



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:53 PM EDT

PDB ID : 3ABK / pdb_00003abk
Title : Bovine heart cytochrome c oxidase at the NO-bound fully reduced state (50K)
Authors : Ohta, K.; Muramoto, K.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.;
Tsukihara, T.
Deposited on : 2009-12-16
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

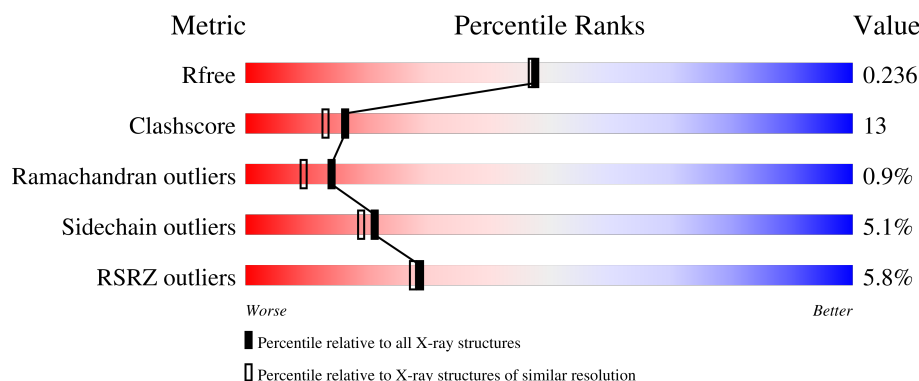
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	68% 27% 5%
1	N	514	% 69% 27% ..
2	B	227	4% 69% 26% ..
2	O	227	4% 67% 27% ..
3	C	261	% 77% 20% ...

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Mol	Chain	Length	Quality of chain
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
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	P	1271	X	-	-	-
23	CHD	P	1525	X	-	-	-
23	CHD	W	1059	X	-	-	-
24	UNX	C	262	-	-	-	X
24	UNX	P	262	-	-	-	X
26	CDL	G	269	-	-	X	-
26	CDL	P	1270	-	-	X	-
26	CDL	T	1269	-	-	X	-
27	DMU	C	272	X	-	-	-
27	DMU	M	526	X	-	-	-
27	DMU	P	272	X	-	-	-
27	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32382 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	5	0
			4060	2712	628	684	36			
1	N	514	Total	C	N	O	S	0	5	0
			4060	2712	628	684	36			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

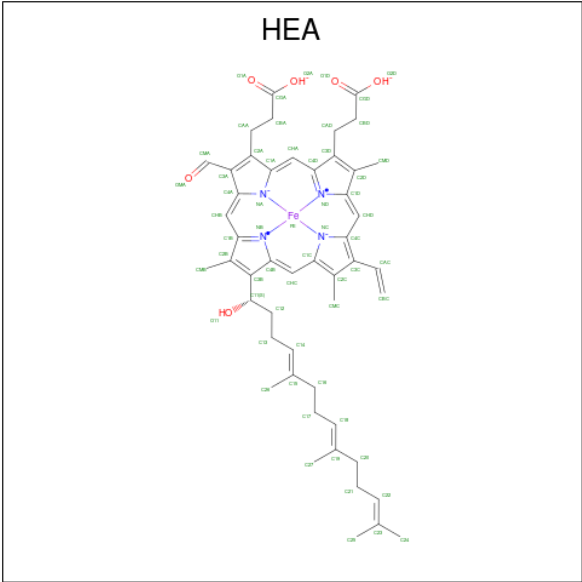
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

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

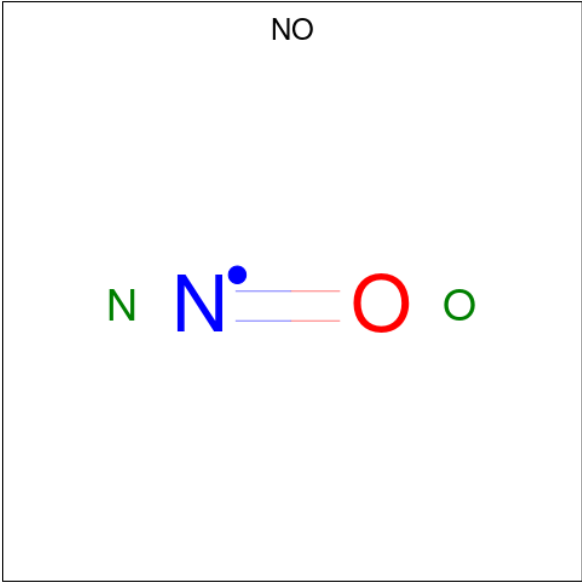
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 15 is NITRIC OXIDE (CCD ID: NO) (formula: NO).



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

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

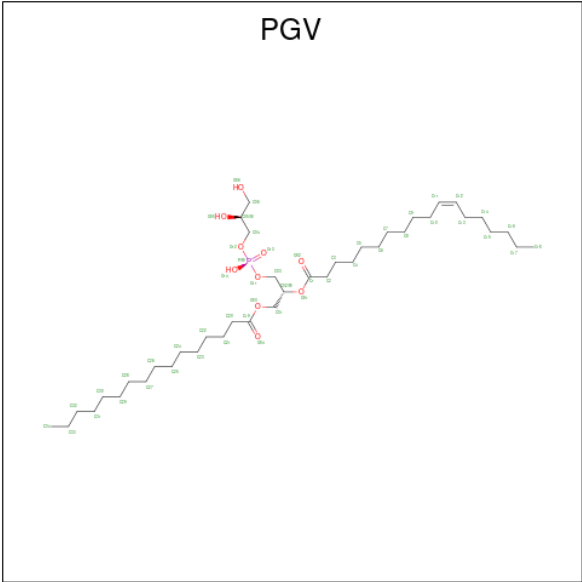
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (CCD ID: NA) (formula: Na).

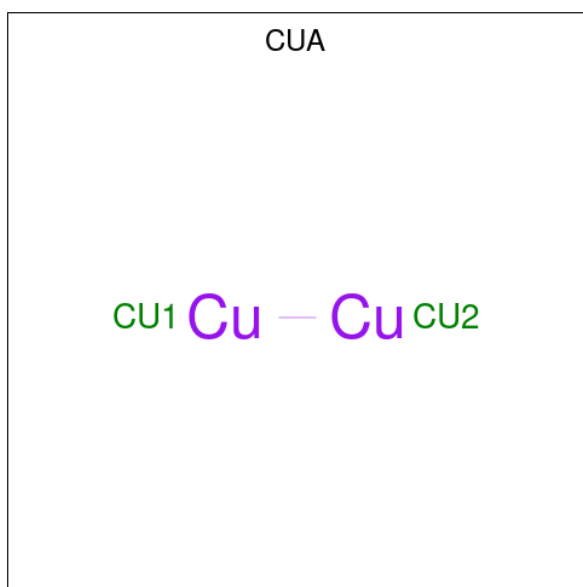
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

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



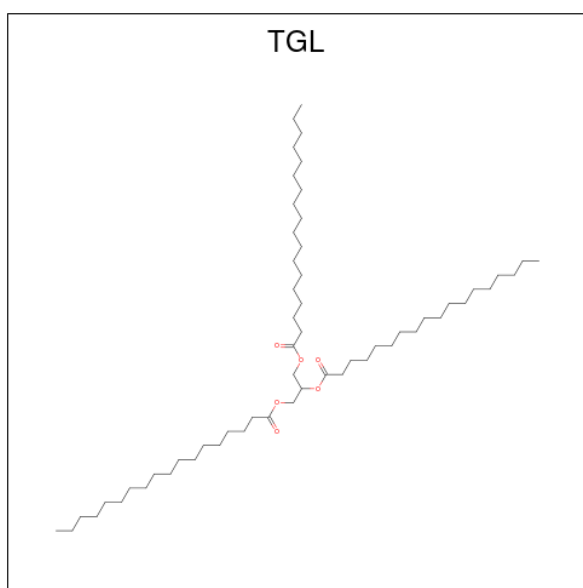
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

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



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

- Molecule 21 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



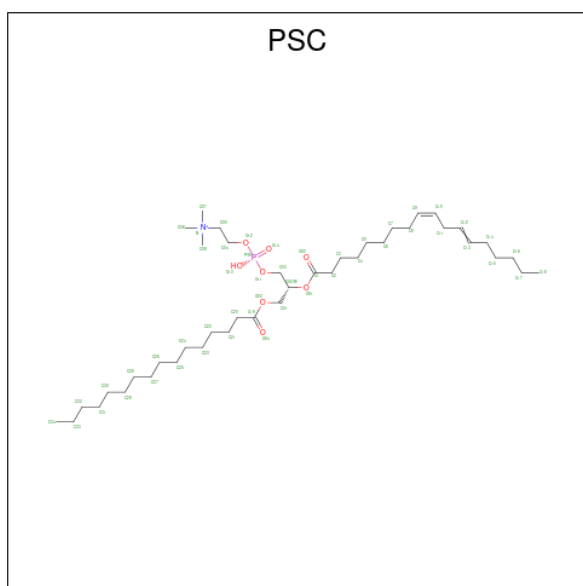
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		

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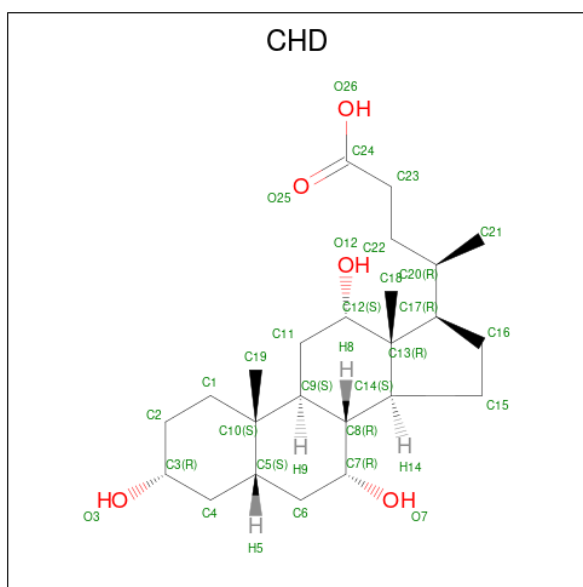
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 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: $C_{42}H_{81}NO_8P$).



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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).

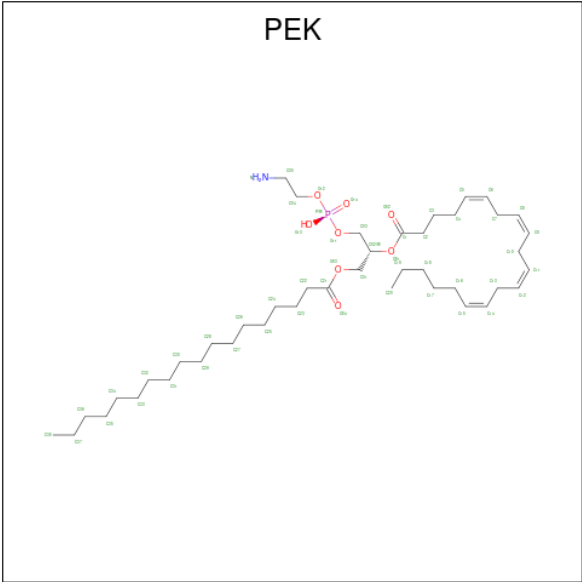


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	O	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0

- Molecule 24 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

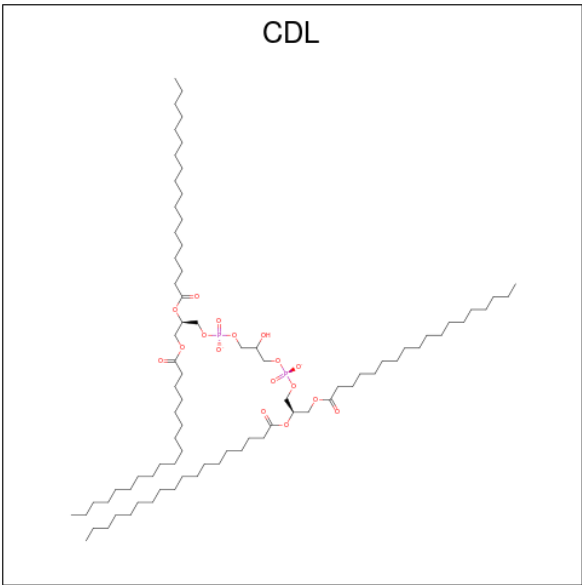
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total X 1 1	0	0
24	P	1	Total X 1 1	0	0

- Molecule 25 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).



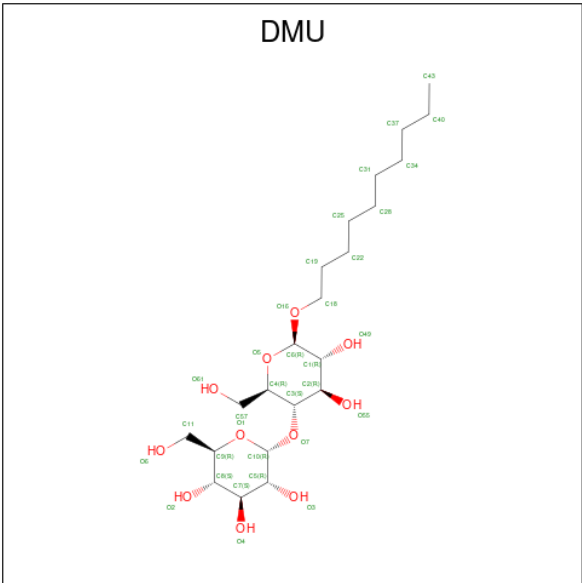
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	217	Total O 217 217	0	0
29	B	127	Total O 127 127	0	0
29	C	93	Total O 93 93	0	0
29	D	86	Total O 86 86	0	0
29	E	52	Total O 52 52	0	0
29	F	72	Total O 72 72	0	0
29	G	42	Total O 42 42	0	0
29	H	46	Total O 46 46	0	0
29	I	31	Total O 31 31	0	0
29	J	28	Total O 28 28	0	0
29	K	27	Total O 27 27	0	0
29	L	16	Total O 16 16	0	0

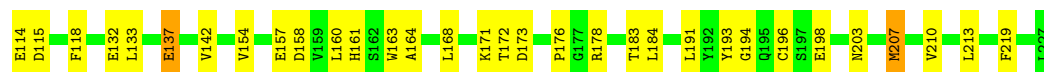
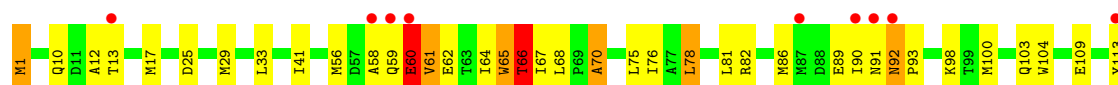
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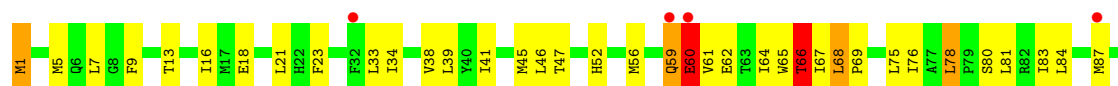
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	M	20	Total 20	O 20	0	0
29	N	207	Total 207	O 207	0	0
29	O	105	Total 105	O 105	0	0
29	P	96	Total 96	O 96	0	0
29	Q	57	Total 57	O 57	0	0
29	R	35	Total 35	O 35	0	0
29	S	63	Total 63	O 63	0	0
29	T	44	Total 44	O 44	0	0
29	U	43	Total 43	O 43	0	0
29	V	20	Total 20	O 20	0	0
29	W	17	Total 17	O 17	0	0
29	X	13	Total 13	O 13	0	0
29	Y	12	Total 12	O 12	0	0
29	Z	11	Total 11	O 11	0	0



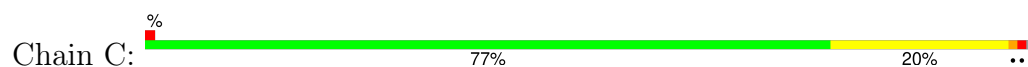
• Molecule 2: Cytochrome c oxidase subunit 2



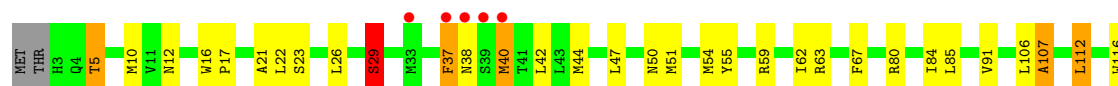
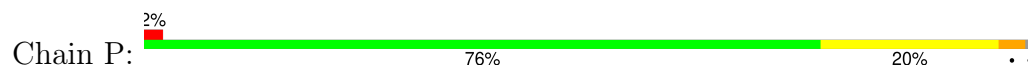
• Molecule 2: Cytochrome c oxidase subunit 2



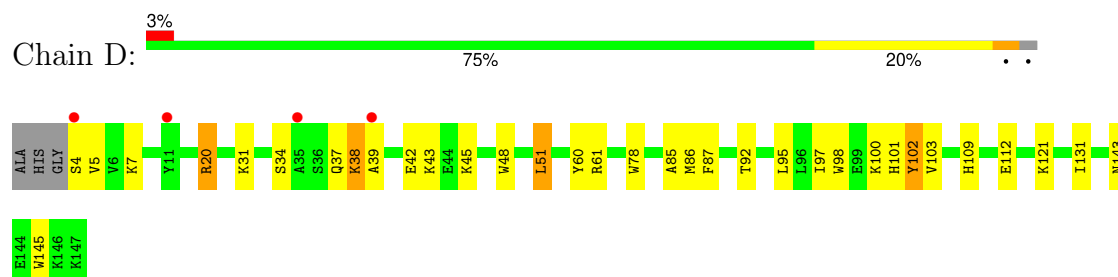
• Molecule 3: Cytochrome c oxidase subunit 3



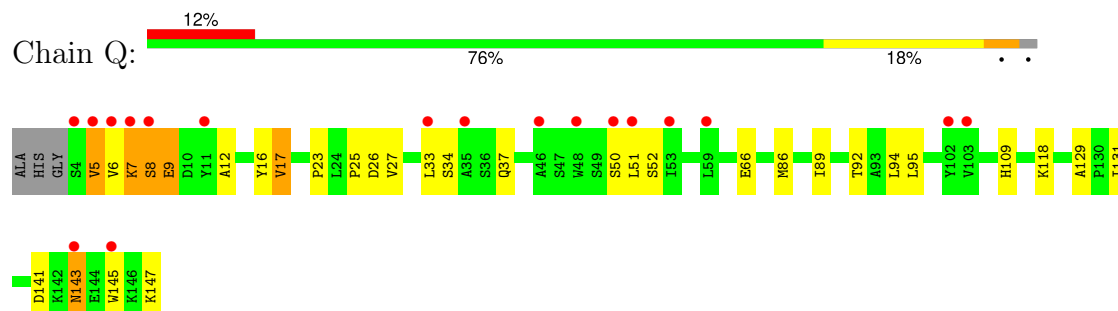
• Molecule 3: Cytochrome c oxidase subunit 3



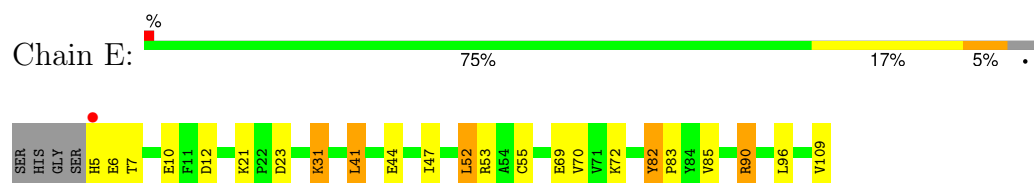
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



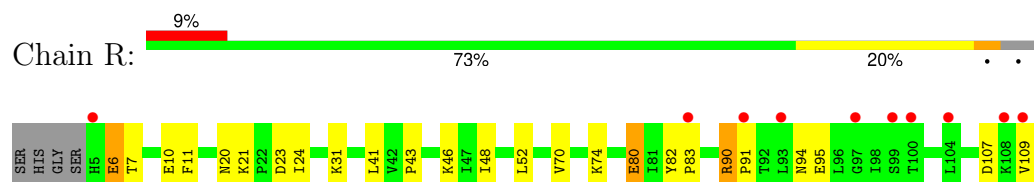
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



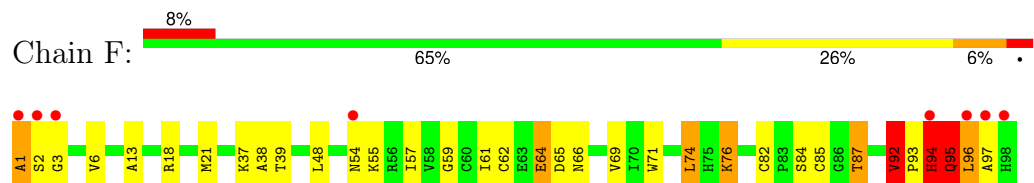
- Molecule 5: Cytochrome c oxidase subunit 5A



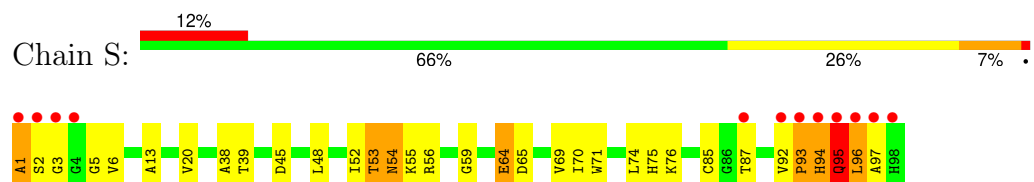
- Molecule 5: Cytochrome c oxidase subunit 5A



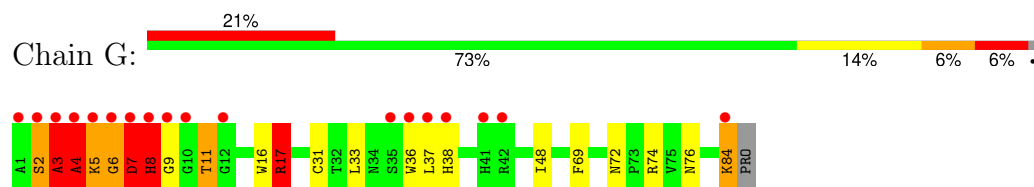
- Molecule 6: Cytochrome c oxidase subunit 5B



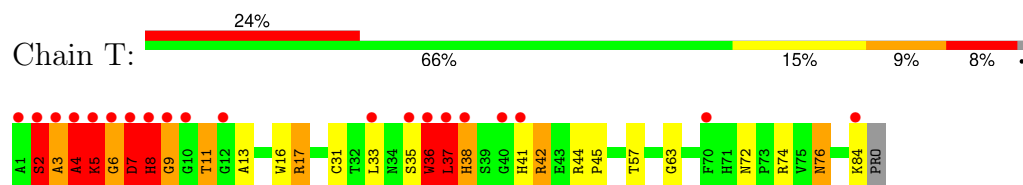
- Molecule 6: Cytochrome c oxidase subunit 5B



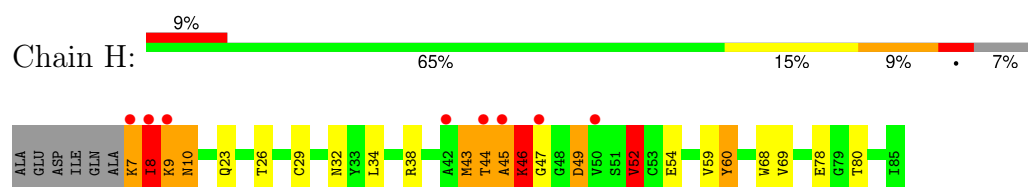
- Molecule 7: Cytochrome c oxidase subunit 6A2



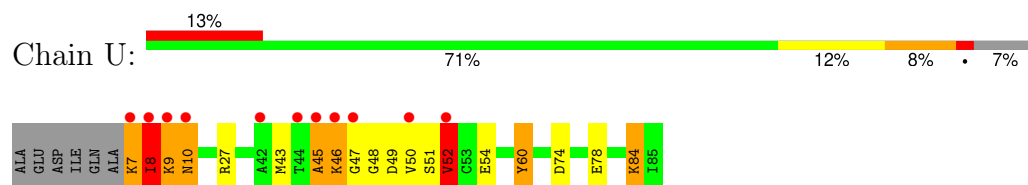
- Molecule 7: Cytochrome c oxidase subunit 6A2



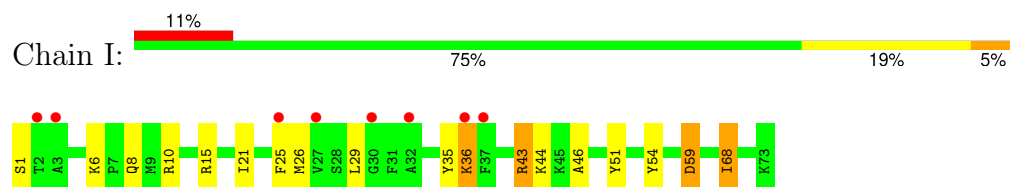
- Molecule 8: Cytochrome c oxidase subunit 6B1



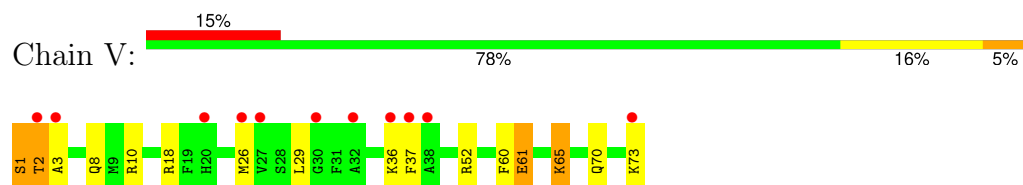
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 9: Cytochrome c oxidase subunit 6C

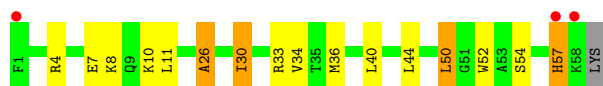


- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase polypeptide 7A1

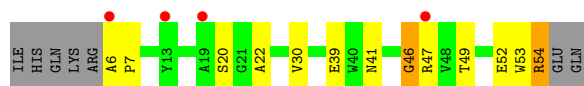




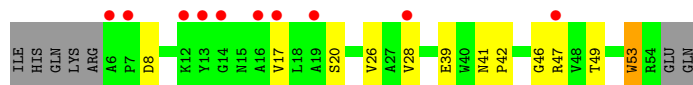
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 11: Cytochrome c oxidase subunit 7B



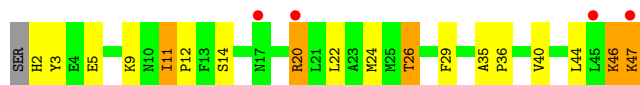
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



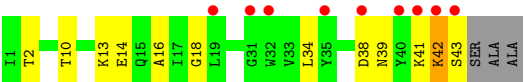
- Molecule 12: Cytochrome c oxidase subunit 7C



- 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	182.25Å 207.94Å 178.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.00) 98.7 (40.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.183 , 0.219 0.201 , 0.236	Depositor DCC
R_{free} test set	22073 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32382	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: NO, CUA, PEK, PGV, ZN, CHD, NA, TPO, PSC, UNX, CU, FME, CDL, DMU, MG, TGL, SAC, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.99	77/4189 (1.8%)	1.57	43/5722 (0.8%)
1	N	1.77	43/4189 (1.0%)	1.50	56/5722 (1.0%)
2	B	1.83	28/1860 (1.5%)	1.57	21/2534 (0.8%)
2	O	1.59	10/1860 (0.5%)	1.37	9/2534 (0.4%)
3	C	1.66	15/2197 (0.7%)	1.39	16/3005 (0.5%)
3	P	1.62	16/2197 (0.7%)	1.43	20/3005 (0.7%)
4	D	1.58	5/1229 (0.4%)	1.34	8/1658 (0.5%)
4	Q	1.45	7/1229 (0.6%)	1.30	6/1658 (0.4%)
5	E	1.61	6/871 (0.7%)	1.30	3/1182 (0.3%)
5	R	1.37	0/871	1.30	3/1182 (0.3%)
6	F	1.88	15/765 (2.0%)	1.63	8/1038 (0.8%)
6	S	1.70	11/765 (1.4%)	1.52	9/1038 (0.9%)
7	G	1.64	7/690 (1.0%)	1.40	6/937 (0.6%)
7	T	1.65	9/690 (1.3%)	1.46	10/937 (1.1%)
8	H	1.61	7/682 (1.0%)	1.44	9/921 (1.0%)
8	U	1.46	4/682 (0.6%)	1.27	1/921 (0.1%)
9	I	1.44	3/605 (0.5%)	1.38	6/802 (0.7%)
9	V	1.37	0/605	1.22	0/802
10	J	1.50	4/471 (0.8%)	1.39	2/636 (0.3%)
10	W	1.44	2/471 (0.4%)	1.47	5/636 (0.8%)
11	K	1.64	1/398 (0.3%)	1.56	9/546 (1.6%)
11	X	1.35	4/398 (1.0%)	1.38	4/546 (0.7%)
12	L	1.67	5/393 (1.3%)	1.47	3/526 (0.6%)
12	Y	1.61	2/393 (0.5%)	1.33	3/526 (0.6%)
13	M	1.73	3/345 (0.9%)	1.49	1/470 (0.2%)
13	Z	1.41	1/345 (0.3%)	1.30	0/470
All	All	1.69	285/29390 (1.0%)	1.45	261/39954 (0.7%)

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
5	E	0	1
6	F	0	1
6	S	0	2
12	Y	0	1
All	All	0	5

All (285) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	198	GLU	C-O	14.52	1.40	1.23
1	A	83	VAL	CA-CB	12.32	1.61	1.54
1	N	297	MET	SD-CE	12.21	2.10	1.79
1	N	188	VAL	N-CA	11.60	1.60	1.46
6	F	3	GLY	C-O	9.88	1.32	1.23
1	A	162	ILE	CA-CB	9.69	1.66	1.54
4	Q	6	VAL	CA-CB	9.46	1.65	1.54
1	A	467	LEU	N-CA	-9.13	1.35	1.46
1	A	113	LEU	CB-CG	8.95	1.71	1.53
1	A	193	VAL	CA-CB	8.84	1.65	1.54
6	S	2	SER	N-CA	8.62	1.56	1.46
2	O	64	ILE	CA-CB	8.49	1.64	1.54
5	E	85	VAL	CA-CB	8.47	1.64	1.54
1	A	397	PHE	CA-C	8.36	1.61	1.52
6	S	70	ILE	CA-CB	-8.22	1.44	1.54
3	P	107	ALA	CA-CB	8.18	1.63	1.53
1	A	439	ARG	C-O	7.99	1.35	1.23
6	F	92	VAL	CA-CB	7.96	1.64	1.54
6	S	69	VAL	CA-CB	-7.96	1.44	1.54
1	N	199	LEU	C-O	7.94	1.32	1.24
1	A	189	MET	C-O	-7.93	1.14	1.24
1	A	190	ILE	CA-CB	7.87	1.64	1.54
1	A	189	MET	CG-SD	-7.86	1.61	1.80
1	N	419	VAL	CA-CB	7.84	1.63	1.54
3	C	214	PHE	CA-C	7.83	1.62	1.52
1	N	157	SER	N-CA	7.80	1.56	1.46
1	N	113	LEU	CB-CG	7.76	1.69	1.53
4	D	103	VAL	CA-CB	7.76	1.63	1.55
6	F	2	SER	N-CA	7.74	1.56	1.46
2	B	59	GLN	CG-CD	7.58	1.71	1.52
2	B	137	GLU	C-O	7.58	1.33	1.23
1	A	500	PRO	CA-C	7.54	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	7.50	1.32	1.23
1	A	436	MET	N-CA	7.46	1.59	1.46
1	A	285	PHE	N-CA	7.45	1.56	1.46
1	N	240	HIS	N-CA	7.36	1.51	1.46
7	G	17	ARG	CD-NE	-7.33	1.35	1.46
13	M	21	VAL	N-CA	7.33	1.55	1.46
3	P	91	VAL	CA-CB	-7.31	1.45	1.54
8	U	52	VAL	CA-CB	7.31	1.65	1.54
1	A	93	ALA	CA-CB	7.26	1.64	1.53
1	A	173	PRO	CA-C	7.16	1.55	1.51
7	T	3	ALA	N-CA	7.15	1.55	1.46
7	T	3	ALA	CA-C	7.13	1.62	1.52
5	E	47	ILE	N-CA	7.12	1.54	1.46
1	A	281	GLY	C-O	7.11	1.32	1.23
1	N	64	VAL	CA-C	7.11	1.61	1.52
2	O	201	GLY	C-O	7.11	1.31	1.23
1	A	199	LEU	N-CA	7.08	1.53	1.46
1	A	61	HIS	ND1-CE1	7.05	1.39	1.32
1	A	193	VAL	CA-C	7.04	1.61	1.52
1	N	86	MET	N-CA	7.04	1.55	1.46
1	A	248	LEU	C-O	-6.95	1.17	1.24
2	B	219	PHE	C-O	6.95	1.32	1.24
1	N	415	ALA	CA-CB	6.93	1.64	1.53
6	S	2	SER	CA-C	6.87	1.61	1.52
1	A	240	HIS	CA-C	6.82	1.60	1.52
2	B	198	GLU	C-N	6.81	1.42	1.33
2	B	142	VAL	CA-CB	6.78	1.60	1.53
6	F	61	ILE	CA-CB	6.78	1.60	1.53
1	N	310	MET	SD-CE	-6.78	1.62	1.79
1	A	512	ASN	CB-CG	-6.77	1.35	1.52
1	N	103	TRP	C-O	6.73	1.32	1.24
2	B	207	MET	N-CA	6.72	1.54	1.46
3	P	246	ASP	CG-OD2	6.70	1.38	1.25
1	A	189	MET	CB-CG	6.70	1.72	1.52
7	T	2	SER	CA-C	6.68	1.61	1.52
7	T	17	ARG	CD-NE	-6.68	1.36	1.46
1	A	203	ALA	C-O	6.67	1.31	1.24
7	G	4	ALA	CA-CB	-6.65	1.42	1.53
2	B	113	TYR	C-O	-6.64	1.15	1.24
6	F	59	GLY	CA-C	-6.61	1.47	1.52
10	J	26	ALA	CA-CB	6.61	1.64	1.53
6	S	3	GLY	N-CA	6.60	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	8	ILE	CA-CB	6.58	1.63	1.54
5	E	82	TYR	CA-C	6.58	1.60	1.52
3	C	139	ALA	CA-CB	6.56	1.63	1.53
1	N	276	ALA	N-CA	6.56	1.54	1.46
2	B	191	LEU	N-CA	6.55	1.54	1.46
1	A	160	GLY	N-CA	6.54	1.53	1.45
3	C	217	VAL	CA-CB	6.46	1.61	1.54
3	C	11	VAL	CA-CB	6.42	1.62	1.54
4	Q	6	VAL	CA-C	6.41	1.61	1.52
6	F	74	LEU	N-CA	6.40	1.54	1.46
6	F	3	GLY	N-CA	6.40	1.50	1.45
1	N	199	LEU	N-CA	6.38	1.53	1.46
1	A	251	PHE	C-O	-6.36	1.16	1.24
1	A	294	THR	CA-CB	6.33	1.63	1.53
6	F	57	ILE	CA-CB	6.32	1.61	1.54
6	F	95	GLN	N-CA	6.31	1.54	1.46
1	N	287	VAL	N-CA	6.27	1.51	1.46
12	L	15	VAL	CA-C	6.22	1.60	1.53
3	P	62	ILE	CA-C	6.21	1.60	1.52
3	P	230	ASN	CA-CB	-6.21	1.45	1.54
1	N	210	LEU	C-O	6.16	1.31	1.24
3	P	5	THR	CA-CB	6.15	1.61	1.53
1	A	297	MET	CB-CG	6.14	1.70	1.52
7	G	36	TRP	CB-CG	6.13	1.69	1.50
1	A	410	ALA	CA-CB	6.10	1.63	1.53
3	P	50	ASN	N-CA	6.08	1.53	1.46
3	P	245	VAL	CA-C	6.08	1.60	1.52
7	T	36	TRP	CB-CG	6.07	1.69	1.50
4	D	5	VAL	N-CA	6.06	1.54	1.46
1	N	295	VAL	CA-CB	6.06	1.61	1.54
2	O	97	VAL	CA-CB	6.04	1.62	1.54
2	B	171	LYS	C-O	6.04	1.31	1.24
1	A	281	GLY	N-CA	6.01	1.53	1.45
11	K	39	GLU	CA-CB	5.99	1.60	1.53
9	I	25	PHE	CA-C	5.97	1.60	1.52
4	Q	7	LYS	N-CA	5.96	1.53	1.46
1	A	419	VAL	CA-CB	5.95	1.61	1.54
1	A	493	GLU	CA-CB	5.95	1.63	1.53
4	D	98	TRP	N-CA	5.94	1.53	1.46
1	A	126	TRP	CA-C	5.93	1.60	1.52
1	A	314	ILE	CA-CB	5.93	1.61	1.54
1	A	372	TYR	CA-C	5.93	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	34	VAL	CA-C	5.92	1.60	1.52
1	A	511	VAL	CA-CB	5.92	1.61	1.54
8	H	26	THR	C-O	5.90	1.31	1.24
1	N	438	ARG	N-CA	-5.89	1.38	1.45
1	A	203	ALA	N-CA	5.86	1.53	1.46
6	F	6	VAL	CA-C	5.85	1.58	1.53
1	N	434	SER	CA-C	5.84	1.60	1.52
1	N	236	TRP	C-O	5.83	1.31	1.24
8	H	8	ILE	CA-C	5.81	1.60	1.52
8	H	68	TRP	N-CA	5.81	1.53	1.46
2	O	38	VAL	CA-CB	5.80	1.61	1.54
8	U	74	ASP	C-O	-5.79	1.17	1.24
2	B	12	ALA	CA-C	5.78	1.60	1.52
1	A	259	THR	N-CA	5.77	1.53	1.46
1	N	469	VAL	CA-CB	-5.76	1.46	1.54
8	U	9	LYS	N-CA	5.74	1.52	1.45
12	Y	40	VAL	CA-C	5.74	1.59	1.52
2	B	10	GLN	N-CA	5.72	1.53	1.46
3	C	95	THR	CA-C	5.71	1.60	1.52
4	Q	129	ALA	C-O	-5.71	1.21	1.23
1	N	502	TYR	CA-C	5.70	1.60	1.52
1	A	113	LEU	CG-CD1	5.70	1.71	1.52
1	A	180	GLN	CA-C	-5.70	1.45	1.52
13	M	32	TRP	N-CA	-5.68	1.39	1.46
12	L	32	GLY	N-CA	5.66	1.52	1.45
6	S	39	THR	CA-CB	-5.66	1.44	1.53
1	A	236	TRP	N-CA	5.64	1.53	1.46
12	L	26	THR	CA-CB	5.64	1.62	1.53
1	A	255	SER	CA-C	5.63	1.60	1.52
2	B	176	PRO	CA-C	5.62	1.59	1.52
1	A	9	SER	N-CA	-5.62	1.39	1.46
2	B	154	VAL	CA-CB	5.60	1.61	1.54
12	L	40	VAL	C-O	-5.59	1.17	1.24
2	B	59	GLN	CB-CG	5.58	1.69	1.52
1	N	162	ILE	CG1-CD1	5.58	1.73	1.51
6	F	2	SER	CA-C	5.58	1.60	1.52
3	P	190	ASP	C-O	5.58	1.29	1.23
1	A	191	THR	CA-C	-5.56	1.45	1.52
5	E	90	ARG	CA-C	5.55	1.59	1.52
1	N	460	ILE	CA-CB	-5.53	1.47	1.54
6	F	21	MET	C-O	5.53	1.30	1.24
3	P	131	LEU	CA-C	-5.53	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	2	SER	CA-C	5.53	1.60	1.52
1	N	189	MET	CB-CG	5.52	1.69	1.52
9	I	59	ASP	C-O	-5.51	1.17	1.24
13	M	6	ALA	CA-CB	5.51	1.62	1.53
1	A	125	GLY	N-CA	5.50	1.53	1.45
11	X	17	VAL	N-CA	5.49	1.53	1.46
2	B	90	ILE	C-O	5.48	1.29	1.24
1	A	3	ILE	CA-CB	-5.46	1.48	1.54
13	Z	16	ALA	CA-CB	5.46	1.61	1.53
3	P	246	ASP	CG-OD1	5.45	1.35	1.25
2	O	123	ILE	N-CA	5.44	1.53	1.46
1	N	203	ALA	N-CA	5.44	1.53	1.46
3	C	97	PHE	N-CA	5.44	1.53	1.46
6	S	56	ARG	C-O	-5.43	1.16	1.23
4	D	43	LYS	CA-C	5.42	1.60	1.52
3	C	38	ASN	N-CA	-5.41	1.38	1.46
1	A	75	ILE	CG1-CD1	5.41	1.72	1.51
4	Q	8	SER	N-CA	5.41	1.53	1.45
6	S	2	SER	C-N	5.40	1.38	1.33
3	C	160	LEU	CA-C	-5.40	1.46	1.52
1	A	67	PHE	N-CA	-5.39	1.39	1.46
8	U	8	ILE	CA-CB	5.39	1.61	1.54
1	N	268	PHE	CA-C	5.38	1.59	1.52
7	T	7	ASP	N-CA	5.38	1.53	1.46
2	O	90	ILE	N-CA	5.38	1.53	1.46
1	A	38	ARG	CA-C	5.38	1.60	1.52
1	A	220	PHE	N-CA	5.38	1.52	1.46
1	A	99	ASN	CA-C	5.37	1.60	1.52
1	A	494	TRP	CA-C	5.37	1.60	1.52
1	N	130	PRO	CA-C	5.37	1.57	1.52
2	B	173	ASP	CA-C	-5.36	1.45	1.52
7	G	3	ALA	CA-C	5.36	1.59	1.52
3	P	84	ILE	CA-CB	-5.36	1.48	1.54
2	B	61	VAL	N-CA	-5.36	1.39	1.46
1	A	368	HIS	CB-CG	5.36	1.57	1.50
10	W	19	PRO	C-O	5.35	1.30	1.23
1	N	185	VAL	CA-C	5.35	1.59	1.52
6	S	20	VAL	CA-CB	5.34	1.61	1.54
2	B	184	LEU	CA-C	5.34	1.59	1.52
3	P	12	ASN	N-CA	-5.34	1.38	1.45
1	A	96	ARG	CA-C	5.33	1.60	1.52
3	C	162	ALA	CA-CB	-5.33	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	475	ALA	CA-CB	5.33	1.61	1.53
1	A	406	ASN	CA-CB	5.32	1.59	1.53
7	T	4	ALA	CA-CB	-5.32	1.44	1.53
6	F	1	ALA	C-O	5.32	1.34	1.23
8	H	32	ASN	N-CA	5.32	1.52	1.46
11	X	41	ASN	C-O	5.32	1.26	1.23
4	D	100	LYS	C-O	-5.31	1.18	1.24
2	B	103	GLN	CA-CB	5.31	1.59	1.53
4	Q	7	LYS	CA-C	5.31	1.59	1.52
1	N	168	ILE	CB-CG2	5.30	1.70	1.52
1	A	258	VAL	CA-CB	-5.30	1.47	1.54
8	H	69	VAL	N-CA	5.30	1.52	1.46
2	B	115	ASP	CB-CG	5.30	1.65	1.52
2	B	25	ASP	N-CA	5.29	1.52	1.46
10	J	11	LEU	CA-C	5.29	1.59	1.52
3	P	180	GLU	CD-OE1	5.29	1.35	1.25
1	A	139	ALA	CA-CB	5.28	1.62	1.53
2	B	158	ASP	CA-C	5.27	1.59	1.52
1	N	176	MET	CA-C	5.27	1.59	1.52
2	B	172	THR	C-O	5.26	1.29	1.23
11	X	42	PRO	CA-C	5.26	1.58	1.52
3	C	57	TRP	CD1-NE1	5.26	1.48	1.37
1	A	150	LEU	N-CA	5.25	1.53	1.46
2	B	213	LEU	CA-CB	5.24	1.60	1.53
1	A	167	THR	C-O	5.24	1.30	1.24
1	N	113	LEU	CA-CB	5.24	1.61	1.53
2	B	163	TRP	CA-C	-5.24	1.46	1.52
6	F	76	LYS	N-CA	5.24	1.52	1.46
6	S	1	ALA	C-N	5.23	1.40	1.33
1	A	15	ILE	CA-CB	-5.23	1.48	1.54
1	A	458	SER	C-O	5.23	1.30	1.24
1	N	146	THR	N-CA	5.22	1.52	1.46
12	L	44	LEU	C-O	-5.22	1.17	1.24
3	C	17	PRO	CG-CD	5.22	1.68	1.50
1	N	438	ARG	CB-CG	-5.21	1.36	1.52
1	A	228	PRO	CA-C	-5.21	1.44	1.52
2	O	98	LYS	CA-C	-5.21	1.46	1.52
2	O	34	ILE	CA-C	-5.20	1.46	1.52
3	C	48	THR	CA-C	-5.19	1.46	1.52
9	I	46	ALA	CA-CB	-5.19	1.45	1.53
1	N	99	ASN	CA-C	5.19	1.59	1.52
7	G	7	ASP	N-CA	5.19	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	VAL	CA-CB	-5.18	1.48	1.54
3	C	211	GLY	CA-C	5.18	1.57	1.52
1	N	168	ILE	N-CA	5.17	1.52	1.46
1	A	509	THR	CA-CB	5.17	1.61	1.53
1	N	483	LEU	CA-C	5.17	1.57	1.53
1	A	354	THR	CA-C	5.16	1.59	1.52
1	A	205	GLY	N-CA	5.16	1.52	1.45
1	A	295	VAL	CA-C	5.15	1.58	1.52
1	A	478	SER	N-CA	-5.15	1.39	1.46
1	N	362	SER	N-CA	5.14	1.52	1.46
1	A	258	VAL	C-O	5.13	1.30	1.24
1	A	153	ALA	CA-CB	5.13	1.61	1.53
7	G	48	ILE	N-CA	5.13	1.52	1.46
5	E	52	LEU	N-CA	5.12	1.52	1.46
1	A	28	MET	N-CA	5.12	1.52	1.46
1	N	106	PRO	C-N	5.12	1.41	1.34
11	X	49	THR	CA-CB	5.12	1.61	1.52
10	J	44	LEU	C-O	-5.11	1.18	1.24
3	P	202	GLY	N-CA	5.10	1.52	1.45
2	O	137	GLU	N-CA	5.10	1.52	1.45
3	C	237	ALA	CA-CB	5.09	1.61	1.53
2	B	118	PHE	CA-C	5.08	1.58	1.52
3	P	217	VAL	CA-CB	5.08	1.60	1.54
1	N	510	TYR	C-O	5.07	1.29	1.24
1	A	54	TYR	N-CA	5.07	1.52	1.46
3	C	88	ILE	CA-CB	-5.07	1.48	1.54
7	T	5	LYS	CA-CB	5.07	1.62	1.53
6	S	13	ALA	CA-CB	5.06	1.61	1.53
4	Q	5	VAL	CA-CB	5.06	1.61	1.54
1	A	394	VAL	CB-CG2	-5.06	1.35	1.52
8	H	80	THR	CA-CB	-5.06	1.46	1.53
1	N	228	PRO	CA-C	5.06	1.60	1.52
1	A	275	TRP	CA-CB	5.05	1.61	1.53
1	A	378	HIS	ND1-CE1	5.05	1.37	1.32
6	F	69	VAL	CA-CB	-5.04	1.48	1.54
12	Y	11	ILE	C-N	5.03	1.38	1.33
1	A	289	ALA	CA-CB	5.03	1.62	1.53
1	N	394	VAL	CA-C	5.02	1.59	1.52
10	W	47	LEU	N-CA	5.02	1.52	1.46
7	T	13	ALA	CA-CB	-5.01	1.45	1.53
1	A	457	GLY	N-CA	5.00	1.52	1.45
2	B	161	HIS	CA-CB	5.00	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	53	ARG	N-CA	5.00	1.52	1.46

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	THR	CA-C-N	10.58	130.66	119.76
1	A	181	THR	C-N-CA	10.58	130.66	119.76
1	A	71	MET	CG-SD-CE	-10.51	77.77	100.90
6	S	2	SER	N-CA-C	9.69	121.54	107.88
1	N	278	MET	CG-SD-CE	-8.99	81.12	100.90
1	N	240	HIS	N-CA-CB	8.87	118.82	110.39
1	N	71	MET	CG-SD-CE	-8.80	81.54	100.90
2	B	65	TRP	CB-CA-C	8.72	125.90	110.81
1	N	12	HIS	N-CA-C	8.65	120.71	111.28
2	B	64	ILE	N-CA-C	-8.61	101.83	110.62
6	S	45	ASP	CA-C-N	-8.60	111.88	120.31
6	S	45	ASP	C-N-CA	-8.60	111.88	120.31
8	H	38	ARG	N-CA-C	-8.47	101.99	111.14
3	P	29	SER	CB-CA-C	-8.38	96.88	110.79
1	N	149	SER	N-CA-C	-8.32	102.16	111.14
3	C	91	VAL	N-CA-C	-8.30	102.73	110.53
1	A	373	VAL	N-CA-C	-8.12	102.52	110.72
1	A	52	GLN	N-CA-C	-8.10	102.53	111.36
1	N	466	MET	N-CA-C	-7.92	102.73	111.36
4	Q	9	GLU	N-CA-C	-7.85	103.01	112.59
10	W	18	LEU	CA-C-N	-7.85	112.61	120.31
10	W	18	LEU	C-N-CA	-7.85	112.61	120.31
2	B	17	MET	N-CA-C	-7.82	102.75	111.82
6	F	82	CYS	CA-C-N	7.67	127.30	119.56
6	F	82	CYS	C-N-CA	7.67	127.30	119.56
3	P	16	TRP	CA-C-N	-7.62	111.31	119.24
3	P	16	TRP	C-N-CA	-7.62	111.31	119.24
1	A	240	HIS	N-CA-CB	7.59	119.38	110.42
6	F	95	GLN	N-CA-C	7.53	126.85	110.80
1	N	64	VAL	N-CA-C	-7.48	103.50	110.53
4	Q	17	VAL	CB-CA-C	-7.47	97.72	111.18
1	N	436	MET	CA-C-N	-7.43	112.67	120.03
1	N	436	MET	C-N-CA	-7.43	112.67	120.03
10	J	57	HIS	CB-CA-C	7.32	121.31	111.14
11	K	22	ALA	N-CA-C	7.32	118.90	111.07
1	N	184	PHE	N-CA-C	-7.15	103.56	111.36
1	N	310	MET	CG-SD-CE	-7.12	85.24	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	46	GLY	N-CA-C	-7.08	105.94	115.36
1	N	169	ILE	CB-CA-C	-7.03	102.53	112.22
1	N	332	ILE	CB-CA-C	-6.99	102.06	111.15
9	I	21	ILE	N-CA-C	-6.98	103.97	110.53
3	C	127	LEU	N-CA-C	-6.96	104.41	113.17
12	L	33	PHE	N-CA-C	6.88	118.77	111.28
1	A	512	ASN	CB-CA-C	-6.87	96.09	109.76
8	U	54	GLU	N-CA-C	6.84	118.73	111.28
7	G	7	ASP	N-CA-C	6.78	125.24	110.80
7	G	17	ARG	NE-CZ-NH2	-6.77	113.11	119.20
10	J	10	LYS	N-CA-C	6.75	118.29	111.07
2	B	114	GLU	CA-C-N	-6.72	112.08	122.16
2	B	114	GLU	C-N-CA	-6.72	112.08	122.16
1	A	266	GLU	CA-C-N	6.67	126.43	119.76
1	A	266	GLU	C-N-CA	6.67	126.43	119.76
1	N	239	GLY	CA-C-N	-6.61	112.50	119.83
1	N	239	GLY	C-N-CA	-6.61	112.50	119.83
1	N	83	VAL	CA-C-N	-6.60	111.66	118.85
1	N	83	VAL	C-N-CA	-6.60	111.66	118.85
1	A	189	MET	N-CA-C	-6.59	104.17	111.36
3	P	80	ARG	CG-CD-NE	-6.57	97.55	112.00
13	M	42	LYS	N-CA-C	6.55	121.25	111.81
3	P	221	ARG	NE-CZ-NH1	-6.51	114.99	121.50
2	O	226	MET	N-CA-C	-6.47	105.39	113.28
11	K	41	ASN	CA-C-N	-6.46	114.07	120.98
11	K	41	ASN	C-N-CA	-6.46	114.07	120.98
2	O	16	ILE	N-CA-C	6.43	116.59	110.42
1	A	391	GLY	N-CA-C	-6.38	104.61	112.77
2	B	66	THR	OG1-CB-CG2	6.36	122.01	109.30
1	A	248	LEU	CA-C-N	-6.33	113.10	119.56
1	A	248	LEU	C-N-CA	-6.33	113.10	119.56
1	N	141	ALA	N-CA-C	6.32	120.25	112.54
9	I	43	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	N	438	ARG	N-CA-CB	-6.29	100.89	110.45
5	E	21	LYS	CA-C-N	-6.26	112.46	118.97
5	E	21	LYS	C-N-CA	-6.26	112.46	118.97
3	C	203	PHE	N-CA-C	-6.23	104.59	111.82
10	W	42	GLY	N-CA-C	-6.23	105.27	112.50
1	A	282	PHE	N-CA-C	6.20	117.73	110.97
2	B	60	GLU	N-CA-C	-6.19	97.62	110.80
2	B	66	THR	CB-CA-C	6.18	120.51	110.37
1	N	254	ILE	N-CA-C	-6.17	104.49	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	66	THR	CB-CA-C	6.15	119.74	110.08
11	K	30	VAL	N-CA-C	-6.14	104.52	110.72
7	T	41	HIS	N-CA-C	6.13	118.44	108.63
1	A	425	PHE	CA-C-N	-6.11	112.51	120.58
1	A	425	PHE	C-N-CA	-6.11	112.51	120.58
9	I	6	LYS	CA-C-N	-6.11	112.20	119.84
9	I	6	LYS	C-N-CA	-6.11	112.20	119.84
2	B	59	GLN	CB-CG-CD	6.10	122.97	112.60
1	A	343	GLY	N-CA-C	-6.09	105.21	113.37
1	N	125	GLY	N-CA-C	-6.06	105.15	112.48
1	N	327	LEU	N-CA-C	-6.04	104.78	111.36
3	P	37	PHE	N-CA-C	-6.02	103.44	112.54
3	P	112	LEU	N-CA-C	-6.02	105.93	113.28
6	S	59	GLY	N-CA-C	-6.01	101.51	110.71
7	T	17	ARG	CB-CG-CD	-6.01	97.47	111.30
1	N	103	TRP	N-CA-C	6.00	120.21	113.01
1	N	224	GLY	N-CA-C	-5.99	105.37	115.80
2	B	66	THR	N-CA-C	-5.99	105.05	112.72
6	F	39	THR	N-CA-C	-5.99	100.53	109.94
2	B	82	ARG	CG-CD-NE	-5.97	98.87	112.00
1	A	147	ILE	N-CA-C	-5.95	104.71	110.42
3	P	129	VAL	N-CA-CB	5.93	114.24	110.50
3	P	29	SER	N-CA-C	-5.92	104.83	111.28
2	O	67	ILE	CB-CA-C	-5.92	104.15	112.14
1	A	240	HIS	CA-CB-CG	-5.91	107.89	113.80
3	C	87	ILE	N-CA-C	-5.88	104.62	110.62
12	Y	29	PHE	N-CA-C	5.88	117.69	111.28
1	A	280	ILE	N-CA-C	-5.87	104.79	110.72
1	A	192	ALA	N-CA-C	5.86	117.67	111.28
1	N	102	PHE	N-CA-CB	5.85	118.45	109.91
6	S	5	GLY	CA-C-N	-5.84	117.67	123.04
6	S	5	GLY	C-N-CA	-5.84	117.67	123.04
1	A	362	SER	CA-CB-OG	-5.83	99.43	111.10
4	D	85	ALA	N-CA-C	-5.82	104.93	111.28
1	A	83	VAL	O-C-N	5.82	124.14	120.42
8	H	52	VAL	CB-CA-C	-5.82	98.57	111.77
11	X	49	THR	CA-C-N	5.79	125.72	119.76
11	X	49	THR	C-N-CA	5.79	125.72	119.76
1	A	278	MET	CG-SD-CE	-5.78	88.19	100.90
4	D	143	ASN	N-CA-C	5.76	119.34	111.39
3	P	47	LEU	N-CA-C	-5.76	105.00	111.28
2	B	184	LEU	N-CA-C	-5.76	99.26	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	53	TRP	N-CA-C	-5.75	106.91	114.04
1	A	251	PHE	CB-CA-C	-5.75	101.25	110.79
3	P	107	ALA	CA-C-N	-5.74	113.88	119.90
3	P	107	ALA	C-N-CA	-5.74	113.88	119.90
1	A	51	ASP	N-CA-C	-5.73	106.29	113.28
7	G	17	ARG	CB-CG-CD	-5.71	98.16	111.30
2	B	161	HIS	N-CA-C	-5.70	100.87	108.34
12	Y	35	ALA	CA-C-N	-5.69	113.02	119.28
12	Y	35	ALA	C-N-CA	-5.69	113.02	119.28
1	A	510	TYR	N-CA-C	-5.67	99.66	108.90
2	O	92	ASN	CB-CA-C	5.67	121.34	110.17
1	N	204	ALA	N-CA-C	-5.67	105.02	111.14
5	R	90	ARG	CA-C-N	5.66	125.33	119.05
5	R	90	ARG	C-N-CA	5.66	125.33	119.05
3	P	206	LEU	N-CA-C	-5.65	105.20	111.36
1	N	483	LEU	CA-C-N	5.64	131.67	122.81
1	N	483	LEU	C-N-CA	5.64	131.67	122.81
8	H	59	VAL	N-CA-C	5.64	116.28	110.36
2	O	161	HIS	N-CA-C	-5.63	100.96	108.34
4	Q	143	ASN	N-CA-C	5.63	119.11	111.17
1	A	250	GLY	N-CA-C	-5.63	105.56	112.77
1	N	438	ARG	CG-CD-NE	-5.63	99.61	112.00
1	A	136	LEU	CB-CG-CD1	-5.63	93.81	110.70
6	F	66	ASN	N-CA-C	-5.62	102.09	110.23
2	B	64	ILE	CB-CA-C	-5.61	104.57	112.14
3	C	80	ARG	CG-CD-NE	-5.59	99.71	112.00
1	N	493	GLU	N-CA-C	-5.58	105.73	112.54
9	I	68	ILE	CG1-CB-CG2	5.58	127.45	110.70
3	C	108	PRO	CA-C-N	-5.58	113.44	122.48
3	C	108	PRO	C-N-CA	-5.58	113.44	122.48
2	B	160	LEU	CA-C-O	-5.57	115.49	121.56
4	D	5	VAL	N-CA-C	5.57	116.45	108.93
1	N	342	LEU	N-CA-C	-5.57	104.84	111.69
1	N	437	PRO	N-CA-C	5.56	119.76	111.41
6	S	53	THR	CB-CA-C	-5.56	99.36	110.42
1	N	299	VAL	N-CA-C	5.54	116.27	110.62
2	O	202	SER	CB-CA-C	-5.53	99.42	110.42
8	H	8	ILE	CB-CA-C	5.52	120.35	111.29
4	Q	89	ILE	N-CA-C	-5.52	105.34	110.53
4	Q	8	SER	N-CA-C	5.51	120.88	113.72
7	T	8	HIS	N-CA-C	5.51	122.53	110.80
7	G	8	HIS	N-CA-C	5.50	122.51	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	30	GLY	N-CA-C	-5.49	106.02	113.37
6	F	59	GLY	N-CA-C	-5.48	102.33	110.71
3	C	150	SER	N-CA-C	5.47	117.67	111.11
1	N	10	THR	N-CA-C	-5.46	103.78	110.61
1	A	259	THR	N-CA-C	-5.46	105.23	111.07
3	P	186	PHE	N-CA-C	-5.46	101.67	110.14
1	N	189	MET	CA-CB-CG	-5.46	103.18	114.10
7	T	57	THR	N-CA-C	-5.44	106.81	113.50
7	T	76	ASN	CA-C-N	-5.43	114.36	119.85
7	T	76	ASN	C-N-CA	-5.43	114.36	119.85
4	D	102	TYR	CA-C-N	-5.43	117.60	123.08
4	D	102	TYR	C-N-CA	-5.43	117.60	123.08
2	B	70	ALA	N-CA-C	-5.42	105.45	111.36
1	N	233	HIS	N-CA-C	-5.42	105.28	111.14
1	A	371	TYR	CA-CB-CG	-5.42	104.14	113.90
1	N	273	MET	N-CA-C	-5.42	105.45	111.36
6	S	2	SER	CA-C-N	5.41	128.24	120.56
6	S	2	SER	C-N-CA	5.41	128.24	120.56
5	E	72	LYS	N-CA-C	-5.40	105.40	111.28
3	C	6	HIS	N-CA-C	-5.39	102.21	110.14
7	T	3	ALA	N-CA-C	5.39	122.27	110.80
8	H	38	ARG	NE-CZ-NH1	-5.38	116.12	121.50
7	T	44	ARG	N-CA-C	5.37	116.46	109.64
1	N	172	LYS	N-CA-C	-5.37	103.17	110.36
1	N	469	VAL	N-CA-C	-5.36	104.35	111.05
9	I	15	ARG	N-CA-C	-5.34	105.53	111.36
11	K	53	TRP	N-CA-C	-5.34	107.42	114.31
8	H	54	GLU	N-CA-C	5.34	117.79	111.33
1	N	202	LEU	N-CA-C	-5.34	104.87	111.33
2	B	67	ILE	CB-CA-C	-5.34	104.85	112.22
1	A	189	MET	CA-CB-CG	-5.33	103.43	114.10
12	L	11	ILE	N-CA-C	-5.32	104.83	109.19
3	P	23	SER	CA-CB-OG	-5.32	100.47	111.10
1	N	438	ARG	CB-CA-C	-5.31	99.19	109.76
1	N	372	TYR	N-CA-C	-5.31	105.57	111.36
3	P	23	SER	N-CA-C	-5.31	105.54	112.23
1	N	217	THR	N-CA-C	-5.31	103.68	110.53
8	H	34	LEU	N-CA-C	-5.30	105.42	111.14
1	A	230	LEU	N-CA-C	-5.27	105.54	111.28
1	N	408	THR	N-CA-C	-5.26	105.22	111.69
7	T	2	SER	CA-C-N	5.26	131.59	121.54
7	T	2	SER	C-N-CA	5.26	131.59	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	38	LYS	N-CA-C	5.26	117.69	111.33
3	P	38	ASN	N-CA-C	5.25	118.44	111.30
1	A	189	MET	CG-SD-CE	-5.24	89.37	100.90
2	B	92	ASN	N-CA-C	5.24	121.39	109.81
7	G	17	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	A	394	VAL	N-CA-CB	5.22	118.41	110.58
1	N	43	GLN	CA-C-N	5.22	125.13	119.76
1	N	43	GLN	C-N-CA	5.22	125.13	119.76
3	C	248	VAL	N-CA-C	-5.21	105.31	110.62
6	F	64	GLU	CA-C-N	-5.21	116.03	125.66
6	F	64	GLU	C-N-CA	-5.21	116.03	125.66
3	P	246	ASP	CB-CA-C	-5.21	102.71	110.88
3	P	40	MET	CB-CG-SD	-5.20	97.10	112.70
2	O	90	ILE	N-CA-CB	5.20	116.47	110.49
1	A	224	GLY	N-CA-C	-5.19	106.77	115.80
3	P	169	LEU	N-CA-C	5.18	116.62	111.07
7	G	5	LYS	N-CA-C	-5.18	99.77	110.80
1	A	474	GLU	N-CA-C	-5.18	105.81	111.82
2	B	64	ILE	CA-C-N	-5.18	114.06	122.65
2	B	64	ILE	C-N-CA	-5.18	114.06	122.65
3	C	215	LEU	N-CA-C	-5.17	105.33	111.69
1	A	251	PHE	N-CA-C	-5.17	105.65	111.28
11	X	39	GLU	CB-CA-C	-5.16	102.32	111.05
1	A	456	MET	CG-SD-CE	-5.16	89.56	100.90
1	N	407	ASP	N-CA-C	5.16	117.64	111.71
1	A	190	ILE	N-CA-C	5.14	115.92	110.72
3	C	71	HIS	N-CA-C	5.14	117.50	108.56
1	N	105	LEU	N-CA-C	5.14	119.74	112.75
4	Q	26	ASP	N-CA-C	5.14	117.62	111.71
1	N	146	THR	N-CA-C	-5.13	105.76	111.36
1	A	438	ARG	N-CA-C	-5.13	103.15	110.59
1	A	399	LEU	N-CA-C	-5.10	105.63	111.14
1	N	513	LEU	CA-C-N	-5.10	112.52	121.70
1	N	513	LEU	C-N-CA	-5.10	112.52	121.70
4	D	97	ILE	N-CA-C	-5.10	105.53	110.42
2	O	121	TYR	CB-CA-C	-5.09	100.89	109.50
5	R	6	GLU	N-CA-C	-5.09	99.95	110.80
11	K	49	THR	CA-C-N	5.09	125.00	119.76
11	K	49	THR	C-N-CA	5.09	125.00	119.76
1	N	113	LEU	CB-CA-C	5.09	119.23	110.79
3	C	23	SER	CA-CB-OG	-5.08	100.94	111.10
3	C	37	PHE	N-CA-C	-5.08	105.39	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	33	MET	CB-CG-SD	5.08	127.93	112.70
4	D	112	GLU	CA-CB-CG	-5.07	103.96	114.10
1	A	284	GLY	N-CA-C	-5.07	109.10	114.67
11	K	54	ARG	CA-C-O	5.07	129.41	120.80
1	N	484	THR	CB-CA-C	-5.05	99.38	109.33
10	W	57	HIS	N-CA-C	5.03	121.16	113.61
1	N	354	THR	N-CA-C	-5.03	106.41	112.54
8	H	78	GLU	N-CA-C	-5.03	106.66	112.89
3	C	136	VAL	N-CA-C	-5.02	105.81	110.53
2	B	178	ARG	NE-CZ-NH1	-5.02	116.48	121.50
12	L	29	PHE	N-CA-C	5.00	116.74	111.28
1	N	236	TRP	N-CA-C	5.00	117.62	111.82
10	W	39	CYS	N-CA-C	5.00	116.43	111.07
8	H	49	ASP	N-CA-C	5.00	116.55	108.34

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	5	HIS	Peptide
6	F	93	PRO	Peptide
6	S	93	PRO	Peptide
6	S	95	GLN	Peptide
12	Y	46	LYS	Peptide

5.2 Too-close contacts [i](#)

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	4060	0	4037	82	0
1	N	4060	0	4037	94	0
2	B	1824	0	1833	31	0
2	O	1824	0	1833	56	0
3	C	2110	0	2027	25	0
3	P	2110	0	2027	38	0
4	D	1195	0	1183	20	0
4	Q	1195	0	1183	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	852	0	845	10	0
5	R	852	0	845	21	0
6	F	748	0	728	22	0
6	S	748	0	728	39	0
7	G	675	0	643	46	0
7	T	675	0	643	43	0
8	H	662	0	623	21	0
8	U	662	0	623	23	0
9	I	601	0	613	9	0
9	V	601	0	613	9	0
10	J	460	0	459	14	0
10	W	460	0	459	12	0
11	K	384	0	366	3	0
11	X	384	0	366	5	0
12	L	380	0	380	17	0
12	Y	380	0	380	20	0
13	M	335	0	352	13	0
13	Z	335	0	352	6	0
14	A	120	0	108	12	0
14	N	120	0	108	5	0
15	A	2	0	0	0	0
15	N	2	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	102	0	152	16	0
19	C	102	0	152	10	0
19	N	102	0	152	7	0
19	P	51	0	76	3	0
19	U	51	0	76	4	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	63	0	110	4	0
21	D	63	0	110	10	0
21	L	63	0	110	15	0
21	N	63	0	110	14	0
21	O	63	0	110	5	0
21	Y	63	0	110	20	0
22	B	52	0	80	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	R	52	0	80	20	0
23	B	29	0	37	4	0
23	C	58	0	71	4	0
23	J	29	0	36	8	0
23	O	29	0	37	3	0
23	P	58	0	72	5	0
23	W	29	0	35	3	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	22	0
25	G	53	0	77	19	0
25	P	53	0	77	6	0
25	T	106	0	154	33	0
26	C	100	0	156	20	0
26	G	100	0	156	34	0
26	P	100	0	156	27	0
26	T	100	0	156	30	0
27	C	33	0	39	4	0
27	M	33	0	39	0	0
27	P	33	0	38	2	0
27	Z	33	0	38	0	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	217	0	0	5	0
29	B	127	0	0	3	0
29	C	93	0	0	4	0
29	D	86	0	0	6	0
29	E	52	0	0	0	0
29	F	72	0	0	3	0
29	G	42	0	0	7	0
29	H	46	0	0	1	0
29	I	31	0	0	3	0
29	J	28	0	0	4	0
29	K	27	0	0	2	0
29	L	16	0	0	1	0
29	M	20	0	0	0	0
29	N	207	0	0	6	0
29	O	105	0	0	2	0
29	P	96	0	0	3	0
29	Q	57	0	0	4	0
29	R	35	0	0	1	0
29	S	63	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	T	44	0	0	5	0
29	U	43	0	0	5	0
29	V	20	0	0	0	0
29	W	17	0	0	2	0
29	X	13	0	0	1	0
29	Y	12	0	0	1	0
29	Z	11	0	0	1	0
All	All	32382	0	31350	808	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 13.

