-C4D-C3D	-4.65	117.99	124.77
22	J	60	CHD	C19-C10-C5	-4.64	102.68	110.44
22	J	60	CHD	C9-C10-C5	4.61	114.91	108.51
20	A	524	PGV	C02-O01-C1	4.59	128.79	117.80
25	P	1270	CDL	OB8-CB7-C71	4.59	125.84	111.83
22	P	1525	CHD	C16-C17-C20	4.59	119.12	112.18
18	N	516	HEA	CAD-C3D-C2D	-4.58	119.28	127.87
25	C	270	CDL	OB8-CB7-OB9	-4.58	112.18	123.63
24	P	1264	PEK	O01-C1-O02	-4.56	113.03	123.70
28	G	272	DMU	C6-C1-C2	4.54	119.56	110.01
24	G	265	PEK	O03-C21-C22	4.53	125.64	111.83
18	A	515	HEA	C27-C19-C18	-4.53	112.00	123.63
18	N	516	HEA	CHD-C1D-ND	4.52	129.96	124.37
25	C	270	CDL	OB8-CB7-C71	4.50	125.57	111.83
28	M	526	DMU	O5-C4-C57	4.49	117.57	106.44
28	M	526	DMU	C8-C7-C5	4.49	118.71	110.83
18	A	515	HEA	CAD-C3D-C2D	4.47	136.24	127.87
18	N	516	HEA	C4C-CHD-C1D	-4.47	115.75	126.25
19	A	521	TGL	OG1-CA1-CA2	4.45	125.42	111.83
28	G	272	DMU	O7-C3-C2	4.45	118.55	107.23
22	C	271	CHD	C4-C5-C10	4.45	117.39	112.66
18	A	516	HEA	C1D-ND-C4D	-4.45	99.94	105.21
19	O	1523	TGL	OG2-CB1-CB2	4.44	121.08	111.48
22	C	525	CHD	C5-C6-C7	4.43	119.66	114.40
18	N	516	HEA	C3A-C2A-C1A	-4.41	102.87	107.05
22	P	1525	CHD	C11-C12-C13	4.41	115.75	111.26
25	G	269	CDL	CB6-CB4-CB3	-4.41	101.51	111.78
22	B	1086	CHD	C15-C14-C13	4.40	107.81	103.54
19	D	523	TGL	OG2-CB1-CB2	-4.40	101.96	111.48
22	P	1525	CHD	O12-C12-C11	-4.40	100.17	109.12
19	D	523	TGL	OG1-CA1-CA2	4.40	125.25	111.83
22	P	1271	CHD	C13-C17-C20	4.40	124.81	119.48
22	C	525	CHD	C4-C5-C10	-4.39	107.99	112.66
22	P	1525	CHD	C22-C20-C17	-4.38	101.25	110.33
22	O	229	CHD	C16-C17-C20	4.38	118.80	112.18
22	W	1060	CHD	C11-C9-C8	4.37	117.36	110.89
18	A	515	HEA	C4C-C3C-C2C	-4.37	101.87	107.30
22	J	60	CHD	C4-C5-C10	4.35	117.29	112.66
28	P	1272	DMU	C6-C1-C2	4.34	119.14	110.01
19	A	521	TGL	OG3-CC1-OC1	-4.34	112.77	123.63
22	C	525	CHD	C1-C10-C9	-4.33	104.61	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	CHC-C4B-NB	4.33	129.72	124.37
22	J	60	CHD	C22-C20-C17	4.31	119.26	110.33
24	T	1265	PEK	O03-C21-C22	4.29	124.93	111.83
18	A	516	HEA	CHD-C4C-NC	4.29	131.64	123.86
18	A	515	HEA	CHB-C1B-NB	-4.29	119.81	124.42
22	C	525	CHD	C18-C13-C14	-4.28	104.50	111.20
18	A	516	HEA	CHA-C1A-NA	4.28	129.11	124.45
22	W	1060	CHD	C6-C5-C4	-4.27	106.34	111.23
28	M	526	DMU	C7-C8-C9	4.27	117.97	110.23
18	A	516	HEA	C3C-C4C-NC	-4.25	106.22	109.80
22	J	60	CHD	C18-C13-C14	-4.23	104.57	111.20
19	D	523	TGL	CG1-OG1-CA1	4.23	132.59	117.12
18	N	515	HEA	C3C-C2C-C1C	-4.23	102.18	107.17
22	P	1271	CHD	C9-C11-C12	4.21	119.81	114.29
22	C	271	CHD	C9-C11-C12	4.21	119.81	114.29
22	P	1525	CHD	O7-C7-C6	-4.21	99.39	109.86
18	N	515	HEA	CHA-C4D-ND	4.21	128.95	124.42
28	P	1272	DMU	C6-O5-C4	4.18	121.89	113.72
18	N	516	HEA	O1D-CGD-CBD	-4.18	109.83	123.09
24	G	265	PEK	O01-C1-C2	4.17	120.51	111.48
22	C	271	CHD	C17-C13-C14	4.16	104.28	100.11
28	G	272	DMU	C7-C8-C9	4.15	117.76	110.23
18	N	515	HEA	CHA-C4D-C3D	-4.15	118.72	124.77
26	E	230	PSC	O01-C1-C2	4.11	120.38	111.48
22	W	1060	CHD	C18-C13-C14	-4.11	104.76	111.20
18	A	515	HEA	CHC-C4B-C3B	-4.10	115.47	125.80
28	P	1272	DMU	O5-C6-C1	4.09	118.78	110.37
28	P	1272	DMU	C18-O16-C6	4.09	120.66	113.68
22	B	1086	CHD	C14-C8-C9	4.08	115.45	109.75
18	A	516	HEA	CHB-C4A-NA	4.08	128.90	124.45
22	J	60	CHD	C19-C10-C9	-4.05	105.73	111.18
22	B	1086	CHD	O7-C7-C6	-4.05	99.79	109.86
28	P	1272	DMU	O1-C9-C11	4.04	116.45	106.44
19	O	1521	TGL	OG1-CA1-CA2	4.04	124.15	111.83
19	O	1521	TGL	OG2-CB1-CB2	4.04	120.21	111.48
22	W	1060	CHD	C18-C13-C17	-4.03	104.89	111.20
22	C	525	CHD	C14-C8-C9	4.03	115.37	109.75
20	A	522	PGV	O03-C01-C02	3.99	119.91	108.40
22	P	1271	CHD	O12-C12-C11	-3.97	101.04	109.12
22	W	1060	CHD	C22-C20-C17	3.95	118.51	110.33
18	N	516	HEA	C13-C12-C11	-3.94	108.11	114.39
24	G	1263	PEK	O01-C1-O02	-3.93	114.51	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	1263	PEK	O03-C21-C22	3.93	123.82	111.83
28	P	1272	DMU	C2-C3-C4	3.93	119.64	110.93
22	O	229	CHD	C13-C17-C20	3.92	124.23	119.48
25	T	1269	CDL	OA6-CA5-C11	3.92	119.95	111.48
28	Z	1526	DMU	O7-C3-C2	3.91	117.18	107.23
22	C	525	CHD	C9-C11-C12	3.90	119.40	114.29
28	M	526	DMU	O3-C5-C7	3.90	119.57	110.38
20	N	1268	PGV	C03-C02-C01	-3.89	102.73	111.78
22	P	1525	CHD	C2-C1-C10	3.88	119.28	112.74
20	A	522	PGV	O03-C19-C20	3.87	123.63	111.83
19	O	1521	TGL	CG3-OG3-CC1	3.87	131.25	117.12
19	O	1523	TGL	OG3-CC1-CC2	3.86	123.62	111.83
28	P	1272	DMU	C1-C2-C3	3.86	118.44	109.68
20	A	524	PGV	C4-C3-C2	-3.86	98.95	113.13
19	A	521	TGL	CB7-CB6-CB5	-3.85	94.88	114.37
18	A	516	HEA	C4C-CHD-C1D	-3.84	117.21	126.25
22	P	1525	CHD	C1-C10-C9	-3.84	105.37	111.34
28	Z	1526	DMU	C7-C8-C9	3.84	117.19	110.23
28	M	526	DMU	O1-C9-C11	3.83	115.93	106.44
22	B	1086	CHD	O7-C7-C8	-3.82	100.76	109.52
18	A	515	HEA	C3B-C4B-NB	3.82	114.24	109.84
22	W	1060	CHD	O7-C7-C6	-3.81	100.38	109.86
20	A	522	PGV	O03-C19-O04	-3.80	114.13	123.63
18	A	515	HEA	C27-C19-C20	3.79	121.81	115.23
22	C	525	CHD	O7-C7-C6	-3.78	100.46	109.86
20	A	524	PGV	O03-C19-C20	3.78	123.35	111.83
22	C	271	CHD	C6-C5-C4	-3.77	106.92	111.23
22	P	1525	CHD	C6-C7-C8	3.76	115.61	111.50
22	B	1086	CHD	C16-C17-C13	3.76	107.19	103.54
22	O	229	CHD	C14-C8-C9	3.76	115.00	109.75
22	W	1060	CHD	C9-C10-C5	3.76	113.73	108.51
24	G	265	PEK	O03-C21-O04	-3.73	114.30	123.63
28	G	272	DMU	C6-O5-C4	3.72	120.99	113.72
24	P	1264	PEK	O03-C01-C02	-3.72	97.69	108.40
22	P	1525	CHD	C4-C5-C10	-3.71	108.71	112.66
18	A	515	HEA	CAD-C3D-C4D	-3.69	118.27	124.70
22	C	525	CHD	C2-C1-C10	3.67	118.94	112.74
20	N	1524	PGV	O01-C1-O02	-3.66	115.14	123.70
22	P	1271	CHD	C18-C13-C17	-3.64	105.50	111.20
22	P	1525	CHD	O7-C7-C8	-3.63	101.20	109.52
24	C	264	PEK	O03-C01-C02	-3.63	97.93	108.40
18	A	516	HEA	C20-C19-C18	-3.62	113.04	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	229	CHD	O7-C7-C8	-3.61	101.24	109.52
22	J	60	CHD	C17-C13-C14	3.61	103.74	100.11
22	B	1086	CHD	O12-C12-C13	-3.60	104.95	111.02
18	A	516	HEA	C12-C13-C14	-3.59	102.73	112.16
22	B	1086	CHD	C18-C13-C14	-3.59	105.58	111.20
22	P	1271	CHD	C2-C1-C10	3.58	118.78	112.74
18	N	516	HEA	C3D-C4D-ND	3.58	113.81	110.35
28	P	1272	DMU	C10-C5-C7	3.57	117.52	110.01
22	B	1086	CHD	C16-C17-C20	3.56	117.56	112.18
22	P	1525	CHD	C19-C10-C5	-3.56	104.49	110.44
24	P	1264	PEK	O01-C1-C2	3.55	119.17	111.48
18	A	516	HEA	CMD-C2D-C1D	3.55	130.59	125.03
18	A	516	HEA	CMB-C2B-C1B	3.54	130.56	125.03
25	P	1270	CDL	C53-C52-C51	-3.53	100.14	113.13
26	R	1230	PSC	O01-C1-C2	3.53	119.12	111.48
22	P	1271	CHD	C17-C13-C14	3.52	103.65	100.11
19	Y	1522	TGL	CG2-OG2-CB1	3.52	126.22	117.80
19	A	521	TGL	OG1-CA1-OA1	-3.51	114.84	123.63
19	Y	1522	TGL	OG1-CA1-CA2	3.51	122.54	111.83
20	N	1524	PGV	O03-C19-C20	3.50	122.52	111.83
24	T	1265	PEK	O03-C21-O04	-3.50	114.87	123.63
24	C	264	PEK	C24-C23-C22	-3.50	100.27	113.13
18	N	516	HEA	C2A-C1A-NA	3.49	113.69	110.32
22	P	1525	CHD	C13-C14-C8	3.49	119.13	114.72
18	A	515	HEA	C16-C17-C18	3.48	129.25	112.02
22	J	60	CHD	O7-C7-C6	-3.47	101.22	109.86
26	R	1230	PSC	O03-C19-C20	3.45	122.36	111.83
28	Z	1526	DMU	C6-O5-C4	3.44	120.44	113.72
18	A	516	HEA	O11-C11-C3B	-3.43	104.97	111.26
25	G	269	CDL	OB8-CB7-OB9	-3.43	115.06	123.63
28	Z	1526	DMU	C1-C2-C3	3.42	117.43	109.68
22	J	60	CHD	C18-C13-C17	-3.42	105.85	111.20
20	A	524	PGV	O02-C1-C2	-3.41	110.43	123.78
20	A	522	PGV	O01-C1-C2	3.40	118.84	111.48
18	A	515	HEA	CHD-C1D-ND	-3.40	120.17	124.37
20	A	522	PGV	O01-C1-O02	-3.38	115.79	123.70
22	P	1525	CHD	C14-C8-C9	3.38	114.47	109.75
20	C	267	PGV	O03-C19-O04	-3.37	115.20	123.63
22	C	525	CHD	C11-C9-C10	3.37	117.12	113.70
20	P	1267	PGV	C8-C9-C10	-3.37	97.68	113.86
19	O	1523	TGL	OG3-CC1-OC1	-3.35	115.26	123.63
22	C	271	CHD	C14-C8-C9	3.35	114.42	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	1268	PGV	O03-C19-O04	-3.34	115.26	123.63
22	O	229	CHD	C6-C7-C8	3.34	115.14	111.50
24	T	263	PEK	O01-C1-O02	-3.34	115.90	123.70
28	P	1272	DMU	C10-O1-C9	3.33	120.23	113.72
19	O	1521	TGL	OG3-CC1-CC2	3.32	121.97	111.83
20	N	1266	PGV	O03-C01-C02	3.32	117.97	108.40
20	A	524	PGV	O01-C1-O02	3.30	131.43	123.70
25	T	1269	CDL	CB2-C1-CA2	-3.30	103.14	112.65
18	A	516	HEA	CHD-C1D-C2D	-3.30	117.56	126.95
28	Z	1526	DMU	C10-O1-C9	3.30	120.17	113.72
18	A	515	HEA	C20-C21-C22	-3.30	95.69	112.02
22	C	525	CHD	O3-C3-C4	3.30	116.42	109.84
20	C	267	PGV	C27-C26-C25	-3.30	97.69	114.37
18	N	516	HEA	CAA-CBA-CGA	-3.30	104.92	113.67
19	L	522	TGL	OG1-CA1-CA2	3.29	121.87	111.83
22	B	1086	CHD	O25-C24-C23	-3.28	112.69	123.09
22	O	229	CHD	C2-C1-C10	3.27	118.25	112.74
18	A	516	HEA	C2A-C1A-NA	3.26	113.47	110.32
22	C	525	CHD	C11-C9-C8	3.25	115.70	110.89
28	P	1272	DMU	C7-C8-C9	3.25	116.12	110.23
20	P	1267	PGV	C27-C26-C25	-3.24	97.97	114.37
19	Y	1522	TGL	CG3-OG3-CC1	3.24	128.97	117.12
28	G	272	DMU	C10-C5-C7	3.23	116.81	110.01
25	C	270	CDL	C53-C52-C51	-3.23	101.27	113.13
24	P	1264	PEK	C30-C29-C28	-3.22	98.08	114.37
20	P	1267	PGV	C02-O01-C1	3.22	125.50	117.80
22	C	525	CHD	C18-C13-C17	-3.22	106.16	111.20
19	A	521	TGL	OG3-CC1-CC2	3.21	121.63	111.83
28	M	526	DMU	C18-O16-C6	3.21	119.16	113.68
18	A	516	HEA	C4B-NB-C1B	-3.20	101.42	105.21
22	B	1086	CHD	C11-C9-C8	3.18	115.61	110.89
19	L	522	TGL	OG3-CG3-CG2	3.18	117.57	108.40
22	J	60	CHD	C6-C5-C4	-3.18	107.59	111.23
20	C	267	PGV	O14-P-O13	3.17	127.19	112.44
20	P	1267	PGV	O03-C19-O04	-3.17	115.70	123.63
24	G	1263	PEK	O03-C01-C02	3.16	117.50	108.40
22	P	1525	CHD	C15-C16-C17	3.16	111.33	105.14
22	C	525	CHD	C13-C14-C8	3.15	118.71	114.72
25	T	1269	CDL	C83-C82-C81	3.15	130.27	114.37
22	P	1271	CHD	C21-C20-C17	3.14	117.59	112.88
18	N	515	HEA	C17-C18-C19	-3.14	120.45	127.62
18	A	515	HEA	CHB-C4A-C3A	-3.13	119.93	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	525	CHD	C19-C10-C5	-3.13	105.21	110.44
19	Y	1522	TGL	OG3-CC1-OC1	-3.12	115.81	123.63
22	C	525	CHD	O12-C12-C11	-3.12	102.77	109.12
28	M	526	DMU	C31-C28-C25	-3.11	98.64	114.37
18	N	516	HEA	C26-C15-C16	3.11	120.63	115.23
19	O	1523	TGL	CG3-CG2-CG1	-3.10	104.55	111.78
22	W	1060	CHD	C14-C8-C9	3.10	114.07	109.75
22	O	229	CHD	O26-C24-C23	3.09	123.76	114.00
19	D	523	TGL	C10-CB9-CB8	3.08	129.95	114.37
22	P	1525	CHD	C23-C22-C20	-3.08	108.70	114.46
28	M	526	DMU	C1-C2-C3	3.08	116.66	109.68
19	Y	1522	TGL	OG3-CC1-CC2	3.07	121.21	111.83
18	A	516	HEA	C27-C19-C20	3.07	120.55	115.23
18	N	515	HEA	CHC-C4B-NB	3.07	128.16	124.37
28	M	526	DMU	C11-C9-C8	3.06	120.53	113.02
22	C	525	CHD	C15-C16-C17	3.06	111.13	105.14
25	C	270	CDL	O1-C1-CB2	3.05	120.25	109.70
28	G	272	DMU	O5-C6-O16	3.05	117.26	110.04
18	N	515	HEA	CHC-C1C-NC	-3.05	118.33	123.86
28	M	526	DMU	C57-C4-C3	3.05	121.96	113.38
18	N	516	HEA	CHD-C1D-C2D	-3.05	118.28	126.95
22	B	1086	CHD	C9-C8-C7	3.05	115.69	111.86
18	A	516	HEA	C4C-NC-C1C	3.03	110.77	105.82
18	A	515	HEA	C25-C23-C24	3.02	121.55	114.59
19	L	522	TGL	CB4-CB3-CB2	-3.02	102.03	113.13
22	W	1060	CHD	C17-C13-C14	3.01	103.14	100.11
25	C	270	CDL	OB6-CB5-C51	3.01	117.99	111.48
19	O	1523	TGL	OG1-CA1-CA2	2.99	120.96	111.83
26	E	230	PSC	C02-O01-C1	2.99	124.95	117.80
19	D	523	TGL	OG2-CB1-OB1	2.99	130.69	123.70
19	A	521	TGL	OB1-CB1-CB2	-2.98	112.11	123.78
22	O	229	CHD	C5-C6-C7	2.98	117.94	114.40
19	L	522	TGL	CC3-CC2-CC1	2.97	124.59	113.69
18	A	515	HEA	OMA-CMA-C3A	-2.97	118.91	125.62
19	D	523	TGL	CB3-CB2-CB1	2.97	124.57	113.69
20	A	524	PGV	O01-C1-C2	2.97	117.90	111.48
18	N	516	HEA	CHC-C4B-NB	-2.97	120.70	124.37
22	C	271	CHD	C22-C23-C24	2.96	120.39	112.49
19	D	523	TGL	CG2-OG2-CB1	2.96	124.88	117.80
25	C	270	CDL	OB6-CB5-OB7	-2.96	116.79	123.70
25	T	1269	CDL	OB8-CB6-CB4	2.95	116.91	108.40
22	P	1525	CHD	C9-C11-C12	2.95	118.16	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	C4A-C3A-C2A	2.95	109.37	106.81
19	O	1523	TGL	OG1-CG1-CG2	2.95	116.90	108.40
19	L	522	TGL	CA4-CA3-CA2	-2.94	102.32	113.13
19	D	523	TGL	CG3-OG3-CC1	2.94	127.86	117.12
25	G	269	CDL	OA8-CA7-C31	2.94	120.79	111.83
20	C	267	PGV	O06-C06-C05	-2.93	97.17	110.38
24	C	264	PEK	O01-C1-O02	-2.93	116.85	123.70
22	C	271	CHD	O12-C12-C11	-2.92	103.17	109.12
20	N	1268	PGV	O01-C1-C2	2.92	117.81	111.48
24	C	264	PEK	C02-O01-C1	2.92	124.79	117.80
26	E	230	PSC	O03-C19-C20	2.92	120.74	111.83
28	M	526	DMU	C6-C1-C2	2.92	116.15	110.01
28	G	272	DMU	C10-O1-C9	2.91	119.41	113.72
19	D	523	TGL	C21-C20-CA9	2.91	129.07	114.37
20	N	1268	PGV	O04-C19-C20	-2.91	112.41	123.78
18	A	515	HEA	C1A-CHA-C4D	-2.91	119.84	126.02
22	O	229	CHD	O12-C12-C11	-2.90	103.21	109.12
18	N	516	HEA	CBD-CAD-C3D	2.90	120.55	112.53
24	T	263	PEK	O03-C01-C02	2.90	116.75	108.40
19	A	521	TGL	CA3-CA2-CA1	-2.89	103.11	113.69
19	L	522	TGL	OG1-CG1-CG2	2.88	116.69	108.40
24	G	265	PEK	C10-C9-C8	-2.88	99.30	123.57
28	G	272	DMU	C1-C2-C3	2.87	116.20	109.68
22	P	1525	CHD	C5-C6-C7	2.87	117.81	114.40
20	A	524	PGV	C8-C9-C10	-2.86	100.09	113.86
18	N	516	HEA	CHB-C4A-C3A	2.86	130.03	125.21
18	A	515	HEA	C3C-C4C-NC	2.86	112.21	109.80
28	Z	1526	DMU	O3-C5-C7	2.86	117.11	110.38
28	G	272	DMU	O7-C3-C4	2.85	116.97	109.48
20	A	524	PGV	O01-C02-C03	2.85	118.58	108.34
18	A	515	HEA	O2D-CGD-O1D	-2.84	116.04	123.33
20	P	1267	PGV	O03-C19-C20	2.83	120.46	111.83
18	A	516	HEA	C17-C18-C19	2.82	134.09	127.62
24	G	265	PEK	C8-C7-C6	-2.82	98.16	112.02
20	H	268	PGV	O04-C19-C20	-2.81	112.78	123.78
20	P	1267	PGV	C4-C3-C2	-2.81	102.81	113.13
28	M	526	DMU	O49-C1-C2	2.81	116.99	110.38
22	C	525	CHD	C21-C20-C22	-2.81	106.00	110.34
18	A	515	HEA	C4A-CHB-C1B	-2.81	120.06	126.02
18	A	516	HEA	C4A-CHB-C1B	-2.80	120.06	126.02
18	A	515	HEA	C17-C18-C19	-2.80	121.22	127.62
22	C	271	CHD	C19-C10-C5	-2.80	105.76	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	522	TGL	OG2-CB1-CB2	2.79	117.52	111.48
18	A	516	HEA	CMB-C2B-C3B	-2.79	124.88	130.28
19	L	522	TGL	C22-C21-C20	-2.79	100.27	114.37
19	L	522	TGL	C26-C25-C24	-2.78	100.33	114.37
25	P	1270	CDL	OB8-CB7-OB9	-2.76	116.72	123.63
28	Z	1526	DMU	C22-C19-C18	-2.75	101.50	113.47
22	O	229	CHD	C1-C10-C9	-2.75	107.07	111.34
19	O	1523	TGL	CG3-OG3-CC1	2.75	127.17	117.12
28	Z	1526	DMU	O5-C6-O16	2.74	116.51	110.04
22	B	1086	CHD	C1-C10-C9	-2.73	107.09	111.34
28	P	1272	DMU	C11-C9-C8	2.73	119.71	113.02
22	O	229	CHD	C11-C9-C10	2.72	116.47	113.70
20	N	1524	PGV	C02-O01-C1	2.72	124.31	117.80
28	M	526	DMU	C10-C5-C7	2.71	115.72	110.01
18	A	516	HEA	O2A-CGA-CBA	2.71	122.57	114.00
19	Y	1522	TGL	CB3-CB2-CB1	2.70	123.60	113.69
24	T	263	PEK	C14-C13-C12	2.70	125.32	112.02
25	C	270	CDL	C73-C72-C71	-2.70	103.22	113.13
18	N	515	HEA	CAD-C3D-C4D	-2.70	120.00	124.70
22	B	1086	CHD	C2-C1-C10	2.70	117.29	112.74
20	N	1266	PGV	O14-P-O11	2.69	119.76	107.57
19	Y	1522	TGL	OG1-CG1-CG2	2.69	116.15	108.40
22	C	271	CHD	C14-C8-C7	2.69	115.42	111.85
18	A	516	HEA	CHB-C1B-C2B	-2.68	120.79	125.03
18	A	516	HEA	C3D-C4D-ND	2.68	112.94	110.35
18	A	515	HEA	C26-C15-C16	2.67	119.86	115.23
18	N	516	HEA	C1D-ND-C4D	-2.67	102.05	105.21
25	T	1269	CDL	OA6-CA5-OA7	-2.67	117.47	123.70
22	C	271	CHD	C23-C22-C20	2.66	119.44	114.46
25	P	1270	CDL	OA6-CA5-OA7	-2.65	117.50	123.70
25	C	270	CDL	OA8-CA6-CA4	2.65	116.04	108.40
24	C	264	PEK	C25-C24-C23	-2.65	100.96	114.37
25	G	269	CDL	C40-C39-C38	2.65	127.77	114.37
18	N	516	HEA	C3B-C4B-NB	2.65	112.88	109.84
19	L	522	TGL	OG2-CG2-CG3	2.64	117.83	108.34
18	A	515	HEA	CHC-C1C-NC	-2.63	119.09	123.86
18	A	515	HEA	C4B-C3B-C2B	-2.62	103.03	107.44
24	C	264	PEK	O11-P-O14	-2.61	98.58	108.94
18	A	515	HEA	O2A-CGA-CBA	2.61	122.26	114.00
25	T	1269	CDL	OA8-CA7-C31	2.61	119.80	111.83
18	N	515	HEA	CHB-C4A-NA	2.61	127.30	124.45
28	Z	1526	DMU	C18-O16-C6	2.61	118.14	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	M	526	DMU	O5-C6-O16	2.61	116.21	110.04
18	N	515	HEA	C4B-NB-C1B	-2.60	102.13	105.21
25	T	1269	CDL	OB4-PB2-OB3	2.60	124.52	112.44
25	T	1269	CDL	C40-C39-C38	2.59	127.47	114.37
19	O	1521	TGL	CG1-OG1-CA1	2.59	126.57	117.12
28	P	1272	DMU	O3-C5-C10	-2.57	103.95	110.08
28	P	1272	DMU	O61-C57-C4	2.57	120.08	111.33
25	G	269	CDL	C58-C57-C56	-2.57	101.39	114.37
20	N	1266	PGV	O01-C1-C2	2.57	117.03	111.48
18	A	516	HEA	O1A-CGA-CBA	-2.56	114.96	123.09
19	L	522	TGL	CA5-CA4-CA3	-2.56	101.41	114.37
24	T	263	PEK	O03-C21-C22	2.56	119.65	111.83
24	C	264	PEK	O13-P-O14	2.56	124.36	112.44
20	N	1524	PGV	O03-C19-O04	-2.56	117.23	123.63
19	O	1521	TGL	OG3-CG3-CG2	2.55	115.76	108.40
28	M	526	DMU	O16-C18-C19	-2.55	100.71	109.37
18	N	516	HEA	CAD-CBD-CGD	-2.55	106.90	113.67
18	A	515	HEA	O1A-CGA-CBA	-2.54	115.02	123.09
28	G	272	DMU	O3-C5-C10	-2.53	104.04	110.08
19	Y	1522	TGL	CC3-CC2-CC1	2.53	122.97	113.69
25	G	269	CDL	C39-C38-C37	2.52	127.12	114.37
24	P	1264	PEK	C02-O01-C1	2.52	123.83	117.80
25	P	1270	CDL	CA6-OA8-CA7	2.52	126.31	117.12
22	B	1086	CHD	O3-C3-C4	2.51	114.85	109.84
18	A	515	HEA	C2D-C1D-ND	2.51	112.73	109.84
28	G	272	DMU	O61-C57-C4	2.51	119.89	111.33
19	L	522	TGL	OB1-CB1-CB2	-2.49	114.05	123.78
26	R	1230	PSC	C29-C28-C27	-2.49	101.80	114.37
19	L	522	TGL	CA3-CA2-CA1	-2.49	104.59	113.69
25	C	270	CDL	C42-C41-C40	2.48	126.93	114.37
20	A	524	PGV	O03-C19-O04	-2.48	117.43	123.63
25	T	1269	CDL	OA8-CA7-OA9	-2.48	117.44	123.63
19	L	522	TGL	CA7-CA6-CA5	-2.47	101.86	114.37
25	T	1269	CDL	OB6-CB5-OB7	-2.47	117.92	123.70
25	P	1270	CDL	OB2-PB2-OB3	2.47	118.74	108.94
20	P	1267	PGV	O01-C02-C03	-2.47	99.48	108.34
25	P	1270	CDL	OB6-CB4-CB6	2.47	117.20	108.34
19	O	1523	TGL	C24-C23-C22	2.46	126.78	114.37
20	P	1267	PGV	O01-C1-C2	2.45	116.78	111.48
22	O	229	CHD	C14-C8-C7	2.45	115.10	111.85
28	Z	1526	DMU	C28-C25-C22	-2.44	102.03	114.37
19	O	1521	TGL	OG1-CA1-OA1	-2.43	117.54	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	229	CHD	C13-C14-C8	2.43	117.80	114.72
24	T	1265	PEK	C03-C02-C01	-2.43	106.12	111.78
20	H	268	PGV	O14-P-O13	2.43	123.73	112.44
24	G	1263	PEK	C01-O03-C21	2.43	125.98	117.12
25	G	269	CDL	CA6-OA8-CA7	2.42	125.97	117.12
20	N	1268	PGV	C02-O01-C1	2.42	123.58	117.80
22	C	271	CHD	C9-C10-C5	2.41	111.87	108.51
18	N	515	HEA	CHC-C4B-C3B	-2.41	119.72	125.80
18	A	516	HEA	C1A-CHA-C4D	-2.41	120.90	126.02
25	P	1270	CDL	O1-C1-CA2	-2.41	101.37	109.70
24	C	264	PEK	O01-C1-C2	2.40	116.68	111.48
24	P	1264	PEK	C24-C23-C22	-2.40	104.30	113.13
22	J	60	CHD	O12-C12-C13	-2.40	106.96	111.02
25	P	1270	CDL	C42-C41-C40	2.40	126.50	114.37
18	A	516	HEA	CHA-C4D-C3D	-2.40	121.28	124.77
28	P	1272	DMU	O7-C10-O1	2.39	116.99	110.69
18	A	515	HEA	C17-C16-C15	2.39	121.10	113.19
25	G	269	CDL	CB4-OB6-CB5	2.39	123.51	117.80
19	A	521	TGL	OG2-CG2-CG1	2.38	116.87	108.34
19	O	1521	TGL	CB7-CB6-CB5	-2.37	102.38	114.37
18	A	515	HEA	C12-C13-C14	-2.37	105.93	112.16
22	J	60	CHD	O7-C7-C8	-2.36	104.10	109.52
25	P	1270	CDL	C79-C78-C77	2.36	126.31	114.37
19	A	521	TGL	CG3-OG3-CC1	2.36	125.74	117.12
25	G	269	CDL	C43-C42-C41	2.36	126.28	114.37
25	P	1270	CDL	OA8-CA7-C31	2.36	119.02	111.83
18	N	515	HEA	C16-C17-C18	2.35	123.65	112.02
25	P	1270	CDL	C39-C38-C37	2.35	126.23	114.37
19	Y	1522	TGL	C15-CC9-CC8	2.35	126.23	114.37
20	H	268	PGV	O01-C02-C03	2.35	116.76	108.34
22	C	525	CHD	O7-C7-C8	-2.34	104.15	109.52
18	A	516	HEA	O1D-CGD-CBD	-2.34	115.67	123.09
18	N	515	HEA	C17-C16-C15	-2.34	105.43	113.19
25	C	270	CDL	OA8-CA7-C31	2.34	118.97	111.83
25	C	270	CDL	O1-C1-CA2	-2.34	101.62	109.70
22	P	1525	CHD	O3-C3-C4	2.33	114.49	109.84
19	A	521	TGL	C15-CC9-CC8	2.33	126.14	114.37
22	P	1525	CHD	C21-C20-C22	2.32	113.93	110.34
24	P	1264	PEK	C03-C02-C01	-2.32	106.38	111.78
22	J	60	CHD	C9-C8-C7	2.32	114.77	111.86
25	G	269	CDL	C80-C79-C78	2.32	126.07	114.37
19	O	1523	TGL	C21-C20-CA9	2.31	126.03	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	516	HEA	O2D-CGD-CBD	2.30	121.27	114.00
28	M	526	DMU	O55-C2-C1	2.30	115.79	110.38
18	N	516	HEA	C4B-C3B-C2B	-2.30	103.58	107.44
20	N	1266	PGV	O01-C1-O02	-2.30	118.34	123.70
18	N	516	HEA	C12-C11-C3B	-2.29	108.54	112.12
28	Z	1526	DMU	C6-C1-C2	2.29	114.84	110.01
19	Y	1522	TGL	C26-C25-C24	-2.29	102.77	114.37
25	T	1269	CDL	C82-C81-C80	2.29	125.96	114.37
28	P	1272	DMU	O16-C18-C19	2.29	117.14	109.37
22	B	1086	CHD	C22-C23-C24	-2.29	106.38	112.49
18	N	516	HEA	C4A-C3A-C2A	2.29	108.80	106.81
25	T	1269	CDL	C19-C18-C17	2.28	125.88	114.37
22	O	229	CHD	O3-C3-C2	2.27	116.11	110.17
19	Y	1522	TGL	C24-C23-C22	-2.27	102.88	114.37
19	D	523	TGL	C16-C15-CC9	2.27	125.83	114.37
24	C	264	PEK	C26-C25-C24	-2.27	102.92	114.37
19	D	523	TGL	OG1-CG1-CG2	2.26	114.90	108.40
25	G	269	CDL	OB7-CB5-C51	-2.25	114.98	123.78
19	O	1523	TGL	OG1-CA1-OA1	-2.25	118.00	123.63
24	T	263	PEK	C01-O03-C21	2.25	125.34	117.12
28	P	1272	DMU	O7-C3-C2	2.25	112.95	107.23
18	N	515	HEA	CAD-C3D-C2D	2.25	132.07	127.87
18	A	515	HEA	CAA-C2A-C1A	2.24	129.40	124.85
20	P	1267	PGV	O06-C06-C05	-2.24	100.31	110.38
18	N	516	HEA	C4C-C3C-C2C	-2.23	104.53	107.30
19	O	1521	TGL	OB1-CB1-CB2	-2.23	115.05	123.78
25	C	270	CDL	OB6-CB4-CB3	-2.23	100.36	108.34
19	L	522	TGL	C15-CC9-CC8	2.23	125.62	114.37
20	A	522	PGV	C01-O03-C19	-2.22	109.00	117.12
18	A	515	HEA	C20-C19-C18	2.22	126.14	121.17
22	B	1086	CHD	C13-C17-C20	2.22	122.17	119.48
20	P	1267	PGV	O01-C1-O02	-2.22	118.52	123.70
22	B	1086	CHD	C23-C22-C20	2.21	118.59	114.46
28	M	526	DMU	O4-C7-C8	2.21	115.58	110.38
24	C	264	PEK	C32-C31-C30	-2.21	103.21	114.37
19	Y	1522	TGL	CA9-CA8-CA7	-2.21	103.22	114.37
19	Y	1522	TGL	OG2-CG2-CG3	2.20	116.25	108.34
22	J	60	CHD	O3-C3-C2	-2.20	104.41	110.17
18	N	515	HEA	CHD-C1D-C2D	-2.20	120.70	126.95
22	C	271	CHD	O26-C24-C23	-2.20	107.06	114.00
28	G	272	DMU	O7-C10-O1	2.20	116.47	110.69
19	O	1521	TGL	C15-CC9-CC8	2.19	125.46	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	1269	CDL	CB6-OB8-CB7	2.19	125.12	117.12
18	N	515	HEA	CAA-C2A-C1A	2.19	129.30	124.85
24	T	1265	PEK	C33-C32-C31	-2.19	103.32	114.37
28	G	272	DMU	C11-C9-C8	2.18	118.38	113.02
24	P	1264	PEK	C26-C25-C24	-2.18	103.33	114.37
19	D	523	TGL	CC3-CC2-CC1	-2.18	105.71	113.69
18	A	516	HEA	C3B-C4B-NB	2.18	112.34	109.84
22	B	1086	CHD	C19-C10-C5	-2.18	106.80	110.44
19	Y	1522	TGL	OG1-CA1-OA1	-2.17	118.20	123.63
25	C	270	CDL	CA6-OA8-CA7	2.16	125.03	117.12
20	H	268	PGV	O02-C1-C2	-2.16	115.32	123.78
18	N	516	HEA	CHB-C1B-C2B	-2.16	121.62	125.03
19	D	523	TGL	C20-CA9-CA8	2.16	125.28	114.37
24	T	1265	PEK	C35-C34-C33	-2.16	103.47	114.37
26	E	230	PSC	C08-N-C06	2.15	114.63	108.98
24	P	1264	PEK	C01-O03-C21	2.15	124.98	117.12
25	T	1269	CDL	C20-C19-C18	2.15	125.23	114.37
25	T	1269	CDL	C80-C79-C78	2.15	125.23	114.37
22	C	525	CHD	C19-C10-C1	2.15	111.72	108.31
20	H	268	PGV	C3-C2-C1	2.15	121.56	113.69
25	G	269	CDL	C72-C71-CB7	2.15	121.56	113.69
19	O	1521	TGL	C16-C15-CC9	2.15	125.21	114.37
22	C	271	CHD	O25-C24-C23	2.14	129.89	123.09
19	D	523	TGL	C15-CC9-CC8	2.14	125.21	114.37
25	P	1270	CDL	C62-C61-C60	2.14	125.19	114.37
18	N	515	HEA	C1D-ND-C4D	-2.13	102.68	105.21
22	C	525	CHD	C22-C23-C24	-2.13	106.81	112.49
18	N	515	HEA	C13-C12-C11	2.12	117.79	114.39
25	G	269	CDL	OA6-CA5-OA7	-2.12	118.74	123.70
22	W	1060	CHD	O3-C3-C2	-2.12	104.62	110.17
26	R	1230	PSC	O01-C1-O02	-2.12	118.75	123.70
22	O	229	CHD	C4-C5-C10	-2.11	110.41	112.66
25	G	269	CDL	OB8-CB7-C71	2.11	118.27	111.83
24	C	264	PEK	O04-C21-C22	2.11	132.03	123.78
25	G	269	CDL	C79-C78-C77	2.11	125.01	114.37
20	C	267	PGV	O01-C02-C03	-2.10	100.80	108.34
18	N	516	HEA	CHA-C1A-C2A	-2.10	121.55	124.86
20	A	522	PGV	C21-C20-C19	-2.09	106.04	113.69
19	D	523	TGL	OG3-CC1-OC1	-2.09	118.41	123.63
20	N	1266	PGV	C01-O03-C19	-2.08	109.50	117.12
18	N	516	HEA	C12-C13-C14	-2.08	106.69	112.16
18	N	516	HEA	O2D-CGD-O1D	2.08	128.67	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	272	DMU	O4-C7-C5	2.08	115.27	110.38
20	A	524	PGV	C01-O03-C19	2.07	124.70	117.12
26	E	230	PSC	C27-C26-C25	-2.07	103.89	114.37
28	Z	1526	DMU	C31-C28-C25	-2.07	103.89	114.37
22	P	1271	CHD	C16-C15-C14	2.07	109.19	105.14
22	C	525	CHD	C6-C7-C8	2.07	113.76	111.50
22	C	525	CHD	C15-C14-C8	2.07	121.19	118.36
20	H	268	PGV	O12-P-O13	-2.06	100.75	108.94
19	Y	1522	TGL	OB1-CB1-CB2	-2.06	115.71	123.78
25	C	270	CDL	C19-C18-C17	2.06	124.79	114.37
19	D	523	TGL	OG1-CA1-OA1	-2.06	118.48	123.63
18	A	516	HEA	CAA-C2A-C1A	2.05	129.02	124.85
24	G	265	PEK	C7-C8-C9	-2.05	106.27	123.57
26	R	1230	PSC	C07-N-C06	-2.05	103.60	108.98
18	N	515	HEA	C4A-NA-C1A	2.04	109.15	105.82
22	O	229	CHD	C15-C16-C17	2.04	109.13	105.14
20	N	1524	PGV	O01-C02-C03	2.04	115.65	108.34
25	T	1269	CDL	OB2-PB2-OB3	-2.04	100.86	108.94
18	N	516	HEA	CMB-C2B-C1B	-2.03	121.86	125.03
18	N	516	HEA	C2B-C1B-NB	2.03	112.25	109.90
18	N	515	HEA	CHA-C1A-NA	-2.03	122.25	124.45
28	Z	1526	DMU	C10-C5-C7	2.02	114.27	110.01
18	N	515	HEA	C2C-C1C-NC	2.02	113.38	110.14
18	A	516	HEA	C26-C15-C14	2.02	128.80	123.63
25	T	1269	CDL	CA6-CA4-CA3	-2.01	107.10	111.78
24	T	1265	PEK	O01-C02-C03	2.00	115.53	108.34

