



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 PM UTC

PDB ID : 2EIN / pdb_00002ein
Title : Zinc ion binding structure of bovine heart cytochrome C oxidase in the fully oxidized state
Authors : Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-o, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2007-03-13
Resolution : 2.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

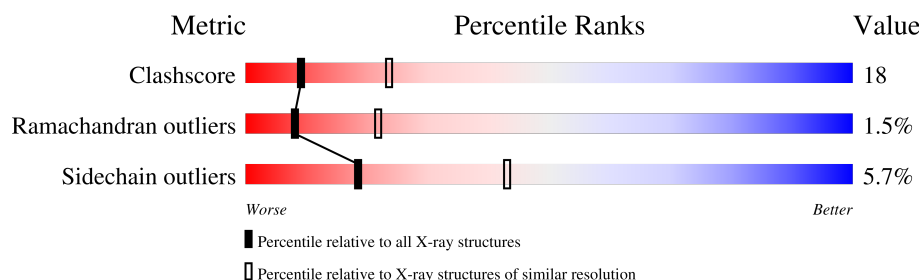
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

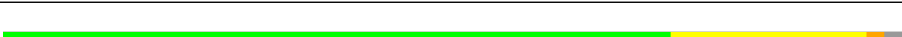
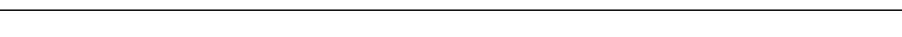
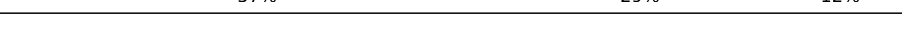
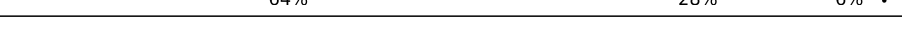
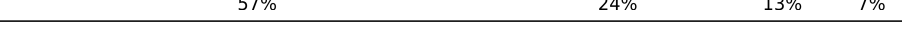
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	
4	D	147	
4	Q	147	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	PSC	B	230	-	-	X	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 31815 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

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 polypeptide Vb.

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 polypeptide VIa-heart.

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 VIb isoform 1.

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 polypeptide VIc.

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 VIIa-heart.

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 polypeptide VIIb.

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 polypeptide VIIc.

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 polypeptide VIII-heart.

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

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

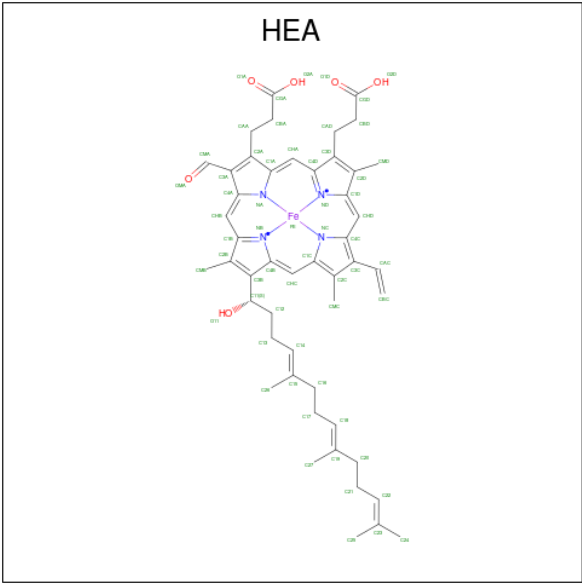
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

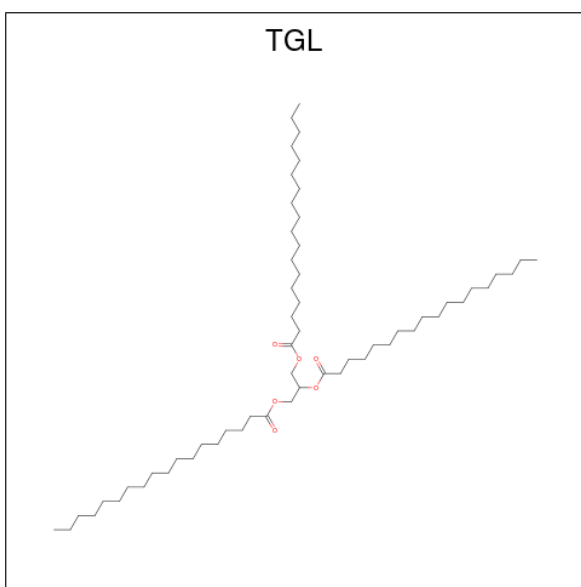
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



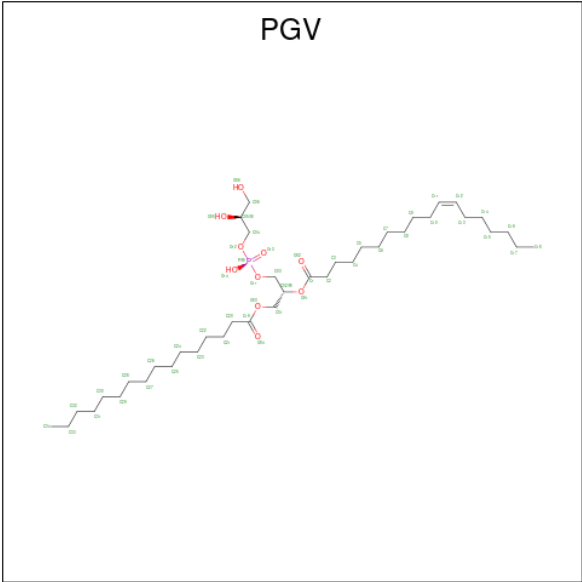
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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



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

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



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

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

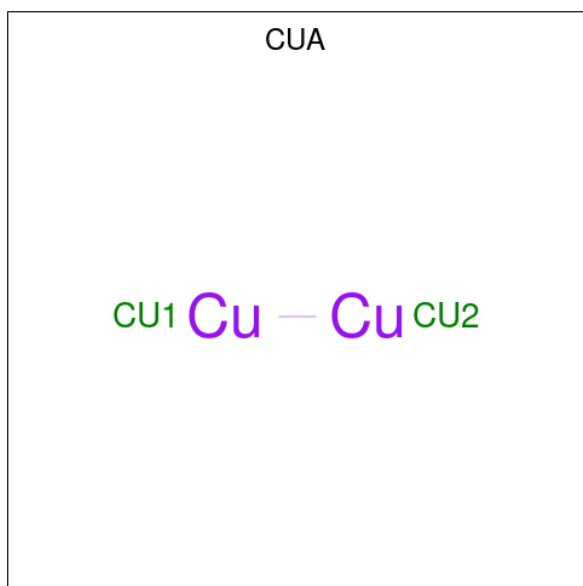
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Zn	0	0
			1	1		
20	C	1	Total	Zn	0	0
			1	1		
20	D	1	Total	Zn	0	0
			1	1		
20	F	2	Total	Zn	0	0
			2	2		

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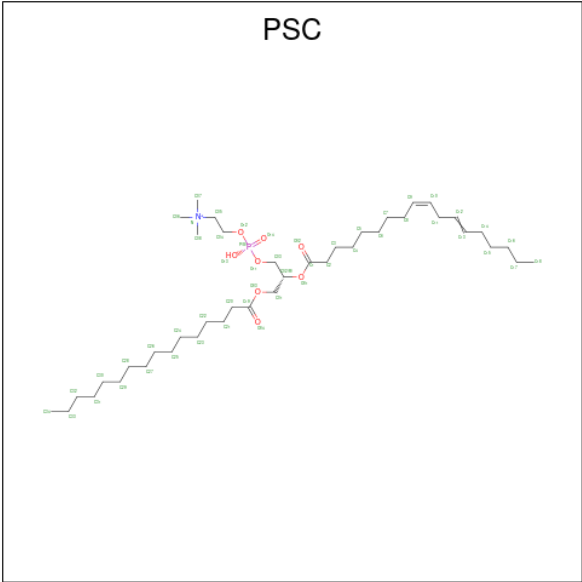
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	G	1	Total 1	Zn 1	0	0
20	L	1	Total 1	Zn 1	0	0
20	N	2	Total 2	Zn 2	0	0
20	O	1	Total 1	Zn 1	0	0
20	P	2	Total 2	Zn 2	0	0
20	S	1	Total 1	Zn 1	0	0
20	T	1	Total 1	Zn 1	0	0

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



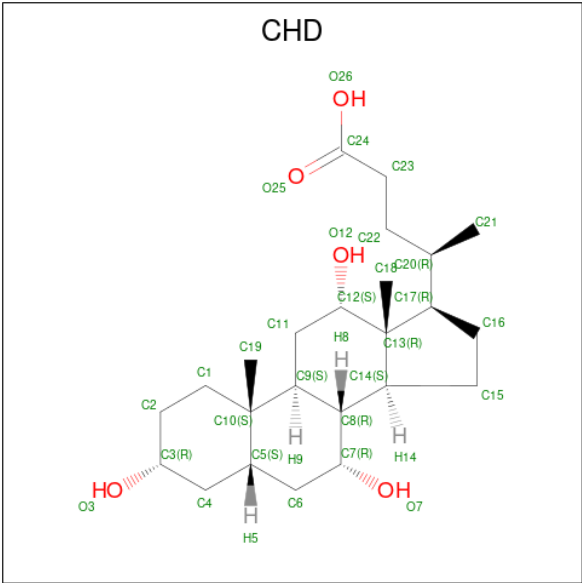
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total 2	Cu 2	0	0
21	O	1	Total 2	Cu 2	0	0

- 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: C₄₂H₈₁NO₈P).



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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



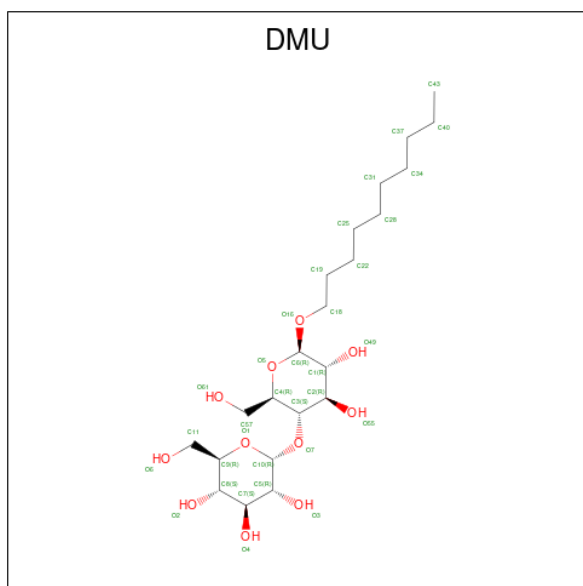
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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

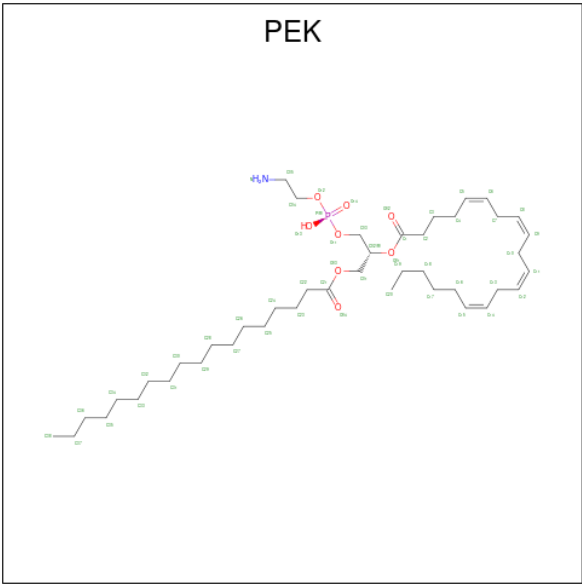
- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

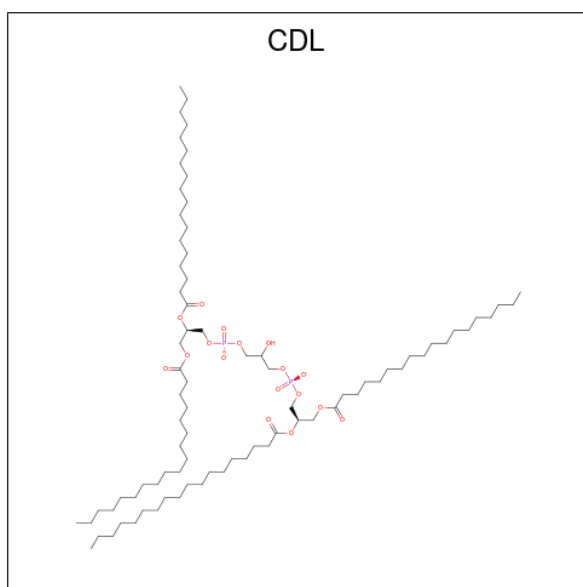
- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(ST

EAROYLOXY)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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	160	Total	O	0	0
			160	160		
27	B	86	Total	O	0	0
			86	86		
27	C	73	Total	O	0	0
			73	73		
27	D	38	Total	O	0	0
			38	38		
27	E	23	Total	O	0	0
			23	23		
27	F	37	Total	O	0	0
			37	37		
27	G	29	Total	O	0	0
			29	29		
27	H	31	Total	O	0	0
			31	31		

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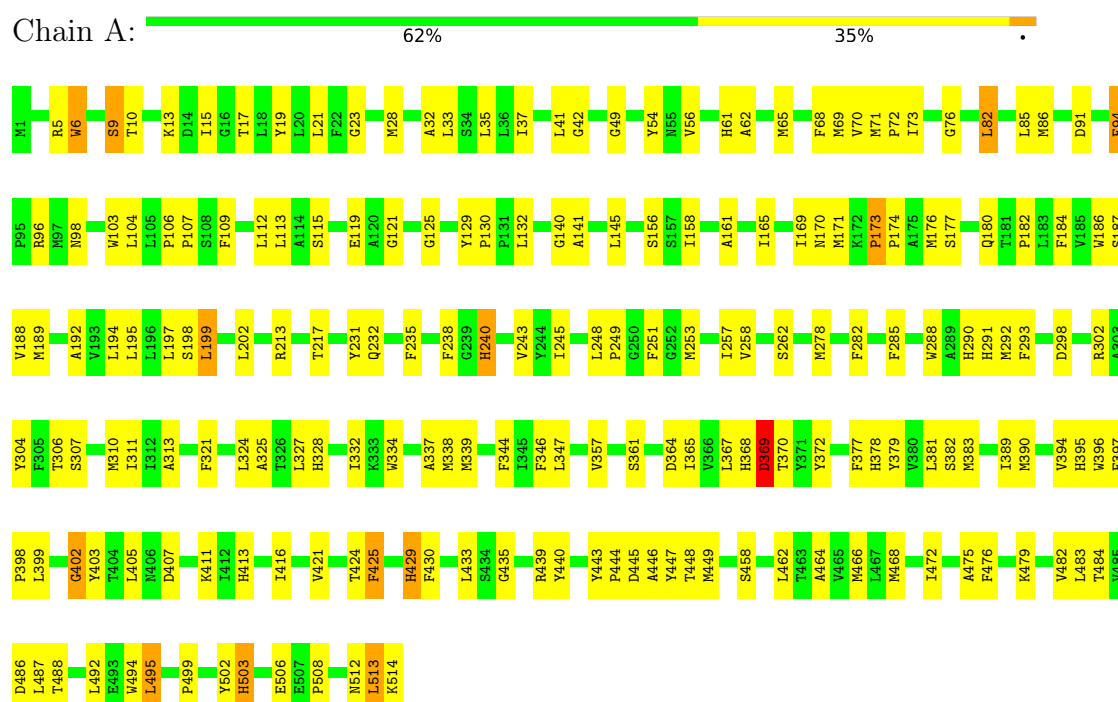
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	I	18	Total 18	O 18	0	0
27	J	9	Total 9	O 9	0	0
27	K	20	Total 20	O 20	0	0
27	L	12	Total 12	O 12	0	0
27	M	11	Total 11	O 11	0	0
27	N	161	Total 161	O 161	0	0
27	O	77	Total 77	O 77	0	0
27	P	72	Total 72	O 72	0	0
27	Q	42	Total 42	O 42	0	0
27	R	22	Total 22	O 22	0	0
27	S	39	Total 39	O 39	0	0
27	T	26	Total 26	O 26	0	0
27	U	28	Total 28	O 28	0	0
27	V	17	Total 17	O 17	0	0
27	W	13	Total 13	O 13	0	0
27	X	13	Total 13	O 13	0	0
27	Y	11	Total 11	O 11	0	0
27	Z	5	Total 5	O 5	0	0