All (808) 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)
25:T:1265:PEK:H383	26:T:1269:CDL:C27	1.34	1.51
1:N:297:MET:SD	1:N:297:MET:CE	2.10	1.40
25:T:1265:PEK:C38	26:T:1269:CDL:H273	1.51	1.36
10:W:2:GLU:HB2	10:W:4:ARG:NH1	1.50	1.26
25:T:1265:PEK:C38	26:T:1269:CDL:C27	2.12	1.18
7:G:5:LYS:HD2	25:G:1263:PEK:C37	1.73	1.18
19:A:524:PGV:H311	13:M:19:LEU:HD23	1.24	1.16
19:U:1268:PGV:H032	29:U:4495:HOH:O	1.43	1.14
25:C:264:PEK:H162	25:C:264:PEK:H101	1.17	1.14
7:G:5:LYS:CD	25:G:1263:PEK:H371	1.78	1.13
26:C:270:CDL:HB22	10:J:8:LYS:NZ	1.62	1.13
29:B:2562:HOH:O	21:D:523:TGL:HC61	1.50	1.11
26:C:270:CDL:HB22	10:J:8:LYS:HZ2	1.09	1.10
7:G:84:LYS:H	7:G:84:LYS:HD2	1.03	1.10
12:L:20:ARG:NH2	21:L:522:TGL:HC32	1.64	1.10
25:T:1265:PEK:H383	26:T:1269:CDL:H271	1.23	1.10
26:G:269:CDL:H561	26:G:269:CDL:H762	1.33	1.09
8:H:52:VAL:HG12	8:U:46:LYS:HB2	1.17	1.09
21:N:1523:TGL:HC21	21:N:1523:TGL:HG11	1.31	1.08
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.26	1.06
26:G:269:CDL:H522	26:G:269:CDL:H222	1.39	1.04
1:N:513:LEU:O	1:N:514:LYS:HB2	1.55	1.04
7:G:5:LYS:CG	25:G:1263:PEK:H371	1.88	1.03
6:S:94:HIS:CD2	6:S:95:GLN:N	2.26	1.03
26:C:270:CDL:H212	26:C:270:CDL:H631	1.05	1.02
1:A:513:LEU:O	1:A:514:LYS:HB2	1.60	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:9:LYS:HG3	8:U:10:ASN:H	1.21	1.01
2:O:59:GLN:O	2:O:59:GLN:HG3	1.59	0.98
6:S:94:HIS:CD2	6:S:95:GLN:H	1.80	0.98
22:R:1229:PSC:H142	22:R:1229:PSC:C34	1.94	0.98
19:N:1524:PGV:H012	19:N:1524:PGV:H221	1.45	0.97
7:G:84:LYS:HD2	7:G:84:LYS:N	1.78	0.95
19:N:1524:PGV:H221	19:N:1524:PGV:C01	1.96	0.94
26:P:1270:CDL:HB21	26:P:1270:CDL:CB3	1.98	0.94
10:W:2:GLU:HB2	10:W:4:ARG:HH12	1.32	0.94
22:B:229:PSC:H212	22:B:229:PSC:O01	1.67	0.94
19:C:267:PGV:H181	26:C:270:CDL:H652	1.48	0.93
7:G:2:SER:OG	25:G:1263:PEK:H291	1.66	0.93
6:F:94:HIS:HB3	6:F:95:GLN:OE1	1.68	0.93
7:G:72:ASN:H	7:G:76:ASN:HD22	0.99	0.93
26:P:1270:CDL:HB21	26:P:1270:CDL:HB32	1.49	0.93
25:T:1265:PEK:H383	26:T:1269:CDL:H273	1.00	0.92
6:F:85:CYS:SG	6:F:87:THR:HG23	2.09	0.92
26:G:269:CDL:H112	26:G:269:CDL:HA21	1.52	0.92
25:T:1265:PEK:H381	26:T:1269:CDL:H273	1.48	0.92
10:W:2:GLU:HB2	10:W:4:ARG:HH11	1.35	0.92
22:B:229:PSC:H072	9:I:10:ARG:HH21	1.32	0.91
6:S:85:CYS:SG	6:S:87:THR:HG23	2.10	0.91
26:T:1269:CDL:H531	26:T:1269:CDL:H241	1.53	0.90
25:P:1264:PEK:H71	25:P:1264:PEK:H32	1.55	0.89
3:P:29:SER:HB2	3:P:42:LEU:HD13	1.53	0.89
25:T:1265:PEK:H71	29:T:4407:HOH:O	1.73	0.89
8:H:9:LYS:O	8:H:10:ASN:HB2	1.71	0.88
7:T:7:ASP:O	7:T:8:HIS:HB2	1.73	0.88
1:A:513:LEU:O	1:A:514:LYS:CB	2.22	0.87
7:G:84:LYS:H	7:G:84:LYS:CD	1.87	0.87
1:A:282:PHE:HA	7:T:4:ALA:CB	2.04	0.87
26:C:270:CDL:H212	26:C:270:CDL:C63	1.99	0.87
12:L:20:ARG:HH22	21:L:522:TGL:HC32	1.38	0.87
1:N:513:LEU:O	1:N:514:LYS:CB	2.23	0.86
7:G:2:SER:OG	25:G:1263:PEK:C29	2.22	0.86
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.41	0.86
12:Y:20:ARG:HH21	21:Y:1522:TGL:HC32	1.39	0.86
19:A:524:PGV:H22	19:A:524:PGV:H011	1.59	0.85
3:C:63:ARG:HH21	26:C:270:CDL:HA21	1.38	0.85
2:B:81:LEU:HD12	26:T:1269:CDL:H351	1.57	0.85
7:G:2:SER:O	25:G:1263:PEK:H331	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:44:LYS:HE2	29:I:4717:HOH:O	1.77	0.84
8:H:52:VAL:HG12	8:U:46:LYS:CB	2.06	0.83
19:A:524:PGV:H311	13:M:19:LEU:CD2	2.09	0.83
21:D:523:TGL:HG32	29:D:4105:HOH:O	1.76	0.83
6:F:97:ALA:CB	29:F:4782:HOH:O	2.26	0.83
7:G:5:LYS:HG3	25:G:1263:PEK:H371	1.60	0.82
7:G:3:ALA:HB1	25:G:1263:PEK:H383	1.61	0.82
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.60	0.82
12:Y:20:ARG:HH21	21:Y:1522:TGL:CC3	1.93	0.82
3:C:246:ASP:HB2	29:C:4124:HOH:O	1.81	0.81
7:G:72:ASN:H	7:G:76:ASN:ND2	1.78	0.81
8:U:9:LYS:HG3	8:U:10:ASN:N	1.94	0.81
6:S:76:LYS:HE2	29:S:4790:HOH:O	1.80	0.81
7:T:2:SER:OG	25:T:263:PEK:H301	1.79	0.81
5:R:7:THR:OG1	5:R:10:GLU:HG3	1.80	0.81
1:N:351:GLY:HA3	1:N:380[A]:VAL:HG13	1.62	0.81
22:B:229:PSC:C07	9:I:10:ARG:HH21	1.93	0.81
4:D:45:LYS:HB3	29:D:4504:HOH:O	1.81	0.81
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.63	0.80
22:B:229:PSC:H343	22:B:229:PSC:H142	1.62	0.80
8:U:45:ALA:O	8:U:47:GLY:N	2.14	0.80
6:S:94:HIS:HD2	6:S:95:GLN:N	1.80	0.80
26:C:270:CDL:H631	26:C:270:CDL:C21	2.01	0.80
21:N:1523:TGL:HC21	21:N:1523:TGL:CG1	2.12	0.80
25:C:264:PEK:H162	25:C:264:PEK:C10	2.07	0.79
26:T:1269:CDL:CA2	26:T:1269:CDL:H111	2.11	0.79
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.61	0.79
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.48	0.79
19:N:1524:PGV:H321	19:N:1524:PGV:H151	1.64	0.79
7:G:31:CYS:SG	26:G:269:CDL:H532	2.22	0.78
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.63	0.78
22:R:1229:PSC:H142	22:R:1229:PSC:H343	1.63	0.78
12:L:20:ARG:HH21	21:L:522:TGL:HC32	1.48	0.78
8:U:9:LYS:O	8:U:10:ASN:HB2	1.82	0.77
10:W:33:ARG:HG2	23:W:1059:CHD:H152	1.66	0.77
6:F:97:ALA:HB3	29:F:4782:HOH:O	1.84	0.77
3:P:107:ALA:HB2	19:U:1268:PGV:H031	1.66	0.77
6:S:94:HIS:HD2	6:S:95:GLN:CA	1.97	0.77
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.67	0.77
1:A:351:GLY:HA3	1:A:380[A]:VAL:HG13	1.67	0.76
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:1522:TGL:H231	21:Y:1522:TGL:CA9	2.14	0.76
7:T:72:ASN:H	7:T:76:ASN:HD22	1.33	0.76
25:C:264:PEK:H101	25:C:264:PEK:C16	2.08	0.76
2:O:227:LEU:OXT	2:O:227:LEU:HD13	1.86	0.76
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.21	0.75
26:G:269:CDL:H372	2:O:78:LEU:CD1	2.16	0.75
1:A:484:THR:HB	13:M:2:THR:OG1	1.87	0.75
22:B:229:PSC:O02	22:B:229:PSC:H032	1.85	0.75
22:B:229:PSC:H142	22:B:229:PSC:C34	2.17	0.75
6:F:1:ALA:HB3	6:S:65:ASP:OD1	1.87	0.74
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.84	0.74
4:D:20:ARG:HG3	29:D:4132:HOH:O	1.86	0.74
19:A:521:PGV:H183	25:C:264:PEK:H332	1.68	0.74
2:B:56:MET:HA	22:B:229:PSC:H201	1.68	0.74
26:T:1269:CDL:H111	26:T:1269:CDL:HA22	1.67	0.74
22:R:1229:PSC:H221	22:R:1229:PSC:H22	1.70	0.74
7:G:5:LYS:HD2	25:G:1263:PEK:H372	1.69	0.73
2:B:70:ALA:HB1	26:T:1269:CDL:H451	1.70	0.73
26:G:269:CDL:H522	26:G:269:CDL:C22	2.18	0.73
6:S:95:GLN:CG	29:S:4728:HOH:O	2.36	0.73
19:C:267:PGV:C18	26:C:270:CDL:H652	2.18	0.72
21:N:1523:TGL:H231	21:N:1523:TGL:HA81	1.71	0.72
19:C:268:PGV:H061	29:C:4333:HOH:O	1.89	0.72
3:C:95:THR:HG21	19:C:268:PGV:H282	1.71	0.72
26:G:269:CDL:H171	29:G:4479:HOH:O	1.90	0.71
8:H:43:MET:HE3	8:H:49:ASP:H	1.55	0.71
1:N:351:GLY:C	1:N:380[A]:VAL:CG1	2.62	0.71
3:P:54:MET:HE3	26:P:1270:CDL:H601	1.72	0.71
7:G:72:ASN:N	7:G:76:ASN:HD22	1.83	0.71
22:R:1229:PSC:H343	22:R:1229:PSC:C14	2.20	0.71
9:V:61:GLU:HG3	9:V:65:LYS:NZ	2.06	0.71
12:Y:20:ARG:NH2	21:Y:1522:TGL:HC32	2.05	0.71
6:S:52:ILE:O	6:S:94:HIS:ND1	2.25	0.70
12:Y:20:ARG:NH2	21:Y:1522:TGL:CC3	2.54	0.70
26:C:270:CDL:HA22	29:J:4496:HOH:O	1.92	0.70
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.27	0.70
25:C:265:PEK:H041	7:G:17:ARG:HH22	1.57	0.69
7:G:3:ALA:CB	25:G:1263:PEK:H383	2.22	0.69
1:N:351:GLY:CA	1:N:380[A]:VAL:HG13	2.21	0.69
19:N:1524:PGV:H012	19:N:1524:PGV:C22	2.22	0.69
6:S:94:HIS:HD2	6:S:95:GLN:HA	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:12:PRO:HB2	21:Y:1522:TGL:HG11	1.72	0.69
21:B:521:TGL:HA91	21:B:521:TGL:H252	1.75	0.69
22:B:229:PSC:H041	5:E:41:LEU:HD23	1.73	0.69
7:T:3:ALA:CB	25:T:263:PEK:H383	2.22	0.69
21:D:523:TGL:H242	21:D:523:TGL:HA91	1.74	0.69
25:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.39	0.68
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.75	0.68
10:J:4:ARG:HD3	10:J:7:GLU:OE2	1.94	0.68
10:J:26:ALA:O	10:J:30:ILE:HD12	1.94	0.68
7:T:2:SER:O	25:T:263:PEK:H331	1.93	0.68
7:G:5:LYS:HB3	1:N:278:MET:SD	2.34	0.68
7:T:7:ASP:CG	7:T:8:HIS:N	2.51	0.68
7:T:45:PRO:HD2	29:T:3099:HOH:O	1.94	0.68
26:C:270:CDL:H222	26:C:270:CDL:H661	1.76	0.68
2:O:59:GLN:C	2:O:60:GLU:HG3	2.19	0.68
6:S:94:HIS:CD2	6:S:95:GLN:CA	2.73	0.67
21:N:1523:TGL:HG11	21:N:1523:TGL:CC2	2.18	0.67
7:T:37:LEU:HD21	26:T:1269:CDL:H361	1.76	0.67
7:G:7:ASP:O	7:G:9:GLY:N	2.22	0.67
1:N:378:HIS:HA	1:N:382[A]:SER:OG	1.93	0.67
26:T:1269:CDL:OB4	26:T:1269:CDL:H1	1.94	0.67
19:C:268:PGV:H102	29:C:4697:HOH:O	1.94	0.67
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.82	0.67
29:A:4171:HOH:O	22:B:229:PSC:H32	1.96	0.66
2:O:52:HIS:CE1	22:R:1229:PSC:H202	2.31	0.66
21:Y:1522:TGL:OC1	21:Y:1522:TGL:HC51	1.96	0.66
2:B:183:THR:CG2	29:B:4424:HOH:O	2.43	0.66
25:C:265:PEK:H371	26:G:269:CDL:C27	2.26	0.66
2:O:227:LEU:HB2	29:O:4695:HOH:O	1.96	0.66
1:A:282:PHE:HA	7:T:4:ALA:HB1	1.76	0.66
10:J:33:ARG:HG2	23:J:60:CHD:C15	2.25	0.66
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.77	0.66
25:C:265:PEK:H042	6:F:1:ALA:H1	1.61	0.66
1:N:351:GLY:C	1:N:380[A]:VAL:HG13	2.21	0.66
22:B:229:PSC:H31	22:B:229:PSC:H221	1.78	0.66
8:H:9:LYS:O	8:H:10:ASN:CB	2.43	0.65
29:N:4633:HOH:O	2:O:87:MET:SD	2.53	0.65
26:G:269:CDL:H752	1:N:282:PHE:HZ	1.62	0.65
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.79	0.65
26:T:1269:CDL:H111	26:T:1269:CDL:HA21	1.78	0.65
6:S:94:HIS:CG	6:S:95:GLN:H	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:87:THR:HG21	29:F:4730:HOH:O	1.97	0.65
19:P:1267:PGV:H181	26:P:1270:CDL:H651	1.79	0.65
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.62	0.64
4:D:86:MET:CE	29:K:4243:HOH:O	2.44	0.64
12:L:11:ILE:CG2	21:L:522:TGL:H272	2.27	0.64
1:A:351:GLY:C	1:A:380[A]:VAL:CG1	2.70	0.64
1:N:407:ASP:O	1:N:411:LYS:HG3	1.97	0.64
12:Y:47:LYS:HE2	12:Y:47:LYS:OXT	1.97	0.64
25:C:265:PEK:H6	25:C:265:PEK:H222	1.80	0.64
26:T:1269:CDL:H241	26:T:1269:CDL:C53	2.27	0.64
1:A:51:ASP:OD1	1:A:441:SER:OG	2.12	0.64
12:Y:22:LEU:O	12:Y:26:THR:HB	1.96	0.64
4:Q:94:LEU:HD23	11:X:28:VAL:HG21	1.79	0.64
1:N:87:ILE:O	1:N:173:PRO:HD3	1.99	0.63
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.63	0.63
8:H:43:MET:CE	8:H:49:ASP:H	2.11	0.63
1:N:113:LEU:HD12	21:Y:1522:TGL:C13	2.28	0.63
8:H:46:LYS:HE2	8:U:8:ILE:CG2	2.27	0.63
25:C:264:PEK:HN2	7:G:76:ASN:HD21	1.46	0.63
6:F:64:GLU:O	6:F:65:ASP:HB2	1.97	0.63
8:H:43:MET:HE3	8:H:49:ASP:N	2.12	0.63
4:Q:92:THR:O	4:Q:95:LEU:HB2	1.99	0.63
10:W:2:GLU:HG2	29:W:4564:HOH:O	1.98	0.63
4:D:78:TRP:HB3	21:D:523:TGL:HB22	1.81	0.62
10:J:33:ARG:HG2	23:J:60:CHD:H151	1.80	0.62
1:A:485:VAL:HG22	13:M:1:ILE:HG13	1.82	0.62
25:P:1264:PEK:H12	25:P:1264:PEK:H242	1.80	0.62
6:S:94:HIS:CG	6:S:95:GLN:N	2.66	0.62
12:Y:2:HIS:CG	12:Y:3:TYR:H	2.17	0.62
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.82	0.62
13:M:10:THR:HA	13:M:14:GLU:OE2	2.00	0.62
26:P:1270:CDL:PA1	26:P:1270:CDL:HB22	2.40	0.62
22:R:1229:PSC:H071	9:V:10:ARG:HE	1.65	0.62
26:G:269:CDL:H351	2:O:78:LEU:HD12	1.80	0.61
3:P:29:SER:CB	3:P:42:LEU:HD13	2.28	0.61
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.83	0.61
1:N:488:THR:HB	1:N:495:LEU:HD13	1.82	0.61
23:P:1271:CHD:C16	23:P:1271:CHD:H232	2.31	0.61
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.15	0.61
26:T:1269:CDL:H582	26:T:1269:CDL:H751	1.83	0.61
19:A:524:PGV:H012	19:A:524:PGV:H221	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:ARG:NH2	26:C:270:CDL:HA21	2.15	0.61
2:O:62:GLU:O	2:O:66:THR:HB	2.01	0.61
10:W:2:GLU:CB	10:W:4:ARG:HH12	2.10	0.60
26:G:269:CDL:H362	2:O:81:LEU:HD12	1.83	0.60
1:N:113:LEU:HD12	21:Y:1522:TGL:C14	2.31	0.60
8:U:48:GLY:HA2	29:U:4792:HOH:O	2.00	0.60
1:N:484:THR:HB	13:Z:2:THR:OG1	2.02	0.60
4:Q:66:GLU:HG2	29:Q:4646:HOH:O	2.02	0.60
7:G:2:SER:OG	25:G:1263:PEK:H292	2.00	0.60
6:F:1:ALA:CB	6:S:65:ASP:OD1	2.49	0.60
2:O:66:THR:HG21	23:O:229:CHD:H3	1.84	0.60
6:S:54:ASN:HD22	6:S:54:ASN:C	2.09	0.60
12:L:2:HIS:CG	12:L:3:TYR:H	2.19	0.59
6:S:1:ALA:H2	25:T:1265:PEK:H041	1.67	0.59
7:G:6:GLY:O	25:G:1263:PEK:H311	2.03	0.59
29:A:2527:HOH:O	12:L:7:PRO:HG3	2.03	0.59
1:A:351:GLY:CA	1:A:380[A]:VAL:HG13	2.33	0.59
3:P:210:ILE:HG12	19:P:1267:PGV:H132	1.85	0.59
21:B:521:TGL:C28	21:B:521:TGL:H101	2.33	0.58
2:O:56:MET:HA	22:R:1229:PSC:H201	1.83	0.58
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.38	0.58
3:C:80:ARG:NH1	3:C:236:GLU:OE2	2.34	0.58
1:N:177:SER:H	1:N:180:GLN:NE2	2.00	0.58
1:N:377:PHE:O	1:N:381[B]:LEU:HB3	2.03	0.58
25:G:1263:PEK:HN1	25:G:1263:PEK:H221	1.68	0.58
21:N:1523:TGL:H231	21:N:1523:TGL:CA9	2.33	0.58
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.84	0.58
1:N:113:LEU:CD1	21:Y:1522:TGL:H292	2.33	0.58
21:N:1523:TGL:HC61	29:O:3562:HOH:O	2.03	0.58
4:Q:109:HIS:HD2	29:Q:3122:HOH:O	1.86	0.58
26:C:270:CDL:OA3	26:C:270:CDL:O1	2.11	0.58
1:N:377:PHE:O	1:N:381[B]:LEU:HB2	2.04	0.58
2:O:59:GLN:O	2:O:59:GLN:CG	2.40	0.58
7:T:8:HIS:O	7:T:9:GLY:C	2.46	0.58
1:A:400:PHE:HB3	21:L:522:TGL:H283	1.86	0.58
19:A:524:PGV:H142	19:A:524:PGV:C30	2.34	0.58
23:O:229:CHD:H12	23:O:229:CHD:H212	1.85	0.58
3:C:55:TYR:CE1	26:C:270:CDL:H512	2.38	0.58
23:C:525:CHD:H152	19:C:268:PGV:H11	1.86	0.58
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.39	0.58
9:V:10:ARG:HG3	9:V:10:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:61:GLU:HG3	9:V:65:LYS:HZ1	1.69	0.58
1:N:113:LEU:HD13	21:Y:1522:TGL:H292	1.85	0.57
25:C:265:PEK:H371	26:G:269:CDL:H273	1.86	0.57
26:C:270:CDL:CB2	10:J:8:LYS:HZ2	2.01	0.57
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.69	0.57
21:B:521:TGL:HC21	29:I:2606:HOH:O	2.04	0.57
25:C:265:PEK:H042	6:F:1:ALA:N	2.20	0.57
1:N:400:PHE:HB3	21:Y:1522:TGL:H283	1.87	0.57
8:U:43:MET:HE3	8:U:49:ASP:N	2.19	0.57
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.87	0.57
1:N:449:MET:SD	2:O:5:MET:HG2	2.44	0.57
25:T:1265:PEK:C37	26:T:1269:CDL:C27	2.82	0.57
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.86	0.57
8:H:45:ALA:C	8:H:47:GLY:H	2.12	0.57
9:V:2:THR:HG22	9:V:3:ALA:H	1.69	0.57
7:G:7:ASP:HB3	29:N:4167:HOH:O	2.02	0.57
8:H:45:ALA:O	8:H:47:GLY:N	2.37	0.57
1:A:28:MET:HE2	14:A:515:HEA:H271	1.86	0.57
3:P:223:LEU:HD21	23:P:1271:CHD:H183	1.87	0.57
1:N:514:LYS:HA	6:S:38:ALA:CB	2.35	0.56
26:C:270:CDL:HB22	10:J:8:LYS:HZ1	1.65	0.56
1:A:307:SER:HB3	26:T:1269:CDL:H171	1.86	0.56
22:R:1229:PSC:C2	22:R:1229:PSC:H011	2.35	0.56
7:G:11:TPO:CG2	7:G:11:TPO:O	2.53	0.56
29:N:4604:HOH:O	11:X:8:ASP:HB2	2.05	0.56
2:O:13:THR:HB	2:O:168:LEU:HD23	1.88	0.56
21:O:1521:TGL:H241	21:O:1521:TGL:H201	1.87	0.56
19:C:268:PGV:C06	29:C:4333:HOH:O	2.52	0.56
2:O:52:HIS:HE1	22:R:1229:PSC:H202	1.68	0.56
5:R:23:ASP:O	5:R:24:ILE:C	2.49	0.56
6:S:64:GLU:O	6:S:65:ASP:HB2	2.05	0.56
19:A:524:PGV:H312	13:M:16:ALA:HA	1.88	0.56
2:O:146:MET:HA	2:O:213:LEU:HD12	1.88	0.56
9:V:52:ARG:CZ	9:V:52:ARG:HB2	2.36	0.55
23:P:1271:CHD:H232	23:P:1271:CHD:H162	1.87	0.55
7:T:35:SER:HB3	7:T:36:TRP:CE3	2.42	0.55
4:Q:86:MET:HE1	29:X:4493:HOH:O	2.06	0.55
7:T:5:LYS:CG	25:T:263:PEK:H371	2.36	0.55
7:G:2:SER:HG	25:G:1263:PEK:H291	1.71	0.55
12:L:14:SER:H	21:L:522:TGL:HC31	1.72	0.55
25:P:1264:PEK:H71	25:P:1264:PEK:C3	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:229:PSC:H42	29:I:2588:HOH:O	2.07	0.55
2:O:84:LEU:HA	2:O:87:MET:CE	2.36	0.55
3:P:40:MET:O	3:P:44:MET:HG2	2.07	0.55
6:S:92:VAL:O	6:S:92:VAL:HG23	2.06	0.55
1:A:382[A]:SER:O	1:A:386:VAL:HB	2.06	0.55
26:G:269:CDL:HA21	26:G:269:CDL:C11	2.33	0.55
2:O:164:ALA:O	2:O:194:GLY:HA3	2.07	0.55
21:D:523:TGL:OA1	21:D:523:TGL:HG31	2.07	0.55
21:N:1523:TGL:H231	21:N:1523:TGL:CA8	2.36	0.55
25:T:1265:PEK:C38	26:T:1269:CDL:H271	2.11	0.55
1:A:310:MET:HE1	2:B:76:ILE:HG21	1.89	0.54
4:D:34:SER:O	4:D:38:LYS:HG3	2.07	0.54
7:G:7:ASP:CB	29:N:4167:HOH:O	2.55	0.54
8:H:23:GLN:HG3	29:H:4128:HOH:O	2.07	0.54
5:R:48:ILE:O	5:R:52:LEU:HG	2.07	0.54
19:U:1268:PGV:C03	29:U:4495:HOH:O	2.22	0.54
7:T:5:LYS:HG3	25:T:263:PEK:H371	1.90	0.54
8:H:43:MET:HE1	8:U:43:MET:HE1	1.90	0.54
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.22	0.54
6:S:95:GLN:HG2	29:S:4728:HOH:O	2.05	0.54
2:B:29:MET:HE1	9:I:36:LYS:HE2	1.90	0.54
23:W:1059:CHD:H41	29:W:4647:HOH:O	2.07	0.54
1:A:381[A]:LEU:HB2	14:A:516:HEA:CAC	2.38	0.54
6:S:95:GLN:HG3	29:S:4728:HOH:O	2.03	0.54
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.48	0.54
1:A:1:FME:HE2	12:L:3:TYR:HE1	1.73	0.54
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.43	0.54
7:T:7:ASP:O	7:T:8:HIS:CB	2.53	0.54
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.43	0.53
3:C:59:ARG:HA	26:C:270:CDL:H522	1.90	0.53
9:V:1:SAC:OAC	9:V:1:SAC:HB3	2.09	0.53
21:D:523:TGL:CG3	29:D:4105:HOH:O	2.42	0.53
2:O:84:LEU:HA	2:O:87:MET:HE2	1.90	0.53
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.44	0.53
3:P:51:MET:HB3	26:P:1270:CDL:H392	1.90	0.53
26:P:1270:CDL:H352	26:P:1270:CDL:H162	1.90	0.53
1:N:297:MET:CE	1:N:297:MET:HB2	2.39	0.53
26:T:1269:CDL:HA22	26:T:1269:CDL:C11	2.36	0.53
1:A:383[A]:MET:O	1:A:384[A]:GLY:C	2.48	0.53
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.91	0.53
19:N:1524:PGV:H221	19:N:1524:PGV:H011	1.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:MET:HE3	29:J:4237:HOH:O	2.08	0.53
21:N:1523:TGL:H231	21:N:1523:TGL:HA92	1.91	0.53
10:W:3:ASN:OD1	10:W:3:ASN:C	2.51	0.53
1:A:47:LEU:O	13:M:41:LYS:HE3	2.09	0.53
3:C:106:LEU:HD13	19:C:268:PGV:H22	1.90	0.53
4:D:121:LYS:HD3	11:K:52:GLU:HA	1.91	0.53
7:T:42:ARG:HB2	29:T:4747:HOH:O	2.09	0.53
2:B:58:ALA:O	2:B:62:GLU:HG3	2.09	0.53
25:C:265:PEK:C37	26:G:269:CDL:C27	2.86	0.53
12:L:20:ARG:HH12	21:L:522:TGL:HC61	1.74	0.53
6:S:1:ALA:N	25:T:1265:PEK:C04	2.72	0.53
22:B:229:PSC:C07	9:I:10:ARG:NH2	2.69	0.52
26:G:269:CDL:H471	29:G:4791:HOH:O	2.08	0.52
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.56	0.52
6:S:1:ALA:N	25:T:1265:PEK:H041	2.22	0.52
19:A:524:PGV:H012	19:A:524:PGV:C22	2.39	0.52
2:B:183:THR:HG23	29:B:4424:HOH:O	2.04	0.52
1:N:352:GLY:N	1:N:380[A]:VAL:CG1	2.72	0.52
1:A:87:ILE:O	1:A:173:PRO:HD3	2.10	0.52
1:A:310:MET:HE3	1:A:356:ILE:HG23	1.91	0.52
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.74	0.52
2:B:89:GLU:O	2:B:91:ASN:ND2	2.42	0.52
7:G:11:TPO:CG2	7:G:16:TRP:HE1	2.19	0.52
26:C:270:CDL:HB21	26:C:270:CDL:PA1	2.50	0.52
5:E:52:LEU:O	5:E:55:CYS:HB2	2.09	0.52
2:O:222:TRP:O	2:O:226:MET:HB2	2.10	0.52
6:F:55:LYS:HA	6:F:74:LEU:O	2.10	0.52
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.45	0.52
8:U:45:ALA:C	8:U:47:GLY:H	2.13	0.52
19:A:524:PGV:H142	19:A:524:PGV:H301	1.90	0.52
8:U:9:LYS:CG	8:U:10:ASN:H	2.09	0.52
25:C:264:PEK:H32	25:C:264:PEK:H71	1.93	0.51
4:D:61:ARG:HD2	29:D:2674:HOH:O	2.10	0.51
8:H:43:MET:O	8:H:44:THR:C	2.53	0.51
29:L:4557:HOH:O	13:M:32:TRP:HH2	1.94	0.51
6:S:76:LYS:HG3	6:S:93:PRO:HG2	1.92	0.51
6:S:94:HIS:O	6:S:95:GLN:HB2	2.09	0.51
6:S:95:GLN:O	6:S:97:ALA:N	2.43	0.51
7:G:3:ALA:HB3	25:G:1263:PEK:H362	1.91	0.51
1:N:240:HIS:O	1:N:241:PRO:C	2.51	0.51
1:N:290:HIS:HD2	1:N:291:HIS:CD2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.98	0.51
12:L:20:ARG:HH22	21:L:522:TGL:CC3	2.19	0.51
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.92	0.51
8:H:7:LYS:O	8:H:8:ILE:HG22	2.10	0.51
1:N:381[A]:LEU:O	1:N:385:ALA:HB3	2.11	0.51
3:P:131:LEU:HD21	26:T:1269:CDL:HB61	1.91	0.51
6:S:55:LYS:HA	6:S:74:LEU:O	2.11	0.51
1:A:177:SER:H	1:A:180:GLN:NE2	2.08	0.51
2:B:62:GLU:O	2:B:66:THR:HB	2.11	0.51
8:H:46:LYS:HE2	8:U:8:ILE:HG21	1.92	0.51
3:P:59:ARG:HA	26:P:1270:CDL:H522	1.93	0.51
7:T:38:HIS:NE2	26:T:1269:CDL:HA21	2.26	0.51
8:U:43:MET:HG3	8:U:49:ASP:O	2.11	0.51
26:P:1270:CDL:H112	26:P:1270:CDL:OB7	2.10	0.51
25:C:265:PEK:C04	6:F:1:ALA:N	2.74	0.51
7:T:17:ARG:NH1	25:T:1265:PEK:O13	2.43	0.51
5:E:31:LYS:HE3	6:F:84:SER:O	2.12	0.50
25:G:1263:PEK:H281	3:P:85:LEU:HD21	1.93	0.50
2:O:83:ILE:O	2:O:87:MET:HG3	2.11	0.50
3:P:116:TRP:HA	3:P:117:PRO:C	2.36	0.50
1:A:351:GLY:HA3	1:A:380[A]:VAL:CG1	2.39	0.50
26:G:269:CDL:C37	2:O:78:LEU:CD1	2.88	0.50
3:C:65:SER:HB2	19:C:267:PGV:H041	1.94	0.50
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.93	0.50
26:G:269:CDL:H112	26:G:269:CDL:CA2	2.33	0.50
2:O:226:MET:O	2:O:227:LEU:C	2.55	0.50
8:U:27:ARG:HG2	29:U:4672:HOH:O	2.12	0.50
1:A:377:PHE:O	1:A:381[A]:LEU:HB3	2.11	0.50
1:N:381[A]:LEU:HD13	14:N:516:HEA:HBC2	1.94	0.50
9:V:61:GLU:HG3	9:V:65:LYS:HZ2	1.75	0.50
1:A:240:HIS:C	1:A:240:HIS:CD2	2.89	0.50
2:B:78:LEU:HD12	26:T:1269:CDL:H352	1.93	0.50
2:O:100:MET:HE3	2:O:157:GLU:HG3	1.93	0.50
12:Y:2:HIS:N	29:Y:4665:HOH:O	2.44	0.50
7:T:8:HIS:O	7:T:9:GLY:O	2.30	0.49
12:Y:14:SER:H	21:Y:1522:TGL:HC31	1.77	0.49
3:P:59:ARG:HG3	26:P:1270:CDL:H511	1.93	0.49
1:A:347:LEU:HD22	1:A:383[B]:MET:SD	2.51	0.49
2:B:68:LEU:HB3	22:B:229:PSC:H182	1.92	0.49
7:G:5:LYS:HB2	25:G:1263:PEK:H351	1.95	0.49
10:J:36:MET:HG2	23:J:60:CHD:H221	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.49
21:N:1523:TGL:HG32	21:N:1523:TGL:OB1	2.11	0.49
26:G:269:CDL:H182	1:N:307:SER:CB	2.42	0.49
8:H:7:LYS:O	8:H:8:ILE:HB	2.12	0.49
1:A:21:LEU:CD2	21:L:522:TGL:HA81	2.43	0.49
7:T:5:LYS:HG3	25:T:263:PEK:C37	2.42	0.49
1:A:115:SER:O	1:A:121:GLY:HA2	2.12	0.49
6:F:54:ASN:OD1	6:F:76:LYS:HD2	2.12	0.49
1:N:489:THR:HA	6:S:71:TRP:O	2.12	0.49
29:N:4743:HOH:O	23:W:1059:CHD:H212	2.12	0.49
1:A:489:THR:HA	6:F:71:TRP:O	2.12	0.49
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.77	0.49
3:C:191:GLY:HA3	29:G:2132:HOH:O	2.13	0.49
5:R:80:GLU:H	5:R:80:GLU:CD	2.21	0.49
12:Y:20:ARG:NH2	21:Y:1522:TGL:HC31	2.25	0.49
3:C:33:MET:CE	29:J:4237:HOH:O	2.61	0.49
3:C:84:ILE:HD13	25:T:263:PEK:H241	1.95	0.49
7:G:17:ARG:HD2	29:G:2446:HOH:O	2.12	0.49
3:C:210:ILE:HG21	19:C:267:PGV:H282	1.95	0.49
25:C:265:PEK:C36	26:G:269:CDL:H271	2.42	0.49
4:D:86:MET:HE2	29:K:4243:HOH:O	2.10	0.49
1:A:351:GLY:C	1:A:380[A]:VAL:HG13	2.38	0.48
4:D:60:TYR:OH	5:E:69:GLU:OE1	2.22	0.48
1:N:53:ILE:HD12	12:Y:44:LEU:HD23	1.95	0.48
21:N:1523:TGL:HC81	2:O:47:THR:HA	1.95	0.48
5:R:41:LEU:HD22	22:R:1229:PSC:H072	1.95	0.48
1:A:310:MET:CE	1:A:356:ILE:HG23	2.43	0.48
1:N:362:SER:HA	2:O:87:MET:HE1	1.94	0.48
1:N:381[A]:LEU:HB2	14:N:516:HEA:CAC	2.43	0.48
7:T:5:LYS:HG3	25:T:263:PEK:C38	2.42	0.48
7:T:72:ASN:H	7:T:76:ASN:ND2	2.06	0.48
1:A:50:ASP:C	1:A:50:ASP:OD1	2.54	0.48
7:G:11:TPO:O	7:G:11:TPO:HG23	2.14	0.48
21:Y:1522:TGL:OC1	21:Y:1522:TGL:CC5	2.61	0.48
1:A:478:SER:O	13:M:6:ALA:HB1	2.13	0.48
22:B:229:PSC:H041	5:E:41:LEU:CD2	2.41	0.48
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.13	0.48
23:C:271:CHD:H112	23:C:271:CHD:H12A	1.61	0.48
19:A:524:PGV:H011	19:A:524:PGV:C2	2.38	0.48
7:G:17:ARG:CD	29:G:2446:HOH:O	2.60	0.48
27:C:272:DMU:H1	7:G:69:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLY:O	7:T:4:ALA:HB1	2.14	0.48
7:G:4:ALA:CB	1:N:282:PHE:HA	2.39	0.48
1:N:248:LEU:O	1:N:251:PHE:HB2	2.13	0.48
7:T:38:HIS:HE1	26:T:1269:CDL:OA7	1.95	0.48
1:A:409:TRP:HB3	1:A:471:ILE:HG12	1.95	0.48
8:H:60:TYR:CD1	8:H:60:TYR:C	2.91	0.48
5:R:41:LEU:HD23	22:R:1229:PSC:H041	1.95	0.48
26:G:269:CDL:H762	26:G:269:CDL:C56	2.25	0.48
1:N:155:VAL:CG2	25:P:1264:PEK:H382	2.44	0.48
1:N:390:MET:O	1:N:394:VAL:HG13	2.13	0.48
4:Q:12:ALA:O	6:S:75:HIS:NE2	2.46	0.48
1:A:406:ASN:HD21	19:A:524:PGV:H21	1.78	0.47
25:C:265:PEK:H362	26:G:269:CDL:C27	2.44	0.47
7:G:5:LYS:HG3	25:G:1263:PEK:C37	2.40	0.47
3:P:22:LEU:O	3:P:26:LEU:HG	2.14	0.47
8:U:60:TYR:CD1	8:U:60:TYR:C	2.92	0.47
21:O:1521:TGL:H301	21:O:1521:TGL:HA82	1.96	0.47
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.97	0.47
6:F:62:CYS:HB3	6:F:85:CYS:HB3	1.96	0.47
1:N:382[A]:SER:O	1:N:383[A]:MET:C	2.58	0.47
1:N:498:CYS:HA	1:N:499:PRO:HA	1.74	0.47
2:B:41:ILE:HD13	22:B:229:PSC:H342	1.97	0.47
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.97	0.47
14:N:515:HEA:H11	14:N:515:HEA:HHC	1.63	0.47
3:P:63:ARG:HE	26:P:1270:CDL:CA2	2.28	0.47
5:R:80:GLU:CD	5:R:80:GLU:N	2.73	0.47
7:T:17:ARG:HD2	29:T:3446:HOH:O	2.13	0.47
2:B:13:THR:HB	2:B:168:LEU:HD23	1.97	0.47
25:C:265:PEK:C36	26:G:269:CDL:C27	2.93	0.47
27:C:272:DMU:H29	27:C:272:DMU:O1	2.15	0.47
10:J:40:LEU:HD12	23:J:60:CHD:H183	1.97	0.47
26:C:270:CDL:HA4	26:C:270:CDL:H131	1.97	0.47
4:D:109:HIS:HD2	29:D:2122:HOH:O	1.97	0.47
1:N:321:PHE:CD2	22:R:1229:PSC:H341	2.49	0.47
22:R:1229:PSC:H212	22:R:1229:PSC:O01	2.15	0.47
7:T:6:GLY:O	7:T:7:ASP:O	2.32	0.47
21:B:521:TGL:H211	21:B:521:TGL:H241	1.59	0.47
10:J:52:TRP:O	10:J:57:HIS:HE1	1.98	0.47
21:Y:1522:TGL:OC1	21:Y:1522:TGL:CC4	2.63	0.47
2:B:196:CYS:CB	2:B:207:MET:HG3	2.45	0.47
26:T:1269:CDL:H732	26:T:1269:CDL:H541	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:36:MET:HG3	10:W:40:LEU:HD12	1.97	0.47
1:A:28:MET:CE	14:A:515:HEA:H271	2.45	0.46
7:G:38:HIS:CE1	26:G:269:CDL:H111	2.50	0.46
13:M:13:LYS:HD2	13:M:13:LYS:C	2.40	0.46
21:Y:1522:TGL:H231	21:Y:1522:TGL:HA92	1.92	0.46
1:A:383[B]:MET:HG2	1:A:421:VAL:HG21	1.95	0.46
25:C:265:PEK:H362	26:G:269:CDL:H272	1.97	0.46
5:E:6:GLU:HB2	5:E:10:GLU:OE1	2.15	0.46
1:N:430:PHE:HE1	21:O:1521:TGL:HB21	1.79	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.97	0.46
23:O:229:CHD:H112	23:O:229:CHD:H12A	1.67	0.46
12:Y:47:LYS:HE3	13:Z:42:LYS:NZ	2.30	0.46
26:P:1270:CDL:H152	26:P:1270:CDL:H202	1.97	0.46
6:S:54:ASN:C	6:S:54:ASN:ND2	2.73	0.46
6:S:94:HIS:CD2	6:S:95:GLN:HA	2.44	0.46
1:A:380[A]:VAL:HG23	1:A:381[A]:LEU:N	2.30	0.46
2:B:66:THR:HG21	23:B:1085:CHD:H42	1.97	0.46
26:C:270:CDL:HA4	26:C:270:CDL:C13	2.45	0.46
27:C:272:DMU:H1	7:G:69:PHE:CZ	2.51	0.46
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.98	0.46
8:U:78:GLU:O	8:U:78:GLU:HG2	2.15	0.46
10:W:4:ARG:HD2	10:W:7:GLU:OE2	2.16	0.46
12:Y:2:HIS:NE2	12:Y:5:GLU:OE1	2.48	0.46
5:E:23:ASP:OD2	5:E:23:ASP:N	2.49	0.46
2:O:65:TRP:O	2:O:69:PRO:HG2	2.15	0.46
4:Q:33:LEU:HA	4:Q:37:GLN:HE21	1.78	0.46
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.46	0.46
3:P:55:TYR:OH	26:P:1270:CDL:H121	2.15	0.46
19:P:1267:PGV:C18	26:P:1270:CDL:H651	2.46	0.46
1:A:379:TYR:CZ	1:A:383[B]:MET:HE1	2.51	0.46
2:B:92:ASN:HA	2:B:93:PRO:HD2	1.87	0.46
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.16	0.46
6:S:1:ALA:H2	25:T:1265:PEK:C04	2.29	0.46
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.80	0.46
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.98	0.46
8:H:43:MET:HE1	8:U:43:MET:CE	2.46	0.46
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.98	0.46
1:N:346:PHE:CE2	21:O:1521:TGL:H271	2.50	0.46
3:P:10:MET:HA	3:P:10:MET:HE2	1.97	0.46
7:T:2:SER:O	25:T:263:PEK:C33	2.62	0.46
1:N:310:MET:HE1	2:O:76:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:1270:CDL:H632	26:P:1270:CDL:H181	1.97	0.45
4:Q:94:LEU:CD2	11:X:28:VAL:HG21	2.46	0.45
1:A:399:LEU:O	1:A:499:PRO:HA	2.17	0.45
4:D:34:SER:H	4:D:37:GLN:NE2	2.14	0.45
23:J:60:CHD:H112	23:J:60:CHD:H12A	1.54	0.45
4:Q:131:ILE:N	4:Q:131:ILE:HD12	2.32	0.45
5:R:23:ASP:OD2	5:R:23:ASP:N	2.34	0.45
1:A:170:ASN:OD1	3:C:77:LYS:HD2	2.17	0.45
5:R:11:PHE:CG	22:R:1229:PSC:H073	2.51	0.45
1:A:40:GLU:HG2	1:A:54:TYR:CD2	2.52	0.45
14:A:516:HEA:HHa	14:A:516:HEA:HAD2	1.79	0.45
25:C:265:PEK:C37	26:G:269:CDL:H271	2.45	0.45
5:R:31:LYS:HD2	5:R:31:LYS:O	2.16	0.45
7:T:3:ALA:O	7:T:4:ALA:HB2	2.16	0.45
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.15	0.45
1:A:1:FME:HE2	12:L:3:TYR:CE1	2.51	0.45
3:C:226:HIS:CE1	26:C:270:CDL:HB31	2.52	0.45
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.98	0.45
29:P:4419:HOH:O	25:T:1265:PEK:H41	2.17	0.45
7:T:17:ARG:CD	29:T:3446:HOH:O	2.65	0.45
1:A:71:MET:N	1:A:72:PRO:CD	2.80	0.45
26:G:269:CDL:C47	29:G:4791:HOH:O	2.64	0.45
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.48	0.45
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.79	0.45
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.99	0.45
1:A:461:SER:HB2	29:A:2700:HOH:O	2.16	0.45
2:B:66:THR:HG21	23:B:1085:CHD:H3	1.97	0.45
4:D:34:SER:H	4:D:37:GLN:HE21	1.65	0.45
21:L:522:TGL:H202	21:L:522:TGL:H231	1.27	0.45
3:P:51:MET:HG3	26:P:1270:CDL:H672	1.99	0.45
26:P:1270:CDL:H652	26:P:1270:CDL:H612	1.98	0.45
25:T:1265:PEK:H6	25:T:1265:PEK:H222	1.99	0.45
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.51	0.45
3:P:63:ARG:HE	26:P:1270:CDL:HA21	1.82	0.45
7:G:3:ALA:O	7:G:4:ALA:HB2	2.16	0.44
13:Z:39:ASN:O	13:Z:43:SER:OG	2.27	0.44
1:N:100:MET:N	3:P:17:PRO:HB3	2.32	0.44
2:O:121:TYR:O	2:O:138:VAL:HA	2.17	0.44
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.00	0.44
19:A:524:PGV:H152	4:D:87:PHE:CZ	2.53	0.44
1:N:310:MET:HE1	2:O:76:ILE:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:7:LEU:HD12	21:O:1521:TGL:HC31	1.98	0.44
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.98	0.44
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.18	0.44
1:N:113:LEU:HD12	21:Y:1522:TGL:H131	1.98	0.44
26:P:1270:CDL:H362	26:P:1270:CDL:H432	1.99	0.44
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.47	0.44
8:H:7:LYS:O	8:H:8:ILE:CB	2.65	0.44
3:C:16:TRP:N	3:C:17:PRO:CD	2.80	0.44
4:D:145:TRP:CG	11:K:46:GLY:H	2.36	0.44
2:B:56:MET:CA	22:B:229:PSC:H201	2.42	0.44
23:C:271:CHD:H232	23:C:271:CHD:H162	1.98	0.44
12:L:2:HIS:CG	12:L:3:TYR:N	2.85	0.44
1:N:179:TYR:CD1	1:N:271:MET:HE1	2.53	0.44
21:N:1523:TGL:H181	2:O:47:THR:HB	2.00	0.44
26:P:1270:CDL:HB32	26:P:1270:CDL:CB2	2.36	0.44
8:U:7:LYS:C	8:U:9:LYS:H	2.26	0.44
1:A:377:PHE:CD1	14:A:516:HEA:HAD1	2.52	0.44
22:B:229:PSC:H212	22:B:229:PSC:C02	2.46	0.44
7:G:84:LYS:NZ	29:G:4536:HOH:O	2.48	0.44
8:H:49:ASP:O	8:H:52:VAL:HG22	2.18	0.44
9:I:54:TYR:OH	9:I:59:ASP:OD1	2.27	0.44
2:O:59:GLN:C	2:O:60:GLU:CG	2.91	0.44
3:P:37:PHE:HD1	29:P:4771:HOH:O	2.00	0.44
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.99	0.44
1:A:486:ASP:HB2	29:A:2142:HOH:O	2.18	0.44
3:C:15:PRO:O	3:C:19:THR:HG23	2.18	0.44
26:G:269:CDL:C11	26:G:269:CDL:CA2	2.95	0.44
1:N:378:HIS:O	1:N:382[A]:SER:HB2	2.18	0.44
8:U:50:VAL:O	8:U:51:SER:C	2.57	0.44
19:A:524:PGV:H12	4:D:87:PHE:CD2	2.53	0.43
9:I:43:ARG:HH11	9:I:43:ARG:HD3	1.62	0.43
11:K:6:ALA:HA	11:K:7:PRO:HD2	1.78	0.43
4:Q:12:ALA:CB	6:S:55:LYS:HE3	2.48	0.43
1:A:28:MET:HE2	14:A:515:HEA:C27	2.48	0.43
22:B:229:PSC:H062	22:B:229:PSC:H042	1.75	0.43
26:G:269:CDL:H182	1:N:307:SER:HB2	2.00	0.43
25:P:1264:PEK:H32	25:P:1264:PEK:C7	2.38	0.43
1:A:34:SER:HB2	14:A:515:HEA:C2B	2.49	0.43
1:A:181:THR:HA	1:A:182:PRO:HD3	1.78	0.43
1:A:383[A]:MET:HE2	1:A:425:PHE:HD1	1.83	0.43
14:A:515:HEA:HBC1	14:A:515:HEA:HMC3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:521:PGV:C18	25:C:264:PEK:H332	2.42	0.43
27:C:272:DMU:H29	27:C:272:DMU:C10	2.47	0.43
1:N:514:LYS:H	6:S:38:ALA:H	1.67	0.43
21:N:1523:TGL:H222	2:O:39:LEU:CD1	2.48	0.43
1:A:408:THR:HB	19:A:524:PGV:H32	2.01	0.43
3:C:109:THR:HB	3:C:110:PRO:CD	2.48	0.43
21:L:522:TGL:HC62	21:L:522:TGL:HC22	1.99	0.43
3:P:165:ILE:HG12	25:T:1265:PEK:H102	2.01	0.43
5:R:107:ASP:OD2	5:R:107:ASP:N	2.45	0.43
8:U:49:ASP:O	8:U:52:VAL:HG13	2.18	0.43
6:F:65:ASP:OD1	6:S:1:ALA:HB3	2.18	0.43
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.53	0.43
1:N:512:ASN:HB2	29:N:4003:HOH:O	2.18	0.43
21:Y:1522:TGL:HA92	21:Y:1522:TGL:C23	2.49	0.43
1:A:450:TRP:HA	1:A:450:TRP:CE3	2.54	0.43
12:L:46:LYS:O	12:L:47:LYS:HB2	2.18	0.43
1:N:473:TRP:CZ3	13:Z:18:GLY:HA3	2.53	0.43
3:P:224:LYS:O	3:P:225:PHE:HB2	2.18	0.43
26:P:1270:CDL:H222	26:P:1270:CDL:H191	1.77	0.43
12:Y:2:HIS:CG	12:Y:3:TYR:N	2.85	0.43
6:F:13:ALA:O	6:F:18:ARG:HD2	2.19	0.43
9:I:51:TYR:HA	9:I:54:TYR:HB2	2.00	0.43
1:N:312:ILE:HG22	1:N:312:ILE:O	2.17	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.19	0.43
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.76	0.43
27:P:272:DMU:H34	7:T:63:GLY:HA2	2.00	0.43
5:R:20:ASN:O	5:R:21:LYS:C	2.62	0.43
1:A:500:PRO:HB2	1:A:504:THR:HG21	2.00	0.43
26:G:269:CDL:H241	26:G:269:CDL:H531	1.99	0.43
5:R:41:LEU:CD2	22:R:1229:PSC:H041	2.48	0.43
5:R:74:LYS:HD2	5:R:74:LYS:HA	1.85	0.43
6:S:1:ALA:N	25:T:1265:PEK:H042	2.33	0.43
1:A:21:LEU:HD23	21:L:522:TGL:HA81	2.00	0.43
1:A:344:PHE:CD2	1:A:384[B]:GLY:O	2.72	0.43
23:B:1085:CHD:H12	23:B:1085:CHD:H212	2.00	0.43
21:D:523:TGL:HB31	21:D:523:TGL:OG1	2.18	0.43
12:Y:11:ILE:CG2	21:Y:1522:TGL:H272	2.48	0.43
23:B:1085:CHD:H112	23:B:1085:CHD:H12A	1.69	0.42
4:Q:109:HIS:CD2	29:Q:3122:HOH:O	2.68	0.42
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.01	0.42
23:J:60:CHD:H211	23:J:60:CHD:H232	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:68:LEU:HD12	2:O:68:LEU:HA	1.73	0.42
4:Q:33:LEU:HD22	4:Q:37:GLN:HB3	2.01	0.42
5:R:11:PHE:CD1	22:R:1229:PSC:H073	2.54	0.42
22:R:1229:PSC:H042	29:R:3664:HOH:O	2.19	0.42
1:A:246:LEU:HD13	1:A:381[A]:LEU:HD11	2.01	0.42
2:B:78:LEU:CD1	26:T:1269:CDL:H352	2.50	0.42
3:C:109:THR:HB	3:C:110:PRO:HD2	1.99	0.42
3:C:202:GLY:HA3	25:C:264:PEK:H21	2.01	0.42
2:O:202:SER:HB3	2:O:203:ASN:HD22	1.84	0.42
4:Q:145:TRP:CG	11:X:46:GLY:H	2.36	0.42
4:Q:7:LYS:HB3	4:Q:8:SER:H	1.68	0.42
26:T:1269:CDL:H581	26:T:1269:CDL:H552	1.94	0.42
10:W:57:HIS:O	10:W:58:LYS:HB2	2.18	0.42
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.48	0.42
1:A:382[B]:SER:OG	14:A:515:HEA:H121	2.20	0.42
1:N:438:ARG:O	1:N:439:ARG:HB2	2.19	0.42
2:O:52:HIS:HE1	22:R:1229:PSC:H02	1.84	0.42
26:P:1270:CDL:CB3	26:P:1270:CDL:CB2	2.85	0.42
7:T:3:ALA:O	7:T:4:ALA:CB	2.67	0.42
7:G:31:CYS:HG	26:G:269:CDL:H532	1.80	0.42
12:L:20:ARG:HH22	21:L:522:TGL:CC5	2.33	0.42
3:P:40:MET:HE2	27:P:272:DMU:H30	2.02	0.42
3:P:106:LEU:HD13	19:U:1268:PGV:H21	2.01	0.42
7:G:3:ALA:O	7:G:4:ALA:CB	2.67	0.42
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	2.02	0.42
1:N:335:SER:HB2	1:N:336:PRO:HD2	2.00	0.42
3:P:40:MET:HE3	3:P:40:MET:HB2	1.69	0.42
5:R:90:ARG:HB3	5:R:91:PRO:CD	2.43	0.42
5:R:94:ASN:O	5:R:95:GLU:C	2.60	0.42
2:B:100:MET:HE3	2:B:157:GLU:HG3	2.00	0.42
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.55	0.42
21:D:523:TGL:HA91	21:D:523:TGL:C24	2.47	0.42
7:T:7:ASP:CG	7:T:8:HIS:H	2.24	0.42
4:D:101:HIS:CD2	4:D:102:TYR:CE2	3.08	0.42
1:N:127:THR:HB	1:N:129:TYR:CE2	2.55	0.42
1:N:514:LYS:HE2	29:S:3514:HOH:O	2.18	0.42
6:F:92:VAL:HG23	6:F:92:VAL:O	2.18	0.41
7:G:9:GLY:HA3	1:N:178:GLN:HE21	1.85	0.41
26:G:269:CDL:H311	26:G:269:CDL:OA7	2.20	0.41
10:J:50:LEU:HD22	10:J:54:SER:OG	2.20	0.41
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:41:LYS:NZ	29:Z:3672:HOH:O	2.53	0.41
1:A:364:ASP:OD2	14:A:516:HEA:O1A	2.38	0.41
1:N:240:HIS:CD2	1:N:240:HIS:C	2.98	0.41
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.02	0.41
21:D:523:TGL:HA52	21:D:523:TGL:HB71	2.01	0.41
12:L:24:MET:SD	21:L:522:TGL:H161	2.60	0.41
1:N:119:GLU:O	12:Y:46:LYS:HE2	2.21	0.41
29:P:4425:HOH:O	7:T:11:TPO:CG2	2.68	0.41
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.51	0.41
1:N:71:MET:HE2	1:N:71:MET:HB3	1.75	0.41
1:N:377:PHE:HA	1:N:380[B]:VAL:HG22	2.02	0.41
8:U:84:LYS:HA	29:U:3538:HOH:O	2.21	0.41
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.88	0.41
1:A:177:SER:H	1:A:180:GLN:HE21	1.68	0.41
23:C:525:CHD:H112	23:C:525:CHD:H12A	1.81	0.41
4:D:39:ALA:O	4:D:42:GLU:HB2	2.21	0.41
26:G:269:CDL:H542	26:G:269:CDL:C24	2.51	0.41
26:G:269:CDL:H782	26:G:269:CDL:H571	2.01	0.41
26:G:269:CDL:H791	26:G:269:CDL:H821	1.50	0.41
1:N:60:ALA:O	1:N:61:HIS:C	2.64	0.41
1:A:382[A]:SER:HB3	14:A:515:HEA:C2C	2.50	0.41
12:L:20:ARG:HH22	21:L:522:TGL:CC6	2.33	0.41
13:M:17:ILE:HD13	13:M:17:ILE:HG21	1.87	0.41
1:N:379:TYR:CZ	1:N:383[B]:MET:HE1	2.55	0.41
2:B:1:FME:HE1	2:B:133:LEU:HD22	2.02	0.41
22:B:229:PSC:H271	22:B:229:PSC:H242	1.01	0.41
8:H:46:LYS:HE2	8:U:8:ILE:HG22	1.99	0.41
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.74	0.41
4:Q:52:SER:HB2	29:Q:4686:HOH:O	2.19	0.41
7:T:3:ALA:HB1	25:T:263:PEK:H383	2.00	0.41
10:W:55:PHE:HA	10:W:56:PRO:HD3	1.83	0.41
1:A:195:LEU:HD23	1:A:245:ILE:HD13	2.02	0.41
1:A:510:TYR:CD1	1:A:510:TYR:C	2.99	0.41
1:A:514:LYS:NZ	29:A:2645:HOH:O	2.34	0.41
1:N:318:VAL:HG22	2:O:65:TRP:HD1	1.85	0.41
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.51	0.41
1:N:334:TRP:CE3	21:N:1523:TGL:HA31	2.56	0.41
5:R:90:ARG:CB	5:R:91:PRO:HD3	2.44	0.41
1:A:190:ILE:CD1	1:A:278:MET:HG2	2.51	0.41
19:A:524:PGV:H012	19:A:524:PGV:C21	2.51	0.41
3:C:155:ASP:C	3:C:155:ASP:OD1	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:92:VAL:O	6:F:92:VAL:CG2	2.69	0.41
10:J:36:MET:HE2	10:J:36:MET:HB2	1.95	0.41
23:J:60:CHD:H161	29:J:4539:HOH:O	2.21	0.41
1:N:66:ILE:HG23	1:N:246:LEU:HD21	2.03	0.41
21:N:1523:TGL:OB1	21:N:1523:TGL:CG3	2.68	0.41
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.85	0.41
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.02	0.41
22:R:1229:PSC:H042	22:R:1229:PSC:H063	1.76	0.41
1:A:514:LYS:HG3	6:F:38:ALA:HB2	2.02	0.41
1:N:103:TRP:O	3:P:21:ALA:HB1	2.21	0.41
2:O:226:MET:O	2:O:227:LEU:O	2.38	0.41
26:P:1270:CDL:HB21	26:P:1270:CDL:CB4	2.51	0.41
7:T:3:ALA:CB	25:T:263:PEK:C38	2.95	0.41
25:T:1265:PEK:H282	25:T:1265:PEK:H311	1.84	0.41
1:A:60:ALA:O	1:A:61:HIS:C	2.64	0.40
1:A:141:ALA:O	1:A:142:SER:C	2.63	0.40
25:C:264:PEK:H32	25:C:264:PEK:C7	2.51	0.40
22:R:1229:PSC:H212	22:R:1229:PSC:C02	2.51	0.40
26:T:1269:CDL:OA7	26:T:1269:CDL:H342	2.21	0.40
22:B:229:PSC:H142	22:B:229:PSC:H341	2.00	0.40
10:J:33:ARG:HG2	23:J:60:CHD:H152	2.01	0.40
19:N:1524:PGV:C01	19:N:1524:PGV:H22	2.52	0.40
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.56	0.40
3:P:226:HIS:CE1	26:P:1270:CDL:HB31	2.57	0.40
7:T:3:ALA:HB3	25:T:263:PEK:H383	2.01	0.40
4:D:92:THR:O	4:D:95:LEU:HB2	2.21	0.40
1:N:37:ILE:HD11	1:N:58:VAL:HA	2.03	0.40
1:N:68:PHE:HA	1:N:72:PRO:HG2	2.03	0.40
1:N:374:VAL:HG13	1:N:378:HIS:CE1	2.56	0.40
2:O:116:LEU:HD13	2:O:226:MET:HG3	2.03	0.40
2:B:98:LYS:HB2	2:B:109:GLU:HB2	2.02	0.40
2:B:164:ALA:O	2:B:194:GLY:HA3	2.21	0.40
21:D:523:TGL:CA9	21:D:523:TGL:H231	2.51	0.40
1:N:34:SER:HB2	14:N:515:HEA:C2B	2.51	0.40
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.54	0.40
4:Q:16:TYR:HB2	4:Q:27:VAL:HG23	2.04	0.40
1:A:240:HIS:O	1:A:241:PRO:C	2.63	0.40
1:A:403:TYR:HA	1:A:480:ARG:O	2.21	0.40
3:C:207:HIS:HD2	3:C:241:TYR:OH	2.05	0.40
4:D:48:TRP:HB2	5:E:96:LEU:O	2.21	0.40
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:240:HIS:CE1	1:N:244:TYR:OH	2.74	0.40
3:P:131:LEU:CD2	26:T:1269:CDL:HB61	2.51	0.40
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.85	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	517/514 (101%)	502 (97%)	15 (3%)	0	100	100
1	N	517/514 (101%)	495 (96%)	22 (4%)	0	100	100
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	30	27
2	O	225/227 (99%)	219 (97%)	5 (2%)	1 (0%)	30	27
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	8 (6%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	100 (97%)	2 (2%)	1 (1%)	12	8
6	F	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	3	1
6	S	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	3	1
7	G	81/85 (95%)	68 (84%)	7 (9%)	6 (7%)	1	0
7	T	81/85 (95%)	67 (83%)	6 (7%)	8 (10%)	0	0
8	H	77/85 (91%)	68 (88%)	3 (4%)	6 (8%)	1	0
8	U	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	1	0
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	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%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3514/3614 (97%)	3356 (96%)	125 (4%)	33 (1%)	14	9