All (25) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	1086	CHD	C9
22	C	271	CHD	C9
22	J	60	CHD	C9
22	J	60	CHD	C17
22	P	1271	CHD	C9
22	W	1060	CHD	C9
22	W	1060	CHD	C17
28	G	272	DMU	C5
28	G	272	DMU	C9
28	G	272	DMU	C6
28	G	272	DMU	C4
28	G	272	DMU	C2

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Mol	Chain	Res	Type	Atom
28	M	526	DMU	C9
28	M	526	DMU	C4
28	M	526	DMU	C5
28	M	526	DMU	C2
28	P	1272	DMU	C9
28	P	1272	DMU	C4
28	P	1272	DMU	C5
28	P	1272	DMU	C2
28	Z	1526	DMU	C5
28	Z	1526	DMU	C9
28	Z	1526	DMU	C6
28	Z	1526	DMU	C4
28	Z	1526	DMU	C2

All (961) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	515	HEA	C2A-C3A-CMA-OMA
18	A	515	HEA	C4A-C3A-CMA-OMA
18	A	516	HEA	C2A-C3A-CMA-OMA
18	N	515	HEA	C16-C17-C18-C19
18	N	516	HEA	C2A-C3A-CMA-OMA
19	A	521	TGL	CB2-CB1-OG2-CG2
19	A	521	TGL	OB1-CB1-OG2-CG2
19	D	523	TGL	OG1-CG1-CG2-OG2
19	Y	1522	TGL	CB2-CB1-OG2-CG2
20	A	524	PGV	C02-C03-O11-P
20	A	524	PGV	O12-C04-C05-C06
20	A	524	PGV	O04-C19-O03-C01
20	A	524	PGV	C20-C19-O03-C01
20	H	268	PGV	C03-O11-P-O12
20	H	268	PGV	C03-O11-P-O13
20	H	268	PGV	C2-C1-O01-C02
20	N	1524	PGV	C03-O11-P-O13
20	N	1524	PGV	C04-O12-P-O11
20	N	1524	PGV	C02-C03-O11-P
20	N	1524	PGV	C04-C05-C06-O06
20	N	1524	PGV	O02-C1-O01-C02
20	N	1524	PGV	C2-C1-O01-C02
20	N	1524	PGV	C20-C19-O03-C01
20	N	1268	PGV	C03-O11-P-O13
20	N	1268	PGV	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
20	N	1268	PGV	C02-C03-O11-P
22	W	1060	CHD	C16-C17-C20-C21
24	C	264	PEK	C11-C10-C9-C8
24	C	264	PEK	C11-C12-C13-C14
24	C	264	PEK	C13-C14-C15-C16
24	G	265	PEK	C03-O11-P-O12
24	G	265	PEK	C03-O11-P-O13
24	G	265	PEK	C03-O11-P-O14
24	G	265	PEK	O12-C04-C05-N
24	G	265	PEK	C5-C6-C7-C8
24	G	1263	PEK	C03-O11-P-O12
24	G	1263	PEK	C03-O11-P-O13
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	O12-C04-C05-N
24	T	263	PEK	C2-C3-C4-C5
24	T	1265	PEK	C03-O11-P-O14
24	T	1265	PEK	C04-O12-P-O11
24	T	1265	PEK	C04-O12-P-O13
24	T	1265	PEK	C04-O12-P-O14
24	T	1265	PEK	O01-C02-C03-O11
24	T	1265	PEK	O12-C04-C05-N
24	T	1265	PEK	C2-C1-O01-C02
24	T	1265	PEK	C9-C10-C11-C12
25	C	270	CDL	CB2-C1-CA2-OA2
25	C	270	CDL	CA2-OA2-PA1-OA3
25	C	270	CDL	CA2-OA2-PA1-OA5
25	C	270	CDL	CA3-OA5-PA1-OA2
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	C	270	CDL	CB3-OB5-PB2-OB2
25	C	270	CDL	CB3-OB5-PB2-OB3
25	G	269	CDL	CA2-C1-CB2-OB2
25	G	269	CDL	CA3-OA5-PA1-OA4
25	G	269	CDL	C1-CB2-OB2-PB2
25	G	269	CDL	CB2-OB2-PB2-OB5
25	G	269	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
25	G	269	CDL	CB3-OB5-PB2-OB3
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	P	1270	CDL	OB7-CB5-OB6-CB4
25	T	1269	CDL	CA2-C1-CB2-OB2
25	T	1269	CDL	CA2-OA2-PA1-OA3
25	T	1269	CDL	CA3-OA5-PA1-OA4
25	T	1269	CDL	C1-CB2-OB2-PB2
25	T	1269	CDL	CB3-OB5-PB2-OB2
25	T	1269	CDL	CB3-OB5-PB2-OB4
26	E	230	PSC	C03-O11-P-O12
26	E	230	PSC	C03-O11-P-O14
26	E	230	PSC	C04-O12-P-O11
26	E	230	PSC	C04-O12-P-O13
26	R	1230	PSC	C04-O12-P-O11
26	R	1230	PSC	C04-O12-P-O14
26	R	1230	PSC	C10-C11-C12-C13
28	P	1272	DMU	C1-C6-O16-C18
28	Z	1526	DMU	O5-C6-O16-C18
20	N	1524	PGV	O04-C19-O03-C01
26	E	230	PSC	C02-C01-O03-C19
19	D	523	TGL	OC1-CC1-OG3-CG3
19	O	1523	TGL	OC1-CC1-OG3-CG3
22	W	1060	CHD	C16-C17-C20-C22
19	Y	1522	TGL	OB1-CB1-OG2-CG2
20	A	524	PGV	O02-C1-O01-C02
24	T	1265	PEK	O02-C1-O01-C02
25	C	270	CDL	OA7-CA5-OA6-CA4
25	P	1270	CDL	OA7-CA5-OA6-CA4
19	D	523	TGL	CC2-CC1-OG3-CG3
19	O	1523	TGL	CC2-CC1-OG3-CG3
26	E	230	PSC	C20-C19-O03-C01
26	R	1230	PSC	C20-C19-O03-C01
25	P	1270	CDL	C51-CB5-OB6-CB4
22	J	60	CHD	C16-C17-C20-C22
28	M	526	DMU	O5-C4-C57-O61
22	C	271	CHD	C20-C22-C23-C24
19	L	522	TGL	CA2-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
24	C	264	PEK	C10-C11-C12-C13
24	G	265	PEK	C13-C14-C15-C16
24	P	1264	PEK	C7-C8-C9-C10
24	P	1264	PEK	C10-C11-C12-C13
24	T	263	PEK	C4-C5-C6-C7
24	T	263	PEK	C7-C8-C9-C10
26	E	230	PSC	C11-C12-C13-C14
28	G	272	DMU	O6-C11-C9-O1
19	L	522	TGL	OA1-CA1-OG1-CG1
26	R	1230	PSC	O04-C19-O03-C01
20	H	268	PGV	O02-C1-O01-C02
25	G	269	CDL	OA7-CA5-OA6-CA4
26	E	230	PSC	C22-C23-C24-C25
20	N	1524	PGV	O12-C04-C05-O05
25	G	269	CDL	O1-C1-CB2-OB2
25	P	1270	CDL	O1-C1-CB2-OB2
28	Z	1526	DMU	O5-C4-C57-O61
28	Z	1526	DMU	O6-C11-C9-O1
26	E	230	PSC	O04-C19-O03-C01
20	A	524	PGV	C2-C1-O01-C02
25	G	269	CDL	C11-CA5-OA6-CA4
19	L	522	TGL	C20-C21-C22-C23
19	Y	1522	TGL	CC3-CC4-CC5-CC6
20	H	268	PGV	C6-C7-C8-C9
25	T	1269	CDL	C56-C57-C58-C59
28	G	272	DMU	O5-C6-O16-C18
28	P	1272	DMU	O5-C6-O16-C18
19	O	1521	TGL	CA9-C20-C21-C22
19	Y	1522	TGL	CA2-CA1-OG1-CG1
19	L	522	TGL	CC1-CC2-CC3-CC4
24	C	264	PEK	C7-C8-C9-C10
24	G	265	PEK	C10-C11-C12-C13
24	G	1263	PEK	C13-C14-C15-C16
24	T	1265	PEK	C13-C14-C15-C16
26	E	230	PSC	C11-C10-C9-C8
26	R	1230	PSC	C11-C12-C13-C14
24	T	263	PEK	C33-C34-C35-C36
25	P	1270	CDL	C82-C83-C84-C85
25	T	1269	CDL	C15-C16-C17-C18
25	T	1269	CDL	C73-C74-C75-C76
19	Y	1522	TGL	OA1-CA1-OG1-CG1
20	N	1524	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	CB2-C1-CA2-OA2
25	P	1270	CDL	CA2-C1-CB2-OB2
19	O	1521	TGL	CC2-CC1-OG3-CG3
25	T	1269	CDL	C71-CB7-OB8-CB6
26	E	230	PSC	C20-C21-C22-C23
20	H	268	PGV	C20-C21-C22-C23
25	C	270	CDL	C83-C84-C85-C86
24	G	265	PEK	C28-C29-C30-C31
24	T	1265	PEK	C28-C29-C30-C31
28	P	1272	DMU	O6-C11-C9-O1
22	C	271	CHD	C17-C20-C22-C23
19	D	523	TGL	CB9-C10-C11-C12
19	L	522	TGL	CC3-CC4-CC5-CC6
18	N	515	HEA	C26-C15-C16-C17
18	N	515	HEA	C14-C15-C16-C17
25	T	1269	CDL	C22-C23-C24-C25
19	Y	1522	TGL	CC1-CC2-CC3-CC4
25	C	270	CDL	CB7-C71-C72-C73
25	G	269	CDL	O1-C1-CA2-OA2
25	T	1269	CDL	O1-C1-CB2-OB2
19	A	521	TGL	CA9-C20-C21-C22
28	P	1272	DMU	C3-C4-C57-O61
25	G	269	CDL	CA5-C11-C12-C13
24	T	263	PEK	O03-C01-C02-O01
20	A	524	PGV	C19-C20-C21-C22
25	G	269	CDL	C15-C16-C17-C18
28	M	526	DMU	O6-C11-C9-C8
28	M	526	DMU	C19-C22-C25-C28
20	A	522	PGV	C10-C11-C12-C13
20	C	267	PGV	C10-C11-C12-C13
22	P	1271	CHD	C13-C17-C20-C21
19	O	1521	TGL	C22-C23-C24-C25
18	A	515	HEA	C15-C16-C17-C18
26	E	230	PSC	C04-C05-N-C08
19	Y	1522	TGL	CB1-CB2-CB3-CB4
24	G	1263	PEK	C21-C22-C23-C24
25	G	269	CDL	CA7-C31-C32-C33
25	P	1270	CDL	CB7-C71-C72-C73
25	T	1269	CDL	CA7-C31-C32-C33
26	R	1230	PSC	C1-C2-C3-C4
22	J	60	CHD	C13-C17-C20-C22
19	O	1523	TGL	CB1-CB2-CB3-CB4

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Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C19-C20-C21-C22
24	C	264	PEK	C1-C2-C3-C4
19	O	1521	TGL	OC1-CC1-OG3-CG3
25	T	1269	CDL	OB9-CB7-OB8-CB6
25	G	269	CDL	C59-C60-C61-C62
20	A	524	PGV	O12-C04-C05-O05
20	N	1268	PGV	O12-C04-C05-O05
25	C	270	CDL	O1-C1-CA2-OA2
22	J	60	CHD	C13-C17-C20-C21
20	H	268	PGV	C1-C2-C3-C4
24	G	265	PEK	C1-C2-C3-C4
20	P	1267	PGV	C12-C13-C14-C15
22	C	271	CHD	C21-C20-C22-C23
24	G	1263	PEK	C10-C11-C12-C13
24	P	1264	PEK	C13-C14-C15-C16
28	M	526	DMU	O6-C11-C9-O1
25	G	269	CDL	C60-C61-C62-C63
28	P	1272	DMU	O16-C18-C19-C22
22	J	60	CHD	C16-C17-C20-C21
20	P	1267	PGV	C1-C2-C3-C4
25	P	1270	CDL	CA7-C31-C32-C33
19	A	521	TGL	C12-C13-C14-C29
20	N	1268	PGV	C1-C2-C3-C4
20	N	1268	PGV	O12-C04-C05-C06
24	T	263	PEK	C22-C21-O03-C01
26	R	1230	PSC	C04-C05-N-C06
26	R	1230	PSC	C04-C05-N-C08
24	G	265	PEK	C22-C21-O03-C01
25	G	269	CDL	C39-C40-C41-C42
20	A	524	PGV	C10-C11-C12-C13
20	N	1268	PGV	C10-C11-C12-C13
25	P	1270	CDL	C61-C62-C63-C64
25	P	1270	CDL	O1-C1-CA2-OA2
24	T	263	PEK	O04-C21-O03-C01
20	H	268	PGV	C02-C03-O11-P
20	A	524	PGV	C04-C05-C06-O06
28	G	272	DMU	C3-C4-C57-O61
19	A	521	TGL	CG1-CG2-OG2-CB1
28	Z	1526	DMU	O16-C18-C19-C22
28	G	272	DMU	O5-C4-C57-O61
25	T	1269	CDL	C11-CA5-OA6-CA4
19	O	1523	TGL	OG1-CG1-CG2-OG2

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Mol	Chain	Res	Type	Atoms
22	W	1060	CHD	C13-C17-C20-C21
26	R	1230	PSC	C04-C05-N-C07
20	A	522	PGV	C19-C20-C21-C22
24	G	1263	PEK	C31-C32-C33-C34
24	T	1265	PEK	C29-C30-C31-C32
25	C	270	CDL	C39-C40-C41-C42
25	G	269	CDL	C75-C76-C77-C78
19	O	1521	TGL	CB9-C10-C11-C12
19	O	1521	TGL	CC5-CC6-CC7-CC8
20	N	1266	PGV	C6-C7-C8-C9
25	C	270	CDL	C61-C62-C63-C64
25	G	269	CDL	C56-C57-C58-C59
25	P	1270	CDL	C62-C63-C64-C65
26	E	230	PSC	C24-C25-C26-C27
26	E	230	PSC	C19-C20-C21-C22
20	H	268	PGV	C24-C25-C26-C27
20	N	1266	PGV	C7-C8-C9-C10
20	N	1268	PGV	C13-C14-C15-C16
26	R	1230	PSC	C24-C25-C26-C27
19	L	522	TGL	CA5-CA6-CA7-CA8
19	O	1523	TGL	CA9-C20-C21-C22
19	Y	1522	TGL	CC6-CC7-CC8-CC9
20	C	267	PGV	C7-C8-C9-C10
20	N	1268	PGV	C22-C23-C24-C25
25	C	270	CDL	C58-C59-C60-C61
25	G	269	CDL	C38-C39-C40-C41
25	P	1270	CDL	C36-C37-C38-C39
25	P	1270	CDL	C37-C38-C39-C40
20	N	1524	PGV	O05-C05-C06-O06
28	Z	1526	DMU	C19-C18-O16-C6
19	L	522	TGL	CC6-CC7-CC8-CC9
20	H	268	PGV	C28-C29-C30-C31
24	P	1264	PEK	C23-C24-C25-C26
25	G	269	CDL	C22-C23-C24-C25
25	G	269	CDL	C36-C37-C38-C39
28	G	272	DMU	C28-C31-C34-C37
19	O	1523	TGL	C15-C16-C17-C18
19	Y	1522	TGL	C22-C23-C24-C25
19	Y	1522	TGL	C19-C33-C34-C35
28	Z	1526	DMU	C25-C28-C31-C34
24	T	1265	PEK	C15-C16-C17-C18
20	N	1268	PGV	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	C77-C78-C79-C80
26	E	230	PSC	C01-C02-C03-O11
25	C	270	CDL	C51-CB5-OB6-CB4
19	L	522	TGL	C16-C15-CC9-CC8
25	C	270	CDL	C57-C58-C59-C60
25	T	1269	CDL	C82-C83-C84-C85
26	E	230	PSC	C1-C2-C3-C4
19	A	521	TGL	C13-C14-C29-C30
19	D	523	TGL	C16-C15-CC9-CC8
20	N	1524	PGV	C2-C3-C4-C5
25	C	270	CDL	C38-C39-C40-C41
25	P	1270	CDL	C12-C13-C14-C15
19	A	521	TGL	C20-C21-C22-C23
19	A	521	TGL	C21-C22-C23-C24
24	G	1263	PEK	C27-C28-C29-C30
24	P	1264	PEK	C31-C32-C33-C34
25	C	270	CDL	C16-C17-C18-C19
25	P	1270	CDL	C64-C65-C66-C67
24	G	265	PEK	O04-C21-O03-C01
25	T	1269	CDL	C36-C37-C38-C39
22	W	1060	CHD	C13-C17-C20-C22
25	T	1269	CDL	OA7-CA5-OA6-CA4
20	H	268	PGV	C4-C5-C6-C7
19	L	522	TGL	CC4-CC5-CC6-CC7
19	O	1523	TGL	CA4-CA5-CA6-CA7
19	O	1523	TGL	CC4-CC5-CC6-CC7
20	A	524	PGV	C14-C15-C16-C17
24	G	265	PEK	C24-C25-C26-C27
25	G	269	CDL	C77-C78-C79-C80
26	R	1230	PSC	C21-C22-C23-C24
19	D	523	TGL	C11-C10-CB9-CB8
19	O	1521	TGL	C17-C18-C19-C33
25	C	270	CDL	C17-C18-C19-C20
25	G	269	CDL	C73-C74-C75-C76
25	T	1269	CDL	C18-C19-C20-C21
25	T	1269	CDL	C31-C32-C33-C34
25	T	1269	CDL	C11-C12-C13-C14
19	A	521	TGL	C24-C25-C26-C27
19	D	523	TGL	C21-C20-CA9-CA8
25	G	269	CDL	C80-C81-C82-C83
25	P	1270	CDL	C63-C64-C65-C66
22	P	1525	CHD	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
19	A	521	TGL	CC5-CC6-CC7-CC8
19	Y	1522	TGL	C21-C22-C23-C24
25	T	1269	CDL	C75-C76-C77-C78
19	D	523	TGL	CB1-CB2-CB3-CB4
19	O	1521	TGL	CA1-CA2-CA3-CA4
20	N	1524	PGV	C1-C2-C3-C4
25	T	1269	CDL	CB7-C71-C72-C73
19	Y	1522	TGL	C11-C10-CB9-CB8
19	A	521	TGL	CC2-CC1-OG3-CG3
24	G	1263	PEK	C4-C5-C6-C7
24	T	1265	PEK	C7-C8-C9-C10
19	O	1521	TGL	C10-C11-C12-C13
19	O	1523	TGL	CB9-C10-C11-C12
19	O	1523	TGL	CC9-C15-C16-C17
25	C	270	CDL	C52-C53-C54-C55
20	N	1268	PGV	C23-C24-C25-C26
24	T	263	PEK	C16-C17-C18-C19
24	T	1265	PEK	C25-C26-C27-C28
25	P	1270	CDL	C53-C54-C55-C56
25	T	1269	CDL	C60-C61-C62-C63
20	H	268	PGV	C19-C20-C21-C22
19	L	522	TGL	C21-C22-C23-C24
19	O	1521	TGL	C18-C19-C33-C34
20	A	524	PGV	C26-C27-C28-C29
20	N	1524	PGV	C24-C25-C26-C27
24	T	1265	PEK	C16-C17-C18-C19
25	C	270	CDL	C11-C12-C13-C14
19	Y	1522	TGL	C16-C17-C18-C19
19	O	1521	TGL	C25-C26-C27-C28
25	C	270	CDL	OB7-CB5-OB6-CB4
19	Y	1522	TGL	CB9-C10-C11-C12
20	N	1524	PGV	C3-C4-C5-C6
25	T	1269	CDL	C38-C39-C40-C41
19	O	1521	TGL	CA4-CA5-CA6-CA7
19	Y	1522	TGL	CB4-CB5-CB6-CB7
25	G	269	CDL	C16-C17-C18-C19
25	G	269	CDL	C55-C56-C57-C58
19	O	1521	TGL	C16-C17-C18-C19
19	Y	1522	TGL	C14-C29-C30-C31
20	P	1267	PGV	C28-C29-C30-C31
25	G	269	CDL	C62-C63-C64-C65
28	M	526	DMU	O5-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
19	D	523	TGL	C23-C24-C25-C26
20	N	1268	PGV	C24-C25-C26-C27
28	G	272	DMU	C1-C6-O16-C18
19	Y	1522	TGL	C18-C19-C33-C34
25	G	269	CDL	C42-C43-C44-C45
19	O	1523	TGL	CC2-CC3-CC4-CC5
25	C	270	CDL	C71-C72-C73-C74
25	C	270	CDL	C72-C73-C74-C75
24	C	264	PEK	C3-C4-C5-C6
19	O	1521	TGL	C14-C29-C30-C31
24	P	1264	PEK	C24-C25-C26-C27
24	T	1265	PEK	C33-C34-C35-C36
25	P	1270	CDL	C42-C43-C44-C45
25	T	1269	CDL	C61-C62-C63-C64
28	P	1272	DMU	C31-C34-C37-C40
19	D	523	TGL	CB2-CB1-OG2-CG2
19	L	522	TGL	CB2-CB1-OG2-CG2
19	O	1521	TGL	CB2-CB1-OG2-CG2
20	N	1268	PGV	C31-C32-C33-C34
19	L	522	TGL	OB1-CB1-OG2-CG2
19	Y	1522	TGL	CB5-CB6-CB7-CB8
24	P	1264	PEK	C26-C27-C28-C29
24	T	1265	PEK	C34-C35-C36-C37
24	G	265	PEK	C2-C3-C4-C5
24	P	1264	PEK	C15-C16-C17-C18
24	T	1265	PEK	C2-C3-C4-C5
19	A	521	TGL	CA1-CA2-CA3-CA4
20	C	267	PGV	C1-C2-C3-C4
24	G	1263	PEK	C25-C26-C27-C28
24	G	1263	PEK	C29-C30-C31-C32
25	P	1270	CDL	C73-C74-C75-C76
25	P	1270	CDL	C81-C82-C83-C84
26	E	230	PSC	C26-C27-C28-C29
25	T	1269	CDL	CB5-C51-C52-C53
19	Y	1522	TGL	CC9-C15-C16-C17
25	C	270	CDL	C21-C22-C23-C24
26	R	1230	PSC	C29-C30-C31-C32
19	O	1523	TGL	CC5-CC6-CC7-CC8
19	A	521	TGL	CB3-CB4-CB5-CB6
20	N	1266	PGV	C5-C6-C7-C8
25	G	269	CDL	C18-C19-C20-C21
25	G	269	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	O	1521	TGL	OB1-CB1-OG2-CG2
20	H	268	PGV	O01-C02-C03-O11
25	P	1270	CDL	C74-C75-C76-C77
28	G	272	DMU	C31-C34-C37-C40
19	A	521	TGL	CC4-CC5-CC6-CC7
25	P	1270	CDL	C16-C17-C18-C19
19	A	521	TGL	OC1-CC1-OG3-CG3
25	T	1269	CDL	C55-C56-C57-C58
26	R	1230	PSC	C5-C6-C7-C8
20	H	268	PGV	O03-C01-C02-O01
20	N	1268	PGV	C12-C13-C14-C15
26	E	230	PSC	C13-C14-C15-C16
20	A	524	PGV	C25-C26-C27-C28
25	T	1269	CDL	C57-C58-C59-C60
19	A	521	TGL	CA7-CA8-CA9-C20
19	A	521	TGL	C21-C20-CA9-CA8
19	D	523	TGL	C17-C18-C19-C33
20	P	1267	PGV	C22-C23-C24-C25
24	T	263	PEK	C29-C30-C31-C32
19	O	1523	TGL	CA6-CA7-CA8-CA9
19	Y	1522	TGL	C23-C24-C25-C26
20	P	1267	PGV	C24-C25-C26-C27
24	C	264	PEK	C27-C28-C29-C30
19	O	1523	TGL	C11-C12-C13-C14
19	O	1523	TGL	C16-C15-CC9-CC8
25	C	270	CDL	C36-C37-C38-C39
19	A	521	TGL	C16-C15-CC9-CC8
20	N	1268	PGV	C14-C15-C16-C17
25	C	270	CDL	C53-C54-C55-C56
25	G	269	CDL	C33-C34-C35-C36
25	T	1269	CDL	C59-C60-C61-C62
26	E	230	PSC	C5-C6-C7-C8
19	O	1523	TGL	C21-C20-CA9-CA8
25	C	270	CDL	C35-C36-C37-C38
25	T	1269	CDL	C40-C41-C42-C43
18	A	515	HEA	C27-C19-C20-C21
20	A	522	PGV	C23-C24-C25-C26
20	P	1267	PGV	C10-C11-C12-C13
19	Y	1522	TGL	C24-C25-C26-C27
19	A	521	TGL	CA5-CA6-CA7-CA8
28	M	526	DMU	O16-C18-C19-C22
24	C	264	PEK	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
19	D	523	TGL	C15-C16-C17-C18
20	N	1266	PGV	C23-C24-C25-C26
24	C	264	PEK	C28-C29-C30-C31
25	G	269	CDL	C71-C72-C73-C74
28	M	526	DMU	C25-C28-C31-C34
20	H	268	PGV	C01-C02-C03-O11
20	N	1268	PGV	C01-C02-C03-O11
24	T	1265	PEK	C01-C02-C03-O11
25	C	270	CDL	OA5-CA3-CA4-CA6
25	P	1270	CDL	OA5-CA3-CA4-CA6
19	O	1521	TGL	CB1-CB2-CB3-CB4
24	C	264	PEK	C23-C24-C25-C26
19	L	522	TGL	C17-C18-C19-C33
20	H	268	PGV	C30-C31-C32-C33
19	O	1523	TGL	CC6-CC7-CC8-CC9
19	A	521	TGL	CC7-CC8-CC9-C15
25	G	269	CDL	C20-C21-C22-C23
19	O	1521	TGL	CC4-CC5-CC6-CC7
24	T	1265	PEK	C22-C21-O03-C01
24	P	1264	PEK	C3-C4-C5-C6
19	O	1523	TGL	C18-C19-C33-C34
20	P	1267	PGV	C7-C8-C9-C10
19	D	523	TGL	OB1-CB1-OG2-CG2
20	N	1524	PGV	C10-C11-C12-C13
24	T	1265	PEK	C4-C5-C6-C7
20	N	1266	PGV	C29-C30-C31-C32
25	T	1269	CDL	C71-C72-C73-C74
19	D	523	TGL	OG1-CG1-CG2-CG3
19	O	1523	TGL	OG1-CG1-CG2-CG3
24	G	1263	PEK	O03-C01-C02-C03
24	T	263	PEK	O03-C01-C02-C03
20	A	522	PGV	C26-C27-C28-C29
25	C	270	CDL	C79-C80-C81-C82
20	N	1524	PGV	C12-C13-C14-C15
19	D	523	TGL	CA6-CA7-CA8-CA9
19	O	1521	TGL	C16-C15-CC9-CC8
19	L	522	TGL	CC2-CC3-CC4-CC5
25	C	270	CDL	C56-C57-C58-C59
25	C	270	CDL	CB5-C51-C52-C53
19	Y	1522	TGL	CC4-CC5-CC6-CC7
19	L	522	TGL	C21-C20-CA9-CA8
25	G	269	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
19	L	522	TGL	C11-C12-C13-C14
26	E	230	PSC	C04-C05-N-C07
24	P	1264	PEK	C1-C2-C3-C4
25	G	269	CDL	CB7-C71-C72-C73
25	C	270	CDL	C78-C79-C80-C81
25	P	1270	CDL	C71-C72-C73-C74
19	O	1523	TGL	CA5-CA6-CA7-CA8
26	R	1230	PSC	C26-C27-C28-C29
20	A	524	PGV	C21-C22-C23-C24
24	G	1263	PEK	C22-C23-C24-C25
19	D	523	TGL	CB2-CB3-CB4-CB5
26	R	1230	PSC	C23-C24-C25-C26
20	N	1268	PGV	C19-C20-C21-C22
20	C	267	PGV	C20-C21-C22-C23
20	C	267	PGV	C29-C30-C31-C32
25	G	269	CDL	C78-C79-C80-C81
19	D	523	TGL	CG3-CG2-OG2-CB1
19	O	1523	TGL	CG3-CG2-OG2-CB1
20	A	524	PGV	C03-C02-O01-C1
26	E	230	PSC	C03-C02-O01-C1
26	R	1230	PSC	C03-C02-O01-C1
20	H	268	PGV	C13-C14-C15-C16
20	N	1524	PGV	C22-C23-C24-C25
25	C	270	CDL	C42-C43-C44-C45
24	G	265	PEK	C30-C31-C32-C33
26	E	230	PSC	C27-C28-C29-C30
19	Y	1522	TGL	C15-C16-C17-C18
20	N	1524	PGV	C30-C31-C32-C33
22	C	271	CHD	C13-C17-C20-C22
19	O	1523	TGL	C14-C29-C30-C31
25	P	1270	CDL	C51-C52-C53-C54
28	G	272	DMU	C25-C28-C31-C34
18	A	515	HEA	C16-C17-C18-C19
19	A	521	TGL	C16-C17-C18-C19
20	N	1524	PGV	C5-C6-C7-C8
28	Z	1526	DMU	C22-C25-C28-C31
25	G	269	CDL	C17-C18-C19-C20
25	T	1269	CDL	C72-C73-C74-C75
25	C	270	CDL	OA6-CA4-CA6-OA8
25	G	269	CDL	OA6-CA4-CA6-OA8
25	G	269	CDL	OB6-CB4-CB6-OB8
25	P	1270	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
20	P	1267	PGV	C15-C16-C17-C18
19	O	1521	TGL	CB4-CB5-CB6-CB7
19	O	1523	TGL	CC7-CC8-CC9-C15
24	C	264	PEK	C17-C18-C19-C20
28	Z	1526	DMU	C34-C37-C40-C43
25	G	269	CDL	C74-C75-C76-C77
25	T	1269	CDL	C24-C25-C26-C27
26	R	1230	PSC	C31-C32-C33-C34
25	G	269	CDL	C32-C31-CA7-OA8
20	A	522	PGV	C24-C25-C26-C27
20	H	268	PGV	C11-C10-C9-C8
24	C	264	PEK	C15-C16-C17-C18
24	G	265	PEK	C35-C36-C37-C38
20	N	1266	PGV	C31-C32-C33-C34
24	T	263	PEK	C26-C27-C28-C29
19	D	523	TGL	C16-C17-C18-C19
20	A	524	PGV	C24-C25-C26-C27
20	A	522	PGV	C31-C32-C33-C34
20	H	268	PGV	C10-C11-C12-C13
24	G	265	PEK	C4-C5-C6-C7
19	O	1521	TGL	C20-C21-C22-C23
24	P	1264	PEK	C35-C36-C37-C38
24	P	1264	PEK	C25-C26-C27-C28
25	C	270	CDL	C18-C19-C20-C21
25	G	269	CDL	C35-C36-C37-C38
25	G	269	CDL	C61-C62-C63-C64
25	C	270	CDL	C1-CA2-OA2-PA1
19	Y	1522	TGL	CA9-C20-C21-C22
20	A	522	PGV	C5-C6-C7-C8
26	E	230	PSC	C31-C32-C33-C34
19	L	522	TGL	OG2-CB1-CB2-CB3
24	T	1265	PEK	C30-C31-C32-C33
19	D	523	TGL	CA5-CA6-CA7-CA8
19	Y	1522	TGL	C17-C18-C19-C33
20	C	267	PGV	C24-C25-C26-C27
20	P	1267	PGV	C25-C26-C27-C28
25	T	1269	CDL	C34-C35-C36-C37
20	A	524	PGV	C28-C29-C30-C31
25	C	270	CDL	C82-C83-C84-C85
26	E	230	PSC	C3-C4-C5-C6
28	M	526	DMU	C34-C37-C40-C43
25	G	269	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	OA5-CA3-CA4-CA6
20	C	267	PGV	C31-C32-C33-C34
20	H	268	PGV	C15-C16-C17-C18
19	A	521	TGL	CA4-CA5-CA6-CA7
25	T	1269	CDL	O1-C1-CA2-OA2
25	P	1270	CDL	C57-C58-C59-C60
24	T	1265	PEK	O04-C21-O03-C01
25	C	270	CDL	C37-C38-C39-C40
26	R	1230	PSC	C28-C29-C30-C31
19	L	522	TGL	CB7-CB8-CB9-C10
19	O	1523	TGL	CA7-CA8-CA9-C20
20	H	268	PGV	C25-C26-C27-C28
25	C	270	CDL	CA3-CA4-CA6-OA8
25	C	270	CDL	CB3-CB4-CB6-OB8
25	G	269	CDL	CA3-CA4-CA6-OA8
25	P	1270	CDL	CB3-CB4-CB6-OB8
19	L	522	TGL	C13-C14-C29-C30
26	R	1230	PSC	C2-C3-C4-C5
20	N	1524	PGV	C28-C29-C30-C31
25	P	1270	CDL	C13-C14-C15-C16
20	N	1524	PGV	C31-C32-C33-C34
25	C	270	CDL	C84-C85-C86-C87
24	G	1263	PEK	C26-C27-C28-C29
19	O	1521	TGL	CB6-CB7-CB8-CB9
24	T	263	PEK	O01-C02-C03-O11
25	C	270	CDL	OA5-CA3-CA4-OA6
25	G	269	CDL	C52-C53-C54-C55
25	P	1270	CDL	C24-C25-C26-C27
20	C	267	PGV	C02-C03-O11-P
25	P	1270	CDL	CA4-CA3-OA5-PA1
25	P	1270	CDL	C72-C73-C74-C75
20	H	268	PGV	C23-C24-C25-C26
25	G	269	CDL	C34-C35-C36-C37
24	P	1264	PEK	C17-C18-C19-C20
19	D	523	TGL	CA4-CA5-CA6-CA7
19	L	522	TGL	C22-C23-C24-C25
20	N	1524	PGV	C20-C21-C22-C23
19	L	522	TGL	OG2-CG2-CG3-OG3
24	C	264	PEK	C9-C10-C11-C12
24	C	264	PEK	C12-C13-C14-C15
24	G	265	PEK	C11-C10-C9-C8
24	G	265	PEK	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	G	1263	PEK	C9-C10-C11-C12
24	G	1263	PEK	C11-C12-C13-C14
24	P	1264	PEK	C11-C10-C9-C8
24	P	1264	PEK	C9-C10-C11-C12
24	T	263	PEK	C6-C7-C8-C9
24	T	263	PEK	C11-C12-C13-C14
24	T	263	PEK	C12-C13-C14-C15
24	T	1265	PEK	C5-C6-C7-C8
24	T	1265	PEK	C6-C7-C8-C9
26	R	1230	PSC	C9-C10-C11-C12
25	P	1270	CDL	C59-C60-C61-C62
20	H	268	PGV	C21-C22-C23-C24
25	G	269	CDL	C31-C32-C33-C34
20	N	1524	PGV	C26-C27-C28-C29
25	P	1270	CDL	C52-C53-C54-C55
19	L	522	TGL	C11-C10-CB9-CB8
19	A	521	TGL	CB9-C10-C11-C12
25	C	270	CDL	C54-C55-C56-C57
26	E	230	PSC	C04-C05-N-C06
20	A	524	PGV	O05-C05-C06-O06
19	D	523	TGL	OG2-CB1-CB2-CB3
19	O	1521	TGL	CC7-CC8-CC9-C15
19	Y	1522	TGL	C11-C12-C13-C14
28	P	1272	DMU	C28-C31-C34-C37
20	H	268	PGV	C20-C19-O03-C01
20	P	1267	PGV	C13-C14-C15-C16
20	N	1524	PGV	C01-C02-C03-O11
19	A	521	TGL	C14-C29-C30-C31
20	H	268	PGV	C5-C6-C7-C8
26	E	230	PSC	C29-C30-C31-C32
20	A	524	PGV	C31-C32-C33-C34
19	L	522	TGL	OG1-CA1-CA2-CA3
28	Z	1526	DMU	C19-C22-C25-C28
19	D	523	TGL	C13-C14-C29-C30
26	R	1230	PSC	C27-C28-C29-C30
19	D	523	TGL	CC6-CC7-CC8-CC9
28	M	526	DMU	C22-C25-C28-C31
20	A	524	PGV	C11-C10-C9-C8
20	A	522	PGV	C11-C10-C9-C8
19	A	521	TGL	CB6-CB7-CB8-CB9
25	P	1270	CDL	C84-C85-C86-C87
20	H	268	PGV	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
24	T	263	PEK	C25-C26-C27-C28
19	D	523	TGL	OG1-CA1-CA2-CA3
25	P	1270	CDL	OB5-CB3-CB4-OB6
19	L	522	TGL	C12-C13-C14-C29
19	Y	1522	TGL	CG1-CG2-CG3-OG3
26	E	230	PSC	O03-C01-C02-C03
26	R	1230	PSC	O03-C01-C02-C03
19	O	1521	TGL	C19-C33-C34-C35
25	C	270	CDL	C40-C41-C42-C43
20	H	268	PGV	C22-C23-C24-C25
24	G	1263	PEK	C16-C17-C18-C19
20	C	267	PGV	C12-C13-C14-C15
26	E	230	PSC	C6-C7-C8-C9
25	C	270	CDL	C59-C60-C61-C62
24	G	265	PEK	C26-C27-C28-C29
25	G	269	CDL	C54-C55-C56-C57
20	P	1267	PGV	C14-C15-C16-C17
20	N	1268	PGV	C4-C5-C6-C7
28	P	1272	DMU	O6-C11-C9-C8
20	N	1266	PGV	C25-C26-C27-C28
26	E	230	PSC	O12-C04-C05-N
26	R	1230	PSC	O12-C04-C05-N
20	H	268	PGV	O04-C19-O03-C01
28	P	1272	DMU	C34-C37-C40-C43
20	C	267	PGV	C28-C29-C30-C31
20	A	524	PGV	C7-C8-C9-C10
24	G	265	PEK	C25-C26-C27-C28
20	P	1267	PGV	C31-C32-C33-C34
19	O	1521	TGL	C23-C24-C25-C26
19	D	523	TGL	C18-C19-C33-C34
20	N	1268	PGV	C3-C4-C5-C6
24	G	265	PEK	C29-C30-C31-C32
24	T	263	PEK	C01-C02-C03-O11
25	T	1269	CDL	OB5-CB3-CB4-CB6
24	T	1265	PEK	C14-C15-C16-C17
20	N	1268	PGV	C05-C04-O12-P
19	Y	1522	TGL	CA5-CA6-CA7-CA8
26	R	1230	PSC	O02-C1-O01-C02
25	T	1269	CDL	OA5-CA3-CA4-OA6
26	E	230	PSC	O01-C02-C03-O11
24	T	263	PEK	C32-C33-C34-C35
25	P	1270	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
19	L	522	TGL	CC7-CC8-CC9-C15
24	T	263	PEK	C28-C29-C30-C31
25	P	1270	CDL	C83-C84-C85-C86
18	N	515	HEA	C4A-C3A-CMA-OMA
19	O	1521	TGL	CA3-CA4-CA5-CA6
24	G	1263	PEK	C32-C33-C34-C35
25	C	270	CDL	OB6-CB4-CB6-OB8
20	N	1266	PGV	C10-C11-C12-C13
19	L	522	TGL	C10-C11-C12-C13
19	L	522	TGL	CG1-CG2-CG3-OG3
25	G	269	CDL	CB3-CB4-CB6-OB8
25	P	1270	CDL	C31-C32-C33-C34
28	G	272	DMU	C34-C37-C40-C43
20	N	1266	PGV	C9-C10-C11-C12
25	C	270	CDL	C34-C35-C36-C37
19	D	523	TGL	CC7-CC8-CC9-C15
19	O	1521	TGL	C12-C13-C14-C29
19	Y	1522	TGL	CB7-CB8-CB9-C10
20	H	268	PGV	C03-O11-P-O14
20	H	268	PGV	C04-O12-P-O13
20	N	1524	PGV	C04-O12-P-O13
20	N	1266	PGV	C04-O12-P-O13
24	G	265	PEK	C04-O12-P-O14
24	G	1263	PEK	C04-O12-P-O11
24	G	1263	PEK	C04-O12-P-O13
24	G	1263	PEK	C04-O12-P-O14
24	T	1265	PEK	C03-O11-P-O12
25	C	270	CDL	CA2-OA2-PA1-OA4
25	C	270	CDL	CA3-OA5-PA1-OA3
25	C	270	CDL	CB2-OB2-PB2-OB5
25	C	270	CDL	CB3-OB5-PB2-OB4
25	G	269	CDL	CA3-OA5-PA1-OA2
25	G	269	CDL	CA3-OA5-PA1-OA3
25	G	269	CDL	CB3-OB5-PB2-OB4
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-OA4
25	T	1269	CDL	CA3-OA5-PA1-OA2
25	T	1269	CDL	CA3-OA5-PA1-OA3
25	T	1269	CDL	CB2-OB2-PB2-OB3
26	E	230	PSC	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
26	R	1230	PSC	C04-O12-P-O13
20	P	1267	PGV	C02-C03-O11-P
24	G	1263	PEK	C02-C03-O11-P
25	T	1269	CDL	CA4-CA3-OA5-PA1
19	Y	1522	TGL	CA4-CA5-CA6-CA7
24	C	264	PEK	C34-C35-C36-C37
20	N	1524	PGV	C11-C12-C13-C14
20	A	522	PGV	C7-C8-C9-C10
19	O	1521	TGL	CG1-CG2-OG2-CB1
25	T	1269	CDL	C14-C15-C16-C17
19	L	522	TGL	CB6-CB7-CB8-CB9
20	N	1266	PGV	C26-C27-C28-C29
24	G	265	PEK	C23-C24-C25-C26
25	G	269	CDL	C32-C33-C34-C35
25	T	1269	CDL	C80-C81-C82-C83
26	E	230	PSC	O01-C1-C2-C3
25	P	1270	CDL	OA5-CA3-CA4-OA6
25	G	269	CDL	C23-C24-C25-C26
18	N	516	HEA	O11-C11-C12-C13
24	C	264	PEK	C2-C3-C4-C5
20	N	1268	PGV	O02-C1-O01-C02
20	A	522	PGV	O03-C19-C20-C21
19	A	521	TGL	CA6-CA7-CA8-CA9
25	G	269	CDL	C14-C15-C16-C17
25	G	269	CDL	C76-C77-C78-C79
25	T	1269	CDL	C20-C21-C22-C23
26	R	1230	PSC	C2-C1-O01-C02
25	G	269	CDL	OB7-CB5-OB6-CB4
20	A	522	PGV	C12-C13-C14-C15
20	N	1268	PGV	C15-C16-C17-C18
19	Y	1522	TGL	CC2-CC1-OG3-CG3
24	G	1263	PEK	C17-C18-C19-C20
19	Y	1522	TGL	OG2-CB1-CB2-CB3
25	G	269	CDL	C51-CB5-OB6-CB4
20	A	522	PGV	C29-C30-C31-C32
25	T	1269	CDL	C44-C45-C46-C47
20	H	268	PGV	C2-C3-C4-C5
25	G	269	CDL	C57-C58-C59-C60
25	G	269	CDL	C32-C31-CA7-OA9
20	A	524	PGV	O01-C1-C2-C3
19	Y	1522	TGL	C16-C15-CC9-CC8
25	T	1269	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
24	C	264	PEK	C24-C25-C26-C27
24	G	265	PEK	C17-C18-C19-C20
25	G	269	CDL	C53-C54-C55-C56
20	A	522	PGV	C9-C10-C11-C12
24	P	1264	PEK	C14-C15-C16-C17
25	C	270	CDL	C60-C61-C62-C63
25	G	269	CDL	C12-C13-C14-C15
25	G	269	CDL	C40-C41-C42-C43
28	G	272	DMU	C5-C10-O7-C3
25	C	270	CDL	C51-C52-C53-C54
20	C	267	PGV	C30-C31-C32-C33
20	P	1267	PGV	C23-C24-C25-C26
19	O	1523	TGL	C22-C23-C24-C25
24	T	263	PEK	O01-C1-C2-C3
19	Y	1522	TGL	OC1-CC1-OG3-CG3
19	L	522	TGL	C29-C30-C31-C32
25	P	1270	CDL	C19-C20-C21-C22
20	N	1266	PGV	C24-C25-C26-C27
25	T	1269	CDL	C37-C38-C39-C40
25	G	269	CDL	CB4-CB3-OB5-PB2
18	A	516	HEA	CAD-CBD-CGD-O1D
22	W	1060	CHD	C22-C23-C24-O26
22	O	229	CHD	C22-C23-C24-O25
20	A	522	PGV	C11-C12-C13-C14
24	T	1265	PEK	O03-C01-C02-C03
25	P	1270	CDL	CA3-CA4-CA6-OA8
20	N	1524	PGV	C03-C02-O01-C1
20	A	522	PGV	C28-C29-C30-C31
18	N	516	HEA	CAD-CBD-CGD-O2D
19	O	1523	TGL	C12-C13-C14-C29
25	T	1269	CDL	OA9-CA7-OA8-CA6
19	Y	1522	TGL	C33-C34-C35-C36
25	C	270	CDL	C43-C44-C45-C46
25	T	1269	CDL	C16-C17-C18-C19
19	D	523	TGL	C29-C30-C31-C32
22	W	1060	CHD	C22-C23-C24-O25
22	C	271	CHD	C22-C23-C24-O25
20	A	524	PGV	C9-C10-C11-C12
25	C	270	CDL	C1-CB2-OB2-PB2
18	A	516	HEA	CAA-CBA-CGA-O1A
22	J	60	CHD	C22-C23-C24-O25
22	O	229	CHD	C22-C23-C24-O26