3 Residue-property plots

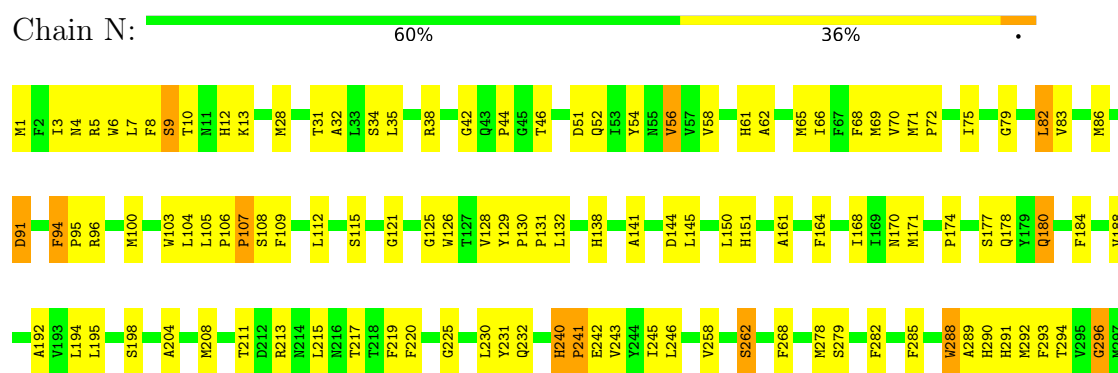
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

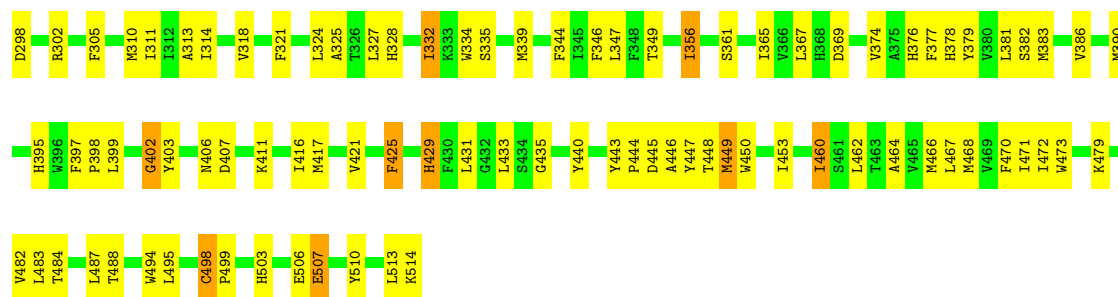
Note EDS was not executed.

• Molecule 1: Cytochrome c oxidase subunit 1



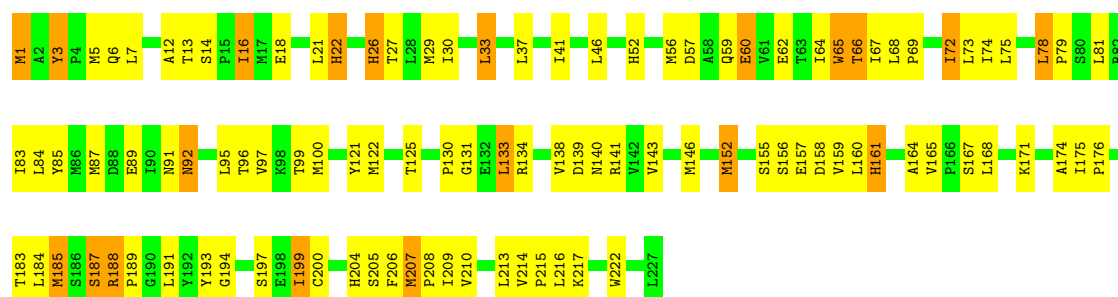
• Molecule 1: Cytochrome c oxidase subunit 1





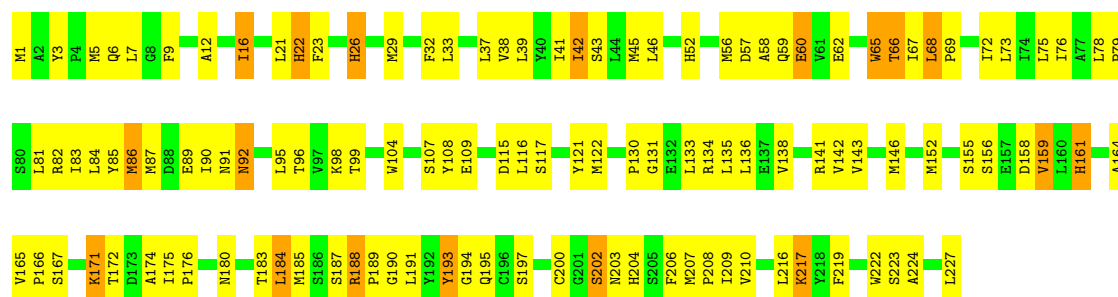
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B: 54% 37% 9%



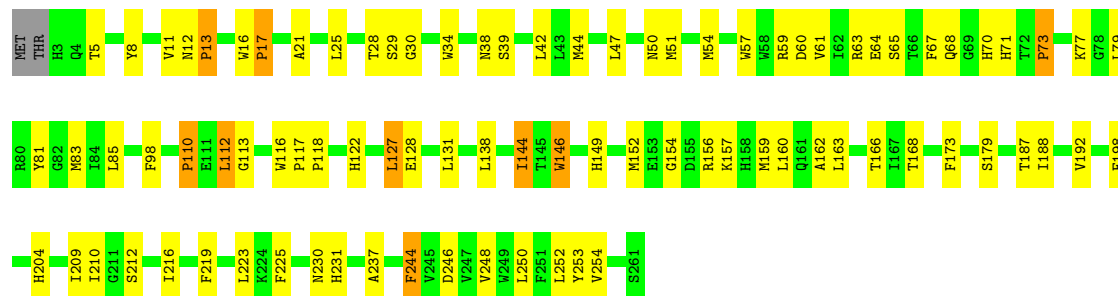
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O: 47% 45% 8%



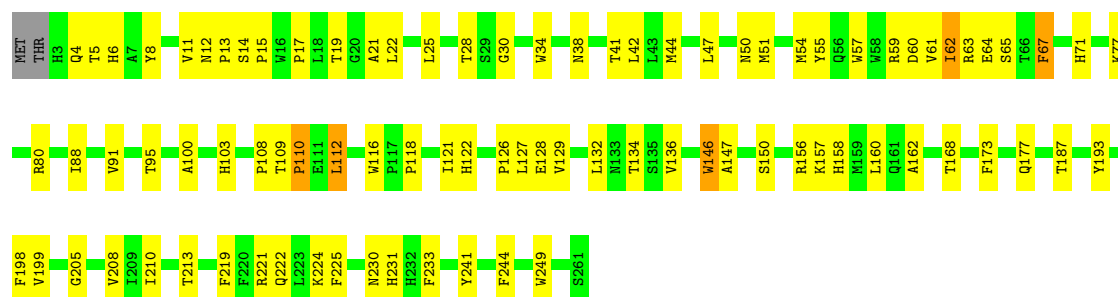
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 66% 30% 4%



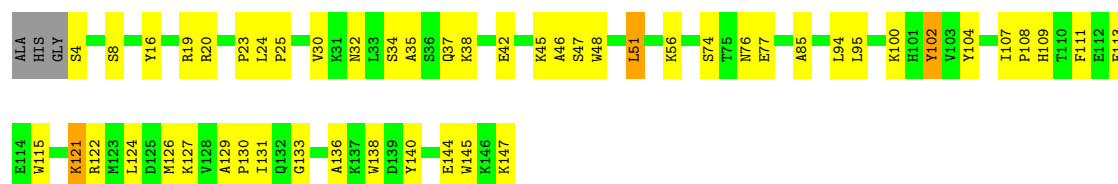
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:  66% 32% ..



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:  63% 33% ..



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:  64% 31% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:  68% 28% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:  66% 29% ..



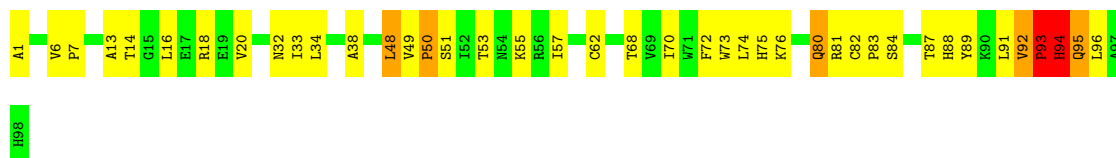
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  69% 23% 7%



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  58% 35% 5%



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  59% 29% 9%



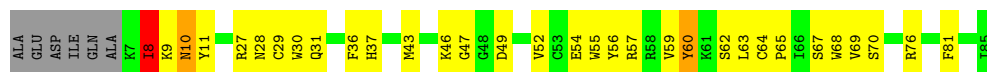
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  61% 26% 9%



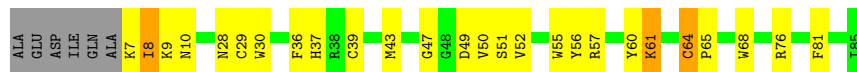
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:  55% 34% 7%



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:  62% 27% 7%



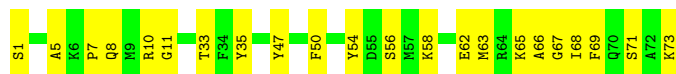
- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  73% 25% 2%



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  70% 30%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  75% 22% ..



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  75% 22% ..



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  64% 21% • 12%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  57% 29% • 12%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  64% 28% 6% •



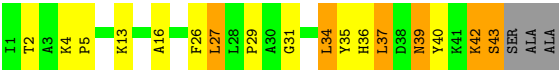
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  62% 30% 6% •



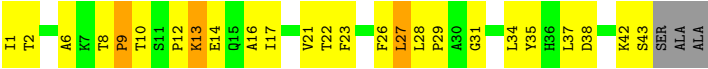
- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M: 57% 24% 13% 7%



● Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z: 39% 48% 7% 7%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.81Å 203.58Å 177.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.208 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31815	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.86	1/4156 (0.0%)	1.19	35/5678 (0.6%)
1	N	0.72	1/4156 (0.0%)	1.14	32/5678 (0.6%)
2	B	0.88	2/1860 (0.1%)	1.26	16/2534 (0.6%)
2	O	0.86	2/1860 (0.1%)	1.21	16/2534 (0.6%)
3	C	0.83	0/2197	1.02	9/3005 (0.3%)
3	P	0.72	0/2197	1.07	11/3005 (0.4%)
4	D	0.72	0/1229	1.07	7/1658 (0.4%)
4	Q	0.73	2/1229 (0.2%)	1.04	4/1658 (0.2%)
5	E	0.74	0/871	1.08	4/1182 (0.3%)
5	R	0.67	0/871	1.07	3/1182 (0.3%)
6	F	0.79	0/765	1.27	6/1038 (0.6%)
6	S	0.82	0/765	1.25	8/1038 (0.8%)
7	G	0.83	0/690	1.15	3/937 (0.3%)
7	T	0.90	1/690 (0.1%)	1.12	3/937 (0.3%)
8	H	0.75	1/682 (0.1%)	1.15	6/921 (0.7%)
8	U	0.70	0/682	1.11	4/921 (0.4%)
9	I	0.70	0/605	0.99	1/802 (0.1%)
9	V	0.65	0/605	0.95	2/802 (0.2%)
10	J	0.69	0/471	1.02	0/636
10	W	0.64	0/471	1.07	0/636
11	K	0.75	0/398	1.23	3/546 (0.5%)
11	X	0.64	0/398	1.25	5/546 (0.9%)
12	L	0.98	2/393 (0.5%)	1.18	5/526 (1.0%)
12	Y	0.83	1/393 (0.3%)	1.16	4/526 (0.8%)
13	M	0.86	0/345	1.13	1/470 (0.2%)
13	Z	0.74	1/345 (0.3%)	1.17	1/470 (0.2%)
All	All	0.78	14/29324 (0.0%)	1.14	189/39866 (0.5%)

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
1	A	0	3
1	N	0	1
2	B	0	1
2	O	0	1
All	All	0	6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	HIS	CD2-NE2	12.73	1.51	1.37
2	O	26	HIS	CD2-NE2	11.10	1.50	1.37
1	N	83	VAL	CA-CB	7.19	1.57	1.54
2	O	22	HIS	ND1-CE1	6.43	1.39	1.32
12	Y	2	HIS	CD2-NE2	6.41	1.45	1.37
4	Q	6	VAL	CA-CB	6.33	1.62	1.54
7	T	51	HIS	CD2-NE2	6.07	1.44	1.37
13	Z	8	THR	CA-CB	5.88	1.60	1.53
1	A	130	PRO	CA-C	5.75	1.57	1.52
8	H	8	ILE	CA-CB	5.66	1.62	1.54
4	Q	5	VAL	CA-CB	5.38	1.59	1.53
2	B	22	HIS	CD2-NE2	5.25	1.43	1.37
12	L	11	ILE	CA-CB	-5.21	1.50	1.55
12	L	2	HIS	CD2-NE2	5.11	1.43	1.37