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
8	H	8	ILE
8	H	44	THR
8	H	46	LYS
2	O	60	GLU
5	R	6	GLU
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	37	LEU
7	T	38	HIS
8	U	10	ASN
8	U	45	ALA
8	U	46	LYS
7	G	3	ALA
7	G	37	LEU
7	T	9	GLY
8	U	8	ILE

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Mol	Chain	Res	Type
2	B	60	GLU
6	F	96	LEU
8	H	10	ASN
8	H	43	MET
7	T	5	LYS
7	G	6	GLY
8	H	45	ALA
7	T	6	GLY

5.3.2 Protein sidechains [i](#)

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	430/426 (101%)	420 (98%)	10 (2%)	44	49
1	N	430/426 (101%)	416 (97%)	14 (3%)	33	34
2	B	210/210 (100%)	202 (96%)	8 (4%)	29	29
2	O	210/210 (100%)	197 (94%)	13 (6%)	16	13
3	C	224/226 (99%)	218 (97%)	6 (3%)	39	42
3	P	224/226 (99%)	219 (98%)	5 (2%)	45	50
4	D	128/129 (99%)	122 (95%)	6 (5%)	23	22
4	Q	128/129 (99%)	120 (94%)	8 (6%)	16	13
5	E	92/95 (97%)	86 (94%)	6 (6%)	15	12
5	R	92/95 (97%)	88 (96%)	4 (4%)	26	25
6	F	81/81 (100%)	74 (91%)	7 (9%)	10	6
6	S	81/81 (100%)	77 (95%)	4 (5%)	22	20
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	9
7	T	67/68 (98%)	59 (88%)	8 (12%)	5	3
8	H	71/75 (95%)	64 (90%)	7 (10%)	7	4
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	16
9	I	57/57 (100%)	52 (91%)	5 (9%)	9	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	V	57/57 (100%)	46 (81%)	11 (19%)	1	1
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	26
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	54
11	K	39/46 (85%)	36 (92%)	3 (8%)	12	8
11	X	39/46 (85%)	36 (92%)	3 (8%)	12	8
12	L	39/40 (98%)	36 (92%)	3 (8%)	12	8
12	Y	39/40 (98%)	35 (90%)	4 (10%)	7	4
13	M	37/38 (97%)	34 (92%)	3 (8%)	11	7
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	3
All	All	3048/3082 (99%)	2894 (95%)	154 (5%)	21	19

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	A	180	GLN
1	A	265	LYS
1	A	297	MET
1	A	333	LYS
1	A	369	ASP
1	A	444	PRO
1	A	484	THR
1	A	486	ASP
1	A	512	ASN
2	B	33	LEU
2	B	60	GLU
2	B	61	VAL
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
3	C	17	PRO
3	C	33	MET
3	C	127	LEU
3	C	161	GLN
3	C	180	GLU
3	C	230	ASN
4	D	4	SER

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Mol	Chain	Res	Type
4	D	7	LYS
4	D	20	ARG
4	D	31	LYS
4	D	51	LEU
4	D	131	ILE
5	E	7	THR
5	E	31	LYS
5	E	41	LEU
5	E	70	VAL
5	E	90	ARG
5	E	109	VAL
6	F	37	LYS
6	F	48	LEU
6	F	87	THR
6	F	92	VAL
6	F	94	HIS
6	F	95	GLN
6	F	96	LEU
7	G	8	HIS
7	G	17	ARG
7	G	33	LEU
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	29	CYS
8	H	46	LYS
8	H	52	VAL
8	H	60	TYR
9	I	8	GLN
9	I	26	MET
9	I	29	LEU
9	I	36	LYS
9	I	68	ILE
10	J	30	ILE
10	J	50	LEU
11	K	20	SER
11	K	47	ARG
11	K	54	ARG
12	L	11	ILE
12	L	26	THR

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Mol	Chain	Res	Type
12	L	47	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
1	N	136	LEU
1	N	152	LEU
1	N	169	ILE
1	N	178	GLN
1	N	180	GLN
1	N	278	MET
1	N	297	MET
1	N	333	LYS
1	N	369	ASP
1	N	394	VAL
1	N	484	THR
1	N	495	LEU
1	N	504	THR
1	N	512	ASN
2	O	18	GLU
2	O	33	LEU
2	O	59	GLN
2	O	60	GLU
2	O	61	VAL
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	171	LYS
2	O	217	LYS
2	O	227	LEU
3	P	29	SER
3	P	127	LEU
3	P	159	MET
3	P	180	GLU
3	P	246	ASP
4	Q	5	VAL
4	Q	9	GLU
4	Q	17	VAL
4	Q	50	SER
4	Q	51	LEU
4	Q	141	ASP

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Mol	Chain	Res	Type
4	Q	143	ASN
4	Q	147	LYS
5	R	46	LYS
5	R	70	VAL
5	R	80	GLU
5	R	109	VAL
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	64	GLU
7	T	2	SER
7	T	8	HIS
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
7	T	42	ARG
7	T	74	ARG
7	T	84	LYS
8	U	7	LYS
8	U	52	VAL
8	U	60	TYR
8	U	84	LYS
9	V	2	THR
9	V	8	GLN
9	V	18	ARG
9	V	26	MET
9	V	29	LEU
9	V	36	LYS
9	V	37	PHE
9	V	61	GLU
9	V	65	LYS
9	V	70	GLN
9	V	73	LYS
10	W	50	LEU
11	X	20	SER
11	X	26	VAL
11	X	47	ARG
12	Y	9	LYS
12	Y	20	ARG
12	Y	26	THR
12	Y	47	LYS
13	Z	13	LYS

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Mol	Chain	Res	Type
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	512	ASN
3	C	3	HIS
3	C	56	GLN
3	C	68	GLN
3	C	70	HIS
3	C	76	GLN
3	C	122	HIS
3	C	230	ASN
4	D	29	HIS
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
5	E	78	HIS
5	E	94	ASN
7	G	34	ASN
7	G	76	ASN
8	H	10	ASN
8	H	32	ASN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	43	GLN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	406	ASN
1	N	422	ASN

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Mol	Chain	Res	Type
1	N	512	ASN
2	O	22	HIS
2	O	52	HIS
2	O	91	ASN
2	O	181	GLN
2	O	203	ASN
3	P	50	ASN
3	P	68	GLN
3	P	70	HIS
3	P	76	GLN
4	Q	37	GLN
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	54	ASN
6	S	94	HIS
6	S	95	GLN
6	S	98	HIS
7	T	8	HIS
7	T	41	HIS
7	T	76	ASN
8	U	12	GLN
8	U	31	GLN
8	U	32	ASN
9	V	8	GLN
10	W	57	HIS
13	Z	36	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	O	1	2	8,9,10	1.05	0	8,9,11	4.87	2 (25%)
9	SAC	I	1	9	7,8,9	2.65	2 (28%)	7,9,11	2.10	3 (42%)
9	SAC	V	1	9	7,8,9	3.34	2 (28%)	7,9,11	1.80	2 (28%)
1	FME	N	1	1	8,9,10	0.59	0	8,9,11	5.70	1 (12%)
2	FME	B	1	2	8,9,10	1.91	3 (37%)	8,9,11	7.60	5 (62%)
1	FME	A	1	1	8,9,10	0.59	0	8,9,11	5.13	4 (50%)
7	TPO	T	11	7	8,10,11	3.18	4 (50%)	10,14,16	2.00	3 (30%)
7	TPO	G	11	7	8,10,11	2.96	4 (50%)	10,14,16	1.55	3 (30%)

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

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-OG1	6.97	1.71	1.59
9	V	1	SAC	CA-N	6.07	1.55	1.46
9	V	1	SAC	OAC-C1A	5.84	1.36	1.23
7	G	11	TPO	P-OG1	5.67	1.69	1.59
9	I	1	SAC	OAC-C1A	5.38	1.35	1.23
7	G	11	TPO	P-O1P	4.35	1.64	1.50
9	I	1	SAC	CA-N	3.94	1.52	1.46
7	T	11	TPO	P-O1P	3.78	1.62	1.50
2	B	1	FME	O1-CN	-3.45	1.08	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O2P	2.60	1.64	1.54
2	B	1	FME	CA-N	2.54	1.50	1.46
2	B	1	FME	CG-SD	-2.42	1.68	1.81
7	T	11	TPO	P-O3P	2.36	1.63	1.54
7	T	11	TPO	P-O2P	2.14	1.62	1.54
7	G	11	TPO	CG2-CB	2.00	1.56	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.70	90.98	122.82
1	N	1	FME	CA-N-CN	-15.77	98.57	122.82
1	A	1	FME	CA-N-CN	-13.36	102.27	122.82
2	O	1	FME	CA-N-CN	-13.30	102.36	122.82
1	A	1	FME	CB-CA-N	4.12	118.02	110.52
9	V	1	SAC	C-CA-N	3.91	117.05	109.50
7	T	11	TPO	O3P-P-OG1	3.85	120.87	105.85
2	B	1	FME	CG-CB-CA	-3.71	101.51	112.87
9	I	1	SAC	C-CA-N	3.55	116.34	109.50
7	T	11	TPO	P-OG1-CB	3.36	132.46	123.33
1	A	1	FME	CE-SD-CG	3.07	116.22	100.32
9	I	1	SAC	OG-CB-CA	-3.01	102.83	111.13
2	B	1	FME	C-CA-N	2.96	115.22	109.50
7	G	11	TPO	O2P-P-OG1	2.95	117.36	105.85
7	G	11	TPO	O-C-CA	-2.35	118.74	124.77
2	B	1	FME	O-C-CA	-2.32	118.80	124.77
7	T	11	TPO	O-C-CA	-2.23	119.03	124.77
2	O	1	FME	O1-CN-N	-2.18	119.68	125.32
7	G	11	TPO	P-OG1-CB	2.16	129.20	123.33
2	B	1	FME	CB-CG-SD	-2.11	99.92	113.82
9	V	1	SAC	O-C-CA	-2.10	119.37	124.77
9	I	1	SAC	OAC-C1A-N	2.03	125.57	121.98
1	A	1	FME	O-C-CA	-2.03	119.55	124.77

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

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

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	1	0
9	V	1	SAC	1	0
2	B	1	FME	2	0
1	A	1	FME	2	0
7	T	11	TPO	2	0
7	G	11	TPO	4	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
25	PEK	C	265	-	52,52,52	1.63	6 (11%)	55,57,57	1.64	8 (14%)
21	TGL	N	1523	-	62,62,62	1.47	7 (11%)	65,65,65	1.43	10 (15%)
23	CHD	O	229	-	32,32,32	1.64	5 (15%)	51,51,51	5.57	32 (62%)
27	DMU	C	272	-	34,34,34	1.53	4 (11%)	45,45,45	3.45	25 (55%)
19	PGV	N	1524	-	50,50,50	1.10	2 (4%)	53,56,56	1.31	6 (11%)
25	PEK	P	1264	-	52,52,52	0.93	3 (5%)	55,57,57	1.75	15 (27%)
27	DMU	P	272	-	34,34,34	1.69	5 (14%)	45,45,45	3.40	25 (55%)
15	NO	N	520	14,16	0,1,1	-	-	-	-	-
27	DMU	Z	1526	-	34,34,34	1.12	2 (5%)	45,45,45	3.19	25 (55%)
26	CDL	G	269	-	99,99,99	1.52	12 (12%)	105,111,111	1.54	20 (19%)
26	CDL	C	270	-	99,99,99	1.58	15 (15%)	105,111,111	1.48	17 (16%)
14	HEA	A	515	1	67,67,67	2.16	23 (34%)	81,103,103	1.74	20 (24%)
23	CHD	B	1085	-	32,32,32	1.90	7 (21%)	51,51,51	5.60	35 (68%)
23	CHD	P	1525	-	32,32,32	1.70	8 (25%)	51,51,51	5.51	39 (76%)
25	PEK	T	263	-	52,52,52	1.47	4 (7%)	55,57,57	1.32	7 (12%)
23	CHD	W	1059	-	32,32,32	1.29	3 (9%)	51,51,51	5.28	32 (62%)
23	CHD	C	271	-	32,32,32	0.88	1 (3%)	51,51,51	4.86	34 (66%)
22	PSC	R	1229	-	51,51,51	1.35	3 (5%)	57,59,59	1.31	3 (5%)
23	CHD	P	1271	-	32,32,32	0.89	1 (3%)	51,51,51	4.95	34 (66%)
19	PGV	N	1266	-	50,50,50	1.00	2 (4%)	53,56,56	1.58	11 (20%)
14	HEA	N	516	15,1	67,67,67	1.99	20 (29%)	81,103,103	2.48	35 (43%)
15	NO	A	520	16	0,1,1	-	-	-	-	-
27	DMU	M	526	-	34,34,34	1.11	4 (11%)	45,45,45	3.41	26 (57%)
21	TGL	Y	1522	-	62,62,62	1.75	10 (16%)	65,65,65	2.20	18 (27%)
23	CHD	J	60	-	32,32,32	1.01	0	51,51,51	5.18	35 (68%)
22	PSC	B	229	-	51,51,51	1.22	3 (5%)	57,59,59	1.36	6 (10%)
19	PGV	U	1268	-	50,50,50	1.60	4 (8%)	53,56,56	1.87	10 (18%)
19	PGV	C	267	-	50,50,50	0.90	3 (6%)	53,56,56	1.38	9 (16%)
21	TGL	B	521	-	62,62,62	1.36	6 (9%)	65,65,65	1.91	14 (21%)
25	PEK	G	1263	-	52,52,52	1.34	3 (5%)	55,57,57	1.41	5 (9%)
19	PGV	P	1267	-	50,50,50	0.94	3 (6%)	53,56,56	1.55	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEK	T	1265	-	52,52,52	1.44	5 (9%)	55,57,57	1.53	7 (12%)
21	TGL	D	523	-	62,62,62	1.65	8 (12%)	65,65,65	1.56	13 (20%)
26	CDL	P	1270	-	99,99,99	1.54	12 (12%)	105,111,111	1.71	21 (20%)
19	PGV	A	521	-	50,50,50	1.28	6 (12%)	53,56,56	1.72	14 (26%)
25	PEK	C	264	-	52,52,52	0.92	2 (3%)	55,57,57	1.76	15 (27%)
19	PGV	A	524	-	50,50,50	1.36	3 (6%)	53,56,56	1.64	9 (16%)
21	TGL	O	1521	-	62,62,62	1.42	6 (9%)	65,65,65	1.62	11 (16%)
20	CUA	B	228	2	0,1,1	-	-	-	-	-
21	TGL	L	522	-	62,62,62	1.64	7 (11%)	65,65,65	2.12	16 (24%)
26	CDL	T	1269	-	99,99,99	1.50	12 (12%)	105,111,111	1.55	15 (14%)
14	HEA	A	516	1	67,67,67	2.00	23 (34%)	81,103,103	2.57	34 (41%)
19	PGV	C	268	-	50,50,50	1.43	4 (8%)	53,56,56	1.67	7 (13%)
14	HEA	N	515	1	67,67,67	2.13	21 (31%)	81,103,103	1.86	24 (29%)
23	CHD	C	525	-	32,32,32	1.63	6 (18%)	51,51,51	5.37	38 (74%)
20	CUA	O	228	2	0,1,1	-	-	-	-	-

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
25	PEK	C	265	-	-	25/56/56/56	-
21	TGL	N	1523	-	-	36/65/65/65	-
27	DMU	C	272	-	6/6/10/10	12/19/59/59	0/2/2/2
23	CHD	O	229	-	-	3/9/74/74	0/4/4/4
19	PGV	N	1524	-	-	31/55/55/55	-
27	DMU	P	272	-	6/6/10/10	8/19/59/59	0/2/2/2
25	PEK	P	1264	-	-	28/56/56/56	-
26	CDL	G	269	-	-	61/110/110/110	-
26	CDL	C	270	-	-	58/110/110/110	-
14	HEA	A	515	1	-	7/36/76/76	-
23	CHD	B	1085	-	-	2/9/74/74	0/4/4/4
23	CHD	P	1525	-	1/1/12/12	2/9/74/74	0/4/4/4
25	PEK	T	263	-	-	25/56/56/56	-
23	CHD	W	1059	-	1/1/12/12	6/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	C	271	-	1/1/12/12	4/9/74/74	0/4/4/4
22	PSC	R	1229	-	-	34/55/55/55	-
23	CHD	P	1271	-	1/1/12/12	3/9/74/74	0/4/4/4
19	PGV	N	1266	-	-	14/55/55/55	-
14	HEA	N	516	15,1	-	6/36/76/76	-
27	DMU	M	526	-	4/4/10/10	8/19/59/59	0/2/2/2
21	TGL	Y	1522	-	-	37/65/65/65	-
23	CHD	J	60	-	2/2/12/12	7/9/74/74	0/4/4/4
22	PSC	B	229	-	-	35/55/55/55	-
19	PGV	U	1268	-	-	30/55/55/55	-
19	PGV	C	267	-	-	13/55/55/55	-
21	TGL	B	521	-	-	34/65/65/65	-
25	PEK	G	1263	-	-	26/56/56/56	-
19	PGV	P	1267	-	-	15/55/55/55	-
25	PEK	T	1265	-	-	25/56/56/56	-
21	TGL	D	523	-	-	34/65/65/65	-
26	CDL	P	1270	-	-	67/110/110/110	-
19	PGV	A	521	-	-	10/55/55/55	-
25	PEK	C	264	-	-	25/56/56/56	-
19	PGV	A	524	-	-	35/55/55/55	-
21	TGL	O	1521	-	-	35/65/65/65	-
21	TGL	L	522	-	-	37/65/65/65	-
26	CDL	T	1269	-	-	63/110/110/110	-
14	HEA	A	516	1	-	9/36/76/76	-
19	PGV	C	268	-	-	30/55/55/55	-
14	HEA	N	515	1	-	7/36/76/76	-
23	CHD	C	525	-	-	2/9/74/74	0/4/4/4
27	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2

All (284) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	1522	TGL	OG2-CB1	7.88	1.56	1.34
19	U	1268	PGV	O01-C1	7.26	1.54	1.34
21	L	522	TGL	OG2-CB1	7.25	1.54	1.34
27	P	272	DMU	O16-C6	7.18	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	268	PGV	O01-C1	6.57	1.52	1.34
25	C	265	PEK	O03-C21	6.47	1.52	1.33
14	N	515	HEA	FE-NC	6.42	2.16	1.95
27	C	272	DMU	O16-C6	6.17	1.50	1.40
23	B	1085	CHD	C18-C13	5.92	1.63	1.54
25	C	265	PEK	O01-C1	5.80	1.50	1.34
25	T	1265	PEK	O01-C1	5.73	1.50	1.34
26	P	1270	CDL	OA6-CA5	5.64	1.50	1.34
26	G	269	CDL	OA6-CA5	5.64	1.50	1.34
26	C	270	CDL	OA8-CA7	5.63	1.49	1.33
19	A	524	PGV	O03-C19	5.61	1.49	1.33
26	T	1269	CDL	OA6-CA5	5.58	1.50	1.34
22	R	1229	PSC	O01-C1	5.57	1.50	1.34
25	G	1263	PEK	O03-C21	5.57	1.49	1.33
25	G	1263	PEK	O01-C1	5.55	1.49	1.34
25	T	1265	PEK	O03-C21	5.51	1.49	1.33
14	N	515	HEA	FE-ND	5.47	2.11	1.94
21	D	523	TGL	OG2-CB1	5.46	1.49	1.34
25	T	263	PEK	O03-C21	5.43	1.49	1.33
21	N	1523	TGL	OG2-CB1	5.42	1.49	1.34
21	D	523	TGL	OG1-CA1	5.38	1.49	1.33
26	P	1270	CDL	OA8-CA7	5.32	1.48	1.33
21	O	1521	TGL	OG1-CA1	5.26	1.48	1.33
25	T	263	PEK	C05-C04	5.24	1.71	1.49
21	Y	1522	TGL	OG3-CC1	5.23	1.48	1.33
19	N	1524	PGV	O03-C19	5.20	1.48	1.33
21	D	523	TGL	OB1-CB1	5.20	1.38	1.22
19	U	1268	PGV	O03-C19	5.16	1.48	1.33
23	B	1085	CHD	C10-C5	-5.12	1.47	1.55
26	G	269	CDL	OB6-CB5	5.11	1.48	1.34
26	C	270	CDL	OB8-CB7	5.06	1.48	1.33
26	P	1270	CDL	OB8-CB7	5.01	1.47	1.33
21	B	521	TGL	OG1-CA1	4.97	1.47	1.33
26	G	269	CDL	OA8-CA7	4.96	1.47	1.33
21	O	1521	TGL	OG2-CB1	4.94	1.48	1.34
26	P	1270	CDL	OB6-CB5	4.94	1.48	1.34
21	L	522	TGL	OG1-CA1	4.86	1.47	1.33
26	T	1269	CDL	OB6-CB5	4.84	1.47	1.34
21	N	1523	TGL	OG1-CA1	4.76	1.47	1.33
21	D	523	TGL	OG3-CC1	4.73	1.47	1.33
21	B	521	TGL	OG2-CB1	4.71	1.47	1.34
25	T	263	PEK	O01-C1	4.70	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	1525	CHD	C13-C12	-4.68	1.47	1.54
26	T	1269	CDL	OB8-CB7	4.68	1.47	1.33
22	B	229	PSC	O03-C19	4.62	1.46	1.33
26	C	270	CDL	OB6-CB5	4.54	1.47	1.34
14	A	515	HEA	FE-NA	4.54	2.10	1.95
22	B	229	PSC	O01-C1	4.48	1.46	1.34
26	T	1269	CDL	OA8-CA7	4.46	1.46	1.33
14	A	516	HEA	C11-C3B	4.42	1.56	1.51
19	A	524	PGV	O01-C1	4.41	1.46	1.34
14	A	516	HEA	FE-NA	4.41	2.09	1.95
26	C	270	CDL	OA6-CA5	4.37	1.46	1.34
14	A	515	HEA	C4B-C3B	-4.37	1.37	1.44
19	A	521	PGV	O01-C1	4.30	1.46	1.34
23	O	229	CHD	C18-C13	4.30	1.61	1.54
21	N	1523	TGL	OG3-CC1	4.28	1.45	1.33
14	A	515	HEA	FE-ND	4.26	2.08	1.94
23	W	1059	CHD	C20-C17	4.23	1.61	1.54
22	R	1229	PSC	O03-C19	4.23	1.45	1.33
19	C	268	PGV	O03-C19	4.22	1.45	1.33
14	N	516	HEA	C4D-C3D	-4.21	1.37	1.45
22	R	1229	PSC	C13-C12	4.19	1.55	1.31
14	N	516	HEA	CHD-C1D	4.19	1.46	1.38
14	A	515	HEA	CHA-C1A	4.17	1.46	1.38
14	N	516	HEA	FE-NC	4.17	2.08	1.95
23	O	229	CHD	C13-C14	-4.15	1.48	1.55
19	A	521	PGV	O03-C19	4.14	1.45	1.33
14	A	515	HEA	C1D-ND	-4.11	1.33	1.40
14	A	515	HEA	C1A-C2A	-4.08	1.38	1.45
21	L	522	TGL	C20-CA9	-4.08	1.31	1.51
14	N	515	HEA	CHA-C4D	4.07	1.48	1.39
26	G	269	CDL	OB8-CB7	4.04	1.45	1.33
21	O	1521	TGL	OG3-CC1	4.01	1.45	1.33
14	A	515	HEA	CHC-C1C	3.96	1.48	1.39
21	Y	1522	TGL	OG1-CA1	3.95	1.44	1.33
26	G	269	CDL	C59-C58	-3.94	1.32	1.51
14	N	516	HEA	CHB-C4A	3.92	1.46	1.38
14	A	515	HEA	C4C-NC	-3.90	1.32	1.39
14	A	516	HEA	CHA-C1A	3.88	1.46	1.38
21	Y	1522	TGL	C20-CA9	-3.87	1.32	1.51
14	N	515	HEA	CHD-C1D	3.87	1.46	1.38
14	A	515	HEA	FE-NC	3.86	2.07	1.95
26	C	270	CDL	C18-C17	3.84	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	522	TGL	OG3-CC1	3.82	1.44	1.33
14	A	516	HEA	CMD-C2D	3.82	1.58	1.50
14	A	516	HEA	CHC-C4B	3.81	1.46	1.38
26	C	270	CDL	C59-C58	-3.76	1.33	1.51
14	N	515	HEA	C3A-C4A	-3.76	1.39	1.46
14	N	516	HEA	CHA-C1A	3.75	1.45	1.38
23	C	525	CHD	O12-C12	3.74	1.49	1.43
14	N	515	HEA	CHC-C4B	3.70	1.45	1.38
14	N	516	HEA	C4B-NB	-3.69	1.33	1.40
22	B	229	PSC	C13-C12	3.68	1.52	1.31
14	A	516	HEA	C4C-NC	-3.67	1.32	1.39
25	C	265	PEK	O03-C01	3.67	1.53	1.45
19	N	1266	PGV	O01-C1	3.65	1.44	1.34
26	T	1269	CDL	C62-C61	-3.62	1.33	1.51
21	O	1521	TGL	C10-CB9	-3.62	1.33	1.51
21	O	1521	TGL	C20-CA9	-3.61	1.33	1.51
23	B	1085	CHD	C13-C14	-3.61	1.49	1.55
26	P	1270	CDL	C59-C58	-3.59	1.33	1.51
21	B	521	TGL	C10-CB9	-3.59	1.33	1.51
14	N	516	HEA	CHC-C1C	3.58	1.47	1.39
14	N	515	HEA	CHA-C1A	3.56	1.45	1.38
23	C	525	CHD	C18-C13	3.55	1.60	1.54
14	N	515	HEA	FE-NB	3.54	2.05	1.94
26	T	1269	CDL	C59-C58	-3.54	1.34	1.51
14	N	515	HEA	C1C-NC	-3.50	1.33	1.39
14	N	516	HEA	FE-NB	3.49	2.05	1.94
26	C	270	CDL	C79-C78	-3.49	1.34	1.51
19	C	268	PGV	P-O11	3.49	1.73	1.59
25	C	264	PEK	O01-C1	3.48	1.44	1.34
23	O	229	CHD	C10-C5	-3.47	1.50	1.55
26	G	269	CDL	C42-C41	-3.46	1.34	1.51
14	N	516	HEA	CHD-C4C	3.45	1.47	1.39
19	N	1524	PGV	O01-C1	3.44	1.44	1.34
21	B	521	TGL	OG3-CC1	3.44	1.43	1.33
26	P	1270	CDL	C22-C21	-3.44	1.34	1.51
27	Z	1526	DMU	C3-C4	-3.43	1.43	1.52
26	G	269	CDL	C62-C61	-3.41	1.34	1.51
26	T	1269	CDL	C79-C78	-3.41	1.34	1.51
14	A	516	HEA	C1B-NB	-3.41	1.32	1.38
26	P	1270	CDL	C19-C18	-3.40	1.34	1.51
27	Z	1526	DMU	O16-C6	3.40	1.45	1.40
25	P	1264	PEK	O01-C1	3.39	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	522	TGL	C10-CB9	-3.39	1.34	1.51
21	N	1523	TGL	C10-CB9	-3.37	1.35	1.51
14	N	515	HEA	FE-NA	3.36	2.06	1.95
26	C	270	CDL	C39-C38	-3.35	1.35	1.51
26	C	270	CDL	C62-C61	-3.35	1.35	1.51
21	N	1523	TGL	C20-CA9	-3.34	1.35	1.51
19	N	1266	PGV	O03-C19	3.33	1.43	1.33
21	Y	1522	TGL	C10-CB9	-3.32	1.35	1.51
25	C	265	PEK	P-O12	3.31	1.72	1.59
26	C	270	CDL	C82-C81	-3.31	1.35	1.51
26	P	1270	CDL	C82-C81	-3.30	1.35	1.51
26	G	269	CDL	C39-C38	-3.28	1.35	1.51
14	N	516	HEA	OMA-CMA	3.27	1.29	1.22
14	A	515	HEA	FE-NB	3.27	2.05	1.94
26	P	1270	CDL	C39-C38	-3.27	1.35	1.51
14	A	515	HEA	C3A-C4A	-3.26	1.40	1.46
26	G	269	CDL	C22-C21	-3.26	1.35	1.51
26	T	1269	CDL	C82-C81	-3.26	1.35	1.51
14	A	515	HEA	CHB-C1B	3.24	1.46	1.39
26	G	269	CDL	C19-C18	-3.24	1.35	1.51
26	C	270	CDL	C22-C21	-3.23	1.35	1.51
26	G	269	CDL	C79-C78	-3.23	1.35	1.51
21	D	523	TGL	C15-CC9	-3.22	1.35	1.51
26	P	1270	CDL	C62-C61	-3.22	1.35	1.51
26	T	1269	CDL	C42-C41	-3.21	1.35	1.51
14	N	515	HEA	CHD-C4C	3.20	1.46	1.39
21	N	1523	TGL	C15-CC9	-3.19	1.35	1.51
25	C	265	PEK	P-O11	3.16	1.71	1.59
26	T	1269	CDL	C39-C38	-3.14	1.36	1.51
14	N	516	HEA	C4B-C3B	-3.12	1.39	1.44
14	A	516	HEA	C4B-NB	-3.10	1.34	1.40
14	N	515	HEA	OMA-CMA	3.08	1.28	1.22
26	T	1269	CDL	C19-C18	-3.08	1.36	1.51
23	P	1525	CHD	C6-C5	-3.07	1.48	1.53
26	C	270	CDL	C19-C18	-3.07	1.36	1.51
14	A	515	HEA	CHA-C4D	3.07	1.46	1.39
25	T	1265	PEK	P-O12	3.05	1.71	1.59
21	D	523	TGL	C20-CA9	-3.05	1.36	1.51
23	P	1271	CHD	C20-C17	3.05	1.59	1.54
27	M	526	DMU	C3-C4	-3.05	1.44	1.52
14	A	516	HEA	CHB-C4A	3.05	1.44	1.38
21	Y	1522	TGL	OG2-CG2	3.04	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	1269	CDL	C22-C21	-3.03	1.36	1.51
21	B	521	TGL	C20-CA9	-3.02	1.36	1.51
14	N	516	HEA	C1B-NB	-3.02	1.32	1.38
23	B	1085	CHD	C11-C12	3.01	1.58	1.53
14	A	516	HEA	C3A-C4A	-3.01	1.40	1.46
14	A	516	HEA	FE-NC	3.00	2.05	1.95
23	W	1059	CHD	C11-C9	2.99	1.58	1.53
26	P	1270	CDL	C79-C78	-2.98	1.37	1.51
14	N	515	HEA	CHB-C4A	2.97	1.44	1.38
21	O	1521	TGL	C15-CC9	-2.96	1.37	1.51
14	A	515	HEA	C4A-NA	-2.96	1.34	1.39
14	A	515	HEA	CHB-C4A	2.96	1.44	1.38
26	P	1270	CDL	C42-C41	-2.95	1.37	1.51
26	C	270	CDL	C42-C41	-2.93	1.37	1.51
14	N	516	HEA	C4A-NA	-2.91	1.34	1.39
14	A	516	HEA	CHB-C1B	2.91	1.45	1.39
19	P	1267	PGV	O01-C1	2.89	1.42	1.34
21	L	522	TGL	C15-CC9	-2.89	1.37	1.51
21	Y	1522	TGL	C15-CC9	-2.88	1.37	1.51
25	T	1265	PEK	P-O11	2.87	1.70	1.59
26	G	269	CDL	C82-C81	-2.87	1.37	1.51
14	A	515	HEA	CHD-C1D	2.87	1.44	1.38
14	N	515	HEA	CHC-C1C	2.85	1.45	1.39
19	A	521	PGV	C03-C02	2.84	1.59	1.50
14	N	515	HEA	C3B-C2B	2.79	1.41	1.34
14	N	516	HEA	C1A-C2A	-2.79	1.40	1.45
23	O	229	CHD	C1-C2	-2.78	1.47	1.53
14	A	516	HEA	C1D-ND	-2.77	1.35	1.40
27	P	272	DMU	O5-C6	2.76	1.48	1.41
27	C	272	DMU	O5-C6	2.73	1.48	1.41
14	A	515	HEA	CMC-C2C	2.73	1.56	1.50
14	N	515	HEA	C4B-NB	-2.73	1.35	1.40
21	D	523	TGL	C10-CB9	-2.71	1.38	1.51
19	P	1267	PGV	O03-C19	2.69	1.41	1.33
23	P	1525	CHD	C11-C9	2.66	1.58	1.53
23	W	1059	CHD	C13-C17	2.66	1.60	1.55
21	B	521	TGL	C15-CC9	-2.64	1.38	1.51
23	C	271	CHD	O26-C24	-2.63	1.22	1.30
21	Y	1522	TGL	CG1-CG2	2.63	1.59	1.50
14	A	516	HEA	C1A-C2A	-2.61	1.40	1.45
14	N	516	HEA	C4C-NC	-2.61	1.34	1.39
19	C	267	PGV	O03-C19	2.60	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	1525	CHD	C10-C5	-2.57	1.51	1.55
21	Y	1522	TGL	CG3-CG2	2.56	1.58	1.50
23	C	525	CHD	C13-C12	-2.55	1.50	1.54
19	A	521	PGV	P-O14	-2.55	1.43	1.55
19	A	521	PGV	O01-C02	-2.53	1.40	1.46
23	C	525	CHD	C4-C3	2.52	1.56	1.52
14	A	516	HEA	C4B-C3B	-2.51	1.40	1.44
14	A	516	HEA	C4A-NA	-2.49	1.34	1.39
14	N	515	HEA	CMA-C3A	2.48	1.50	1.45
25	P	1264	PEK	O03-C21	2.48	1.40	1.33
14	N	516	HEA	C1D-C2D	-2.47	1.39	1.44
14	N	516	HEA	FE-NA	2.46	2.03	1.95
14	A	516	HEA	C20-C19	2.46	1.56	1.51
19	A	521	PGV	C01-C02	2.42	1.58	1.50
23	C	525	CHD	C1-C2	-2.38	1.48	1.53
21	L	522	TGL	CC2-CC1	2.37	1.57	1.50
14	A	516	HEA	C1C-NC	-2.37	1.35	1.39
27	P	272	DMU	O5-C4	2.36	1.50	1.44
27	C	272	DMU	O1-C10	2.36	1.47	1.41
27	M	526	DMU	C6-C1	-2.35	1.45	1.52
14	A	515	HEA	C12-C13	2.34	1.61	1.53
27	P	272	DMU	O1-C10	2.33	1.47	1.41
25	C	265	PEK	C22-C21	2.30	1.57	1.50
23	C	525	CHD	C1-C10	-2.28	1.50	1.54
14	N	515	HEA	C4D-C3D	-2.28	1.41	1.45
14	A	515	HEA	C11-C3B	2.27	1.54	1.51
19	U	1268	PGV	C04-C05	2.24	1.58	1.51
14	A	515	HEA	C12-C11	-2.24	1.49	1.53
19	C	267	PGV	C03-C02	2.23	1.57	1.50
26	C	270	CDL	C15-C14	2.22	1.62	1.51
23	O	229	CHD	C6-C7	-2.21	1.48	1.52
14	N	515	HEA	C4B-C3B	-2.21	1.40	1.44
19	C	268	PGV	O04-C19	-2.20	1.15	1.22
23	P	1525	CHD	C16-C17	2.20	1.58	1.54
27	P	272	DMU	O7-C10	2.19	1.47	1.41
23	P	1525	CHD	C13-C14	-2.19	1.51	1.55
23	B	1085	CHD	C8-C7	-2.19	1.49	1.53
19	A	524	PGV	C20-C19	2.18	1.57	1.50
21	Y	1522	TGL	CB2-CB1	2.17	1.57	1.50
25	G	1263	PEK	P-O11	2.16	1.67	1.59
14	A	515	HEA	O2D-CGD	-2.16	1.23	1.30
14	A	516	HEA	CHA-C4D	2.15	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	270	CDL	C17-C16	2.14	1.62	1.51
14	N	516	HEA	CHB-C1B	2.13	1.44	1.39
14	A	516	HEA	FE-NB	2.13	2.01	1.94
14	A	515	HEA	C4D-C3D	-2.12	1.41	1.45
14	N	516	HEA	C14-C15	2.12	1.38	1.33
19	U	1268	PGV	P-O11	2.11	1.67	1.59
14	A	515	HEA	O11-C11	2.09	1.47	1.42
19	P	1267	PGV	P-O14	-2.09	1.45	1.55
25	P	1264	PEK	C2-C1	2.09	1.56	1.50
14	A	516	HEA	C4D-C3D	-2.08	1.41	1.45
23	B	1085	CHD	O12-C12	2.08	1.47	1.43
27	M	526	DMU	O49-C1	-2.08	1.37	1.43
25	C	264	PEK	C2-C1	2.07	1.56	1.50
25	T	263	PEK	O12-C04	2.07	1.53	1.44
14	N	516	HEA	C1C-NC	-2.06	1.35	1.39
21	N	1523	TGL	OB1-CB1	2.06	1.28	1.22
14	N	515	HEA	O2A-CGA	-2.06	1.24	1.30
19	C	267	PGV	O01-C1	2.06	1.40	1.34
23	P	1525	CHD	C11-C12	2.05	1.56	1.53
14	A	516	HEA	CAC-C3C	2.04	1.52	1.47
14	N	515	HEA	CBD-CGD	2.03	1.55	1.50
25	T	1265	PEK	C22-C21	2.02	1.56	1.50
23	B	1085	CHD	C13-C12	-2.01	1.51	1.54
27	M	526	DMU	O16-C6	2.01	1.43	1.40
27	C	272	DMU	C3-C4	-2.01	1.47	1.52
21	D	523	TGL	CB2-CB1	2.01	1.56	1.50
14	A	516	HEA	C1A-NA	-2.01	1.35	1.39
23	P	1525	CHD	O12-C12	2.01	1.46	1.43