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Mol	Chain	Res	Type	Atoms
24	G	1263	PEK	C01-C02-C03-O11
20	N	1268	PGV	C29-C30-C31-C32
18	N	516	HEA	CAA-CBA-CGA-O1A
22	P	1271	CHD	C22-C23-C24-O25
19	L	522	TGL	CA6-CA7-CA8-CA9
19	O	1523	TGL	CB2-CB3-CB4-CB5
24	G	265	PEK	C6-C7-C8-C9
24	G	1263	PEK	C11-C10-C9-C8
24	G	1263	PEK	C12-C13-C14-C15
24	T	263	PEK	C9-C10-C11-C12
19	D	523	TGL	CA2-CA3-CA4-CA5
20	P	1267	PGV	C29-C30-C31-C32
20	N	1266	PGV	O03-C19-C20-C21
18	N	515	HEA	CAA-CBA-CGA-O1A
24	G	1263	PEK	C33-C34-C35-C36
18	A	516	HEA	CAD-CBD-CGD-O2D
19	O	1521	TGL	C11-C10-CB9-CB8
20	N	1266	PGV	C20-C21-C22-C23
20	A	524	PGV	C11-C12-C13-C14
20	N	1268	PGV	C9-C10-C11-C12
22	B	1086	CHD	C22-C23-C24-O25
28	Z	1526	DMU	C28-C31-C34-C37
20	N	1268	PGV	C25-C26-C27-C28
22	C	271	CHD	C22-C23-C24-O26
18	N	515	HEA	CAA-CBA-CGA-O2A
22	B	1086	CHD	C22-C23-C24-O26
25	P	1270	CDL	C1-CA2-OA2-PA1
24	T	1265	PEK	C22-C23-C24-C25
25	T	1269	CDL	C77-C78-C79-C80
18	N	516	HEA	CAA-CBA-CGA-O2A
20	N	1524	PGV	C25-C26-C27-C28
25	P	1270	CDL	C11-C12-C13-C14
20	H	268	PGV	O03-C01-C02-C03
22	P	1525	CHD	C22-C23-C24-O26
22	P	1271	CHD	C22-C23-C24-O26
25	T	1269	CDL	C54-C55-C56-C57
22	J	60	CHD	C22-C23-C24-O26
18	A	515	HEA	C18-C19-C20-C21
20	C	267	PGV	C13-C14-C15-C16
18	A	516	HEA	CAA-CBA-CGA-O2A
24	T	263	PEK	C3-C4-C5-C6
24	G	265	PEK	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
24	T	1265	PEK	C10-C11-C12-C13
25	T	1269	CDL	C79-C80-C81-C82
26	E	230	PSC	C28-C29-C30-C31
24	T	263	PEK	C22-C23-C24-C25
25	P	1270	CDL	C58-C59-C60-C61
19	Y	1522	TGL	OG2-CG2-CG3-OG3
26	E	230	PSC	C7-C8-C9-C10
19	Y	1522	TGL	OG1-CA1-CA2-CA3
19	O	1521	TGL	CB3-CB4-CB5-CB6
20	A	524	PGV	C12-C13-C14-C15
20	A	522	PGV	C4-C5-C6-C7
24	G	265	PEK	C3-C4-C5-C6
22	C	525	CHD	C22-C23-C24-O26
19	Y	1522	TGL	CB6-CB7-CB8-CB9
24	G	265	PEK	C14-C15-C16-C17
20	H	268	PGV	C12-C13-C14-C15
24	G	1263	PEK	C15-C16-C17-C18
24	T	263	PEK	C15-C16-C17-C18
19	A	521	TGL	C18-C19-C33-C34
19	L	522	TGL	C16-C17-C18-C19
18	N	515	HEA	C2A-C3A-CMA-OMA
22	C	525	CHD	C22-C23-C24-O25
24	G	1263	PEK	O01-C02-C03-O11
18	N	516	HEA	CAD-CBD-CGD-O1D
19	L	522	TGL	OA1-CA1-CA2-CA3
20	A	524	PGV	C2-C3-C4-C5
22	P	1525	CHD	C13-C17-C20-C22
26	E	230	PSC	C4-C5-C6-C7
24	T	1265	PEK	C3-C4-C5-C6
20	N	1524	PGV	O01-C1-C2-C3
22	P	1525	CHD	C22-C23-C24-O25
25	G	269	CDL	C83-C84-C85-C86
25	C	270	CDL	C41-C42-C43-C44
20	A	524	PGV	C15-C16-C17-C18
25	T	1269	CDL	C42-C43-C44-C45
25	T	1269	CDL	C35-C36-C37-C38
26	E	230	PSC	C21-C22-C23-C24
26	R	1230	PSC	O03-C19-C20-C21
24	G	265	PEK	O02-C1-O01-C02
20	N	1268	PGV	C2-C1-O01-C02
20	N	1266	PGV	C11-C10-C9-C8
19	O	1523	TGL	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
18	A	516	HEA	C26-C15-C16-C17
18	N	516	HEA	C26-C15-C16-C17
19	D	523	TGL	OG3-CC1-CC2-CC3
24	C	264	PEK	O01-C1-C2-C3
19	Y	1522	TGL	C29-C30-C31-C32
18	A	516	HEA	C4D-C3D-CAD-CBD
19	O	1523	TGL	C17-C18-C19-C33
19	D	523	TGL	OA1-CA1-CA2-CA3
28	P	1272	DMU	C19-C18-O16-C6
18	A	515	HEA	CAA-CBA-CGA-O1A
24	P	1264	PEK	O01-C1-C2-C3
26	E	230	PSC	O03-C19-C20-C21
18	A	515	HEA	CAA-CBA-CGA-O2A
19	D	523	TGL	CC5-CC6-CC7-CC8
25	P	1270	CDL	C52-C51-CB5-OB6
19	O	1521	TGL	OG1-CG1-CG2-OG2
25	P	1270	CDL	C14-C15-C16-C17
19	L	522	TGL	OB1-CB1-CB2-CB3
25	C	270	CDL	C12-C11-CA5-OA6
25	P	1270	CDL	C12-C11-CA5-OA6
19	O	1521	TGL	C21-C22-C23-C24
19	A	521	TGL	CB2-CB3-CB4-CB5
19	O	1523	TGL	C23-C24-C25-C26
18	A	515	HEA	CAD-CBD-CGD-O1D
19	A	521	TGL	C29-C30-C31-C32
24	P	1264	PEK	C16-C17-C18-C19
25	C	270	CDL	C44-C45-C46-C47
19	Y	1522	TGL	C21-C20-CA9-CA8
25	T	1269	CDL	C81-C82-C83-C84
25	C	270	CDL	C81-C82-C83-C84
25	P	1270	CDL	C52-C51-CB5-OB7
22	P	1271	CHD	C16-C17-C20-C22
19	D	523	TGL	OB1-CB1-CB2-CB3
24	P	1264	PEK	O02-C1-C2-C3
20	N	1524	PGV	O02-C1-C2-C3
25	P	1270	CDL	C12-C11-CA5-OA7
19	A	521	TGL	CB5-CB6-CB7-CB8
24	C	264	PEK	C22-C23-C24-C25
28	M	526	DMU	C28-C31-C34-C37
25	C	270	CDL	C12-C11-CA5-OA7
26	R	1230	PSC	O04-C19-C20-C21
24	G	1263	PEK	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
19	D	523	TGL	CC3-CC4-CC5-CC6
19	L	522	TGL	CB4-CB5-CB6-CB7
20	C	267	PGV	C05-C04-O12-P
19	O	1523	TGL	OG1-CA1-CA2-CA3
20	H	268	PGV	C31-C32-C33-C34
19	D	523	TGL	OC1-CC1-CC2-CC3
24	C	264	PEK	O02-C1-C2-C3
26	E	230	PSC	O04-C19-C20-C21
19	A	521	TGL	CA2-CA3-CA4-CA5
25	C	270	CDL	C75-C76-C77-C78
26	E	230	PSC	C2-C3-C4-C5
18	A	515	HEA	CAD-CBD-CGD-O2D

There are no ring outliers.

38 monomers are involved in 342 short contacts:

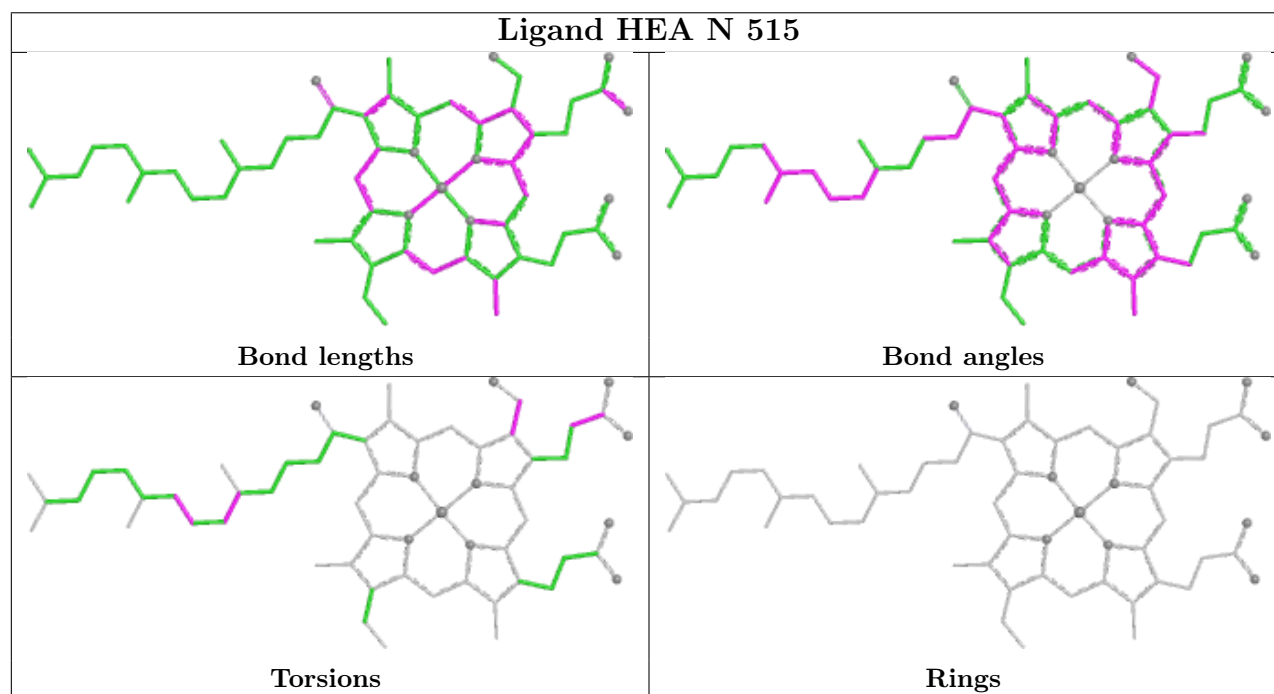
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	515	HEA	13	0
24	T	1265	PEK	8	0
24	G	1263	PEK	15	0
15	N	520	PER	1	0
20	H	268	PGV	3	0
26	E	230	PSC	22	0
22	W	1060	CHD	4	0
26	R	1230	PSC	15	0
28	P	1272	DMU	1	0
24	G	265	PEK	16	0
19	O	1521	TGL	14	0
20	A	522	PGV	2	0
24	C	264	PEK	7	0
19	L	522	TGL	15	0
22	B	1086	CHD	2	0
28	Z	1526	DMU	3	0
24	P	1264	PEK	7	0
25	T	1269	CDL	19	0
22	J	60	CHD	1	0
28	G	272	DMU	5	0
24	T	263	PEK	22	0
22	C	271	CHD	2	0
20	N	1268	PGV	1	0
25	P	1270	CDL	24	0
25	C	270	CDL	19	0

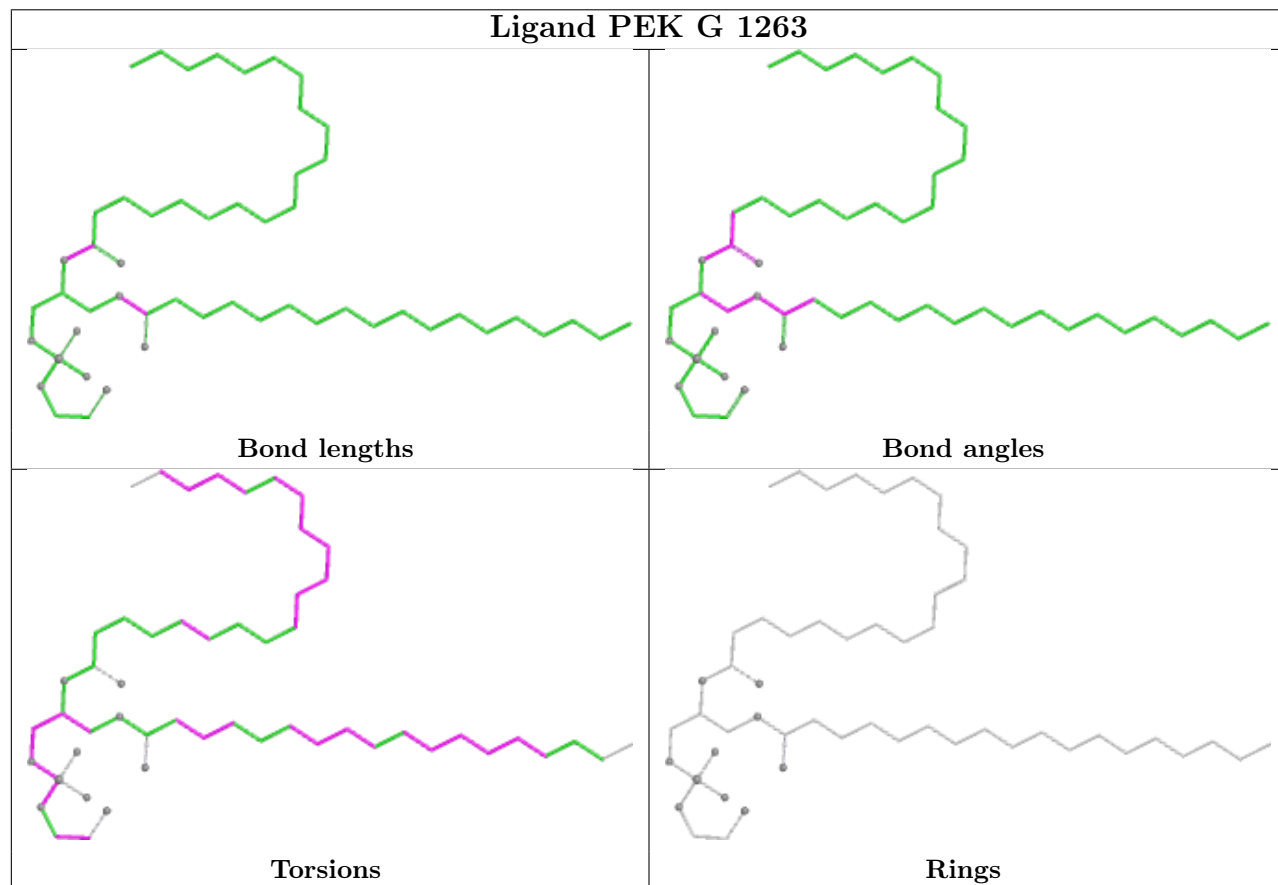
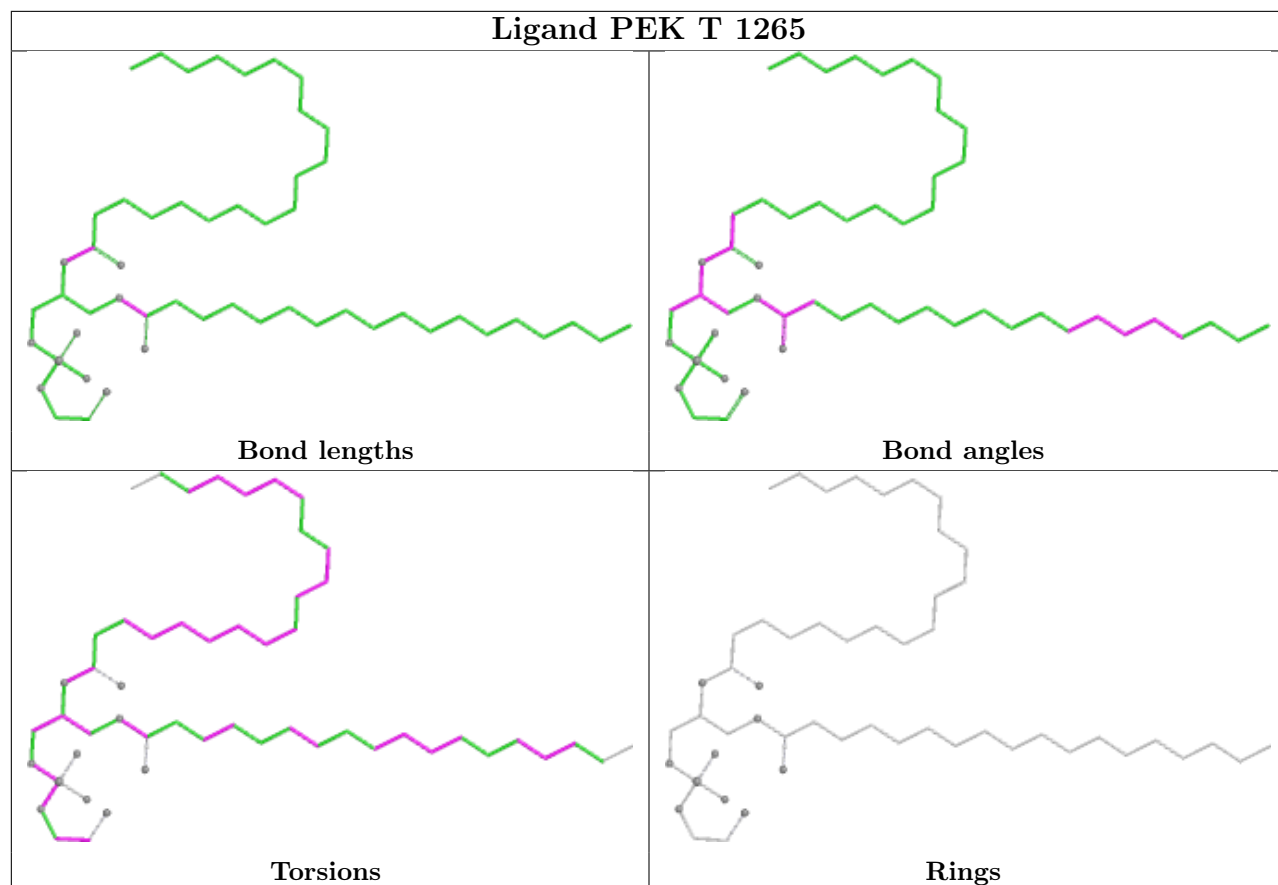
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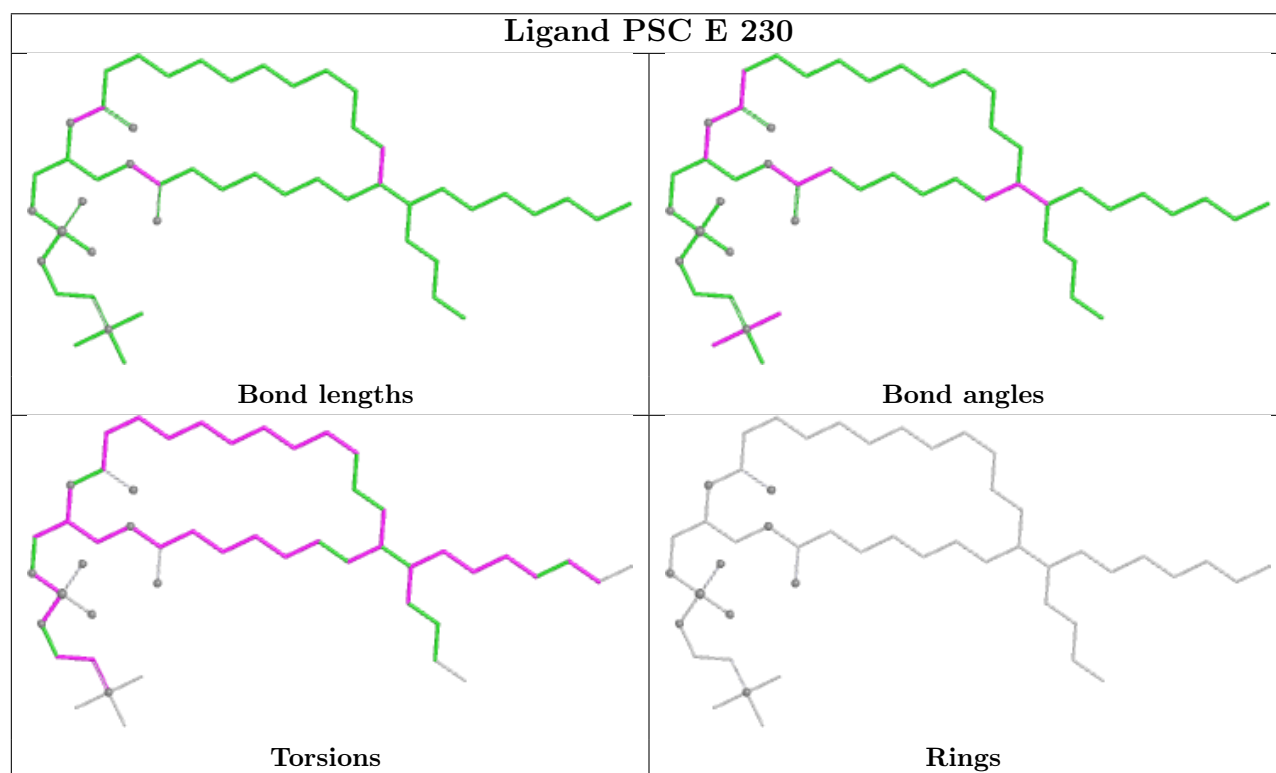
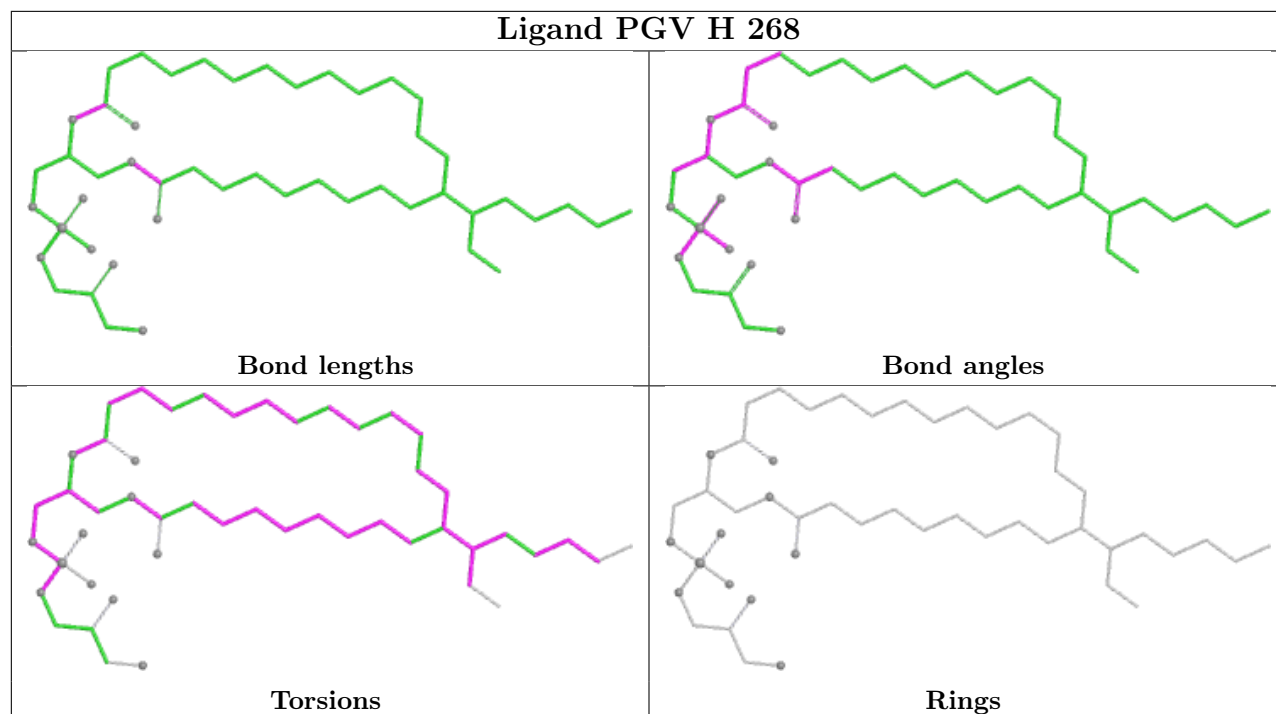
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	P	1271	CHD	1	0
18	A	515	HEA	8	0
22	C	525	CHD	3	0
15	A	520	PER	1	0
20	P	1267	PGV	12	0
19	A	521	TGL	13	0
19	Y	1522	TGL	18	0
19	D	523	TGL	9	0
20	N	1524	PGV	11	0
20	C	267	PGV	5	0
19	O	1523	TGL	9	0
25	G	269	CDL	27	0
20	A	524	PGV	6	0