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	LEU	N-CA-C	10.76	123.09	111.36
1	N	82	LEU	N-CA-C	10.32	122.60	111.36
5	E	81	ILE	N-CA-C	8.75	118.65	110.42
13	Z	27	LEU	N-CA-C	8.71	121.73	111.71
1	A	262	SER	N-CA-C	-8.70	102.45	113.23
1	A	171	MET	N-CA-C	8.45	122.11	112.57
5	E	42	VAL	N-CA-C	-8.35	98.21	107.73
1	N	262	SER	N-CA-C	-8.30	102.94	113.23
8	H	81	PHE	CA-C-N	8.28	128.39	119.28
8	H	81	PHE	C-N-CA	8.28	128.39	119.28
2	B	92	ASN	CA-C-N	8.26	128.19	119.85
2	B	92	ASN	C-N-CA	8.26	128.19	119.85
6	S	94	HIS	N-CA-C	8.23	128.32	110.80
13	M	27	LEU	N-CA-C	8.18	121.11	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	94	HIS	N-CA-C	7.94	127.72	110.80
1	N	171	MET	N-CA-C	7.83	121.42	112.57
11	X	36	ILE	N-CA-C	7.75	119.56	112.43
1	A	70	VAL	N-CA-C	7.71	117.83	110.42
8	U	64	CYS	N-CA-C	7.67	119.32	109.65
1	A	332	ILE	N-CA-C	7.67	118.96	108.84
2	B	206	PHE	N-CA-C	7.52	119.14	108.54
1	N	506	GLU	N-CA-C	-7.44	103.17	111.28
5	R	42	VAL	N-CA-C	-7.38	99.85	107.89
2	B	26	HIS	CE1-NE2-CD2	-7.36	101.64	109.00
1	A	125	GLY	N-CA-C	-7.33	103.61	112.48
1	N	125	GLY	N-CA-C	-7.24	103.72	112.48
8	H	64	CYS	N-CA-C	7.23	118.76	109.65
11	K	36	ILE	N-CA-C	7.17	119.02	112.43
2	O	206	PHE	N-CA-C	7.11	118.57	108.54
2	O	65	TRP	N-CA-C	7.06	120.46	112.97
3	P	8	TYR	N-CA-C	7.03	119.06	110.41
4	D	102	TYR	N-CA-C	7.01	121.58	112.89
1	A	130	PRO	N-CA-C	-6.97	102.20	110.70
1	A	435	GLY	N-CA-C	6.89	125.15	115.43
2	B	65	TRP	N-CA-C	6.80	120.18	112.97
4	Q	8	SER	N-CA-C	6.79	119.55	111.33
1	N	332	ILE	N-CA-C	6.79	117.78	109.30
1	A	506	GLU	N-CA-C	-6.77	103.93	111.71
1	N	70	VAL	N-CA-C	6.76	116.91	110.42
6	S	92	VAL	CA-C-N	6.72	128.24	119.84
6	S	92	VAL	C-N-CA	6.72	128.24	119.84
1	N	130	PRO	N-CA-C	-6.71	102.51	110.70
1	A	119	GLU	CB-CA-C	-6.70	108.83	116.54
2	O	26	HIS	CE1-NE2-CD2	-6.70	102.30	109.00
7	T	13	ALA	N-CA-C	6.67	119.40	111.33
3	P	112	LEU	N-CA-C	-6.66	105.31	113.50
1	N	10	THR	N-CA-C	-6.62	102.33	112.99
4	Q	102	TYR	N-CA-C	6.60	120.55	112.23
3	C	112	LEU	N-CA-C	-6.58	105.41	113.50
1	A	487	LEU	N-CA-C	6.57	120.88	112.86
1	A	402	GLY	N-CA-C	-6.54	106.12	114.37
1	N	425	PHE	N-CA-C	6.54	121.34	113.23
1	N	217	THR	N-CA-C	-6.52	102.12	110.53
1	A	10	THR	N-CA-C	-6.51	103.51	112.03
3	P	11	VAL	N-CA-C	6.51	117.48	108.89
6	F	93	PRO	N-CA-C	6.45	125.75	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	93	PRO	N-CA-C	6.41	125.67	112.47
4	D	8	SER	N-CA-C	6.40	119.08	111.33
5	R	76	GLY	CA-C-N	6.39	126.94	120.04
5	R	76	GLY	C-N-CA	6.39	126.94	120.04
2	B	161	HIS	N-CA-C	-6.38	99.93	108.74
1	A	6	TRP	N-CA-C	6.38	121.35	113.50
11	X	49	THR	CA-C-N	6.38	127.38	119.98
11	X	49	THR	C-N-CA	6.38	127.38	119.98
1	N	487	LEU	N-CA-C	6.32	120.57	112.86
1	N	56	VAL	N-CA-C	-6.29	103.23	111.09
1	A	217	THR	N-CA-C	-6.28	101.68	110.35
12	L	46	LYS	N-CA-C	-6.28	105.75	113.41
1	A	288	TRP	N-CA-C	6.27	118.92	111.33
3	C	8	TYR	N-CA-C	6.21	118.05	110.41
1	A	425	PHE	N-CA-C	6.18	120.90	113.23
1	A	198	SER	N-CA-C	6.18	118.09	111.36
1	A	94	PHE	CA-C-N	6.12	127.50	119.84
1	A	94	PHE	C-N-CA	6.12	127.50	119.84
8	H	68	TRP	N-CA-C	-6.09	104.27	111.03
7	G	6	GLY	N-CA-C	6.08	127.59	113.18
2	B	193	TYR	N-CA-C	6.05	119.80	110.42
2	B	207	MET	CA-C-N	6.00	127.33	119.84
2	B	207	MET	C-N-CA	6.00	127.33	119.84
3	P	14	SER	CA-C-N	5.98	125.68	119.64
3	P	14	SER	C-N-CA	5.98	125.68	119.64
1	N	445	ASP	N-CA-C	5.97	118.58	111.71
7	G	13	ALA	N-CA-C	5.95	118.53	111.33
2	O	193	TYR	N-CA-C	5.95	119.64	110.42
1	N	288	TRP	N-CA-C	5.94	118.52	111.33
1	A	170	ASN	N-CA-C	5.91	119.67	112.23
12	Y	2	HIS	CE1-NE2-CD2	-5.91	103.09	109.00
2	O	197	SER	N-CA-C	5.89	119.61	111.55
3	P	67	PHE	N-CA-C	5.86	118.55	111.40
11	K	49	THR	CA-C-N	5.86	126.77	119.98
11	K	49	THR	C-N-CA	5.86	126.77	119.98
1	A	173	PRO	CA-C-N	5.84	127.14	119.84
1	A	173	PRO	C-N-CA	5.84	127.14	119.84
1	N	435	GLY	N-CA-C	5.83	123.66	115.43
7	T	8	HIS	N-CA-C	5.78	123.11	110.80
12	L	11	ILE	CA-C-N	5.76	125.46	119.64
12	L	11	ILE	C-N-CA	5.76	125.46	119.64
2	O	165	VAL	CA-C-N	5.75	127.03	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	165	VAL	C-N-CA	5.75	127.03	119.84
12	L	39	ILE	N-CA-C	-5.75	105.24	110.82
9	I	69	PHE	N-CA-C	5.75	118.99	110.48
8	U	68	TRP	N-CA-C	-5.74	104.66	111.03
4	D	133	GLY	N-CA-C	5.72	126.74	113.18
9	V	69	PHE	N-CA-C	5.70	118.91	110.48
1	A	429	HIS	N-CA-C	-5.67	105.18	111.36
4	Q	133	GLY	N-CA-C	5.64	126.55	113.18
6	S	32	ASN	N-CA-C	5.62	118.94	111.30
5	E	76	GLY	CA-C-N	5.59	126.08	120.04
5	E	76	GLY	C-N-CA	5.59	126.08	120.04
1	N	460	ILE	CB-CA-C	-5.58	104.61	112.14
3	C	11	VAL	N-CA-C	5.55	116.21	108.89
12	Y	46	LYS	N-CA-C	-5.51	106.68	113.41
1	N	83	VAL	N-CA-CB	5.51	114.21	110.52
3	P	122	HIS	CA-C-N	5.51	125.51	119.89
3	P	122	HIS	C-N-CA	5.51	125.51	119.89
1	N	402	GLY	N-CA-C	-5.50	107.77	114.92
2	O	92	ASN	CA-C-N	5.48	125.68	120.31
2	O	92	ASN	C-N-CA	5.48	125.68	120.31
1	N	198	SER	N-CA-C	5.47	117.05	111.14
1	N	170	ASN	N-CA-C	5.47	119.12	112.23
2	B	26	HIS	ND1-CE1-NE2	5.46	113.86	108.40
1	A	448	THR	N-CA-C	5.45	116.90	111.07
3	C	113	GLY	N-CA-C	-5.44	107.09	116.01
11	X	35	GLN	N-CA-C	5.44	120.02	113.17
2	O	136	LEU	N-CA-C	5.42	120.17	113.50
2	B	64	ILE	CB-CA-C	-5.40	104.90	111.87
8	H	63	LEU	N-CA-C	5.40	119.95	112.45
7	G	8	HIS	N-CA-C	5.39	122.28	110.80
1	N	129	TYR	N-CA-C	5.39	116.48	109.64
1	A	199	LEU	N-CA-C	5.38	120.80	113.16
6	F	82	CYS	CA-C-N	5.37	125.04	119.56
6	F	82	CYS	C-N-CA	5.37	125.04	119.56
4	D	76	ASN	N-CA-C	-5.37	106.32	112.92
2	O	161	HIS	ND1-CG-CD2	5.37	111.47	106.10
7	T	6	GLY	N-CA-C	5.37	125.90	113.18
1	A	56	VAL	N-CA-C	-5.35	104.40	111.09
2	B	165	VAL	CA-C-N	5.35	126.53	119.84
2	B	165	VAL	C-N-CA	5.35	126.53	119.84
1	A	495	LEU	N-CA-C	5.34	119.28	112.34
1	N	449	MET	N-CA-C	5.34	117.53	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	62	ILE	N-CA-C	-5.33	105.52	110.53
2	B	197	SER	N-CA-C	5.33	118.85	111.55
4	D	129	ALA	CA-C-N	5.32	124.83	119.19
4	D	129	ALA	C-N-CA	5.32	124.83	119.19
11	X	34	THR	N-CA-C	5.30	120.76	113.97
3	P	129	VAL	N-CA-CB	5.29	113.84	110.50
3	C	146	TRP	N-CA-C	-5.28	105.43	111.14
1	N	6	TRP	N-CA-C	5.28	120.00	113.50
1	N	94	PHE	CA-C-N	5.28	124.95	119.56
1	N	94	PHE	C-N-CA	5.28	124.95	119.56
1	N	429	HIS	N-CA-C	-5.28	105.61	111.36
8	U	81	PHE	CA-C-N	5.26	124.77	119.19
8	U	81	PHE	C-N-CA	5.26	124.77	119.19
1	A	141	ALA	N-CA-C	5.25	117.91	111.82
12	Y	39	ILE	N-CA-C	-5.25	105.73	110.82
3	C	244	PHE	N-CA-C	-5.22	105.48	111.07
2	O	133	LEU	N-CA-C	5.22	117.79	109.96
1	A	389	ILE	CB-CA-C	-5.21	105.30	111.97
2	B	133	LEU	N-CA-C	5.20	117.76	109.96
3	P	146	TRP	N-CA-C	-5.20	105.53	111.14
12	Y	20	ARG	N-CA-C	-5.18	105.63	111.28
6	F	93	PRO	CA-C-N	5.18	131.44	121.54
6	F	93	PRO	C-N-CA	5.18	131.44	121.54
1	N	507	GLU	CA-C-N	5.18	125.17	119.89
1	N	507	GLU	C-N-CA	5.18	125.17	119.89
1	A	49	GLY	N-CA-C	-5.17	103.60	110.58
2	B	188	ARG	N-CA-C	5.16	114.24	108.25
2	O	161	HIS	N-CA-C	-5.16	101.58	108.86
6	S	93	PRO	CA-C-N	5.16	131.39	121.54
6	S	93	PRO	C-N-CA	5.16	131.39	121.54
1	N	107	PRO	N-CA-C	-5.15	106.37	113.53
1	N	129	TYR	CB-CA-C	-5.15	101.38	109.52
2	O	26	HIS	ND1-CE1-NE2	5.15	113.55	108.40
4	D	85	ALA	N-CA-C	-5.15	105.36	110.97
12	L	5	GLU	N-CA-C	5.14	117.49	109.52
2	O	188	ARG	N-CA-C	5.14	114.21	108.25
1	A	445	ASP	N-CA-C	5.13	118.32	111.75
9	V	66	ALA	N-CA-C	-5.13	107.02	113.28
4	Q	89	ILE	N-CA-C	-5.13	105.54	110.72
3	C	122	HIS	CA-C-N	5.12	125.11	119.89
3	C	122	HIS	C-N-CA	5.12	125.11	119.89
1	A	129	TYR	CB-CA-C	-5.11	101.45	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	141	ALA	N-CA-C	5.08	117.71	111.82
1	A	158	ILE	N-CA-C	-5.08	105.75	110.53
1	A	61	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
3	C	159	MET	N-CA-C	-5.05	105.66	111.07
2	O	90	ILE	N-CA-C	-5.01	103.11	109.58
6	S	70	ILE	CB-CA-C	-5.01	104.90	110.96
8	H	11	TYR	N-CA-C	5.00	117.41	109.96

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	372	TYR	Sidechain
1	A	502	TYR	Sidechain
2	B	85	TYR	Sidechain
1	N	240	HIS	Sidechain
2	O	85	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	175	0
1	N	4027	0	4001	177	0
2	B	1824	0	1833	95	0
2	O	1824	0	1833	105	0
3	C	2110	0	2027	84	0
3	P	2110	0	2027	85	0
4	D	1195	0	1183	42	0
4	Q	1195	0	1183	39	0
5	E	852	0	845	16	0
5	R	852	0	845	22	0
6	F	748	0	728	18	0
6	S	748	0	728	26	0
7	G	675	0	644	38	0
7	T	675	0	644	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	662	0	623	21	0
8	U	662	0	623	17	0
9	I	601	0	613	15	0
9	V	601	0	613	20	0
10	J	460	0	459	10	0
10	W	460	0	459	11	0
11	K	384	0	366	12	0
11	X	384	0	366	14	0
12	L	380	0	380	17	0
12	Y	380	0	380	17	0
13	M	335	0	352	19	0
13	Z	335	0	352	13	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	17	0
17	N	120	0	108	18	0
18	A	126	0	220	12	0
18	L	63	0	110	20	0
18	N	63	0	110	9	0
18	O	63	0	110	8	0
18	Y	63	0	110	16	0
19	A	102	0	152	9	0
19	C	102	0	152	7	0
19	N	102	0	152	10	0
19	P	102	0	152	12	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	D	1	0	0	0	0
20	F	2	0	0	0	0
20	G	1	0	0	0	0
20	L	1	0	0	0	0
20	N	2	0	0	0	0
20	O	1	0	0	0	0
20	P	2	0	0	0	0
20	S	1	0	0	0	0
20	T	1	0	0	0	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	52	0	80	21	0
22	O	52	0	80	20	0
23	B	29	0	39	5	0
23	C	58	0	78	5	0
23	G	29	0	39	1	0
23	J	29	0	39	4	0
23	P	58	0	78	6	0
23	W	29	0	39	3	0
24	C	33	0	36	3	0
24	M	33	0	38	2	0
24	P	33	0	38	4	0
24	Z	33	0	38	1	0
25	C	106	0	154	20	0
25	G	53	0	77	10	0
25	P	53	0	77	10	0
25	T	106	0	154	23	0
26	C	100	0	156	17	0
26	G	100	0	156	23	0
26	P	100	0	156	17	0
26	T	100	0	156	32	0
27	A	160	0	0	8	0
27	B	86	0	0	3	0
27	C	73	0	0	5	0
27	D	38	0	0	3	0
27	E	23	0	0	2	0
27	F	37	0	0	1	0
27	G	29	0	0	5	0
27	H	31	0	0	2	0
27	I	18	0	0	1	0
27	J	9	0	0	0	0
27	K	20	0	0	0	0
27	L	12	0	0	0	0
27	M	11	0	0	1	0
27	N	161	0	0	9	0
27	O	77	0	0	5	0
27	P	72	0	0	7	0
27	Q	42	0	0	2	0
27	R	22	0	0	1	0
27	S	39	0	0	1	0
27	T	26	0	0	3	0
27	U	28	0	0	1	0
27	V	17	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	W	13	0	0	1	0
27	X	13	0	0	1	0
27	Y	11	0	0	2	0
27	Z	5	0	0	1	0
All	All	31815	0	31300	1133	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 18.