All (788) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C6-C5-C10	15.27	128.91	112.66
23	O	229	CHD	C18-C13-C12	-14.12	94.92	109.06
23	C	271	CHD	C10-C9-C8	14.09	127.55	111.84
23	P	1525	CHD	C1-C10-C5	13.37	126.94	107.75
23	O	229	CHD	C14-C13-C12	13.19	119.47	107.42
23	O	229	CHD	C6-C5-C10	12.89	126.37	112.66
23	B	1085	CHD	C1-C10-C5	12.88	126.24	107.75
23	P	1525	CHD	C6-C5-C10	12.81	126.30	112.66
23	C	525	CHD	C6-C5-C10	12.54	126.01	112.66
23	J	60	CHD	C10-C9-C8	12.51	125.79	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C1-C10-C5	12.28	125.38	107.75
23	P	1271	CHD	C10-C9-C8	12.24	125.48	111.84
23	P	1525	CHD	C18-C13-C12	-12.17	96.87	109.06
23	O	229	CHD	C1-C10-C5	11.58	124.36	107.75
23	B	1085	CHD	C18-C13-C12	-11.35	97.70	109.06
23	P	1525	CHD	C4-C3-C2	11.26	124.35	110.62
23	B	1085	CHD	C10-C9-C8	10.98	124.08	111.84
23	P	1525	CHD	C14-C13-C12	10.86	117.34	107.42
23	P	1525	CHD	C17-C13-C12	10.51	127.12	117.67
23	W	1059	CHD	C13-C17-C20	10.44	132.12	119.48
23	W	1059	CHD	C14-C8-C7	10.11	125.27	111.85
23	B	1085	CHD	C17-C13-C12	10.04	126.70	117.67
23	W	1059	CHD	C10-C9-C8	9.95	122.93	111.84
23	J	60	CHD	C13-C17-C20	9.93	131.51	119.48
23	W	1059	CHD	C6-C5-C4	-9.85	99.98	111.23
23	C	525	CHD	C4-C3-C2	9.41	122.10	110.62
23	O	229	CHD	C19-C10-C9	-9.41	98.53	111.18
23	C	525	CHD	C19-C10-C9	-9.34	98.63	111.18
23	B	1085	CHD	C14-C13-C12	9.12	115.75	107.42
23	C	525	CHD	C10-C9-C8	9.09	121.97	111.84
23	P	1525	CHD	C19-C10-C9	-9.07	98.98	111.18
23	C	525	CHD	C11-C12-C13	8.99	120.41	111.26
23	P	1271	CHD	C18-C13-C12	-8.95	100.09	109.06
23	P	1525	CHD	C15-C14-C13	8.79	112.07	103.54
23	P	1271	CHD	C6-C7-C8	8.75	121.06	111.50
23	W	1059	CHD	C15-C14-C13	8.69	111.97	103.54
23	W	1059	CHD	C16-C17-C13	8.67	111.95	103.54
14	A	516	HEA	C3C-C4C-NC	8.65	117.09	109.80
23	W	1059	CHD	C11-C12-C13	8.62	120.03	111.26
23	J	60	CHD	C17-C13-C12	8.56	125.37	117.67
23	J	60	CHD	C18-C13-C12	-8.55	100.49	109.06
23	C	525	CHD	C17-C13-C12	8.55	125.36	117.67
23	O	229	CHD	C10-C9-C8	8.52	121.34	111.84
23	B	1085	CHD	C4-C3-C2	8.48	120.97	110.62
23	C	271	CHD	C15-C14-C8	8.40	129.88	118.36
23	J	60	CHD	C1-C10-C5	8.39	119.79	107.75
23	O	229	CHD	C17-C13-C12	8.28	125.11	117.67
23	W	1059	CHD	C1-C10-C9	-8.26	98.51	111.34
23	C	271	CHD	C6-C5-C10	8.21	121.40	112.66
23	W	1059	CHD	C15-C14-C8	8.19	129.59	118.36
23	P	1525	CHD	C10-C9-C8	8.17	120.95	111.84
23	P	1271	CHD	C14-C13-C12	8.17	114.88	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C16-C17-C13	8.09	111.39	103.54
23	C	525	CHD	C18-C13-C17	-8.04	98.60	111.20
23	B	1085	CHD	C19-C10-C9	-7.99	100.44	111.18
21	Y	1522	TGL	OG2-CB1-CB2	7.97	128.72	111.48
27	M	526	DMU	O1-C9-C8	7.86	123.87	109.70
23	C	271	CHD	C16-C17-C13	7.84	111.15	103.54
23	O	229	CHD	C11-C12-C13	7.84	119.24	111.26
23	C	525	CHD	C13-C17-C20	7.83	128.97	119.48
23	P	1271	CHD	C1-C10-C5	7.81	118.96	107.75
23	C	271	CHD	C18-C13-C12	-7.78	101.27	109.06
23	B	1085	CHD	C5-C4-C3	7.77	124.42	112.71
23	J	60	CHD	C4-C3-C2	7.74	120.06	110.62
23	C	525	CHD	C17-C13-C14	7.72	107.85	100.11
23	J	60	CHD	C6-C5-C10	7.66	120.81	112.66
27	P	272	DMU	O1-C9-C8	7.66	123.50	109.70
23	O	229	CHD	C1-C2-C3	7.62	120.58	110.48
26	P	1270	CDL	OA6-CA5-C11	7.61	127.95	111.48
27	Z	1526	DMU	O1-C10-C5	7.57	125.93	110.37
27	Z	1526	DMU	O1-C9-C8	7.57	123.35	109.70
23	P	1271	CHD	C16-C17-C20	7.55	123.60	112.18
23	P	1271	CHD	C6-C5-C10	7.54	120.68	112.66
27	C	272	DMU	O1-C9-C8	7.48	123.18	109.70
23	P	1271	CHD	C15-C14-C8	7.45	128.58	118.36
27	C	272	DMU	O5-C4-C57	7.40	124.79	106.44
27	M	526	DMU	O1-C10-C5	7.39	125.56	110.37
23	C	271	CHD	C5-C6-C7	7.35	123.14	114.40
27	C	272	DMU	O16-C6-C1	7.34	119.42	108.27
23	J	60	CHD	C11-C12-C13	7.31	118.70	111.26
23	W	1059	CHD	C5-C6-C7	7.28	123.06	114.40
23	W	1059	CHD	C5-C4-C3	7.27	123.67	112.71
23	B	1085	CHD	C6-C7-C8	7.26	119.43	111.50
23	C	525	CHD	C23-C22-C20	-7.24	100.94	114.46
21	L	522	TGL	OG3-CC1-OC1	-7.22	105.58	123.63
23	B	1085	CHD	C18-C13-C17	-7.21	99.91	111.20
23	C	271	CHD	C14-C13-C12	7.07	113.87	107.42
21	B	521	TGL	OG2-CB1-CB2	7.05	126.72	111.48
27	M	526	DMU	O5-C4-C57	7.04	123.89	106.44
19	U	1268	PGV	O03-C19-C20	6.99	133.16	111.83
23	C	271	CHD	C16-C17-C20	6.95	122.69	112.18
23	O	229	CHD	O12-C12-C13	-6.91	99.35	111.02
19	U	1268	PGV	O01-C1-C2	6.89	126.40	111.48
19	C	268	PGV	O03-C19-C20	6.89	132.85	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	1059	CHD	C6-C7-C8	6.88	119.01	111.50
14	N	516	HEA	C27-C19-C20	6.88	127.16	115.23
23	J	60	CHD	C6-C7-C8	6.87	119.01	111.50
23	J	60	CHD	C5-C6-C7	6.83	122.53	114.40
23	C	271	CHD	C1-C10-C5	6.80	117.51	107.75
27	Z	1526	DMU	O5-C6-C1	6.79	124.31	110.37
23	C	271	CHD	C1-C2-C3	6.76	119.44	110.48
23	O	229	CHD	C14-C8-C9	6.76	119.19	109.75
23	P	1271	CHD	C11-C9-C8	6.71	120.83	110.89
23	C	525	CHD	C14-C13-C12	6.71	113.55	107.42
23	P	1271	CHD	C16-C17-C13	6.71	110.05	103.54
23	C	271	CHD	C15-C14-C13	6.69	110.03	103.54
23	W	1059	CHD	C2-C1-C10	6.69	124.03	112.74
23	W	1059	CHD	C9-C10-C5	6.65	117.75	108.51
23	P	1271	CHD	C4-C3-C2	6.64	118.72	110.62
23	J	60	CHD	C14-C8-C7	6.63	120.65	111.85
23	B	1085	CHD	C15-C14-C13	6.61	109.95	103.54
23	P	1271	CHD	C14-C8-C7	6.61	120.62	111.85
27	P	272	DMU	C18-O16-C6	6.60	124.95	113.68
23	P	1271	CHD	C1-C2-C3	6.56	119.17	110.48
23	C	271	CHD	C5-C4-C3	6.51	122.53	112.71
23	C	271	CHD	C4-C5-C10	6.47	119.55	112.66
23	J	60	CHD	C6-C5-C4	-6.47	103.84	111.23
26	T	1269	CDL	OA6-CA5-C11	6.46	125.47	111.48
23	P	1271	CHD	C5-C4-C3	6.46	122.45	112.71
23	J	60	CHD	C5-C4-C3	6.46	122.44	112.71
23	J	60	CHD	C9-C11-C12	6.45	122.73	114.29
23	W	1059	CHD	C1-C2-C3	6.44	119.01	110.48
23	C	271	CHD	C6-C7-C8	6.44	118.53	111.50
23	O	229	CHD	C6-C5-C4	-6.43	103.88	111.23
25	C	265	PEK	O03-C21-C22	6.35	131.19	111.83
23	J	60	CHD	C14-C13-C12	6.33	113.20	107.42
23	O	229	CHD	C15-C14-C8	6.29	126.99	118.36
23	C	271	CHD	C4-C3-C2	6.28	118.28	110.62
23	W	1059	CHD	C1-C10-C5	6.28	116.76	107.75
23	B	1085	CHD	O12-C12-C13	-6.27	100.43	111.02
27	C	272	DMU	O1-C10-C5	6.25	123.21	110.37
27	Z	1526	DMU	C2-C3-C4	6.23	124.74	110.93
23	B	1085	CHD	C14-C8-C9	6.23	118.44	109.75
27	P	272	DMU	O1-C10-C5	6.21	123.12	110.37
23	B	1085	CHD	C17-C13-C14	6.20	106.34	100.11
21	Y	1522	TGL	OG1-CG1-CG2	6.17	126.18	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C1-C10-C9	-6.15	101.80	111.34
23	C	271	CHD	C11-C9-C8	6.11	119.93	110.89
25	T	1265	PEK	O03-C21-C22	6.10	130.44	111.83
23	W	1059	CHD	C6-C5-C10	6.08	119.13	112.66
23	O	229	CHD	C5-C4-C3	6.04	121.81	112.71
21	O	1521	TGL	OG2-CB1-CB2	6.03	124.52	111.48
23	P	1525	CHD	C6-C5-C4	-6.02	104.34	111.23
23	P	1525	CHD	C11-C9-C10	6.01	119.80	113.70
23	W	1059	CHD	C4-C3-C2	6.01	117.95	110.62
23	C	525	CHD	C18-C13-C12	-5.99	103.06	109.06
25	G	1263	PEK	O01-C1-C2	5.99	124.43	111.48
23	W	1059	CHD	C14-C13-C12	5.98	112.88	107.42
27	P	272	DMU	O5-C4-C3	5.95	122.02	109.72
14	A	516	HEA	CMD-C2D-C1D	5.94	134.31	125.03
22	R	1229	PSC	O01-C1-C2	5.91	124.26	111.48
23	P	1271	CHD	C17-C13-C12	5.90	122.97	117.67
23	B	1085	CHD	C6-C5-C4	-5.87	104.52	111.23
23	J	60	CHD	C15-C14-C13	5.86	109.22	103.54
23	J	60	CHD	C1-C2-C3	5.86	118.24	110.48
23	P	1271	CHD	C2-C1-C10	5.84	122.60	112.74
23	O	229	CHD	C9-C8-C7	5.82	119.19	111.86
26	C	270	CDL	OA6-CA5-C11	5.81	124.05	111.48
23	J	60	CHD	C2-C1-C10	5.79	122.52	112.74
23	C	525	CHD	C6-C5-C4	-5.78	104.62	111.23
23	B	1085	CHD	C4-C5-C10	-5.73	106.56	112.66
27	P	272	DMU	O5-C4-C57	5.73	120.64	106.44
23	C	525	CHD	C15-C14-C13	5.72	109.08	103.54
23	C	525	CHD	O3-C3-C4	5.70	121.18	109.84
27	P	272	DMU	C6-C1-C2	5.66	121.91	110.01
27	M	526	DMU	C2-C3-C4	5.65	123.46	110.93
23	B	1085	CHD	C11-C12-C13	5.62	116.98	111.26
23	J	60	CHD	C15-C14-C8	5.61	126.05	118.36
23	O	229	CHD	C11-C9-C8	5.60	119.19	110.89
23	C	271	CHD	C2-C1-C10	5.58	122.16	112.74
21	Y	1522	TGL	CG2-OG2-CB1	5.57	131.12	117.80
27	Z	1526	DMU	O5-C4-C57	5.56	120.22	106.44
23	C	525	CHD	O12-C12-C13	-5.54	101.66	111.02
26	G	269	CDL	OB6-CB5-C51	5.54	123.46	111.48
27	P	272	DMU	O16-C6-C1	5.51	116.65	108.27
23	W	1059	CHD	C4-C5-C10	5.50	118.51	112.66
21	L	522	TGL	CA4-CA3-CA2	-5.49	92.94	113.13
23	P	1271	CHD	C9-C11-C12	5.45	121.42	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	516	HEA	C2D-C1D-ND	5.43	116.08	109.84
14	N	516	HEA	CAD-C3D-C4D	5.43	134.15	124.70
27	C	272	DMU	C18-O16-C6	5.42	122.94	113.68
23	P	1525	CHD	O12-C12-C13	-5.39	101.91	111.02
27	C	272	DMU	C6-O5-C4	5.37	124.21	113.72
27	M	526	DMU	O16-C6-C1	5.33	116.37	108.27
26	G	269	CDL	OA6-CA5-C11	5.33	123.01	111.48
23	O	229	CHD	C4-C3-C2	5.32	117.11	110.62
14	A	516	HEA	C27-C19-C20	5.30	124.43	115.23
25	C	265	PEK	O01-C1-C2	5.28	122.90	111.48
23	C	271	CHD	C19-C10-C9	-5.27	104.09	111.18
23	P	1271	CHD	C15-C14-C13	5.26	108.64	103.54
23	P	1271	CHD	C5-C6-C7	5.24	120.63	114.40
14	N	515	HEA	C13-C12-C11	-5.23	106.03	114.39
27	C	272	DMU	C8-C7-C5	5.21	119.98	110.83
25	C	264	PEK	O01-C1-O02	-5.20	111.55	123.70
23	O	229	CHD	O12-C12-C11	-5.19	98.55	109.12
21	L	522	TGL	OG3-CC1-CC2	5.18	127.64	111.83
23	P	1525	CHD	C18-C13-C14	-5.16	103.11	111.20
27	P	272	DMU	C8-C7-C5	5.14	119.85	110.83
23	O	229	CHD	C17-C13-C14	5.11	105.24	100.11
27	C	272	DMU	C2-C3-C4	5.11	122.25	110.93
23	O	229	CHD	C15-C14-C13	5.10	108.49	103.54
27	M	526	DMU	C8-C7-C5	5.06	119.72	110.83
14	A	516	HEA	CHA-C4D-C3D	-5.06	117.40	124.77
26	T	1269	CDL	OB6-CB5-C51	5.03	122.36	111.48
23	C	525	CHD	C19-C10-C5	-4.96	102.14	110.44
14	N	516	HEA	CAD-C3D-C2D	-4.96	118.58	127.87
23	O	229	CHD	C18-C13-C17	-4.96	103.44	111.20
26	C	270	CDL	OB8-CB7-C71	4.94	126.91	111.83
27	M	526	DMU	C6-O5-C4	4.94	123.36	113.72
23	J	60	CHD	C13-C14-C8	4.93	120.97	114.72
23	W	1059	CHD	C17-C13-C12	4.91	122.09	117.67
21	B	521	TGL	OG3-CC1-CC2	4.91	126.81	111.83
14	A	515	HEA	C13-C12-C11	-4.90	106.56	114.39
21	L	522	TGL	CG2-OG2-CB1	4.90	129.53	117.80
27	C	272	DMU	O1-C9-C11	4.90	118.58	106.44
23	P	1271	CHD	C4-C5-C10	4.88	117.86	112.66
23	P	1271	CHD	C19-C10-C9	-4.88	104.62	111.18
19	C	268	PGV	O01-C1-C2	4.84	121.96	111.48
19	A	524	PGV	O03-C19-C20	4.84	126.60	111.83
23	B	1085	CHD	O7-C7-C6	-4.84	97.82	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	O7-C7-C6	-4.84	97.82	109.86
23	B	1085	CHD	C15-C14-C8	4.83	124.98	118.36
23	C	525	CHD	C11-C9-C10	4.83	118.60	113.70
23	C	525	CHD	C14-C8-C9	4.79	116.44	109.75
25	T	1265	PEK	O03-C21-O04	-4.79	111.66	123.63
19	A	524	PGV	C4-C3-C2	-4.79	95.54	113.13
27	M	526	DMU	O5-C6-C1	4.76	120.16	110.37
23	P	1525	CHD	C11-C9-C8	4.72	117.89	110.89
14	N	516	HEA	C13-C12-C11	-4.70	106.89	114.39
14	N	516	HEA	CMD-C2D-C1D	4.68	132.35	125.03
23	W	1059	CHD	C9-C8-C7	4.68	117.74	111.86
23	O	229	CHD	O7-C7-C6	-4.65	98.30	109.86
23	P	1525	CHD	C1-C10-C9	-4.62	104.17	111.34
23	C	271	CHD	C9-C11-C12	4.60	120.32	114.29
21	B	521	TGL	OG3-CC1-OC1	-4.56	112.23	123.63
19	N	1266	PGV	O01-C1-O02	-4.54	113.08	123.70
27	Z	1526	DMU	C8-C7-C5	4.54	118.80	110.83
21	D	523	TGL	CB3-CB2-CB1	4.53	130.31	113.69
21	Y	1522	TGL	OG1-CA1-CA2	4.53	125.65	111.83
27	C	272	DMU	O7-C3-C2	4.49	118.64	107.23
19	P	1267	PGV	O14-P-O13	4.49	133.32	112.44
23	P	1271	CHD	C21-C20-C17	4.47	119.60	112.88
26	P	1270	CDL	OA8-CA7-C31	4.46	125.44	111.83
21	D	523	TGL	CG2-OG2-CB1	4.44	128.42	117.80
23	P	1525	CHD	C9-C8-C7	4.43	117.44	111.86
23	C	525	CHD	O7-C7-C6	-4.43	98.83	109.86
27	P	272	DMU	O7-C10-C5	4.41	118.94	108.09
23	P	1525	CHD	O7-C7-C6	-4.40	98.91	109.86
27	P	272	DMU	O1-C9-C11	4.38	117.30	106.44
21	O	1521	TGL	OG3-CC1-CC2	4.38	125.19	111.83
23	J	60	CHD	C19-C10-C5	-4.38	103.12	110.44
14	A	516	HEA	C20-C19-C18	-4.38	111.34	121.17
14	N	516	HEA	O2A-CGA-CBA	4.38	127.83	114.00
19	P	1267	PGV	O12-P-O13	-4.37	91.61	108.94
21	Y	1522	TGL	OG1-CA1-OA1	-4.36	112.71	123.63
14	A	516	HEA	C1D-ND-C4D	-4.36	100.04	105.21
27	M	526	DMU	O55-C2-C3	4.36	121.10	109.94
23	W	1059	CHD	C22-C20-C17	4.35	119.34	110.33
27	P	272	DMU	O5-C6-O16	4.35	120.31	110.04
23	P	1525	CHD	C9-C11-C12	4.35	119.98	114.29
14	A	516	HEA	C1D-C2D-C3D	-4.34	102.41	106.98
27	Z	1526	DMU	O16-C6-C1	4.34	114.87	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	1270	CDL	OB8-CB7-C71	4.34	125.06	111.83
27	M	526	DMU	C6-C1-C2	4.32	119.09	110.01
26	T	1269	CDL	OA8-CA7-C31	4.31	124.98	111.83
21	N	1523	TGL	OG3-CC1-CC2	4.31	124.97	111.83
14	A	516	HEA	C3D-C4D-ND	4.30	114.50	110.35
21	B	521	TGL	OG2-CG2-CG3	4.29	123.75	108.34
25	P	1264	PEK	O01-C1-O02	-4.29	113.67	123.70
23	P	1271	CHD	C18-C13-C17	-4.28	104.49	111.20
23	O	229	CHD	C18-C13-C14	-4.26	104.53	111.20
23	J	60	CHD	C22-C20-C17	4.26	119.16	110.33
19	A	521	PGV	O03-C19-C20	4.25	124.79	111.83
27	M	526	DMU	O7-C3-C2	4.25	118.02	107.23
26	P	1270	CDL	CB4-OB6-CB5	-4.24	107.64	117.80
23	B	1085	CHD	C2-C1-C10	4.23	119.88	112.74
25	T	263	PEK	O01-C1-C2	4.23	120.62	111.48
23	W	1059	CHD	C11-C9-C10	4.22	117.98	113.70
27	Z	1526	DMU	O1-C9-C11	4.21	116.87	106.44
23	P	1525	CHD	C18-C13-C17	-4.20	104.62	111.20
27	P	272	DMU	C6-O5-C4	4.16	121.85	113.72
14	N	516	HEA	O2D-CGD-CBD	4.16	127.15	114.00
19	U	1268	PGV	O04-C19-C20	-4.15	107.54	123.78
21	B	521	TGL	CG3-OG3-CC1	4.15	132.29	117.12
21	L	522	TGL	CC3-CC2-CC1	4.14	128.87	113.69
27	C	272	DMU	O5-C6-C1	4.13	118.85	110.37
23	P	1271	CHD	C17-C13-C14	4.13	104.25	100.11
27	M	526	DMU	O1-C9-C11	4.12	116.66	106.44
27	Z	1526	DMU	O5-C4-C3	4.11	118.23	109.72
27	C	272	DMU	C6-C1-C2	4.11	118.66	110.01
19	P	1267	PGV	O03-C19-O04	-4.10	113.37	123.63
25	P	1264	PEK	O03-C01-C02	-4.10	96.58	108.40
23	W	1059	CHD	C21-C20-C17	4.08	119.00	112.88
21	N	1523	TGL	CG3-CG2-CG1	-4.08	102.28	111.78
27	P	272	DMU	C1-C2-C3	4.06	118.91	109.68
23	P	1525	CHD	C5-C4-C3	4.06	118.83	112.71
23	C	525	CHD	C9-C8-C7	4.05	116.96	111.86
14	A	516	HEA	C4C-C3C-C2C	-4.05	102.26	107.30
23	C	525	CHD	C6-C7-C8	4.04	115.91	111.50
21	L	522	TGL	OG2-CB1-CB2	4.03	120.20	111.48
19	N	1524	PGV	C4-C3-C2	-4.03	98.33	113.13
21	Y	1522	TGL	OG3-CC1-CC2	4.02	124.10	111.83
27	C	272	DMU	C7-C8-C9	4.02	117.52	110.23
23	P	1271	CHD	C9-C10-C5	4.01	114.08	108.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	1059	CHD	C11-C9-C8	4.00	116.82	110.89
14	A	515	HEA	C26-C15-C16	4.00	122.17	115.23
27	M	526	DMU	O7-C10-C5	-3.98	98.30	108.09
23	C	271	CHD	C17-C13-C12	3.95	121.22	117.67
23	C	271	CHD	C11-C12-C13	3.95	115.28	111.26
23	C	525	CHD	C11-C9-C8	3.95	116.74	110.89
27	Z	1526	DMU	C7-C8-C9	3.94	117.37	110.23
27	M	526	DMU	C7-C8-C9	3.94	117.37	110.23
14	N	516	HEA	C4C-CHD-C1D	-3.93	117.00	126.25
19	A	521	PGV	C8-C9-C10	-3.93	94.96	113.86
23	O	229	CHD	O3-C3-C4	3.93	117.67	109.84
21	N	1523	TGL	OG3-CC1-OC1	-3.93	113.80	123.63
23	J	60	CHD	C4-C5-C10	3.92	116.83	112.66
14	A	516	HEA	O11-C11-C3B	-3.92	104.07	111.26
23	P	1271	CHD	C13-C17-C20	3.91	124.22	119.48
25	C	265	PEK	O03-C21-O04	-3.91	113.85	123.63
23	P	1525	CHD	C21-C20-C17	3.91	118.75	112.88
23	W	1059	CHD	C9-C11-C12	3.91	119.40	114.29
27	C	272	DMU	O5-C4-C3	3.90	117.79	109.72
23	C	525	CHD	O12-C12-C11	-3.89	101.20	109.12
23	P	1525	CHD	C21-C20-C22	-3.89	104.32	110.34
23	P	1525	CHD	C17-C13-C14	3.88	104.01	100.11
14	N	515	HEA	C12-C11-C3B	3.88	118.19	112.12
14	N	516	HEA	C13-C14-C15	-3.88	118.75	127.62
14	A	515	HEA	O11-C11-C3B	-3.88	104.15	111.26
21	L	522	TGL	CA8-CA7-CA6	-3.86	94.88	114.37
27	C	272	DMU	O61-C57-C4	3.85	124.44	111.33
21	O	1521	TGL	OG1-CA1-CA2	3.83	123.52	111.83
23	J	60	CHD	C11-C9-C8	3.83	116.56	110.89
25	P	1264	PEK	O13-P-O14	3.82	130.21	112.44
26	P	1270	CDL	CA4-OA6-CA5	3.82	126.93	117.80
19	N	1524	PGV	O03-C19-C20	3.80	123.43	111.83
25	T	1265	PEK	O01-C1-C2	3.79	119.68	111.48
23	C	525	CHD	C18-C13-C14	-3.78	105.27	111.20
23	P	1525	CHD	C5-C6-C7	3.78	118.90	114.40
25	P	1264	PEK	C2-C3-C4	3.77	121.59	113.35
23	C	271	CHD	C21-C20-C17	3.76	118.53	112.88
14	A	516	HEA	O1A-CGA-CBA	-3.76	111.16	123.09
27	C	272	DMU	C1-C2-C3	3.76	118.20	109.68
21	O	1521	TGL	CG2-OG2-CB1	3.75	126.77	117.80
23	P	1525	CHD	O3-C3-C4	3.74	117.30	109.84
27	P	272	DMU	C7-C8-C9	3.73	116.99	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C9-C11-C12	3.71	119.15	114.29
19	N	1266	PGV	O03-C19-C20	3.71	123.16	111.83
27	P	272	DMU	O7-C3-C4	3.71	119.21	109.48
21	Y	1522	TGL	OG2-CG2-CG1	3.70	121.61	108.34
26	T	1269	CDL	CB6-CB4-CB3	-3.68	103.21	111.78
14	N	516	HEA	C3B-C4B-NB	3.68	114.07	109.84
27	M	526	DMU	O5-C4-C3	3.66	117.30	109.72
21	N	1523	TGL	OG1-CG1-CG2	3.65	118.93	108.40
27	P	272	DMU	C2-C3-C4	3.65	119.03	110.93
14	N	516	HEA	C3D-C4D-ND	3.64	113.87	110.35
23	C	525	CHD	C22-C20-C17	-3.64	102.79	110.33
22	B	229	PSC	O01-C1-C2	3.63	119.33	111.48
27	Z	1526	DMU	C6-O5-C4	3.63	120.80	113.72
19	P	1267	PGV	O03-C19-C20	3.63	122.89	111.83
23	J	60	CHD	O12-C12-C11	-3.61	101.78	109.12
27	C	272	DMU	O5-C6-O16	3.59	118.53	110.04
23	J	60	CHD	C9-C10-C5	3.59	113.50	108.51
23	O	229	CHD	C5-C6-C7	3.59	118.67	114.40
19	C	268	PGV	O04-C19-C20	-3.59	109.74	123.78
19	N	1266	PGV	O01-C1-C2	3.58	119.24	111.48
23	O	229	CHD	C16-C17-C20	3.58	117.60	112.18
23	B	1085	CHD	O12-C12-C11	-3.58	101.84	109.12
23	C	525	CHD	C5-C4-C3	3.57	118.09	112.71
19	A	521	PGV	O01-C1-C2	3.56	119.19	111.48
14	N	516	HEA	O1D-CGD-CBD	-3.56	111.81	123.09
23	P	1525	CHD	C13-C17-C20	3.55	123.78	119.48
25	P	1264	PEK	O01-C1-C2	3.54	119.13	111.48
23	P	1525	CHD	C16-C17-C20	3.51	117.50	112.18
27	Z	1526	DMU	O7-C10-C5	-3.50	99.47	108.09
23	C	525	CHD	C1-C2-C3	3.49	115.11	110.48
19	A	524	PGV	O03-C19-O04	-3.49	114.90	123.63
23	P	1525	CHD	C11-C12-C13	3.48	114.80	111.26
23	P	1271	CHD	C19-C10-C5	-3.48	104.62	110.44
21	B	521	TGL	OG1-CA1-CA2	3.47	122.42	111.83
23	P	1271	CHD	O12-C12-C11	-3.46	102.07	109.12
14	A	515	HEA	C3D-C4D-ND	3.46	113.70	110.35
25	G	1263	PEK	O03-C01-C02	3.46	118.36	108.40
23	C	525	CHD	O26-C24-C23	3.46	124.92	114.00
19	C	268	PGV	P-O11-C03	3.45	141.11	121.35
21	D	523	TGL	OG1-CA1-CA2	3.45	122.35	111.83
21	Y	1522	TGL	CB3-CB2-CB1	3.44	126.28	113.69
23	C	271	CHD	O7-C7-C6	-3.43	101.32	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C22-C23-C24	-3.43	103.35	112.49
23	B	1085	CHD	C11-C9-C8	3.43	115.97	110.89
14	A	516	HEA	CHC-C4B-NB	3.42	128.60	124.37
25	P	1264	PEK	C03-C02-C01	-3.42	103.82	111.78
26	G	269	CDL	OB8-CB7-OB9	-3.41	115.10	123.63
19	A	524	PGV	O01-C02-C01	3.40	120.54	108.34
25	T	263	PEK	O03-C21-C22	3.39	122.17	111.83
26	P	1270	CDL	C53-C52-C51	-3.39	100.67	113.13
21	O	1521	TGL	OG3-CC1-OC1	-3.38	115.17	123.63
23	P	1271	CHD	C11-C12-C13	3.37	114.69	111.26
25	P	1264	PEK	O01-C02-C01	-3.36	96.31	108.34
14	A	515	HEA	CMC-C2C-C1C	3.35	130.52	125.42
23	O	229	CHD	C11-C9-C10	3.35	117.10	113.70
19	N	1524	PGV	O01-C1-C2	3.35	118.73	111.48
23	B	1085	CHD	C14-C8-C7	3.35	116.29	111.85
27	P	272	DMU	C10-C5-C7	3.34	117.04	110.01
14	N	515	HEA	O2D-CGD-O1D	-3.34	114.73	123.33
25	T	263	PEK	O03-C21-O04	-3.34	115.28	123.63
27	P	272	DMU	O16-C18-C19	3.32	120.64	109.37
25	C	264	PEK	O03-C01-C02	-3.32	98.83	108.40
14	N	516	HEA	C2D-C1D-ND	3.32	113.66	109.84
22	R	1229	PSC	O03-C19-C20	3.31	121.94	111.83
26	T	1269	CDL	OA6-CA5-OA7	-3.31	115.96	123.70
21	D	523	TGL	C10-CB9-CB8	3.31	131.11	114.37
14	N	515	HEA	CHC-C4B-NB	3.31	128.46	124.37
14	N	515	HEA	C21-C20-C19	-3.31	102.22	113.19
22	B	229	PSC	C30-C29-C28	-3.31	97.65	114.37
23	P	1525	CHD	C14-C8-C9	3.31	114.37	109.75
23	P	1525	CHD	C16-C17-C13	3.29	106.73	103.54
23	P	1525	CHD	O12-C12-C11	-3.29	102.43	109.12
27	C	272	DMU	C10-C5-C7	3.28	116.92	110.01
19	U	1268	PGV	O02-C1-C2	-3.28	110.95	123.78
14	N	515	HEA	CAD-C3D-C2D	3.28	134.01	127.87
19	A	521	PGV	O01-C1-O02	-3.27	116.05	123.70
27	M	526	DMU	O3-C5-C7	3.27	118.09	110.38
14	N	516	HEA	O1A-CGA-CBA	-3.26	112.74	123.09
23	C	525	CHD	C19-C10-C1	3.26	113.48	108.31
14	N	515	HEA	O2D-CGD-CBD	3.25	124.28	114.00
23	C	271	CHD	C17-C13-C14	3.24	103.36	100.11
23	B	1085	CHD	C11-C9-C10	3.23	116.98	113.70
19	A	524	PGV	C8-C9-C10	-3.22	98.37	113.86
23	P	1525	CHD	C6-C7-C8	3.22	115.02	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	270	CDL	OB8-CB7-OB9	-3.21	115.59	123.63
25	C	264	PEK	C3-C2-C1	-3.20	101.95	113.69
14	A	515	HEA	C17-C18-C19	-3.20	120.30	127.62
27	Z	1526	DMU	C1-C2-C3	3.20	116.94	109.68
23	O	229	CHD	C16-C17-C13	3.19	106.64	103.54
25	C	264	PEK	C03-C02-C01	-3.19	104.34	111.78
27	C	272	DMU	O7-C3-C4	3.18	117.81	109.48
23	C	271	CHD	C19-C10-C1	-3.18	103.26	108.31
14	N	516	HEA	C1D-ND-C4D	-3.17	101.45	105.21
23	C	271	CHD	C6-C5-C4	-3.17	107.61	111.23
14	A	515	HEA	C3C-C4C-NC	3.17	112.47	109.80
14	N	515	HEA	OMA-CMA-C3A	-3.16	118.48	125.62
26	P	1270	CDL	OA8-CA7-OA9	-3.16	115.72	123.63
21	B	521	TGL	C15-CC9-CC8	3.16	130.34	114.37
23	C	271	CHD	O3-C3-C4	-3.15	103.56	109.84
19	A	521	PGV	C7-C6-C5	-3.15	98.44	114.37
19	C	267	PGV	O12-P-O13	-3.15	96.46	108.94
14	N	515	HEA	CMD-C2D-C1D	3.13	129.92	125.03
14	A	516	HEA	O2D-CGD-CBD	3.12	123.87	114.00
23	J	60	CHD	C11-C9-C10	3.12	116.87	113.70
14	A	516	HEA	C12-C13-C14	-3.12	103.97	112.16
25	G	1263	PEK	O03-C21-C22	3.11	121.32	111.83
14	N	516	HEA	O11-C11-C3B	-3.11	105.56	111.26
22	B	229	PSC	O03-C19-C20	3.11	121.31	111.83
19	N	1524	PGV	O03-C01-C02	3.11	117.35	108.40
14	A	516	HEA	CHD-C1D-ND	-3.10	120.53	124.37
21	B	521	TGL	CG2-OG2-CB1	3.10	125.22	117.80
21	L	522	TGL	OG1-CG1-CG2	3.10	117.34	108.40
26	P	1270	CDL	OA6-CA5-OA7	-3.10	116.45	123.70
25	C	264	PEK	C25-C24-C23	-3.10	98.72	114.37
14	A	516	HEA	O2D-CGD-O1D	-3.09	115.38	123.33
14	N	516	HEA	C1D-C2D-C3D	-3.09	103.73	106.98
14	N	516	HEA	CHD-C1D-C2D	-3.08	118.19	126.95
23	B	1085	CHD	C16-C17-C13	3.08	106.53	103.54
14	A	516	HEA	CHC-C4B-C3B	-3.07	118.06	125.80
14	A	516	HEA	C4C-NC-C1C	-3.07	100.82	105.82
27	Z	1526	DMU	O7-C3-C2	3.07	115.03	107.23
23	J	60	CHD	C16-C17-C20	3.06	116.81	112.18
14	A	515	HEA	C3C-C2C-C1C	-3.05	103.58	107.17
14	N	515	HEA	C2A-C1A-NA	-3.05	107.38	110.32
23	C	525	CHD	C15-C14-C8	3.05	122.54	118.36
14	A	516	HEA	C12-C11-C3B	3.04	116.88	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C5-C6-C7	3.04	118.02	114.40
23	O	229	CHD	C6-C7-C8	3.03	114.81	111.50
14	A	516	HEA	CHA-C4D-ND	3.03	127.68	124.42
14	N	516	HEA	CAD-CBD-CGD	-3.03	105.64	113.67
23	B	1085	CHD	C19-C10-C5	-3.01	105.41	110.44
19	A	521	PGV	O03-C19-O04	-3.00	116.12	123.63
27	M	526	DMU	C31-C28-C25	-3.00	99.21	114.37
25	G	1263	PEK	O01-C1-O02	-2.99	116.71	123.70
23	O	229	CHD	C1-C10-C9	-2.99	106.69	111.34
14	N	516	HEA	CHA-C1A-NA	2.99	127.71	124.45
14	N	516	HEA	CHD-C1D-ND	2.98	128.05	124.37
14	N	515	HEA	C13-C14-C15	-2.98	120.81	127.62
14	N	516	HEA	CHA-C1A-C2A	-2.97	120.18	124.86
26	G	269	CDL	C80-C79-C78	2.96	129.35	114.37
27	M	526	DMU	O55-C2-C1	2.96	117.36	110.38
27	Z	1526	DMU	C10-C5-C7	2.96	116.24	110.01
26	C	270	CDL	C42-C41-C40	2.96	129.31	114.37
26	G	269	CDL	OB6-CB5-OB7	-2.95	116.81	123.70
22	B	229	PSC	C32-C31-C30	-2.94	99.49	114.37
26	G	269	CDL	C83-C82-C81	2.94	129.22	114.37
26	C	270	CDL	OA8-CA7-C31	2.94	120.78	111.83
25	T	263	PEK	C01-O03-C21	2.93	127.83	117.12
14	N	516	HEA	C27-C19-C18	-2.93	116.11	123.63
23	C	271	CHD	O12-C12-C11	-2.92	103.17	109.12
23	P	1525	CHD	C22-C20-C17	-2.92	104.28	110.33
23	W	1059	CHD	C18-C13-C14	-2.91	106.64	111.20
23	B	1085	CHD	C16-C17-C20	2.91	116.58	112.18
23	W	1059	CHD	C18-C13-C12	-2.91	106.14	109.06
25	C	264	PEK	C2-C3-C4	2.91	119.70	113.35
22	R	1229	PSC	O01-C1-O02	-2.90	116.92	123.70
27	Z	1526	DMU	C57-C4-C3	2.90	121.54	113.38
23	P	1525	CHD	C13-C14-C8	2.89	118.38	114.72
27	P	272	DMU	C10-O1-C9	2.89	119.36	113.72
23	C	271	CHD	C14-C8-C7	2.89	115.68	111.85
23	B	1085	CHD	C1-C10-C9	-2.89	106.86	111.34
26	P	1270	CDL	C79-C78-C77	2.88	128.95	114.37
26	T	1269	CDL	OA8-CA7-OA9	-2.88	116.42	123.63
23	J	60	CHD	C18-C13-C14	-2.88	106.69	111.20
14	A	516	HEA	C3B-C4B-NB	2.88	113.15	109.84
25	C	264	PEK	O01-C1-C2	2.87	117.70	111.48
19	C	267	PGV	O03-C19-O04	-2.86	116.48	123.63
21	D	523	TGL	OG1-CA1-OA1	-2.86	116.48	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	515	HEA	C3C-C4C-NC	2.85	112.20	109.80
27	P	272	DMU	O5-C6-C1	2.85	116.23	110.37
19	N	1266	PGV	C23-C22-C21	-2.85	99.96	114.37
19	A	521	PGV	C8-C7-C6	2.85	128.77	114.37
19	N	1524	PGV	O01-C1-O02	-2.85	117.05	123.70
19	C	267	PGV	C30-C29-C28	-2.84	100.01	114.37
26	T	1269	CDL	C43-C42-C41	2.83	128.66	114.37
19	A	521	PGV	C23-C22-C21	-2.82	100.09	114.37
19	C	267	PGV	O14-P-O12	2.82	120.35	107.57
14	A	515	HEA	C4D-C3D-C2D	-2.78	102.84	106.89
23	C	525	CHD	C15-C16-C17	2.76	110.55	105.14
14	N	516	HEA	CAA-C2A-C1A	2.76	130.46	124.85
21	L	522	TGL	CB4-CB3-CB2	-2.76	103.00	113.13
23	B	1085	CHD	C18-C13-C14	-2.75	106.89	111.20
26	P	1270	CDL	OB8-CB7-OB9	-2.75	116.75	123.63
27	C	272	DMU	O16-C18-C19	2.75	118.70	109.37
21	L	522	TGL	C22-C21-C20	-2.75	100.49	114.37
25	G	1263	PEK	C01-O03-C21	2.74	127.15	117.12
27	M	526	DMU	O7-C10-O1	-2.74	103.47	110.69
21	Y	1522	TGL	OG2-CG2-CG3	2.74	118.18	108.34
26	T	1269	CDL	OB5-PB2-OB3	-2.74	98.08	108.94
27	C	272	DMU	C10-O1-C9	2.73	119.06	113.72
14	A	515	HEA	O2A-CGA-CBA	2.73	122.62	114.00
25	C	264	PEK	C01-O03-C21	2.73	127.09	117.12
27	P	272	DMU	O55-C2-C3	-2.73	102.94	109.94
19	A	521	PGV	C9-C8-C7	2.73	128.15	114.37
27	Z	1526	DMU	C11-C9-C8	2.72	119.70	113.02
14	N	515	HEA	C3D-C4D-ND	2.72	112.98	110.35
23	B	1085	CHD	O26-C24-C23	2.72	122.59	114.00
26	G	269	CDL	CA6-OA8-CA7	2.71	127.02	117.12
27	P	272	DMU	O7-C10-O1	2.70	117.80	110.69
25	T	263	PEK	C2-C3-C4	2.69	119.23	113.35
23	O	229	CHD	C19-C10-C5	-2.69	105.94	110.44
14	N	515	HEA	C26-C15-C16	2.68	119.89	115.23
23	C	271	CHD	C23-C22-C20	-2.68	109.45	114.46
14	N	516	HEA	C3A-C2A-C1A	-2.68	104.51	107.05
14	N	515	HEA	CHA-C4D-C3D	-2.68	120.87	124.77
26	C	270	CDL	OA6-CA5-OA7	-2.67	117.45	123.70
25	C	264	PEK	C32-C31-C30	-2.67	100.85	114.37
21	O	1521	TGL	CG3-OG3-CC1	2.67	126.89	117.12
21	B	521	TGL	CG1-OG1-CA1	2.67	126.89	117.12
23	C	525	CHD	C1-C10-C9	-2.67	107.19	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	OA6-CA4-CA6	2.67	117.92	108.34
14	A	515	HEA	C21-C20-C19	-2.67	104.34	113.19
25	P	1264	PEK	O11-P-O14	-2.67	98.36	108.94
21	O	1521	TGL	CG1-OG1-CA1	2.67	126.86	117.12
21	Y	1522	TGL	OG2-CB1-OB1	-2.66	117.48	123.70
21	N	1523	TGL	CG3-OG3-CC1	2.66	126.85	117.12
19	N	1524	PGV	O03-C19-O04	-2.66	116.97	123.63
21	Y	1522	TGL	OG3-CC1-OC1	-2.66	116.98	123.63
19	A	524	PGV	O03-C01-C02	2.66	116.06	108.40
27	M	526	DMU	C22-C19-C18	-2.65	101.94	113.47
27	M	526	DMU	O4-C7-C5	-2.65	104.13	110.38
27	M	526	DMU	C1-C2-C3	2.64	115.68	109.68
27	M	526	DMU	C10-C5-C7	2.64	115.56	110.01
26	C	270	CDL	C18-C17-C16	-2.64	101.04	114.37
14	N	515	HEA	CAD-C3D-C4D	-2.63	120.11	124.70
25	T	263	PEK	O01-C1-O02	-2.63	117.55	123.70
14	A	516	HEA	CMC-C2C-C1C	2.63	129.42	125.42
14	A	515	HEA	C26-C15-C14	-2.62	116.90	123.63
27	M	526	DMU	O49-C1-C2	2.62	116.54	110.38
23	J	60	CHD	O7-C7-C6	-2.61	103.37	109.86
23	P	1271	CHD	C6-C5-C4	-2.61	108.25	111.23
21	L	522	TGL	OG1-CA1-CA2	2.61	119.78	111.83
27	Z	1526	DMU	O3-C5-C7	2.60	116.51	110.38
26	G	269	CDL	OA8-CA7-C31	2.60	119.75	111.83
23	P	1525	CHD	C2-C1-C10	2.60	117.12	112.74
25	T	1265	PEK	O03-C01-C02	2.59	115.87	108.40
27	M	526	DMU	C11-C9-C8	2.59	119.37	113.02
14	N	515	HEA	CHB-C1B-NB	-2.58	121.64	124.42
21	L	522	TGL	C26-C25-C24	-2.58	101.31	114.37
19	A	521	PGV	C6-C5-C4	-2.58	101.33	114.37
23	P	1525	CHD	C1-C2-C3	2.58	113.89	110.48
21	O	1521	TGL	OG2-CB1-OB1	-2.57	117.69	123.70
27	Z	1526	DMU	O16-C18-C19	2.57	118.07	109.37
21	N	1523	TGL	OG1-CA1-CA2	2.56	119.65	111.83
21	Y	1522	TGL	OB1-CB1-CB2	-2.55	113.80	123.78
21	B	521	TGL	CC3-CC2-CC1	2.54	123.01	113.69
27	Z	1526	DMU	O5-C6-O16	2.54	116.05	110.04
14	N	516	HEA	CHA-C4D-C3D	-2.54	121.08	124.77
25	C	265	PEK	O12-C04-C05	2.53	118.44	109.17
23	W	1059	CHD	C19-C10-C1	-2.52	104.30	108.31
14	A	516	HEA	CHD-C4C-C3C	-2.52	116.44	127.37
19	C	268	PGV	O03-C19-O04	-2.51	117.34	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	272	DMU	C11-C9-C8	2.51	119.19	113.02
25	P	1264	PEK	O04-C21-C22	2.51	133.59	123.78
19	A	524	PGV	O14-P-O13	2.50	124.09	112.44
14	N	516	HEA	CHC-C4B-C3B	-2.50	119.49	125.80
21	D	523	TGL	OG2-CB1-CB2	-2.50	106.07	111.48
21	L	522	TGL	CA9-CA8-CA7	-2.50	101.75	114.37
25	C	265	PEK	C24-C23-C22	2.50	122.30	113.13
14	A	515	HEA	CAA-CBA-CGA	-2.49	107.05	113.67
21	L	522	TGL	C15-CC9-CC8	2.49	126.97	114.37
23	P	1271	CHD	C23-C22-C20	-2.49	109.81	114.46
23	C	271	CHD	C18-C13-C17	-2.49	107.30	111.20
14	N	515	HEA	CHD-C1D-ND	-2.49	121.29	124.37
26	T	1269	CDL	C82-C81-C80	2.49	126.93	114.37
14	A	516	HEA	CBC-CAC-C3C	-2.49	115.11	127.53
22	B	229	PSC	O01-C1-O02	-2.48	117.91	123.70
21	O	1521	TGL	C15-CC9-CC8	2.47	126.88	114.37
21	L	522	TGL	OG2-CG2-CG1	2.47	117.21	108.34
14	N	516	HEA	O11-C11-C12	2.47	115.69	109.14
26	P	1270	CDL	OB6-CB5-C51	2.47	116.81	111.48
26	G	269	CDL	OA6-CA5-OA7	-2.46	117.95	123.70
26	G	269	CDL	CB2-C1-CA2	-2.46	105.57	112.65
21	D	523	TGL	C11-C10-CB9	2.45	126.76	114.37
26	P	1270	CDL	OB4-PB2-OB3	2.45	123.83	112.44
26	G	269	CDL	C82-C81-C80	2.44	126.72	114.37
27	Z	1526	DMU	O7-C10-O1	-2.44	104.26	110.69
23	W	1059	CHD	C19-C10-C5	-2.44	106.36	110.44
26	P	1270	CDL	OA8-CA6-CA4	2.44	115.43	108.40
26	C	270	CDL	O1-C1-CA2	-2.44	101.28	109.70
14	A	516	HEA	OMA-CMA-C3A	-2.44	120.12	125.62
26	G	269	CDL	OB8-CB7-C71	2.43	119.25	111.83
14	A	516	HEA	C13-C14-C15	-2.42	122.09	127.62
14	A	516	HEA	CHB-C4A-NA	-2.41	121.83	124.45
14	A	516	HEA	CAA-CBA-CGA	-2.41	107.27	113.67
19	P	1267	PGV	C7-C6-C5	-2.40	102.23	114.37
14	A	515	HEA	CHD-C1D-ND	-2.40	121.40	124.37
19	U	1268	PGV	O01-C02-C01	2.40	116.94	108.34
26	C	270	CDL	O1-C1-CB2	2.40	117.97	109.70
14	N	516	HEA	CHC-C1C-C2C	-2.39	120.49	127.43
22	B	229	PSC	C27-C26-C25	-2.39	102.30	114.37
21	Y	1522	TGL	CG3-OG3-CC1	2.39	125.85	117.12
26	P	1270	CDL	C42-C41-C40	2.38	126.42	114.37
23	P	1525	CHD	O26-C24-C23	2.38	121.53	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	1522	TGL	C15-CC9-CC8	2.38	126.39	114.37
26	C	270	CDL	CA6-OA8-CA7	2.38	125.81	117.12
23	J	60	CHD	C9-C8-C7	2.38	114.85	111.86
26	T	1269	CDL	OB8-CB7-OB9	-2.38	117.68	123.63
19	C	268	PGV	O01-C02-C03	2.37	116.86	108.34
14	N	515	HEA	C4A-C3A-C2A	-2.37	104.76	106.81
14	A	516	HEA	CMB-C2B-C3B	-2.37	125.69	130.28
23	C	525	CHD	C9-C11-C12	2.37	117.39	114.29
25	C	265	PEK	O13-P-O11	2.36	118.25	107.57
21	D	523	TGL	CC4-CC3-CC2	-2.35	104.49	113.13
21	Y	1522	TGL	C26-C25-C24	-2.35	102.49	114.37
25	C	264	PEK	C26-C25-C24	-2.35	102.50	114.37
14	A	515	HEA	O1A-CGA-CBA	-2.34	115.66	123.09
21	B	521	TGL	OB1-CB1-CB2	-2.34	114.62	123.78
21	L	522	TGL	OB1-CB1-CB2	-2.34	114.63	123.78
14	A	516	HEA	CBD-CAD-C3D	2.34	118.99	112.53
23	O	229	CHD	C2-C1-C10	2.33	116.68	112.74
19	C	267	PGV	O14-P-O13	2.33	123.29	112.44
25	C	264	PEK	O13-P-O14	2.33	123.28	112.44
19	A	524	PGV	C8-C7-C6	-2.32	102.65	114.37
19	N	1266	PGV	C6-C5-C4	-2.32	102.66	114.37
19	P	1267	PGV	C03-C02-C01	-2.32	106.39	111.78
25	C	265	PEK	P-O11-C03	2.31	134.60	121.35
21	N	1523	TGL	OG1-CA1-OA1	-2.31	117.86	123.63
14	N	516	HEA	C2B-C1B-NB	2.31	112.57	109.90
19	N	1266	PGV	O14-P-O12	-2.30	97.12	107.57
19	N	1266	PGV	C15-C14-C13	-2.30	102.82	113.86
21	D	523	TGL	OG2-CG2-CG3	2.30	116.58	108.34
25	P	1264	PEK	C33-C32-C31	-2.29	102.80	114.37
19	N	1266	PGV	O03-C19-O04	-2.28	117.93	123.63
26	G	269	CDL	O1-C1-CB2	2.28	117.57	109.70
19	C	267	PGV	O03-C19-C20	2.28	118.78	111.83
26	C	270	CDL	OB4-PB2-OB3	2.28	123.04	112.44
21	N	1523	TGL	OG2-CG2-CG3	2.28	116.51	108.34
26	C	270	CDL	C83-C82-C81	2.27	125.86	114.37
26	C	270	CDL	C39-C38-C37	2.27	125.85	114.37
19	A	524	PGV	C02-O01-C1	2.27	123.23	117.80
19	C	268	PGV	O02-C1-C2	-2.27	114.90	123.78
26	C	270	CDL	C53-C52-C51	-2.27	104.79	113.13
21	D	523	TGL	C20-CA9-CA8	2.27	125.83	114.37
14	N	516	HEA	CHD-C4C-NC	2.27	127.97	123.86
25	P	1264	PEK	C24-C23-C22	-2.27	104.80	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	521	TGL	OG1-CG1-CG2	-2.27	101.86	108.40
14	A	515	HEA	C3B-C4B-NB	2.26	112.43	109.84
25	C	265	PEK	O04-C21-C22	-2.25	114.96	123.78
26	P	1270	CDL	C54-C53-C52	-2.25	102.97	114.37
19	N	1266	PGV	O01-C02-C01	-2.25	100.26	108.34
14	A	515	HEA	OMA-CMA-C3A	-2.25	120.54	125.62
25	C	264	PEK	O03-C21-O04	-2.25	118.01	123.63
19	A	521	PGV	C15-C14-C13	-2.25	103.06	113.86
23	P	1525	CHD	C19-C10-C5	-2.24	106.69	110.44
23	B	1085	CHD	C23-C22-C20	-2.24	110.27	114.46
21	N	1523	TGL	OG2-CB1-CB2	2.24	116.33	111.48
14	N	516	HEA	C1A-CHA-C4D	-2.24	121.26	126.02
27	Z	1526	DMU	O55-C2-C3	2.24	115.67	109.94
26	T	1269	CDL	CA4-OA6-CA5	2.24	123.15	117.80
26	T	1269	CDL	C39-C38-C37	2.23	125.66	114.37
26	P	1270	CDL	C56-C55-C54	-2.23	103.08	114.37
21	B	521	TGL	OG2-CB1-OB1	-2.23	118.49	123.70
23	C	525	CHD	C2-C1-C10	2.23	116.50	112.74
26	T	1269	CDL	CB6-OB8-CB7	2.22	125.24	117.12
21	Y	1522	TGL	C10-CB9-CB8	2.22	125.58	114.37
27	Z	1526	DMU	C6-C1-C2	2.22	114.67	110.01
27	Z	1526	DMU	O7-C3-C4	2.22	115.29	109.48
26	G	269	CDL	C23-C22-C21	2.22	125.57	114.37
21	D	523	TGL	C13-C12-C11	2.21	125.56	114.37
21	D	523	TGL	CB5-CB4-CB3	2.21	125.53	114.37
26	T	1269	CDL	C20-C19-C18	2.21	125.53	114.37
21	D	523	TGL	C21-C20-CA9	2.20	125.50	114.37
23	B	1085	CHD	C13-C14-C8	2.19	117.50	114.72
14	N	516	HEA	CHB-C1B-C2B	-2.19	121.57	125.03
23	P	1525	CHD	C4-C5-C10	-2.19	110.33	112.66
23	C	525	CHD	O7-C7-C8	-2.19	104.51	109.52
14	N	515	HEA	O1A-CGA-CBA	-2.18	116.17	123.09
26	G	269	CDL	CB6-CB4-CB3	-2.18	106.70	111.78
25	P	1264	PEK	C3-C2-C1	-2.18	105.71	113.69
21	N	1523	TGL	C21-C20-CA9	2.17	125.36	114.37
26	P	1270	CDL	C40-C39-C38	2.17	125.36	114.37
25	C	264	PEK	C35-C34-C33	-2.17	103.38	114.37
27	C	272	DMU	O7-C10-C5	2.17	113.44	108.09
26	C	270	CDL	C22-C21-C20	2.17	125.35	114.37
27	P	272	DMU	O7-C3-C2	2.16	112.73	107.23
26	G	269	CDL	OA8-CA6-CA4	2.16	114.62	108.40
19	P	1267	PGV	C4-C3-C2	-2.16	105.20	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	O12-C12-C13	-2.15	107.39	111.02
19	N	1266	PGV	C04-C05-C06	-2.15	104.53	111.77
19	U	1268	PGV	C29-C28-C27	2.15	125.21	114.37
27	C	272	DMU	O55-C2-C3	2.14	115.43	109.94
27	Z	1526	DMU	O61-C57-C4	2.14	118.61	111.33
23	P	1271	CHD	C1-C10-C9	-2.13	108.03	111.34
23	C	271	CHD	C19-C10-C5	-2.13	106.87	110.44
25	P	1264	PEK	C37-C36-C35	-2.13	96.58	115.25
26	C	270	CDL	C57-C56-C55	-2.13	103.62	114.37
14	A	516	HEA	CMB-C2B-C1B	2.13	128.36	125.03
23	C	271	CHD	C22-C20-C17	-2.12	105.93	110.33
27	P	272	DMU	O49-C1-C2	-2.12	105.37	110.38
23	J	60	CHD	C14-C8-C9	2.12	112.71	109.75
25	C	264	PEK	C11-C10-C9	2.11	122.44	112.02
14	A	515	HEA	CAD-CBD-CGD	-2.11	108.06	113.67
19	C	267	PGV	O03-C01-C02	-2.11	102.32	108.40
26	P	1270	CDL	CA6-CA4-CA3	-2.10	106.88	111.78
27	C	272	DMU	C11-C9-C8	2.10	118.19	113.02
19	A	521	PGV	C5-C4-C3	-2.10	103.74	114.37
27	C	272	DMU	O2-C8-C7	-2.10	105.42	110.38
21	O	1521	TGL	OG2-CG2-CG3	2.10	115.88	108.34
25	T	1265	PEK	C24-C23-C22	2.10	120.84	113.13
19	N	1266	PGV	C26-C25-C24	2.10	124.97	114.37
26	G	269	CDL	C85-C84-C83	2.10	124.97	114.37
26	T	1269	CDL	C83-C82-C81	2.10	124.96	114.37
26	P	1270	CDL	OA7-CA5-C11	-2.10	115.59	123.78
14	N	516	HEA	C16-C15-C14	2.09	125.87	121.17
14	A	516	HEA	O2A-CGA-O1A	2.09	128.72	123.33
25	T	1265	PEK	C35-C34-C33	-2.09	103.80	114.37
14	N	515	HEA	CHC-C1C-NC	-2.08	120.08	123.86
25	C	264	PEK	C24-C23-C22	-2.08	105.48	113.13
25	P	1264	PEK	O03-C21-C22	-2.08	105.49	111.83
23	B	1085	CHD	O25-C24-C23	-2.08	116.50	123.09
25	T	1265	PEK	C2-C3-C4	-2.07	108.82	113.35
21	O	1521	TGL	OG2-CG2-CG1	2.07	115.77	108.34
19	A	521	PGV	C25-C24-C23	-2.07	103.91	114.37
26	P	1270	CDL	C20-C19-C18	2.07	124.82	114.37
26	P	1270	CDL	C55-C54-C53	-2.07	103.92	114.37
19	P	1267	PGV	C22-C21-C20	-2.06	105.55	113.13
14	A	515	HEA	C16-C17-C18	2.06	122.22	112.02
14	A	515	HEA	CHA-C1A-C2A	2.06	128.12	124.86
14	N	515	HEA	CHC-C4B-C3B	-2.06	120.61	125.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	U	1268	PGV	C24-C23-C22	2.06	124.77	114.37
21	B	521	TGL	C16-C15-CC9	2.05	124.75	114.37
14	N	515	HEA	C4C-C3C-C2C	-2.05	104.75	107.30
19	C	267	PGV	C21-C20-C19	-2.05	106.18	113.69
25	P	1264	PEK	C35-C34-C33	-2.05	104.03	114.37
19	U	1268	PGV	O05-C05-C06	-2.04	100.72	109.18
23	W	1059	CHD	O26-C24-C23	2.04	120.45	114.00
21	Y	1522	TGL	C16-C15-CC9	2.04	124.68	114.37
19	C	267	PGV	O01-C1-O02	-2.04	118.95	123.70
26	C	270	CDL	C80-C79-C78	2.04	124.66	114.37
21	Y	1522	TGL	CG3-CG2-CG1	-2.03	107.04	111.78
26	G	269	CDL	CB6-OB8-CB7	2.03	124.55	117.12
14	A	516	HEA	C4B-C3B-C2B	-2.03	104.03	107.44
14	N	516	HEA	C20-C19-C18	-2.03	116.61	121.17
19	U	1268	PGV	C15-C14-C13	2.03	123.59	113.86
26	G	269	CDL	C62-C61-C60	2.02	124.60	114.37
25	T	263	PEK	O03-C01-C02	2.02	114.23	108.40
19	U	1268	PGV	C01-O03-C19	2.02	124.50	117.12
23	P	1271	CHD	C19-C10-C1	-2.02	105.10	108.31
19	A	521	PGV	O06-C06-C05	-2.01	101.32	110.38
27	M	526	DMU	O49-C1-C6	2.01	114.86	110.08
14	N	515	HEA	C1B-C2B-C3B	-2.00	104.47	106.80

All (27) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	C	271	CHD	C9
23	J	60	CHD	C9
23	J	60	CHD	C17
23	P	1525	CHD	C9
23	P	1271	CHD	C9
23	W	1059	CHD	C17
27	C	272	DMU	C9
27	C	272	DMU	C3
27	C	272	DMU	C4
27	C	272	DMU	C6
27	C	272	DMU	C2
27	C	272	DMU	C5
27	M	526	DMU	C4
27	M	526	DMU	C5
27	M	526	DMU	C2
27	M	526	DMU	C9

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Mol	Chain	Res	Type	Atom
27	P	272	DMU	C9
27	P	272	DMU	C4
27	P	272	DMU	C6
27	P	272	DMU	C2
27	P	272	DMU	C5
27	P	272	DMU	C10
27	Z	1526	DMU	C9
27	Z	1526	DMU	C4
27	Z	1526	DMU	C6
27	Z	1526	DMU	C2
27	Z	1526	DMU	C5