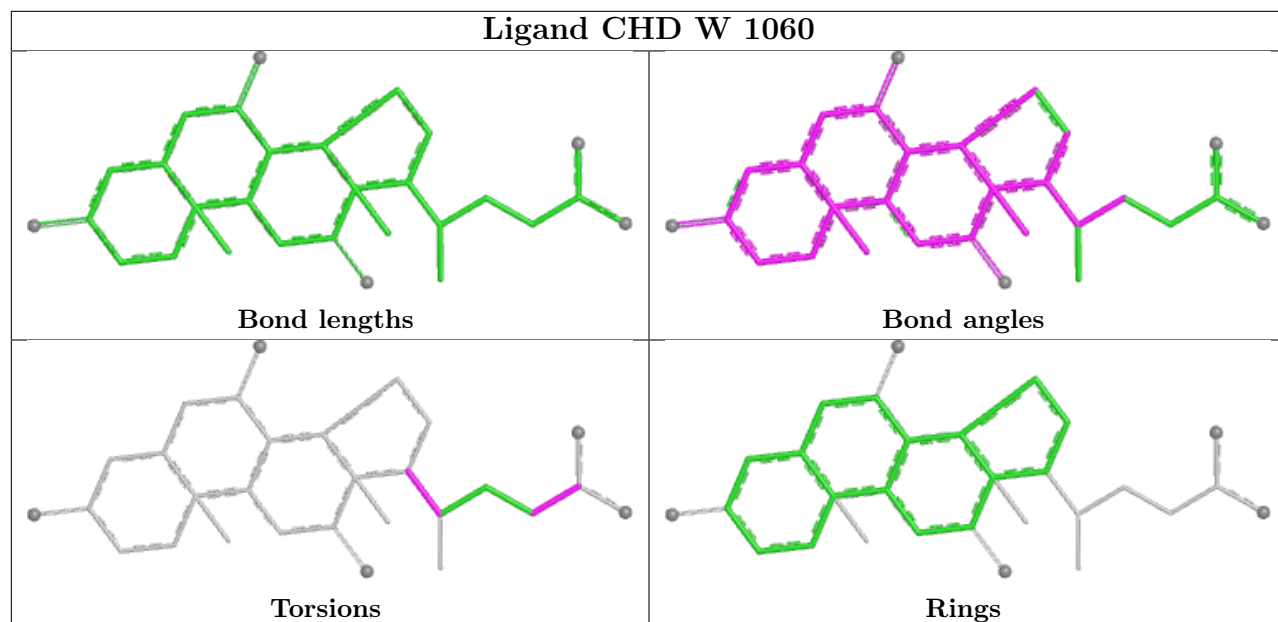
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



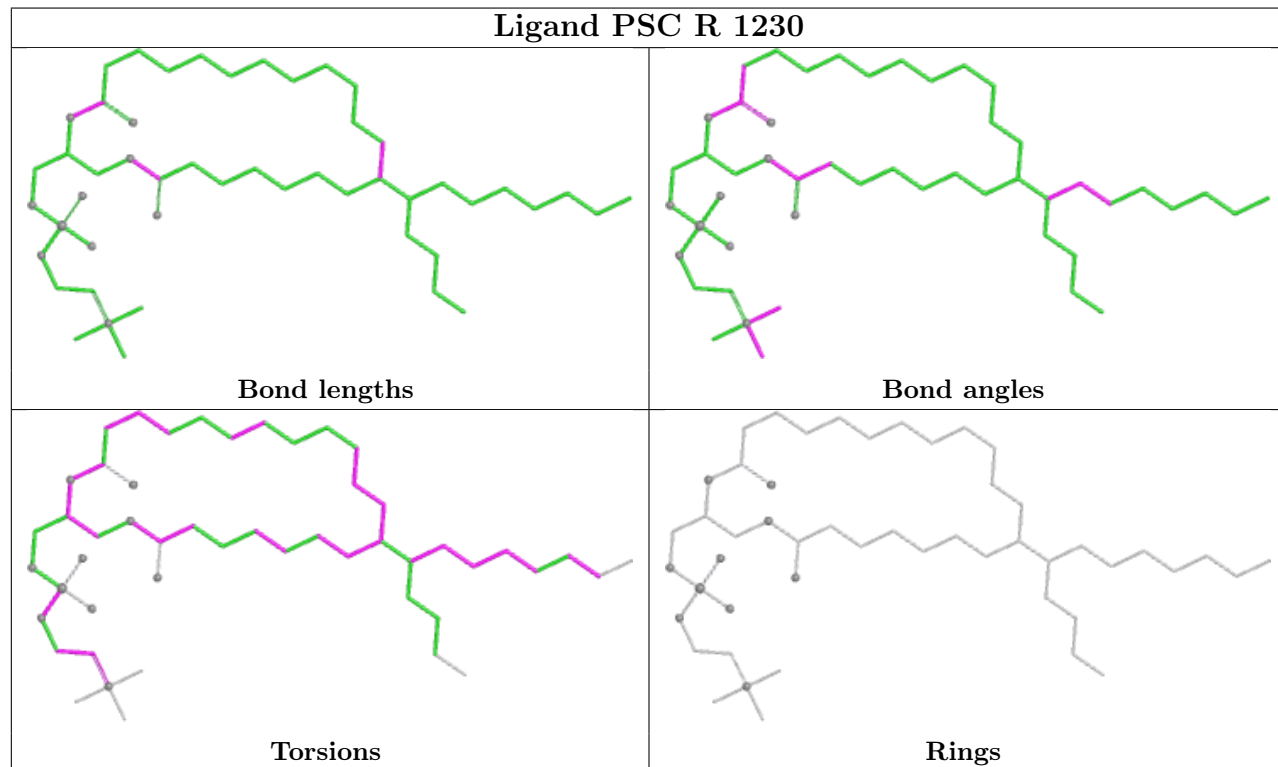




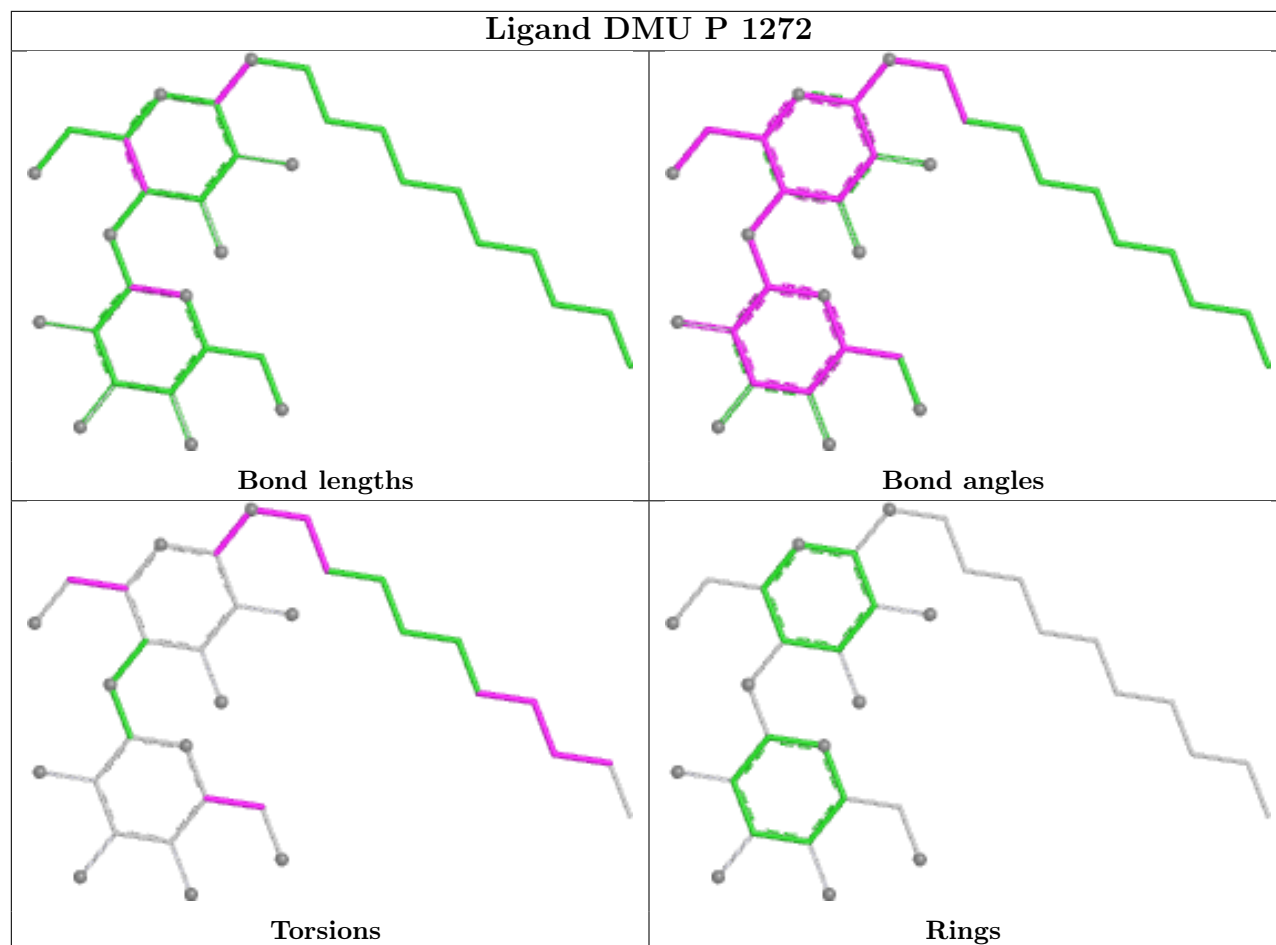
Ligand CHD W 1060



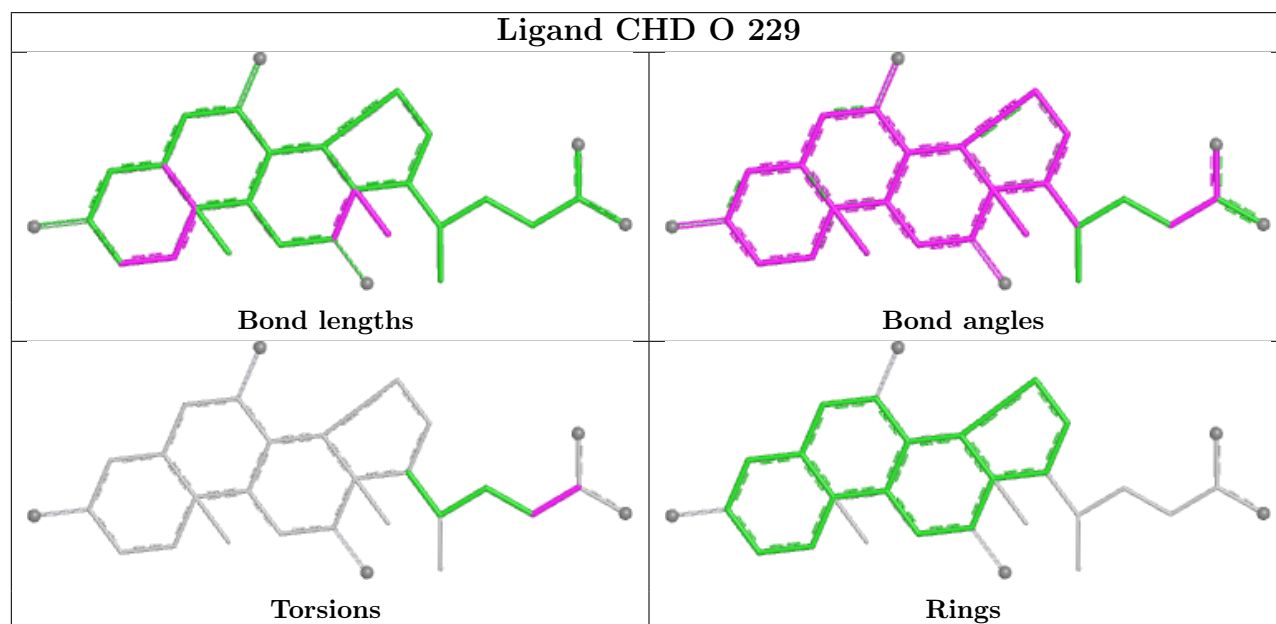
Ligand PSC R 1230

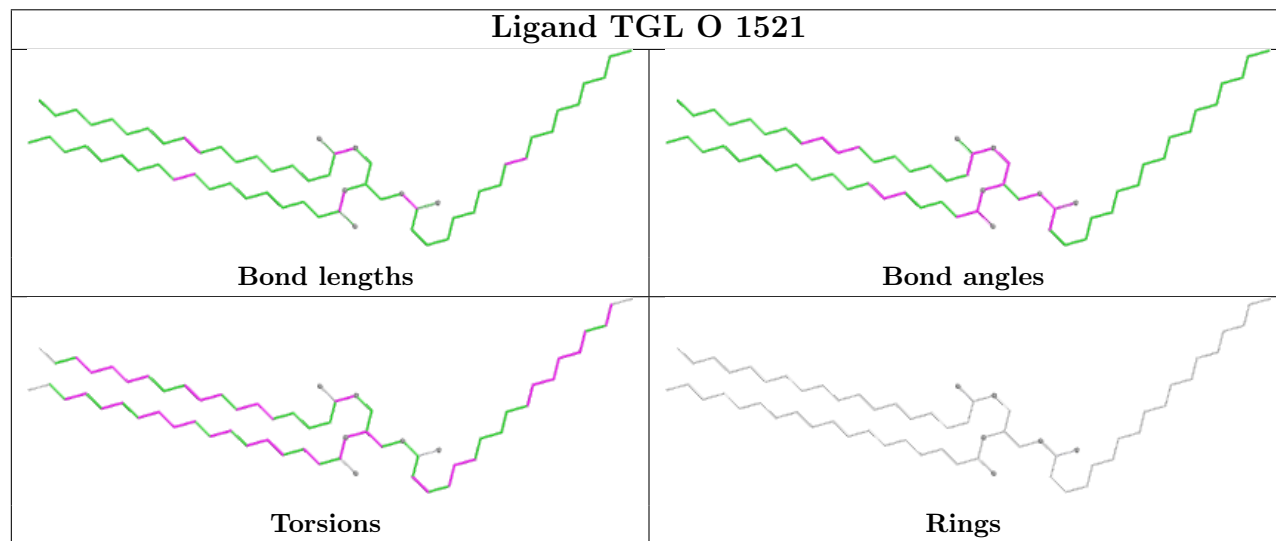
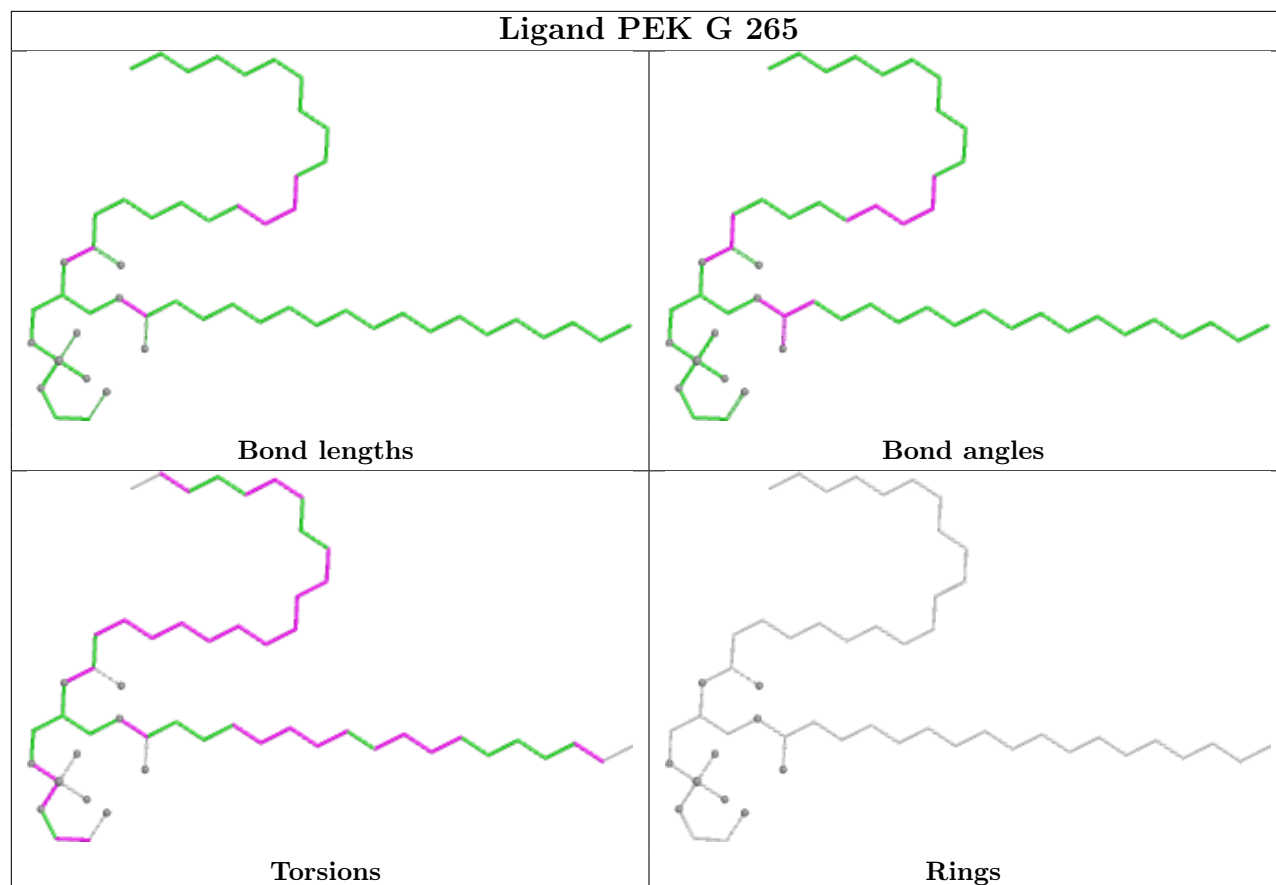


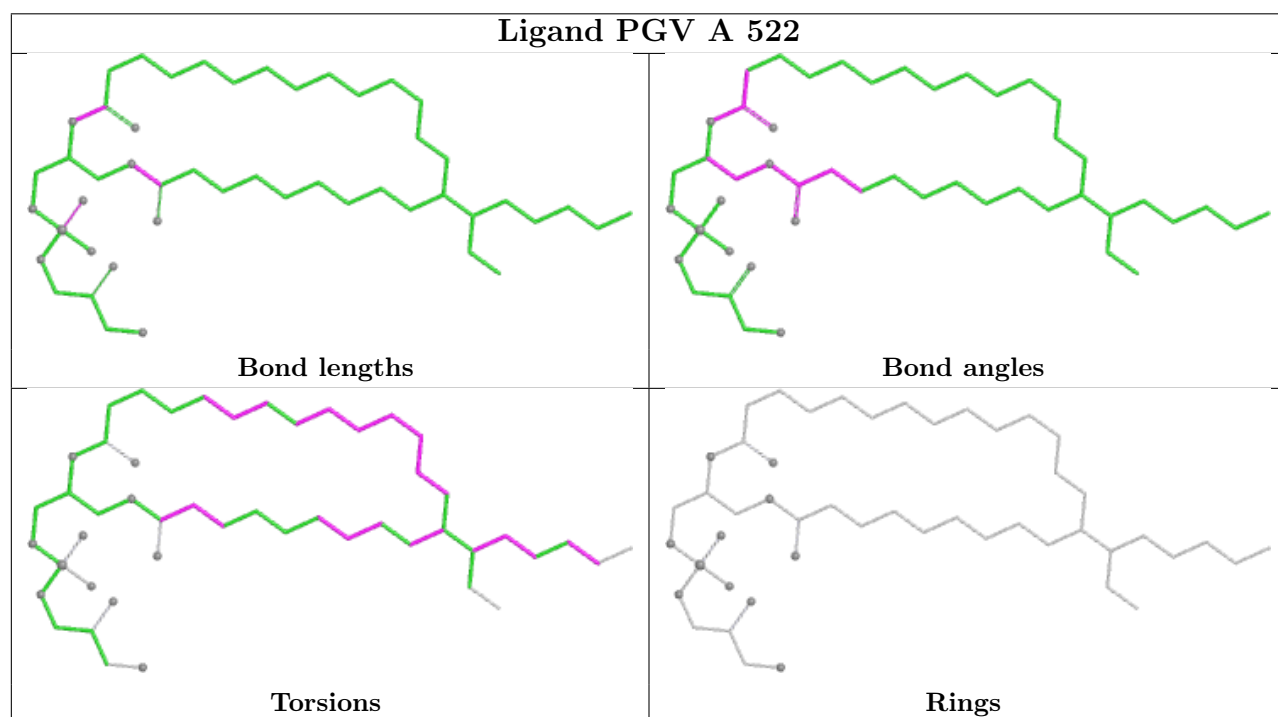
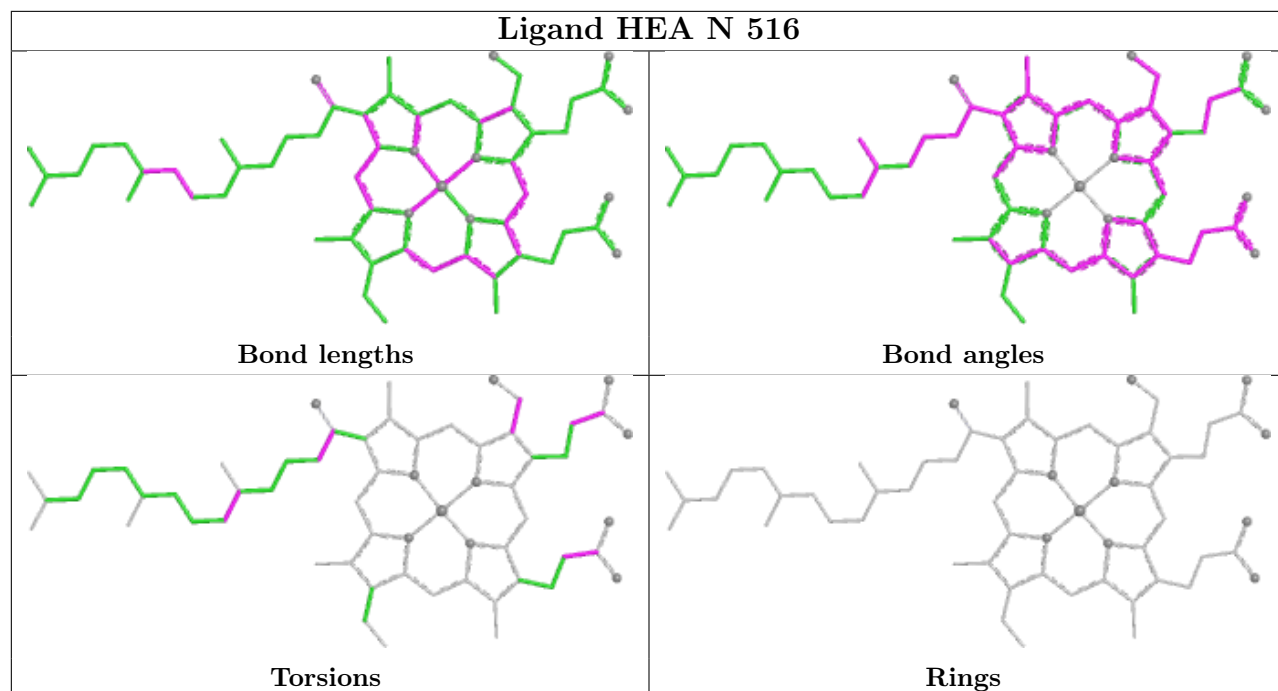
Ligand DMU P 1272