All (1133) 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)
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.12	1.11
25:C:264:PEK:H161	25:C:264:PEK:H102	1.38	1.04
7:T:31:CYS:SG	26:T:1269:CDL:H532	1.98	1.04
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.08	1.01
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.45	0.99
22:B:230:PSC:H343	22:B:230:PSC:H142	1.43	0.97
26:G:269:CDL:H541	26:G:269:CDL:H231	1.46	0.97
25:T:1264:PEK:H161	25:T:1264:PEK:H102	1.48	0.96
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.47	0.95
7:G:84:LYS:H	7:G:84:LYS:HD2	1.33	0.94
18:O:1521:TGL:H102	18:O:1521:TGL:H281	1.50	0.94
1:A:503:HIS:H	1:A:503:HIS:CD2	1.82	0.92
12:L:20:ARG:HH12	18:L:522:TGL:HC61	1.34	0.91
12:L:13:PHE:HA	18:L:522:TGL:HC31	1.52	0.90
26:C:270:CDL:H191	26:C:270:CDL:H642	1.54	0.89
12:Y:13:PHE:HA	18:Y:1522:TGL:HC31	1.54	0.89
18:A:521:TGL:H102	18:A:521:TGL:H281	1.51	0.89
26:P:1270:CDL:H191	26:P:1270:CDL:H642	1.53	0.89
18:L:522:TGL:HC62	18:L:522:TGL:HC22	1.56	0.87
1:A:278:MET:SD	7:T:5:LYS:HB3	2.15	0.87
26:G:269:CDL:H522	26:G:269:CDL:H202	1.57	0.86
3:C:187:THR:HB	7:G:68:THR:HG21	1.59	0.85
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.59	0.84
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.57	0.84
18:O:1521:TGL:H102	18:O:1521:TGL:C28	2.06	0.84
18:A:521:TGL:H102	18:A:521:TGL:C28	2.07	0.84
3:C:54:MET:HE3	26:C:270:CDL:H612	1.60	0.83
18:Y:1522:TGL:HC62	18:Y:1522:TGL:HC22	1.60	0.83
7:G:5:LYS:HB3	1:N:278:MET:SD	2.20	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:84:LYS:HD2	7:T:84:LYS:H	1.42	0.82
1:A:42:GLY:HA3	4:D:104:TYR:OH	1.78	0.82
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.15	0.82
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.44	0.82
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.60	0.82
1:N:488:THR:HB	1:N:495:LEU:HD13	1.62	0.81
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.60	0.80
1:N:42:GLY:HA3	4:Q:104:TYR:OH	1.82	0.79
2:O:57:ASP:H	22:O:1230:PSC:H201	1.45	0.79
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.64	0.78
18:A:523:TGL:HC21	18:A:523:TGL:HG11	1.66	0.78
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.66	0.77
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.67	0.77
1:A:472:ILE:HD13	18:L:522:TGL:HA91	1.65	0.77
26:G:269:CDL:H541	26:G:269:CDL:C23	2.15	0.77
26:G:269:CDL:H622	19:P:1268:PGV:H152	1.66	0.77
1:N:177:SER:H	1:N:180:GLN:HE21	1.34	0.76
1:A:381:LEU:HB3	17:A:515:HEA:HBC1	1.66	0.76
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.15	0.76
1:N:472:ILE:HG21	18:Y:1522:TGL:CA9	2.16	0.75
7:T:34:ASN:HD22	26:T:1269:CDL:H151	1.52	0.75
18:N:1523:TGL:HC21	18:N:1523:TGL:HG11	1.68	0.75
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.84	0.75
1:N:82:LEU:O	1:N:86:MET:HG3	1.86	0.75
3:C:63:ARG:NE	26:C:270:CDL:HA22	1.97	0.74
4:Q:24:LEU:HD12	5:R:30:ARG:HA	1.67	0.74
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.52	0.74
3:P:187:THR:HB	7:T:68:THR:HG21	1.69	0.74
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.68	0.73
1:N:472:ILE:HG21	18:Y:1522:TGL:HA92	1.67	0.73
6:F:54:ASN:OD1	6:F:76:LYS:HD2	1.89	0.73
2:O:65:TRP:CZ3	22:O:1230:PSC:H331	2.23	0.73
7:T:27:SER:OG	26:T:1269:CDL:H792	1.89	0.73
18:A:521:TGL:H241	18:A:521:TGL:H201	1.71	0.72
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.52	0.72
4:D:34:SER:H	4:D:37:GLN:HE21	1.37	0.72
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.54	0.72
7:G:45:PRO:HD2	27:G:2152:HOH:O	1.90	0.72
1:N:334:TRP:CZ3	18:N:1523:TGL:HA51	2.24	0.72
1:A:232:GLN:HB2	1:A:292:MET:HE3	1.72	0.71
19:C:268:PGV:H152	26:T:1269:CDL:H622	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:516:HEA:H241	2:O:72:ILE:CG2	2.21	0.71
3:P:62:ILE:HD11	3:P:221:ARG:HD2	1.72	0.71
6:S:75:HIS:H	6:S:80:GLN:HE22	1.38	0.71
3:P:213:THR:HG21	19:P:1267:PGV:H11	1.72	0.71
2:O:22:HIS:CE1	2:O:26:HIS:HE1	2.09	0.71
27:Y:4268:HOH:O	13:Z:22:THR:HA	1.91	0.71
4:D:127:LYS:O	4:D:130:PRO:HD3	1.91	0.71
7:G:7:ASP:HB2	27:N:4030:HOH:O	1.90	0.70
1:N:195:LEU:HG	1:N:245:ILE:HD13	1.72	0.70
18:Y:1522:TGL:H242	18:Y:1522:TGL:H202	1.73	0.70
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.22	0.70
2:O:224:ALA:O	2:O:227:LEU:HG	1.91	0.70
2:O:22:HIS:NE2	2:O:26:HIS:CE1	2.60	0.70
2:B:22:HIS:CE1	2:B:26:HIS:HE1	2.10	0.70
3:C:160:LEU:HD13	23:C:271:CHD:H181	1.73	0.70
1:A:232:GLN:CB	1:A:292:MET:HE3	2.22	0.70
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.27	0.70
2:B:156:SER:HB3	2:B:176:PRO:HD3	1.72	0.70
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.73	0.69
12:L:20:ARG:NH1	18:L:522:TGL:HC61	2.07	0.69
1:N:298:ASP:HB3	27:N:3389:HOH:O	1.91	0.69
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.57	0.69
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.06	0.69
4:Q:34:SER:N	4:Q:37:GLN:HE21	1.88	0.69
22:B:230:PSC:H222	22:B:230:PSC:H21	1.74	0.69
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.74	0.69
6:S:51:SER:HB2	6:S:91:LEU:HD11	1.74	0.69
2:B:56:MET:HG2	22:B:230:PSC:H211	1.75	0.69
1:N:402:GLY:O	1:N:482:VAL:HG23	1.93	0.69
8:U:7:LYS:O	8:U:8:ILE:HG22	1.94	0.68
1:N:177:SER:H	1:N:180:GLN:NE2	1.91	0.68
3:P:59:ARG:O	3:P:63:ARG:HG3	1.93	0.68
2:B:143:VAL:HB	2:B:222:TRP:CE3	2.29	0.68
7:T:38:HIS:CD2	26:T:1269:CDL:HA21	2.27	0.68
2:B:65:TRP:CZ3	22:B:230:PSC:H331	2.29	0.68
2:B:81:LEU:HD13	26:T:1269:CDL:H122	1.75	0.68
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.76	0.68
18:L:522:TGL:H242	18:L:522:TGL:H202	1.75	0.68
8:H:43:MET:HE1	8:U:43:MET:HE1	1.76	0.68
22:O:1230:PSC:C07	9:V:10:ARG:HE	2.06	0.68
3:C:187:THR:CB	7:G:68:THR:HG21	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:4207:HOH:O	7:T:9:GLY:HA3	1.94	0.67
1:N:232:GLN:HB3	1:N:292:MET:HE3	1.76	0.67
1:A:365:ILE:HD11	27:A:4150:HOH:O	1.94	0.67
26:G:269:CDL:H511	26:G:269:CDL:H172	1.77	0.67
1:N:381:LEU:HB3	17:N:515:HEA:HBC1	1.76	0.67
22:O:1230:PSC:H21	22:O:1230:PSC:H222	1.77	0.67
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.76	0.67
1:A:82:LEU:HB3	1:A:86:MET:HE3	1.77	0.67
2:B:22:HIS:NE2	2:B:26:HIS:CE1	2.63	0.66
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.78	0.66
2:B:68:LEU:O	2:B:72:ILE:HD12	1.95	0.66
7:T:30:LEU:HD12	26:T:1269:CDL:H252	1.77	0.66
7:G:31:CYS:SG	26:G:269:CDL:H532	2.36	0.66
1:N:339:MET:HE2	18:N:1523:TGL:HA52	1.77	0.66
1:N:503:HIS:HB2	27:Y:3093:HOH:O	1.94	0.66
2:O:56:MET:HA	22:O:1230:PSC:C20	2.26	0.66
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.31	0.66
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.30	0.66
26:P:1270:CDL:H431	27:W:4131:HOH:O	1.95	0.66
6:S:94:HIS:CD2	6:S:95:GLN:H	2.14	0.66
1:N:479:LYS:HD3	27:N:4148:HOH:O	1.96	0.65
7:T:70:PHE:HB2	25:T:1264:PEK:H041	1.78	0.65
2:O:7:LEU:HD11	18:O:1521:TGL:H161	1.78	0.65
4:Q:94:LEU:HD23	11:X:28:VAL:HG21	1.79	0.65
18:O:1521:TGL:H241	18:O:1521:TGL:H201	1.78	0.65
6:F:92:VAL:HG23	6:F:92:VAL:O	1.94	0.65
1:N:379:TYR:O	1:N:383:MET:HB2	1.95	0.65
2:B:22:HIS:CE1	2:B:26:HIS:CE1	2.84	0.65
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.01	0.65
1:A:165:ILE:O	1:A:169:ILE:HG12	1.97	0.65
1:N:240:HIS:O	1:N:243:VAL:HG22	1.97	0.65
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.79	0.65
18:A:521:TGL:H161	2:B:7:LEU:HD11	1.79	0.64
25:C:264:PEK:H102	25:C:264:PEK:C16	2.21	0.64
8:H:60:TYR:CD1	8:H:60:TYR:C	2.75	0.64
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.79	0.64
3:P:157:LYS:NZ	25:P:1265:PEK:H052	2.12	0.64
1:A:65:MET:HE3	17:A:515:HEA:CMC	2.28	0.64
3:C:210:ILE:HG23	19:C:267:PGV:H102	1.77	0.64
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.79	0.64
22:B:230:PSC:C07	9:I:10:ARG:HH21	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:209:ILE:HA	27:O:3158:HOH:O	1.98	0.64
1:A:377:PHE:CE2	1:A:378:HIS:CE1	2.86	0.64
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.32	0.64
1:A:298:ASP:HB3	27:A:2389:HOH:O	1.98	0.64
2:O:57:ASP:N	22:O:1230:PSC:H201	2.11	0.64
22:O:1230:PSC:H071	9:V:10:ARG:HE	1.63	0.64
3:C:246:ASP:HB2	27:C:4064:HOH:O	1.97	0.64
10:W:45:TYR:O	10:W:48:TYR:HB3	1.98	0.64
2:O:222:TRP:HB2	9:V:71:SER:HB2	1.79	0.63
19:C:267:PGV:H182	26:C:270:CDL:H673	1.80	0.63
1:A:488:THR:HB	1:A:495:LEU:HD13	1.81	0.63
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.80	0.63
7:T:34:ASN:ND2	26:T:1269:CDL:H151	2.12	0.63
11:X:24:PHE:O	11:X:28:VAL:HG12	1.99	0.63
7:G:4:ALA:CB	1:N:282:PHE:HA	2.29	0.63
2:O:22:HIS:CE1	2:O:26:HIS:CE1	2.86	0.63
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.62	0.63
1:N:232:GLN:CB	1:N:292:MET:HE3	2.28	0.63
6:S:94:HIS:CG	6:S:95:GLN:H	2.17	0.63
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.81	0.63
1:A:466:MET:HG2	13:M:26:PHE:CD2	2.34	0.63
19:C:267:PGV:H172	26:C:270:CDL:H662	1.81	0.62
1:N:69:MET:HE2	17:N:515:HEA:H18	1.82	0.62
26:P:1270:CDL:H112	27:P:4194:HOH:O	1.98	0.62
1:A:347:LEU:HD13	1:A:383:MET:SD	2.38	0.62
4:D:122:ARG:HG2	4:D:126:MET:HE2	1.80	0.62
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.35	0.62
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.34	0.62
1:A:407:ASP:O	1:A:411:LYS:HG3	2.00	0.62
1:N:324:LEU:HD13	2:O:41:ILE:HG21	1.82	0.62
2:O:161:HIS:CE1	2:O:200:CYS:SG	2.92	0.62
2:B:1:FME:SD	2:B:133:LEU:HD11	2.40	0.62
1:N:347:LEU:HD13	1:N:383:MET:SD	2.39	0.62
1:N:449:MET:SD	2:O:5:MET:HG2	2.39	0.62
27:P:4092:HOH:O	6:S:1:ALA:HB2	2.00	0.62
2:O:42:ILE:O	2:O:46:LEU:HG	2.00	0.61
1:A:413:HIS:NE2	1:A:468:MET:HB2	2.15	0.61
2:B:62:GLU:O	2:B:66:THR:HB	2.00	0.61
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	1.81	0.61
5:R:31:LYS:HE2	5:R:35:THR:OG1	2.00	0.61
1:N:416:ILE:HG22	1:N:464:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:112:LEU:HB3	3:P:118:PRO:HB3	1.82	0.61
3:C:44:MET:HE2	3:C:44:MET:HA	1.82	0.61
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.82	0.61
10:W:30:ILE:O	10:W:34:VAL:HG23	2.00	0.61
1:A:112:LEU:C	1:A:112:LEU:HD23	2.26	0.61
1:A:367:LEU:HD21	1:A:433:LEU:HD23	1.82	0.61
1:A:382:SER:HA	17:A:515:HEA:HMC2	1.83	0.61
1:N:103:TRP:O	3:P:21:ALA:HB1	2.01	0.61
3:P:47:LEU:O	3:P:51:MET:HG2	2.01	0.61
3:C:204:HIS:HD2	3:C:248:VAL:HG12	1.65	0.61
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.65	0.61
19:N:1524:PGV:H062	27:Z:3160:HOH:O	2.01	0.61
3:C:212:SER:O	3:C:216:ILE:HG13	2.01	0.60
1:A:112:LEU:HG	27:A:2073:HOH:O	2.00	0.60