All (959) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	515	HEA	C2A-C3A-CMA-OMA
19	A	524	PGV	C02-C03-O11-P
19	A	524	PGV	C04-C05-C06-O06
19	A	524	PGV	O02-C1-O01-C02
19	A	524	PGV	O04-C19-O03-C01
19	A	524	PGV	C20-C19-O03-C01
19	A	521	PGV	C04-O12-P-O13
19	C	268	PGV	O01-C02-C03-O11
19	C	268	PGV	C02-C03-O11-P
19	C	268	PGV	C2-C1-O01-C02
19	N	1524	PGV	C03-O11-P-O12
19	N	1524	PGV	C03-O11-P-O14
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	O02-C1-O01-C02
19	U	1268	PGV	O12-C04-C05-C06
19	U	1268	PGV	C2-C1-O01-C02
21	D	523	TGL	CB2-CB1-OG2-CG2
21	D	523	TGL	CC2-CC1-OG3-CG3
21	D	523	TGL	OC1-CC1-OG3-CG3
21	N	1523	TGL	CC2-CC1-OG3-CG3
21	N	1523	TGL	OC1-CC1-OG3-CG3
21	Y	1522	TGL	CB2-CB1-OG2-CG2
21	Y	1522	TGL	OB1-CB1-OG2-CG2
22	B	229	PSC	O12-C04-C05-N
22	R	1229	PSC	C03-O11-P-O12
22	R	1229	PSC	C03-O11-P-O13
22	R	1229	PSC	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
22	R	1229	PSC	O12-C04-C05-N
22	R	1229	PSC	C2-C1-O01-C02
23	J	60	CHD	C16-C17-C20-C21
23	W	1059	CHD	C13-C17-C20-C22
23	W	1059	CHD	C16-C17-C20-C21
25	C	264	PEK	O12-C04-C05-N
25	C	264	PEK	C11-C12-C13-C14
25	C	264	PEK	C12-C13-C14-C15
25	C	265	PEK	C04-O12-P-O11
25	C	265	PEK	C04-O12-P-O13
25	G	1263	PEK	C03-O11-P-O12
25	G	1263	PEK	C03-O11-P-O14
25	T	263	PEK	C03-O11-P-O12
25	T	263	PEK	C03-O11-P-O13
25	T	263	PEK	C9-C10-C11-C12
25	T	1265	PEK	C03-O11-P-O12
25	T	1265	PEK	C03-O11-P-O13
26	C	270	CDL	C1-CA2-OA2-PA1
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB4
26	G	269	CDL	CA2-C1-CB2-OB2
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB3-OB5-PB2-OB2
26	G	269	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4
26	G	269	CDL	OB6-CB4-CB6-OB8
26	P	1270	CDL	CB2-C1-CA2-OA2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CA3-OA5-PA1-OA2
26	P	1270	CDL	CA3-OA5-PA1-OA3
26	P	1270	CDL	CA3-OA5-PA1-OA4
26	P	1270	CDL	OA7-CA5-OA6-CA4
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CB2-OB2-PB2-OB4
26	P	1270	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	CA3-OA5-PA1-OA2
26	T	1269	CDL	CA3-OA5-PA1-OA4
26	T	1269	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	C11-CA5-OA6-CA4
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB2-OB2-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
27	C	272	DMU	O5-C6-O16-C18
19	N	1524	PGV	O04-C19-O03-C01
26	P	1270	CDL	OA9-CA7-OA8-CA6
26	P	1270	CDL	C31-CA7-OA8-CA6
22	B	229	PSC	O04-C19-O03-C01
22	R	1229	PSC	O04-C19-O03-C01
25	G	1263	PEK	O04-C21-O03-C01
25	T	263	PEK	O04-C21-O03-C01
23	J	60	CHD	C16-C17-C20-C22
19	C	268	PGV	O02-C1-O01-C02
19	U	1268	PGV	O02-C1-O01-C02
21	D	523	TGL	OB1-CB1-OG2-CG2
22	R	1229	PSC	O02-C1-O01-C02
25	C	265	PEK	O02-C1-O01-C02
25	T	1265	PEK	O02-C1-O01-C02
19	N	1524	PGV	C20-C19-O03-C01
22	B	229	PSC	C20-C19-O03-C01
22	R	1229	PSC	C20-C19-O03-C01
25	G	1263	PEK	C22-C21-O03-C01
27	P	272	DMU	O6-C11-C9-O1
19	A	524	PGV	C2-C1-O01-C02
19	N	1524	PGV	C2-C1-O01-C02
14	N	515	HEA	C26-C15-C16-C17
14	N	515	HEA	C14-C15-C16-C17
21	L	522	TGL	CA2-CA1-OG1-CG1
25	T	263	PEK	C22-C21-O03-C01
19	A	521	PGV	C10-C11-C12-C13
19	C	268	PGV	C10-C11-C12-C13
19	N	1524	PGV	C10-C11-C12-C13
25	C	265	PEK	C13-C14-C15-C16
25	G	1263	PEK	C4-C5-C6-C7
25	P	1264	PEK	C7-C8-C9-C10
25	T	263	PEK	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	OA7-CA5-OA6-CA4
21	Y	1522	TGL	C20-C21-C22-C23
26	G	269	CDL	C79-C80-C81-C82
26	P	1270	CDL	C61-C62-C63-C64
19	C	268	PGV	O12-C04-C05-O05
26	G	269	CDL	O1-C1-CB2-OB2
26	T	1269	CDL	O1-C1-CA2-OA2
27	M	526	DMU	O5-C4-C57-O61
27	Z	1526	DMU	O5-C4-C57-O61
27	M	526	DMU	O6-C11-C9-C8
25	C	265	PEK	C2-C1-O01-C02
25	T	1265	PEK	C2-C1-O01-C02
23	P	1271	CHD	C13-C17-C20-C21
23	C	271	CHD	C17-C20-C22-C23
21	L	522	TGL	OA1-CA1-OG1-CG1
19	A	524	PGV	C05-C04-O12-P
21	B	521	TGL	C12-C13-C14-C29
27	Z	1526	DMU	O5-C6-O16-C18
21	Y	1522	TGL	CC1-CC2-CC3-CC4
19	C	267	PGV	C10-C11-C12-C13
19	P	1267	PGV	C10-C11-C12-C13
25	C	264	PEK	C10-C11-C12-C13
25	C	264	PEK	C13-C14-C15-C16
25	C	265	PEK	C7-C8-C9-C10
25	G	1263	PEK	C13-C14-C15-C16
25	P	1264	PEK	C13-C14-C15-C16
19	A	521	PGV	C6-C7-C8-C9
21	B	521	TGL	C21-C22-C23-C24
21	N	1523	TGL	C16-C15-CC9-CC8
27	C	272	DMU	O6-C11-C9-C8
26	T	1269	CDL	CA2-C1-CB2-OB2
19	U	1268	PGV	C20-C19-O03-C01
21	O	1521	TGL	CC2-CC1-OG3-CG3
27	P	272	DMU	C3-C4-C57-O61
26	P	1270	CDL	C19-C20-C21-C22
21	L	522	TGL	C20-C21-C22-C23
19	A	524	PGV	C20-C21-C22-C23
27	P	272	DMU	C1-C6-O16-C18
19	U	1268	PGV	O12-C04-C05-O05
21	Y	1522	TGL	CC3-CC4-CC5-CC6
26	T	1269	CDL	CB7-C71-C72-C73
22	B	229	PSC	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
23	W	1059	CHD	C16-C17-C20-C22
26	G	269	CDL	C11-CA5-OA6-CA4
21	Y	1522	TGL	CA2-CA1-OG1-CG1
19	N	1524	PGV	C19-C20-C21-C22
21	L	522	TGL	CC1-CC2-CC3-CC4
21	Y	1522	TGL	C16-C15-CC9-CC8
26	T	1269	CDL	C40-C41-C42-C43
22	R	1229	PSC	C11-C12-C13-C14
25	C	265	PEK	C10-C11-C12-C13
25	P	1264	PEK	C10-C11-C12-C13
25	T	1265	PEK	C13-C14-C15-C16
19	N	1524	PGV	O05-C05-C06-O06
19	A	524	PGV	C12-C13-C14-C15
27	C	272	DMU	O5-C4-C57-O61
21	D	523	TGL	CB9-C10-C11-C12
25	T	1265	PEK	C28-C29-C30-C31
23	C	271	CHD	C21-C20-C22-C23
19	C	268	PGV	C1-C2-C3-C4
21	L	522	TGL	OB1-CB1-OG2-CG2
26	G	269	CDL	OA7-CA5-OA6-CA4
27	Z	1526	DMU	O6-C11-C9-O1
23	J	60	CHD	C13-C17-C20-C21
21	O	1521	TGL	CA1-CA2-CA3-CA4
25	P	1264	PEK	C1-C2-C3-C4
26	G	269	CDL	CB7-C71-C72-C73
26	G	269	CDL	C31-CA7-OA8-CA6
21	B	521	TGL	CB1-CB2-CB3-CB4
21	N	1523	TGL	CB1-CB2-CB3-CB4
22	R	1229	PSC	C1-C2-C3-C4
26	P	1270	CDL	CB5-C51-C52-C53
21	O	1521	TGL	OC1-CC1-OG3-CG3
19	U	1268	PGV	C20-C21-C22-C23
26	G	269	CDL	C40-C41-C42-C43
26	P	1270	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	O1-C1-CB2-OB2
27	C	272	DMU	O16-C18-C19-C22
21	Y	1522	TGL	C25-C26-C27-C28
19	U	1268	PGV	O04-C19-O03-C01
25	C	264	PEK	C1-C2-C3-C4
25	G	1263	PEK	C21-C22-C23-C24
26	C	270	CDL	CB5-C51-C52-C53
19	U	1268	PGV	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	T	1265	PEK	C4-C5-C6-C7
25	T	1265	PEK	C10-C11-C12-C13
26	G	269	CDL	CA5-C11-C12-C13
21	L	522	TGL	CB2-CB1-OG2-CG2
26	G	269	CDL	C51-CB5-OB6-CB4
26	G	269	CDL	OA9-CA7-OA8-CA6
23	P	1271	CHD	C21-C20-C22-C23
26	T	1269	CDL	C60-C61-C62-C63
21	B	521	TGL	CA1-CA2-CA3-CA4
22	B	229	PSC	O02-C1-O01-C02
26	G	269	CDL	OB7-CB5-OB6-CB4
23	W	1059	CHD	C13-C17-C20-C21
22	B	229	PSC	C04-C05-N-C06
22	B	229	PSC	C04-C05-N-C07
27	Z	1526	DMU	O16-C18-C19-C22
22	B	229	PSC	C2-C1-O01-C02
21	O	1521	TGL	C12-C13-C14-C29
25	C	264	PEK	C7-C8-C9-C10
26	P	1270	CDL	O1-C1-CB2-OB2
26	G	269	CDL	C60-C61-C62-C63
21	Y	1522	TGL	OA1-CA1-OG1-CG1
19	C	268	PGV	C04-C05-C06-O06
19	N	1524	PGV	C04-C05-C06-O06
19	U	1268	PGV	C04-C05-C06-O06
22	B	229	PSC	C03-C02-O01-C1
21	D	523	TGL	CA2-CA1-OG1-CG1
26	G	269	CDL	C55-C56-C57-C58
19	C	267	PGV	C24-C25-C26-C27
21	D	523	TGL	CA6-CA7-CA8-CA9
22	B	229	PSC	C30-C31-C32-C33
26	G	269	CDL	C80-C81-C82-C83
21	D	523	TGL	C10-C11-C12-C13
21	D	523	TGL	CC2-CC3-CC4-CC5
21	L	522	TGL	CA3-CA4-CA5-CA6
21	O	1521	TGL	C11-C10-CB9-CB8
21	O	1521	TGL	C14-C29-C30-C31
21	Y	1522	TGL	C10-C11-C12-C13
21	Y	1522	TGL	C22-C23-C24-C25
22	R	1229	PSC	C20-C21-C22-C23
25	G	1263	PEK	C27-C28-C29-C30
25	P	1264	PEK	C30-C31-C32-C33
25	T	263	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C38-C39-C40-C41
26	C	270	CDL	C77-C78-C79-C80
26	G	269	CDL	C58-C59-C60-C61
26	P	1270	CDL	C74-C75-C76-C77
22	R	1229	PSC	C11-C10-C9-C8
25	T	263	PEK	C10-C11-C12-C13
19	N	1524	PGV	C7-C8-C9-C10
19	N	1266	PGV	C5-C6-C7-C8
21	B	521	TGL	CC7-CC8-CC9-C15
26	T	1269	CDL	C76-C77-C78-C79
22	B	229	PSC	C3-C4-C5-C6
22	B	229	PSC	C25-C26-C27-C28
25	G	1263	PEK	C23-C24-C25-C26
26	C	270	CDL	C57-C58-C59-C60
26	G	269	CDL	C43-C44-C45-C46
26	P	1270	CDL	C16-C17-C18-C19
26	T	1269	CDL	C23-C24-C25-C26
26	T	1269	CDL	C82-C83-C84-C85
21	O	1521	TGL	OB1-CB1-OG2-CG2
19	A	524	PGV	O05-C05-C06-O06
19	U	1268	PGV	O05-C05-C06-O06
27	Z	1526	DMU	C19-C18-O16-C6
21	B	521	TGL	CC5-CC6-CC7-CC8
22	R	1229	PSC	C25-C26-C27-C28
25	C	265	PEK	C32-C33-C34-C35
26	C	270	CDL	C23-C24-C25-C26
26	T	1269	CDL	C32-C33-C34-C35
19	C	268	PGV	C3-C4-C5-C6
21	Y	1522	TGL	C21-C22-C23-C24
21	O	1521	TGL	CB2-CB1-OG2-CG2
22	B	229	PSC	C23-C24-C25-C26
26	C	270	CDL	C19-C20-C21-C22
26	P	1270	CDL	C59-C60-C61-C62
19	C	267	PGV	C7-C8-C9-C10
21	L	522	TGL	CA7-CA8-CA9-C20
21	N	1523	TGL	C21-C20-CA9-CA8
22	R	1229	PSC	C22-C23-C24-C25
26	C	270	CDL	C41-C42-C43-C44
26	G	269	CDL	C22-C23-C24-C25
26	P	1270	CDL	C37-C38-C39-C40
26	P	1270	CDL	C42-C43-C44-C45
26	P	1270	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C36-C37-C38-C39
19	P	1267	PGV	C7-C8-C9-C10
21	N	1523	TGL	CC5-CC6-CC7-CC8
21	O	1521	TGL	CA6-CA7-CA8-CA9
26	P	1270	CDL	C43-C44-C45-C46
26	P	1270	CDL	C71-C72-C73-C74
27	Z	1526	DMU	C22-C25-C28-C31
21	Y	1522	TGL	CB1-CB2-CB3-CB4
21	O	1521	TGL	CC5-CC6-CC7-CC8
21	B	521	TGL	CA5-CA6-CA7-CA8
21	B	521	TGL	CC6-CC7-CC8-CC9
21	N	1523	TGL	C20-C21-C22-C23
26	G	269	CDL	C41-C42-C43-C44
26	P	1270	CDL	C21-C22-C23-C24
26	P	1270	CDL	C81-C82-C83-C84
26	T	1269	CDL	C12-C13-C14-C15
23	J	60	CHD	C13-C17-C20-C22
19	N	1266	PGV	C6-C7-C8-C9
26	G	269	CDL	C71-CB7-OB8-CB6
25	G	1263	PEK	O03-C01-C02-C03
19	U	1268	PGV	C26-C27-C28-C29
21	L	522	TGL	C17-C18-C19-C33
21	O	1521	TGL	CC7-CC8-CC9-C15
26	C	270	CDL	C76-C77-C78-C79
26	G	269	CDL	C59-C60-C61-C62
26	P	1270	CDL	C14-C15-C16-C17
19	U	1268	PGV	C24-C25-C26-C27
21	B	521	TGL	CB3-CB4-CB5-CB6
21	L	522	TGL	C11-C12-C13-C14
21	O	1521	TGL	CC2-CC3-CC4-CC5
22	B	229	PSC	C5-C6-C7-C8
25	P	1264	PEK	C23-C24-C25-C26
25	T	1265	PEK	C29-C30-C31-C32
26	G	269	CDL	C61-C62-C63-C64
26	P	1270	CDL	C20-C21-C22-C23
26	P	1270	CDL	C53-C54-C55-C56
19	N	1524	PGV	C26-C27-C28-C29
19	N	1266	PGV	C26-C27-C28-C29
19	U	1268	PGV	C29-C30-C31-C32
21	B	521	TGL	C22-C23-C24-C25
21	D	523	TGL	CA4-CA5-CA6-CA7
22	B	229	PSC	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	C52-C53-C54-C55
26	G	269	CDL	C57-C58-C59-C60
19	C	267	PGV	C14-C15-C16-C17
22	B	229	PSC	C4-C5-C6-C7
25	G	1263	PEK	C31-C32-C33-C34
22	B	229	PSC	C04-C05-N-C08
19	C	268	PGV	C28-C29-C30-C31
21	B	521	TGL	CA7-CA8-CA9-C20
21	Y	1522	TGL	CB4-CB5-CB6-CB7
26	G	269	CDL	C82-C83-C84-C85
21	L	522	TGL	CC3-CC4-CC5-CC6
22	B	229	PSC	C11-C12-C13-C14
21	B	521	TGL	CA2-CA3-CA4-CA5
21	L	522	TGL	C21-C22-C23-C24
25	C	264	PEK	C28-C29-C30-C31
25	P	1264	PEK	C32-C33-C34-C35
25	T	263	PEK	C30-C31-C32-C33
26	G	269	CDL	C37-C38-C39-C40
25	C	264	PEK	C23-C24-C25-C26
25	G	1263	PEK	C25-C26-C27-C28
21	D	523	TGL	OA1-CA1-OG1-CG1
26	P	1270	CDL	C12-C13-C14-C15
21	N	1523	TGL	CC2-CC3-CC4-CC5
25	P	1264	PEK	C16-C17-C18-C19
26	C	270	CDL	C78-C79-C80-C81
19	C	268	PGV	C20-C19-O03-C01
21	N	1523	TGL	CA2-CA1-OG1-CG1
25	C	264	PEK	C34-C35-C36-C37
25	C	265	PEK	C25-C26-C27-C28
26	C	270	CDL	C40-C41-C42-C43
21	D	523	TGL	C18-C19-C33-C34
26	T	1269	CDL	C11-C12-C13-C14
19	N	1266	PGV	C25-C26-C27-C28
19	U	1268	PGV	C27-C28-C29-C30
26	T	1269	CDL	C58-C59-C60-C61
26	T	1269	CDL	CB5-C51-C52-C53
21	D	523	TGL	C23-C24-C25-C26
21	L	522	TGL	C22-C23-C24-C25
26	C	270	CDL	C36-C37-C38-C39
26	C	270	CDL	C39-C40-C41-C42
26	G	269	CDL	C11-C12-C13-C14
26	G	269	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
21	L	522	TGL	C25-C26-C27-C28
27	Z	1526	DMU	C25-C28-C31-C34
21	B	521	TGL	CB2-CB1-OG2-CG2
26	C	270	CDL	C51-CB5-OB6-CB4
26	P	1270	CDL	C51-CB5-OB6-CB4
26	T	1269	CDL	C51-CB5-OB6-CB4
25	T	263	PEK	C25-C26-C27-C28
21	B	521	TGL	OB1-CB1-OG2-CG2
21	N	1523	TGL	CB9-C10-C11-C12
21	O	1521	TGL	CB5-CB6-CB7-CB8
21	O	1521	TGL	CB6-CB7-CB8-CB9
19	C	268	PGV	C11-C10-C9-C8
25	P	1264	PEK	C15-C16-C17-C18
19	A	524	PGV	C19-C20-C21-C22
26	C	270	CDL	C43-C44-C45-C46
26	G	269	CDL	C33-C34-C35-C36
21	B	521	TGL	C13-C14-C29-C30
19	N	1266	PGV	C4-C5-C6-C7
21	D	523	TGL	C20-C21-C22-C23
26	T	1269	CDL	C80-C81-C82-C83
19	A	521	PGV	C26-C27-C28-C29
27	Z	1526	DMU	C28-C31-C34-C37
26	G	269	CDL	C63-C64-C65-C66
26	G	269	CDL	OB9-CB7-OB8-CB6
21	D	523	TGL	CC5-CC6-CC7-CC8
19	U	1268	PGV	C30-C31-C32-C33
21	B	521	TGL	CC4-CC5-CC6-CC7
26	C	270	CDL	OB7-CB5-OB6-CB4
19	N	1524	PGV	C3-C4-C5-C6
21	Y	1522	TGL	CC7-CC8-CC9-C15
19	U	1268	PGV	C22-C23-C24-C25
25	T	1265	PEK	C16-C17-C18-C19
27	M	526	DMU	C19-C22-C25-C28
21	O	1521	TGL	CC1-CC2-CC3-CC4
26	C	270	CDL	C12-C13-C14-C15
26	C	270	CDL	C73-C74-C75-C76
19	A	521	PGV	C11-C10-C9-C8
22	B	229	PSC	C13-C14-C15-C16
25	G	1263	PEK	O03-C01-C02-O01
25	T	1265	PEK	C2-C3-C4-C5
26	T	1269	CDL	OA6-CA4-CA6-OA8
21	B	521	TGL	CA3-CA4-CA5-CA6

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Mol	Chain	Res	Type	Atoms
21	O	1521	TGL	CA2-CA3-CA4-CA5
26	C	270	CDL	C63-C64-C65-C66
21	O	1521	TGL	C20-C21-C22-C23
21	Y	1522	TGL	C15-C16-C17-C18
26	P	1270	CDL	C36-C37-C38-C39
26	T	1269	CDL	C78-C79-C80-C81
19	A	524	PGV	C13-C14-C15-C16
19	C	268	PGV	C24-C25-C26-C27
21	N	1523	TGL	C21-C22-C23-C24
25	T	263	PEK	C24-C25-C26-C27
26	T	1269	CDL	C59-C60-C61-C62
26	T	1269	CDL	OB7-CB5-OB6-CB4
19	C	268	PGV	O12-C04-C05-C06
21	D	523	TGL	CB2-CB3-CB4-CB5
21	L	522	TGL	C16-C17-C18-C19
21	N	1523	TGL	C19-C33-C34-C35
25	C	264	PEK	C25-C26-C27-C28
22	B	229	PSC	C20-C21-C22-C23
25	T	263	PEK	C34-C35-C36-C37
26	T	1269	CDL	C13-C14-C15-C16
19	N	1266	PGV	C7-C8-C9-C10
21	L	522	TGL	CC4-CC5-CC6-CC7
26	T	1269	CDL	C39-C40-C41-C42
25	P	1264	PEK	C25-C26-C27-C28
26	C	270	CDL	C11-C12-C13-C14
26	C	270	CDL	C17-C18-C19-C20
21	N	1523	TGL	C15-C16-C17-C18
26	P	1270	CDL	C11-C12-C13-C14
22	R	1229	PSC	C2-C3-C4-C5
26	T	1269	CDL	C72-C73-C74-C75
22	B	229	PSC	C26-C27-C28-C29
26	P	1270	CDL	C40-C41-C42-C43
19	A	524	PGV	C11-C10-C9-C8
25	C	264	PEK	C15-C16-C17-C18
25	C	265	PEK	C2-C3-C4-C5
19	C	267	PGV	C13-C14-C15-C16
21	D	523	TGL	C16-C17-C18-C19
21	N	1523	TGL	C10-C11-C12-C13
26	P	1270	CDL	C77-C78-C79-C80
19	C	268	PGV	C01-C02-C03-O11
19	N	1524	PGV	C01-C02-C03-O11
22	B	229	PSC	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	OA5-CA3-CA4-CA6
19	A	524	PGV	C5-C6-C7-C8
21	D	523	TGL	C12-C13-C14-C29
21	N	1523	TGL	C16-C17-C18-C19
26	T	1269	CDL	C71-CB7-OB8-CB6
27	C	272	DMU	C3-C4-C57-O61
26	C	270	CDL	C83-C84-C85-C86
26	C	270	CDL	C34-C35-C36-C37
26	C	270	CDL	C84-C85-C86-C87
22	R	1229	PSC	C24-C25-C26-C27
22	B	229	PSC	C11-C10-C9-C8
26	C	270	CDL	CB7-C71-C72-C73
19	N	1524	PGV	O03-C01-C02-C03
26	P	1270	CDL	CB3-CB4-CB6-OB8
26	T	1269	CDL	CA3-CA4-CA6-OA8
21	O	1521	TGL	CA3-CA4-CA5-CA6
21	D	523	TGL	C21-C20-CA9-CA8
21	Y	1522	TGL	C12-C13-C14-C29
26	T	1269	CDL	C81-C82-C83-C84
19	N	1266	PGV	C29-C30-C31-C32
25	C	265	PEK	C26-C27-C28-C29
26	P	1270	CDL	C34-C35-C36-C37
27	Z	1526	DMU	O6-C11-C9-C8
26	P	1270	CDL	C13-C14-C15-C16
19	C	268	PGV	C6-C7-C8-C9
26	P	1270	CDL	C23-C24-C25-C26
21	N	1523	TGL	OA1-CA1-OG1-CG1
21	D	523	TGL	CA5-CA6-CA7-CA8
27	C	272	DMU	C19-C22-C25-C28
26	G	269	CDL	C78-C79-C80-C81
21	N	1523	TGL	C22-C23-C24-C25
25	P	1264	PEK	C28-C29-C30-C31
25	P	1264	PEK	C27-C28-C29-C30
21	Y	1522	TGL	C21-C20-CA9-CA8
26	P	1270	CDL	C57-C58-C59-C60
27	C	272	DMU	C31-C34-C37-C40
19	C	268	PGV	C23-C24-C25-C26
21	Y	1522	TGL	C18-C19-C33-C34
19	A	524	PGV	C01-C02-O01-C1
21	N	1523	TGL	CG3-CG2-OG2-CB1
21	Y	1522	TGL	CG1-CG2-OG2-CB1
21	O	1521	TGL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C21-C22-C23-C24
19	C	268	PGV	C30-C31-C32-C33
26	P	1270	CDL	CA7-C31-C32-C33
26	T	1269	CDL	OB9-CB7-OB8-CB6
25	C	264	PEK	C4-C5-C6-C7
25	C	265	PEK	C4-C5-C6-C7
25	T	263	PEK	O01-C02-C03-O11
21	B	521	TGL	C11-C12-C13-C14
21	O	1521	TGL	CC3-CC4-CC5-CC6
26	G	269	CDL	C20-C21-C22-C23
26	G	269	CDL	C32-C33-C34-C35
19	A	521	PGV	C25-C26-C27-C28
21	O	1521	TGL	C15-C16-C17-C18
21	B	521	TGL	CB4-CB5-CB6-CB7
21	Y	1522	TGL	C29-C30-C31-C32
26	T	1269	CDL	C53-C54-C55-C56
25	T	263	PEK	O03-C01-C02-O01
19	N	1524	PGV	C15-C16-C17-C18
25	T	1265	PEK	C25-C26-C27-C28
26	P	1270	CDL	C73-C74-C75-C76
26	T	1269	CDL	C44-C45-C46-C47
21	B	521	TGL	CA9-C20-C21-C22
19	C	268	PGV	C31-C32-C33-C34
19	A	521	PGV	C31-C32-C33-C34
25	C	265	PEK	C35-C36-C37-C38
19	U	1268	PGV	C23-C24-C25-C26
21	D	523	TGL	C33-C34-C35-C36
14	A	516	HEA	C3B-C11-C12-C13
26	P	1270	CDL	C24-C25-C26-C27
21	N	1523	TGL	CA6-CA7-CA8-CA9
25	C	264	PEK	C30-C31-C32-C33
19	P	1267	PGV	C25-C26-C27-C28
26	C	270	CDL	C42-C43-C44-C45
14	A	516	HEA	C4D-C3D-CAD-CBD
21	L	522	TGL	CA5-CA6-CA7-CA8
21	O	1521	TGL	CA5-CA6-CA7-CA8
25	C	264	PEK	C24-C25-C26-C27
26	G	269	CDL	CA4-CA3-OA5-PA1
26	P	1270	CDL	C1-CA2-OA2-PA1
19	N	1524	PGV	C31-C32-C33-C34
19	C	268	PGV	O04-C19-O03-C01
19	U	1268	PGV	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	O	1521	TGL	C13-C14-C29-C30
27	P	272	DMU	C31-C34-C37-C40
21	B	521	TGL	C23-C24-C25-C26
27	C	272	DMU	C1-C6-O16-C18
19	A	524	PGV	C15-C16-C17-C18
26	C	270	CDL	OB5-CB3-CB4-CB6
26	P	1270	CDL	OB5-CB3-CB4-CB6
21	B	521	TGL	C24-C25-C26-C27
26	P	1270	CDL	C64-C65-C66-C67
26	G	269	CDL	C36-C37-C38-C39
19	P	1267	PGV	C31-C32-C33-C34
25	G	1263	PEK	C17-C18-C19-C20
19	N	1266	PGV	C31-C32-C33-C34
19	C	268	PGV	C13-C14-C15-C16
21	Y	1522	TGL	CA5-CA6-CA7-CA8
25	P	1264	PEK	C34-C35-C36-C37
26	P	1270	CDL	C52-C53-C54-C55
21	Y	1522	TGL	C17-C18-C19-C33
22	R	1229	PSC	C21-C22-C23-C24
19	A	524	PGV	C14-C15-C16-C17
26	T	1269	CDL	C21-C22-C23-C24
21	D	523	TGL	CC4-CC5-CC6-CC7
25	T	1265	PEK	C22-C23-C24-C25
19	C	267	PGV	C31-C32-C33-C34
23	C	271	CHD	C16-C17-C20-C22
19	N	1524	PGV	C30-C31-C32-C33
25	T	1265	PEK	C30-C31-C32-C33
19	N	1266	PGV	C23-C24-C25-C26
26	T	1269	CDL	C75-C76-C77-C78
21	O	1521	TGL	CB1-CB2-CB3-CB4
25	C	264	PEK	C35-C36-C37-C38
19	N	1524	PGV	C25-C26-C27-C28
19	P	1267	PGV	C20-C21-C22-C23
26	C	270	CDL	C59-C60-C61-C62
21	D	523	TGL	CG1-CG2-CG3-OG3
21	Y	1522	TGL	OG1-CG1-CG2-CG3
25	T	263	PEK	O03-C01-C02-C03
26	C	270	CDL	CB3-CB4-CB6-OB8
26	G	269	CDL	CB3-CB4-CB6-OB8
26	C	270	CDL	C37-C38-C39-C40
21	Y	1522	TGL	CC4-CC5-CC6-CC7
26	G	269	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C38-C39-C40-C41
19	A	524	PGV	C31-C32-C33-C34
27	M	526	DMU	C25-C28-C31-C34
26	P	1270	CDL	OB7-CB5-OB6-CB4
25	C	265	PEK	O01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-OA6
22	R	1229	PSC	C23-C24-C25-C26
26	T	1269	CDL	C52-C53-C54-C55
19	C	267	PGV	C15-C16-C17-C18
26	C	270	CDL	C56-C57-C58-C59
21	L	522	TGL	C16-C15-CC9-CC8
26	G	269	CDL	C34-C35-C36-C37
19	U	1268	PGV	O03-C01-C02-O01
22	B	229	PSC	O03-C01-C02-O01
26	C	270	CDL	OA6-CA4-CA6-OA8
26	P	1270	CDL	OB6-CB4-CB6-OB8
19	N	1524	PGV	C21-C22-C23-C24
22	B	229	PSC	C9-C10-C11-C12
22	R	1229	PSC	C9-C10-C11-C12
25	C	264	PEK	C9-C10-C11-C12
25	C	265	PEK	C5-C6-C7-C8
25	C	265	PEK	C11-C10-C9-C8
25	G	1263	PEK	C6-C7-C8-C9
25	G	1263	PEK	C11-C10-C9-C8
25	G	1263	PEK	C11-C12-C13-C14
25	P	1264	PEK	C6-C7-C8-C9
25	P	1264	PEK	C11-C10-C9-C8
25	P	1264	PEK	C12-C13-C14-C15
25	T	263	PEK	C11-C10-C9-C8
25	T	1265	PEK	C6-C7-C8-C9
25	T	1265	PEK	C11-C10-C9-C8
21	L	522	TGL	CC2-CC3-CC4-CC5
19	P	1267	PGV	C13-C14-C15-C16
26	G	269	CDL	C53-C54-C55-C56
26	G	269	CDL	C62-C63-C64-C65
26	T	1269	CDL	C43-C44-C45-C46
25	P	1264	PEK	C3-C4-C5-C6
21	B	521	TGL	CC2-CC3-CC4-CC5
25	P	1264	PEK	C26-C27-C28-C29
26	C	270	CDL	C15-C16-C17-C18
25	C	265	PEK	C28-C29-C30-C31
21	Y	1522	TGL	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
27	M	526	DMU	O5-C6-O16-C18
19	A	521	PGV	C23-C24-C25-C26
25	G	1263	PEK	C16-C17-C18-C19
21	B	521	TGL	C29-C30-C31-C32
21	B	521	TGL	CC9-C15-C16-C17
21	L	522	TGL	CB4-CB5-CB6-CB7
21	Y	1522	TGL	CC5-CC6-CC7-CC8
25	P	1264	PEK	C22-C23-C24-C25
19	C	268	PGV	C14-C15-C16-C17
26	C	270	CDL	C80-C81-C82-C83
23	P	1525	CHD	C13-C17-C20-C22
21	L	522	TGL	OG1-CA1-CA2-CA3
21	L	522	TGL	CB6-CB7-CB8-CB9
26	T	1269	CDL	C18-C19-C20-C21
19	N	1266	PGV	C24-C25-C26-C27
21	B	521	TGL	C21-C20-CA9-CA8
25	C	265	PEK	C01-C02-C03-O11
26	P	1270	CDL	OA5-CA3-CA4-CA6
26	T	1269	CDL	C83-C84-C85-C86
27	Z	1526	DMU	C34-C37-C40-C43
19	C	268	PGV	C25-C26-C27-C28
26	P	1270	CDL	C22-C23-C24-C25
25	T	1265	PEK	C23-C24-C25-C26
26	C	270	CDL	C58-C59-C60-C61
21	B	521	TGL	C15-C16-C17-C18
21	L	522	TGL	C12-C13-C14-C29
21	N	1523	TGL	C12-C13-C14-C29
27	P	272	DMU	C5-C10-O7-C3
19	N	1524	PGV	C03-C02-O01-C1
21	B	521	TGL	CG1-CG2-OG2-CB1
21	O	1521	TGL	CG1-CG2-OG2-CB1
22	R	1229	PSC	C01-C02-O01-C1
27	M	526	DMU	C22-C25-C28-C31
19	C	268	PGV	C15-C16-C17-C18
25	C	264	PEK	C17-C18-C19-C20
26	G	269	CDL	C35-C36-C37-C38
26	G	269	CDL	C19-C20-C21-C22
25	G	1263	PEK	O01-C02-C03-O11
26	C	270	CDL	OB5-CB3-CB4-OB6
19	U	1268	PGV	C3-C4-C5-C6
25	C	265	PEK	C33-C34-C35-C36
22	B	229	PSC	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
22	R	1229	PSC	O03-C01-C02-C03
21	L	522	TGL	CC7-CC8-CC9-C15
14	A	515	HEA	C14-C15-C16-C17
26	P	1270	CDL	C15-C16-C17-C18
25	C	264	PEK	C32-C33-C34-C35
21	N	1523	TGL	OG2-CG2-CG3-OG3
26	P	1270	CDL	OA6-CA4-CA6-OA8
26	G	269	CDL	CA7-C31-C32-C33
25	T	263	PEK	C23-C24-C25-C26
21	B	521	TGL	C16-C17-C18-C19
21	Y	1522	TGL	C19-C33-C34-C35
21	N	1523	TGL	CC4-CC5-CC6-CC7
21	N	1523	TGL	CC9-C15-C16-C17
21	O	1521	TGL	C10-C11-C12-C13
19	A	524	PGV	C7-C8-C9-C10
21	L	522	TGL	CA2-CA3-CA4-CA5
22	R	1229	PSC	C28-C29-C30-C31
25	P	1264	PEK	C24-C25-C26-C27
21	N	1523	TGL	C24-C25-C26-C27
21	D	523	TGL	C22-C23-C24-C25
23	C	271	CHD	C16-C17-C20-C21
19	C	268	PGV	C27-C28-C29-C30
26	G	269	CDL	C44-C45-C46-C47
26	G	269	CDL	C77-C78-C79-C80
21	O	1521	TGL	C29-C30-C31-C32
27	M	526	DMU	C34-C37-C40-C43
26	T	1269	CDL	C54-C55-C56-C57
19	U	1268	PGV	C01-C02-C03-O11
25	G	1263	PEK	C01-C02-C03-O11
25	T	263	PEK	C01-C02-C03-O11
19	A	524	PGV	C2-C3-C4-C5
19	C	267	PGV	C20-C21-C22-C23
19	P	1267	PGV	C02-C03-O11-P
22	B	229	PSC	C02-C03-O11-P
22	R	1229	PSC	C02-C03-O11-P
21	L	522	TGL	C13-C14-C29-C30
19	U	1268	PGV	C31-C32-C33-C34
21	L	522	TGL	C33-C34-C35-C36
22	B	229	PSC	O01-C02-C03-O11
26	P	1270	CDL	OB5-CB3-CB4-OB6
19	C	267	PGV	C12-C13-C14-C15
19	U	1268	PGV	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C74-C75-C76-C77
26	T	1269	CDL	C32-C31-CA7-OA8
14	A	515	HEA	C4A-C3A-CMA-OMA
14	N	515	HEA	C4A-C3A-CMA-OMA
19	P	1267	PGV	C9-C10-C11-C12
25	C	264	PEK	C3-C4-C5-C6
26	G	269	CDL	C15-C16-C17-C18
19	A	524	PGV	O03-C01-C02-O01
19	N	1524	PGV	O03-C01-C02-O01
21	D	523	TGL	OG2-CG2-CG3-OG3
22	R	1229	PSC	O03-C01-C02-O01
26	C	270	CDL	OB6-CB4-CB6-OB8
19	U	1268	PGV	C14-C15-C16-C17
21	N	1523	TGL	CG1-CG2-CG3-OG3
21	Y	1522	TGL	CG1-CG2-CG3-OG3
26	C	270	CDL	CA3-CA4-CA6-OA8
26	P	1270	CDL	CA3-CA4-CA6-OA8
21	N	1523	TGL	CA3-CA4-CA5-CA6
19	A	524	PGV	C22-C23-C24-C25
25	G	1263	PEK	C24-C25-C26-C27
25	G	1263	PEK	C29-C30-C31-C32
21	O	1521	TGL	C21-C20-CA9-CA8
23	C	525	CHD	C13-C17-C20-C22
21	D	523	TGL	CB5-CB6-CB7-CB8
22	B	229	PSC	C22-C23-C24-C25
19	A	524	PGV	C03-O11-P-O13
19	A	524	PGV	C04-O12-P-O14
19	C	268	PGV	C04-O12-P-O13
19	N	1266	PGV	C04-O12-P-O13
22	B	229	PSC	C03-O11-P-O12
22	B	229	PSC	C03-O11-P-O13
22	R	1229	PSC	C04-O12-P-O11
22	R	1229	PSC	C04-O12-P-O13
22	R	1229	PSC	C04-C05-N-C06
25	C	265	PEK	C04-O12-P-O14
25	G	1263	PEK	C03-O11-P-O13
25	T	1265	PEK	C03-O11-P-O14
25	T	1265	PEK	O12-C04-C05-N
26	T	1269	CDL	CA2-OA2-PA1-OA3
26	T	1269	CDL	CA2-OA2-PA1-OA4
26	T	1269	CDL	CA2-OA2-PA1-OA5
21	Y	1522	TGL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	A	521	PGV	C29-C30-C31-C32
14	A	515	HEA	C26-C15-C16-C17
21	B	521	TGL	C14-C29-C30-C31
21	Y	1522	TGL	C23-C24-C25-C26
19	C	267	PGV	C02-C03-O11-P
25	T	263	PEK	C02-C03-O11-P
26	T	1269	CDL	C33-C34-C35-C36
27	P	272	DMU	C22-C25-C28-C31
26	T	1269	CDL	C63-C64-C65-C66
19	P	1267	PGV	C1-C2-C3-C4
26	P	1270	CDL	CA5-C11-C12-C13
21	D	523	TGL	CG3-CG2-OG2-CB1
19	A	524	PGV	C29-C30-C31-C32
26	G	269	CDL	C71-C72-C73-C74
21	D	523	TGL	C29-C30-C31-C32
14	A	516	HEA	C2D-C3D-CAD-CBD
22	B	229	PSC	C12-C13-C14-C15
21	B	521	TGL	CC3-CC4-CC5-CC6
21	D	523	TGL	CB4-CB5-CB6-CB7
25	C	265	PEK	C31-C32-C33-C34
25	T	263	PEK	C32-C33-C34-C35
27	C	272	DMU	C5-C10-O7-C3
26	T	1269	CDL	C61-C62-C63-C64
25	C	265	PEK	C14-C15-C16-C17
25	P	1264	PEK	O03-C01-C02-O01
21	D	523	TGL	OG1-CA1-CA2-CA3
26	C	270	CDL	C52-C51-CB5-OB6
26	C	270	CDL	C44-C45-C46-C47
26	G	269	CDL	C75-C76-C77-C78
26	C	270	CDL	C18-C19-C20-C21
25	P	1264	PEK	C21-C22-C23-C24
19	U	1268	PGV	C11-C10-C9-C8
25	C	264	PEK	C2-C3-C4-C5
25	T	263	PEK	C15-C16-C17-C18
21	O	1521	TGL	OG3-CC1-CC2-CC3
25	G	1263	PEK	C22-C23-C24-C25
26	P	1270	CDL	C38-C39-C40-C41
25	C	265	PEK	C34-C35-C36-C37
19	A	524	PGV	C1-C2-C3-C4
25	T	1265	PEK	C33-C34-C35-C36
26	C	270	CDL	C20-C21-C22-C23
21	D	523	TGL	OG2-CB1-CB2-CB3

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C79-C80-C81-C82
21	Y	1522	TGL	CB2-CB3-CB4-CB5
25	G	1263	PEK	C30-C31-C32-C33
19	N	1524	PGV	C28-C29-C30-C31
21	Y	1522	TGL	CA6-CA7-CA8-CA9
25	T	1265	PEK	C22-C21-O03-C01
25	P	1264	PEK	C2-C3-C4-C5
19	N	1524	PGV	O01-C02-C03-O11
19	C	267	PGV	C9-C10-C11-C12
26	C	270	CDL	C31-C32-C33-C34
26	T	1269	CDL	C34-C35-C36-C37
23	P	1525	CHD	C13-C17-C20-C21
26	P	1270	CDL	C78-C79-C80-C81
19	N	1524	PGV	C9-C10-C11-C12
25	T	1265	PEK	O04-C21-O03-C01
19	C	268	PGV	O03-C01-C02-O01
27	C	272	DMU	C34-C37-C40-C43
19	N	1524	PGV	C24-C25-C26-C27
21	O	1521	TGL	CA7-CA8-CA9-C20
14	A	516	HEA	CAD-CBD-CGD-O1D
26	G	269	CDL	C74-C75-C76-C77
26	C	270	CDL	CA4-CA3-OA5-PA1
27	C	272	DMU	C4-C3-O7-C10
23	P	1271	CHD	C16-C17-C20-C22
23	O	229	CHD	C22-C23-C24-O25
19	P	1267	PGV	C29-C30-C31-C32
14	N	516	HEA	CAD-CBD-CGD-O2D
21	L	522	TGL	OG2-CB1-CB2-CB3
23	W	1059	CHD	C22-C23-C24-O26
21	N	1523	TGL	CA2-CA3-CA4-CA5
21	B	521	TGL	OC1-CC1-OG3-CG3
23	W	1059	CHD	C22-C23-C24-O25
19	C	267	PGV	C1-C2-C3-C4
26	C	270	CDL	CA7-C31-C32-C33
26	P	1270	CDL	OA5-CA3-CA4-OA6
21	D	523	TGL	CB7-CB8-CB9-C10
26	T	1269	CDL	CA5-C11-C12-C13
23	B	1085	CHD	C22-C23-C24-O25
26	G	269	CDL	C64-C65-C66-C67
19	U	1268	PGV	C02-C03-O11-P
26	P	1270	CDL	CA4-CA3-OA5-PA1
14	A	516	HEA	O11-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	P	1267	PGV	C15-C16-C17-C18
14	A	516	HEA	CAA-CBA-CGA-O1A
23	O	229	CHD	C22-C23-C24-O26
27	M	526	DMU	C28-C31-C34-C37
26	G	269	CDL	OA6-CA4-CA6-OA8
22	B	229	PSC	C10-C11-C12-C13
22	R	1229	PSC	C10-C11-C12-C13
21	N	1523	TGL	CA7-CA8-CA9-C20
21	O	1521	TGL	CB7-CB8-CB9-C10
25	C	265	PEK	C29-C30-C31-C32
19	N	1524	PGV	C20-C21-C22-C23
22	R	1229	PSC	C15-C16-C17-C18
14	A	516	HEA	CAD-CBD-CGD-O2D
26	P	1270	CDL	C39-C40-C41-C42
26	T	1269	CDL	C62-C63-C64-C65
21	D	523	TGL	CC9-C15-C16-C17
25	T	263	PEK	C26-C27-C28-C29
19	N	1266	PGV	C11-C10-C9-C8
14	N	516	HEA	CAD-CBD-CGD-O1D
25	T	1265	PEK	C31-C32-C33-C34
14	N	516	HEA	C26-C15-C16-C17
25	G	1263	PEK	C02-C03-O11-P
26	T	1269	CDL	C17-C18-C19-C20
21	L	522	TGL	CA9-C20-C21-C22
25	T	1265	PEK	C27-C28-C29-C30
19	P	1267	PGV	C28-C29-C30-C31
19	P	1267	PGV	C14-C15-C16-C17
14	A	516	HEA	CAA-CBA-CGA-O2A
26	T	1269	CDL	C56-C57-C58-C59
25	T	263	PEK	C21-C22-C23-C24
19	C	268	PGV	O05-C05-C06-O06
19	U	1268	PGV	O01-C02-C03-O11
26	P	1270	CDL	C44-C45-C46-C47
23	J	60	CHD	C21-C20-C22-C23
21	Y	1522	TGL	CB7-CB8-CB9-C10
23	J	60	CHD	C22-C23-C24-O26
19	A	524	PGV	C24-C25-C26-C27
21	N	1523	TGL	C13-C14-C29-C30
19	A	524	PGV	C26-C27-C28-C29
23	B	1085	CHD	C22-C23-C24-O26
25	T	263	PEK	C4-C5-C6-C7
22	R	1229	PSC	C04-C05-N-C08

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C22-C23-C24-C25
21	N	1523	TGL	OG1-CG1-CG2-OG2
14	N	515	HEA	CAD-CBD-CGD-O1D
19	N	1266	PGV	C9-C10-C11-C12
19	A	521	PGV	C4-C5-C6-C7
21	N	1523	TGL	CA5-CA6-CA7-CA8
23	C	525	CHD	C13-C17-C20-C21
19	N	1524	PGV	C05-C04-O12-P
26	G	269	CDL	C1-CA2-OA2-PA1
23	O	229	CHD	C17-C20-C22-C23
14	A	515	HEA	CAD-CBD-CGD-O2D
21	O	1521	TGL	OG1-CA1-CA2-CA3
26	P	1270	CDL	C55-C56-C57-C58
25	C	264	PEK	C14-C15-C16-C17
25	P	1264	PEK	C14-C15-C16-C17
25	P	1264	PEK	C17-C18-C19-C20
21	B	521	TGL	C20-C21-C22-C23
23	J	60	CHD	C22-C23-C24-O25
21	O	1521	TGL	CC4-CC5-CC6-CC7
25	T	263	PEK	C3-C4-C5-C6
26	G	269	CDL	C52-C51-CB5-OB6
14	A	515	HEA	C2A-C3A-CMA-OMA
19	A	524	PGV	C3-C4-C5-C6
21	N	1523	TGL	C14-C29-C30-C31
22	R	1229	PSC	C12-C13-C14-C15
19	C	267	PGV	C05-C04-O12-P
26	T	1269	CDL	CB4-CB3-OB5-PB2
27	P	272	DMU	C34-C37-C40-C43
27	C	272	DMU	C25-C28-C31-C34
25	C	264	PEK	C16-C17-C18-C19
22	R	1229	PSC	C04-C05-N-C07
21	N	1523	TGL	CA9-C20-C21-C22
21	L	522	TGL	OG3-CC1-CC2-CC3
26	C	270	CDL	C12-C11-CA5-OA6
19	A	524	PGV	C23-C24-C25-C26
25	P	1264	PEK	O01-C1-C2-C3
26	T	1269	CDL	OB5-CB3-CB4-CB6
14	A	515	HEA	CAD-CBD-CGD-O1D
21	L	522	TGL	C21-C20-CA9-CA8
21	Y	1522	TGL	CC6-CC7-CC8-CC9
22	R	1229	PSC	C26-C27-C28-C29
26	G	269	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
14	N	516	HEA	C3B-C11-C12-C13
26	C	270	CDL	O1-C1-CA2-OA2
21	L	522	TGL	C23-C24-C25-C26
21	Y	1522	TGL	C13-C14-C29-C30
19	N	1524	PGV	O01-C1-C2-C3
19	N	1266	PGV	O03-C19-C20-C21
25	C	264	PEK	O01-C1-C2-C3
14	N	516	HEA	CAA-CBA-CGA-O1A
21	B	521	TGL	CB6-CB7-CB8-CB9
19	A	524	PGV	C4-C5-C6-C7
21	D	523	TGL	CB6-CB7-CB8-CB9
19	U	1268	PGV	O01-C1-C2-C3
14	N	515	HEA	CAD-CBD-CGD-O2D
14	A	516	HEA	C26-C15-C16-C17
19	P	1267	PGV	O03-C01-C02-O01
21	O	1521	TGL	OG1-CG1-CG2-OG2
21	Y	1522	TGL	OG1-CG1-CG2-OG2
21	N	1523	TGL	C17-C18-C19-C33
21	N	1523	TGL	CC6-CC7-CC8-CC9
19	A	524	PGV	O12-C04-C05-C06
19	P	1267	PGV	C27-C28-C29-C30
26	P	1270	CDL	C79-C80-C81-C82
21	L	522	TGL	C11-C10-CB9-CB8
19	C	268	PGV	C05-C04-O12-P
19	U	1268	PGV	C05-C04-O12-P
19	N	1524	PGV	O02-C1-C2-C3
22	B	229	PSC	C6-C7-C8-C9
21	O	1521	TGL	C18-C19-C33-C34
22	B	229	PSC	C7-C8-C9-C10
26	G	269	CDL	C32-C31-CA7-OA9
26	C	270	CDL	C12-C11-CA5-OA7
25	C	265	PEK	C24-C25-C26-C27
21	L	522	TGL	OA1-CA1-CA2-CA3
21	L	522	TGL	CB5-CB6-CB7-CB8
25	C	264	PEK	O02-C1-C2-C3
22	R	1229	PSC	O03-C19-C20-C21
21	L	522	TGL	C29-C30-C31-C32
19	A	524	PGV	O03-C01-C02-C03
19	A	524	PGV	C9-C10-C11-C12
25	P	1264	PEK	O03-C01-C02-C03
14	N	515	HEA	CAA-CBA-CGA-O2A
14	N	516	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	A	524	PGV	O03-C19-C20-C21
25	P	1264	PEK	O02-C1-C2-C3
19	U	1268	PGV	O02-C1-C2-C3
27	P	272	DMU	O5-C4-C57-O61
25	T	1265	PEK	C34-C35-C36-C37
21	L	522	TGL	OC1-CC1-CC2-CC3
14	A	515	HEA	CAA-CBA-CGA-O1A
21	N	1523	TGL	CB5-CB6-CB7-CB8

There are no ring outliers.

38 monomers are involved in 366 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	265	PEK	13	0
21	N	1523	TGL	14	0
23	O	229	CHD	3	0
27	C	272	DMU	4	0
19	N	1524	PGV	7	0
25	P	1264	PEK	6	0
27	P	272	DMU	2	0
26	G	269	CDL	34	0
26	C	270	CDL	20	0
14	A	515	HEA	8	0
23	B	1085	CHD	4	0
25	T	263	PEK	14	0
23	W	1059	CHD	3	0
23	C	271	CHD	2	0
22	R	1229	PSC	20	0
23	P	1271	CHD	5	0
14	N	516	HEA	2	0
21	Y	1522	TGL	20	0
23	J	60	CHD	8	0
22	B	229	PSC	20	0
19	U	1268	PGV	4	0
19	C	267	PGV	4	0
21	B	521	TGL	4	0
25	G	1263	PEK	19	0
19	P	1267	PGV	3	0
25	T	1265	PEK	19	0
21	D	523	TGL	10	0
26	P	1270	CDL	27	0
19	A	521	PGV	2	0

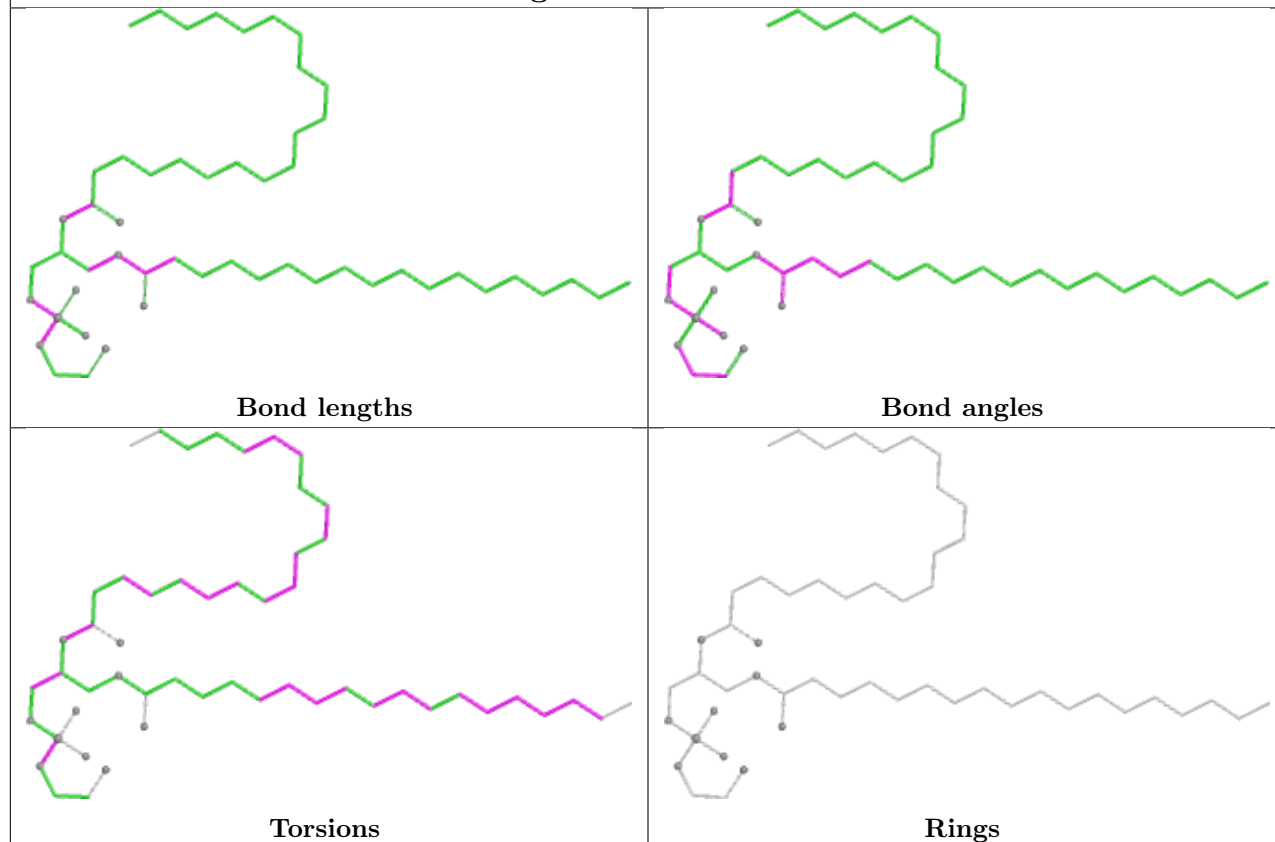
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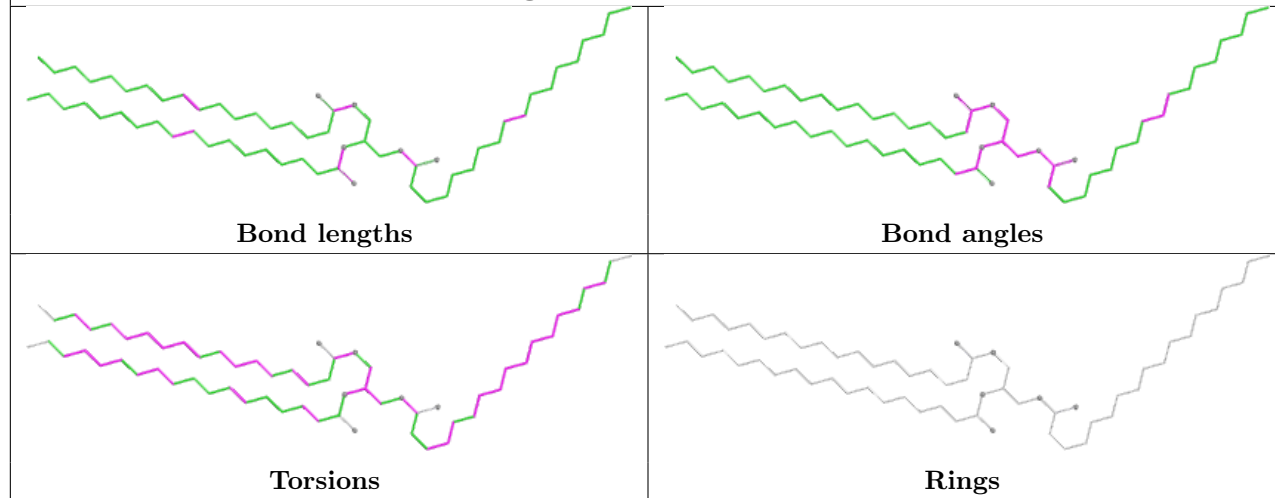
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	264	PEK	9	0
19	A	524	PGV	14	0
21	O	1521	TGL	5	0
21	L	522	TGL	15	0
26	T	1269	CDL	30	0
14	A	516	HEA	4	0
19	C	268	PGV	6	0
14	N	515	HEA	3	0
23	C	525	CHD	2	0

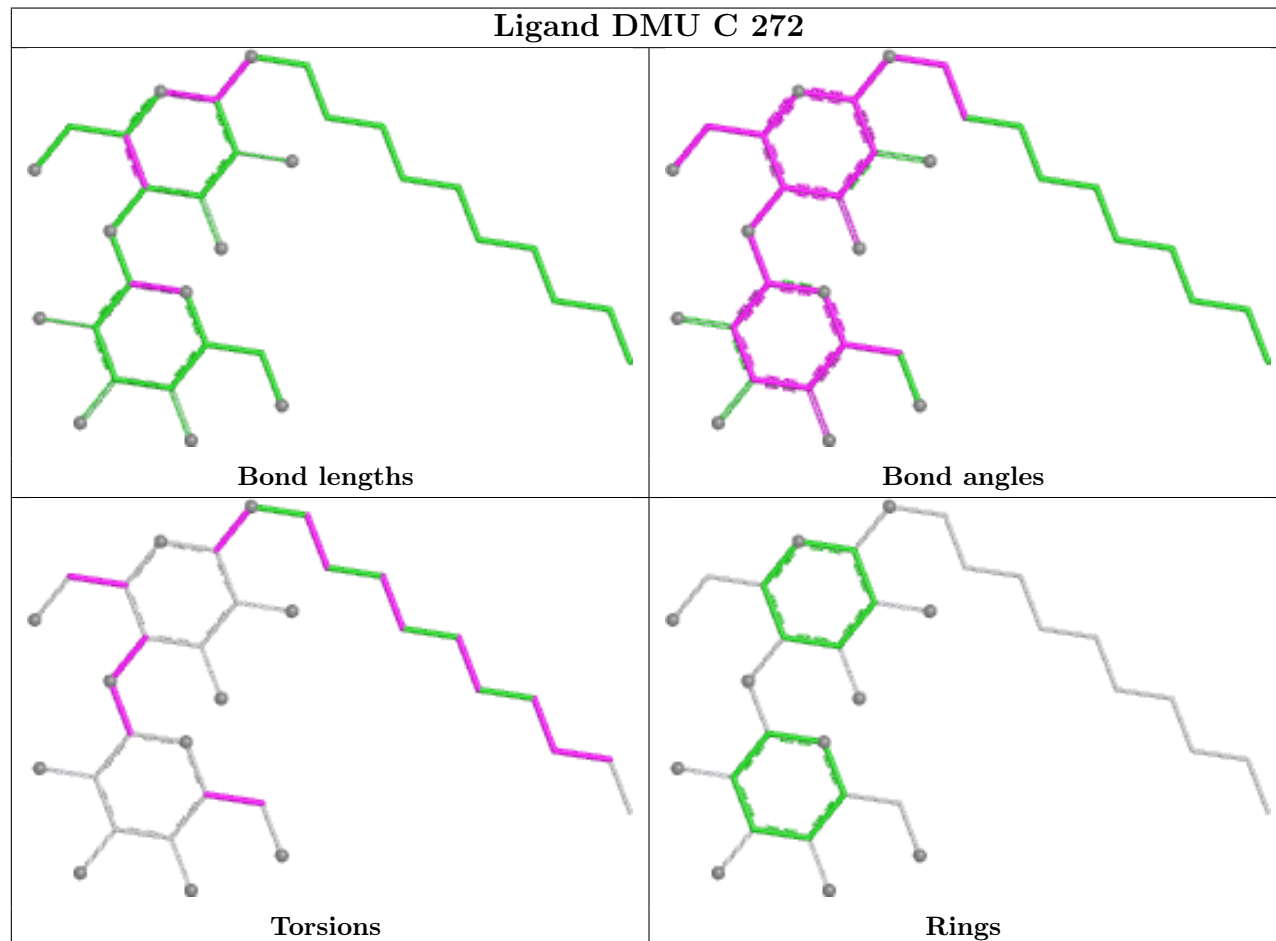
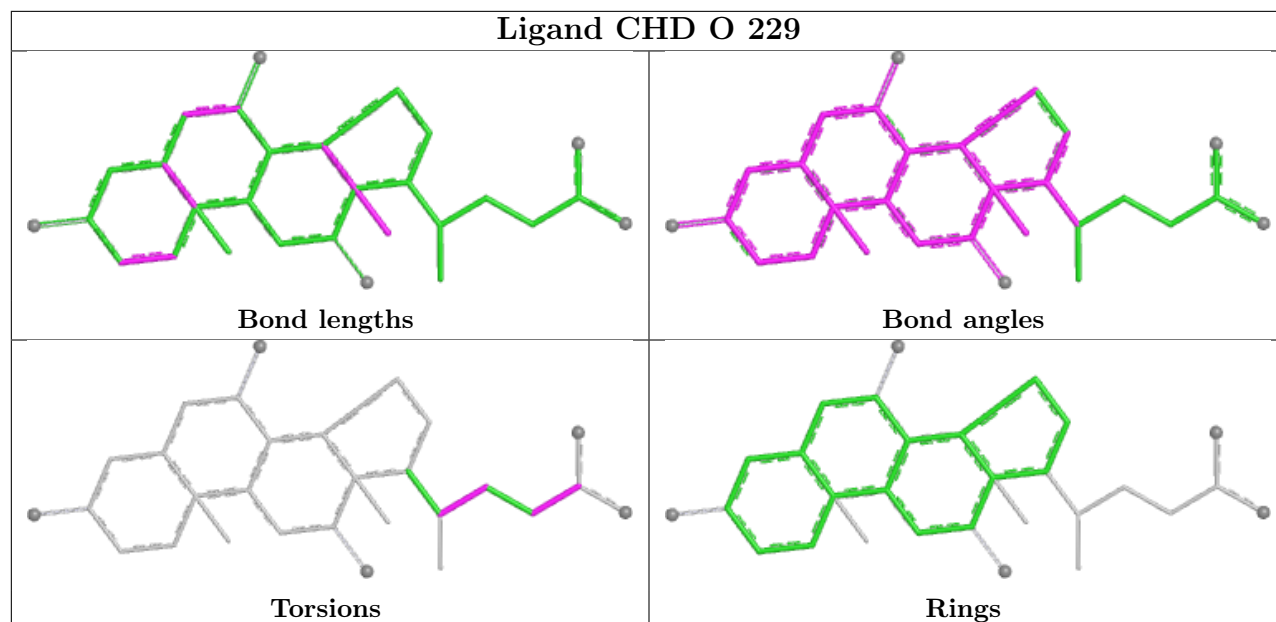
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

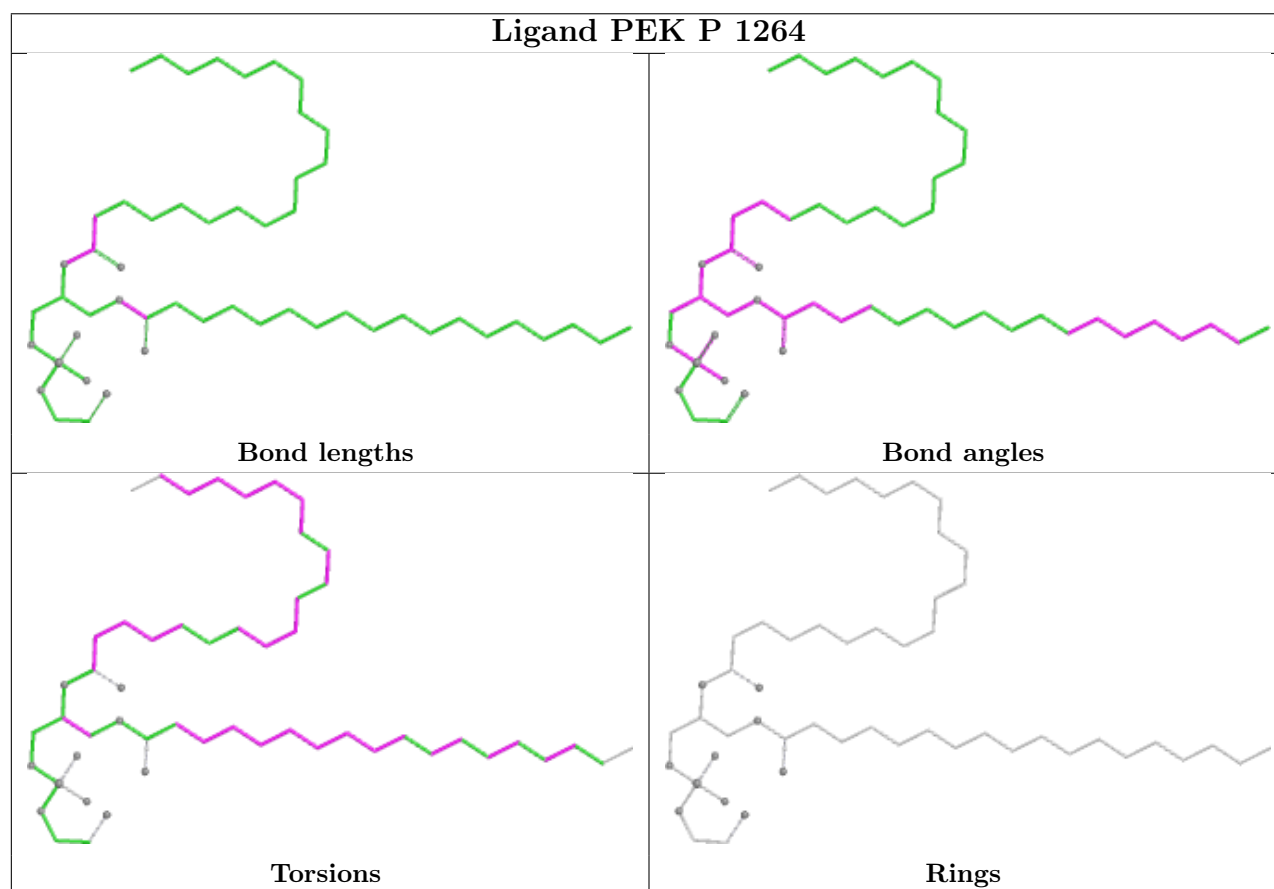
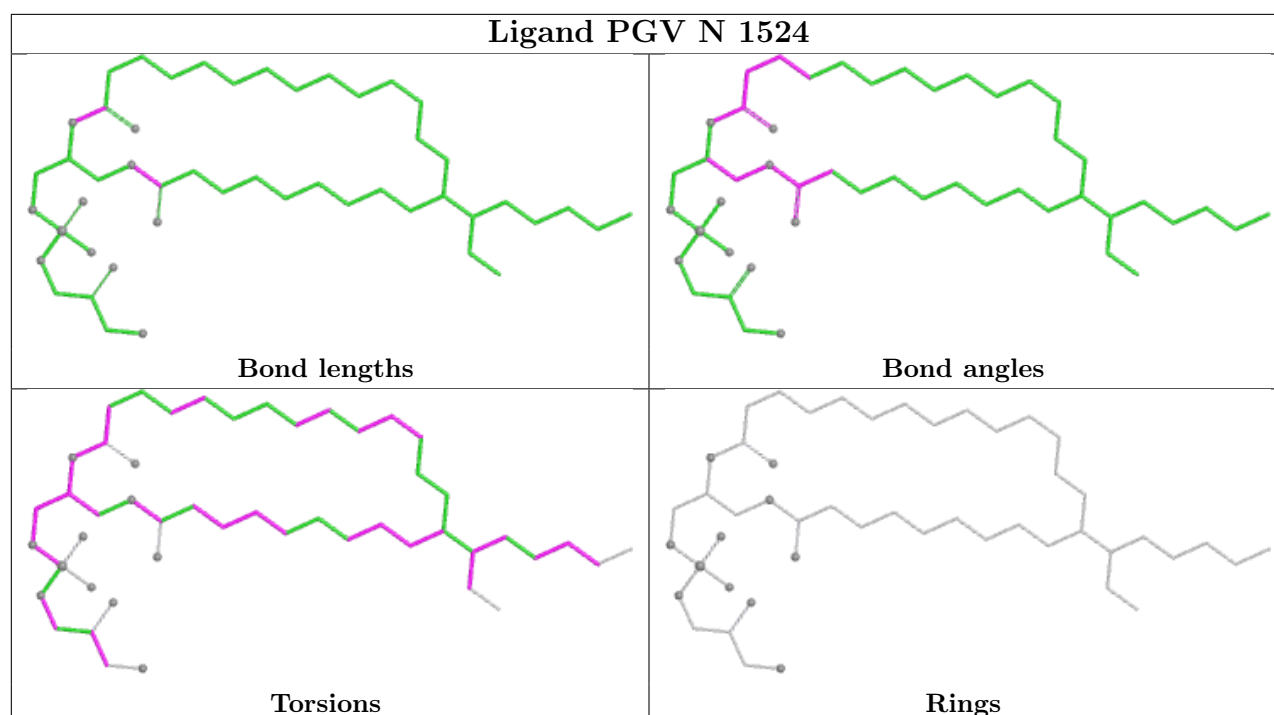
Ligand PEK C 265