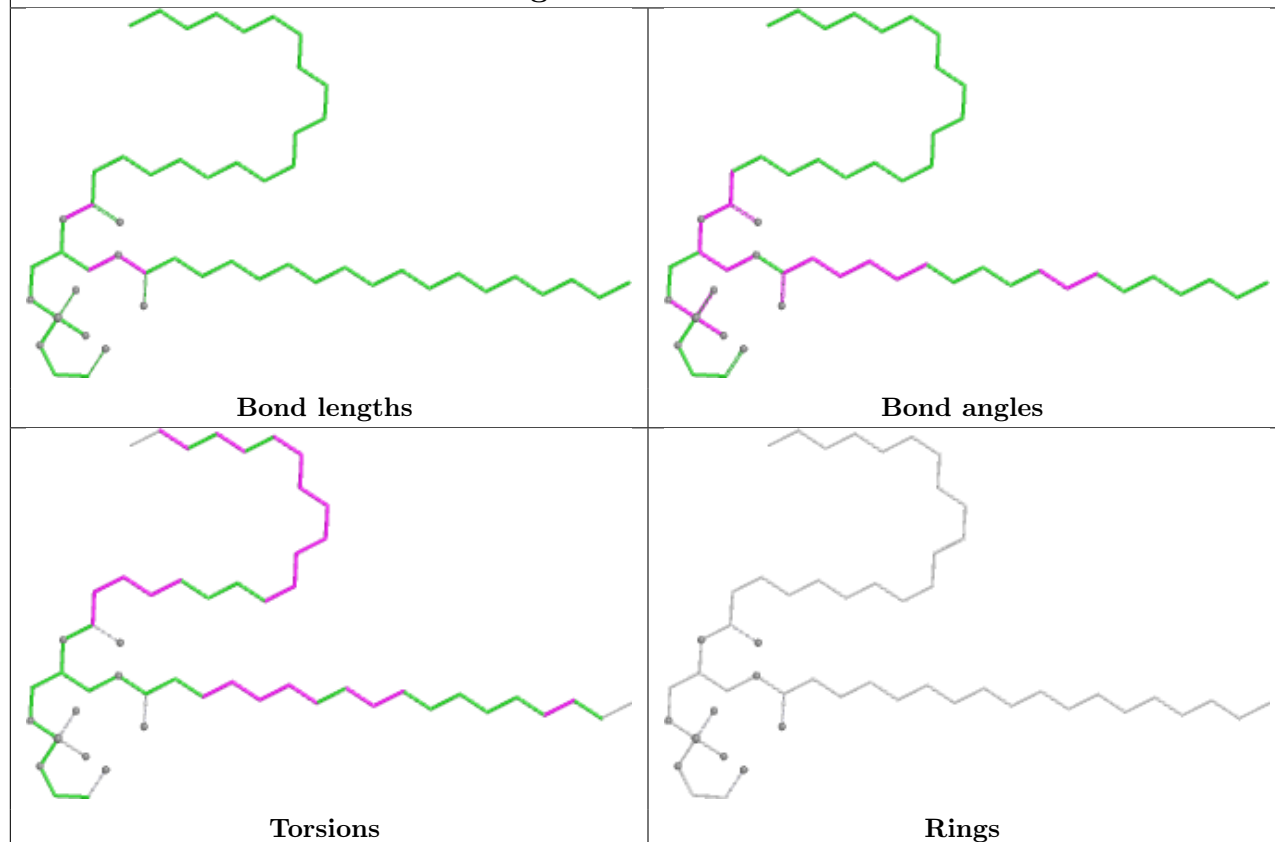
Ligand CHD O 229



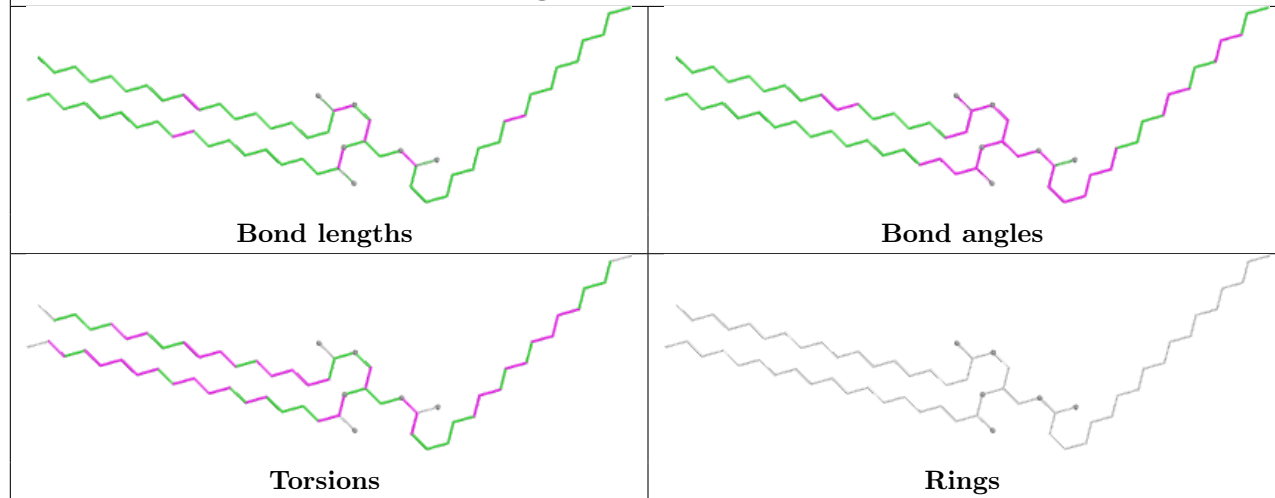




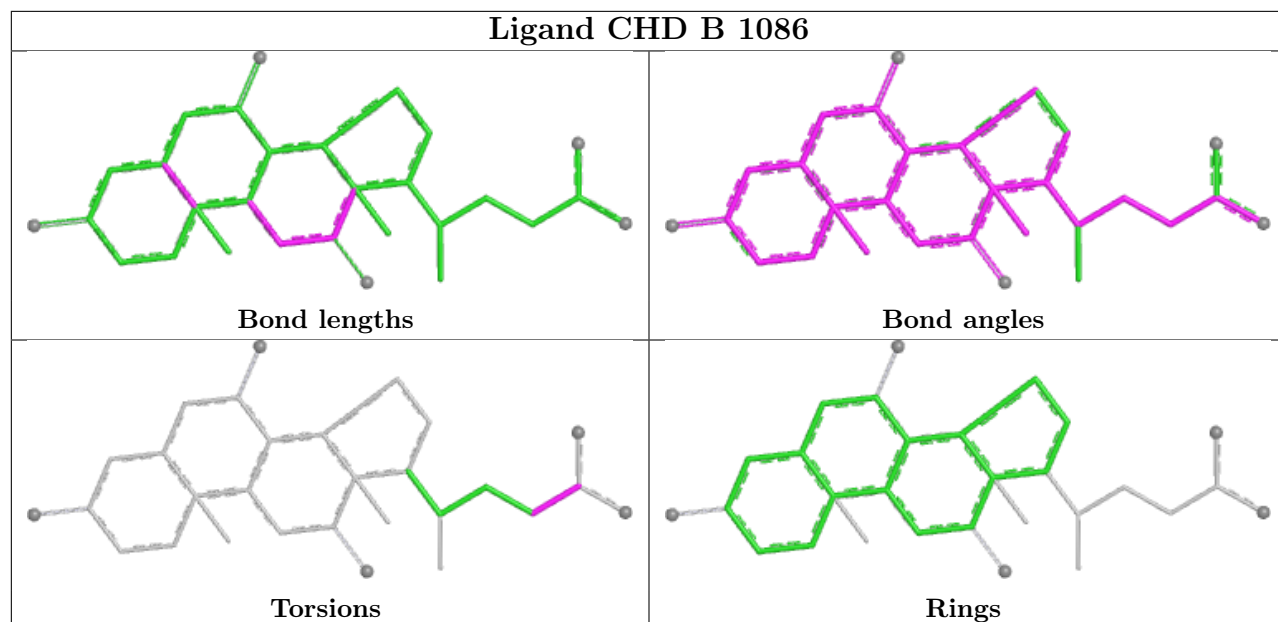
Ligand PEK C 264



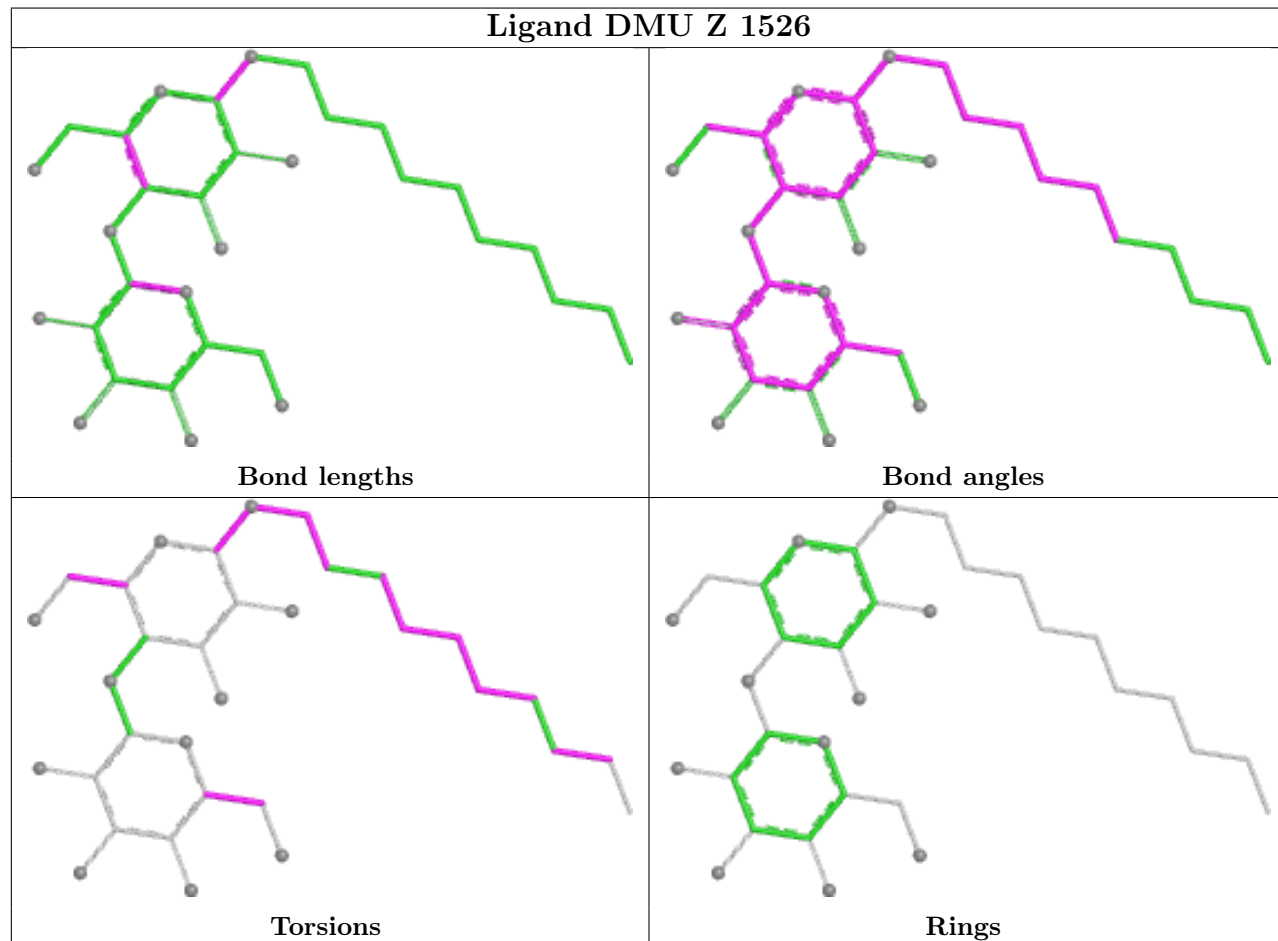
Ligand TGL L 522

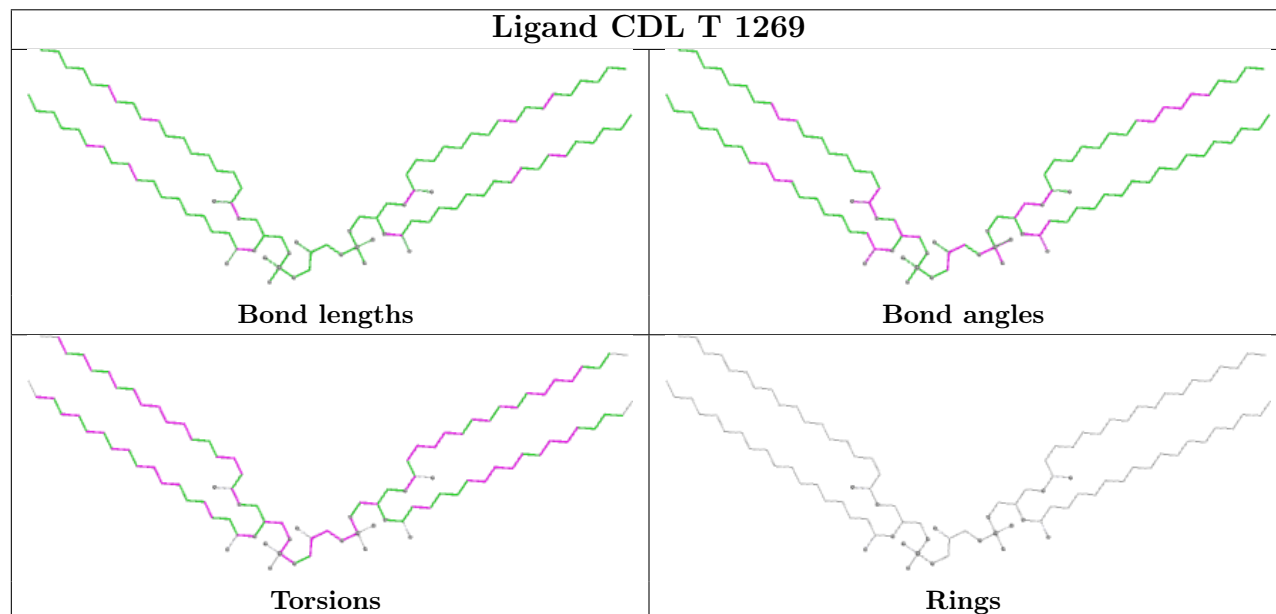
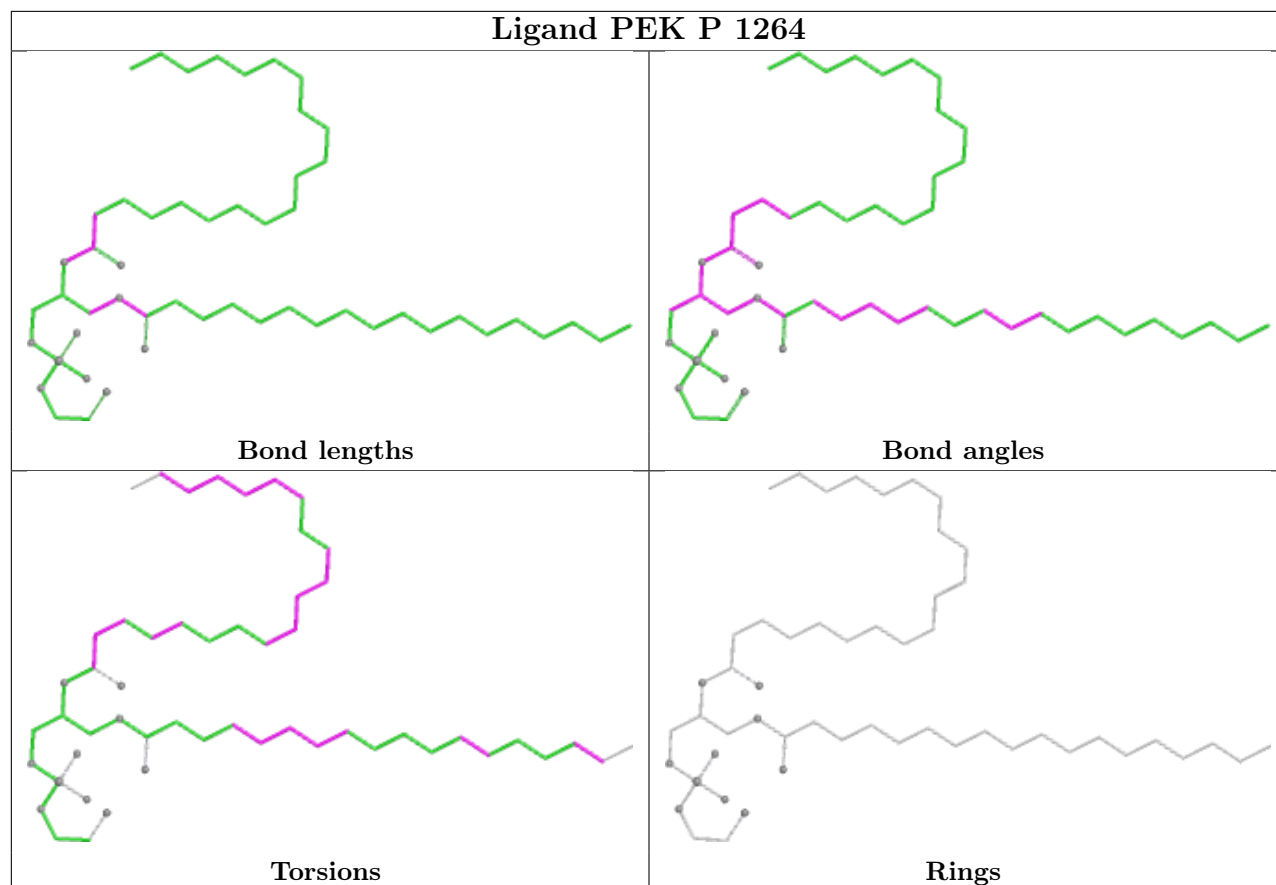


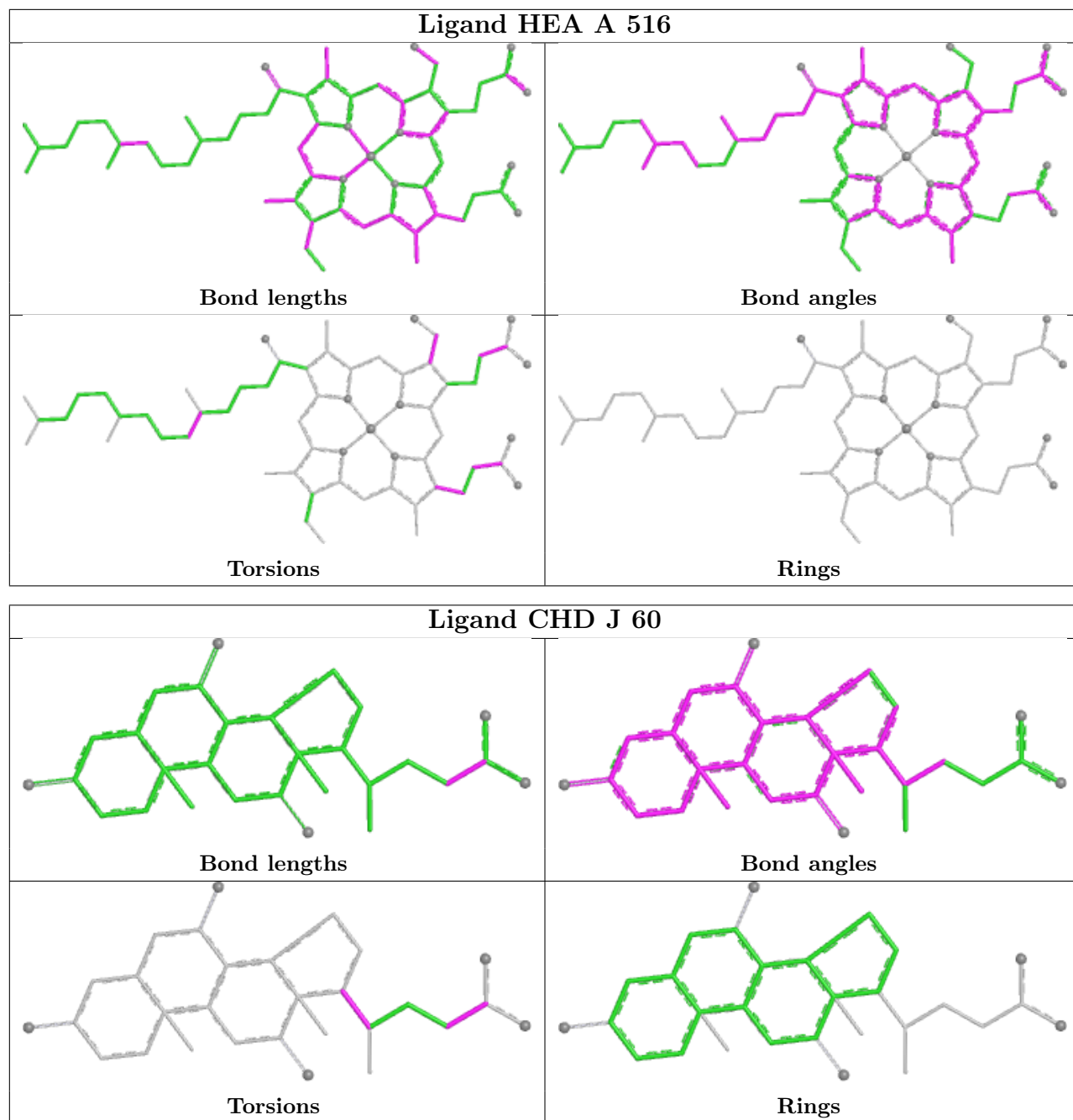
Ligand CHD B 1086

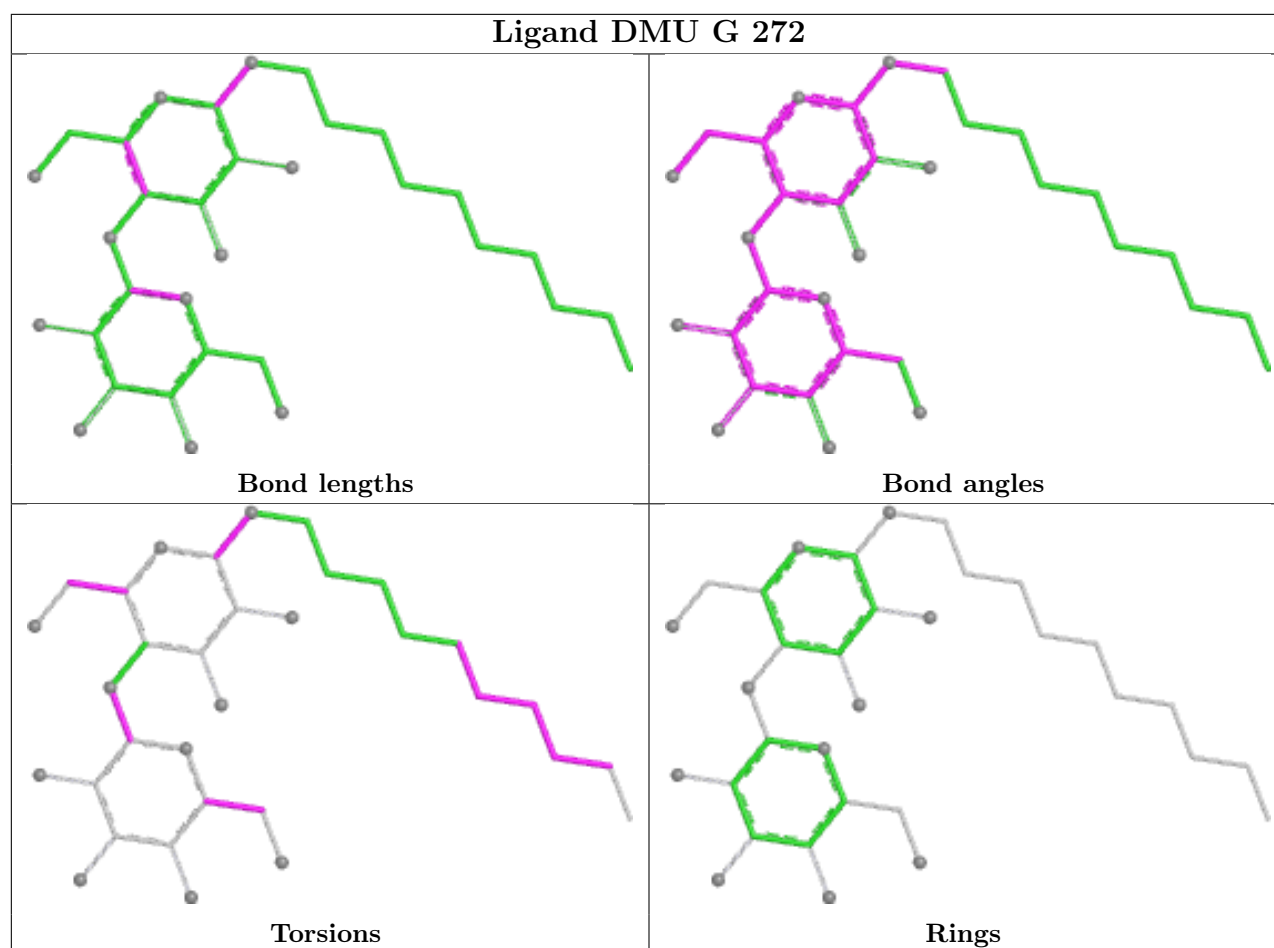


Ligand DMU Z 1526

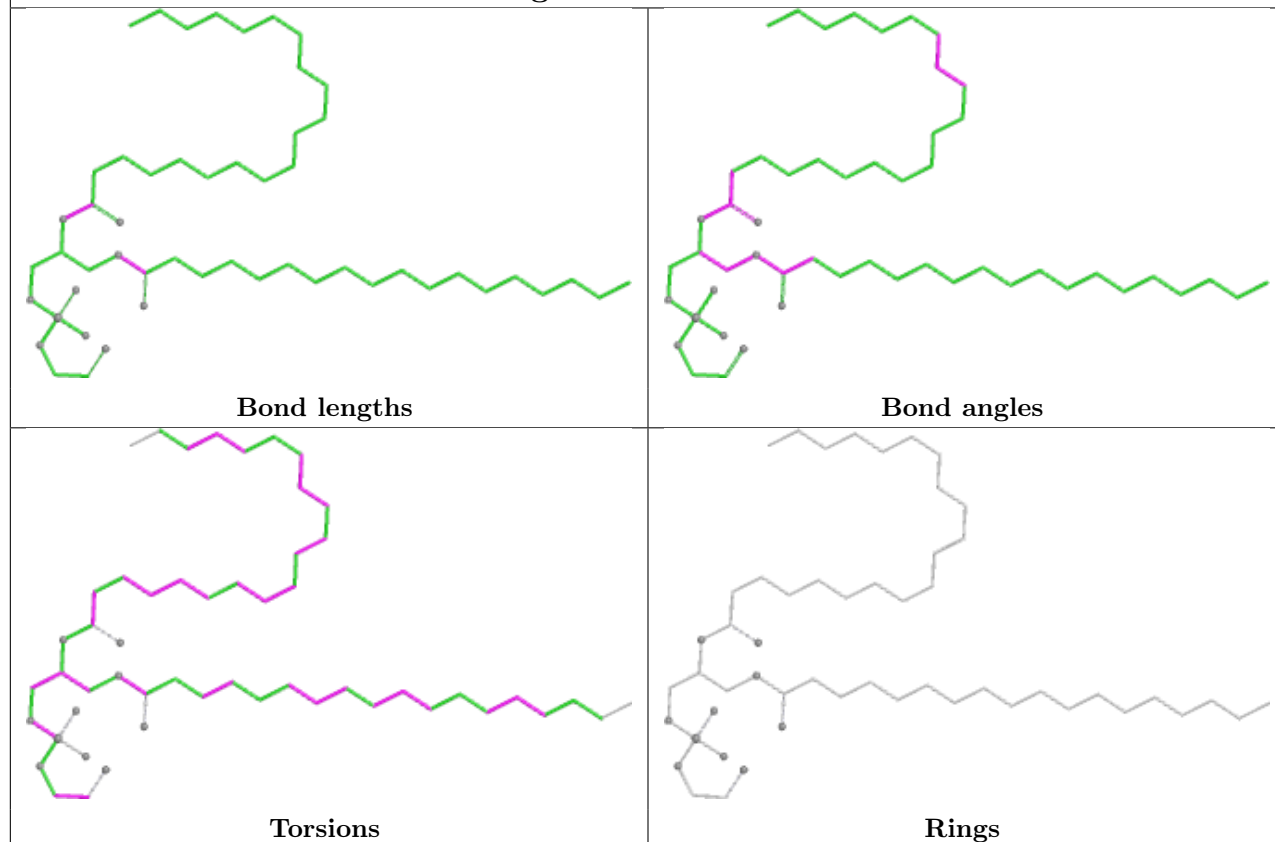




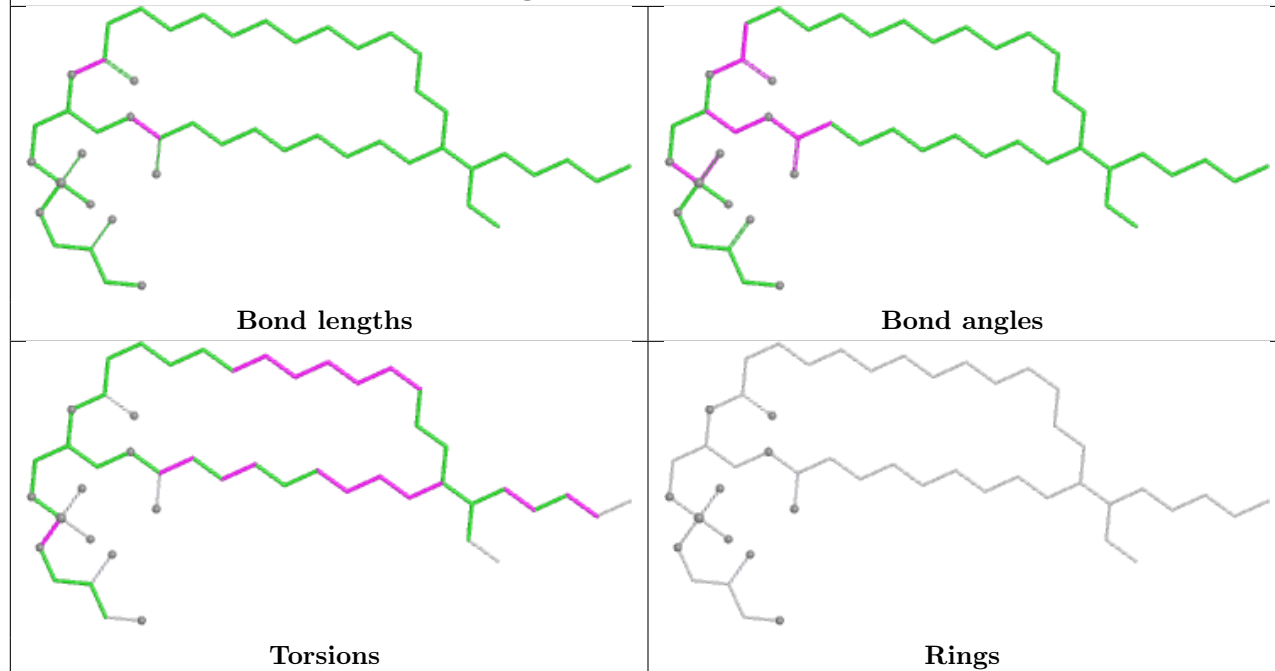


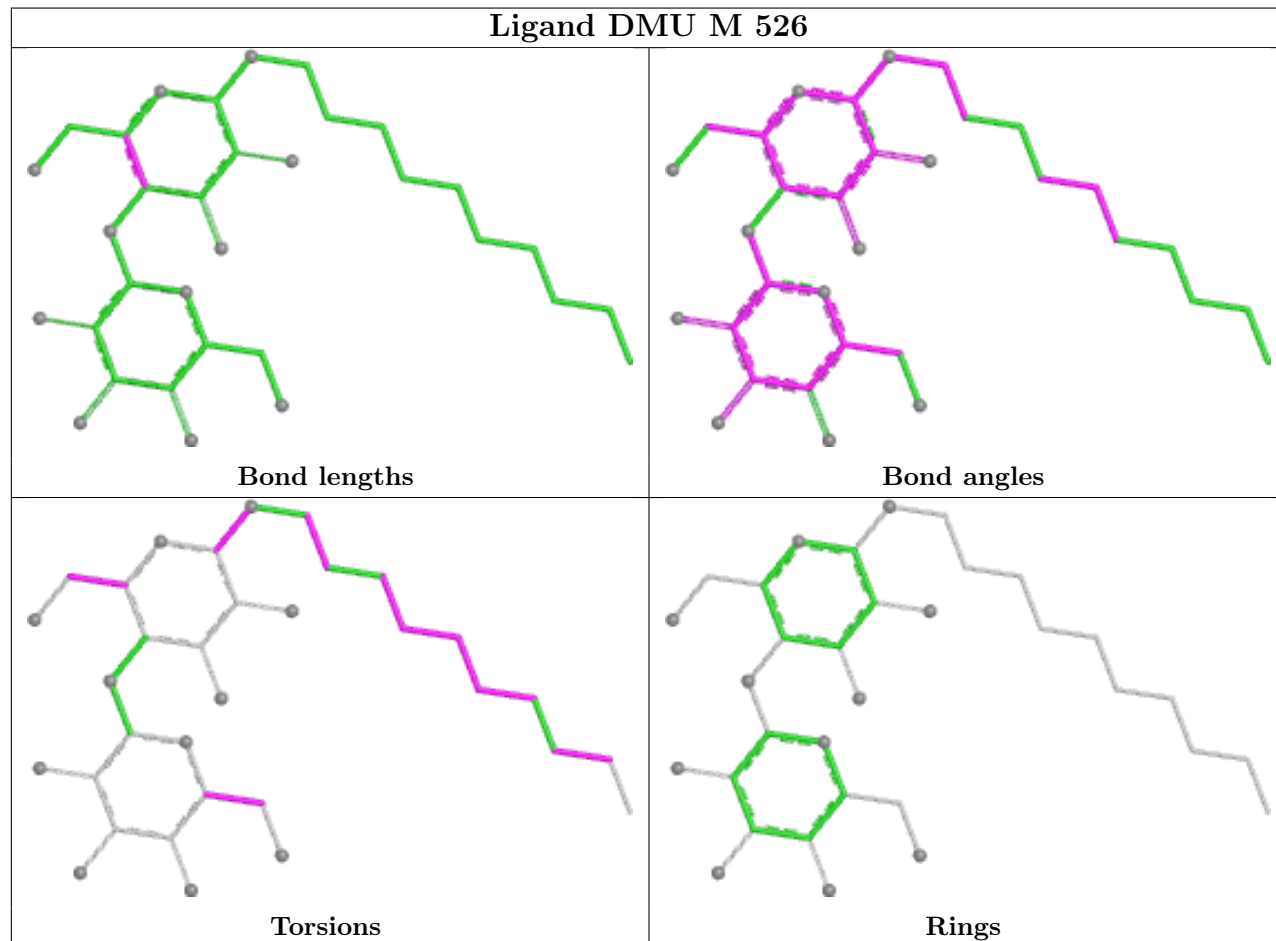
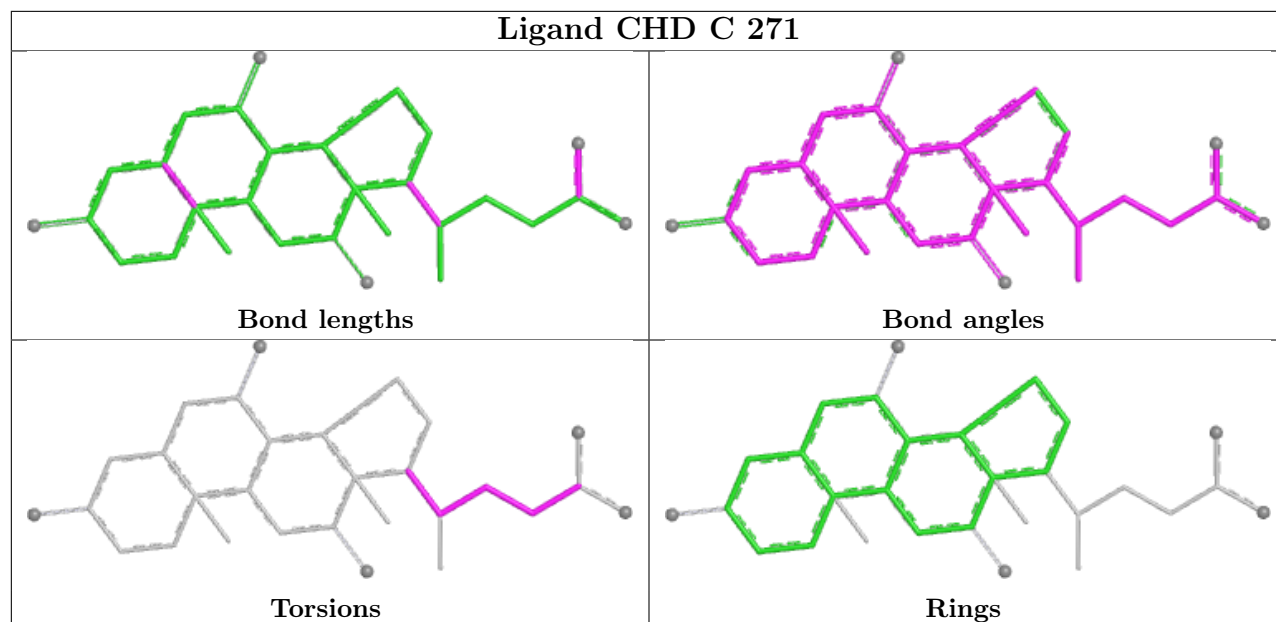


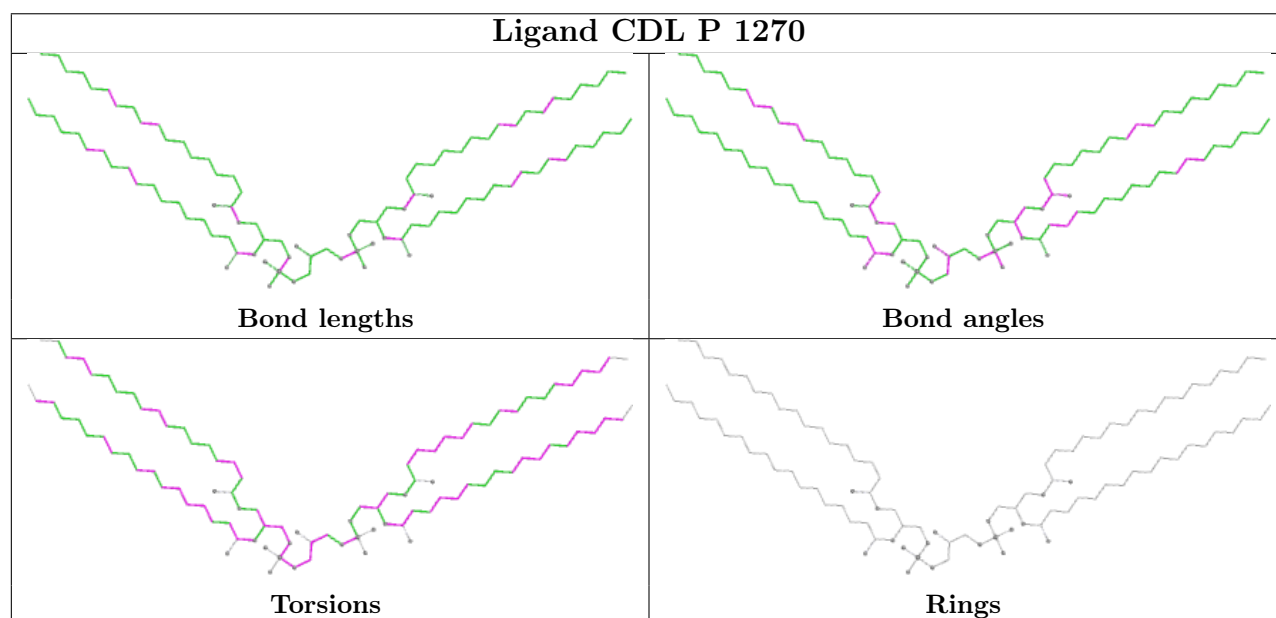
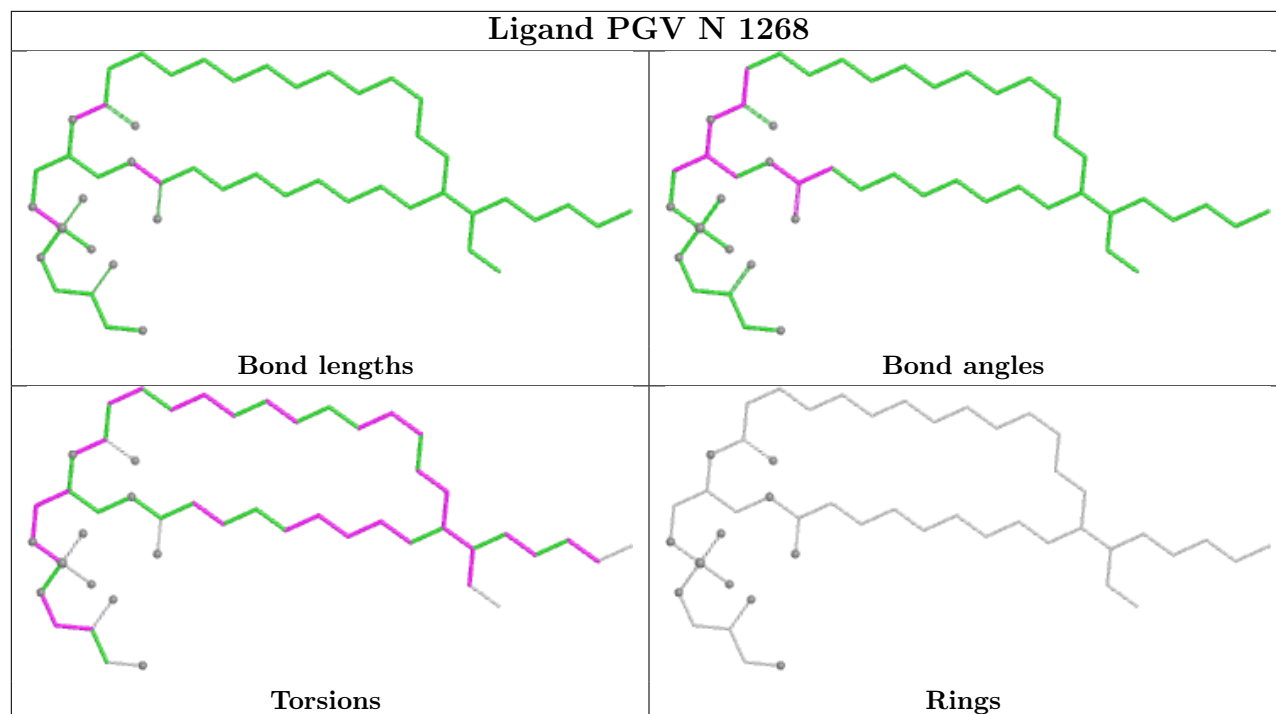
Ligand PEK T 263

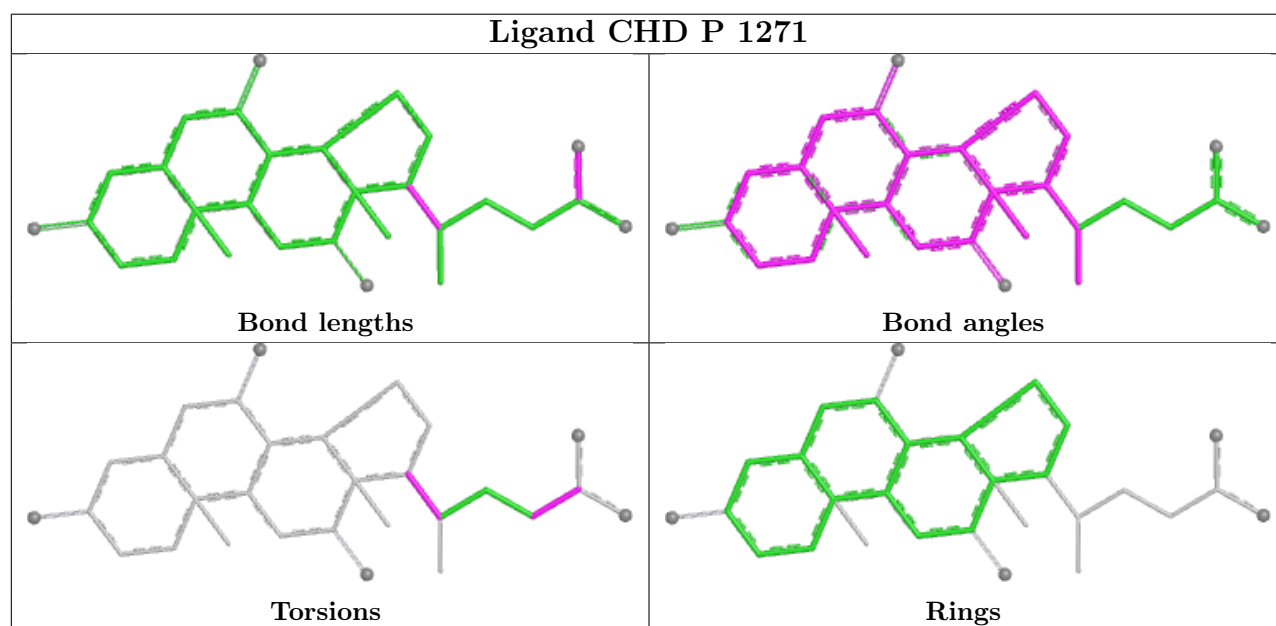
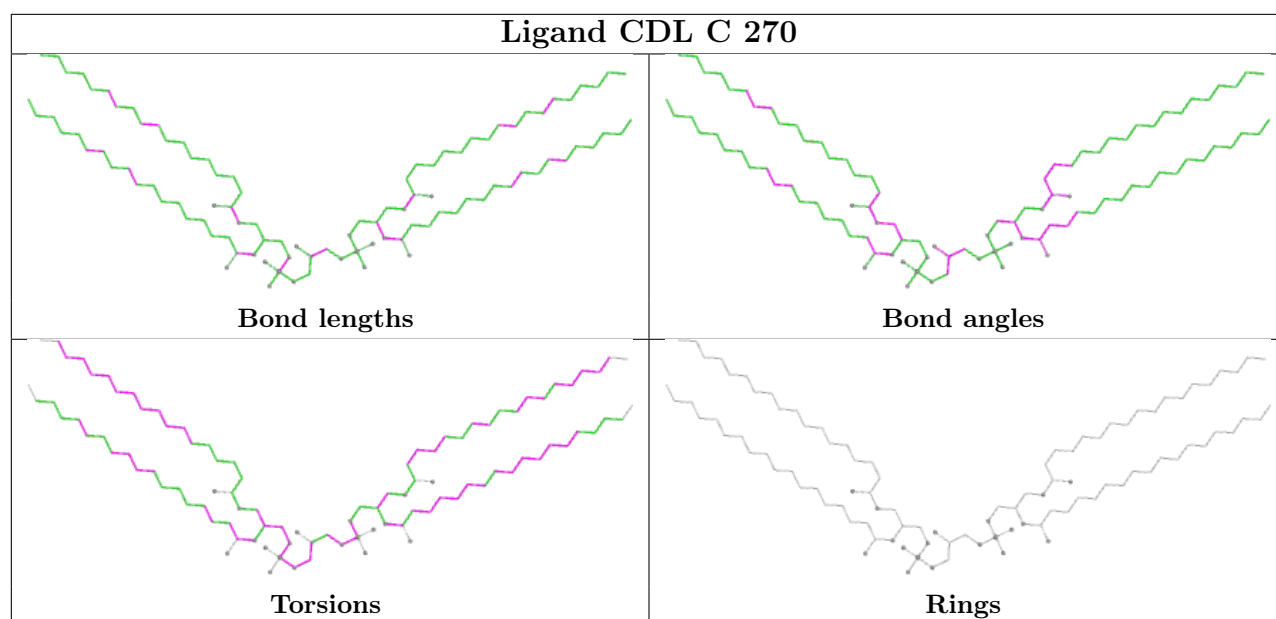