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.83	0.60
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.82	0.60
8:H:36:PHE:CE1	8:H:57:ARG:HB2	2.36	0.60
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.82	0.60
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.82	0.60
1:A:177:SER:H	1:A:180:GLN:HE21	1.49	0.60
19:A:524:PGV:H062	27:M:2160:HOH:O	2.01	0.60
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.37	0.60
3:P:157:LYS:HE2	27:P:3156:HOH:O	2.01	0.60
1:N:54:TYR:HB2	27:N:3113:HOH:O	2.02	0.60
3:C:168:THR:HG22	25:C:265:PEK:H14	1.84	0.59
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.84	0.59
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.84	0.59
6:F:85:CYS:SG	6:F:87:THR:HG23	2.42	0.59
3:C:204:HIS:HD2	3:C:248:VAL:CG1	2.16	0.59
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.83	0.59
7:G:17:ARG:HD2	27:G:2309:HOH:O	2.01	0.59
10:J:21:HIS:CD2	10:J:22:LEU:HG	2.37	0.59
10:J:40:LEU:HD12	23:J:60:CHD:H183	1.85	0.59
1:N:144:ASP:CG	1:N:213:ARG:HH21	2.11	0.59
1:N:339:MET:HE1	18:N:1523:TGL:HB31	1.85	0.59
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.03	0.59
6:S:14:THR:HB	10:W:9:GLN:NE2	2.18	0.59
1:N:406:ASN:ND2	19:N:1524:PGV:H032	2.17	0.59
9:V:65:LYS:O	11:X:54:ARG:NH1	2.36	0.59
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.67	0.59
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:264:PEK:H041	7:G:70:PHE:HB2	1.85	0.59
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.91	0.58
4:D:102:TYR:HD1	13:M:35:TYR:HE1	1.51	0.58
1:N:128:VAL:HG12	1:N:128:VAL:O	2.02	0.58
4:D:34:SER:H	4:D:37:GLN:NE2	2.01	0.58
19:P:1267:PGV:H182	26:P:1270:CDL:H673	1.85	0.58
1:A:240:HIS:O	1:A:243:VAL:HG22	2.03	0.58
2:B:146:MET:HA	2:B:213:LEU:HD12	1.85	0.58
1:N:115:SER:O	1:N:121:GLY:HA2	2.02	0.58
13:Z:17:ILE:O	13:Z:21:VAL:HG23	2.02	0.58
1:A:69:MET:HE2	17:A:515:HEA:H18	1.86	0.58
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.66	0.58
3:C:168:THR:CG2	25:C:265:PEK:H14	2.34	0.58
4:D:131:ILE:HD12	4:D:131:ILE:H	1.68	0.58
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.85	0.58
2:B:157:GLU:HA	27:B:4023:HOH:O	2.02	0.58
18:O:1521:TGL:HA82	18:O:1521:TGL:H222	1.85	0.58
1:A:311:ILE:HD12	26:T:1269:CDL:H212	1.86	0.58
1:A:449:MET:SD	2:B:5:MET:HG2	2.44	0.58
3:P:63:ARG:NH1	10:W:20:VAL:O	2.34	0.58
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.86	0.58
18:L:522:TGL:H202	18:L:522:TGL:C24	2.34	0.58
3:P:30:GLY:HA2	3:P:42:LEU:HB3	1.85	0.58
1:A:514:LYS:NZ	27:A:2395:HOH:O	2.37	0.58
25:T:1264:PEK:H32	25:T:1264:PEK:H71	1.85	0.58
1:A:94:PHE:HE1	3:C:79:LEU:HD23	1.69	0.57
1:N:335:SER:O	1:N:339:MET:HG3	2.03	0.57
2:B:66:THR:HG22	2:B:67:ILE:N	2.17	0.57
2:B:74:ILE:HD11	26:T:1269:CDL:H452	1.86	0.57
3:C:83:MET:HE2	3:C:237:ALA:HB1	1.85	0.57
5:E:43:PRO:HB2	5:E:48:ILE:HD11	1.86	0.57
1:N:344:PHE:CD1	1:N:344:PHE:C	2.81	0.57
7:T:31:CYS:SG	26:T:1269:CDL:C53	2.86	0.57
1:N:290:HIS:CD2	1:N:291:HIS:NE2	2.73	0.57
3:P:15:PRO:O	3:P:19:THR:HG23	2.04	0.57
1:A:282:PHE:HA	7:T:4:ALA:CB	2.34	0.57
2:B:1:FME:SD	2:B:133:LEU:CD1	2.93	0.57
1:A:357:VAL:HG22	2:B:27:THR:HG21	1.86	0.57
25:G:1263:PEK:H9	3:P:244:PHE:HA	1.85	0.57
3:P:126:PRO:HG2	3:P:127:LEU:HD22	1.86	0.57
1:A:327:LEU:CD2	1:A:338:MET:HE1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:47:PHE:HE1	7:T:49:PRO:HG3	1.70	0.57
1:A:13:LYS:HE3	1:A:85:LEU:HD21	1.86	0.57
1:A:41:LEU:HD11	1:A:54:TYR:OH	2.05	0.57
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.40	0.57
3:C:51:MET:SD	26:C:270:CDL:H622	2.44	0.57
3:C:204:HIS:CD2	3:C:248:VAL:HG12	2.39	0.57
1:A:405:LEU:HD23	1:A:475:ALA:HB2	1.87	0.57
18:A:521:TGL:HC22	27:I:2383:HOH:O	2.05	0.57
3:C:54:MET:HE3	26:C:270:CDL:C61	2.31	0.57
1:A:253:MET:O	1:A:257:ILE:HG13	2.04	0.57
2:B:56:MET:HA	22:B:230:PSC:C20	2.35	0.57
2:B:99:THR:HG22	2:B:152:MET:CE	2.35	0.57
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.39	0.57
2:O:56:MET:HA	22:O:1230:PSC:H202	1.87	0.56
1:A:115:SER:O	1:A:121:GLY:HA2	2.06	0.56
1:A:416:ILE:HG22	1:A:464:ALA:HB2	1.87	0.56
1:A:492:LEU:HD12	1:A:492:LEU:O	2.04	0.56
18:A:521:TGL:HA82	18:A:521:TGL:H222	1.86	0.56
3:P:187:THR:CB	7:T:68:THR:HG21	2.34	0.56
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.05	0.56
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.39	0.56
2:O:82:ARG:HG2	2:O:86:MET:CE	2.36	0.56
25:C:265:PEK:H371	26:G:269:CDL:H261	1.87	0.56
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.06	0.56
25:C:265:PEK:C38	26:G:269:CDL:H273	2.35	0.56
5:R:67:ILE:O	5:R:71:VAL:HG23	2.06	0.56
23:B:1086:CHD:H14	27:B:2112:HOH:O	2.05	0.56
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.87	0.56
6:S:48:LEU:O	6:S:50:PRO:HD3	2.06	0.56
1:A:103:TRP:O	3:C:21:ALA:HB1	2.05	0.56
1:A:484:THR:HB	13:M:2:THR:OG1	2.06	0.56
1:N:31:THR:HG23	17:N:515:HEA:H14	1.87	0.56
1:N:52:GLN:O	1:N:56:VAL:HG23	2.06	0.56
4:Q:69:ALA:O	5:R:109:VAL:HG12	2.05	0.56
19:P:1267:PGV:H161	19:P:1267:PGV:H12	1.87	0.56
6:S:16:LEU:O	6:S:20:VAL:HG23	2.06	0.56
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.28	0.56
1:A:104:LEU:O	1:A:107:PRO:HD2	2.06	0.55
4:D:102:TYR:CD1	13:M:35:TYR:HE1	2.24	0.55
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.87	0.55
1:N:310:MET:O	2:O:73:LEU:HD13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:GLU:HB2	10:J:4:ARG:NH1	2.21	0.55
7:T:23:LEU:C	7:T:26:PRO:HD2	2.31	0.55
1:A:399:LEU:HB2	1:A:494:TRP:CE3	2.41	0.55
6:F:16:LEU:O	6:F:16:LEU:HD12	2.06	0.55
2:O:23:PHE:CE2	2:O:79:PRO:HG2	2.42	0.55
1:A:381:LEU:HB3	17:A:515:HEA:CB3	2.35	0.55
7:G:2:SER:O	25:G:1263:PEK:H322	2.07	0.55
19:N:1266:PGV:H182	3:P:28:THR:HG22	1.89	0.55
18:Y:1522:TGL:H231	18:Y:1522:TGL:H272	1.87	0.55
2:B:57:ASP:H	22:B:230:PSC:H201	1.71	0.55
1:A:173:PRO:HD2	1:A:176:MET:SD	2.45	0.55
12:Y:40:VAL:O	12:Y:44:LEU:HG	2.07	0.55
3:C:57:TRP:O	3:C:61:VAL:HG23	2.07	0.55
2:O:193:TYR:CD1	2:O:210:VAL:HG22	2.42	0.55
19:P:1267:PGV:H172	26:P:1270:CDL:H662	1.87	0.55
1:A:113:LEU:HD12	18:L:522:TGL:H292	1.89	0.55
1:A:324:LEU:HD13	2:B:41:ILE:HG21	1.89	0.55
1:A:398:PRO:HA	1:A:403:TYR:O	2.07	0.55
7:G:66:ASN:HD21	7:G:79:PRO:HD2	1.72	0.55
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.72	0.55
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.88	0.55
3:P:213:THR:CG2	19:P:1267:PGV:H11	2.36	0.55
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.89	0.54
3:C:149:HIS:HA	3:C:152:MET:HE2	1.89	0.54
1:N:184:PHE:O	1:N:188:VAL:HG23	2.07	0.54
2:O:217:LYS:HA	2:O:217:LYS:HE2	1.89	0.54
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.89	0.54
2:B:158:ASP:O	2:B:176:PRO:HG3	2.06	0.54
19:A:524:PGV:H311	13:M:16:ALA:HA	1.89	0.54
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.23	0.54
1:N:367:LEU:HD21	1:N:433:LEU:HD23	1.89	0.54
26:T:1269:CDL:H322	26:T:1269:CDL:HA62	1.89	0.54
25:C:265:PEK:H22	27:G:4145:HOH:O	2.07	0.54
1:N:100:MET:HE1	19:N:1266:PGV:H81	1.90	0.54
7:T:45:PRO:HD2	27:T:3152:HOH:O	2.07	0.54
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.43	0.54
6:F:77:GLY:O	6:F:90:LYS:HE2	2.07	0.54
8:H:46:LYS:NZ	8:U:55:TRP:HB2	2.23	0.54
9:I:23:GLY:O	9:I:27:VAL:HG23	2.08	0.54
2:O:84:LEU:HD12	2:O:87:MET:HE2	1.89	0.54
18:O:1521:TGL:HC22	27:V:3383:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:G:4051:HOH:O	2:O:67:ILE:HD11	2.07	0.54
13:M:39:ASN:O	13:M:43:SER:HB2	2.08	0.54
1:N:324:LEU:HD13	2:O:41:ILE:HG22	1.90	0.54
7:T:2:SER:O	25:T:263:PEK:H322	2.07	0.54
1:A:65:MET:HE3	17:A:515:HEA:C2C	2.38	0.54
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.89	0.54
8:H:43:MET:CE	8:U:43:MET:HE1	2.37	0.54
1:N:104:LEU:O	1:N:107:PRO:HD2	2.08	0.54
1:N:132:LEU:O	1:N:132:LEU:HD12	2.08	0.54
2:O:155:SER:O	2:O:174:ALA:HB1	2.08	0.54
2:B:138:VAL:HG22	2:B:210:VAL:CG2	2.38	0.54
3:C:68:GLN:HB2	3:C:70:HIS:HD2	1.73	0.54
1:N:69:MET:HE2	17:N:515:HEA:C18	2.38	0.54
1:A:5:ARG:O	1:A:9:SER:HB2	2.08	0.54
2:O:216:LEU:O	2:O:219:PHE:HB3	2.08	0.54
1:A:33:LEU:HD23	12:L:36:PRO:HB3	1.89	0.53
1:N:65:MET:HB3	17:N:515:HEA:HAC	1.90	0.53
2:O:121:TYR:O	2:O:138:VAL:HA	2.08	0.53
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.07	0.53
24:P:1272:DMU:H25	25:T:1264:PEK:H341	1.90	0.53
1:A:443:TYR:HD1	1:A:447:TYR:HB2	1.72	0.53
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.43	0.53
18:Y:1522:TGL:H202	18:Y:1522:TGL:C24	2.37	0.53
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.74	0.53
9:V:5:ALA:O	9:V:7:PRO:HD3	2.09	0.53
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.22	0.53
2:B:69:PRO:HG3	22:B:230:PSC:H183	1.91	0.53
4:D:94:LEU:HD23	11:K:28:VAL:HG21	1.89	0.53
4:D:100:LYS:HE2	11:K:37:GLY:O	2.07	0.53
3:P:225:PHE:HA	27:P:3236:HOH:O	2.09	0.53
4:Q:131:ILE:HD12	4:Q:131:ILE:N	2.22	0.53
6:S:62:CYS:SG	6:S:84:SER:HB3	2.49	0.53
1:A:86:MET:HB3	1:A:182:PRO:HG2	1.91	0.53
1:A:503:HIS:CD2	1:A:503:HIS:N	2.58	0.53
3:C:98:PHE:CZ	3:C:252:LEU:HD23	2.44	0.53
1:N:399:LEU:HA	1:N:498:CYS:HB3	1.90	0.53
1:N:35:LEU:HD11	1:N:462:LEU:HD13	1.91	0.53
1:N:466:MET:HG2	13:Z:26:PHE:CD2	2.44	0.53
1:A:306:THR:O	1:A:310:MET:HG3	2.09	0.53
1:A:499:PRO:HD2	12:L:7:PRO:HD3	1.91	0.53
24:C:272:DMU:H25	25:C:264:PEK:H341	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:TYR:HD1	13:M:35:TYR:CE1	2.26	0.53
4:D:107:ILE:HD13	11:K:39:GLU:HB2	1.91	0.53
10:J:56:PRO:HD3	12:L:46:LYS:HE3	1.90	0.53
3:P:118:PRO:HD2	3:P:121:ILE:HG13	1.91	0.53
18:Y:1522:TGL:H211	18:Y:1522:TGL:HA72	1.91	0.53
1:N:472:ILE:HD13	18:Y:1522:TGL:HA91	1.91	0.52
6:S:51:SER:CB	6:S:91:LEU:HD11	2.39	0.52
2:B:216:LEU:O	2:B:216:LEU:HD12	2.09	0.52
2:O:141:ARG:NH1	2:O:191:LEU:HD11	2.24	0.52
19:C:267:PGV:H12	19:C:267:PGV:H161	1.90	0.52
2:O:68:LEU:HB3	22:O:1230:PSC:H182	1.91	0.52
3:C:29:SER:HB3	3:C:42:LEU:CD1	2.40	0.52
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.44	0.52
1:N:407:ASP:O	1:N:411:LYS:HG3	2.09	0.52
4:Q:97:ILE:HG13	11:X:32:MET:HG3	1.92	0.52
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.92	0.52
2:O:108:TYR:CE1	2:O:142:VAL:HG21	2.45	0.52
26:T:1269:CDL:H342	26:T:1269:CDL:OA7	2.10	0.52
22:B:230:PSC:C07	9:I:10:ARG:NH2	2.73	0.52
7:G:34:ASN:HD22	26:G:269:CDL:H151	1.75	0.52
27:O:4075:HOH:O	4:Q:108:PRO:HG3	2.08	0.52
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.91	0.52
25:T:1264:PEK:H102	25:T:1264:PEK:C16	2.32	0.52