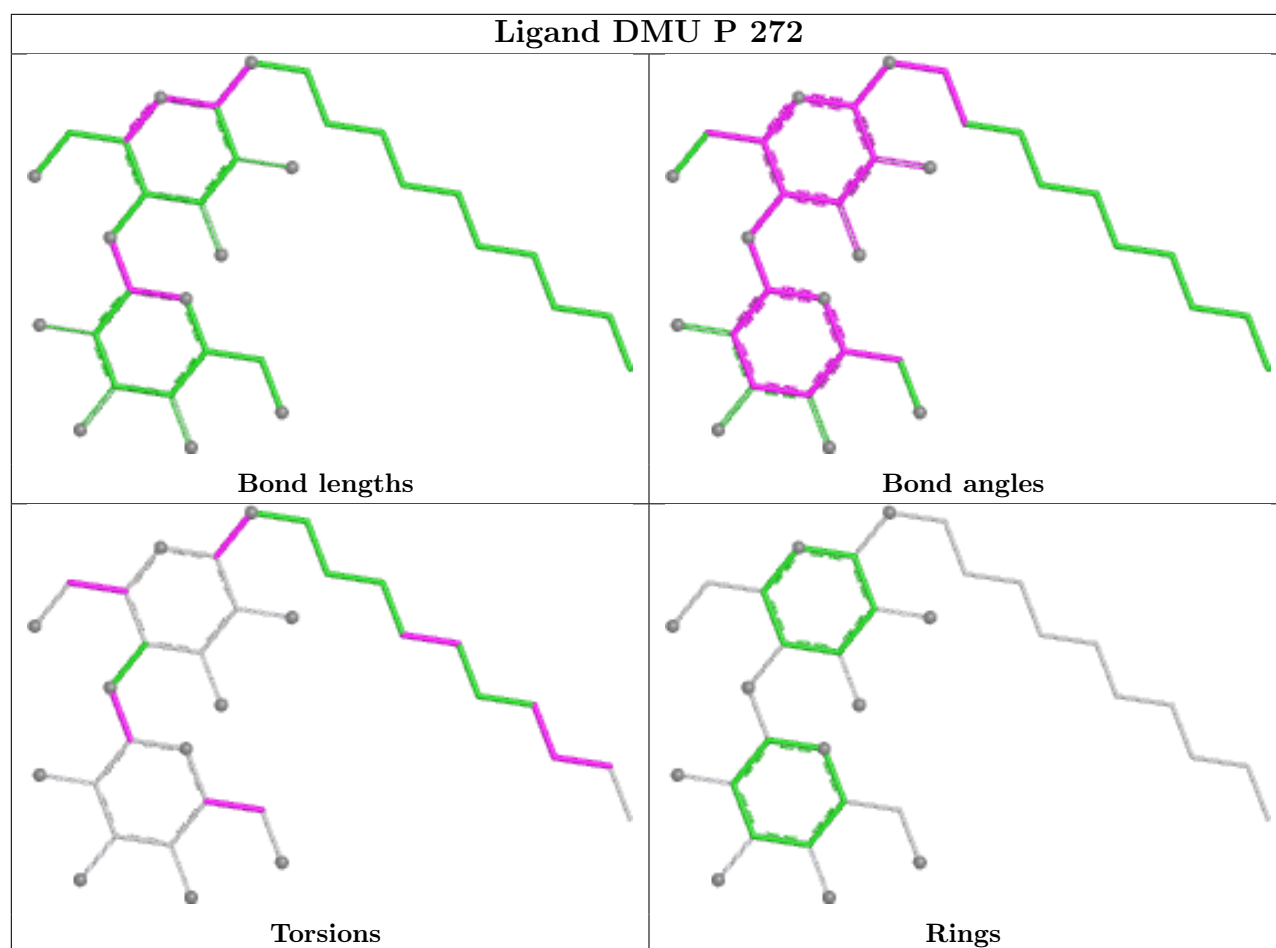


Ligand TGL N 1523

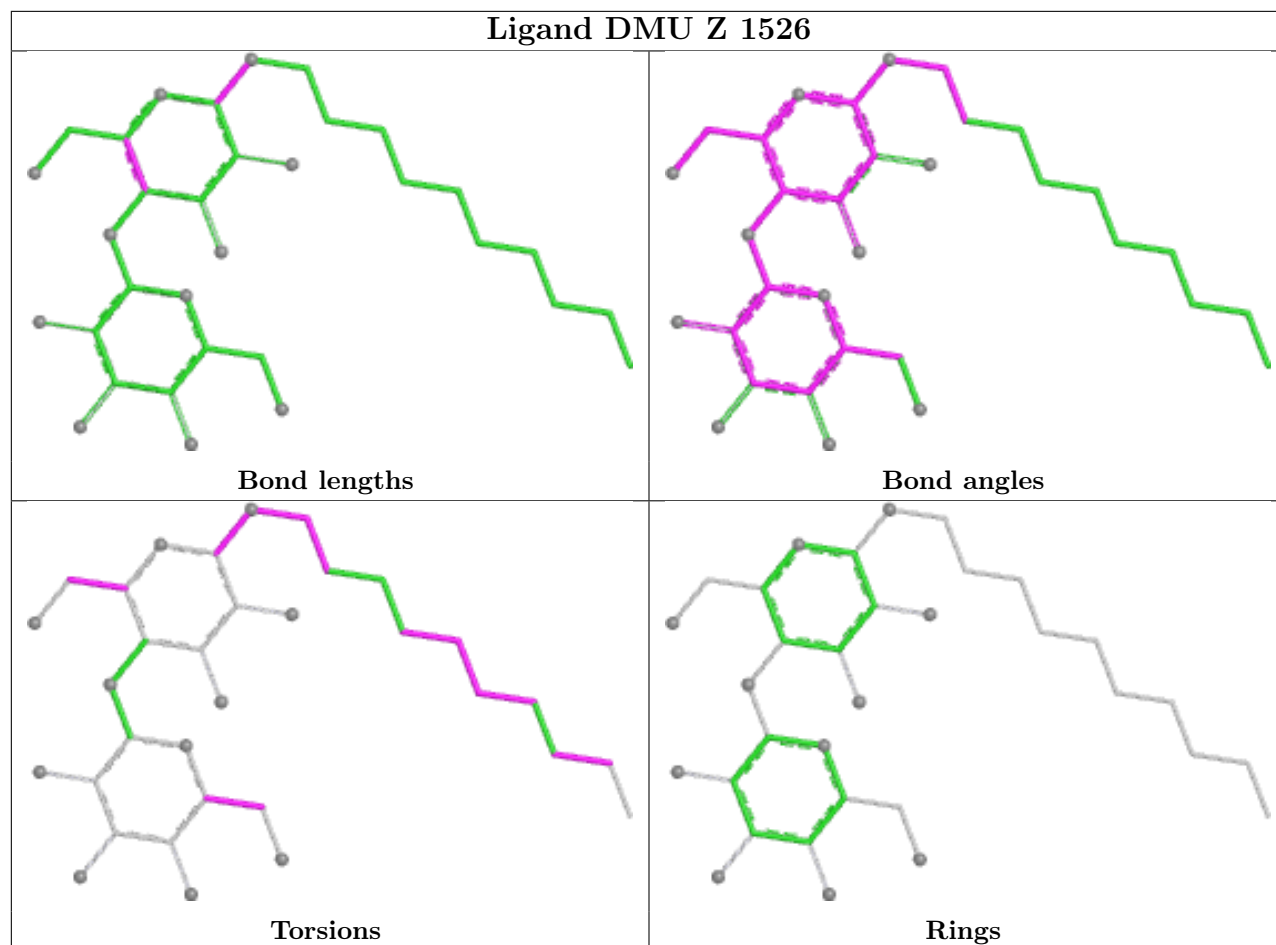




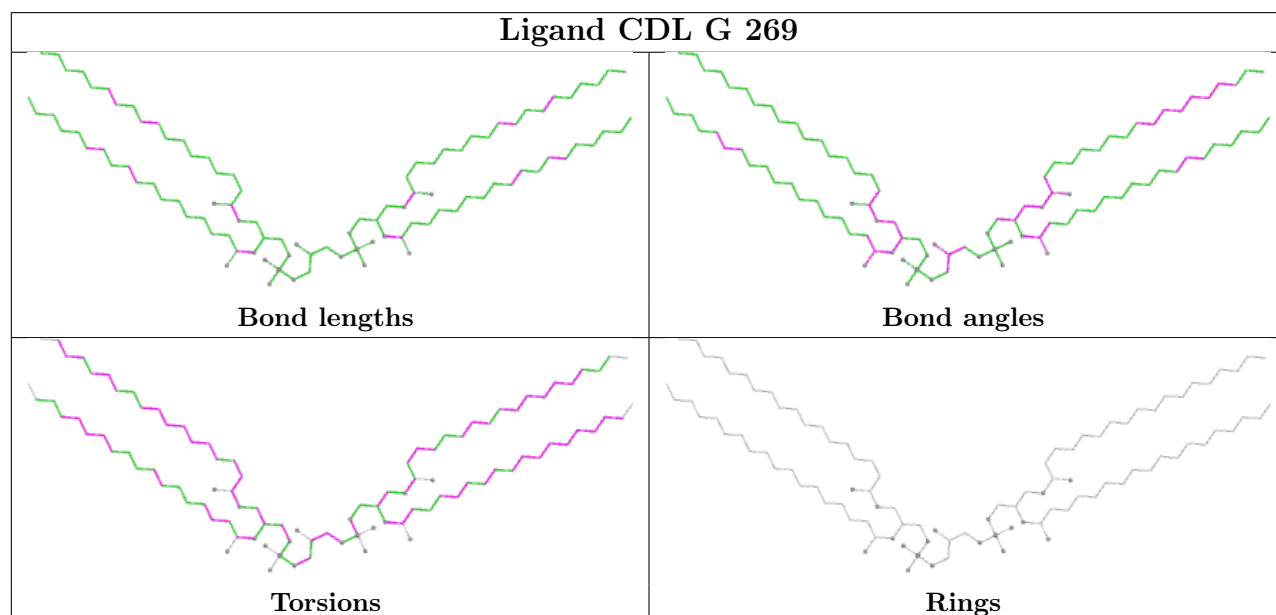


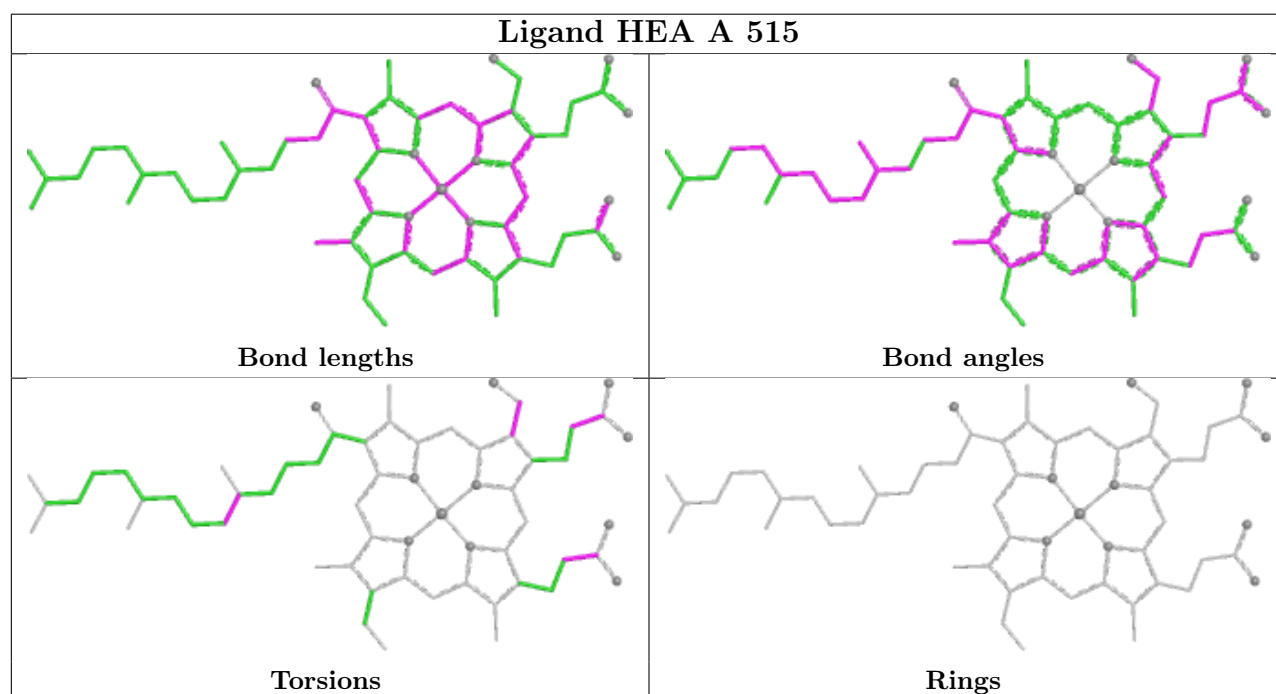
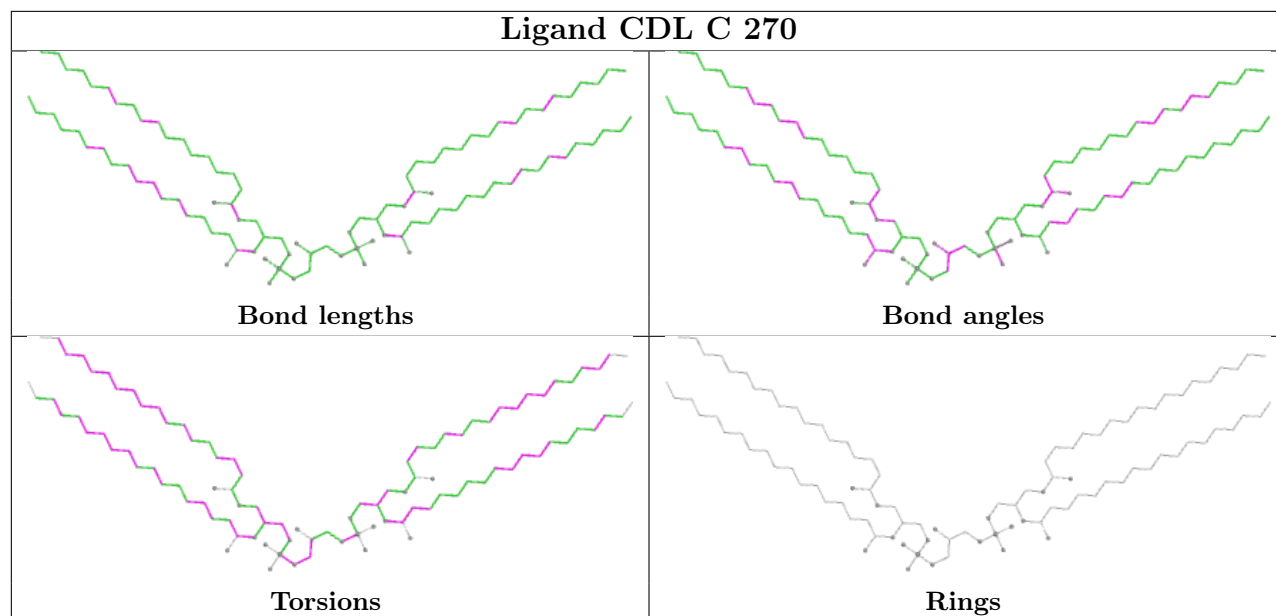


Ligand DMU Z 1526

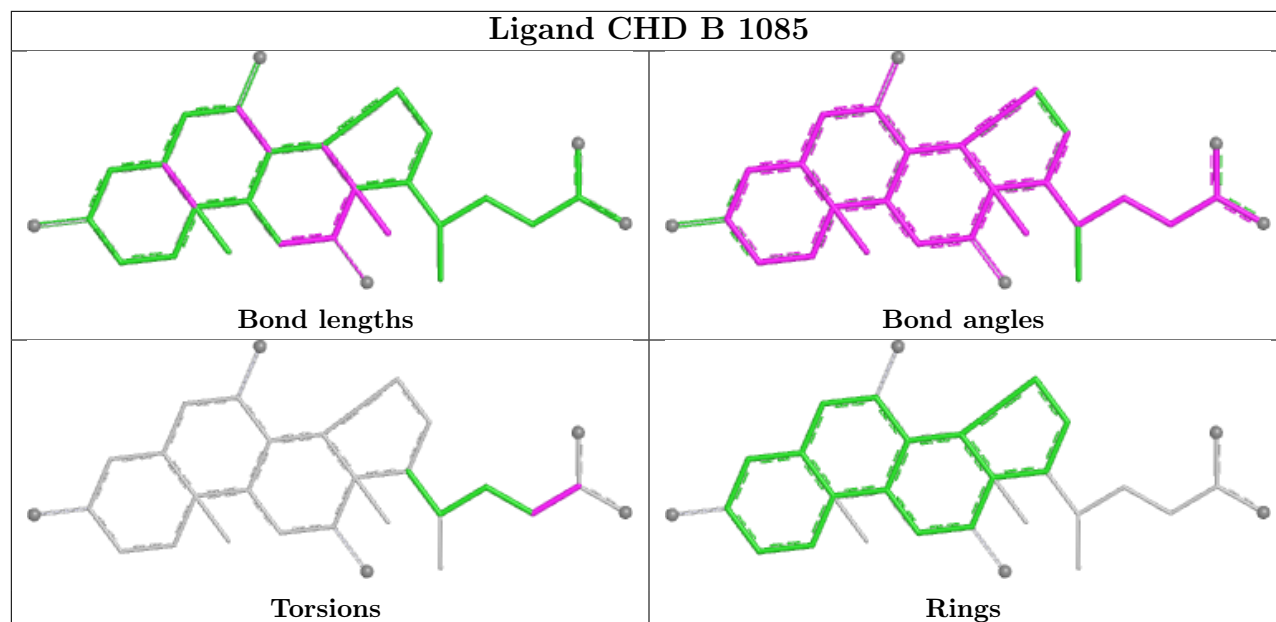


Ligand CDL G 269

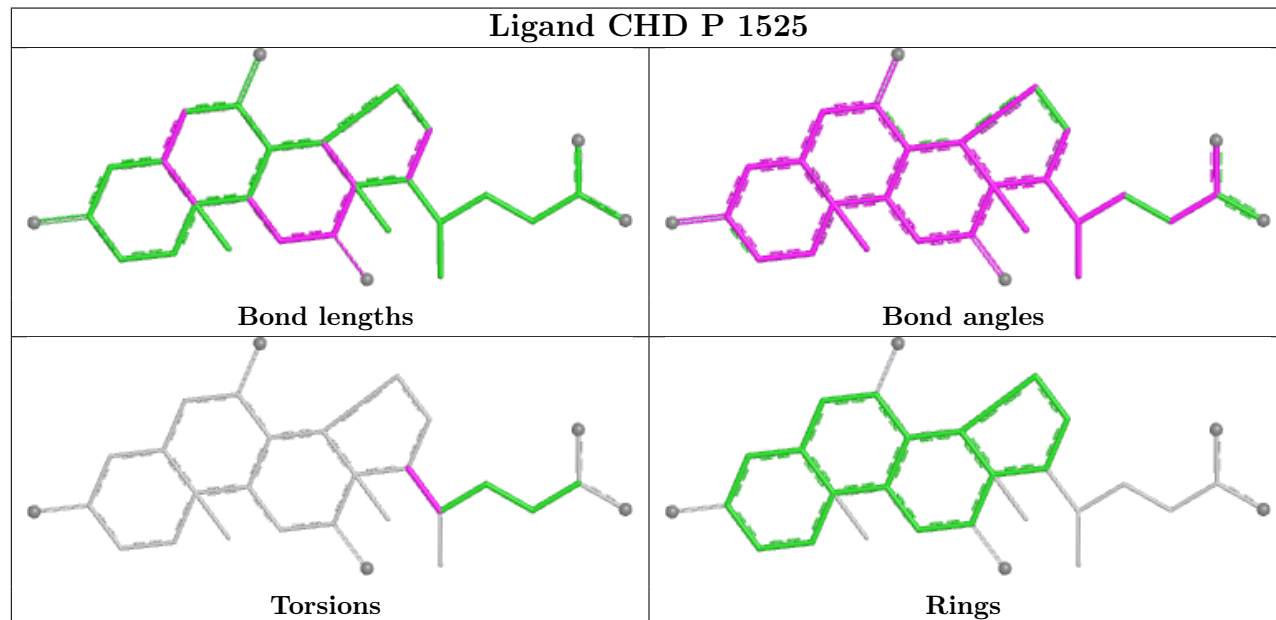




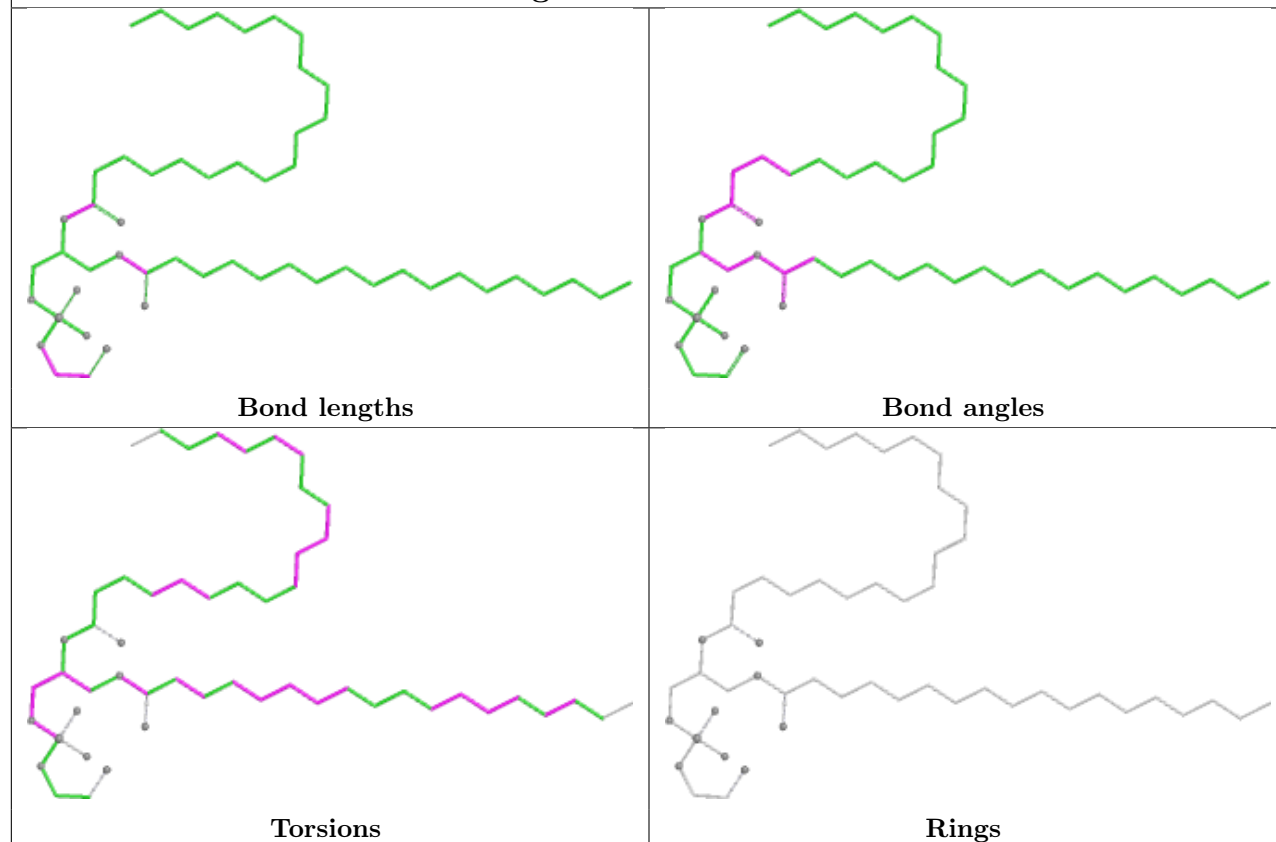
Ligand CHD B 1085



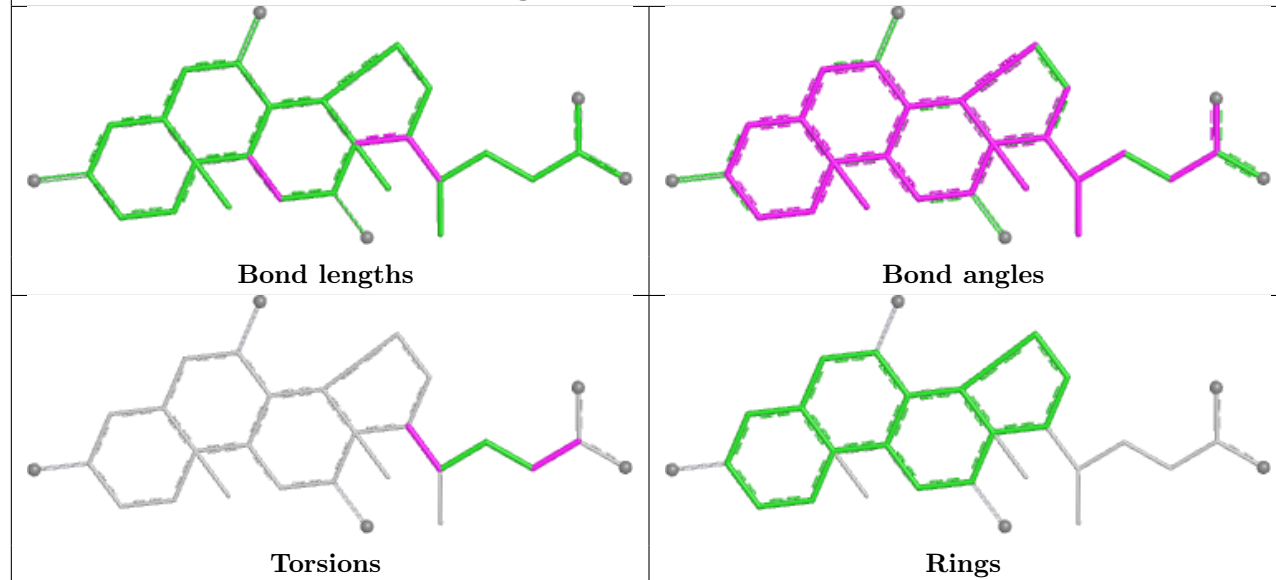
Ligand CHD P 1525

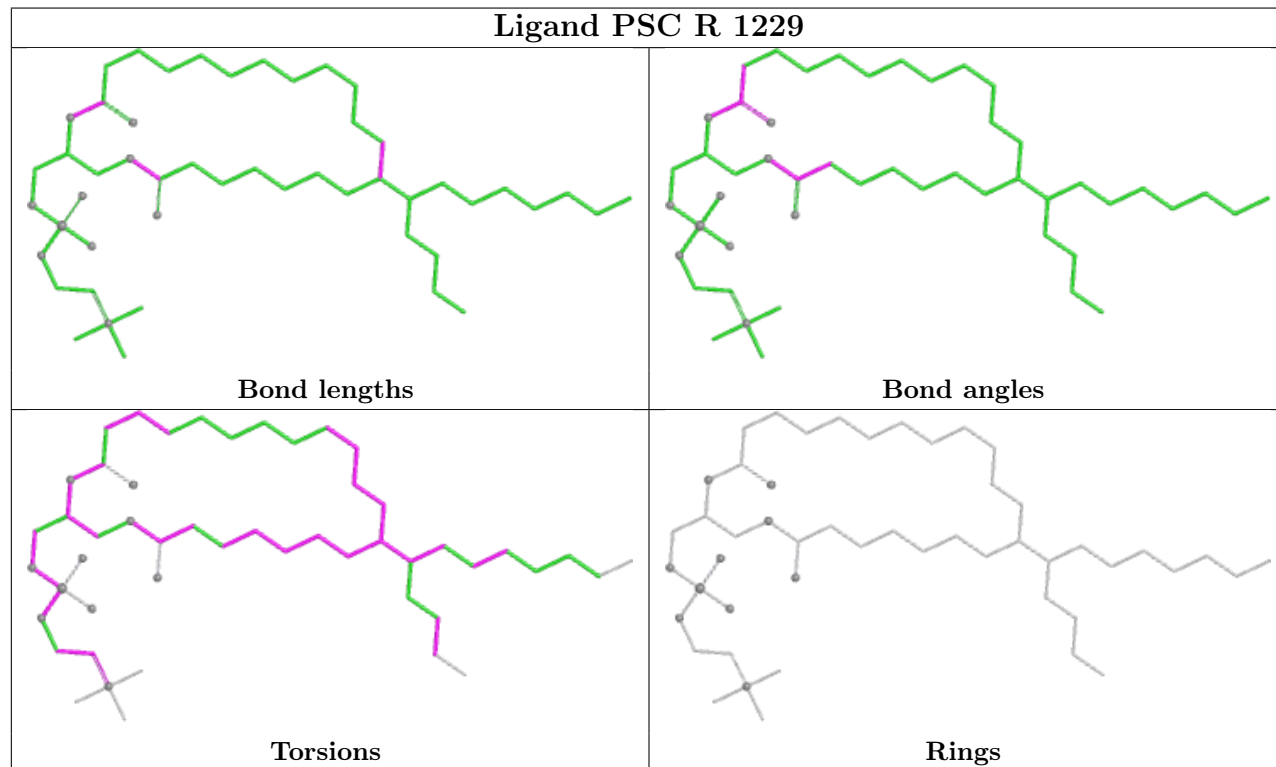
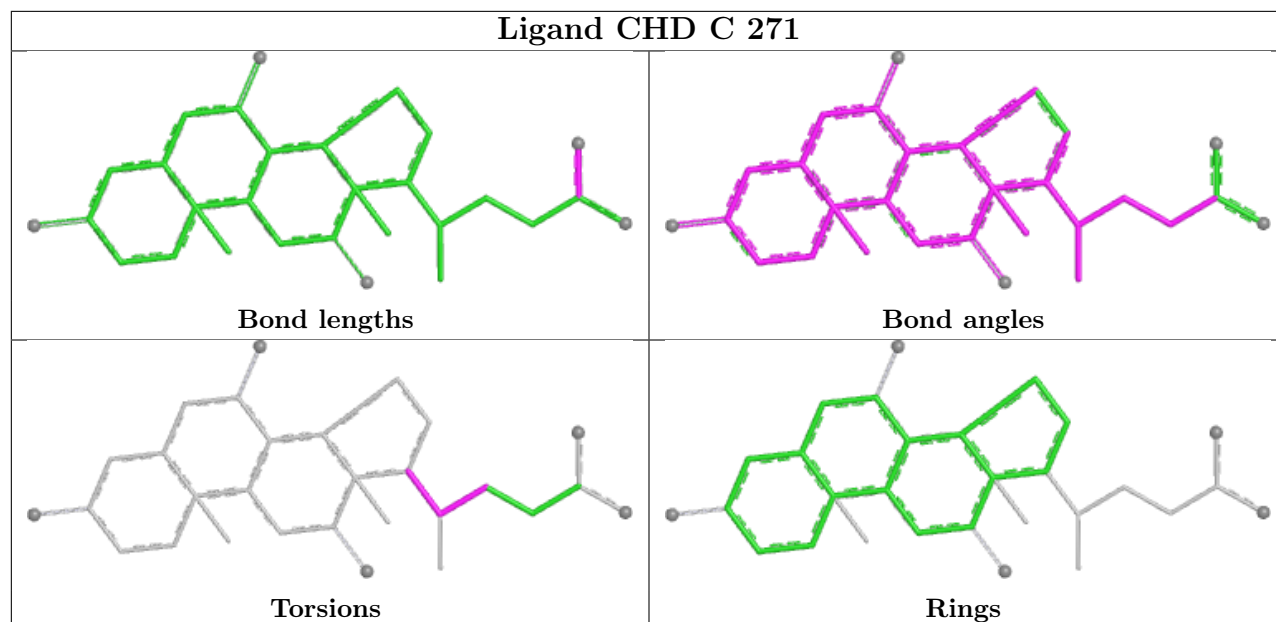


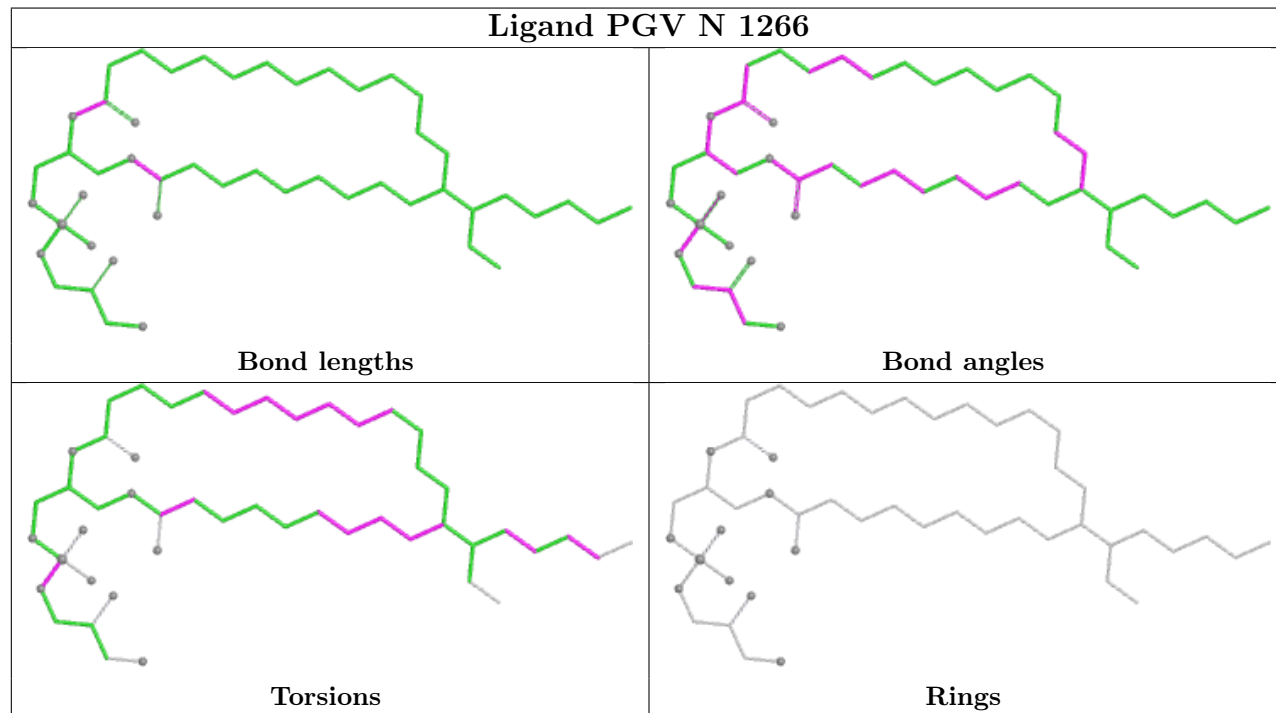
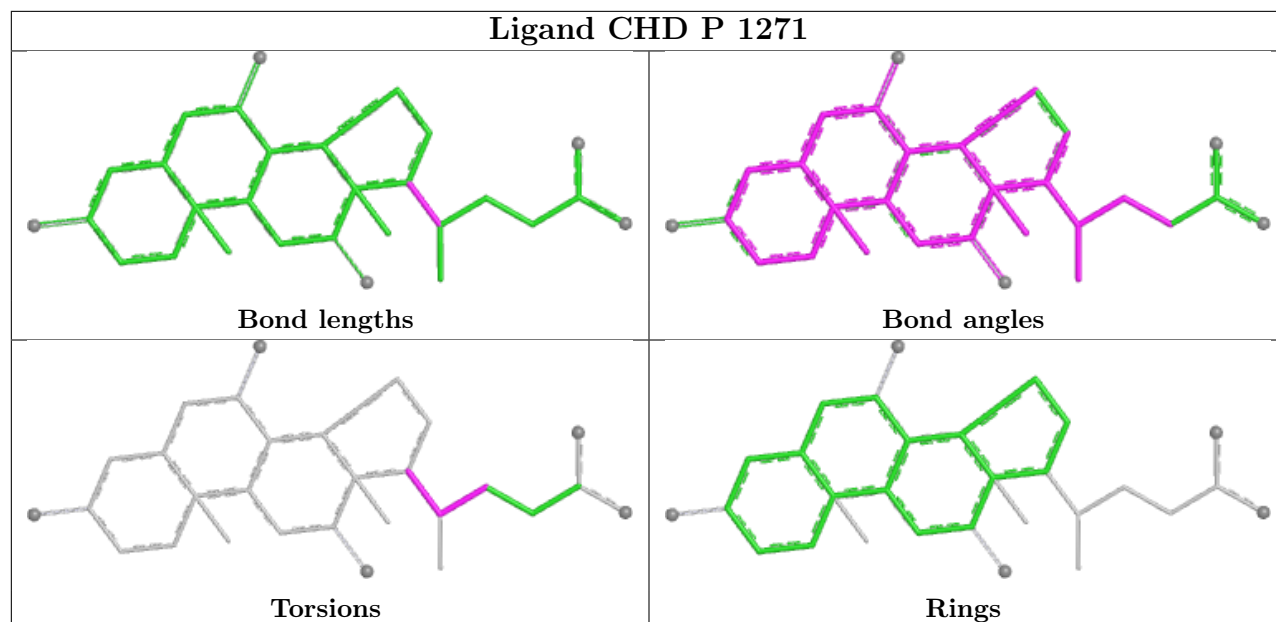
Ligand PEK T 263

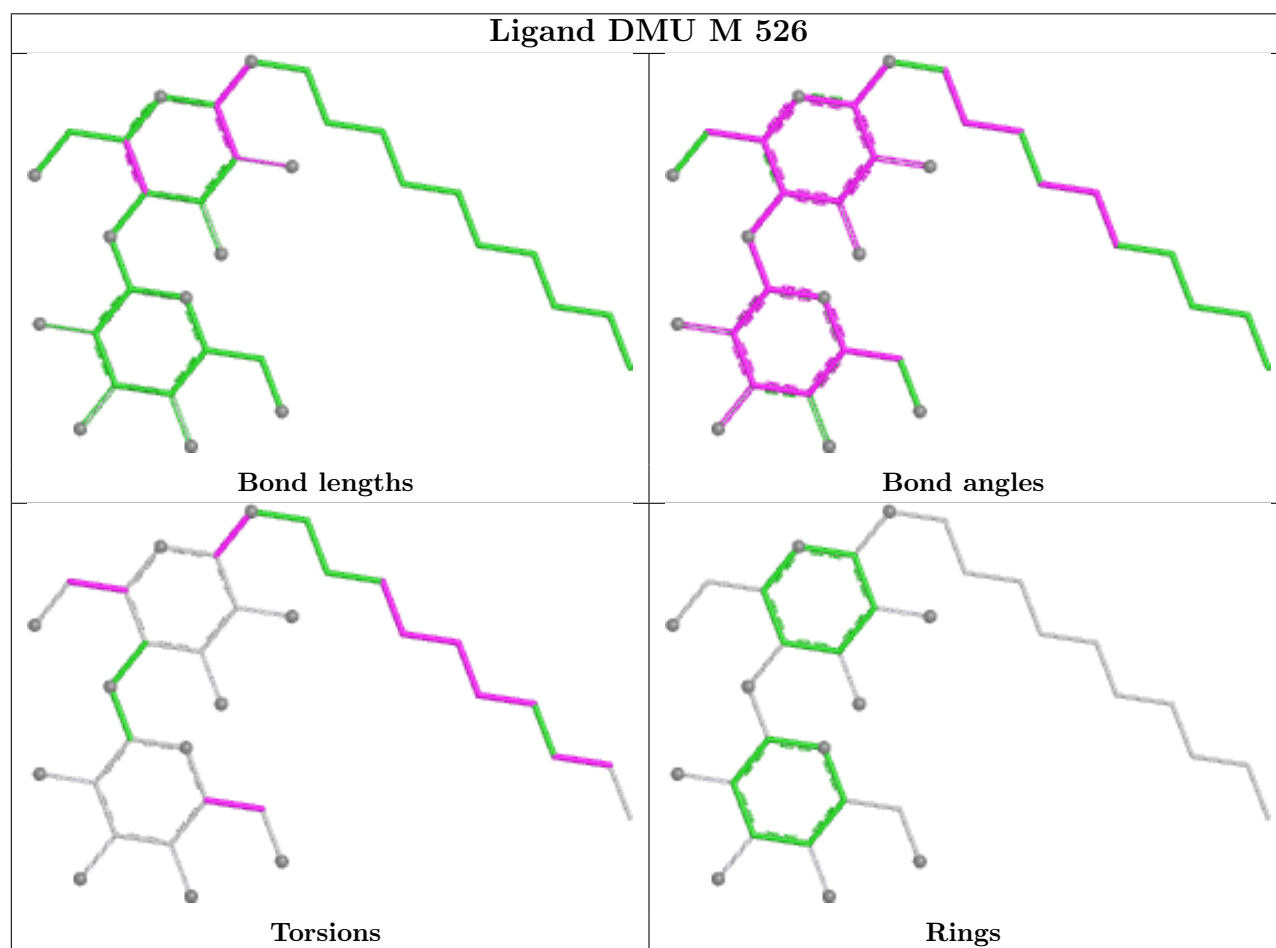
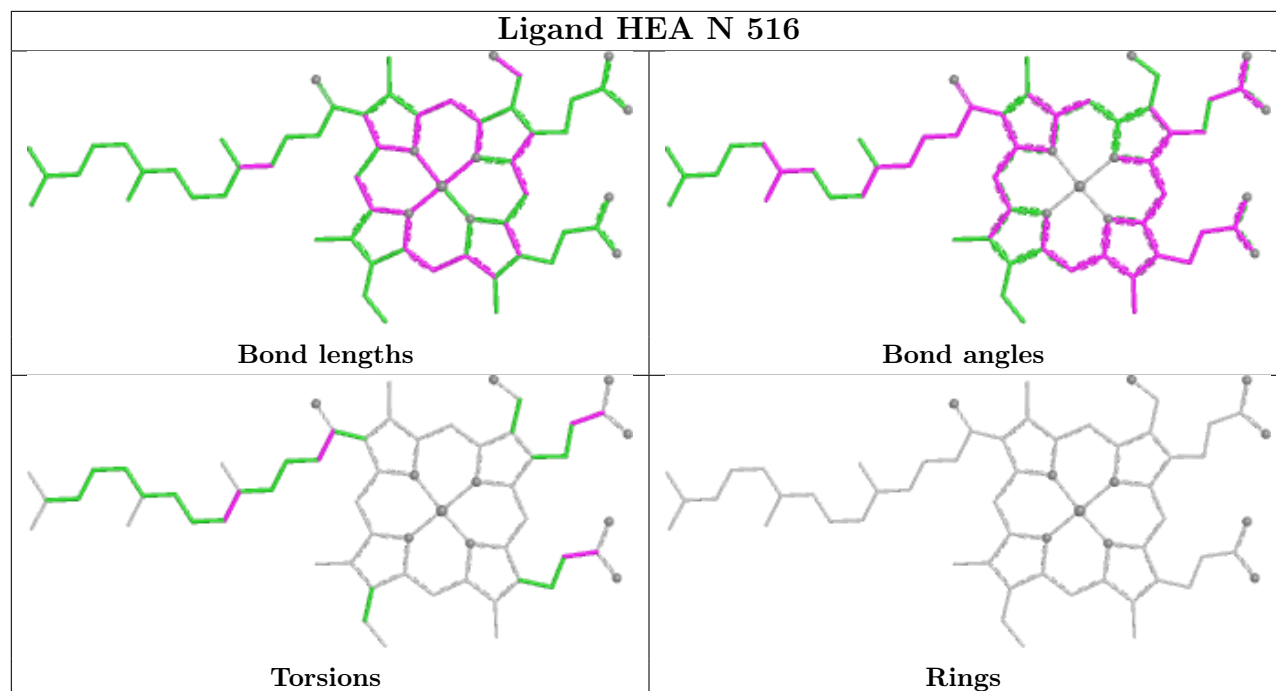


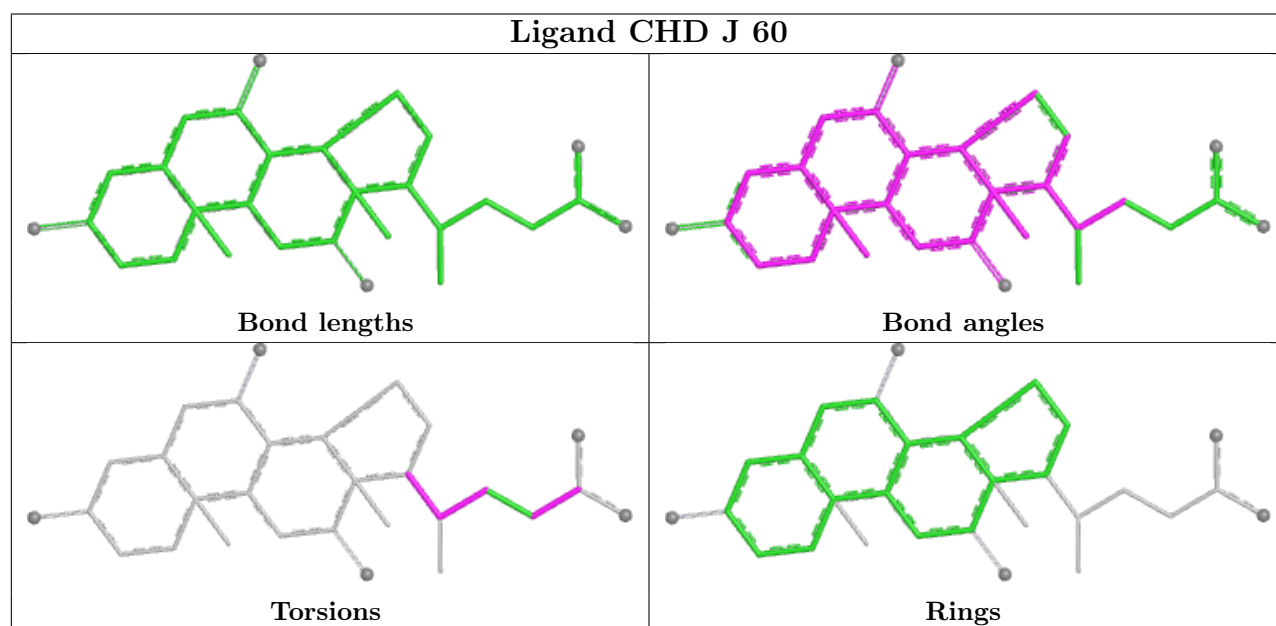
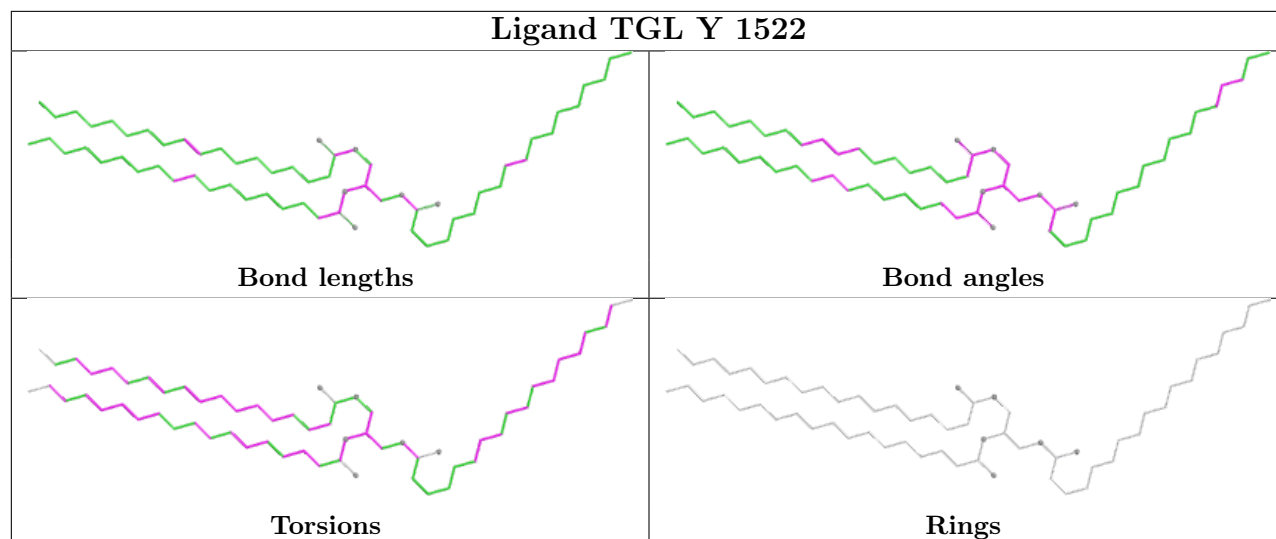
Ligand CHD W 1059



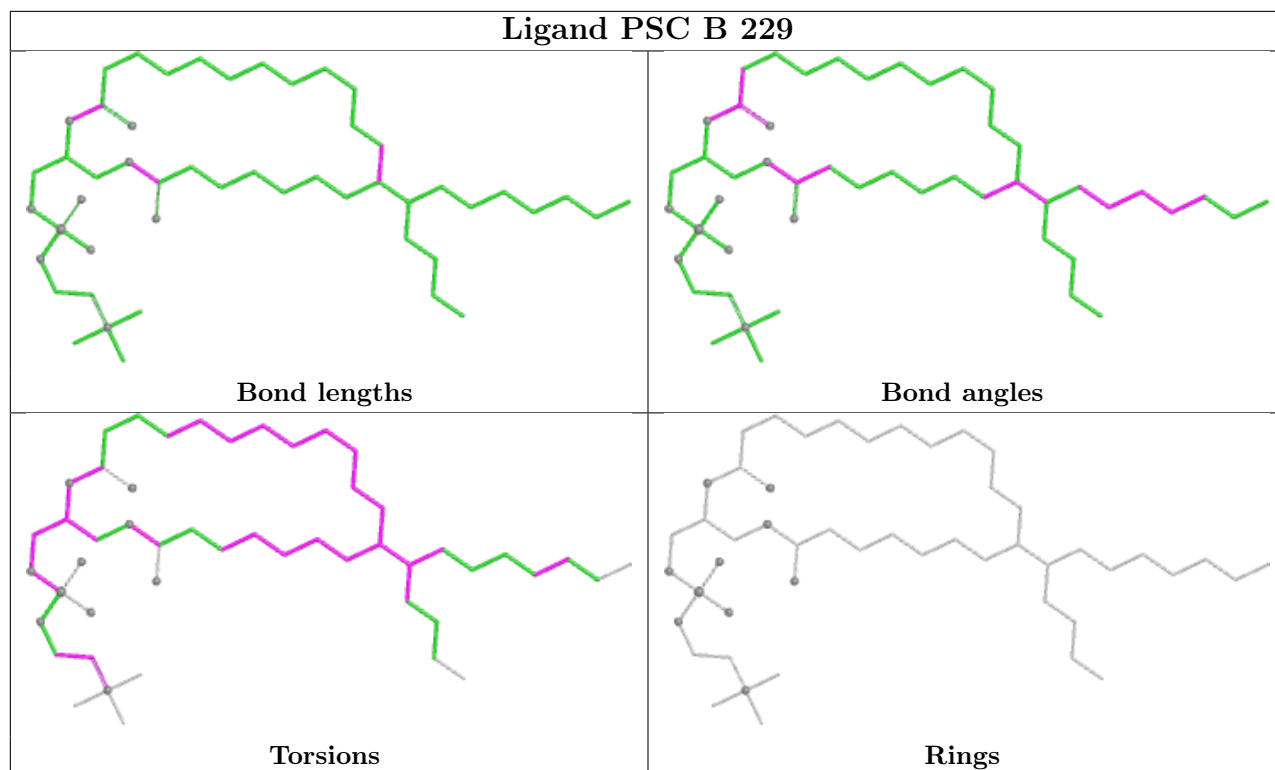




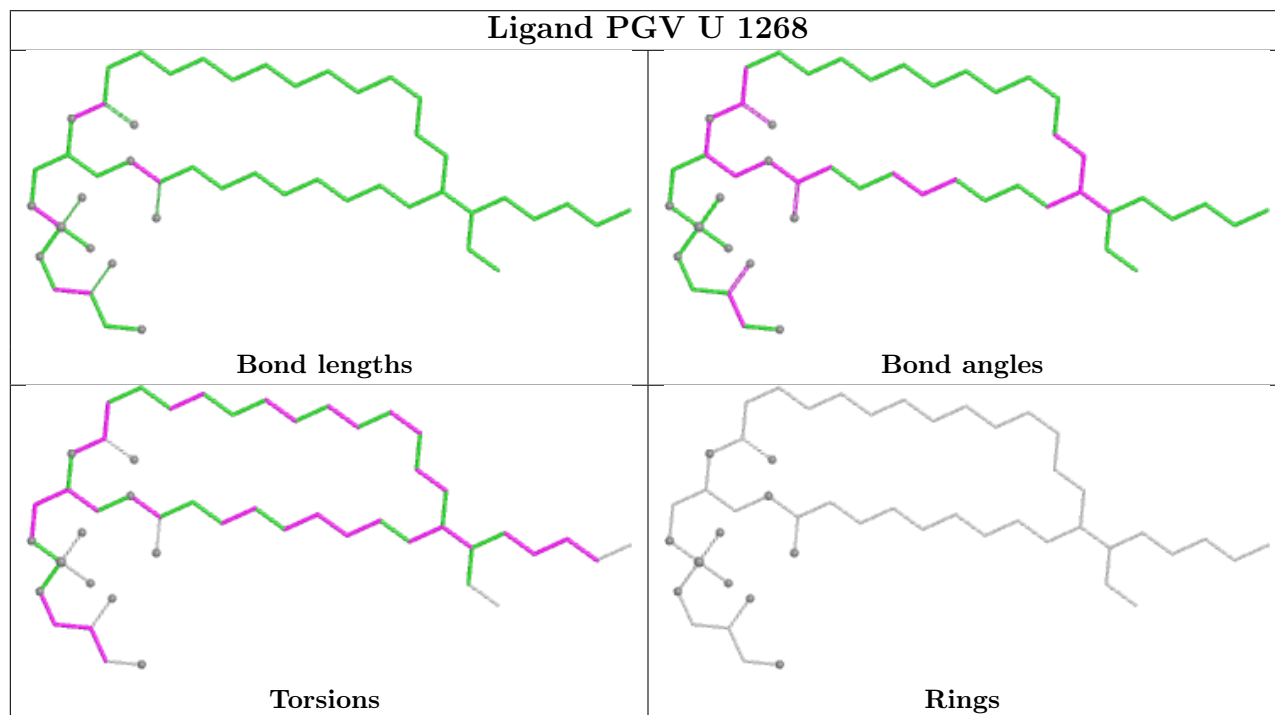


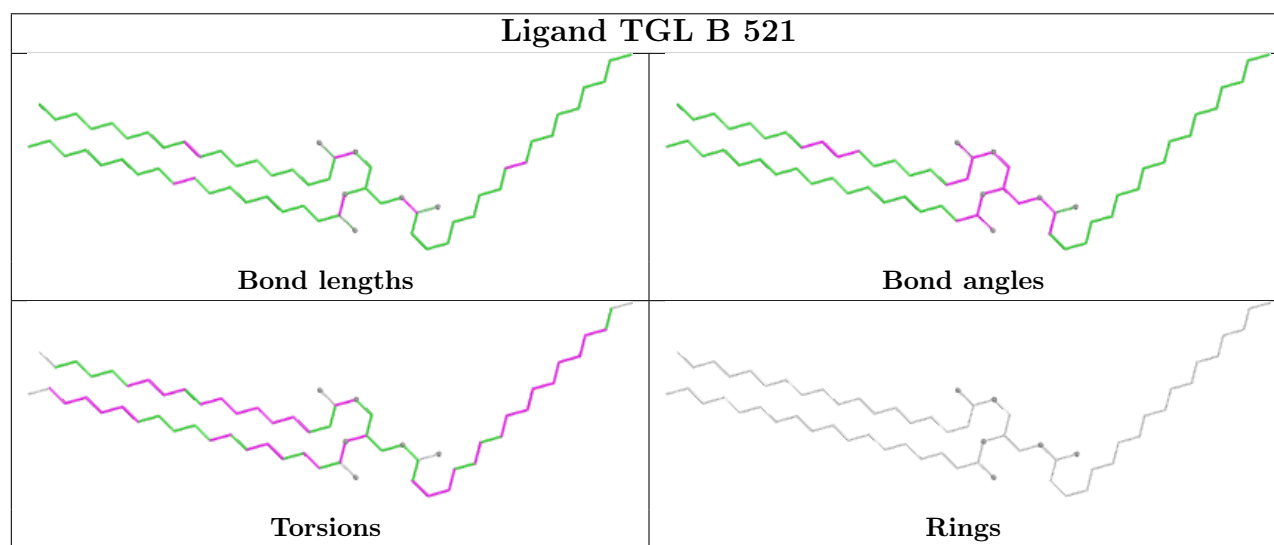
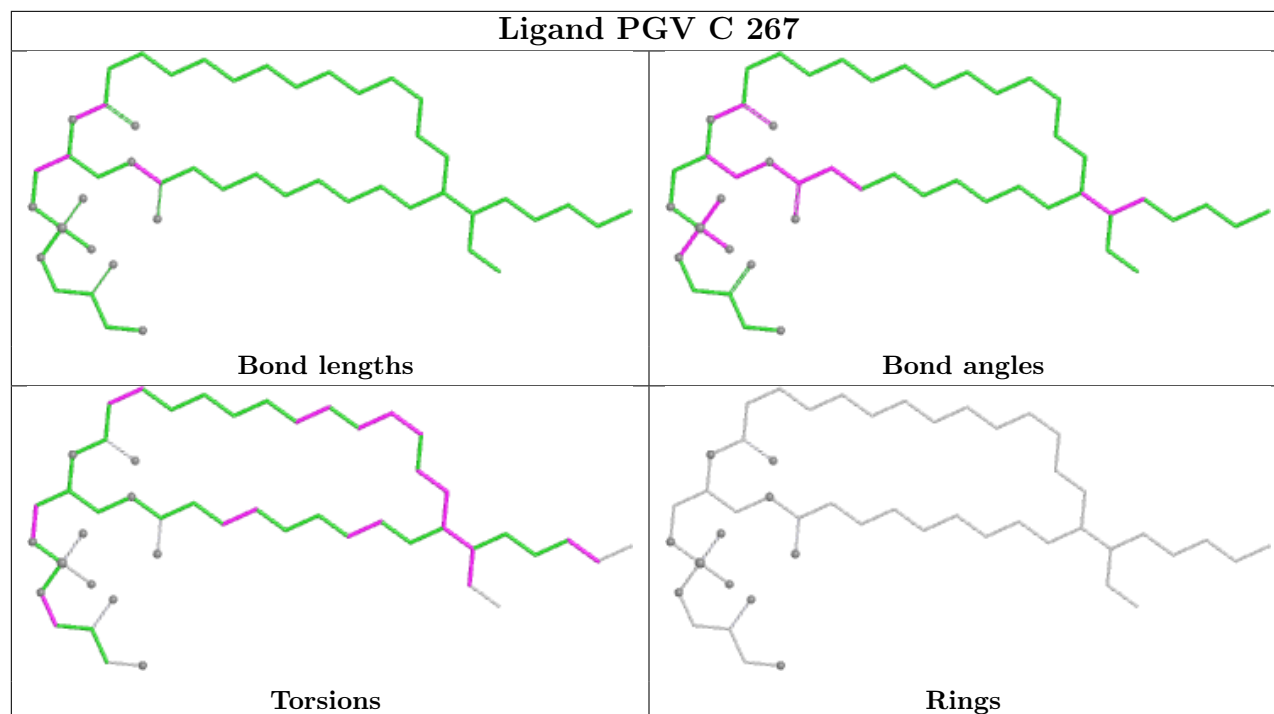