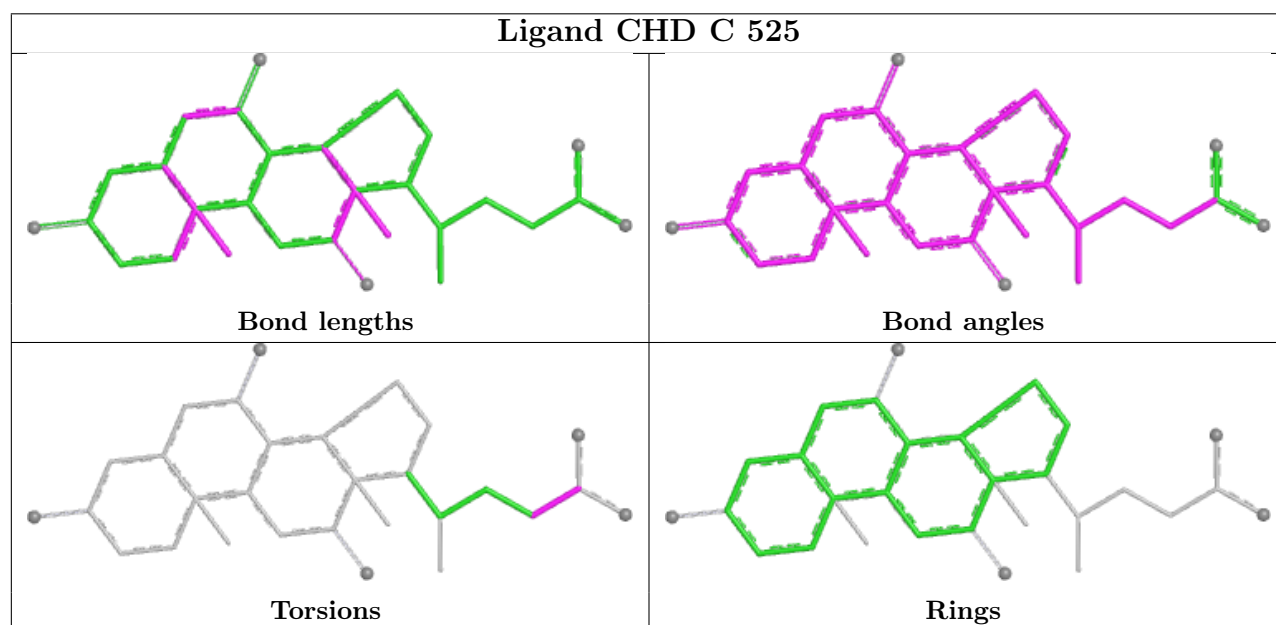
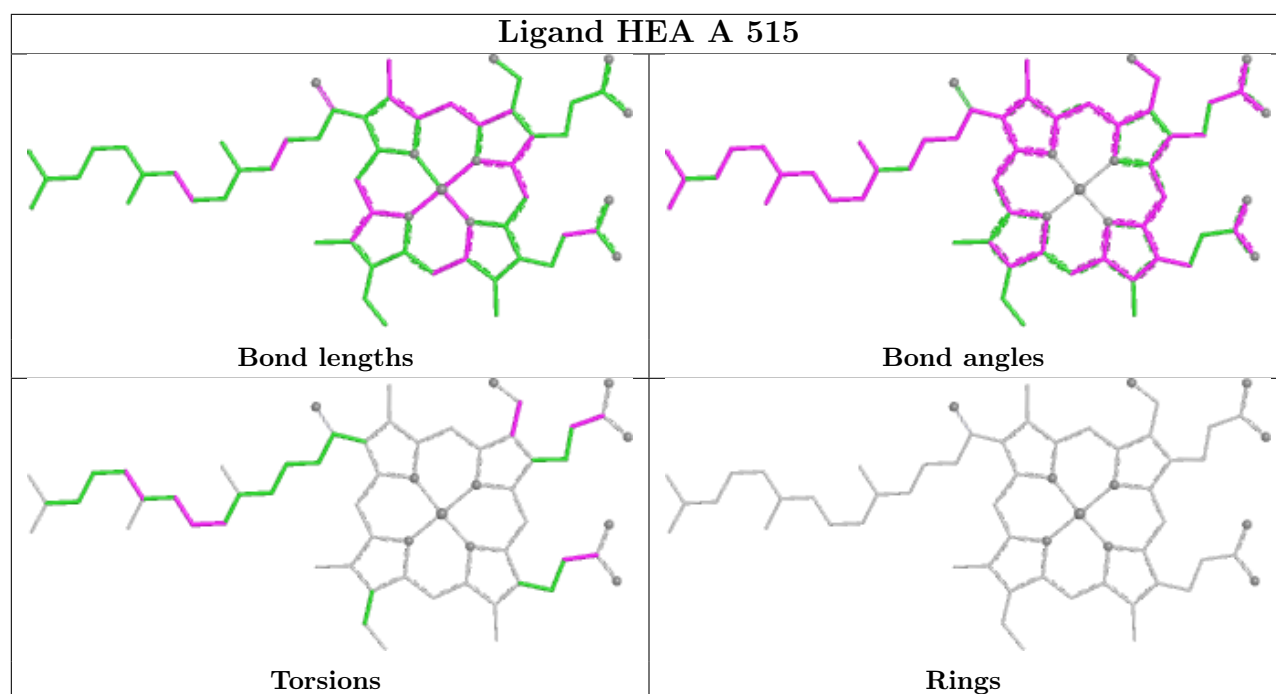
Ligand PGV N 1266

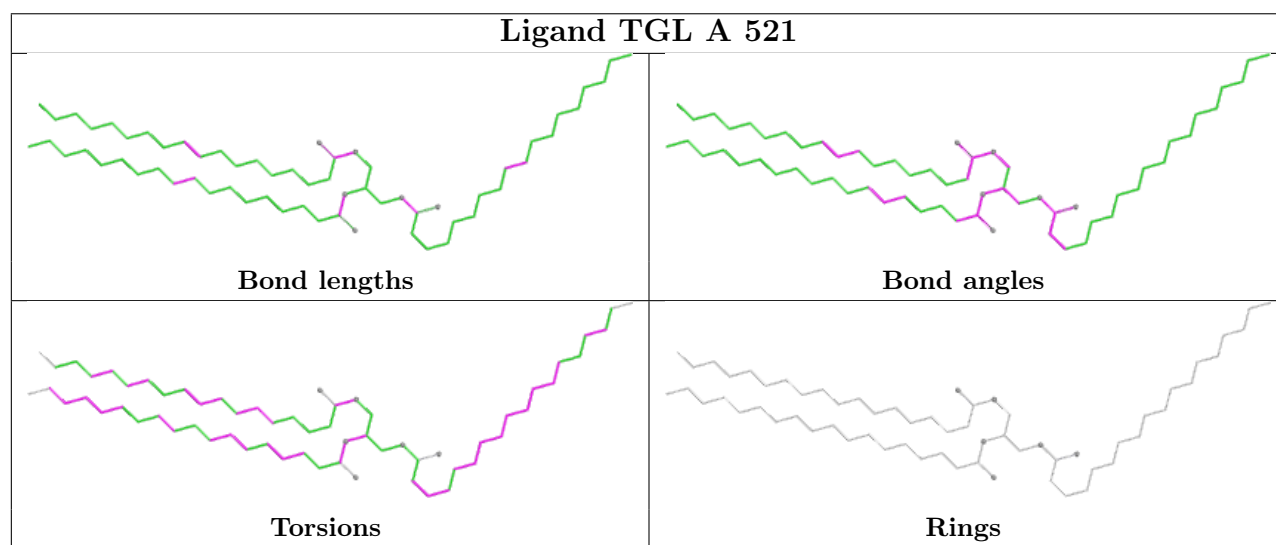
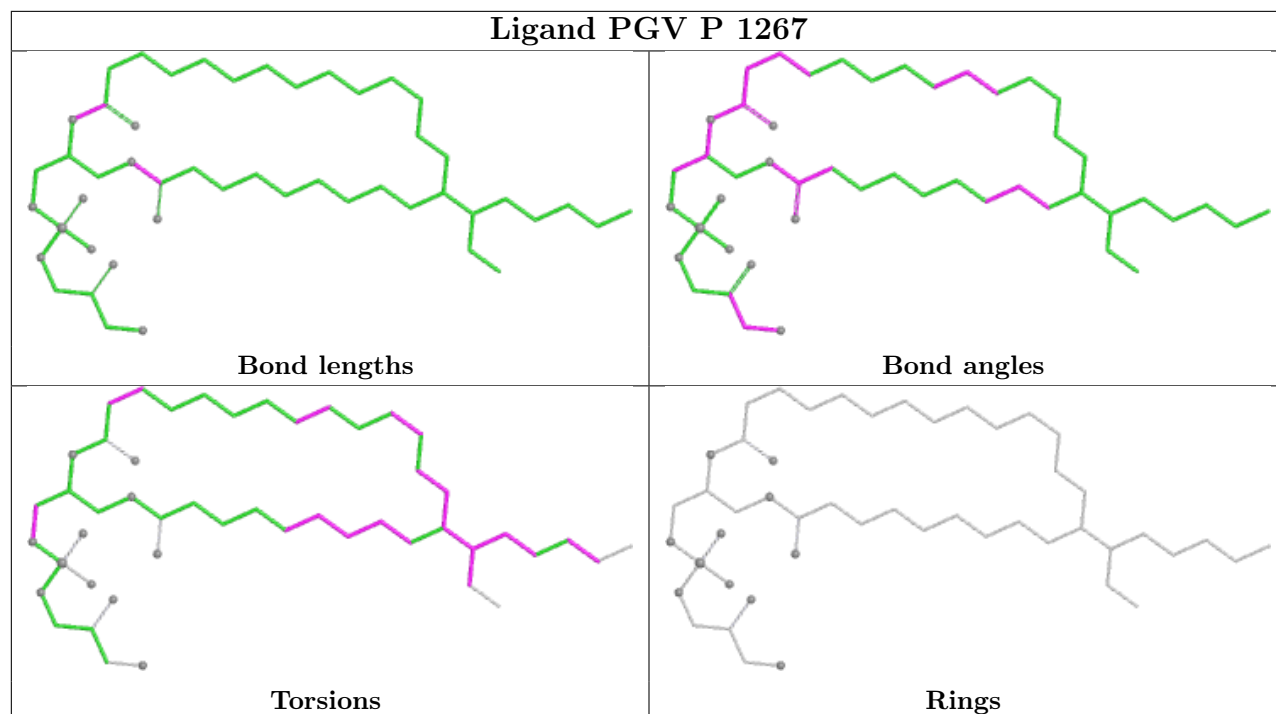


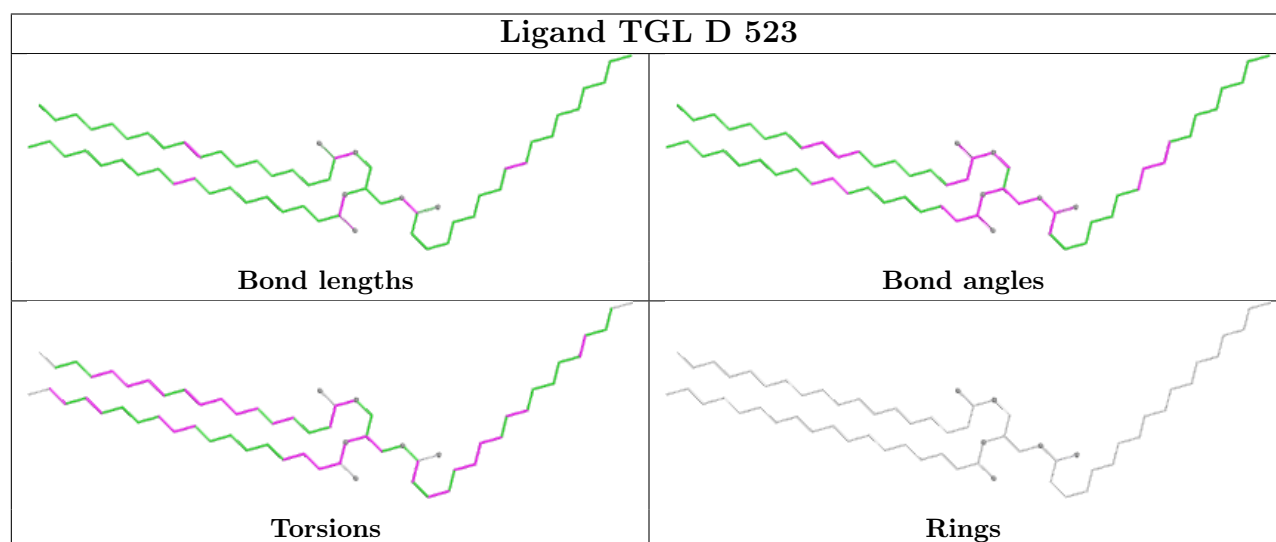
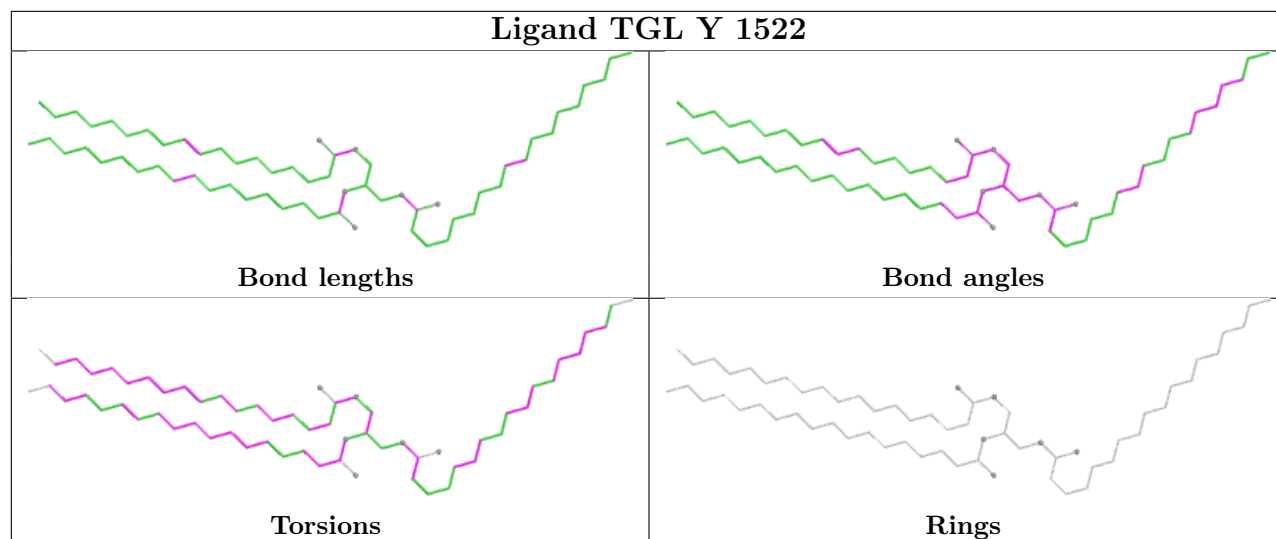




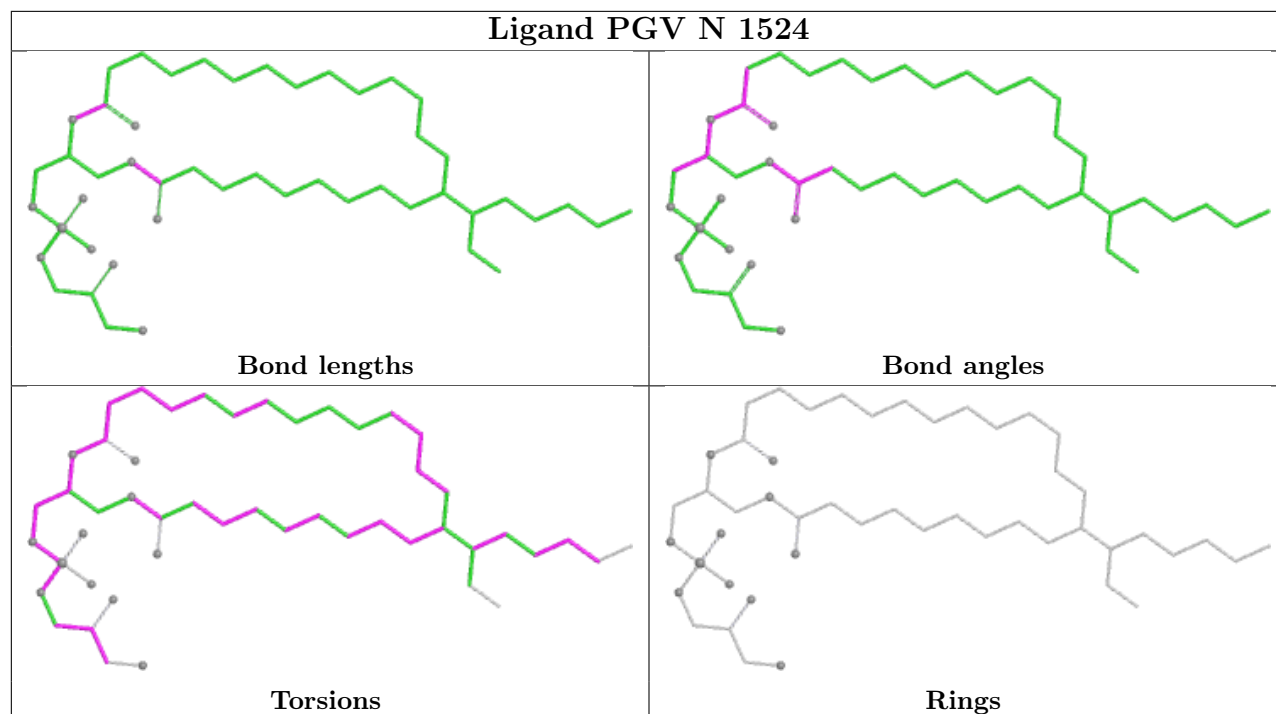




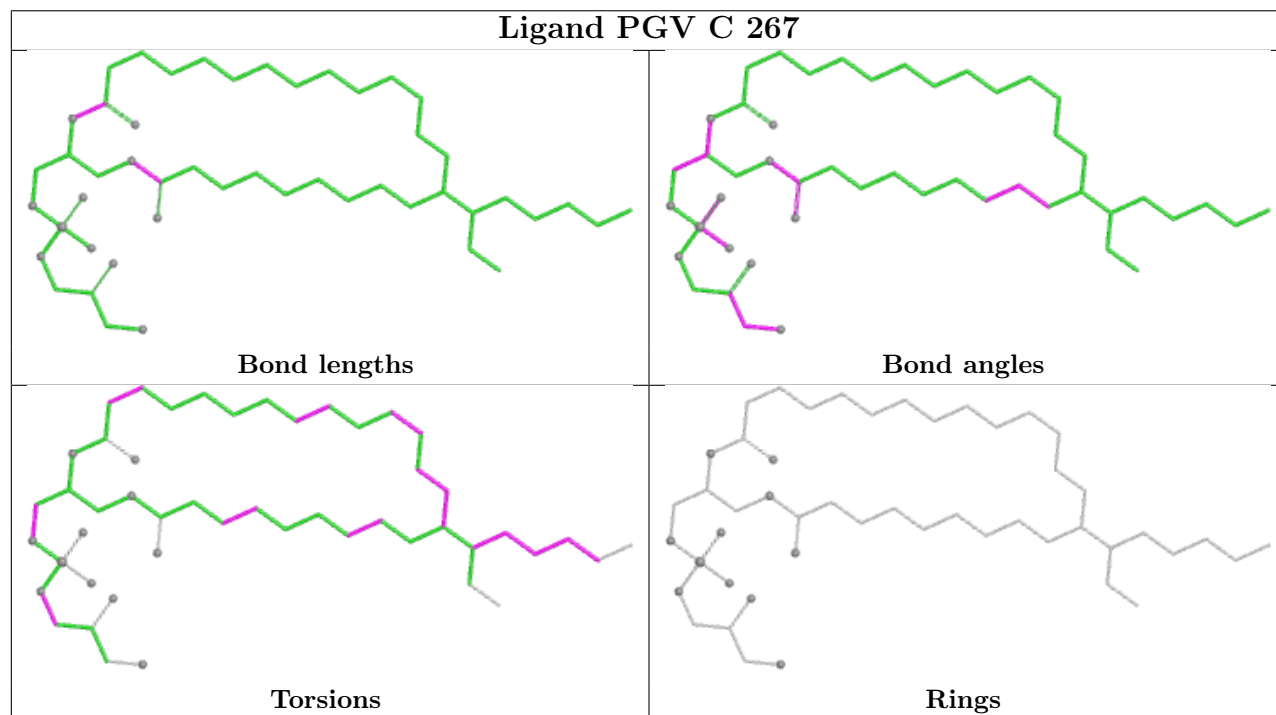


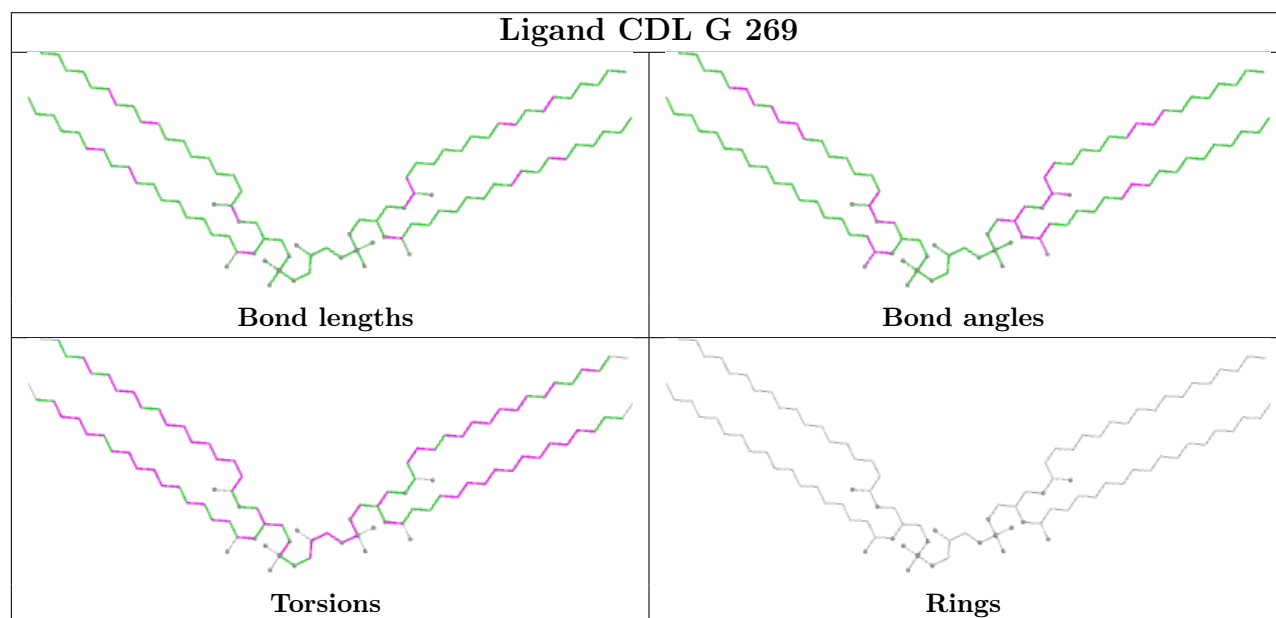
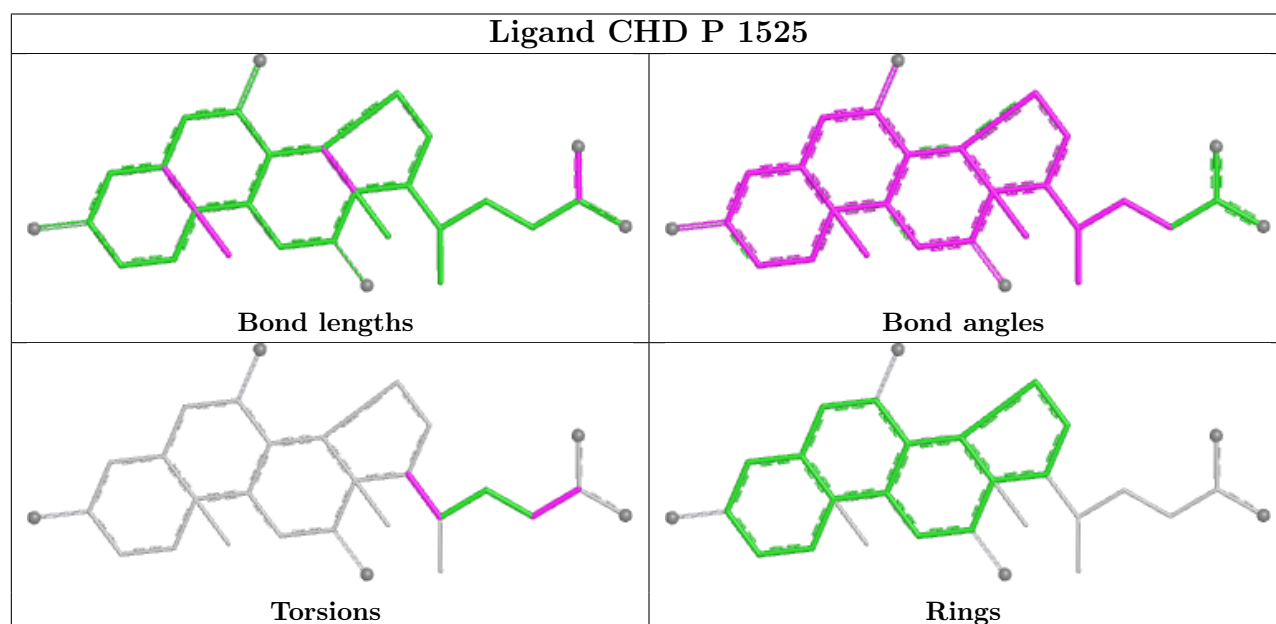
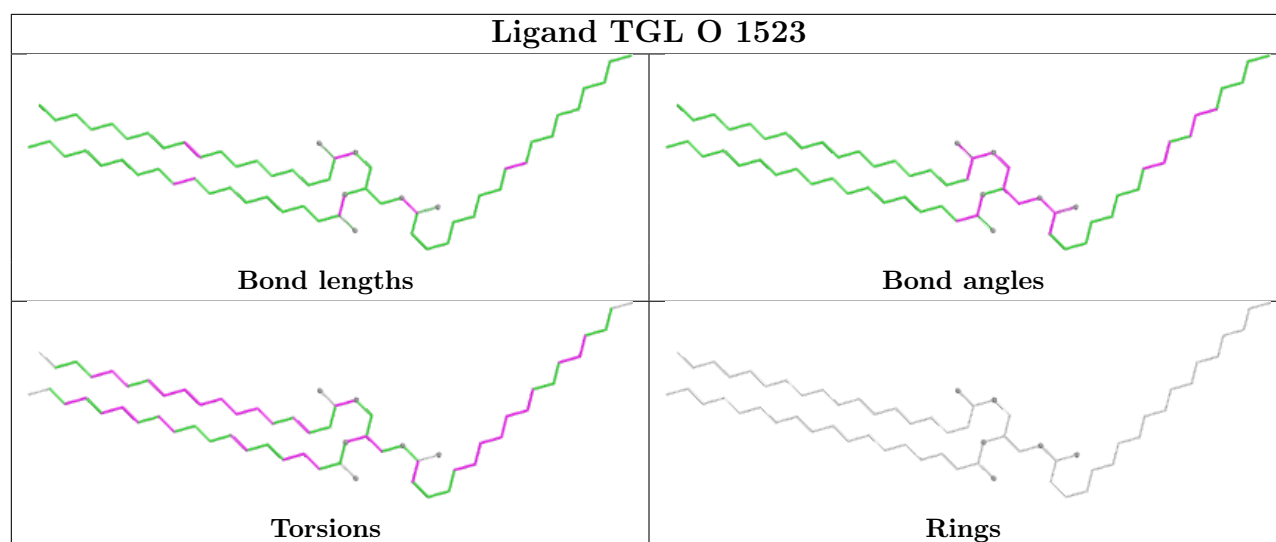


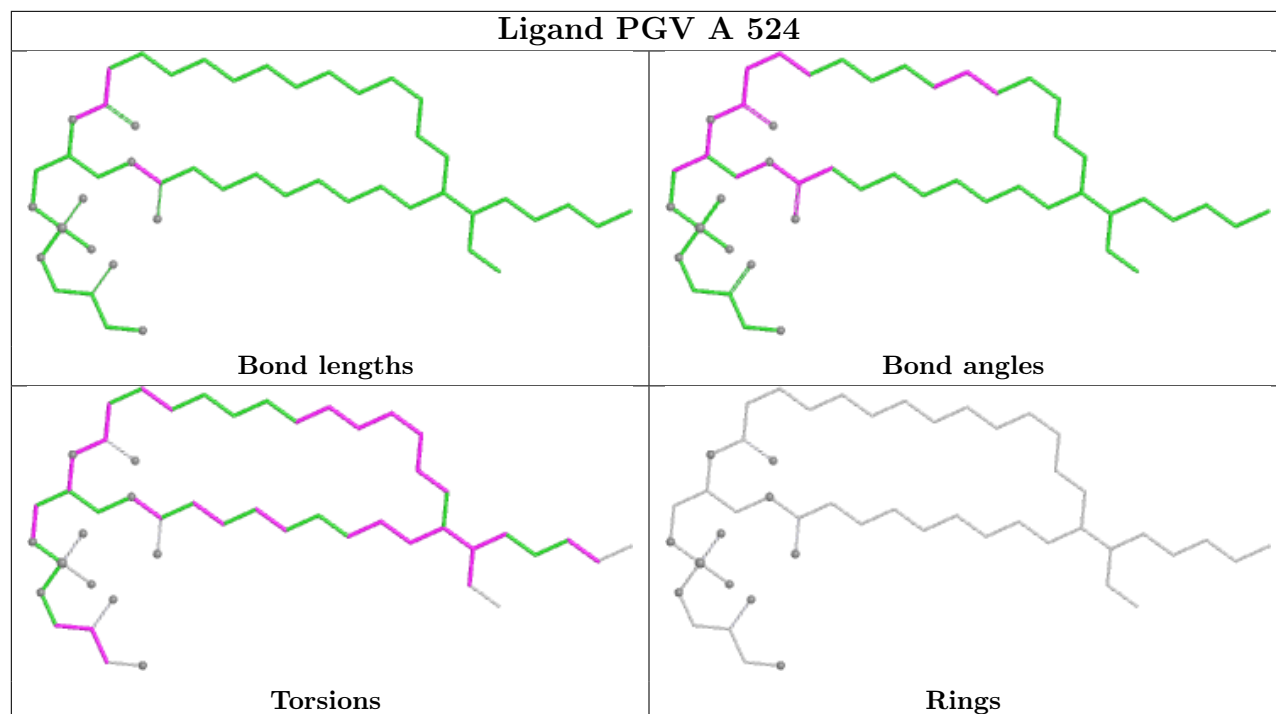
Ligand PGV N 1524



Ligand PGV C 267







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%)	-0.42	2 (0%) 88 91	23, 29, 37, 63	0
1	N	513/514 (99%)	0.07	2 (0%) 88 91	27, 34, 43, 64	0
2	B	226/227 (99%)	0.04	9 (3%) 42 49	24, 34, 56, 82	0
2	O	226/227 (99%)	0.60	12 (5%) 32 37	30, 40, 62, 82	0
3	C	259/261 (99%)	-0.12	3 (1%) 76 82	25, 32, 44, 61	0
3	P	259/261 (99%)	0.22	4 (1%) 72 78	28, 35, 47, 64	0
4	D	144/147 (97%)	0.10	4 (2%) 55 62	29, 35, 50, 65	0
4	Q	144/147 (97%)	1.22	24 (16%) 4 4	36, 50, 70, 109	0
5	E	104/109 (95%)	-0.10	1 (0%) 79 84	29, 35, 54, 70	0
5	R	104/109 (95%)	0.54	1 (0%) 79 84	32, 41, 57, 75	0
6	F	93/98 (94%)	0.28	4 (4%) 40 46	29, 38, 56, 93	0
6	S	93/98 (94%)	0.62	4 (4%) 40 46	32, 40, 62, 87	0
7	G	83/85 (97%)	0.95	17 (20%) 2 2	29, 38, 93, 99	0
7	T	83/85 (97%)	1.30	19 (22%) 2 2	30, 42, 90, 104	0
8	H	75/85 (88%)	0.45	7 (9%) 14 16	30, 41, 77, 83	0
8	U	75/85 (88%)	0.81	9 (12%) 9 10	36, 46, 80, 86	0
9	I	71/73 (97%)	0.71	10 (14%) 6 7	31, 41, 65, 71	0
9	V	71/73 (97%)	1.11	7 (9%) 13 14	36, 51, 66, 75	0
10	J	57/59 (96%)	0.38	0 100 100	32, 41, 58, 73	0
10	W	57/59 (96%)	0.97	4 (7%) 22 26	36, 45, 62, 78	0
11	K	49/56 (87%)	0.38	2 (4%) 41 48	32, 38, 49, 58	0
11	X	49/56 (87%)	1.30	7 (14%) 6 7	42, 47, 62, 69	0
12	L	46/47 (97%)	0.14	2 (4%) 40 46	30, 35, 54, 79	0
12	Y	46/47 (97%)	0.80	4 (8%) 16 18	34, 42, 62, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.62	5 (11%) 9 11	29, 35, 87, 107	0
13	Z	43/46 (93%)	1.30	9 (20%) 2 2	37, 44, 96, 112	0
All	All	3526/3614 (97%)	0.28	172 (4%) 35 41	23, 36, 61, 112	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	9.4
6	S	96	LEU	8.0
4	Q	4	SER	6.8
7	T	4	ALA	6.4
6	S	94	HIS	6.2
6	S	93	PRO	6.1
2	O	227	LEU	6.0
7	T	36	TRP	5.9
6	F	96	LEU	5.9
2	B	59	GLN	5.8
7	G	5	LYS	5.8
7	G	2	SER	5.7
7	T	9	GLY	5.6
7	T	2	SER	5.6
4	Q	5	VAL	5.5
7	G	36	TRP	5.4
2	O	113	TYR	5.4
7	T	5	LYS	5.3
8	U	47	GLY	5.1
7	G	4	ALA	5.1
7	T	12	GLY	5.0
13	Z	40	TYR	5.0
7	T	3	ALA	4.9
13	M	40	TYR	4.9
4	D	4	SER	4.8
7	G	1	ALA	4.7
8	U	46	LYS	4.7
9	V	3	ALA	4.6
9	V	37	PHE	4.6
7	T	8	HIS	4.6
10	W	52	TRP	4.6
7	T	37	LEU	4.5
7	G	3	ALA	4.5
6	F	94	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
4	Q	7	LYS	4.4
8	U	42	ALA	4.4
6	S	95	GLN	4.3
7	G	12	GLY	4.3
13	M	41	LYS	4.2
7	G	10	GLY	4.1
13	M	42	LYS	4.1
4	Q	8	SER	4.1
11	X	47	ARG	3.9
7	G	37	LEU	3.9
7	G	7	ASP	3.9
13	M	43	SER	3.9
7	T	38	HIS	3.9
3	C	38	ASN	3.8
13	Z	42	LYS	3.8
7	T	6	GLY	3.7
7	T	1	ALA	3.7
11	X	6	ALA	3.7
9	I	37	PHE	3.7
8	U	50	VAL	3.7
7	G	9	GLY	3.6
6	F	95	GLN	3.6
9	V	36	LYS	3.6
2	B	91	ASN	3.6
13	Z	43	SER	3.5
2	O	59	GLN	3.5
3	P	3	HIS	3.5
9	I	27	VAL	3.4
8	U	45	ALA	3.4
1	A	298	ASP	3.3
7	T	10	GLY	3.3
2	O	65	TRP	3.3
7	G	6	GLY	3.3
8	H	48	GLY	3.3
12	Y	20	ARG	3.2
12	Y	45	LEU	3.2
2	O	90	ILE	3.2
8	H	50	VAL	3.2
9	I	29	LEU	3.2
13	Z	32	TRP	3.2
11	K	6	ALA	3.2
8	H	44	THR	3.2