1:A:321:PHE:CD2	22:B:230:PSC:H341	2.45	0.52
3:C:73:PRO:HB2	27:C:4140:HOH:O	2.10	0.52
26:C:270:CDL:H112	27:C:4234:HOH:O	2.09	0.52
9:V:58:LYS:O	9:V:62:GLU:HG3	2.09	0.52
19:A:524:PGV:H301	19:A:524:PGV:H152	1.91	0.52
26:G:269:CDL:H122	2:O:81:LEU:HD13	1.91	0.52
13:M:31:GLY:HA3	24:M:526:DMU:H9	1.91	0.52
8:H:43:MET:HE1	8:U:43:MET:CE	2.38	0.52
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.45	0.52
2:B:209:ILE:HA	27:B:2158:HOH:O	2.09	0.52
1:N:443:TYR:HE1	1:N:448:THR:HA	1.73	0.52
1:A:514:LYS:HE2	27:F:2339:HOH:O	2.10	0.51
23:B:1086:CHD:H20	7:T:18:PHE:HD2	1.75	0.51
3:C:127:LEU:HD12	3:C:131:LEU:HD22	1.92	0.51
4:D:107:ILE:CD1	11:K:39:GLU:HB2	2.40	0.51
1:A:177:SER:H	1:A:180:GLN:NE2	2.08	0.51
2:B:222:TRP:HB2	9:I:71:SER:HB2	1.91	0.51
3:C:68:GLN:HE21	3:C:70:HIS:CD2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:243:VAL:HB	17:N:516:HEA:HAC	1.92	0.51
3:P:156:ARG:HE	23:P:1271:CHD:H232	1.76	0.51
7:T:6:GLY:O	25:T:263:PEK:H311	2.11	0.51
11:X:19:ALA:HA	27:X:4125:HOH:O	2.10	0.51
12:Y:11:ILE:HG13	12:Y:13:PHE:O	2.10	0.51
3:C:60:ASP:O	3:C:64:GLU:HG3	2.10	0.51
12:L:20:ARG:HH22	18:L:522:TGL:HC32	1.75	0.51
27:N:3198:HOH:O	3:P:17:PRO:HG2	2.11	0.51
2:O:41:ILE:HD13	22:O:1230:PSC:H342	1.93	0.51
2:O:98:LYS:HE3	2:O:109:GLU:HB2	1.92	0.51
3:C:173:PHE:C	3:C:173:PHE:CD2	2.89	0.51
25:C:265:PEK:H371	26:G:269:CDL:C26	2.41	0.51
1:N:219:PHE:HZ	3:P:199:VAL:HG21	1.76	0.51
1:N:398:PRO:HA	1:N:403:TYR:O	2.10	0.51
1:N:472:ILE:CG2	18:Y:1522:TGL:HA92	2.36	0.51
6:S:55:LYS:HA	6:S:74:LEU:O	2.11	0.51
6:S:94:HIS:CD2	6:S:95:GLN:N	2.79	0.51
2:B:185:MET:SD	2:B:185:MET:C	2.93	0.51
3:P:67:PHE:HA	10:W:9:GLN:HG2	1.92	0.51
3:P:80:ARG:HG2	3:P:233:PHE:CE2	2.46	0.51
3:P:198:PHE:CD2	25:T:1264:PEK:H032	2.46	0.51
2:B:141:ARG:HH11	2:B:191:LEU:HD21	1.75	0.51
26:G:269:CDL:H231	26:G:269:CDL:C54	2.29	0.51
9:I:58:LYS:O	9:I:62:GLU:HG3	2.10	0.51
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.93	0.51
1:A:232:GLN:HB3	1:A:292:MET:HE3	1.93	0.51
18:A:523:TGL:HG11	18:A:523:TGL:CC2	2.39	0.51
2:B:97:VAL:O	2:B:152:MET:HE3	2.10	0.51
3:P:54:MET:HE1	19:P:1267:PGV:H141	1.92	0.51
3:P:116:TRP:CZ2	3:P:193:TYR:HD1	2.29	0.51
1:A:37:ILE:HG21	17:A:515:HEA:HMA	1.93	0.51
1:A:235:PHE:C	1:A:235:PHE:CD2	2.88	0.51
1:A:508:PRO:HD2	3:C:5:THR:OG1	2.10	0.51
2:B:164:ALA:O	2:B:194:GLY:HA3	2.10	0.51
19:C:267:PGV:H182	26:C:270:CDL:C67	2.41	0.51
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.46	0.51
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.93	0.51
3:P:80:ARG:HG2	3:P:233:PHE:HE2	1.76	0.51
1:A:243:VAL:HB	17:A:516:HEA:HAC	1.93	0.51
2:B:3:TYR:N	2:B:3:TYR:CD2	2.79	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:55:LYS:HA	6:F:74:LEU:O	2.10	0.51
1:N:1:FME:HCN	1:N:4:ASN:H	1.76	0.51
1:N:346:PHE:CE1	2:O:39:LEU:HB2	2.46	0.51
1:N:349:THR:HG21	2:O:38:VAL:HG21	1.93	0.51
1:A:82:LEU:O	1:A:86:MET:HG3	2.10	0.50
4:D:113:GLU:HG3	27:D:2281:HOH:O	2.11	0.50
10:J:50:LEU:HD22	10:J:50:LEU:O	2.10	0.50
1:A:429:HIS:HB3	18:A:521:TGL:HB41	1.93	0.50
6:F:72:PHE:CE2	6:F:82:CYS:HA	2.47	0.50
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.34	0.50
1:A:94:PHE:CE1	3:C:79:LEU:HD23	2.46	0.50
1:A:379:TYR:O	1:A:383:MET:HB2	2.11	0.50
23:B:1086:CHD:H162	7:T:18:PHE:CE2	2.46	0.50
1:N:219:PHE:CZ	3:P:199:VAL:HG21	2.47	0.50
1:N:406:ASN:HD21	19:N:1524:PGV:H032	1.75	0.50
1:N:443:TYR:HD1	1:N:447:TYR:HB2	1.77	0.50
1:N:514:LYS:NZ	27:N:3395:HOH:O	2.43	0.50
2:B:184:LEU:HD23	2:B:185:MET:N	2.27	0.50
4:D:35:ALA:HB3	27:D:4135:HOH:O	2.12	0.50
6:F:48:LEU:O	6:F:50:PRO:HD3	2.11	0.50
1:N:302:ARG:NH1	2:O:84:LEU:HD11	2.26	0.50
3:P:173:PHE:C	3:P:173:PHE:CD2	2.88	0.50
25:C:264:PEK:H32	25:C:264:PEK:H71	1.94	0.50
2:O:164:ALA:O	2:O:194:GLY:HA3	2.12	0.50
9:V:67:GLY:HA2	27:V:3310:HOH:O	2.12	0.50
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.10	0.50
2:B:79:PRO:O	2:B:83:ILE:HG13	2.10	0.50
2:B:100:MET:HE3	2:B:157:GLU:HG3	1.93	0.50
2:B:146:MET:SD	2:B:189:PRO:HB3	2.52	0.50
3:C:47:LEU:O	3:C:51:MET:HG2	2.12	0.50
8:H:46:LYS:HZ3	8:U:55:TRP:HB2	1.75	0.50
1:N:382:SER:HA	17:N:515:HEA:HMC2	1.94	0.50
1:N:472:ILE:HG21	18:Y:1522:TGL:HA91	1.91	0.50
2:O:22:HIS:CD2	2:O:26:HIS:CE1	2.99	0.50
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.93	0.50
2:O:65:TRP:HZ3	22:O:1230:PSC:H331	1.72	0.50
1:A:472:ILE:HG21	18:L:522:TGL:CA9	2.41	0.50
11:K:24:PHE:O	11:K:28:VAL:HG12	2.12	0.50
4:Q:78:TRP:O	4:Q:82:VAL:HG23	2.12	0.50
6:S:81:ARG:HG2	6:S:88:HIS:CD2	2.47	0.50
1:A:368:HIS:CD2	1:A:369:ASP:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:MET:O	2:B:207:MET:HG3	2.12	0.49
4:D:51:LEU:HB3	4:D:56:LYS:HG3	1.93	0.49
27:E:2292:HOH:O	9:I:4:LEU:HD13	2.11	0.49
8:H:54:GLU:OE1	8:H:54:GLU:HA	2.11	0.49
13:Z:23:PHE:O	13:Z:27:LEU:HG	2.12	0.49
1:A:483:LEU:HD21	13:M:4:LYS:HD3	1.94	0.49
22:B:230:PSC:H12	22:B:230:PSC:H322	1.94	0.49
23:B:1086:CHD:H20	7:T:18:PHE:CD2	2.47	0.49
23:B:1086:CHD:H212	23:B:1086:CHD:H12	1.94	0.49
5:E:6:GLU:HB2	5:E:10:GLU:OE1	2.12	0.49
5:E:52:LEU:O	5:E:55:CYS:HB2	2.12	0.49
6:F:64:GLU:O	6:F:65:ASP:HB2	2.12	0.49
1:N:35:LEU:CD1	1:N:462:LEU:HD13	2.42	0.49
7:T:38:HIS:CE1	26:T:1269:CDL:H111	2.47	0.49
1:A:15:ILE:HG21	1:A:98:ASN:ND2	2.27	0.49
8:H:36:PHE:HB2	8:H:56:TYR:HB2	1.94	0.49
3:P:157:LYS:HZ2	25:P:1265:PEK:H052	1.77	0.49
1:A:337:ALA:HB2	1:A:394:VAL:CG2	2.42	0.49
2:B:33:LEU:O	2:B:37:LEU:HB2	2.13	0.49
7:G:8:HIS:HD2	25:G:1263:PEK:H232	1.78	0.49
1:N:5:ARG:O	1:N:9:SER:HB2	2.12	0.49
1:N:293:PHE:CE1	1:N:361:SER:HB3	2.48	0.49
1:N:507:GLU:HG3	3:P:5:THR:OG1	2.12	0.49
19:N:1524:PGV:H152	19:N:1524:PGV:H301	1.94	0.49
2:O:134:ARG:HG2	2:O:135:LEU:HG	1.94	0.49
3:P:57:TRP:HD1	3:P:57:TRP:O	1.96	0.49
1:A:17:THR:OG1	18:L:522:TGL:H281	2.11	0.49
2:B:29:MET:HE2	2:B:30:ILE:HG13	1.93	0.49
1:N:115:SER:HB3	1:N:145:LEU:HB2	1.94	0.49
3:P:134:THR:HA	3:P:249:TRP:HE1	1.77	0.49
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.13	0.49
6:S:33:ILE:HG22	6:S:34:LEU:HD23	1.95	0.49
10:W:8:LYS:O	10:W:12:PHE:HD1	1.96	0.49
18:Y:1522:TGL:HC21	18:Y:1522:TGL:OA1	2.12	0.49
22:O:1230:PSC:H322	22:O:1230:PSC:H12	1.95	0.49
3:P:158:HIS:NE2	25:P:1265:PEK:H051	2.28	0.49
1:A:68:PHE:CE2	1:A:109:PHE:HA	2.47	0.49
1:A:69:MET:HE2	17:A:515:HEA:C18	2.43	0.49
2:B:125:THR:HG23	2:B:134:ARG:HG3	1.93	0.49
12:L:20:ARG:HH22	18:L:522:TGL:HC61	1.78	0.49
1:A:472:ILE:HG21	18:L:522:TGL:HA92	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:95:LEU:HG	2:O:96:THR:N	2.28	0.49
3:P:219:PHE:O	3:P:222:GLN:HB3	2.13	0.49
10:W:56:PRO:HD3	12:Y:46:LYS:HE3	1.93	0.49
17:N:516:HEA:H241	2:O:72:ILE:HG22	1.94	0.48
3:P:225:PHE:N	3:P:225:PHE:CD1	2.81	0.48
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.47	0.48
12:L:24:MET:SD	18:L:522:TGL:H162	2.53	0.48
3:P:128:GLU:OE1	7:T:38:HIS:HB3	2.14	0.48
4:Q:129:ALA:HB1	4:Q:133:GLY:HA3	1.96	0.48
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.95	0.48
2:B:56:MET:HA	22:B:230:PSC:H202	1.94	0.48
4:D:121:LYS:HG2	11:K:53:TRP:CD1	2.48	0.48
1:N:443:TYR:CD1	1:N:447:TYR:HB2	2.49	0.48
5:R:40:ASP:CG	9:V:11:GLY:HA2	2.39	0.48
1:A:248:LEU:HB2	1:A:249:PRO:HD3	1.94	0.48
1:A:390:MET:HE1	1:A:468:MET:SD	2.53	0.48
3:C:225:PHE:HA	27:C:2236:HOH:O	2.13	0.48
1:N:65:MET:HB3	17:N:515:HEA:CAC	2.42	0.48
9:I:37:PHE:CD1	9:I:38:ALA:N	2.82	0.48
1:N:5:ARG:HB2	12:Y:3:TYR:CE1	2.49	0.48
7:T:31:CYS:SG	26:T:1269:CDL:H552	2.53	0.48
1:A:476:PHE:CD2	12:L:15:VAL:HG11	2.49	0.48
22:B:230:PSC:H142	22:B:230:PSC:C34	2.31	0.48
1:N:482:VAL:HG13	13:Z:1:ILE:HD11	1.95	0.48
1:N:510:TYR:CG	6:S:49:VAL:HG13	2.48	0.48
2:O:57:ASP:H	22:O:1230:PSC:C20	2.19	0.48
2:O:69:PRO:HA	2:O:72:ILE:HD12	1.95	0.48
22:O:1230:PSC:H072	9:V:10:ARG:HE	1.77	0.48
7:T:84:LYS:H	7:T:84:LYS:CD	2.19	0.48
1:A:104:LEU:C	1:A:107:PRO:HD2	2.39	0.48
2:B:95:LEU:HD12	2:B:96:THR:H	1.79	0.48
2:B:100:MET:CE	2:B:157:GLU:HG3	2.44	0.48
2:B:143:VAL:HB	2:B:222:TRP:CZ3	2.49	0.48
2:B:155:SER:OG	2:B:156:SER:N	2.46	0.48
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.67	0.48
5:R:14:ARG:HH11	5:R:14:ARG:HB3	1.79	0.48
1:A:361:SER:O	1:A:365:ILE:HG12	2.13	0.48
2:B:188:ARG:HB3	2:B:189:PRO:HD2	1.96	0.48
3:C:144:ILE:HG13	3:C:166:THR:HG21	1.96	0.48
3:C:187:THR:HG22	25:C:264:PEK:H052	1.96	0.48
23:C:271:CHD:H162	23:C:271:CHD:H222	1.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:66:ILE:HG23	1:N:246:LEU:HD21	1.96	0.48
1:N:94:PHE:HB3	19:N:1266:PGV:O11	2.14	0.48
2:O:66:THR:HG22	2:O:67:ILE:N	2.28	0.48
1:A:161:ALA:HB1	1:A:192:ALA:O	2.14	0.48
18:N:1523:TGL:HG32	27:Q:4216:HOH:O	2.12	0.48
2:O:52:HIS:ND1	5:R:40:ASP:HB2	2.28	0.48
13:Z:13:LYS:O	13:Z:17:ILE:HG13	2.13	0.48
1:A:397:PHE:HB3	1:A:398:PRO:HD3	1.96	0.48
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.01	0.48
2:B:121:TYR:O	2:B:138:VAL:HA	2.14	0.47
7:G:26:PRO:O	7:G:29:ALA:HB3	2.14	0.47
3:P:4:GLN:NE2	3:P:6:HIS:O	2.43	0.47
7:T:8:HIS:HD2	25:T:263:PEK:H232	1.79	0.47
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.14	0.47
19:N:1524:PGV:H311	13:Z:16:ALA:HA	1.97	0.47
3:P:88:ILE:O	3:P:91:VAL:HB	2.14	0.47
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.95	0.47
19:A:524:PGV:H152	19:A:524:PGV:H321	1.96	0.47
3:C:131:LEU:HD13	3:C:253:TYR:OH	2.14	0.47
3:C:198:PHE:O	25:C:264:PEK:H22	2.15	0.47
8:H:49:ASP:O	8:H:52:VAL:HG22	2.14	0.47
1:N:44:PRO:HB3	2:O:134:ARG:NH2	2.29	0.47
1:N:468:MET:O	1:N:472:ILE:HG13	2.14	0.47
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.25	0.47
1:A:310:MET:O	2:B:73:LEU:HD13	2.14	0.47
1:A:344:PHE:CD1	1:A:344:PHE:C	2.92	0.47
19:A:524:PGV:H321	19:A:524:PGV:C15	2.45	0.47
6:F:96:LEU:HD23	6:F:97:ALA:N	2.29	0.47
7:G:23:LEU:C	7:G:26:PRO:HD2	2.39	0.47
18:L:522:TGL:H231	18:L:522:TGL:H272	1.96	0.47
1:A:357:VAL:HG22	2:B:27:THR:CG2	2.44	0.47
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.49	0.47
18:L:522:TGL:HC21	18:L:522:TGL:OA1	2.15	0.47
13:M:35:TYR:HD2	13:M:36:HIS:ND1	2.12	0.47
4:Q:109:HIS:C	4:Q:111:PHE:H	2.22	0.47
5:R:21:LYS:HE3	27:R:3128:HOH:O	2.13	0.47
8:U:49:ASP:O	8:U:52:VAL:HG22	2.14	0.47
11:X:47:ARG:HG3	11:X:48:VAL:N	2.29	0.47
1:A:104:LEU:HB2	1:A:156:SER:HB2	1.97	0.47
6:F:74:LEU:HD12	6:F:80:GLN:OE1	2.14	0.47
7:G:84:LYS:HD2	7:G:84:LYS:N	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:522:TGL:H211	18:L:522:TGL:HA72	1.97	0.47
2:O:65:TRP:CE3	22:O:1230:PSC:H331	2.50	0.47