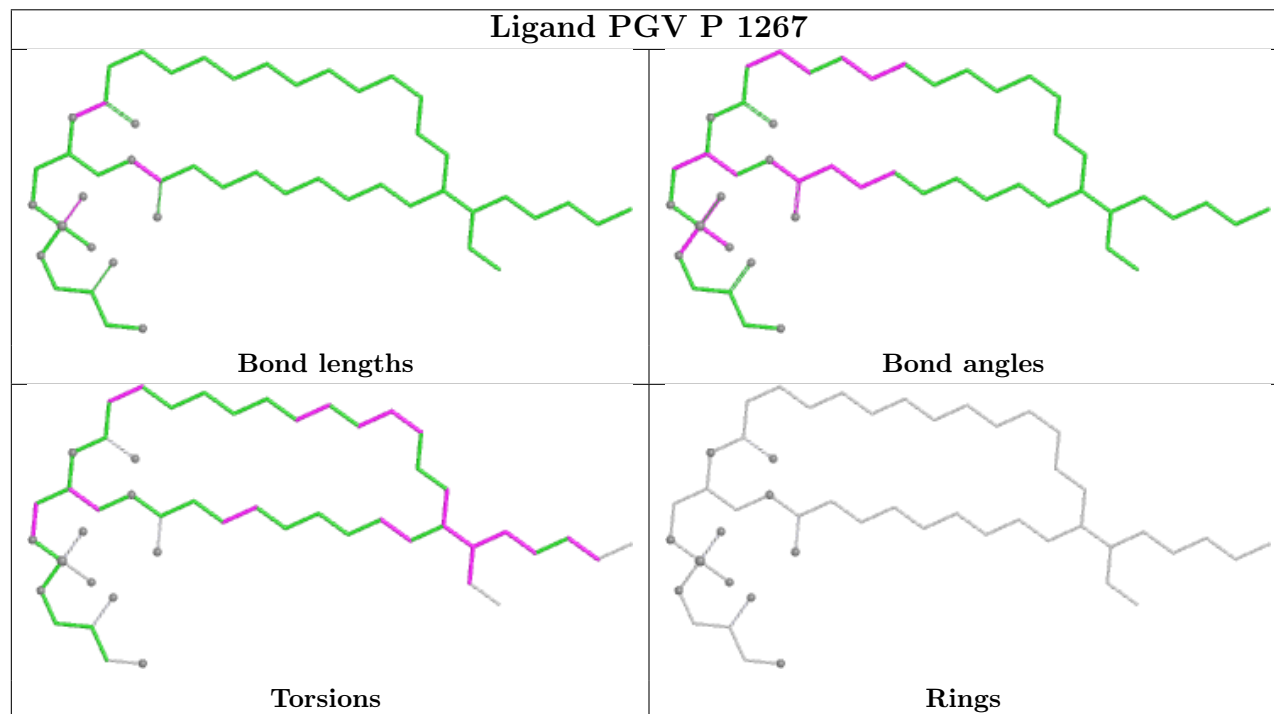
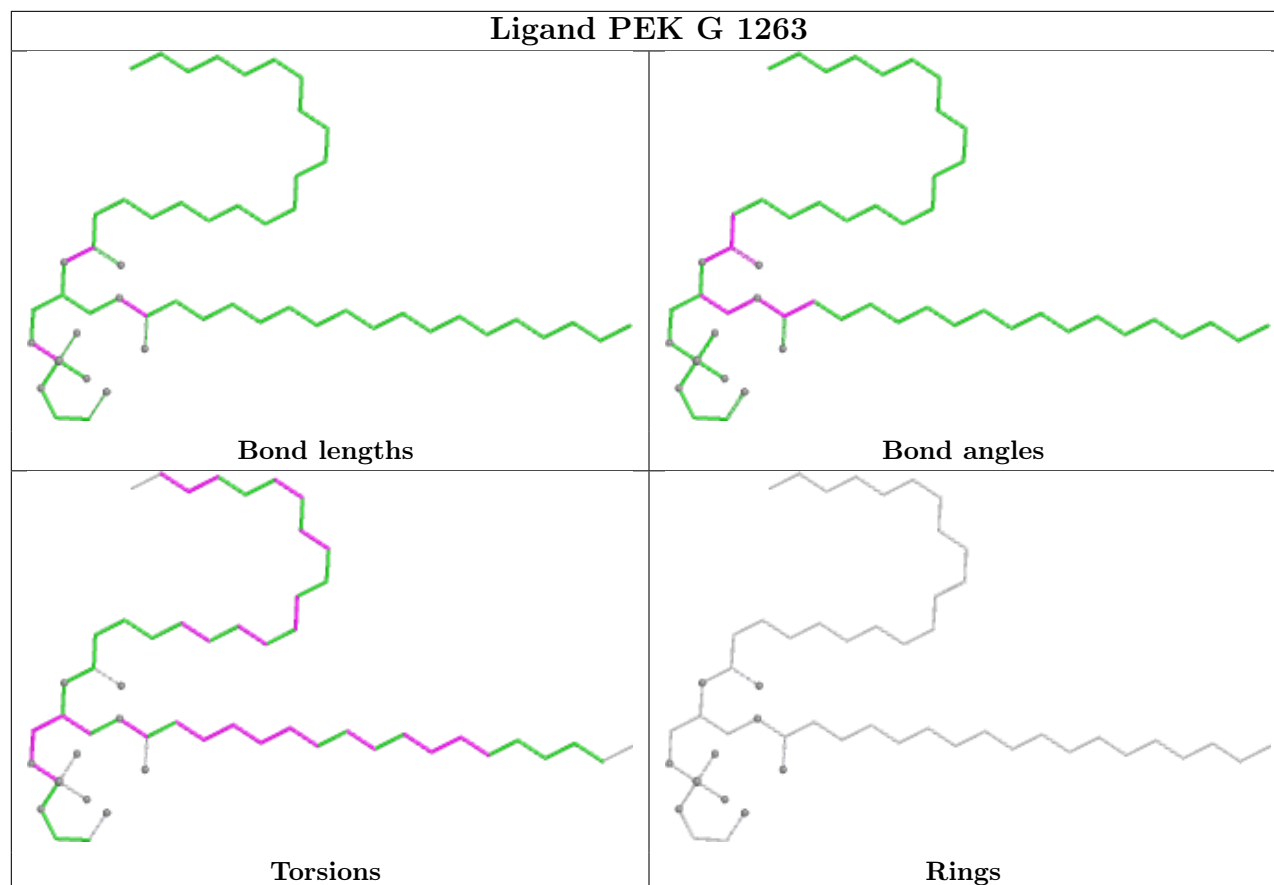
Ligand PSC B 229

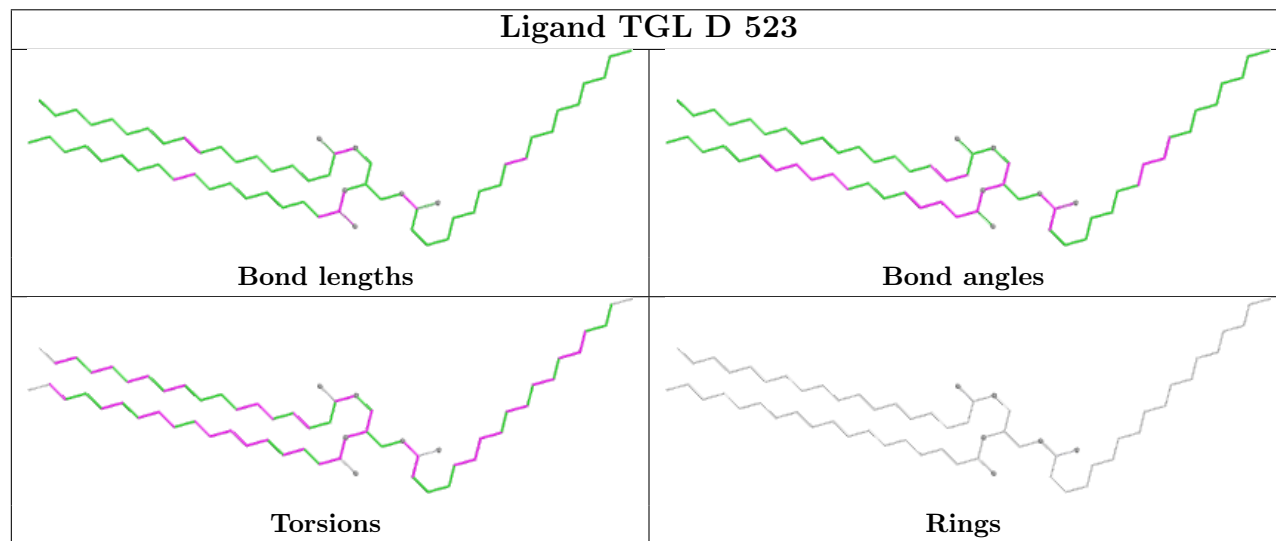
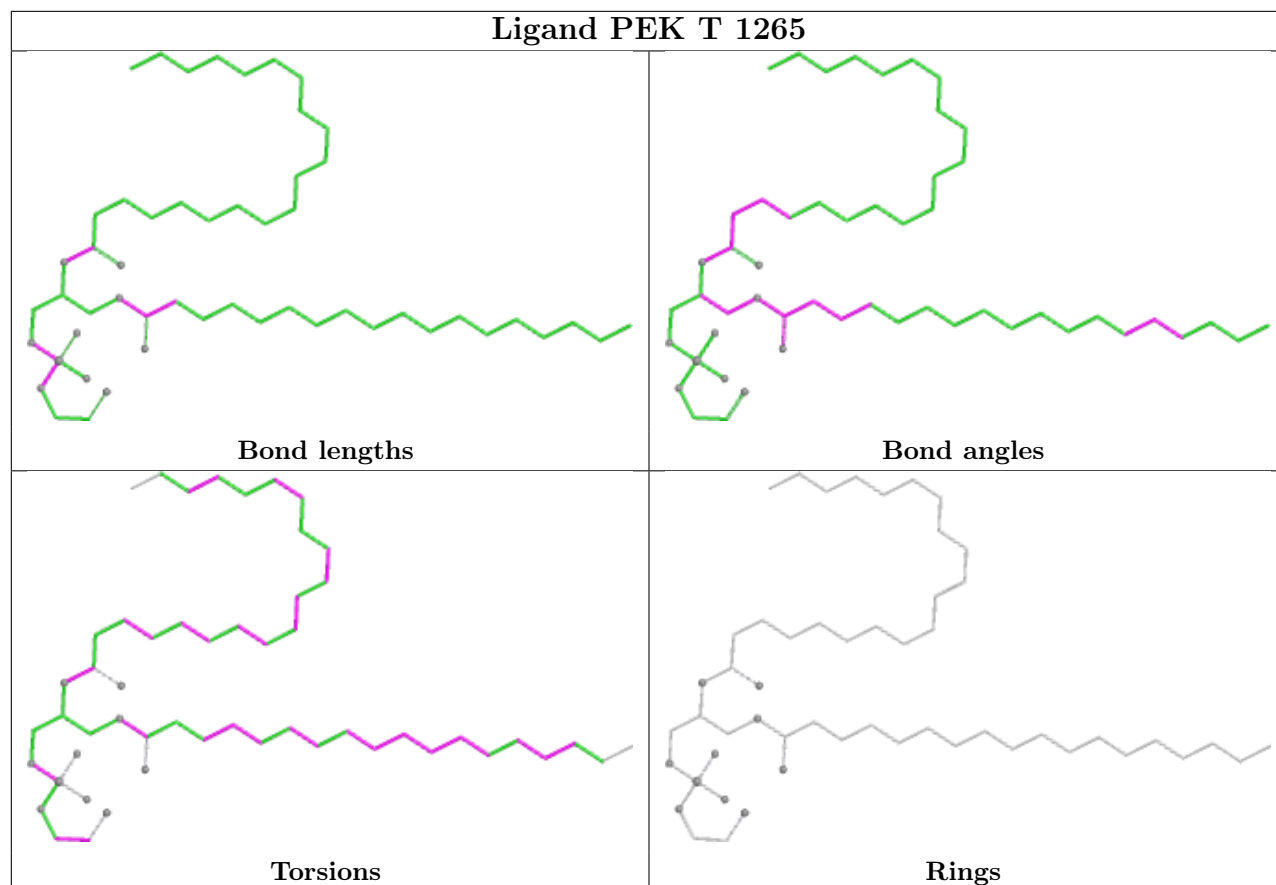


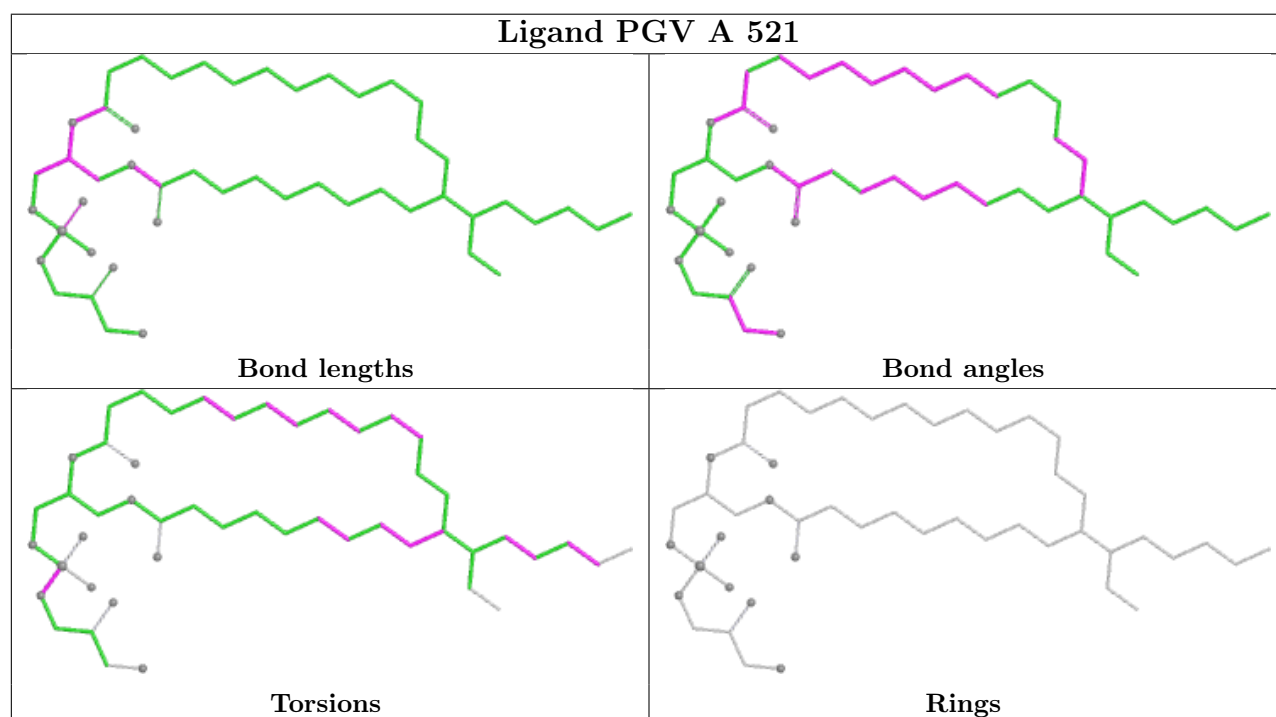
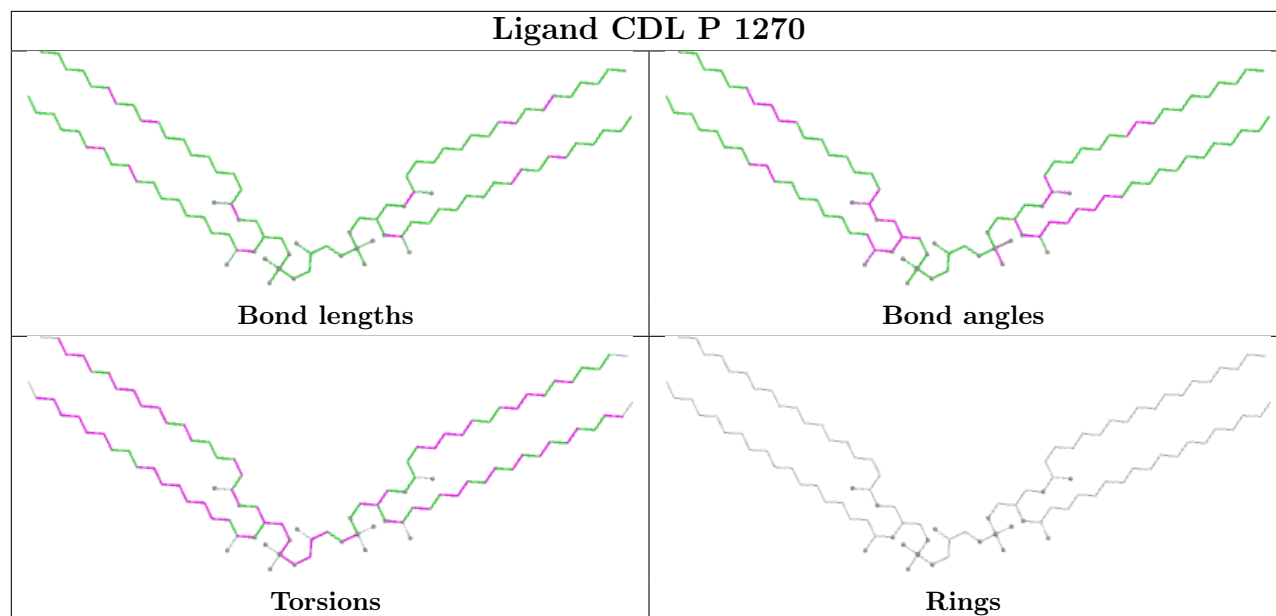
Ligand PGV U 1268



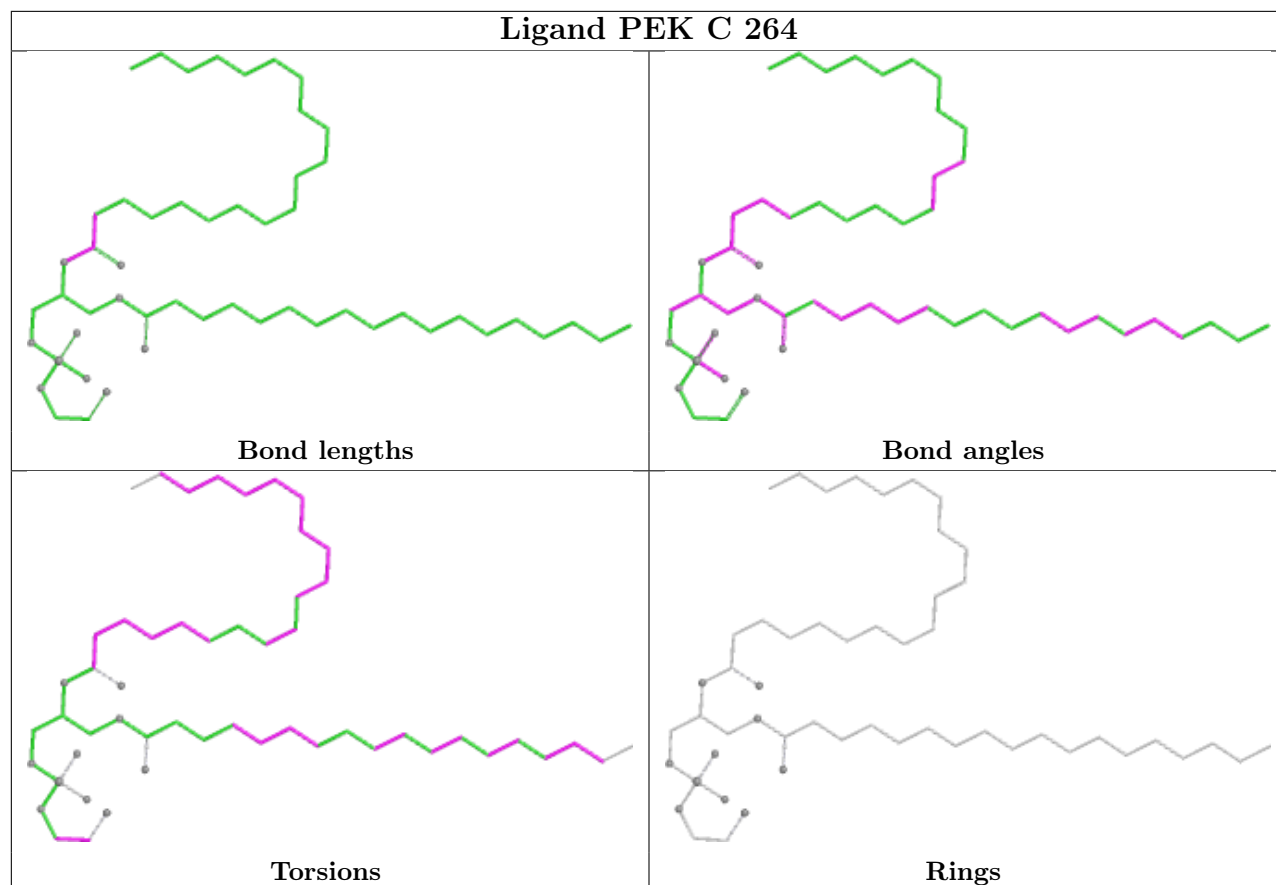




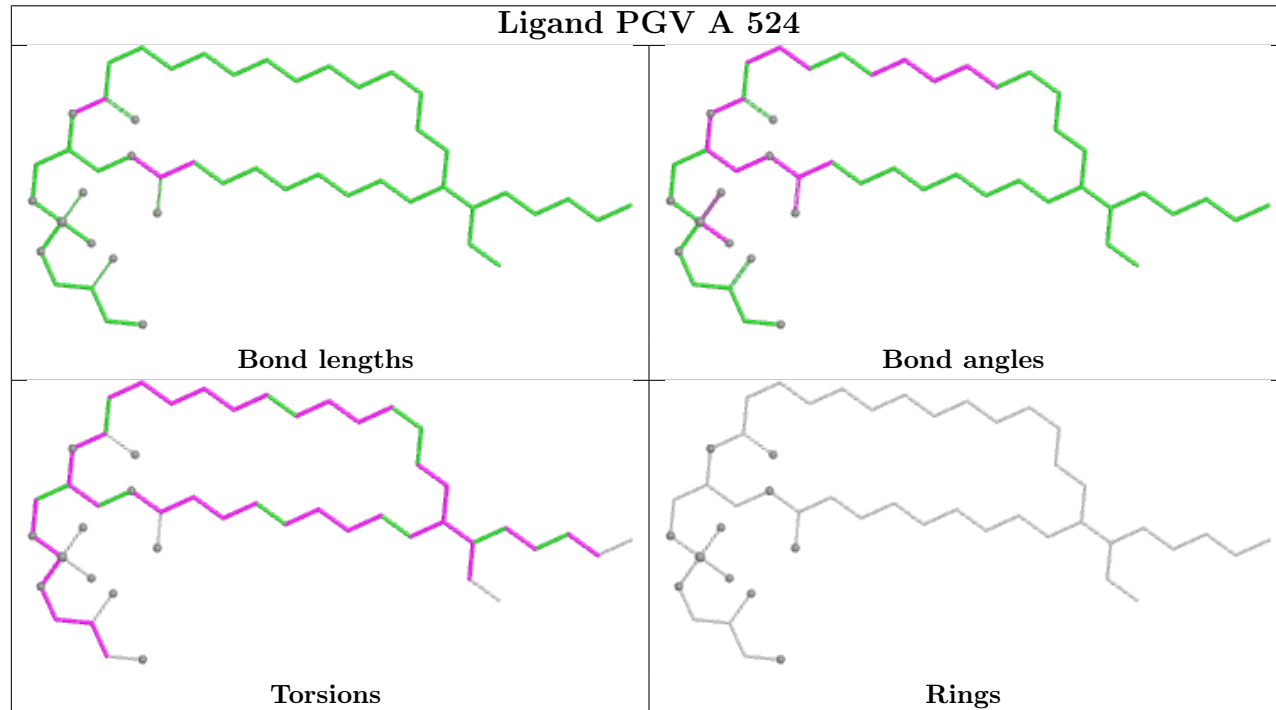


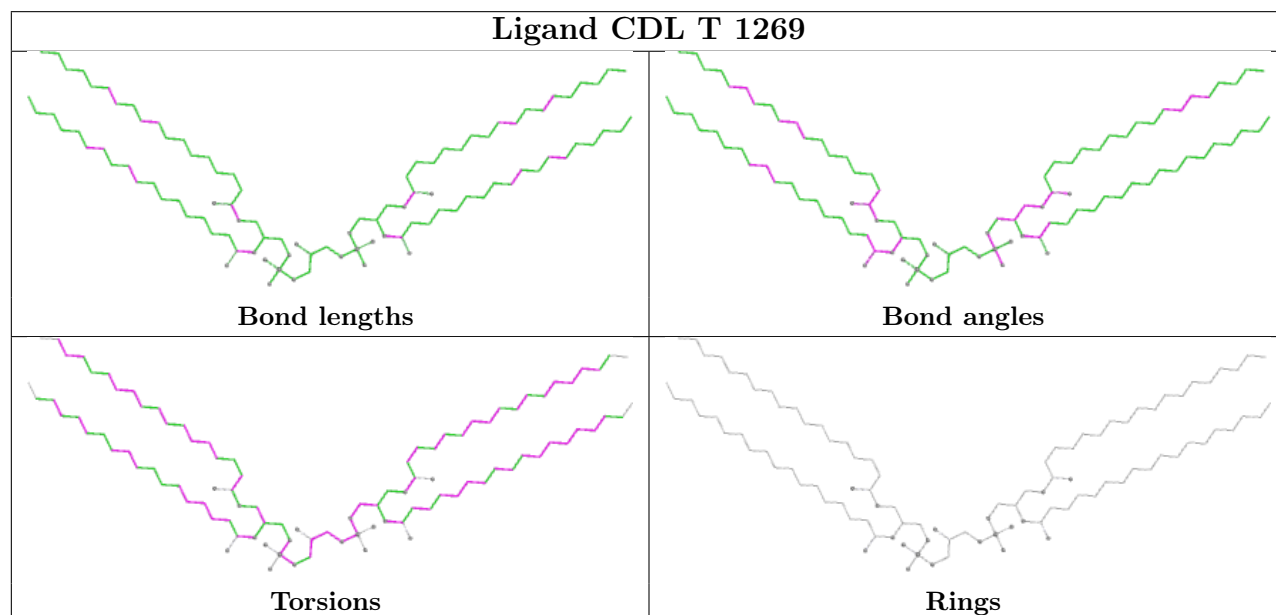
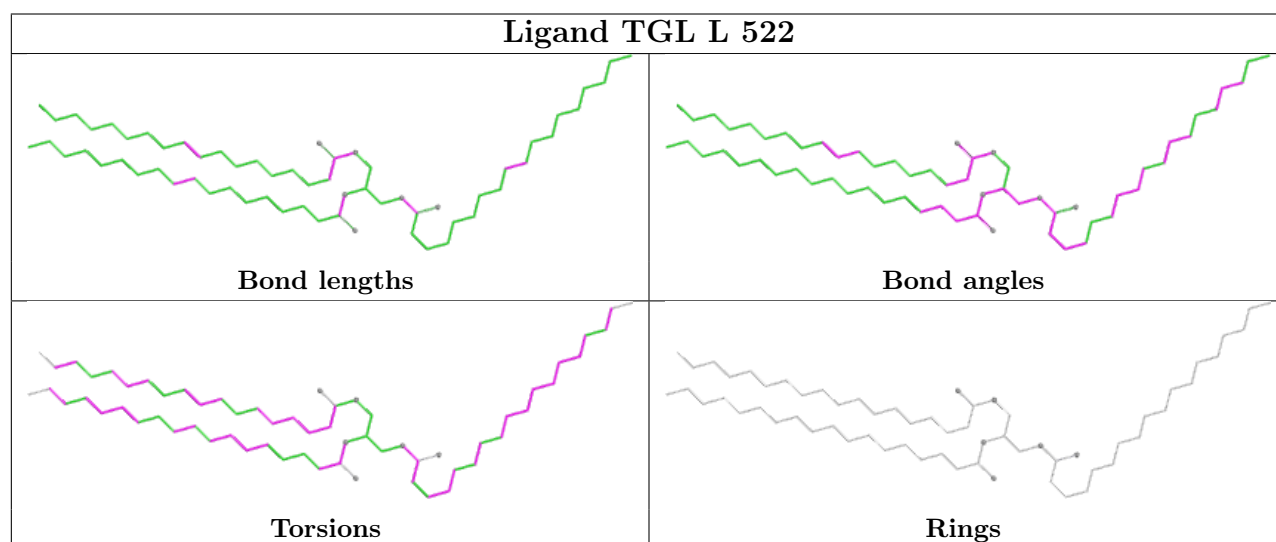
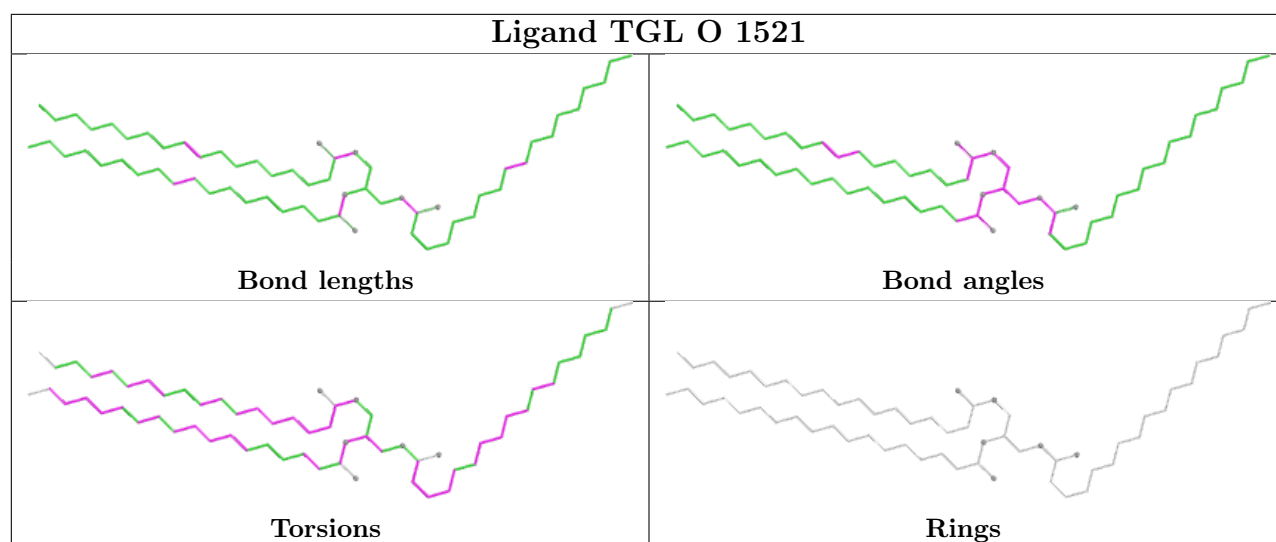


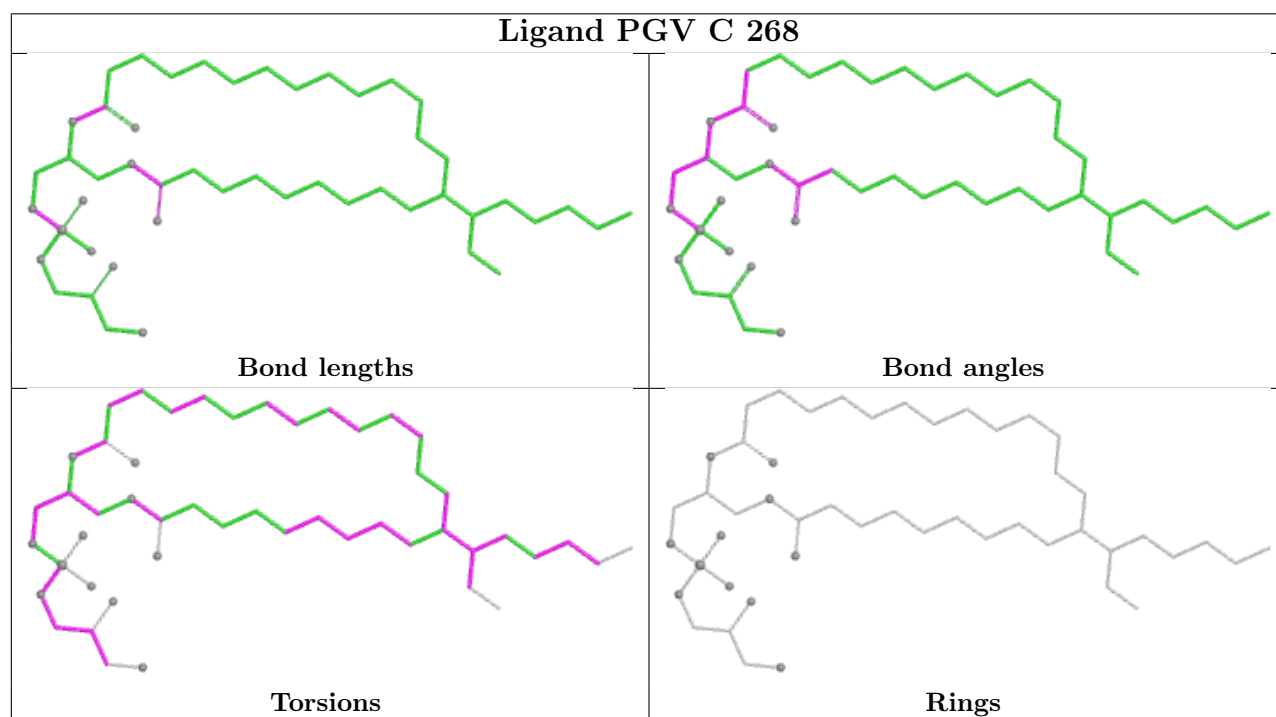
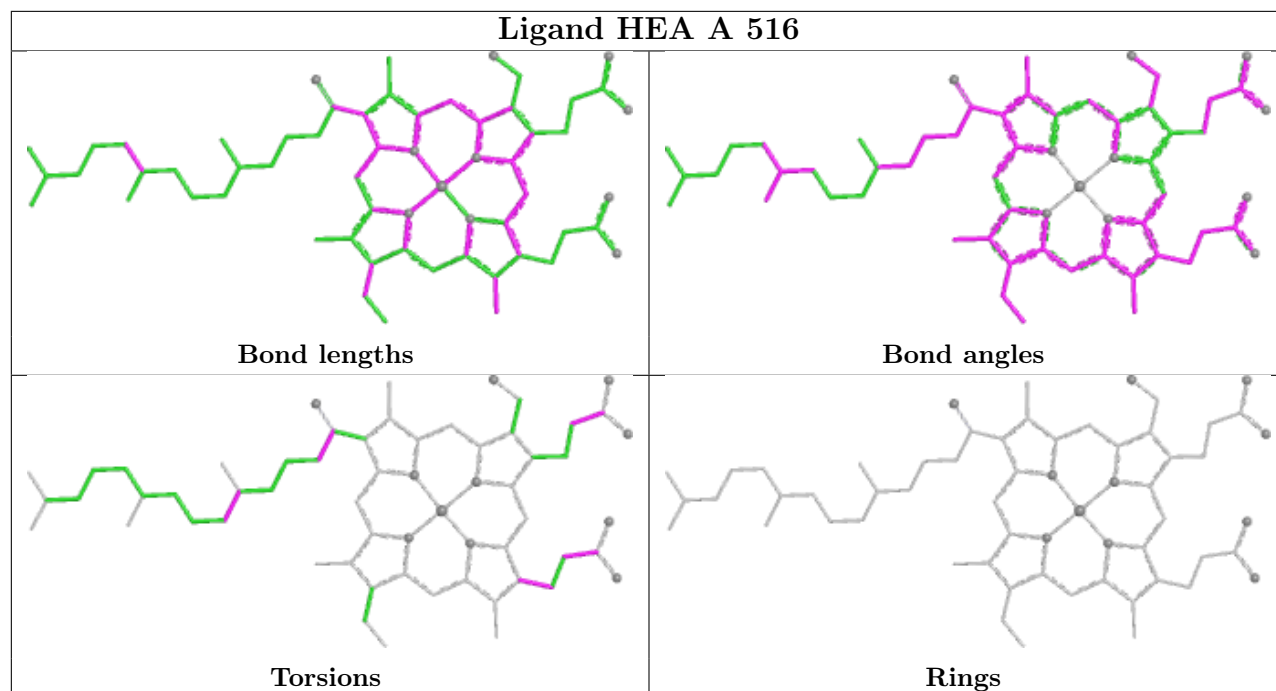
Ligand PEK C 264

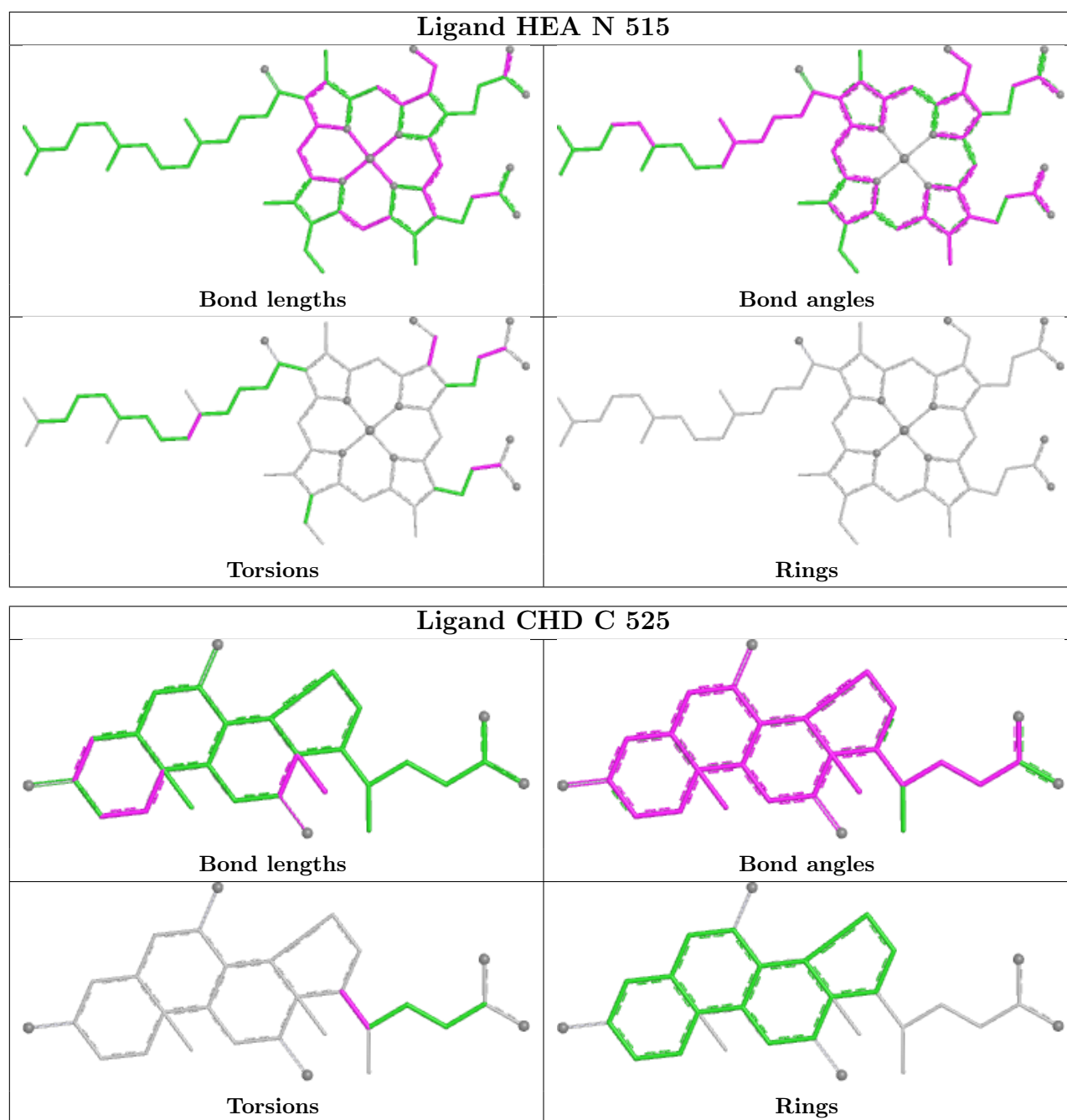


Ligand PGV A 524









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%)	-0.44	2 (0%) 88 88	13, 29, 38, 65	5 (0%)
1	N	513/514 (99%)	0.15	5 (0%) 79 79	16, 35, 44, 71	5 (0%)
2	B	226/227 (99%)	0.01	9 (3%) 42 41	24, 33, 53, 72	0
2	O	226/227 (99%)	0.56	10 (4%) 39 38	31, 42, 64, 81	0
3	C	259/261 (99%)	-0.21	2 (0%) 82 82	26, 32, 43, 66	0
3	P	259/261 (99%)	0.20	5 (1%) 66 66	30, 36, 48, 67	0
4	D	144/147 (97%)	0.36	4 (2%) 55 54	30, 40, 53, 66	0
4	Q	144/147 (97%)	1.20	18 (12%) 8 7	39, 50, 71, 105	0
5	E	105/109 (96%)	0.50	1 (0%) 79 79	33, 40, 64, 97	0
5	R	105/109 (96%)	0.95	10 (9%) 14 12	36, 46, 70, 97	0
6	F	98/98 (100%)	0.69	8 (8%) 17 16	30, 41, 80, 117	0
6	S	98/98 (100%)	0.87	12 (12%) 8 7	34, 46, 80, 113	0
7	G	83/85 (97%)	0.84	18 (21%) 2 2	29, 38, 90, 106	0
7	T	83/85 (97%)	1.11	20 (24%) 2 2	32, 41, 91, 106	0
8	H	79/85 (92%)	0.51	8 (10%) 12 11	29, 41, 81, 101	0
8	U	79/85 (92%)	0.83	11 (13%) 6 5	37, 47, 85, 106	0
9	I	72/73 (98%)	0.76	8 (11%) 10 9	31, 46, 65, 70	0
9	V	72/73 (98%)	1.19	11 (15%) 5 4	36, 52, 67, 77	0
10	J	58/59 (98%)	0.50	3 (5%) 33 31	32, 41, 66, 95	0
10	W	58/59 (98%)	1.10	7 (12%) 8 8	36, 45, 67, 97	0
11	K	49/56 (87%)	0.67	4 (8%) 17 16	31, 39, 54, 64	0
11	X	49/56 (87%)	1.44	10 (20%) 3 2	42, 50, 66, 78	0
12	L	46/47 (97%)	-0.01	2 (4%) 40 39	29, 34, 51, 77	0
12	Y	46/47 (97%)	0.93	4 (8%) 16 15	35, 43, 60, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.48	6 (13%) 6 5	31, 34, 72, 96	0
13	Z	43/46 (93%)	1.26	9 (20%) 2 2	39, 44, 81, 104	0
All	All	3550/3614 (98%)	0.35	207 (5%) 29 27	13, 38, 64, 117	10 (0%)

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	13.5
6	F	1	ALA	12.6
4	Q	6	VAL	8.3
6	S	98	HIS	7.5
6	S	97	ALA	7.5
4	Q	5	VAL	6.5
6	S	94	HIS	6.2
8	H	8	ILE	5.9
7	G	2	SER	5.9
7	T	36	TRP	5.9
7	T	4	ALA	5.6
7	T	3	ALA	5.5
7	T	9	GLY	5.5
2	B	59	GLN	5.5
6	F	96	LEU	5.4
2	O	113	TYR	5.4
7	T	8	HIS	5.4
6	S	96	LEU	5.4
7	G	36	TRP	5.3
9	I	37	PHE	5.2
7	G	4	ALA	5.0
8	U	8	ILE	4.8
6	F	3	GLY	4.7
9	V	2	THR	4.7
7	G	8	HIS	4.7
6	F	2	SER	4.6
7	G	1	ALA	4.5
7	T	10	GLY	4.5
6	F	97	ALA	4.5
7	G	10	GLY	4.4
9	V	37	PHE	4.4
9	V	3	ALA	4.4
7	T	5	LYS	4.4
7	G	3	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
6	F	94	HIS	4.2
2	B	90	ILE	4.1
13	M	40	TYR	4.1
6	S	93	PRO	4.1
9	I	2	THR	4.0
8	H	47	GLY	3.9
9	V	36	LYS	3.9
2	B	60	GLU	3.9
3	P	33	MET	3.9
7	T	2	SER	3.8
7	G	37	LEU	3.8
5	E	5	HIS	3.8
7	T	38	HIS	3.8
11	X	7	PRO	3.8
4	Q	51	LEU	3.8
8	U	9	LYS	3.8
9	V	27	VAL	3.8
11	X	19	ALA	3.7
4	Q	4	SER	3.7
11	X	16	ALA	3.7
13	Z	42	LYS	3.6
5	R	109	VAL	3.6
10	W	1	PHE	3.6
13	M	42	LYS	3.6
7	T	12	GLY	3.6
13	M	43	SER	3.6
7	T	7	ASP	3.5
11	X	6	ALA	3.5
4	Q	35	ALA	3.5
8	U	44	THR	3.5
6	S	2	SER	3.4
7	G	7	ASP	3.4
7	G	38	HIS	3.4
6	S	3	GLY	3.4
13	Z	40	TYR	3.4
12	L	2	HIS	3.3
10	W	55	PHE	3.3
10	W	58	LYS	3.3
7	T	37	LEU	3.3
12	L	47	LYS	3.2
3	C	3	HIS	3.2
7	T	84	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
9	I	32	ALA	3.1
2	O	131	GLY	3.1
7	G	12	GLY	3.1
10	J	58	LYS	3.1
2	B	113	TYR	3.0
13	M	41	LYS	3.0
2	O	90	ILE	3.0
2	O	60	GLU	3.0
10	J	1	PHE	3.0
12	Y	20	ARG	3.0
1	N	113	LEU	3.0
11	X	12	LYS	3.0
3	P	37	PHE	3.0
7	T	1	ALA	2.9
2	O	227	LEU	2.9
1	A	298	ASP	2.9
8	H	42	ALA	2.9
2	B	92	ASN	2.9
4	Q	7	LYS	2.9
8	U	42	ALA	2.9
8	U	45	ALA	2.9
5	R	5	HIS	2.9
10	W	52	TRP	2.9
2	O	116	LEU	2.8
8	H	50	VAL	2.8
8	H	7	LYS	2.8
7	G	9	GLY	2.8
4	Q	48	TRP	2.8
2	B	58	ALA	2.8
1	A	514	LYS	2.8
3	P	38	ASN	2.8
4	Q	11	TYR	2.8
4	Q	145	TRP	2.8
7	T	40	GLY	2.7
8	U	47	GLY	2.7
7	G	5	LYS	2.7
8	H	45	ALA	2.7
3	P	40	MET	2.7
9	I	27	VAL	2.7
8	U	46	LYS	2.7
7	T	6	GLY	2.7
1	N	513	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
4	Q	33	LEU	2.6
12	Y	45	LEU	2.6
4	D	4	SER	2.6
7	G	42	ARG	2.6
11	K	19	ALA	2.6
1	N	484	THR	2.6
2	O	32	PHE	2.6
11	K	6	ALA	2.6
11	X	14	GLY	2.6
7	G	41	HIS	2.6
2	B	91	ASN	2.6
8	U	50	VAL	2.5
8	U	52	VAL	2.5
2	O	87	MET	2.5
13	Z	32	TRP	2.5
4	Q	102	TYR	2.4
10	W	41	GLY	2.4
4	Q	46	ALA	2.4
9	I	3	ALA	2.4
6	S	4	GLY	2.4
7	G	6	GLY	2.4
6	F	54	ASN	2.4
6	S	95	GLN	2.4
4	Q	53	ILE	2.4
6	S	92	VAL	2.4
11	X	28	VAL	2.4
4	Q	8	SER	2.4
10	W	32	TYR	2.3
12	Y	17	ASN	2.3
13	Z	41	LYS	2.3
9	I	25	PHE	2.3
9	V	20	HIS	2.3
8	H	44	THR	2.3
9	V	32	ALA	2.3
5	R	97	GLY	2.3
3	C	38	ASN	2.3
13	M	39	ASN	2.3
8	U	7	LYS	2.3
9	I	30	GLY	2.3
4	Q	59	LEU	2.3
6	F	98	HIS	2.2
7	T	70	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
4	Q	143	ASN	2.2
9	I	36	LYS	2.2
9	V	30	GLY	2.2
13	Z	31	GLY	2.2
4	D	11	TYR	2.2
11	X	47	ARG	2.2
4	Q	103	VAL	2.2
9	V	26	MET	2.2
13	Z	38	ASP	2.2
9	V	38	ALA	2.2
13	Z	35	TYR	2.2
5	R	99	SER	2.2
8	U	10	ASN	2.2
2	O	59	GLN	2.2
4	D	35	ALA	2.2
5	R	93	LEU	2.2
11	K	47	ARG	2.2
11	X	13	TYR	2.2
8	H	9	LYS	2.2
5	R	83	PRO	2.1
13	M	38	ASP	2.2
5	R	104	LEU	2.1
3	P	39	SER	2.1
4	Q	50	SER	2.1
1	N	514	LYS	2.1
5	R	108	LYS	2.1
12	Y	47	LYS	2.1
1	N	297	MET	2.1
2	B	87	MET	2.1
2	B	13	THR	2.1
2	O	130	PRO	2.1
7	T	41	HIS	2.1
7	T	35	SER	2.1
5	R	100	THR	2.1
11	X	17	VAL	2.1
9	V	73	LYS	2.1
13	Z	19	LEU	2.1
13	Z	43	SER	2.1
5	R	91	PRO	2.1
6	S	87	THR	2.1
4	D	39	ALA	2.1
7	G	35	SER	2.1

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Mol	Chain	Res	Type	RSRZ
7	T	33	LEU	2.0
10	W	57	HIS	2.0
7	G	84	LYS	2.0
10	J	57	HIS	2.0
11	K	13	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.34	0.24	83,84,85,86	0
9	SAC	I	1	9/10	0.63	0.23	73,76,78,80	0
7	TPO	T	11	11/12	0.66	0.25	75,82,102,103	0
7	TPO	G	11	11/12	0.67	0.29	69,76,102,102	0
1	FME	N	1	10/11	0.83	0.19	46,53,78,82	0
1	FME	A	1	10/11	0.89	0.15	44,51,71,75	0
2	FME	B	1	10/11	0.96	0.08	33,33,41,48	0
2	FME	O	1	10/11	0.96	0.09	40,42,47,55	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(Å ²)	Q<0.9
24	UNX	C	262	1/1	0.42	0.59	80,80,80,80	0
24	UNX	P	262	1/1	0.47	0.48	79,79,79,79	0
27	DMU	C	272	33/33	0.74	0.20	68,100,115,116	0
27	DMU	P	272	33/33	0.74	0.22	77,107,124,124	0
25	PEK	T	1265	53/53	0.76	0.23	49,79,110,118	0

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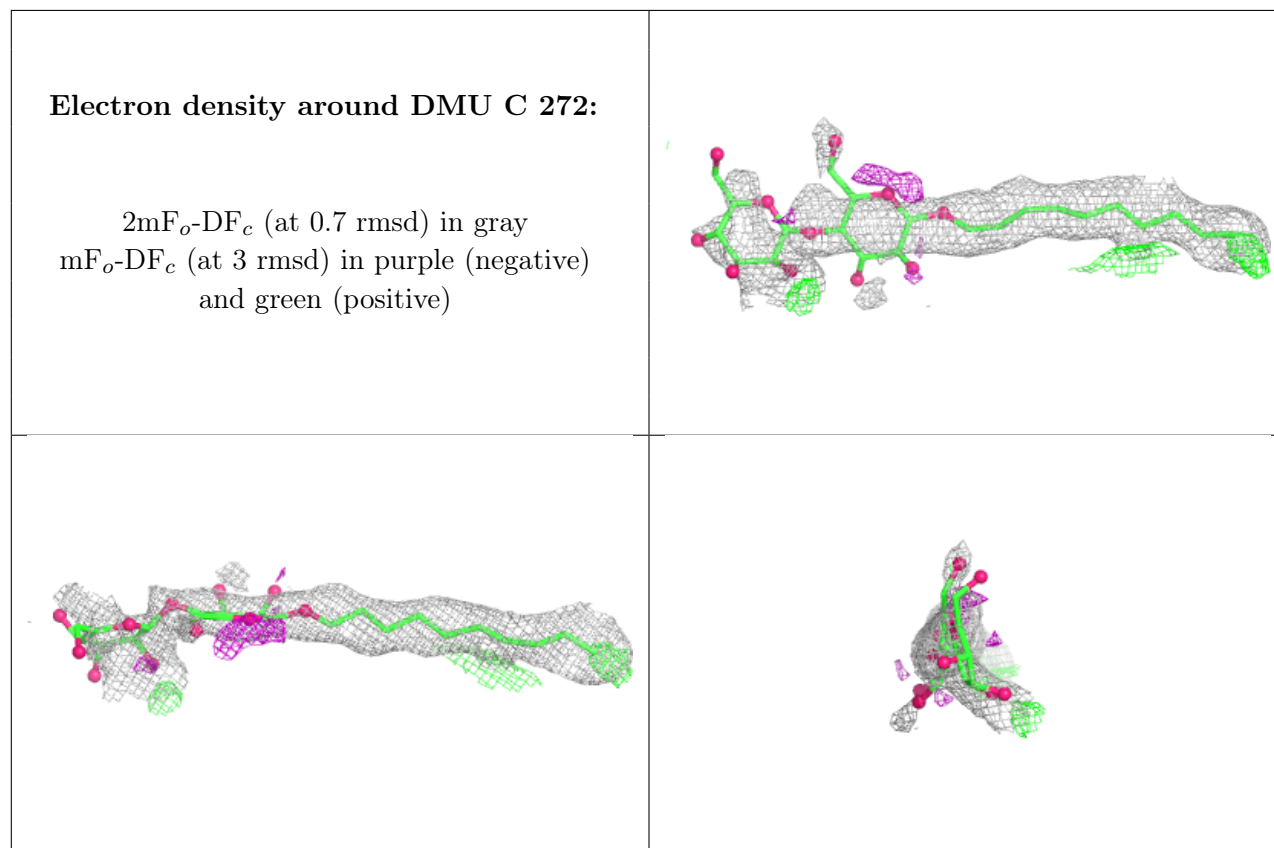
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CHD	J	60	29/29	0.77	0.23	99,105,108,110	0
19	PGV	U	1268	51/51	0.77	0.24	60,84,103,105	0
23	CHD	W	1059	29/29	0.78	0.23	101,109,113,115	0
19	PGV	A	524	51/51	0.78	0.20	44,72,112,114	0
21	TGL	Y	1522	63/63	0.79	0.21	51,73,89,92	0
25	PEK	C	265	53/53	0.79	0.23	49,83,106,107	0
25	PEK	T	263	53/53	0.79	0.23	52,103,125,127	0
19	PGV	N	1524	51/51	0.79	0.20	54,74,103,105	0
21	TGL	D	523	63/63	0.79	0.20	48,69,91,91	0
21	TGL	N	1523	63/63	0.79	0.22	61,79,97,99	0
26	CDL	T	1269	100/100	0.80	0.20	58,86,114,118	0
19	PGV	C	268	51/51	0.80	0.23	53,81,98,102	0
21	TGL	O	1521	63/63	0.80	0.20	58,80,95,96	0
22	PSC	R	1229	52/52	0.81	0.21	48,99,136,139	0
26	CDL	G	269	100/100	0.82	0.20	62,86,116,120	0
25	PEK	G	1263	53/53	0.82	0.24	52,103,133,134	0
21	TGL	L	522	63/63	0.82	0.20	43,66,82,89	0
21	TGL	B	521	63/63	0.82	0.21	53,74,88,90	0
26	CDL	P	1270	100/100	0.83	0.20	36,94,119,119	0
26	CDL	C	270	100/100	0.83	0.20	41,91,129,130	0
22	PSC	B	229	52/52	0.84	0.21	43,92,139,143	0
23	CHD	C	271	29/29	0.84	0.17	79,83,85,85	0
23	CHD	P	1271	29/29	0.85	0.20	78,92,94,95	0
27	DMU	Z	1526	33/33	0.86	0.14	49,57,70,70	0
17	MG	N	518	1/1	0.93	0.07	34,34,34,34	0
27	DMU	M	526	33/33	0.93	0.10	33,47,65,71	0
25	PEK	C	264	53/53	0.94	0.12	30,46,78,80	0
25	PEK	P	1264	53/53	0.94	0.13	35,50,86,88	0
23	CHD	O	229	29/29	0.94	0.08	27,32,38,40	0
19	PGV	N	1266	51/51	0.95	0.10	30,42,65,69	0
19	PGV	P	1267	51/51	0.95	0.11	29,40,82,87	0
18	NA	N	519	1/1	0.95	0.15	39,39,39,39	0
15	NO	N	520	2/2	0.95	0.17	39,39,39,42	0
23	CHD	C	525	29/29	0.96	0.06	26,33,39,41	0
23	CHD	P	1525	29/29	0.96	0.08	32,37,43,47	0
19	PGV	C	267	51/51	0.96	0.10	28,40,73,76	0
23	CHD	B	1085	29/29	0.96	0.06	27,31,36,42	0
15	NO	A	520	2/2	0.97	0.12	32,32,32,36	0
19	PGV	A	521	51/51	0.97	0.09	23,35,63,67	0
18	NA	A	519	1/1	0.97	0.10	32,32,32,32	0
17	MG	A	518	1/1	0.97	0.06	23,23,23,23	0
14	HEA	N	516	60/60	0.98	0.07	27,33,37,40	0

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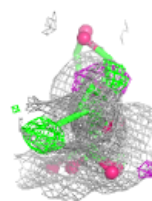
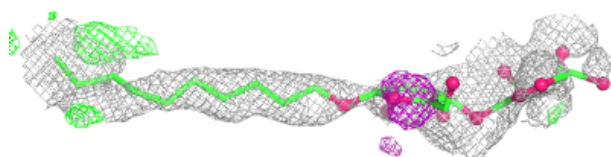
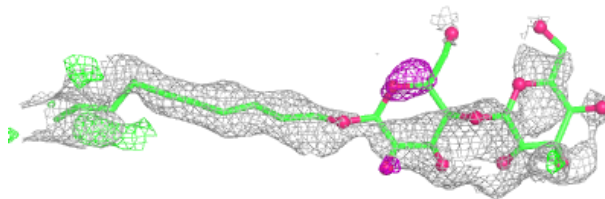
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	HEA	A	515	60/60	0.98	0.06	22,28,41,42	0
14	HEA	N	515	60/60	0.98	0.07	28,36,45,49	0
20	CUA	O	228	2/2	0.98	0.04	34,34,34,36	0
28	ZN	F	99	1/1	0.98	0.03	37,37,37,37	0
16	CU	N	517	1/1	0.99	0.04	35,35,35,35	0
20	CUA	B	228	2/2	0.99	0.03	27,27,27,28	0
14	HEA	A	516	60/60	0.99	0.05	18,26,31,36	0
28	ZN	S	99	1/1	0.99	0.03	43,43,43,43	0
16	CU	A	517	1/1	1.00	0.03	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.