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Mol	Chain	Res	Type	RSRZ
9	I	26	MET	3.1
5	R	109	VAL	3.1
7	G	38	HIS	3.1
2	B	113	TYR	3.1
12	L	2	HIS	3.1
7	T	7	ASP	3.0
4	Q	48	TRP	3.0
13	Z	39	ASN	3.0
2	O	60	GLU	3.0
8	U	44	THR	3.0
1	N	513	LEU	2.9
4	Q	51	LEU	2.9
7	G	8	HIS	2.9
4	Q	111	PHE	2.9
9	I	3	ALA	2.9
12	Y	2	HIS	2.9
13	M	39	ASN	2.9
1	N	113	LEU	2.9
2	B	32	PHE	2.8
10	W	57	HIS	2.8
7	T	84	LYS	2.7
5	E	109	VAL	2.7
2	O	91	ASN	2.7
8	H	43	MET	2.7
2	B	60	GLU	2.7
8	H	47	GLY	2.6
9	I	30	GLY	2.6
4	D	5	VAL	2.6
2	O	32	PHE	2.6
3	C	37	PHE	2.6
4	Q	59	LEU	2.6
4	Q	9	GLU	2.6
2	B	58	ALA	2.6
7	G	41	HIS	2.5
4	D	11	TYR	2.5
1	A	514	LYS	2.5
3	P	33	MET	2.5
3	P	44	MET	2.5
6	F	93	PRO	2.5
10	W	44	LEU	2.5
4	Q	138	TRP	2.5
11	X	13	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
13	Z	37	LEU	2.5
7	T	42	ARG	2.5
2	B	90	ILE	2.5
2	O	67	ILE	2.5
4	Q	115	TRP	2.5
8	H	45	ALA	2.5
4	Q	121	LYS	2.5
3	P	37	PHE	2.4
4	Q	107	ILE	2.4
2	O	217	LYS	2.4
9	I	25	PHE	2.4
9	V	33	THR	2.4
13	Z	41	LYS	2.4
9	I	33	THR	2.4
9	V	72	ALA	2.4
7	T	40	GLY	2.4
2	B	57	ASP	2.3
4	D	19	ARG	2.3
4	Q	95	LEU	2.3
11	X	7	PRO	2.3
4	Q	17	VAL	2.3
4	Q	87	PHE	2.3
9	I	15	ARG	2.3
11	K	47	ARG	2.3
7	T	39	SER	2.3
2	O	138	VAL	2.3
2	O	226	MET	2.3
4	Q	10	ASP	2.2
11	X	27	ALA	2.2
2	B	61	VAL	2.2
8	U	48	GLY	2.2
4	Q	53	ILE	2.2
12	L	47	LYS	2.2
12	Y	47	LYS	2.2
4	Q	57	VAL	2.2
3	C	3	HIS	2.1
10	W	55	PHE	2.1
11	X	49	THR	2.1
7	T	35	SER	2.1
9	V	30	GLY	2.1
4	Q	35	ALA	2.1
4	Q	39	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
8	H	42	ALA	2.1
9	I	32	ALA	2.1
13	Z	35	TYR	2.1
4	Q	147	LYS	2.1
4	Q	11	TYR	2.1
7	G	39	SER	2.1
8	U	27	ARG	2.1
8	U	79	GLY	2.1
13	Z	3	ALA	2.1
7	G	84	LYS	2.0
9	V	63	MET	2.0
11	X	23	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	TPO	T	11	11/12	0.56	0.22	71,78,95,96	0
7	TPO	G	11	11/12	0.60	0.27	71,78,96,97	0
1	FME	A	1	10/11	0.88	0.13	48,51,72,78	0
1	FME	N	1	10/11	0.89	0.16	47,49,70,71	0
2	FME	O	1	10/11	0.94	0.11	39,40,48,52	0
2	FME	B	1	10/11	0.94	0.09	32,33,40,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	DMU	P	1272	33/33	0.72	0.21	80,103,111,112	0
22	CHD	W	1060	29/29	0.73	0.21	87,91,96,97	0
24	PEK	T	263	53/53	0.74	0.26	55,95,117,119	0
25	CDL	G	269	100/100	0.75	0.23	64,87,115,118	0
28	DMU	G	272	33/33	0.75	0.18	65,94,105,105	0
24	PEK	G	265	53/53	0.75	0.24	45,82,114,116	0
25	CDL	T	1269	100/100	0.77	0.21	61,84,108,111	0
26	PSC	R	1230	52/52	0.77	0.26	43,96,122,124	0
20	PGV	H	268	51/51	0.77	0.25	59,84,110,112	0
24	PEK	G	1263	53/53	0.77	0.25	60,95,118,119	0
19	TGL	O	1523	63/63	0.78	0.25	54,76,89,94	0
19	TGL	Y	1522	63/63	0.78	0.23	45,72,86,88	0
24	PEK	T	1265	53/53	0.78	0.23	44,79,110,112	0
20	PGV	A	524	51/51	0.78	0.22	33,74,105,108	0
25	CDL	P	1270	100/100	0.80	0.23	41,85,115,120	0
22	CHD	J	60	29/29	0.81	0.21	77,83,93,94	0
19	TGL	D	523	63/63	0.81	0.21	44,63,81,82	0
20	PGV	N	1268	51/51	0.81	0.23	67,91,112,114	0
19	TGL	L	522	63/63	0.82	0.19	38,59,77,79	0
19	TGL	O	1521	63/63	0.82	0.19	53,77,88,89	0
26	PSC	E	230	52/52	0.82	0.22	58,99,125,127	0
19	TGL	A	521	63/63	0.82	0.20	48,69,84,89	0
25	CDL	C	270	100/100	0.82	0.21	41,84,118,119	0
20	PGV	N	1524	51/51	0.82	0.19	41,75,113,114	0
23	UNX	C	262	1/1	0.86	0.49	28,28,28,28	0
28	DMU	Z	1526	33/33	0.86	0.12	39,54,67,69	0
17	NA	A	519	1/1	0.89	0.17	42,42,42,42	0
23	UNX	P	1262	1/1	0.91	0.48	22,22,22,22	0
22	CHD	C	271	29/29	0.91	0.11	46,51,53,55	0
17	NA	N	1519	1/1	0.92	0.20	45,45,45,45	0
22	CHD	P	1271	29/29	0.93	0.10	48,53,56,58	0
28	DMU	M	526	33/33	0.93	0.10	39,47,65,67	0
22	CHD	C	525	29/29	0.94	0.08	28,33,40,45	0
24	PEK	C	264	53/53	0.95	0.11	29,47,73,75	0
22	CHD	O	229	29/29	0.95	0.08	23,31,37,37	0
22	CHD	P	1525	29/29	0.95	0.08	29,36,42,44	0
24	PEK	P	1264	53/53	0.95	0.12	29,48,75,78	0
20	PGV	C	267	51/51	0.96	0.10	25,36,67,70	0
22	CHD	B	1086	29/29	0.96	0.06	26,30,37,47	0
20	PGV	N	1266	51/51	0.96	0.10	31,42,67,71	0
20	PGV	P	1267	51/51	0.97	0.09	28,40,72,79	0
20	PGV	A	522	51/51	0.97	0.09	25,39,65,66	0
15	PER	N	520	2/2	0.97	0.08	31,31,31,34	0

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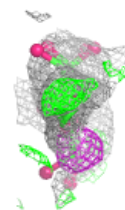
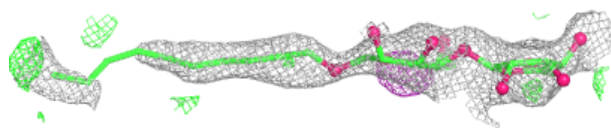
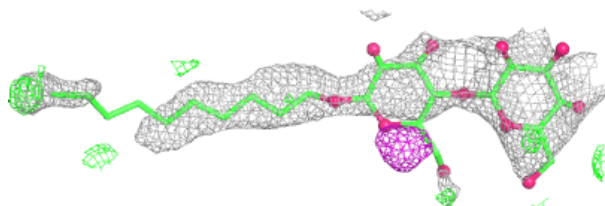
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	HEA	N	516	60/60	0.98	0.07	26,32,39,41	0
15	PER	A	520	2/2	0.98	0.05	25,25,25,32	0
16	MG	N	1518	1/1	0.98	0.04	34,34,34,34	0
21	CUA	O	228	2/2	0.98	0.04	36,36,36,37	0
18	HEA	N	515	60/60	0.98	0.07	23,32,51,54	0
18	HEA	A	515	60/60	0.99	0.06	19,26,50,53	0
27	ZN	S	99	1/1	0.99	0.03	38,38,38,38	0
18	HEA	A	516	60/60	0.99	0.05	20,26,33,36	0
21	CUA	B	228	2/2	0.99	0.03	27,27,27,30	0
16	MG	A	518	1/1	0.99	0.03	27,27,27,27	0
14	CU	N	517	1/1	0.99	0.04	32,32,32,32	0
27	ZN	F	99	1/1	1.00	0.01	34,34,34,34	0
14	CU	A	517	1/1	1.00	0.02	29,29,29,29	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.

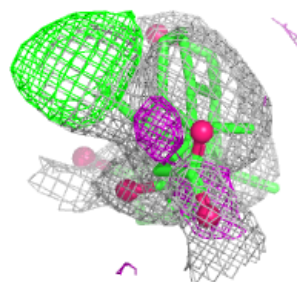
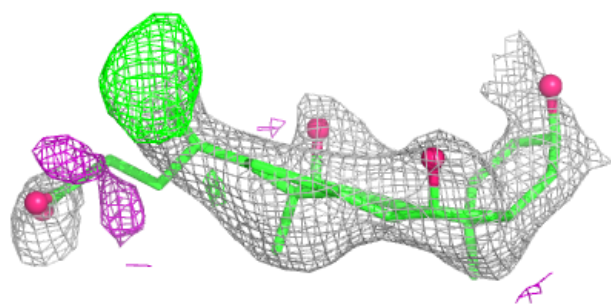
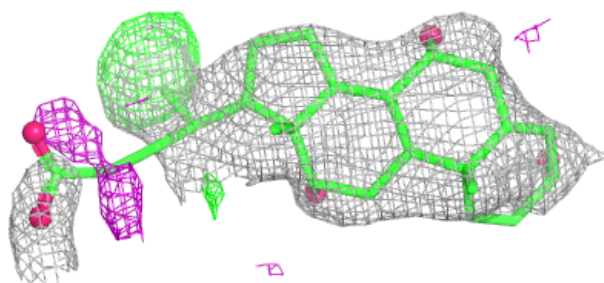
Electron density around DMU P 1272:

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



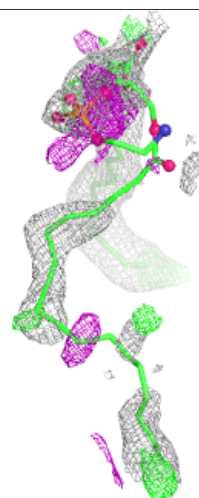
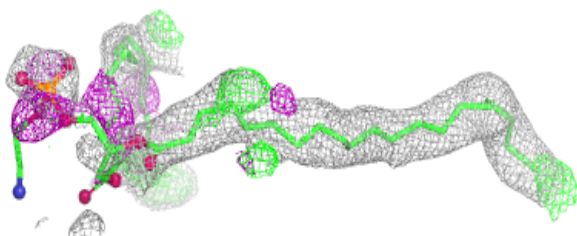
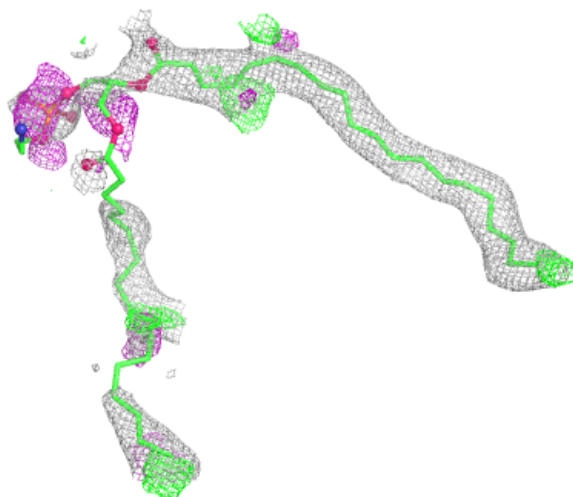
Electron density around CHD W 1060:

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



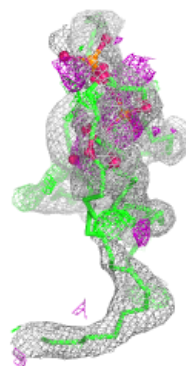
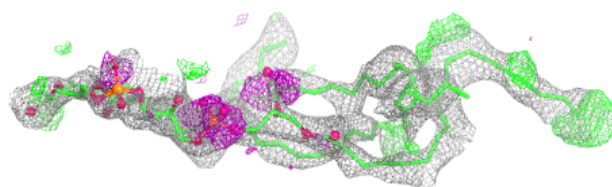
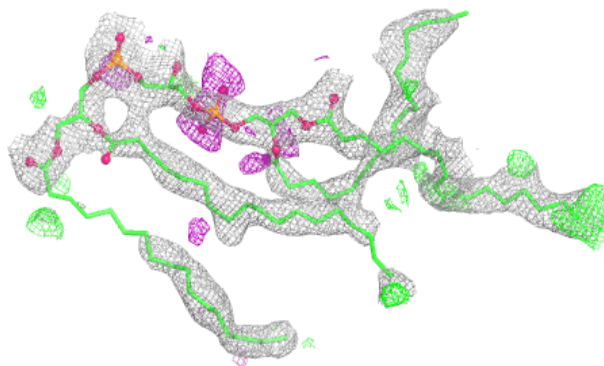
Electron density around PEK T 263:

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

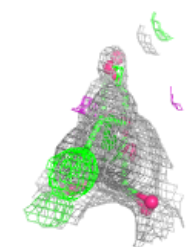
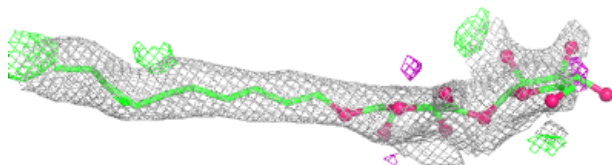
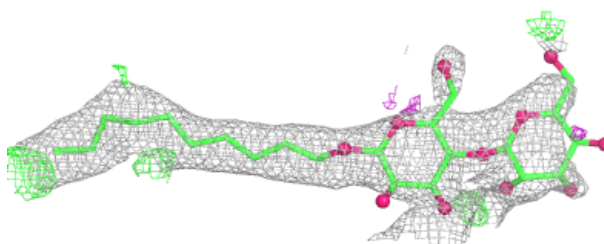


Electron density around CDL G 269:

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

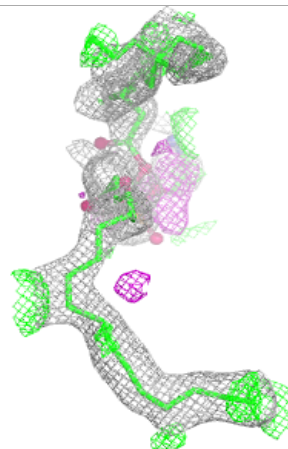
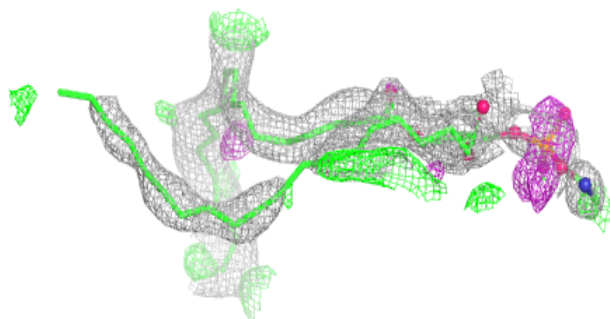
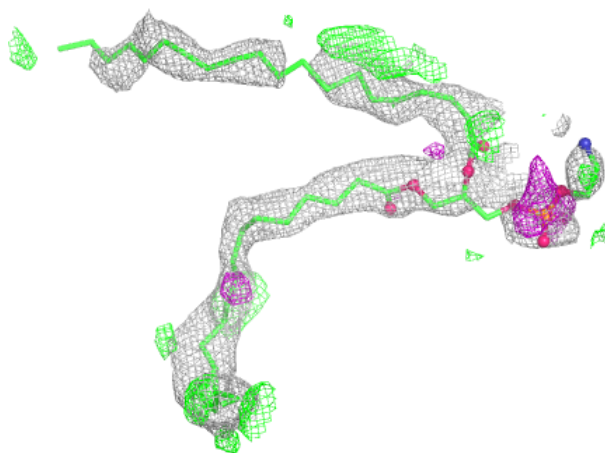
**Electron density around DMU G 272:**

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



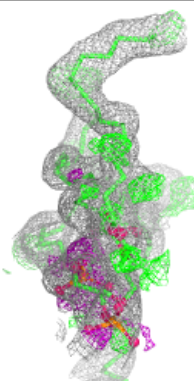
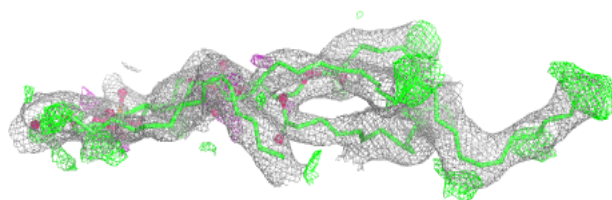
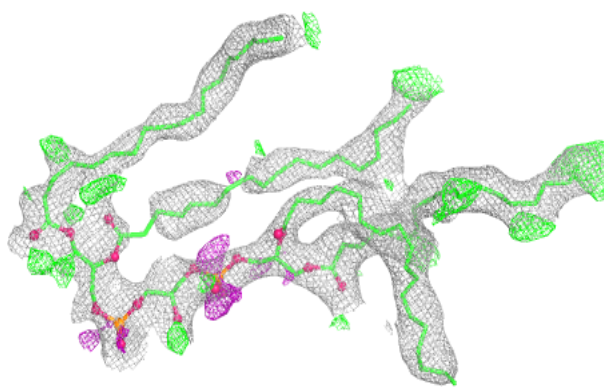
Electron density around PEK G 265:

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

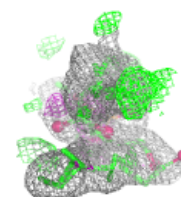
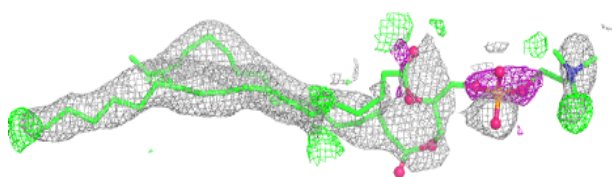
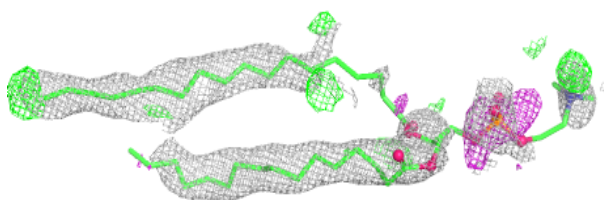


Electron density around CDL T 1269:

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

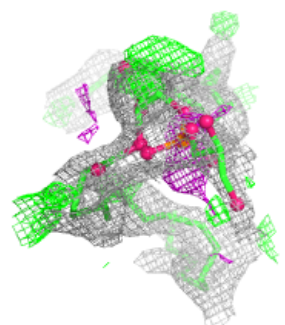
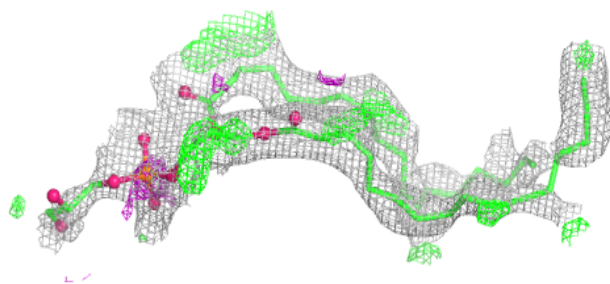
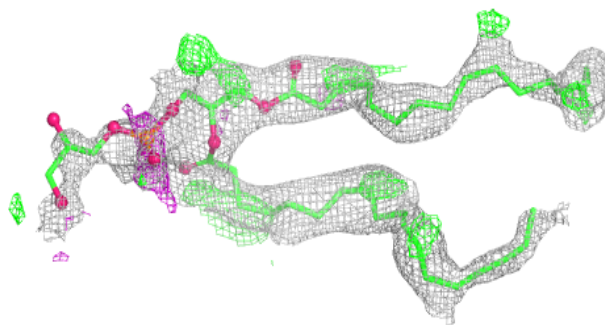
**Electron density around PSC R 1230:**

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



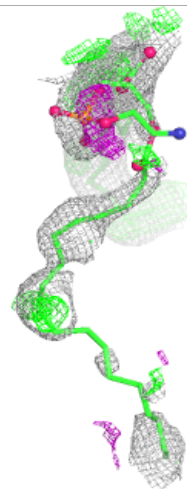
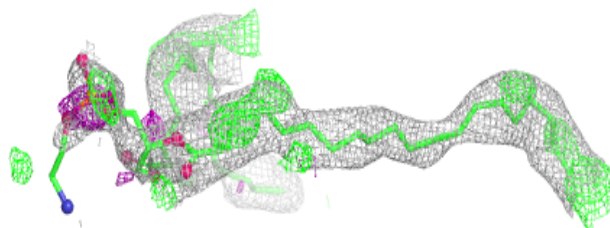
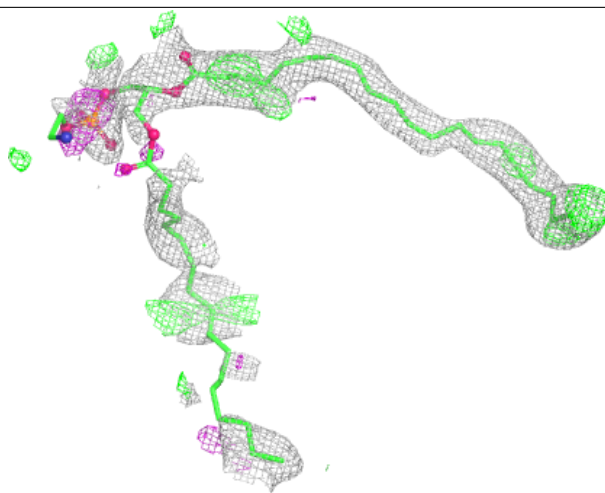
Electron density around PGV H 268:

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



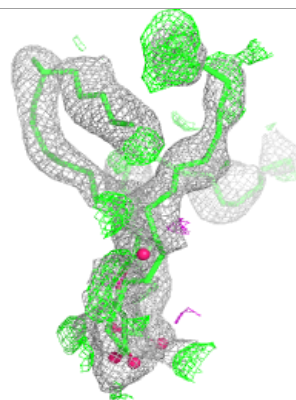
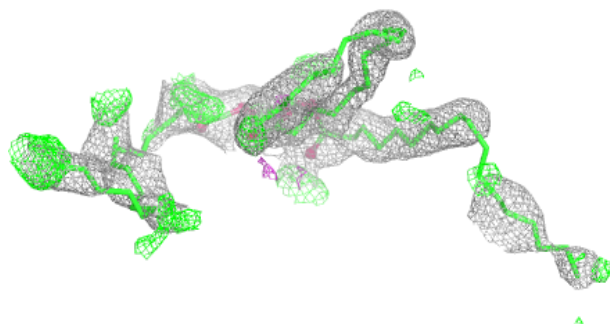
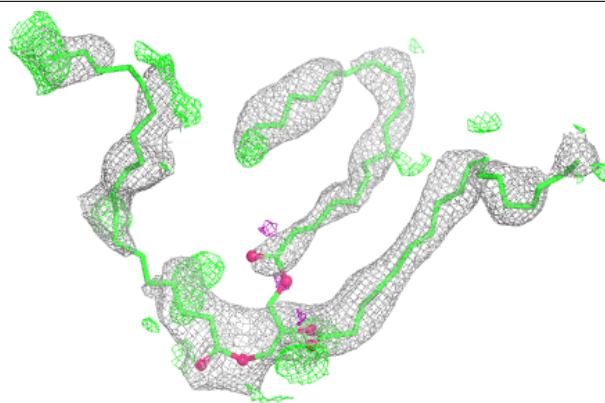
Electron density around PEK G 1263:

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

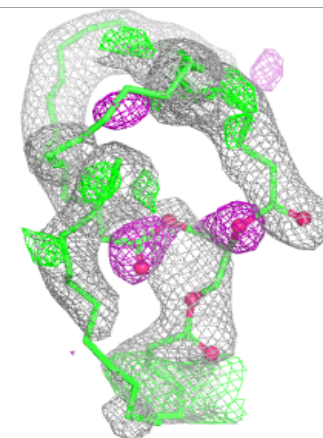
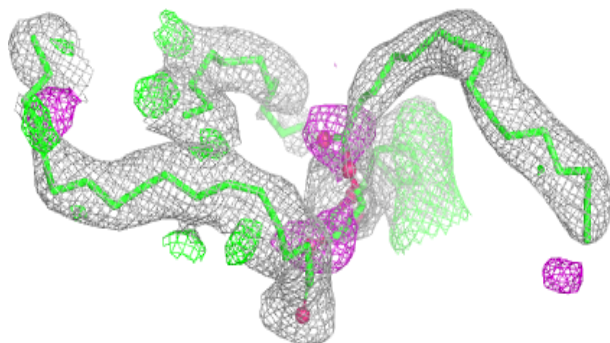
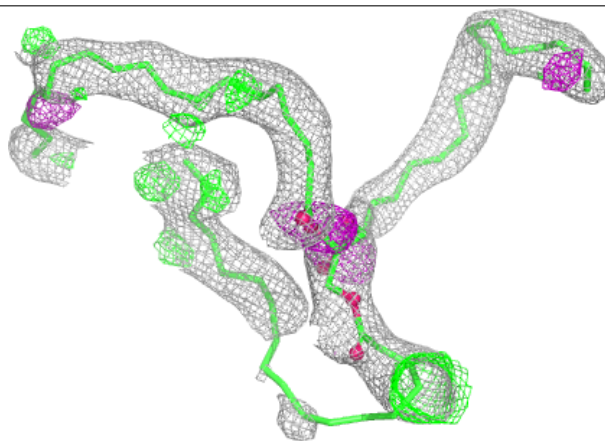


Electron density around TGL O 1523:

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

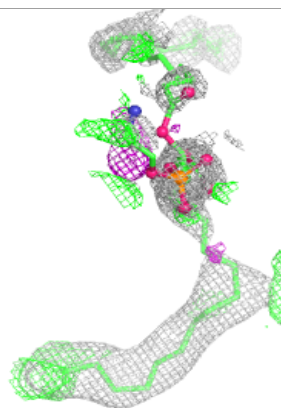
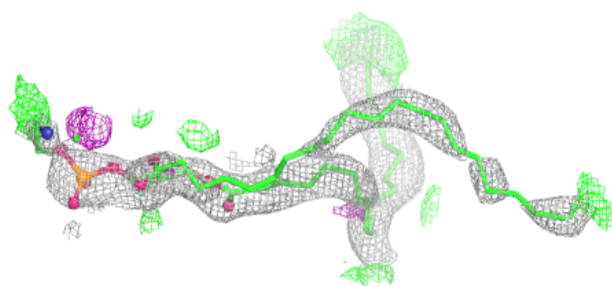
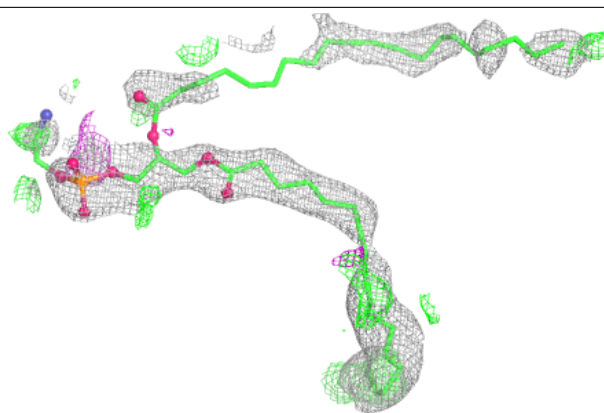
**Electron density around TGL Y 1522:**

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

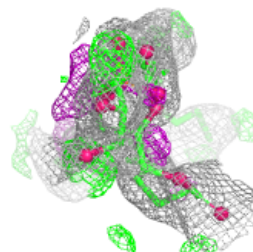
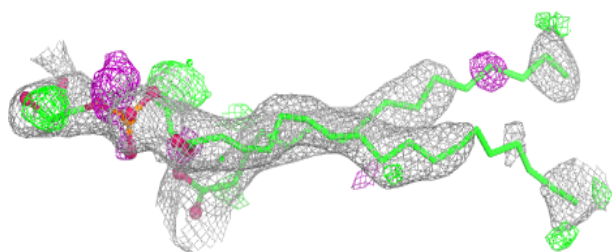
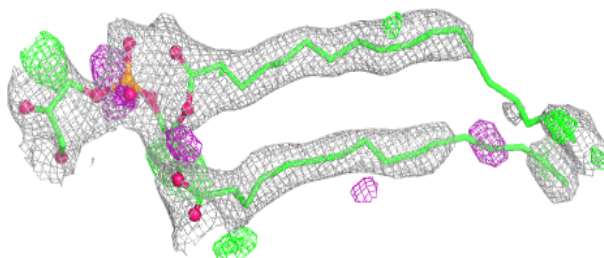


Electron density around PEK T 1265:

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

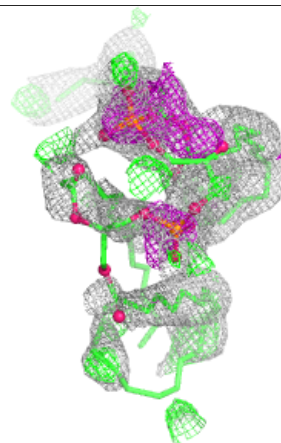
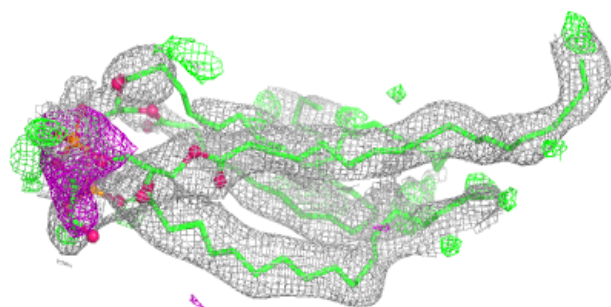
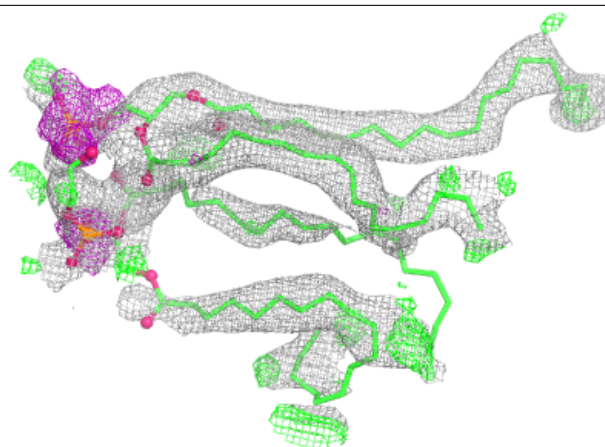
**Electron density around PGV A 524:**

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



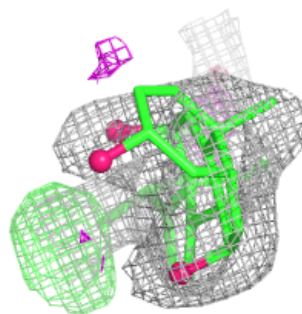
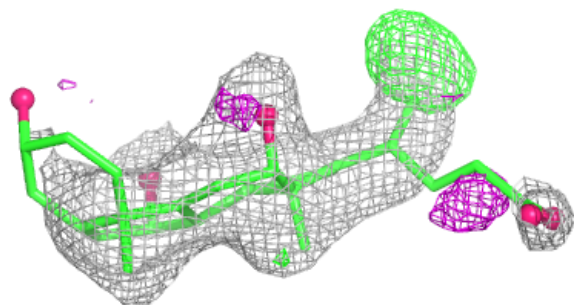
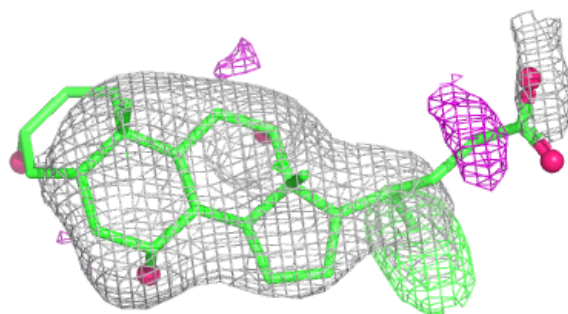
Electron density around CDL P 1270:

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

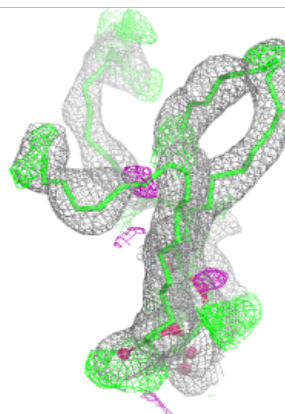
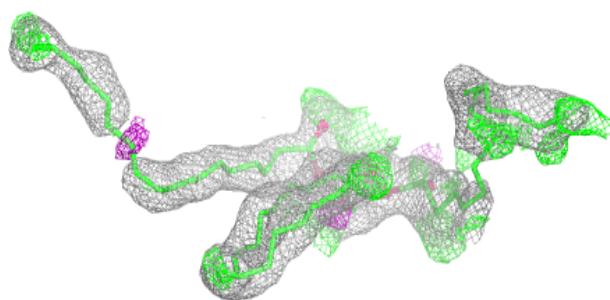
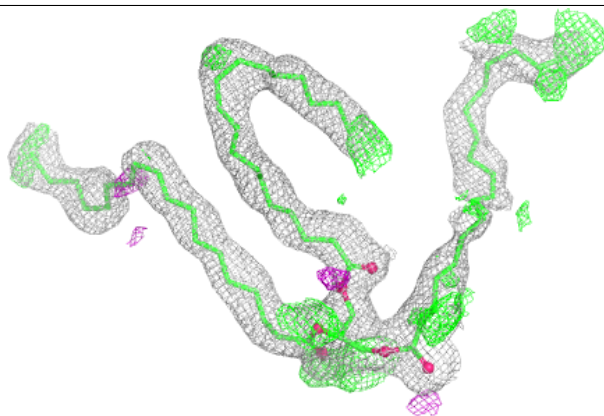


Electron density around CHD J 60:

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

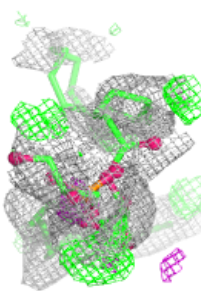
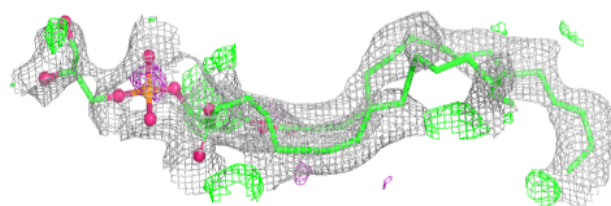
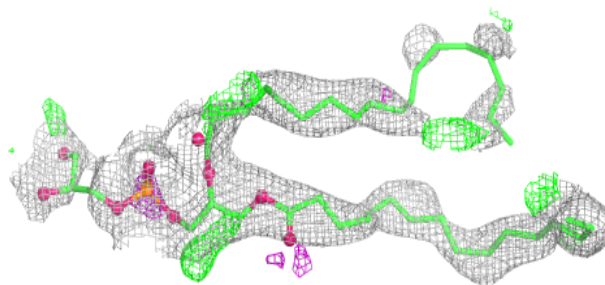
**Electron density around TGL D 523:**

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



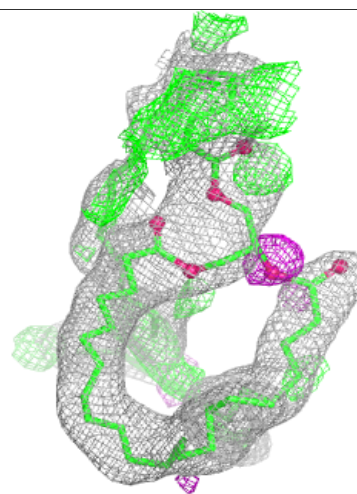
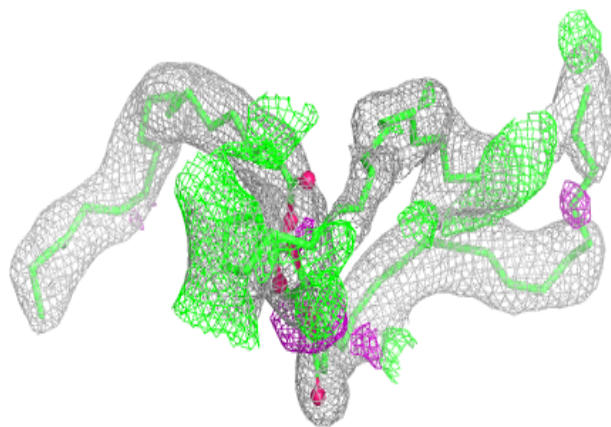
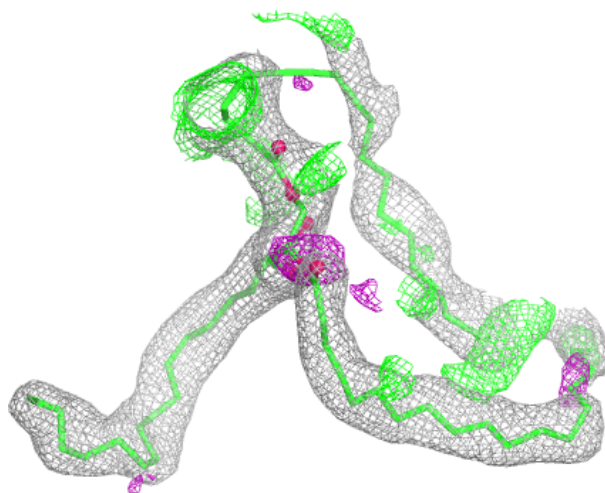
Electron density around PGV N 1268:

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



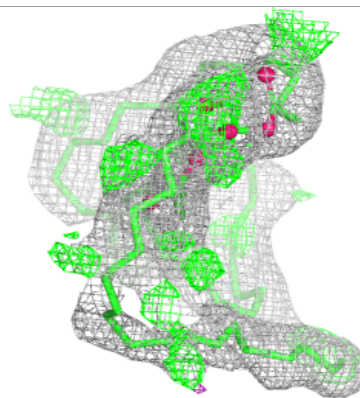
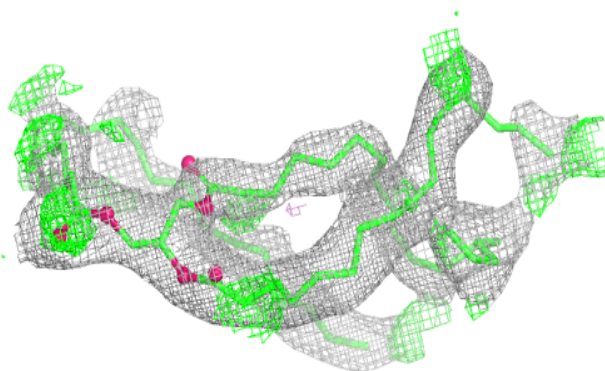
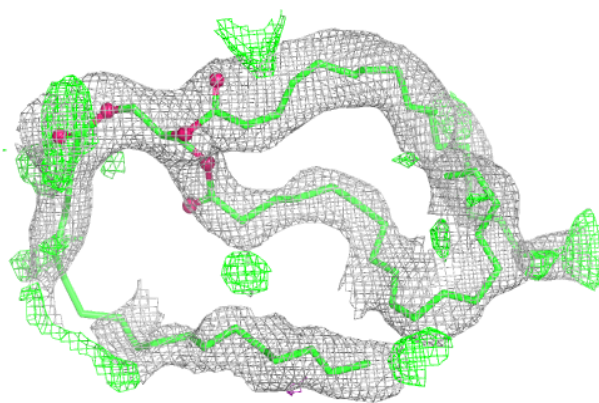
Electron density around TGL L 522:

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

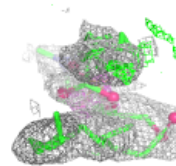
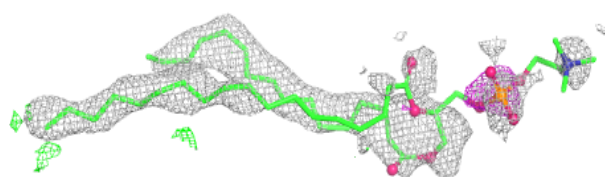
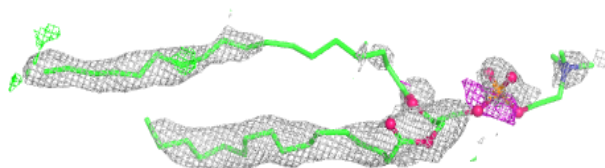


Electron density around TGL O 1521:

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

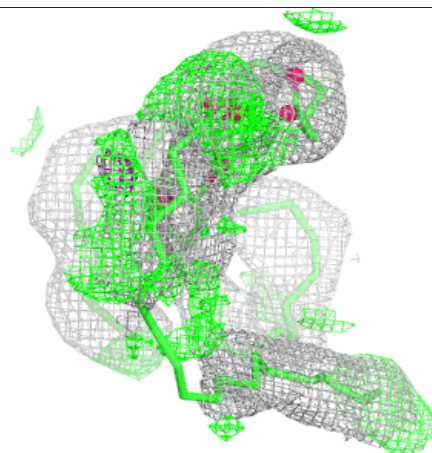
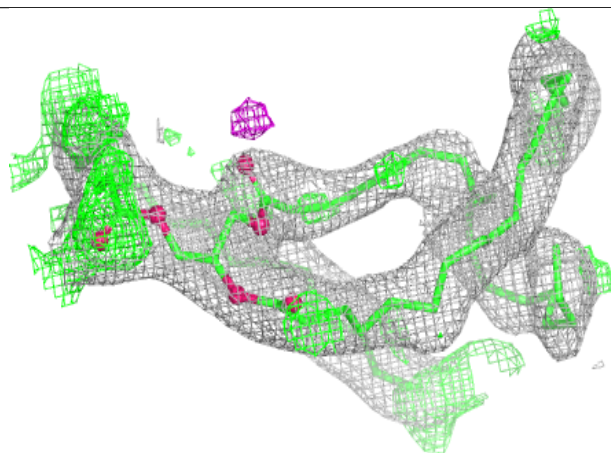
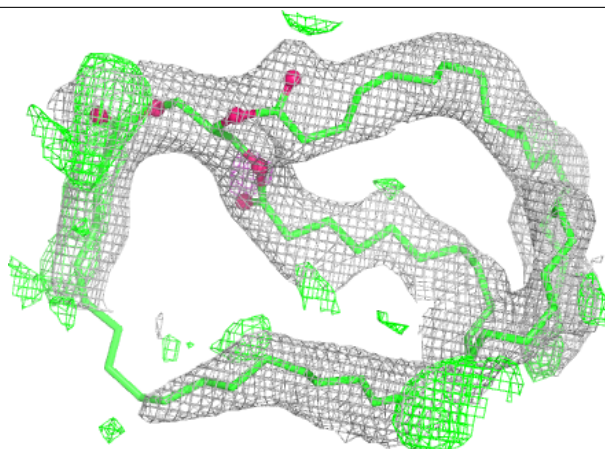
**Electron density around PSC E 230:**

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



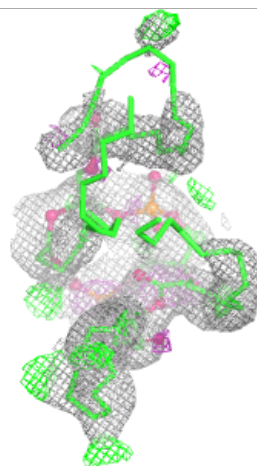
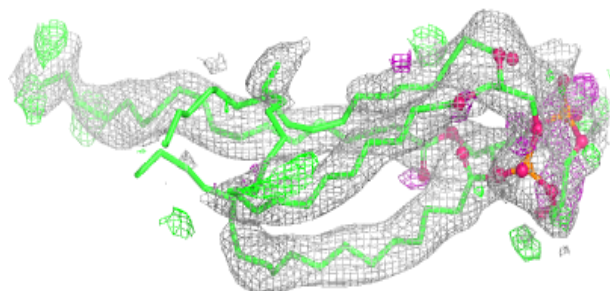
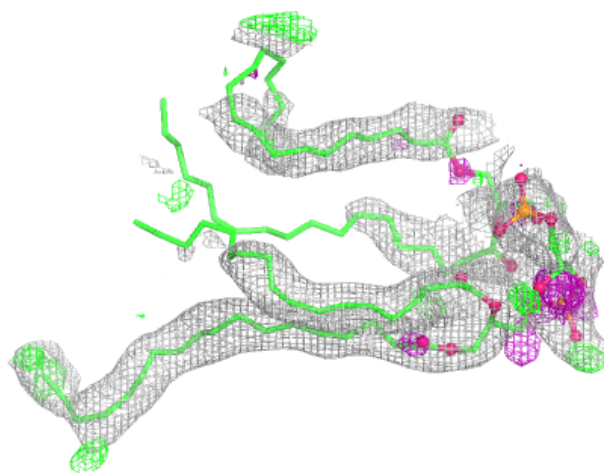
Electron density around TGL A 521:

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



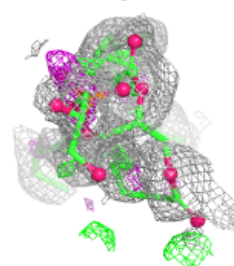
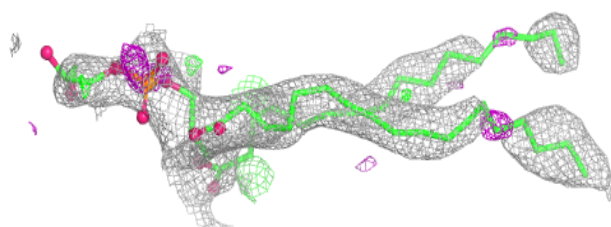
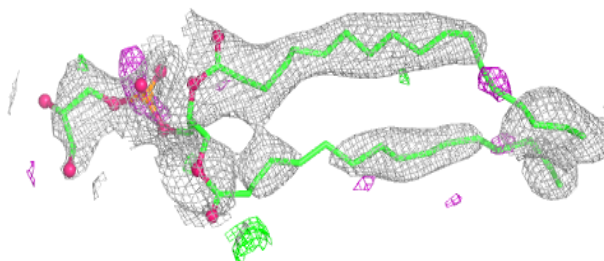
Electron density around CDL C 270:

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

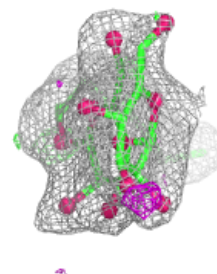
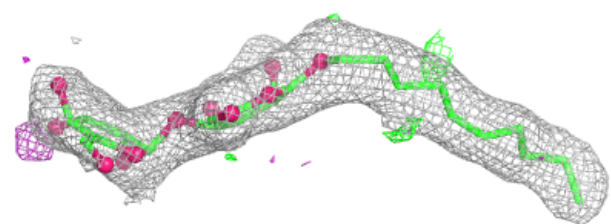
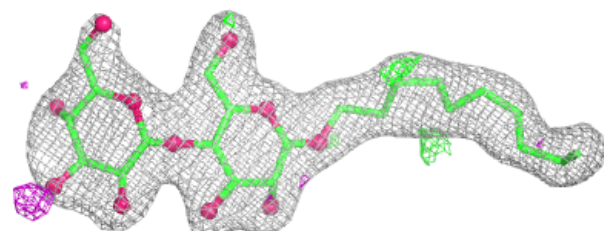


Electron density around PGV N 1524:

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

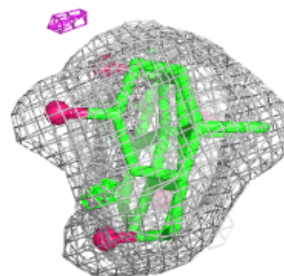
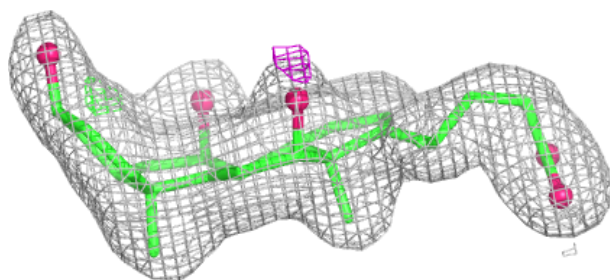
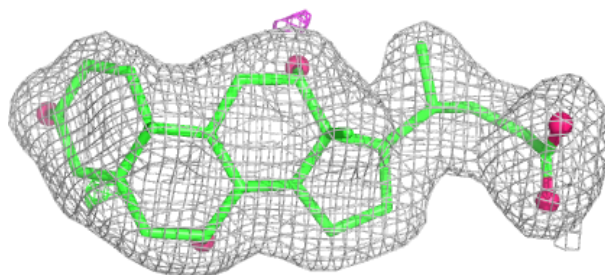
**Electron density around DMU Z 1526:**

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

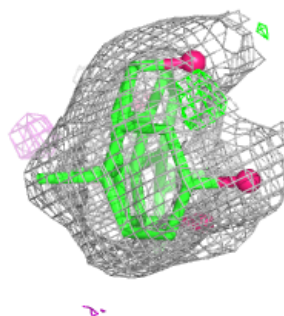
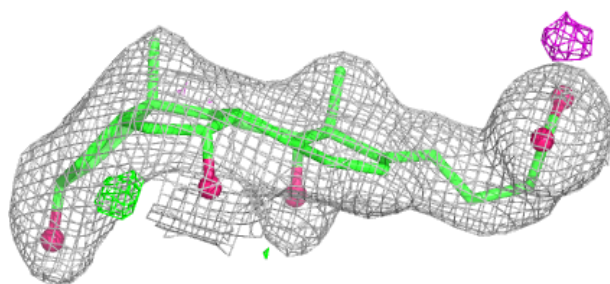
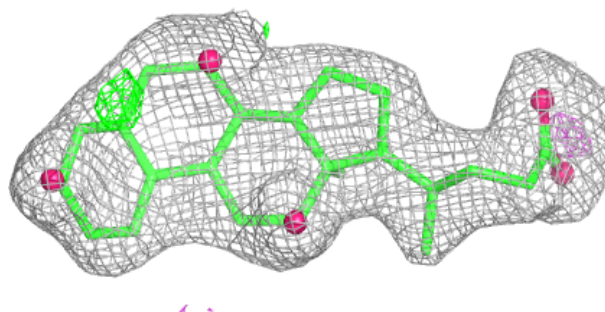


Electron density around CHD C 271:

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

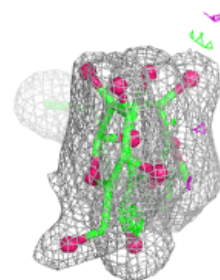
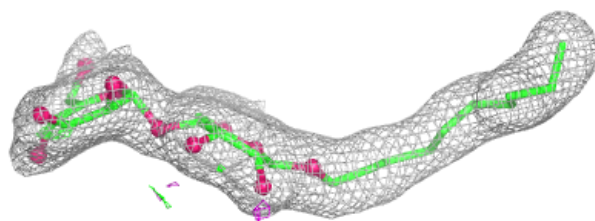
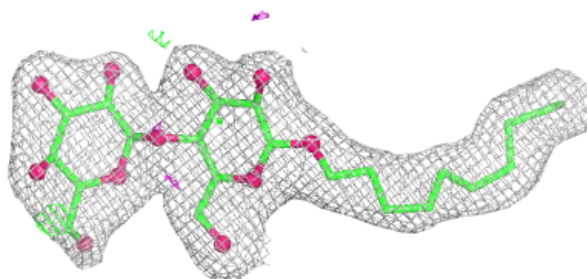
**Electron density around CHD P 1271:**

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

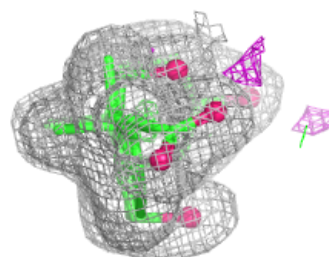
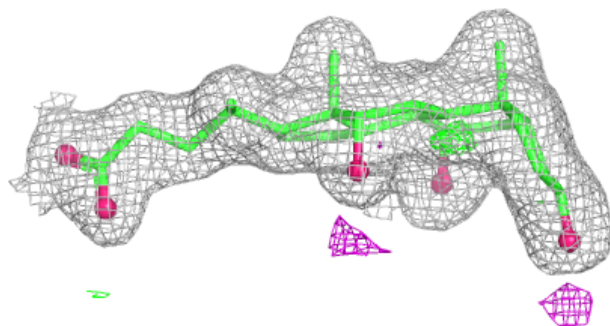
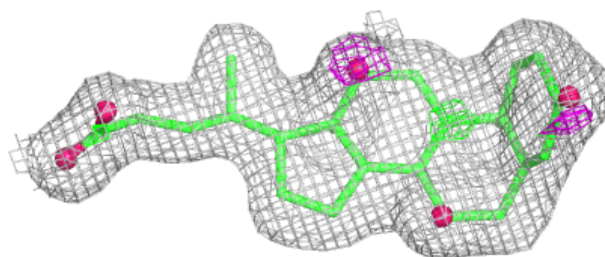


Electron density around DMU M 526:

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

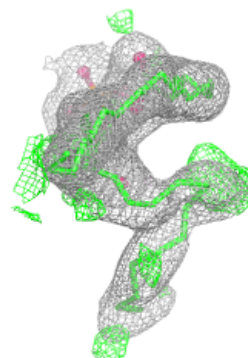
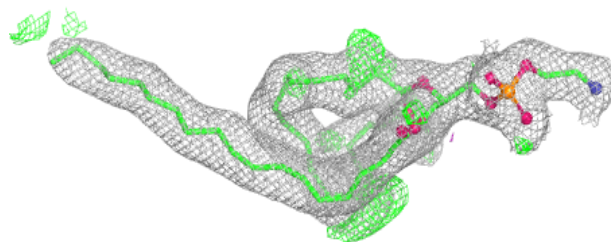
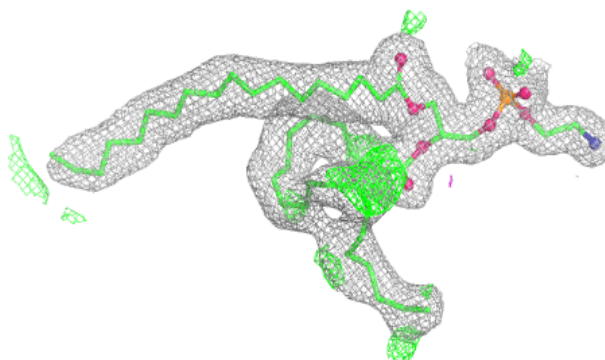
**Electron density around CHD C 525:**

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

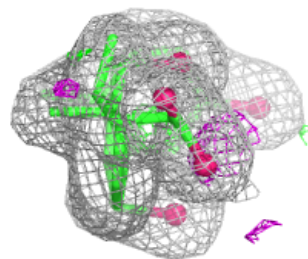
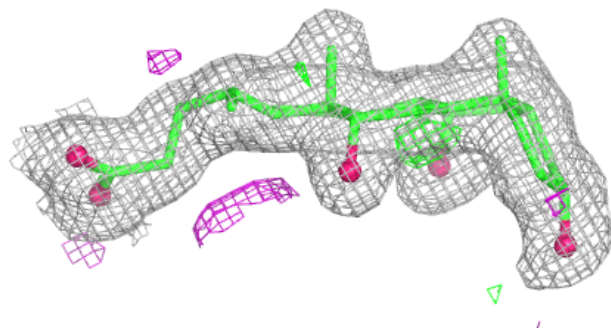
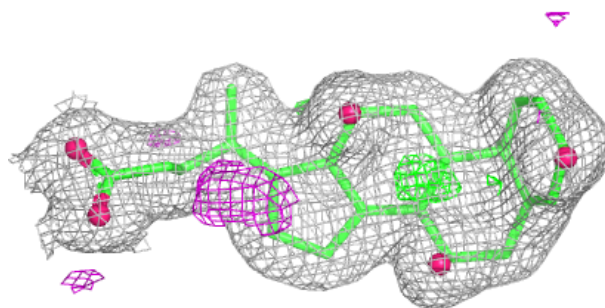


Electron density around PEK C 264:

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

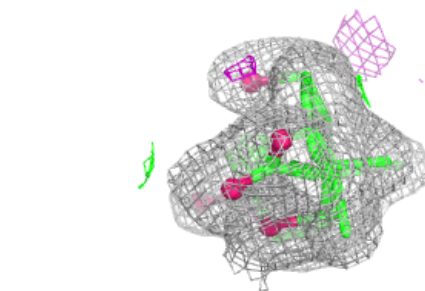
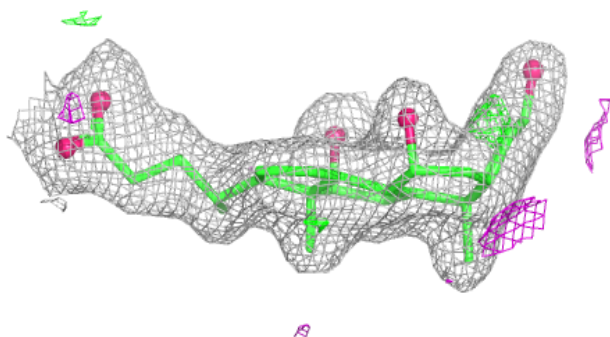
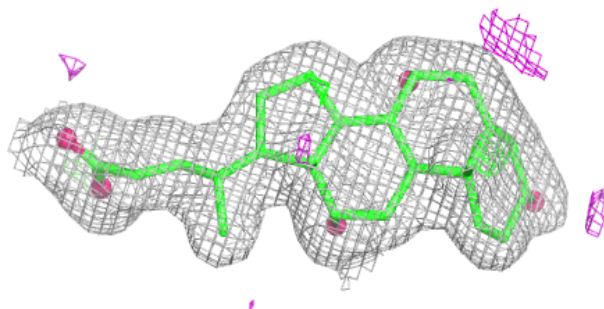
**Electron density around CHD O 229:**

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

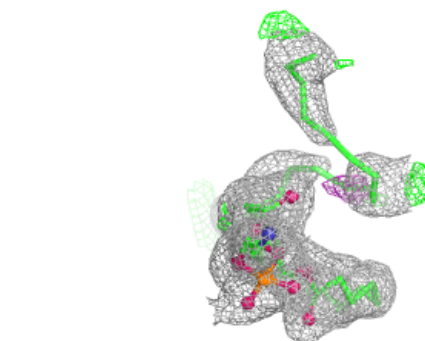
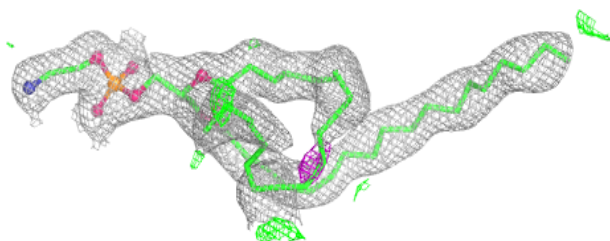
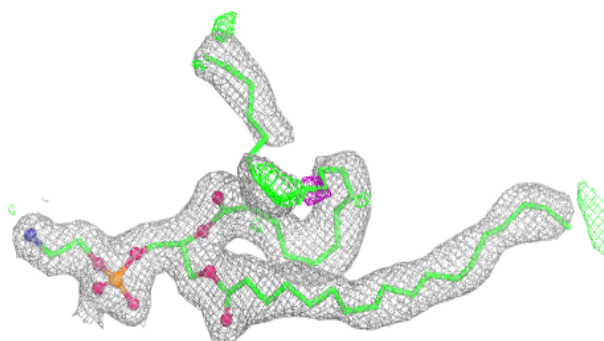


Electron density around CHD P 1525:

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

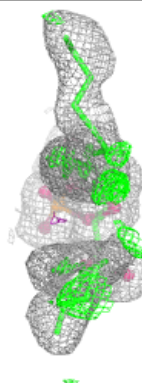
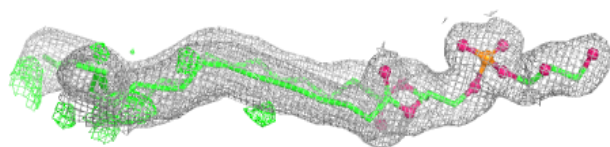
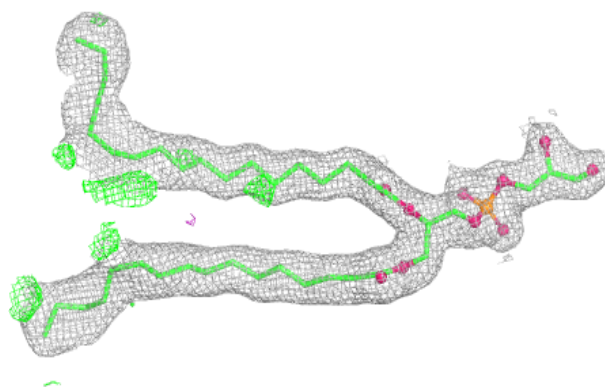
**Electron density around PEK P 1264:**

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

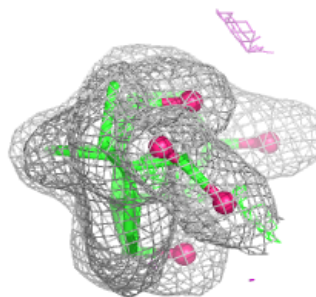
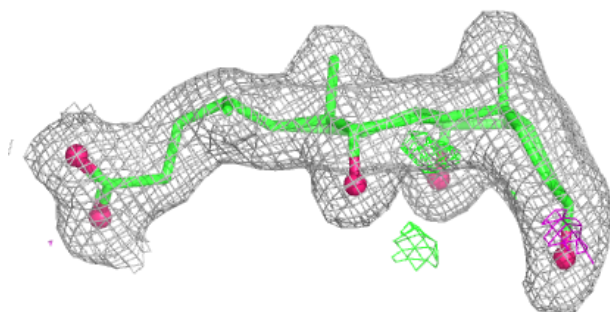
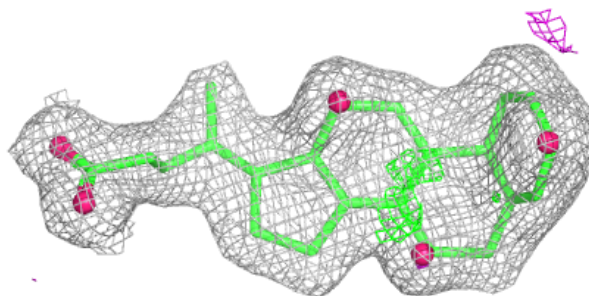


Electron density around PGV C 267:

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

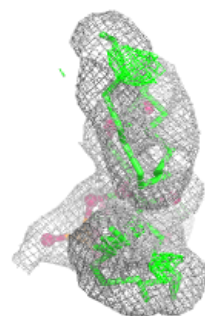
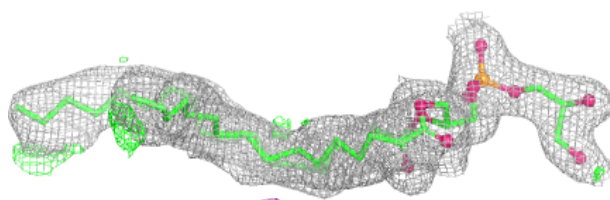
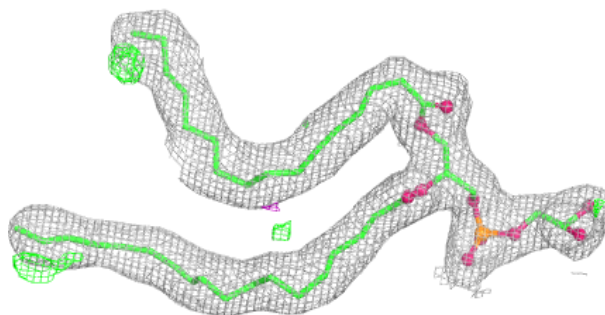
**Electron density around CHD B 1086:**

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

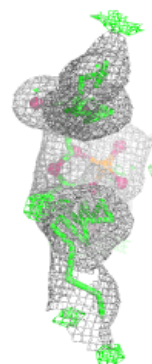
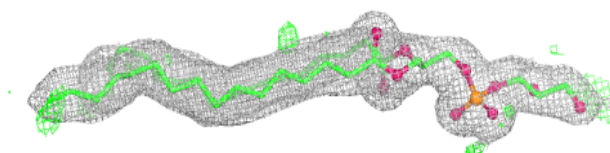
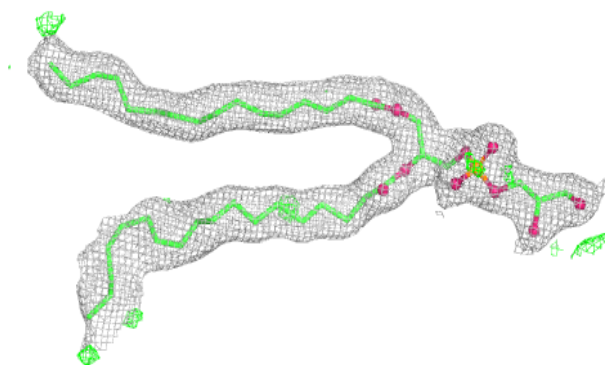


Electron density around PGV N 1266:

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

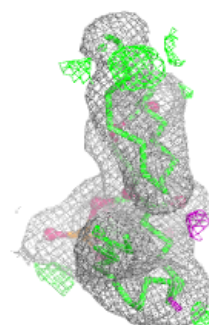
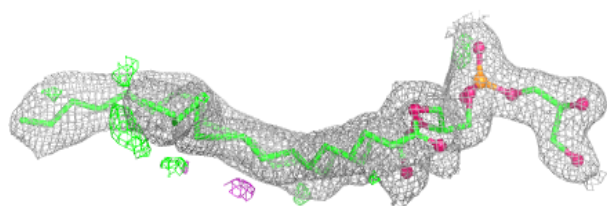
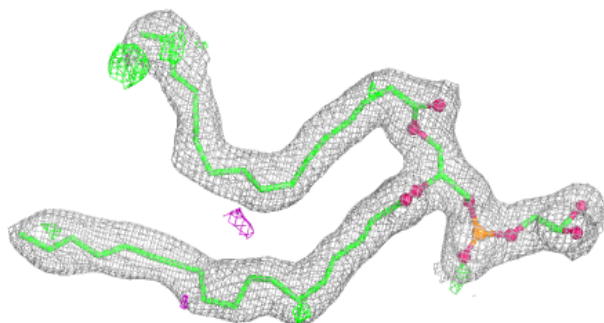
**Electron density around PGV P 1267:**

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

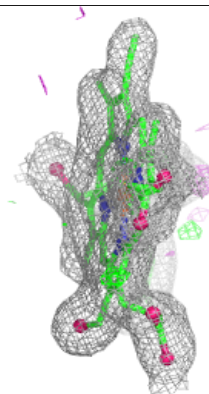
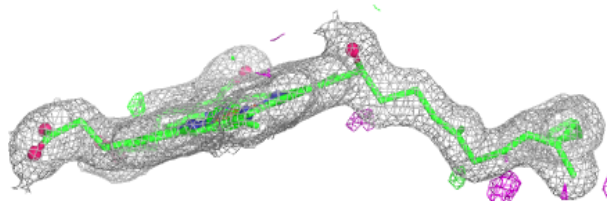
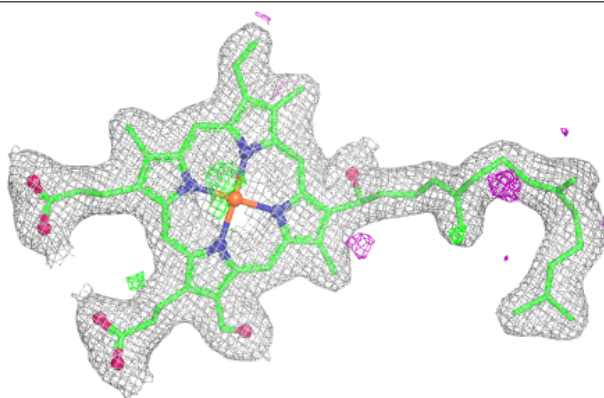


Electron density around PGV A 522:

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

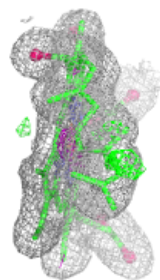
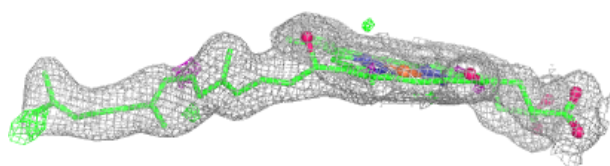
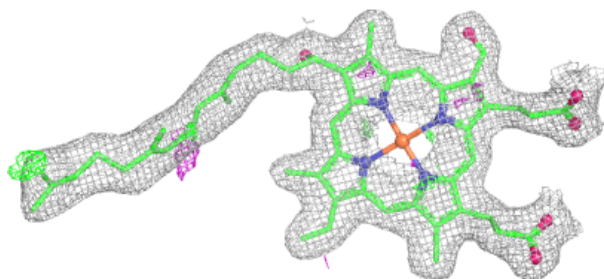
**Electron density around HEA N 516:**

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

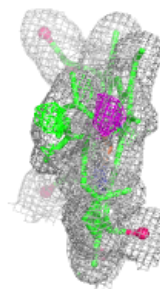
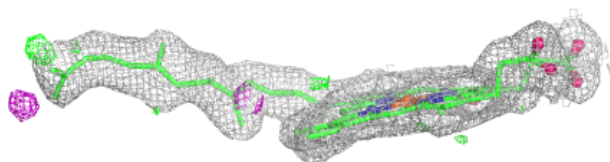
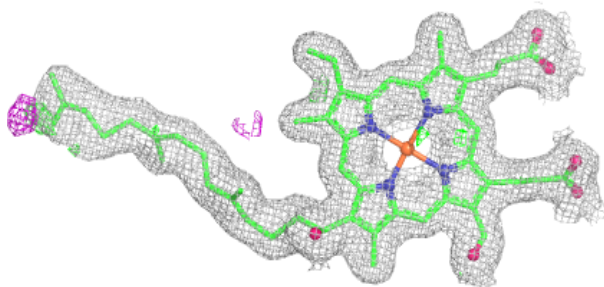


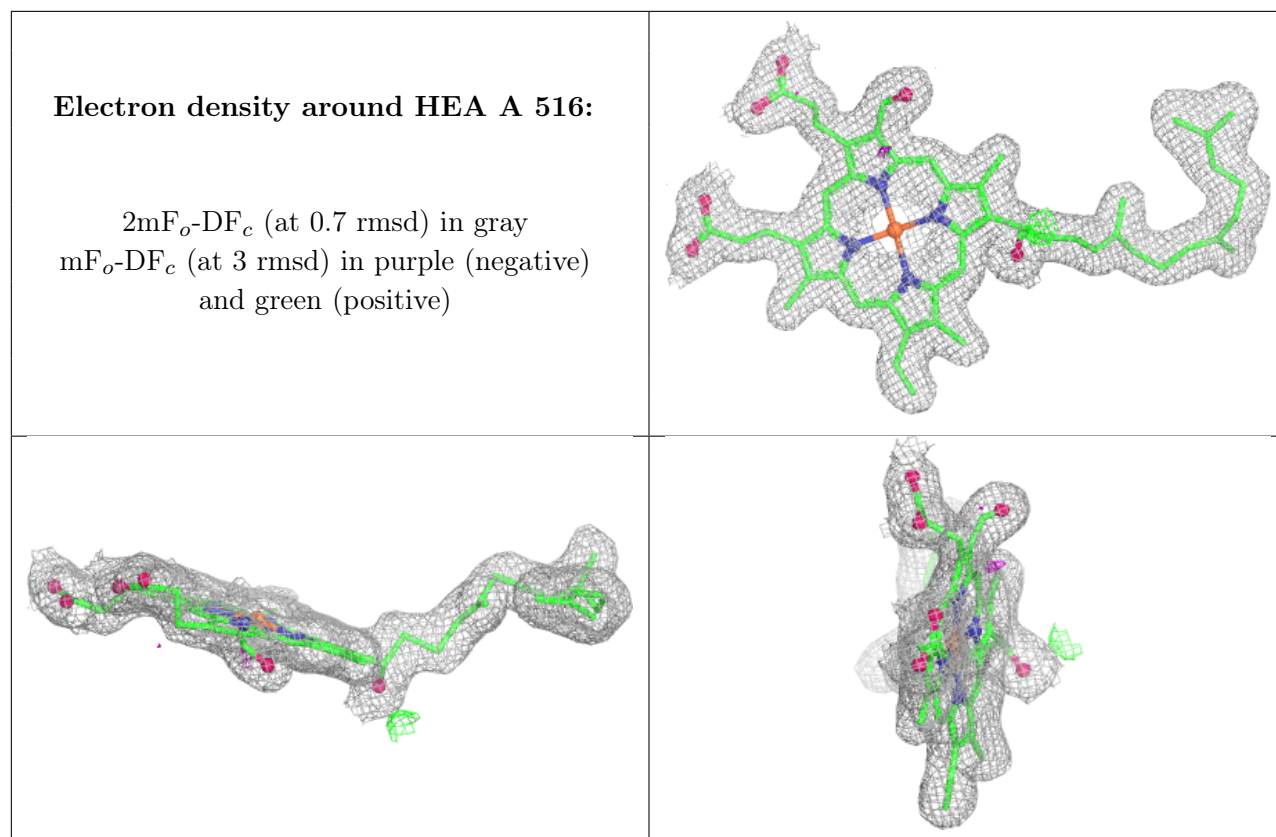
Electron density around HEA N 515:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.