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.50	0.47
26:C:270:CDL:H642	26:C:270:CDL:C19	2.35	0.47
4:D:109:HIS:C	4:D:111:PHE:H	2.22	0.47
8:H:55:TRP:O	8:H:59:VAL:HG23	2.14	0.47
19:N:1524:PGV:H321	19:N:1524:PGV:C15	2.44	0.47
5:R:43:PRO:HB2	5:R:48:ILE:CD1	2.42	0.47
1:A:132:LEU:HD12	1:A:132:LEU:O	2.15	0.47
7:G:3:ALA:O	7:G:4:ALA:HB2	2.15	0.47
1:N:356:ILE:HD13	1:N:356:ILE:HA	1.74	0.47
3:P:50:ASN:O	3:P:54:MET:HG3	2.14	0.47
3:P:157:LYS:HZ1	25:P:1265:PEK:H052	1.78	0.47
1:A:231:TYR:CD1	1:A:231:TYR:C	2.92	0.47
3:C:67:PHE:N	3:C:67:PHE:CD2	2.82	0.47
1:N:164:PHE:O	1:N:168:ILE:HG13	2.15	0.47
1:N:376:HIS:HA	27:N:3228:HOH:O	2.14	0.47
4:Q:131:ILE:HG23	9:V:50:PHE:HB2	1.97	0.47
25:T:1264:PEK:H71	25:T:1264:PEK:C3	2.45	0.47
2:B:3:TYR:CZ	2:B:6:GLN:HG3	2.50	0.47
7:G:3:ALA:HB3	25:G:1263:PEK:H361	1.97	0.47
1:N:3:ILE:HG23	1:N:7:LEU:HD22	1.97	0.47
1:N:365:ILE:O	2:O:171:LYS:NZ	2.47	0.47
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.45	0.47
13:M:42:LYS:HA	13:M:42:LYS:CE	2.41	0.46
1:N:513:LEU:O	1:N:514:LYS:HB2	2.13	0.46
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.50	0.46
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.71	0.46
1:N:12:HIS:CE1	1:N:13:LYS:HG2	2.51	0.46
1:N:429:HIS:HB3	18:O:1521:TGL:HB41	1.96	0.46
8:U:28:ASN:ND2	27:U:3134:HOH:O	2.40	0.46
1:A:378:HIS:CG	1:A:425:PHE:CE2	3.03	0.46
11:K:32:MET:HE2	11:K:32:MET:HB3	1.84	0.46
1:N:211:THR:HG22	1:N:215:LEU:HD12	1.97	0.46
6:S:13:ALA:O	6:S:18:ARG:HD2	2.15	0.46
8:U:36:PHE:HB2	8:U:56:TYR:HB2	1.98	0.46
23:C:271:CHD:H112	23:C:271:CHD:H12A	1.67	0.46
13:M:26:PHE:O	13:M:29:PRO:HD2	2.15	0.46
6:S:72:PHE:CE2	6:S:83:PRO:HD3	2.49	0.46
1:A:413:HIS:HE2	1:A:468:MET:HB2	1.79	0.46
3:C:51:MET:SD	26:C:270:CDL:C62	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.46
3:P:59:ARG:HG3	26:P:1270:CDL:H512	1.96	0.46
3:P:147:ALA:HB2	3:P:162:ALA:CB	2.46	0.46
24:P:1272:DMU:H30	24:P:1272:DMU:O1	2.16	0.46
5:R:9:GLU:CD	5:R:9:GLU:H	2.23	0.46
1:A:140:GLY:O	1:A:213:ARG:NH2	2.49	0.46
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.51	0.46
7:G:2:SER:OG	25:G:1263:PEK:H301	2.16	0.46
19:P:1267:PGV:H181	26:P:1270:CDL:H812	1.96	0.46
4:Q:87:PHE:C	4:Q:87:PHE:CD2	2.94	0.46
1:A:346:PHE:CD2	1:A:347:LEU:HD23	2.50	0.46
1:A:446:ALA:HB1	2:B:3:TYR:C	2.41	0.46
12:L:11:ILE:HG13	12:L:13:PHE:O	2.16	0.46
7:T:70:PHE:O	25:T:1264:PEK:N	2.48	0.46
8:H:46:LYS:HE2	27:H:4276:HOH:O	2.16	0.46
1:N:417:MET:O	1:N:421:VAL:HG22	2.16	0.46
3:P:224:LYS:C	3:P:225:PHE:HD1	2.24	0.46
19:P:1267:PGV:H182	26:P:1270:CDL:C67	2.45	0.46
17:A:515:HEA:H261	17:A:515:HEA:H171	1.72	0.46
19:A:525:PGV:H21	3:C:57:TRP:CZ2	2.51	0.46
3:C:112:LEU:HA	7:G:52:HIS:CD2	2.50	0.46
27:C:4266:HOH:O	25:T:263:PEK:H042	2.15	0.46
7:T:11:TPO:CG2	7:T:11:TPO:O	2.64	0.46
1:A:395:HIS:HD2	1:A:396:TRP:CD2	2.34	0.45
2:B:139:ASP:OD2	2:B:140:ASN:N	2.49	0.45
2:B:217:LYS:HA	2:B:217:LYS:HD3	1.79	0.45
3:C:156:ARG:HE	23:C:271:CHD:H232	1.80	0.45
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.98	0.45
18:N:1523:TGL:H271	2:O:46:LEU:HD12	1.97	0.45
1:A:377:PHE:HE2	1:A:378:HIS:CE1	2.34	0.45
25:C:265:PEK:H041	6:F:1:ALA:N	2.32	0.45
12:L:20:ARG:HH12	18:L:522:TGL:CC6	2.16	0.45
2:O:72:ILE:HG13	27:O:4128:HOH:O	2.15	0.45
5:R:12:ASP:CG	9:V:10:ARG:HH22	2.24	0.45
23:W:1060:CHD:H212	23:W:1060:CHD:H161	1.84	0.45
1:A:21:LEU:HD23	18:L:522:TGL:H221	1.98	0.45
19:A:525:PGV:H42	19:A:525:PGV:H251	1.98	0.45
2:B:22:HIS:NE2	2:B:26:HIS:NE2	2.64	0.45
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.97	0.45
1:N:230:LEU:HD21	3:P:100:ALA:HA	1.97	0.45
1:A:195:LEU:HD23	1:A:245:ILE:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:HIS:CD2	2:B:26:HIS:CE1	3.04	0.45
23:G:86:CHD:H212	23:G:86:CHD:H12	1.97	0.45
13:M:34:LEU:HD12	13:M:34:LEU:HA	1.68	0.45
1:N:367:LEU:CD2	1:N:433:LEU:HD23	2.46	0.45
26:T:1269:CDL:H202	26:T:1269:CDL:C52	2.40	0.45
1:A:115:SER:HA	1:A:145:LEU:HD12	1.99	0.45
1:A:248:LEU:O	1:A:251:PHE:HB2	2.15	0.45
25:C:265:PEK:H371	26:G:269:CDL:H273	1.99	0.45
1:N:450:TRP:CE3	1:N:453:ILE:HD12	2.52	0.45
2:O:62:GLU:O	2:O:66:THR:HB	2.16	0.45
2:O:69:PRO:HG3	22:O:1230:PSC:H183	1.98	0.45
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.32	0.45
10:W:32:TYR:CD2	10:W:32:TYR:C	2.94	0.45
1:A:443:TYR:CD1	1:A:447:TYR:HB2	2.50	0.45
1:A:513:LEU:O	1:A:514:LYS:HB2	2.17	0.45
2:B:131:GLY:O	4:D:122:ARG:HD3	2.16	0.45
2:B:161:HIS:CE1	2:B:200:CYS:HB2	2.52	0.45
2:B:215:PRO:HD3	9:I:60:PHE:CD2	2.52	0.45
7:G:44:ARG:HA	7:G:45:PRO:HD2	1.83	0.45
1:N:195:LEU:HG	1:N:245:ILE:CD1	2.42	0.45
1:N:313:ALA:CB	17:N:516:HEA:H262	2.46	0.45
1:N:397:PHE:N	1:N:398:PRO:CD	2.78	0.45
7:T:70:PHE:HD1	25:T:1264:PEK:O11	2.00	0.45
1:A:443:TYR:CD2	1:A:443:TYR:N	2.85	0.45
2:B:14:SER:O	2:B:18:GLU:HG3	2.16	0.45
2:B:16:ILE:HD13	2:B:16:ILE:HA	1.74	0.45
2:B:41:ILE:CD1	22:B:230:PSC:H342	2.47	0.45
2:B:78:LEU:HD12	26:T:1269:CDL:C35	2.47	0.45
3:C:112:LEU:HB3	3:C:118:PRO:HB3	1.98	0.45
4:D:145:TRP:CZ3	11:K:45:VAL:HG22	2.52	0.45
23:J:60:CHD:H212	23:J:60:CHD:H161	1.79	0.45
3:P:160:LEU:HD21	3:P:222:GLN:HG3	1.99	0.45
26:T:1269:CDL:H251	26:T:1269:CDL:H222	1.84	0.45
3:C:16:TRP:HB2	3:C:17:PRO:HD3	1.98	0.45
3:C:163:LEU:HD23	3:C:219:PHE:HA	1.99	0.45
4:D:95:LEU:HD21	13:M:27:LEU:CD1	2.47	0.45
26:G:269:CDL:H251	26:G:269:CDL:H222	1.86	0.45
1:N:8:PHE:N	1:N:8:PHE:CD1	2.85	0.45
1:N:460:ILE:HA	4:Q:92:THR:HG21	1.98	0.45
2:O:32:PHE:HE2	18:O:1521:TGL:HB91	1.80	0.45
6:S:92:VAL:O	6:S:92:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:37:HIS:CD2	8:U:76:ARG:CZ	2.99	0.45
2:B:68:LEU:HB3	22:B:230:PSC:H182	1.99	0.45
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.69	0.45
26:G:269:CDL:H271	1:N:282:PHE:HE2	1.81	0.45
12:L:33:PHE:O	12:L:36:PRO:HD2	2.16	0.45
18:N:1523:TGL:HG11	18:N:1523:TGL:CC2	2.41	0.45
2:O:22:HIS:NE2	2:O:26:HIS:HE1	2.06	0.45
1:A:302:ARG:NH1	27:A:4150:HOH:O	2.49	0.45
1:A:365:ILE:HG13	2:B:87:MET:HE1	1.99	0.45
1:N:91:ASP:OD1	1:N:95:PRO:HB3	2.15	0.45
1:N:467:LEU:O	1:N:470:PHE:HB3	2.17	0.45
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.99	0.45
12:Y:11:ILE:HD12	12:Y:13:PHE:CE1	2.51	0.45
2:B:99:THR:HG22	2:B:152:MET:HE1	1.99	0.44
26:C:270:CDL:H202	26:C:270:CDL:H171	1.77	0.44
1:N:151:HIS:CD2	25:T:1264:PEK:H382	2.51	0.44
6:S:6:VAL:HA	6:S:7:PRO:HD2	1.87	0.44
1:N:220:PHE:CE1	1:N:231:TYR:HB2	2.52	0.44
1:N:507:GLU:OE1	6:S:51:SER:HA	2.18	0.44
2:O:116:LEU:HD12	2:O:117:SER:N	2.33	0.44
2:O:161:HIS:CE1	2:O:200:CYS:CB	3.01	0.44
25:P:1265:PEK:H371	26:T:1269:CDL:H261	1.99	0.44
12:Y:36:PRO:O	12:Y:40:VAL:HG23	2.17	0.44
1:A:449:MET:SD	2:B:5:MET:CG	3.05	0.44
2:B:12:ALA:HB3	9:I:47:TYR:CE2	2.53	0.44
3:C:81:TYR:O	3:C:85:LEU:HG	2.18	0.44
1:N:104:LEU:C	1:N:107:PRO:HD2	2.42	0.44
1:N:381:LEU:HB3	17:N:515:HEA:CB	2.46	0.44
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.83	0.44
4:D:122:ARG:NH1	4:D:126:MET:HE1	2.32	0.44
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.72	0.44
13:M:35:TYR:HD2	13:M:36:HIS:HD1	1.66	0.44
7:T:3:ALA:O	7:T:4:ALA:HB2	2.16	0.44
7:T:8:HIS:CD2	25:T:263:PEK:H232	2.53	0.44
18:Y:1522:TGL:H272	18:Y:1522:TGL:C23	2.47	0.44
1:A:424:THR:OG1	1:A:458:SER:N	2.51	0.44
1:A:439:ARG:HH21	17:A:515:HEA:CGD	2.30	0.44
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.53	0.44
1:N:12:HIS:CD2	1:N:91:ASP:HA	2.53	0.44
1:N:446:ALA:HB1	2:O:3:TYR:C	2.42	0.44
2:O:12:ALA:HB3	9:V:47:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:1230:PSC:H142	22:O:1230:PSC:C34	2.32	0.44
3:P:156:ARG:HE	23:P:1271:CHD:C23	2.30	0.44
1:A:6:TRP:HH2	12:L:10:ASN:O	2.01	0.44
1:A:35:LEU:CD1	1:A:462:LEU:HD13	2.48	0.44
1:A:96:ARG:NH2	3:C:61:VAL:HG22	2.32	0.44
1:A:397:PHE:N	1:A:398:PRO:CD	2.80	0.44
4:D:32:ASN:HD22	4:D:32:ASN:HA	1.64	0.44
6:F:92:VAL:O	6:F:92:VAL:CG2	2.62	0.44
1:N:314:ILE:O	1:N:318:VAL:HG23	2.18	0.44
1:N:473:TRP:NE1	12:Y:22:LEU:HB2	2.32	0.44
7:T:17:ARG:HD2	27:T:3309:HOH:O	2.17	0.44
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.86	0.44
1:A:397:PHE:HD1	1:A:405:LEU:HG	1.83	0.44
7:G:79:PRO:HD2	27:G:2136:HOH:O	2.17	0.44
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.99	0.44
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.98	0.44
18:N:1523:TGL:HC22	18:N:1523:TGL:HC51	1.78	0.44
2:O:131:GLY:O	4:Q:122:ARG:HD3	2.18	0.44
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.99	0.44
23:P:1525:CHD:H112	23:P:1525:CHD:H12A	1.74	0.44
4:Q:11:TYR:CD1	4:Q:12:ALA:N	2.86	0.44
1:A:98:ASN:HA	27:A:2052:HOH:O	2.17	0.44
2:B:159:VAL:HG23	2:B:160:LEU:N	2.32	0.44
22:B:230:PSC:H032	27:E:2129:HOH:O	2.17	0.44
22:B:230:PSC:H241	22:B:230:PSC:H62	2.00	0.44
5:E:71:VAL:HG11	5:E:85:VAL:HG11	1.98	0.44
7:G:11:TPO:O	7:G:11:TPO:CG2	2.66	0.44
26:G:269:CDL:H571	26:G:269:CDL:H601	1.48	0.44
1:N:361:SER:O	1:N:365:ILE:HG12	2.17	0.44
4:Q:131:ILE:HG23	9:V:50:PHE:CB	2.48	0.44
8:U:39:CYS:O	8:U:43:MET:HG2	2.17	0.44
1:A:19:TYR:CD1	1:A:76:GLY:HA3	2.53	0.44
1:A:397:PHE:CD1	1:A:405:LEU:HG	2.53	0.44
2:B:99:THR:HG22	2:B:152:MET:HE2	1.99	0.44
5:E:19:PHE:O	5:E:57:ARG:NH2	2.51	0.44
8:H:37:HIS:CD2	8:H:76:ARG:CZ	3.01	0.44
1:N:395:HIS:O	1:N:398:PRO:HD2	2.18	0.44
13:Z:31:GLY:C	24:Z:1526:DMU:H1	2.43	0.44
4:D:23:PRO:O	4:D:25:PRO:HD3	2.18	0.43
4:D:48:TRP:O	4:D:51:LEU:HB2	2.18	0.43
8:H:9:LYS:O	8:H:10:ASN:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:1270:CDL:H632	26:P:1270:CDL:H602	1.76	0.43
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.18	0.43
4:D:20:ARG:H	4:D:20:ARG:HG3	1.66	0.43
26:G:269:CDL:H322	26:G:269:CDL:HA62	1.99	0.43
8:H:28:ASN:ND2	27:H:2134:HOH:O	2.50	0.43
1:N:499:PRO:HD2	12:Y:7:PRO:HD3	1.99	0.43
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.87	0.43
3:P:50:ASN:HD22	3:P:51:MET:HE2	1.83	0.43
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.18	0.43
5:R:100:THR:OG1	5:R:103:GLU:HG3	2.17	0.43
8:U:49:ASP:OD1	8:U:51:SER:HB3	2.18	0.43
1:A:368:HIS:O	1:A:370:THR:HG23	2.18	0.43
18:A:523:TGL:H212	18:A:523:TGL:H242	1.78	0.43
23:C:525:CHD:H112	23:C:525:CHD:H12A	1.74	0.43
4:D:42:GLU:OE2	4:D:45:LYS:HE2	2.18	0.43
1:N:9:SER:HB3	27:N:4019:HOH:O	2.18	0.43
2:O:23:PHE:HE2	2:O:79:PRO:HG2	1.82	0.43
2:O:161:HIS:CE1	2:O:200:CYS:HB2	2.53	0.43
8:U:57:ARG:O	8:U:61:LYS:HB2	2.18	0.43
1:A:440:TYR:HE2	2:B:204:HIS:CE1	2.37	0.43
1:A:486:ASP:OD2	4:D:19:ARG:HD3	2.19	0.43
2:B:189:PRO:HD2	9:I:54:TYR:OH	2.18	0.43