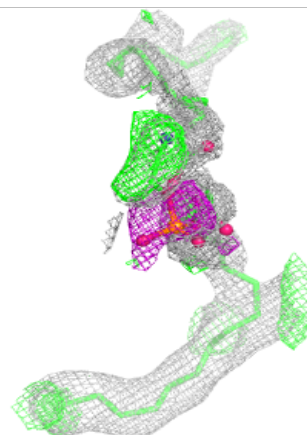
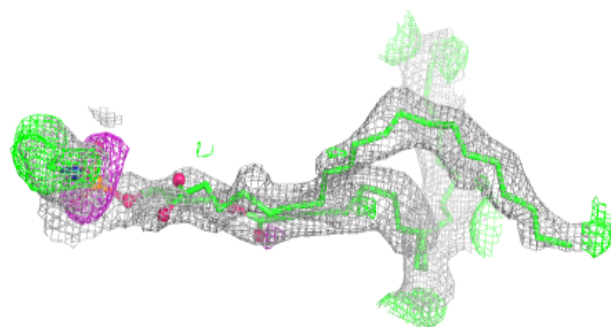
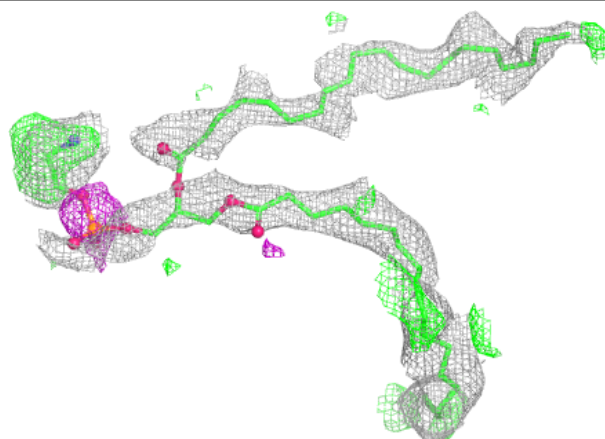


Electron density around DMU P 272:

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

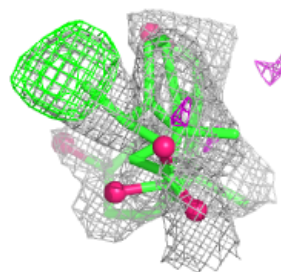
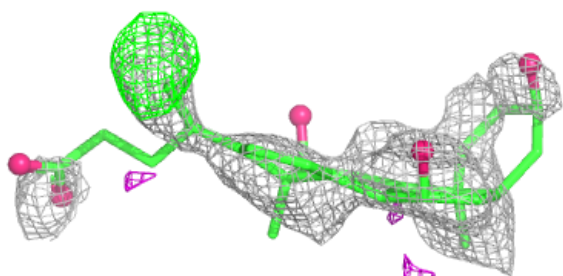
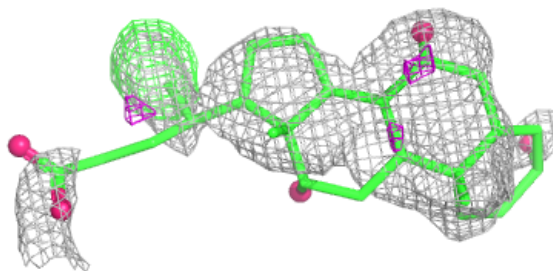
**Electron density around PEK T 1265:**

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

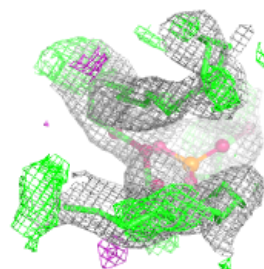
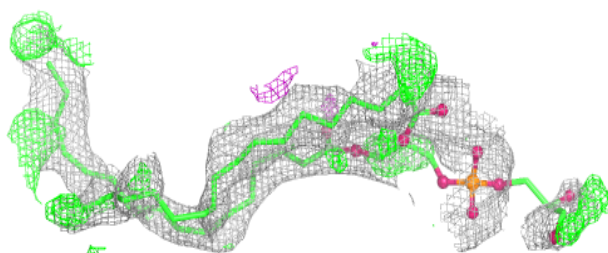
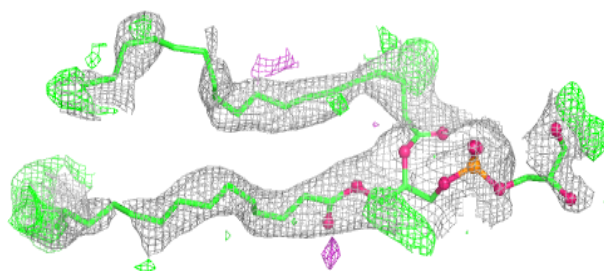


Electron density around CHD J 60:

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

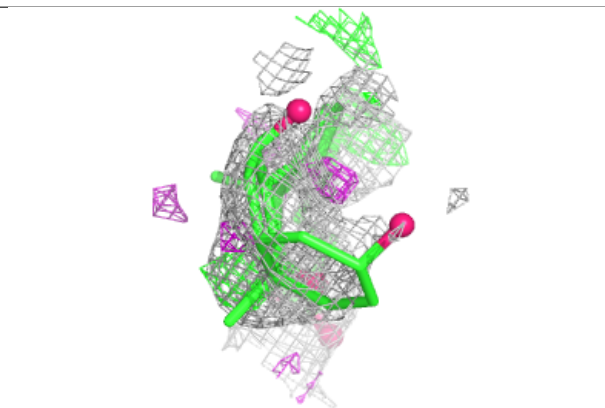
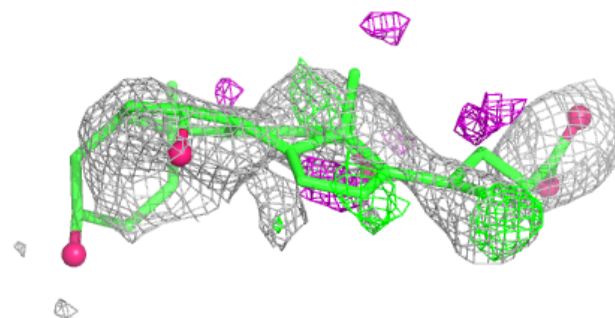
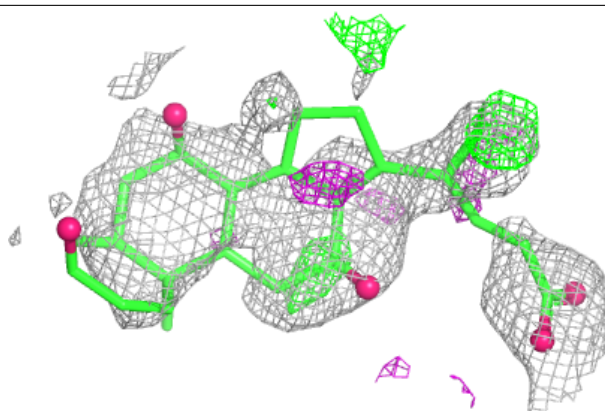
**Electron density around PGV U 1268:**

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

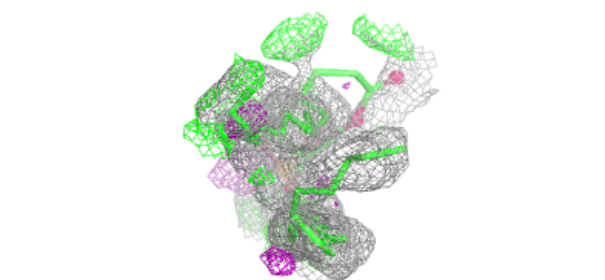
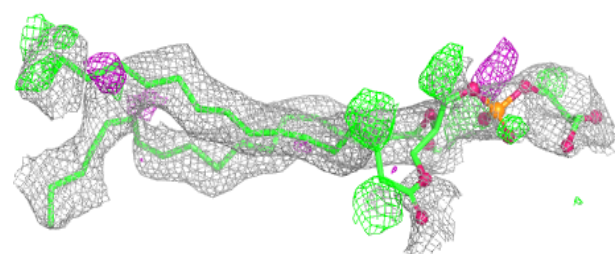
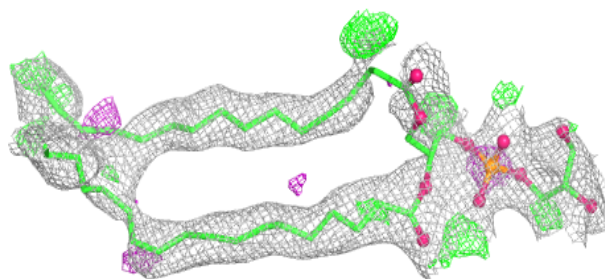


Electron density around CHD W 1059:

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

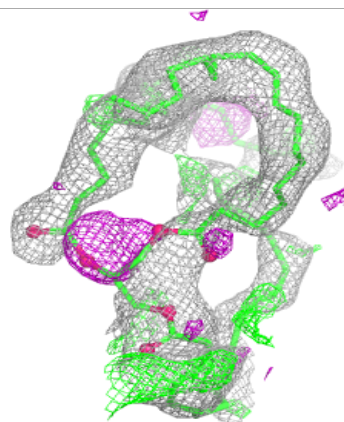
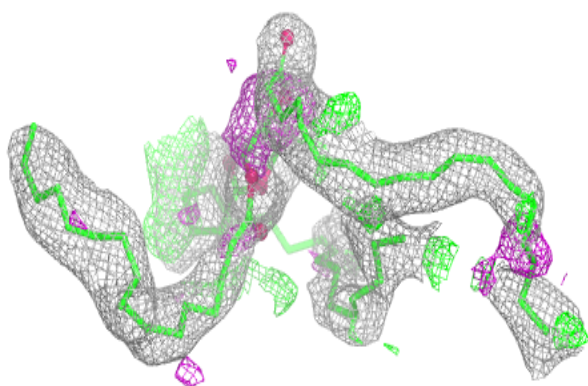
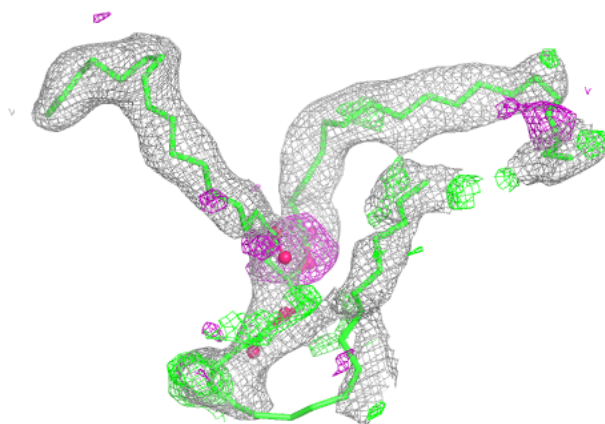
**Electron density around PGV A 524:**

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



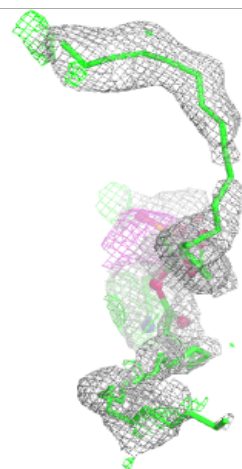
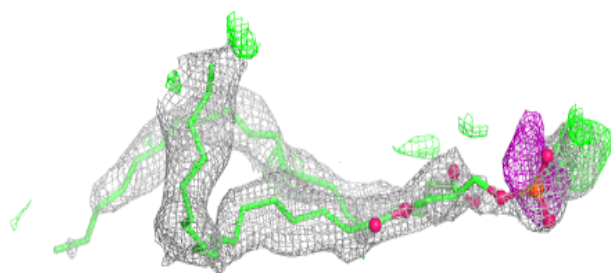
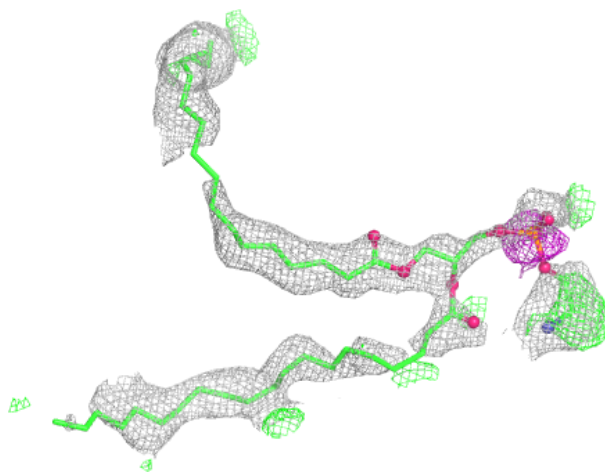
Electron density around TGL Y 1522:

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



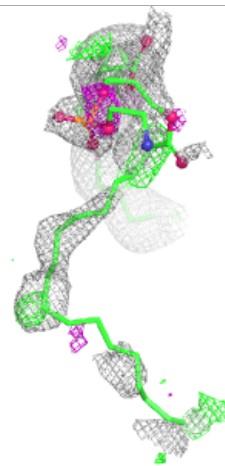
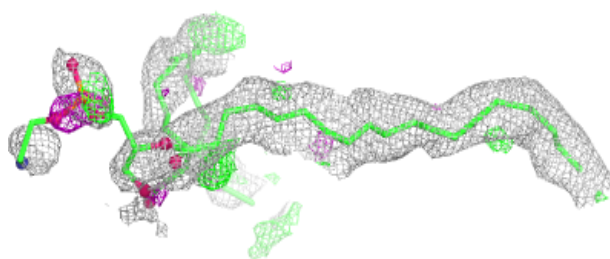
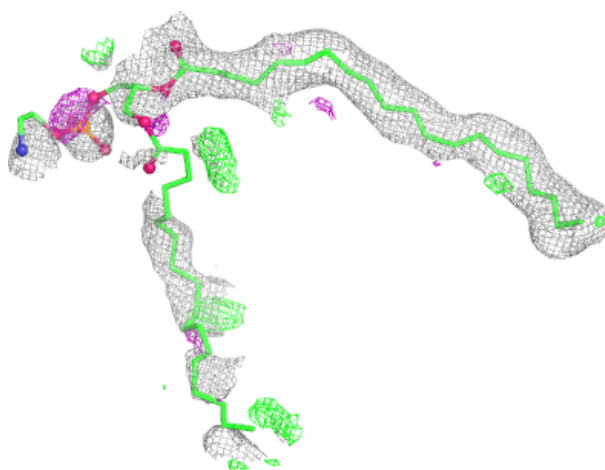
Electron density around PEK C 265:

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



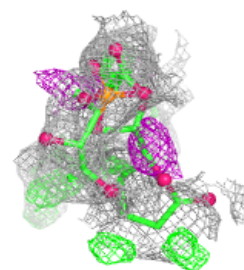
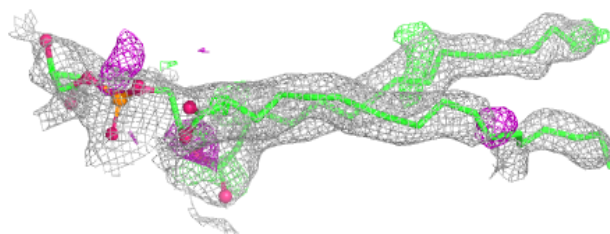
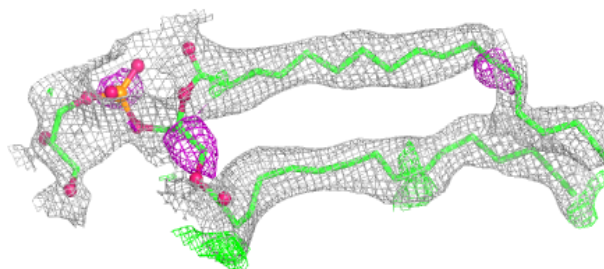
Electron density around PEK T 263:

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and green (positive)

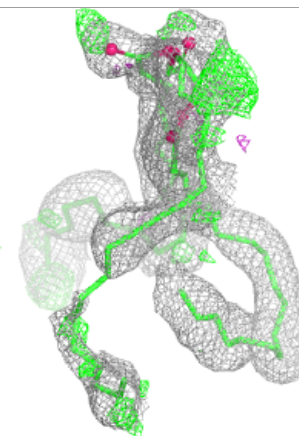
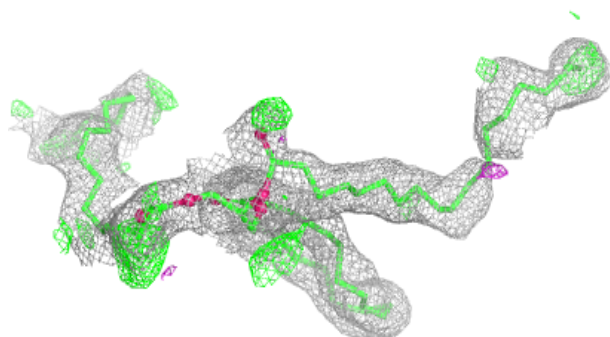
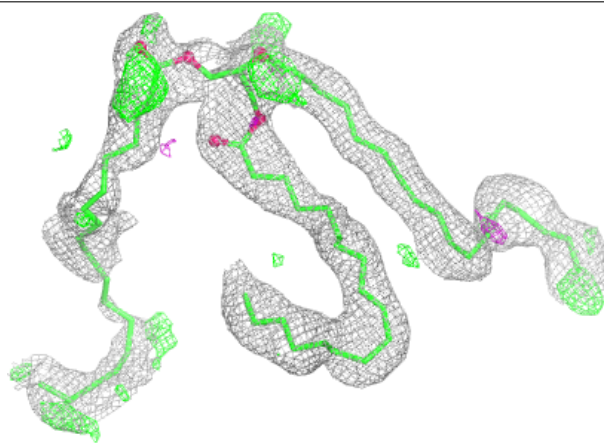


Electron density around PGV N 1524:

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

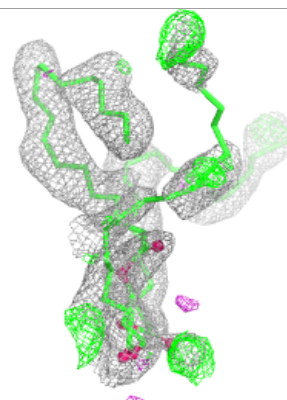
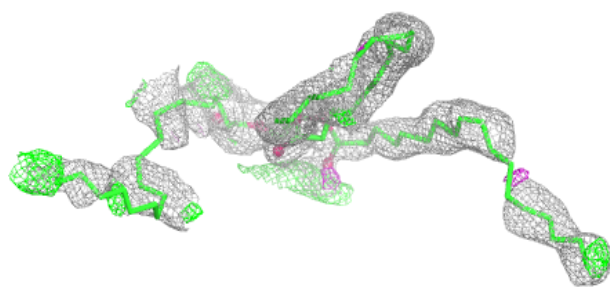
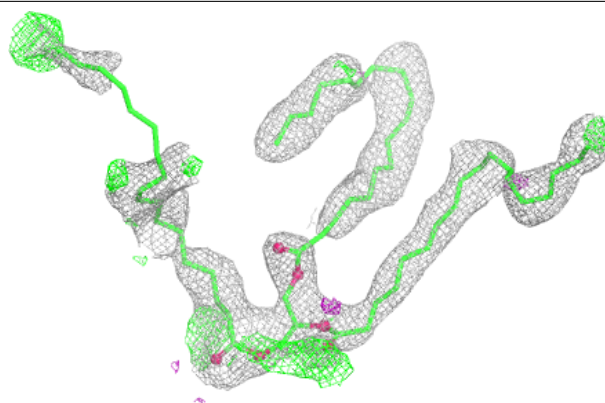
**Electron density around TGL D 523:**

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

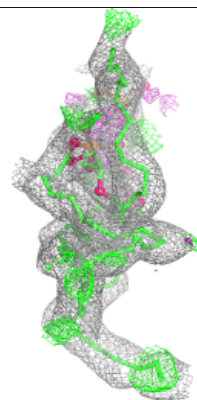
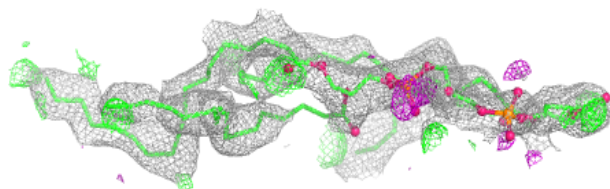
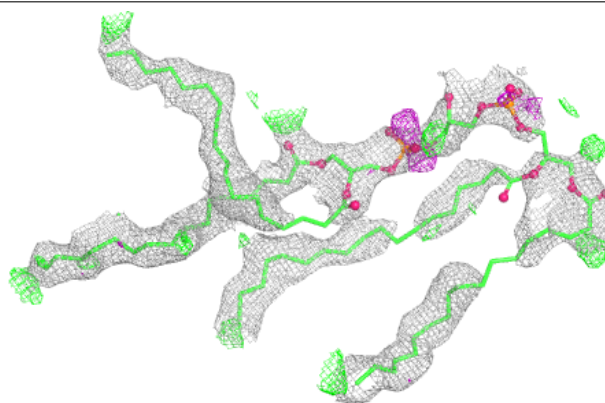


Electron density around TGL N 1523:

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

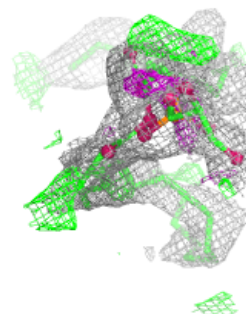
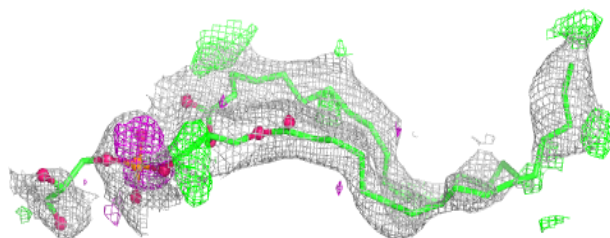
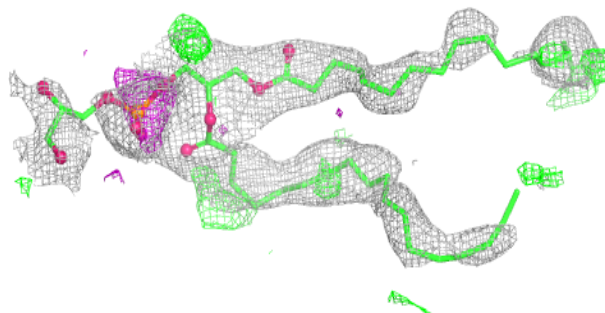
**Electron density around CDL T 1269:**

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

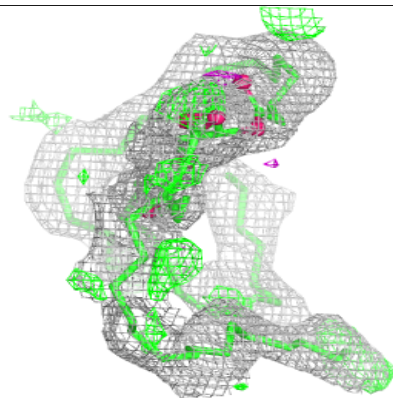
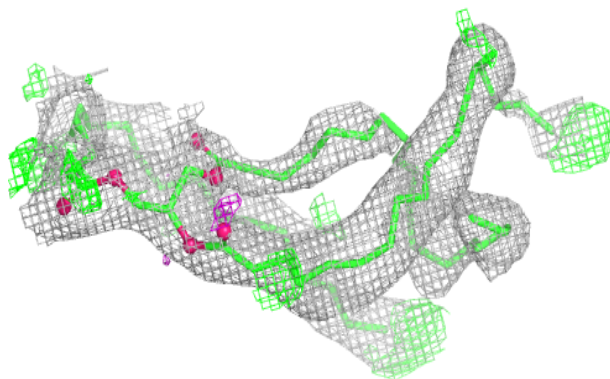
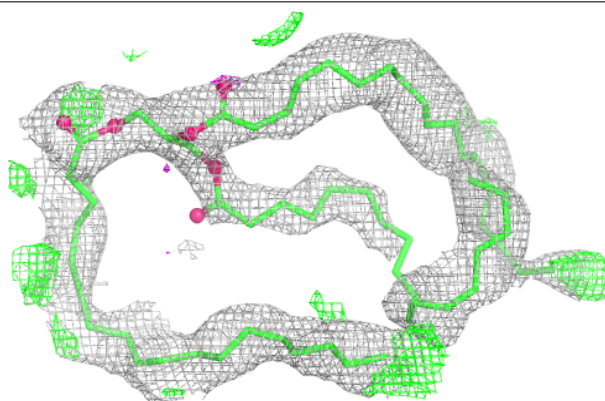


Electron density around PGV C 268:

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

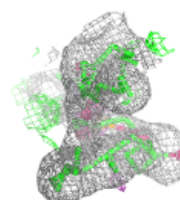
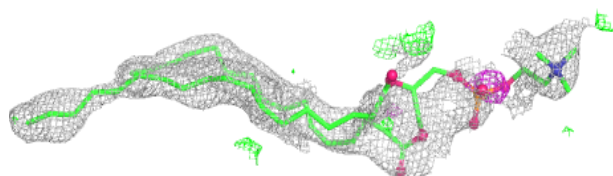
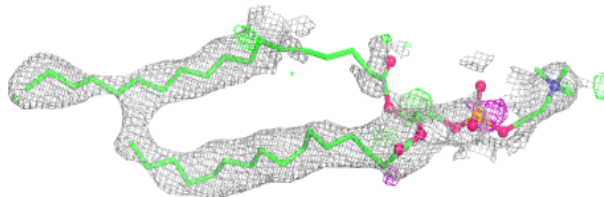
**Electron density around TGL O 1521:**

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

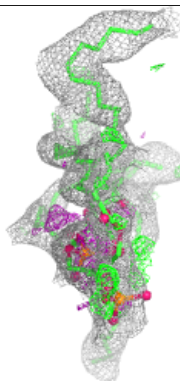
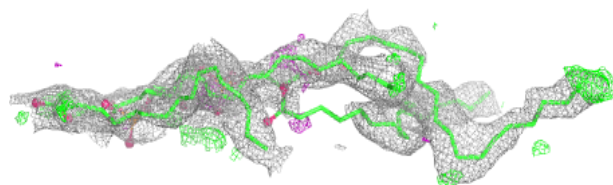
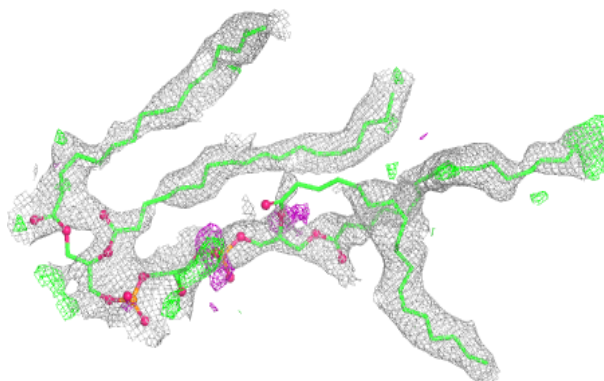


Electron density around PSC R 1229:

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

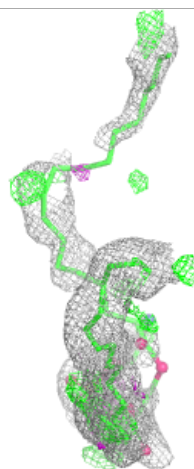
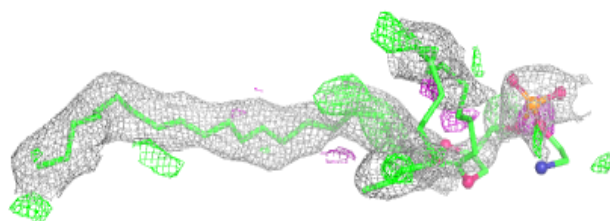
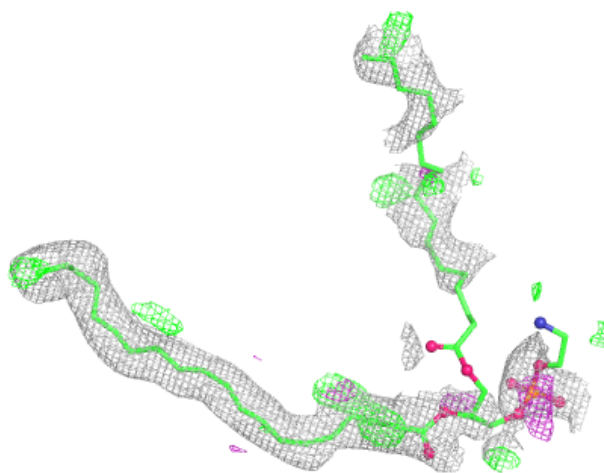
**Electron density around CDL G 269:**

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



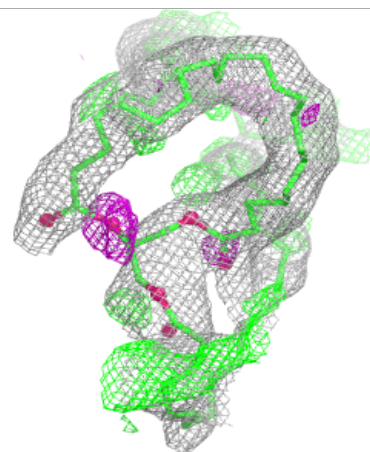
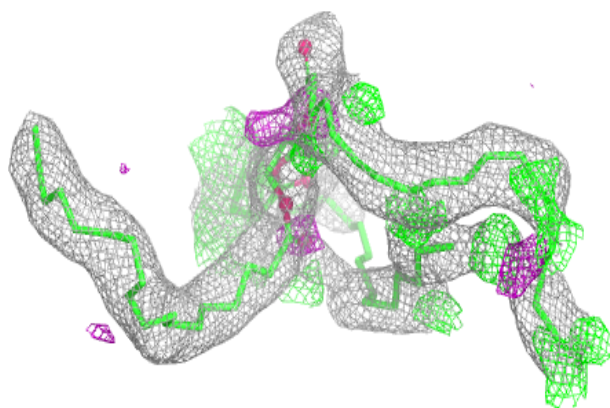
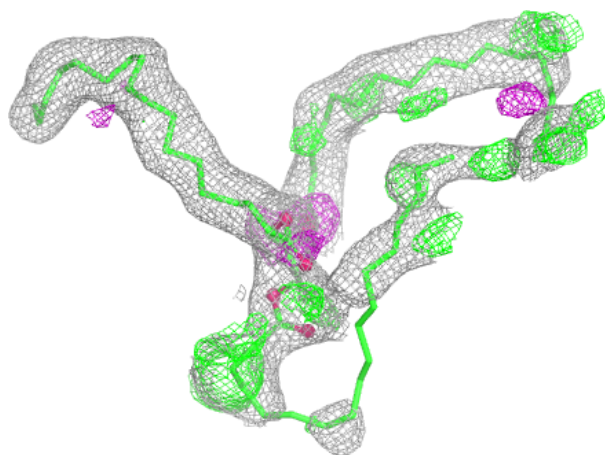
Electron density around PEK G 1263:

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



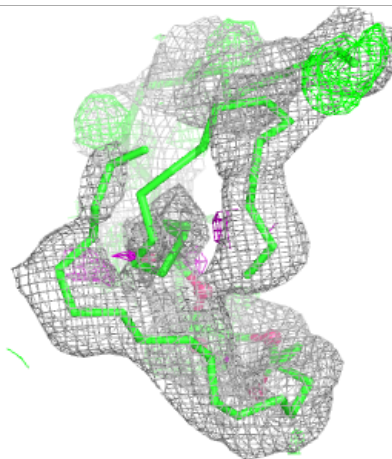
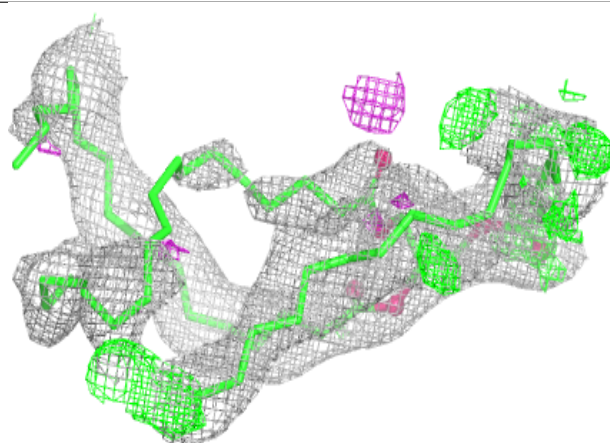
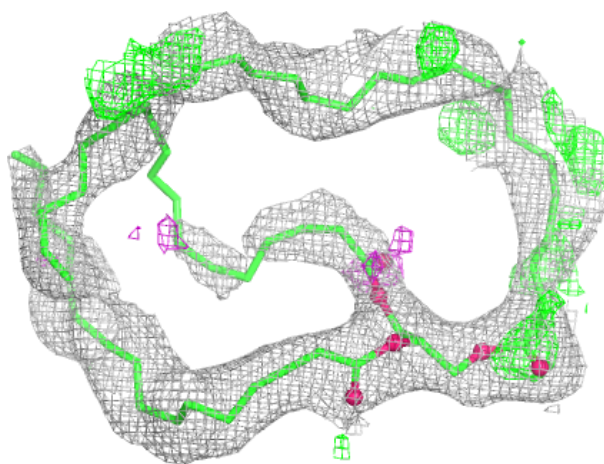
Electron density around TGL L 522:

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



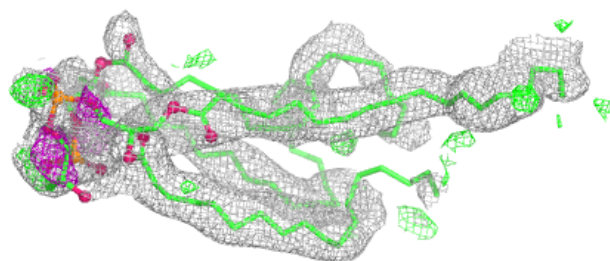
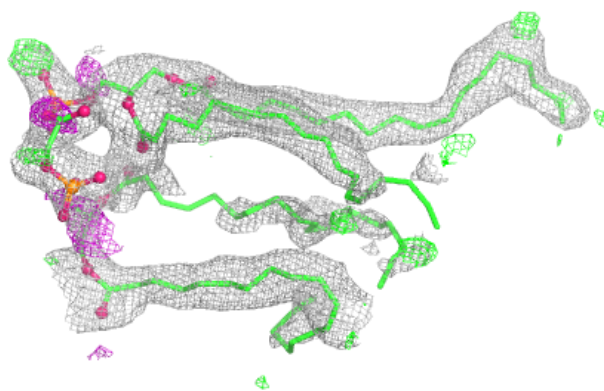
Electron density around TGL B 521:

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



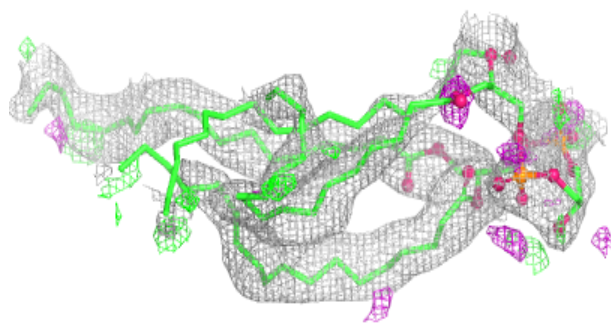
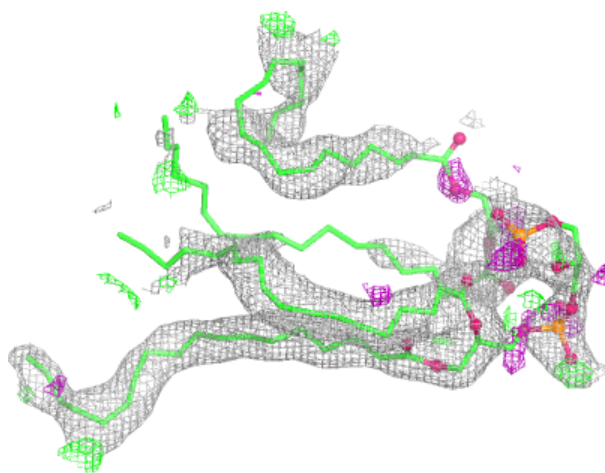
Electron density around CDL P 1270:

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



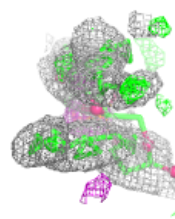
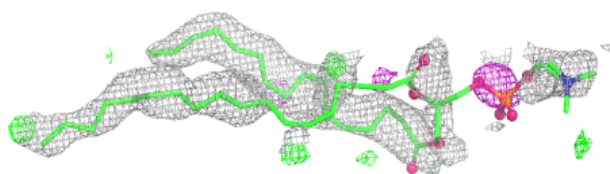
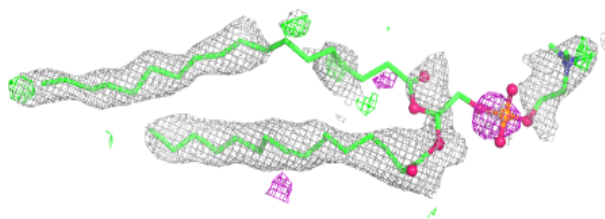
Electron density around CDL C 270:

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

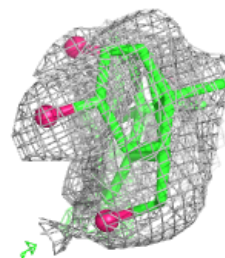
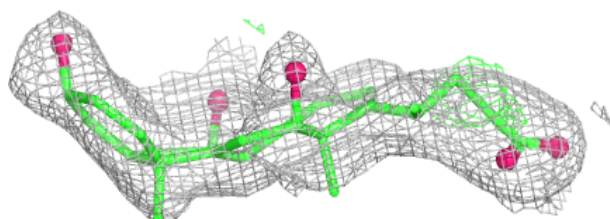
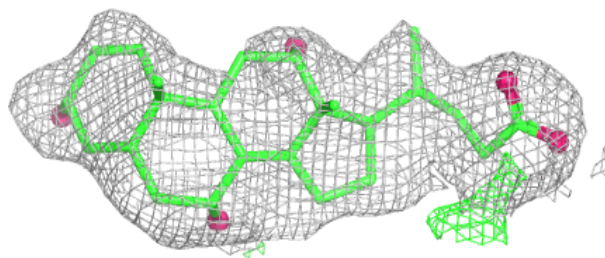


Electron density around PSC B 229:

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

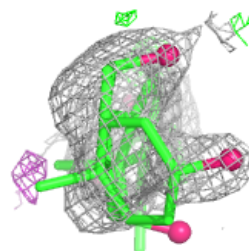
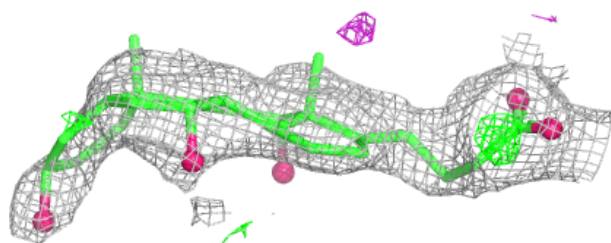
**Electron density around CHD C 271:**

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

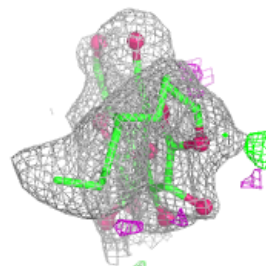
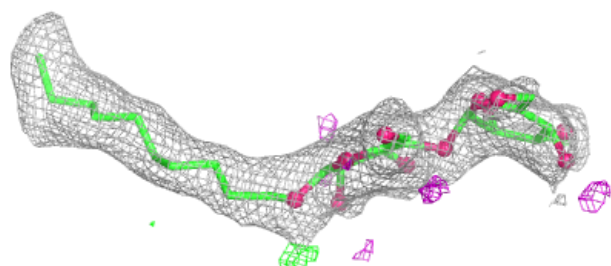
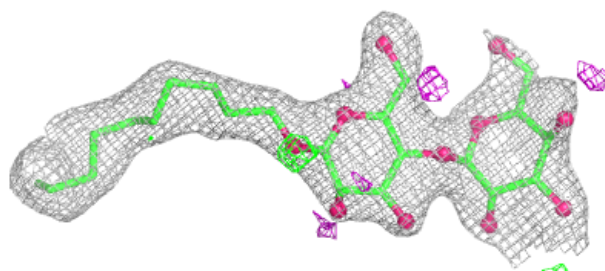


Electron density around CHD P 1271:

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

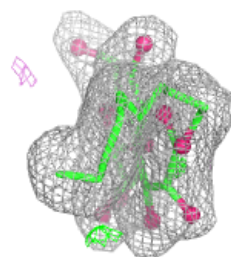
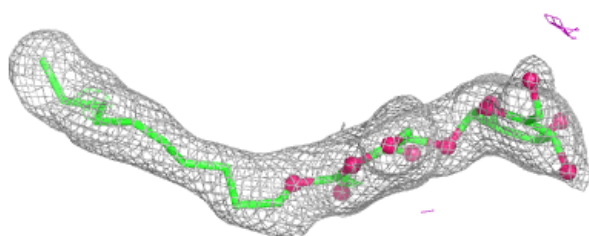
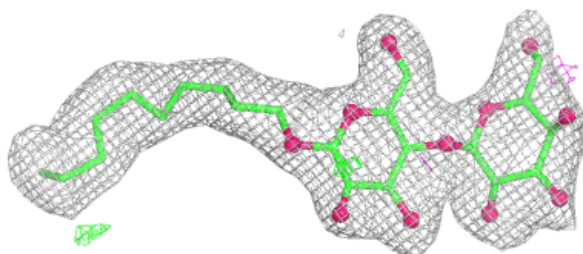
**Electron density around DMU Z 1526:**

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

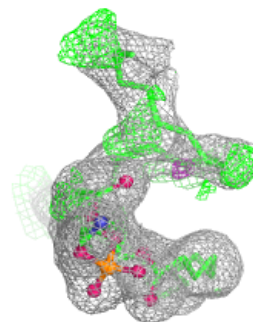
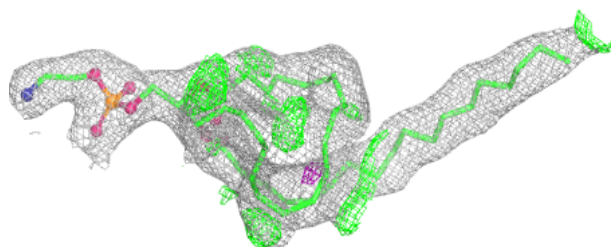
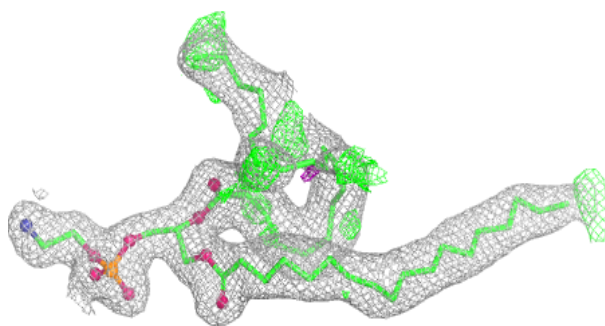


Electron density around DMU M 526:

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

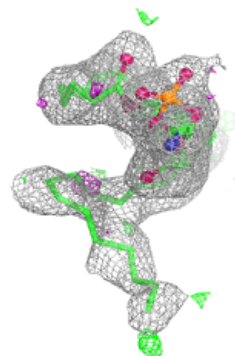
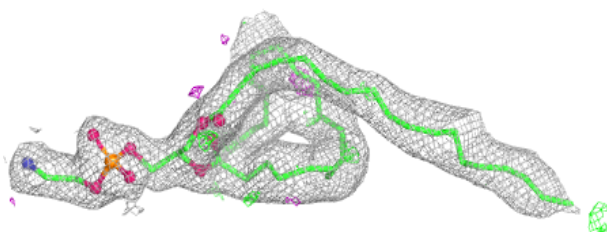
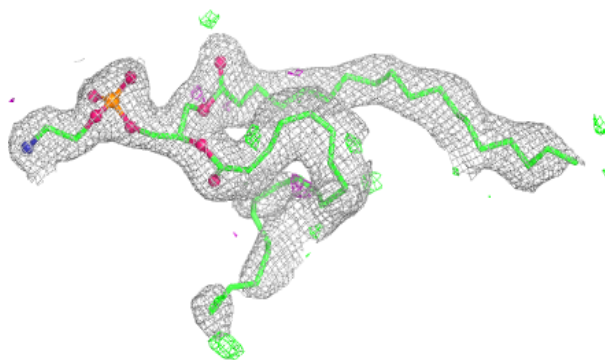
**Electron density around PEK C 264:**

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

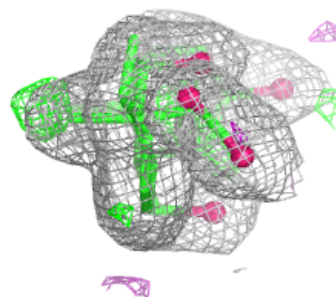
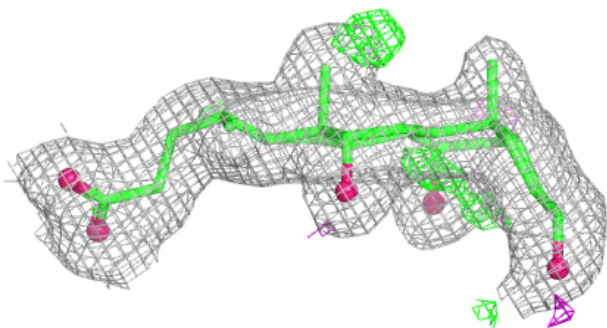
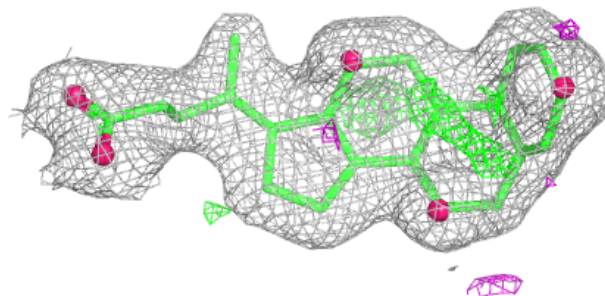


Electron density around PEK P 1264:

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

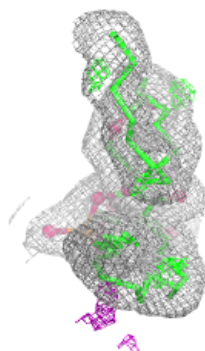
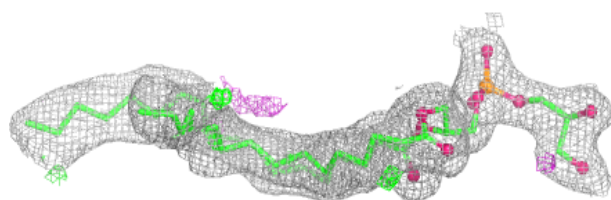
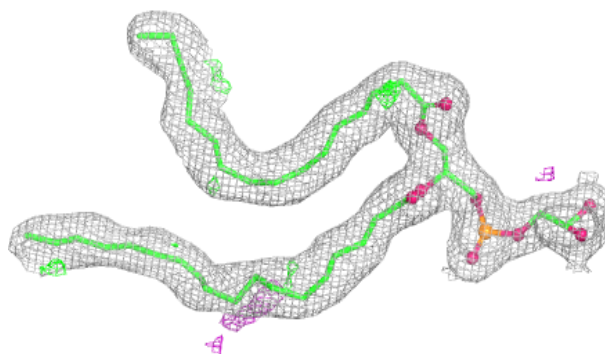
**Electron density around CHD O 229:**

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

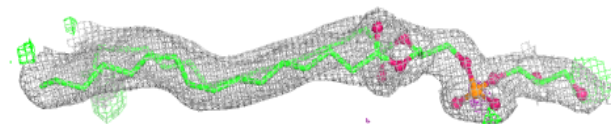
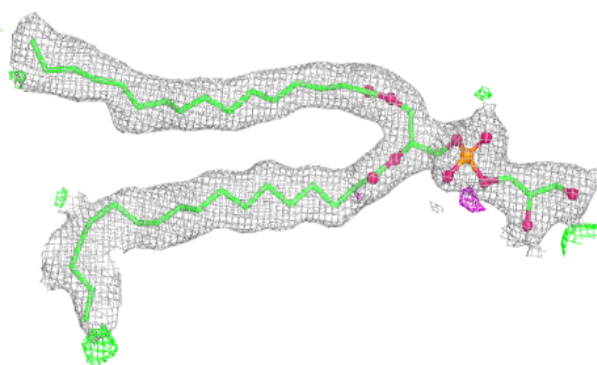


Electron density around PGV N 1266:

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

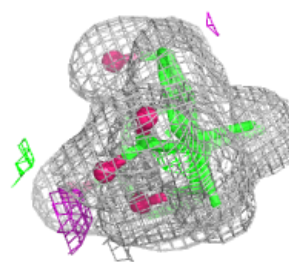
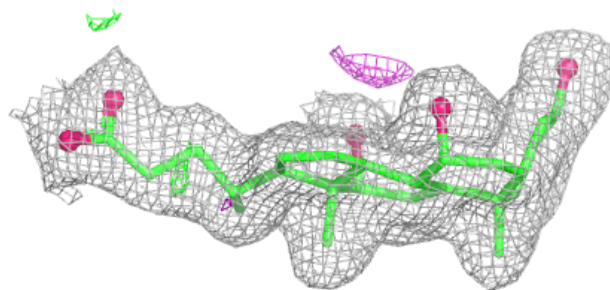
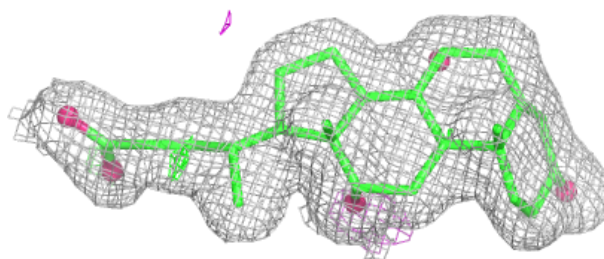
**Electron density around PGV P 1267:**

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

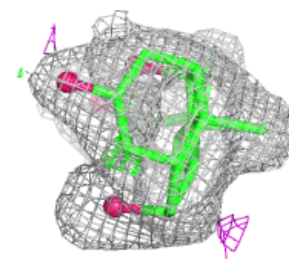
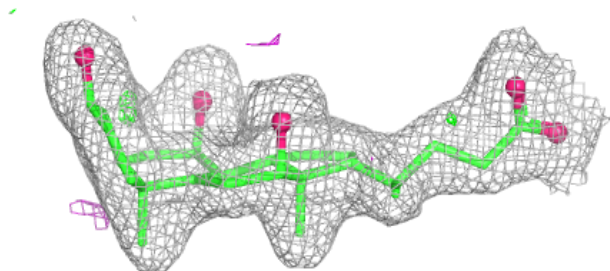
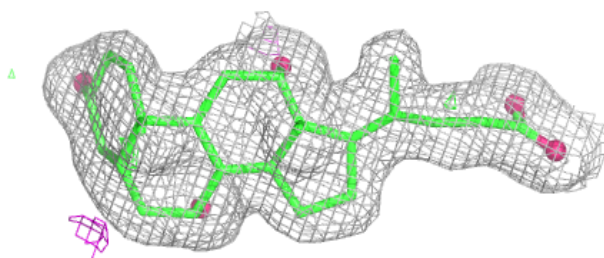


Electron density around CHD C 525:

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

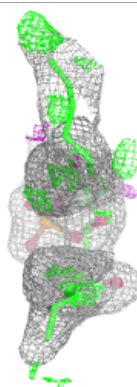
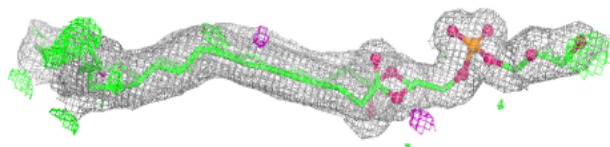
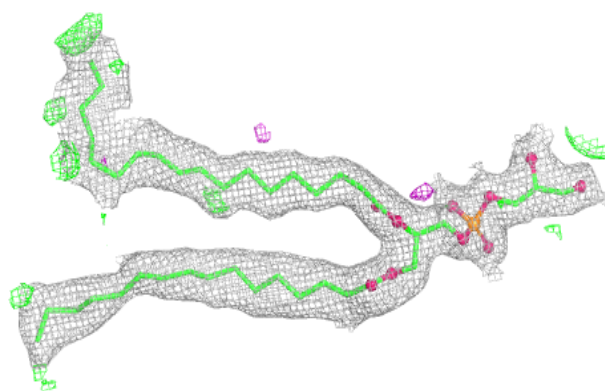
**Electron density around CHD P 1525:**

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

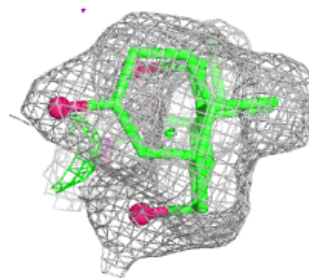
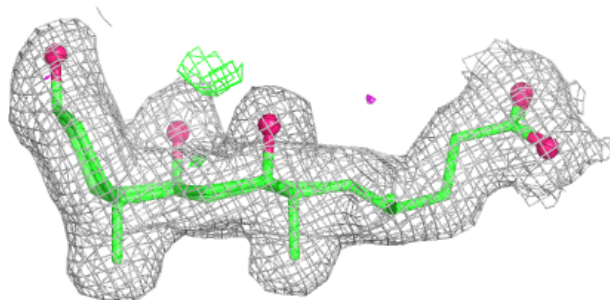
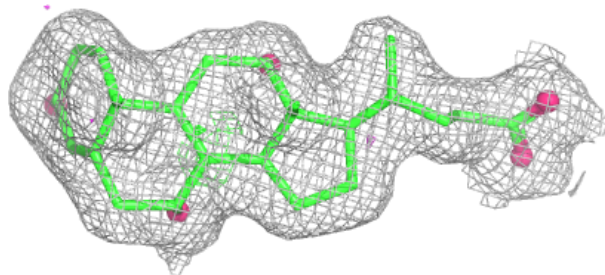


Electron density around PGV C 267:

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

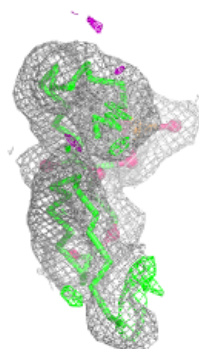
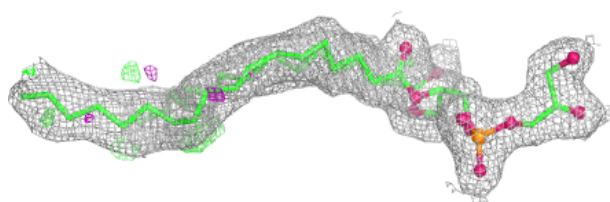
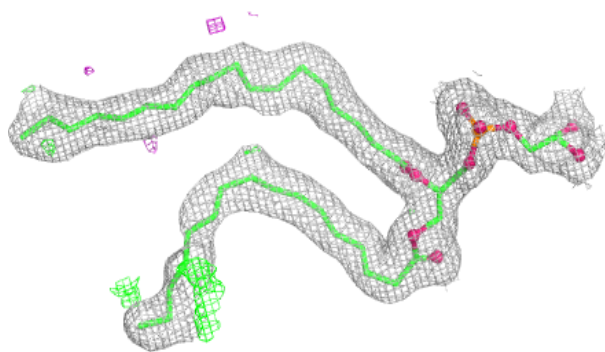
**Electron density around CHD B 1085:**

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

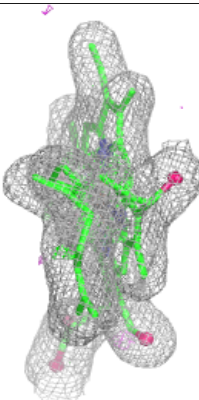
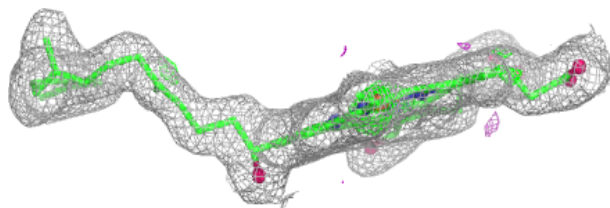
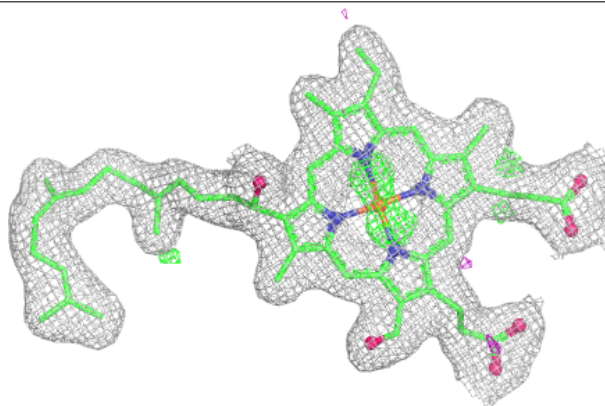


Electron density around PGV A 521:

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

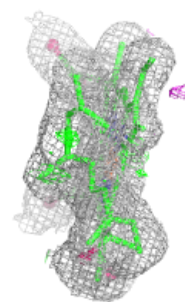
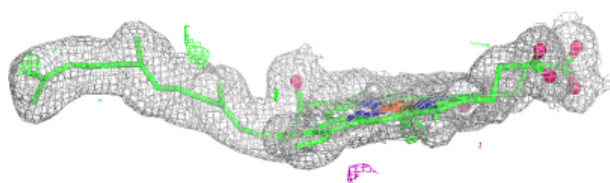
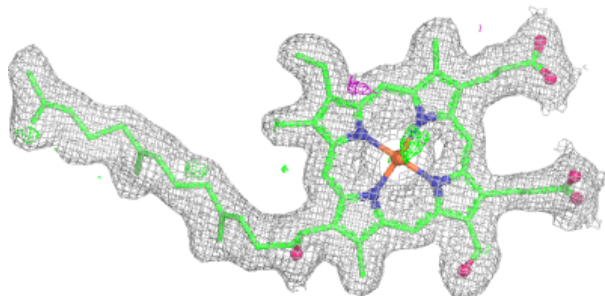
**Electron density around HEA N 516:**

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

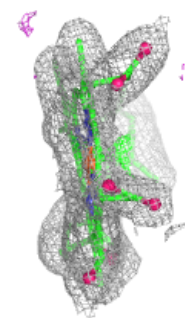
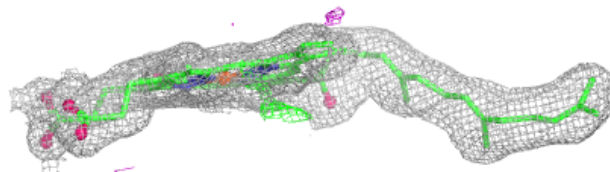
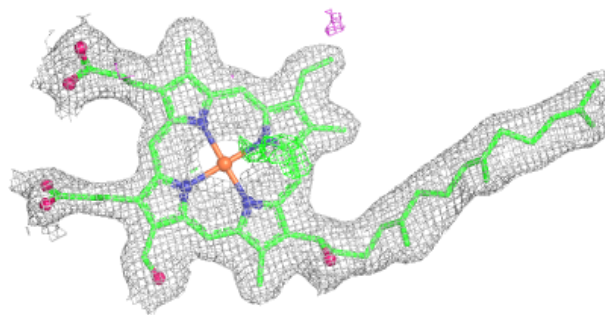


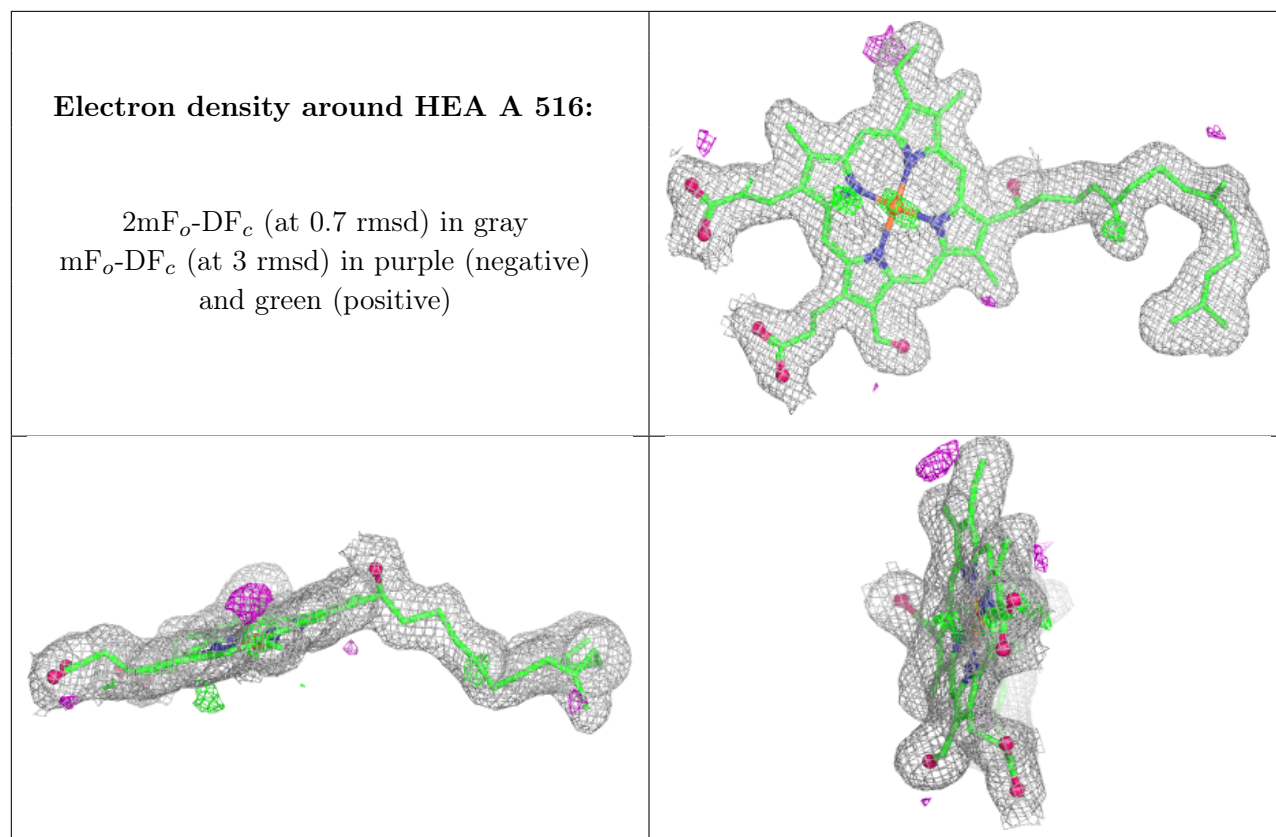
Electron density around HEA A 515:

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

**Electron density around HEA N 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.