11:K:9:PHE:C	11:K:9:PHE:CD2	2.96	0.43
2:O:29:MET:HB2	9:V:35:TYR:CE2	2.53	0.43
2:O:184:LEU:HD23	2:O:185:MET:N	2.33	0.43
22:O:1230:PSC:H251	22:O:1230:PSC:H221	1.77	0.43
3:P:198:PHE:O	25:T:1264:PEK:H22	2.19	0.43
1:A:186:TRP:O	1:A:189:MET:N	2.52	0.43
1:A:325:ALA:HA	22:B:230:PSC:H291	1.99	0.43
26:C:270:CDL:H632	26:C:270:CDL:H602	1.81	0.43
5:E:105:GLY:O	5:E:108:LYS:HE2	2.17	0.43
25:G:1263:PEK:C9	3:P:244:PHE:HA	2.47	0.43
1:N:109:PHE:CE2	1:N:112:LEU:HD22	2.53	0.43
17:N:515:HEA:HHC	17:N:515:HEA:H122	2.00	0.43
9:V:47:TYR:HB2	27:V:4249:HOH:O	2.19	0.43
1:A:302:ARG:NH1	2:B:84:LEU:HD11	2.34	0.43
1:A:440:TYR:CE2	2:B:205:SER:HA	2.53	0.43
1:N:131:PRO:HG2	2:O:159:VAL:HA	2.00	0.43
7:T:31:CYS:SG	26:T:1269:CDL:C55	3.07	0.43
10:W:50:LEU:O	10:W:50:LEU:HD22	2.18	0.43
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:450:TRP:HE3	1:N:453:ILE:HD12	1.83	0.43
1:N:498:CYS:HA	1:N:499:PRO:HA	1.74	0.43
5:R:14:ARG:HB3	5:R:14:ARG:NH1	2.33	0.43
1:A:35:LEU:HD23	1:A:35:LEU:HA	1.78	0.43
1:N:51:ASP:HB2	2:O:202:SER:O	2.19	0.43
4:Q:60:TYR:OH	4:Q:67:SER:HA	2.19	0.43
1:A:35:LEU:HD11	1:A:462:LEU:HD13	2.01	0.43
6:F:14:THR:OG1	6:F:15:GLY:N	2.51	0.43
2:O:3:TYR:CE1	2:O:6:GLN:HG3	2.54	0.43
2:O:190:GLY:HA3	27:O:4222:HOH:O	2.18	0.43
26:T:1269:CDL:H141	27:T:4142:HOH:O	2.17	0.43
1:A:65:MET:HB3	17:A:515:HEA:HAC	2.00	0.43
1:A:293:PHE:HB2	1:A:364:ASP:OD1	2.19	0.43
3:C:50:ASN:HD22	3:C:51:MET:HE2	1.83	0.43
25:C:265:PEK:H382	1:N:279:SER:OG	2.19	0.43
4:D:115:TRP:CD1	4:D:115:TRP:C	2.97	0.43
2:B:12:ALA:HB3	9:I:47:TYR:HE2	1.84	0.42
1:N:75:ILE:O	1:N:79:GLY:HA3	2.18	0.42
1:N:204:ALA:C	1:N:208:MET:HE3	2.44	0.42
1:N:243:VAL:HA	1:N:246:LEU:HD12	1.99	0.42
2:O:188:ARG:HB3	2:O:189:PRO:HD2	2.01	0.42
25:P:1265:PEK:H21	27:P:4191:HOH:O	2.19	0.42
4:Q:102:TYR:HD1	13:Z:35:TYR:HE1	1.67	0.42
6:S:87:THR:HG22	27:S:3350:HOH:O	2.18	0.42
1:A:176:MET:HG3	1:A:180:GLN:HB3	2.00	0.42
1:A:278:MET:HB3	7:T:5:LYS:HD3	2.02	0.42
1:A:324:LEU:HD13	2:B:41:ILE:CG2	2.48	0.42
2:B:13:THR:O	2:B:187:SER:HB2	2.19	0.42
2:B:59:GLN:NE2	25:P:1265:PEK:O04	2.52	0.42
17:N:516:HEA:H241	2:O:72:ILE:HG21	1.98	0.42
2:O:172:THR:CG2	2:O:180:ASN:HB3	2.49	0.42
12:Y:20:ARG:HH11	12:Y:20:ARG:HB3	1.83	0.42
8:H:9:LYS:HB3	8:H:10:ASN:H	1.52	0.42
8:H:65:PRO:O	8:H:69:VAL:HG23	2.19	0.42
1:N:28:MET:HE2	17:N:515:HEA:H271	2.01	0.42
2:O:22:HIS:CD2	2:O:26:HIS:HE1	2.38	0.42
2:O:108:TYR:CE1	2:O:142:VAL:CG2	3.02	0.42
2:O:216:LEU:HB3	27:O:4168:HOH:O	2.18	0.42
3:P:241:TYR:O	3:P:244:PHE:HB3	2.19	0.42
26:P:1270:CDL:PA1	26:P:1270:CDL:HB22	2.59	0.42
26:P:1270:CDL:H202	26:P:1270:CDL:H171	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HD11	1:A:462:LEU:HB2	2.01	0.42
4:D:102:TYR:CD1	13:M:35:TYR:CE1	3.04	0.42
3:P:57:TRP:O	3:P:61:VAL:HG23	2.19	0.42
3:P:198:PHE:CD2	25:T:1264:PEK:C03	3.02	0.42
23:P:1271:CHD:H222	23:P:1271:CHD:H162	1.54	0.42
1:A:327:LEU:HD22	1:A:338:MET:HE1	2.02	0.42
1:A:484:THR:HG22	27:A:4238:HOH:O	2.18	0.42
2:B:41:ILE:HD13	22:B:230:PSC:H342	2.01	0.42
7:G:30:LEU:CD1	26:G:269:CDL:H252	2.49	0.42
1:N:325:ALA:O	1:N:328:HIS:HB3	2.20	0.42
1:N:416:ILE:CG2	1:N:464:ALA:HB2	2.49	0.42
27:N:4241:HOH:O	2:O:58:ALA:HB3	2.20	0.42
2:O:99:THR:HG22	2:O:152:MET:CE	2.49	0.42
2:O:146:MET:CE	9:V:56:SER:HB2	2.49	0.42
5:R:5:HIS:HB3	5:R:6:GLU:H	1.67	0.42
5:R:61:PHE:HE1	5:R:98:ILE:HA	1.83	0.42
6:S:74:LEU:HD11	6:S:89:TYR:O	2.19	0.42
7:T:38:HIS:NE2	26:T:1269:CDL:HA21	2.34	0.42
9:V:73:LYS:HB3	9:V:73:LYS:HE3	1.94	0.42
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	2.00	0.42
2:B:66:THR:CG2	2:B:67:ILE:N	2.80	0.42
2:B:138:VAL:HG22	2:B:210:VAL:HG21	2.02	0.42
3:C:244:PHE:HA	25:T:263:PEK:H9	2.01	0.42
26:C:270:CDL:PA1	26:C:270:CDL:HB22	2.59	0.42
12:L:25:MET:HG2	18:L:522:TGL:HA62	2.02	0.42
2:O:37:LEU:HD12	2:O:37:LEU:HA	1.89	0.42
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.54	0.42
6:S:76:LYS:HE2	6:S:93:PRO:HG3	1.99	0.42
1:A:258:VAL:HG13	1:A:327:LEU:CD2	2.50	0.42
1:A:383:MET:HE2	1:A:421:VAL:HB	2.02	0.42
2:B:3:TYR:CE1	2:B:6:GLN:HG3	2.54	0.42
4:D:94:LEU:HD23	11:K:28:VAL:CG2	2.50	0.42
5:E:52:LEU:HD23	5:E:52:LEU:HA	1.87	0.42
13:M:31:GLY:C	24:M:526:DMU:H1	2.44	0.42
1:N:62:ALA:HB3	1:N:126:TRP:HB3	2.01	0.42
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.54	0.42
26:P:1270:CDL:H561	26:P:1270:CDL:H532	1.88	0.42
4:Q:130:PRO:HG2	4:Q:131:ILE:CD1	2.49	0.42
6:S:57:ILE:HG13	6:S:73:TRP:CZ3	2.55	0.42
7:T:2:SER:O	7:T:3:ALA:HB3	2.20	0.42
1:A:104:LEU:HD23	3:C:21:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:SER:O	2:B:174:ALA:HB1	2.19	0.42
3:C:30:GLY:HA2	3:C:42:LEU:HB3	2.02	0.42
3:C:187:THR:HA	25:C:264:PEK:O12	2.20	0.42
26:G:269:CDL:OA7	26:G:269:CDL:H342	2.19	0.42
10:J:36:MET:O	10:J:40:LEU:HG	2.20	0.42
2:O:143:VAL:HG12	2:O:219:PHE:HD1	1.84	0.42
1:A:430:PHE:HE1	18:A:521:TGL:HB21	1.85	0.42
1:N:34:SER:HB3	1:N:61:HIS:CE1	2.54	0.42
1:N:68:PHE:CE2	1:N:112:LEU:HD13	2.51	0.42
13:Z:6:ALA:O	13:Z:9:PRO:HD3	2.20	0.42
1:A:325:ALA:O	1:A:328:HIS:HB3	2.20	0.42
25:C:265:PEK:H371	26:G:269:CDL:C27	2.50	0.42
1:N:242:GLU:O	1:N:246:LEU:HG	2.20	0.42
1:N:334:TRP:CZ2	2:O:46:LEU:HB3	2.55	0.42
1:N:378:HIS:CG	1:N:425:PHE:CE2	3.08	0.42
3:P:132:LEU:O	3:P:136:VAL:HG23	2.20	0.42
5:R:84:TYR:CZ	5:R:88:GLU:HG3	2.54	0.42
7:T:24:ALA:O	7:T:27:SER:HB2	2.19	0.42
3:C:12:ASN:O	3:C:13:PRO:C	2.62	0.41
3:C:68:GLN:HB2	3:C:70:HIS:CD2	2.55	0.41
3:C:128:GLU:OE1	7:G:38:HIS:HB3	2.20	0.41
4:D:24:LEU:HD12	5:E:30:ARG:HA	2.02	0.41
4:D:46:ALA:O	4:D:47:SER:C	2.62	0.41
5:E:49:ASP:OD2	5:E:92:THR:HG21	2.20	0.41
5:E:89:LEU:O	5:E:93:LEU:HG	2.20	0.41
7:G:25:LEU:HD23	7:G:25:LEU:HA	1.76	0.41
2:O:135:LEU:O	2:O:208:PRO:HG3	2.19	0.41
2:O:224:ALA:O	2:O:227:LEU:CG	2.65	0.41
3:P:60:ASP:HA	3:P:63:ARG:HD2	2.02	0.41
4:Q:46:ALA:O	4:Q:47:SER:C	2.63	0.41
4:Q:84:ALA:O	4:Q:88:PHE:HD1	2.03	0.41
4:Q:130:PRO:O	4:Q:136:ALA:HB2	2.20	0.41
3:C:67:PHE:HA	10:J:9:GLN:HG2	2.03	0.41
12:L:46:LYS:O	12:L:47:LYS:HB2	2.20	0.41
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.20	0.41
2:O:5:MET:HE2	2:O:5:MET:HB3	1.67	0.41
3:P:22:LEU:HD23	3:P:22:LEU:HA	1.91	0.41
3:P:41:THR:O	3:P:44:MET:HB2	2.20	0.41
1:A:28:MET:HE2	17:A:515:HEA:H271	2.02	0.41
2:B:52:HIS:CD2	2:B:52:HIS:C	2.98	0.41
4:D:77:GLU:HA	11:K:10:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:258:VAL:HG13	1:N:327:LEU:CD2	2.51	0.41
3:P:12:ASN:O	3:P:13:PRO:C	2.62	0.41
4:Q:34:SER:OG	4:Q:37:GLN:HG3	2.20	0.41
1:A:243:VAL:HB	17:A:516:HEA:CAC	2.50	0.41
3:C:231:HIS:CG	19:C:267:PGV:H061	2.55	0.41
8:H:27:ARG:O	8:H:31:GLN:N	2.44	0.41
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.81	0.41
10:J:45:TYR:O	10:J:48:TYR:HB3	2.20	0.41
18:N:1523:TGL:H212	18:N:1523:TGL:H242	1.79	0.41
1:A:197:LEU:HB2	1:A:285:PHE:CZ	2.56	0.41
1:A:307:SER:HB3	26:T:1269:CDL:H182	2.02	0.41
1:A:425:PHE:HZ	17:A:515:HEA:C2B	2.34	0.41
1:A:512:ASN:HB3	6:F:38:ALA:HB2	2.01	0.41
3:C:146:TRP:CE3	3:C:162:ALA:HB2	2.56	0.41
3:C:223:LEU:HD23	3:C:223:LEU:HA	1.95	0.41
4:D:124:LEU:O	4:D:140:TYR:OH	2.30	0.41
2:O:79:PRO:O	2:O:83:ILE:HG13	2.20	0.41
2:O:175:ILE:HA	2:O:176:PRO:HD2	1.82	0.41
3:P:30:GLY:CA	3:P:42:LEU:HB3	2.49	0.41
3:P:231:HIS:CG	19:P:1267:PGV:H061	2.56	0.41
8:U:50:VAL:HG12	8:U:50:VAL:O	2.20	0.41
2:O:207:MET:HG3	2:O:207:MET:O	2.21	0.41
3:P:42:LEU:HD23	3:P:42:LEU:HA	1.83	0.41
3:P:108:PRO:HA	27:P:3207:HOH:O	2.20	0.41
7:T:31:CYS:O	7:T:35:SER:HB2	2.21	0.41
12:Y:20:ARG:HB3	12:Y:20:ARG:NH1	2.36	0.41
1:A:184:PHE:O	1:A:188:VAL:HG23	2.21	0.41
19:A:525:PGV:H182	3:C:28:THR:HG22	2.02	0.41
2:B:146:MET:HG2	2:B:214:VAL:O	2.21	0.41
1:N:105:LEU:HA	1:N:108:SER:HB3	2.02	0.41
1:N:268:PHE:CD2	1:N:268:PHE:C	2.99	0.41
1:N:440:TYR:HE1	2:O:195:GLN:NE2	2.17	0.41
1:N:443:TYR:CD2	1:N:443:TYR:N	2.88	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.21	0.41
1:A:94:PHE:HB3	19:A:525:PGV:O11	2.21	0.41
3:C:138:LEU:HD23	3:C:138:LEU:HA	1.93	0.41
7:G:3:ALA:CB	25:G:1263:PEK:H382	2.40	0.41
7:G:33:LEU:HD22	7:G:33:LEU:HA	1.88	0.41
8:H:67:SER:HA	8:H:70:SER:HB3	2.03	0.41
1:N:112:LEU:HD23	1:N:112:LEU:C	2.45	0.41
1:N:161:ALA:HB1	1:N:192:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:289:ALA:HB3	1:N:305:PHE:CD1	2.56	0.41
3:P:205:GLY:O	3:P:208:VAL:HB	2.21	0.41
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.02	0.41
8:U:9:LYS:HB2	8:U:9:LYS:HE2	1.83	0.41
11:X:9:PHE:CD2	11:X:9:PHE:C	2.98	0.41
1:A:65:MET:HE3	17:A:515:HEA:HMC3	2.01	0.41
1:A:240:HIS:CD2	1:A:240:HIS:C	2.99	0.41
3:C:57:TRP:CD1	3:C:57:TRP:C	2.98	0.41
4:D:38:LYS:HE2	27:D:4155:HOH:O	2.21	0.41
6:F:72:PHE:CE2	6:F:83:PRO:HD3	2.56	0.41
1:N:262:SER:HA	1:N:332:ILE:HD13	2.03	0.41
1:N:381:LEU:HD23	1:N:381:LEU:HA	1.92	0.41
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.39	0.41
2:O:12:ALA:HB3	9:V:47:TYR:HE2	1.84	0.41
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.21	0.41
3:P:60:ASP:O	3:P:64:GLU:HG3	2.21	0.41
3:P:103:HIS:HA	19:P:1268:PGV:O04	2.21	0.41
4:Q:31:LYS:HB3	27:Q:4171:HOH:O	2.20	0.41
5:R:86:ILE:HD13	5:R:86:ILE:HA	1.96	0.41
6:S:82:CYS:HA	6:S:83:PRO:HD3	1.93	0.41
12:Y:11:ILE:HG22	18:Y:1522:TGL:H271	2.02	0.41
12:Y:13:PHE:CA	18:Y:1522:TGL:HC31	2.38	0.41
12:Y:24:MET:HE1	18:Y:1522:TGL:H162	2.03	0.41
1:A:403:TYR:CD1	1:A:479:LYS:HA	2.56	0.41
4:D:130:PRO:O	4:D:136:ALA:HB2	2.20	0.41
5:E:53:ARG:O	5:E:57:ARG:HG3	2.21	0.41
1:N:150:LEU:HD23	1:N:150:LEU:HA	1.81	0.41
4:Q:94:LEU:CD2	11:X:28:VAL:HG21	2.49	0.41
1:A:186:TRP:O	1:A:187:SER:C	2.64	0.40
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.84	0.40
1:A:202:LEU:HB2	1:A:238:PHE:CG	2.56	0.40
1:A:313:ALA:HB3	2:B:73:LEU:HD11	2.02	0.40
1:A:378:HIS:CD2	1:A:425:PHE:CE2	3.08	0.40
1:A:402:GLY:O	1:A:482:VAL:HG23	2.21	0.40
22:B:230:PSC:H072	9:I:10:ARG:NH2	2.30	0.40
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.02	0.40
3:C:188:ILE:HG22	25:C:264:PEK:O13	2.21	0.40
3:C:248:VAL:HG22	25:T:263:PEK:H15	2.02	0.40
23:J:60:CHD:H112	23:J:60:CHD:H12A	1.88	0.40
1:N:58:VAL:HG13	17:N:515:HEA:HBA1	2.02	0.40
1:N:294:THR:C	1:N:296:GLY:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:51:LEU:HB3	4:Q:56:LYS:HG3	2.03	0.40
1:A:19:TYR:CG	1:A:76:GLY:HA3	2.55	0.40
1:A:132:LEU:HD23	2:B:199:ILE:HG23	2.03	0.40
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.56	0.40
3:C:250:LEU:HD23	3:C:250:LEU:HA	1.66	0.40
5:E:54:ALA:O	5:E:58:LEU:HD12	2.20	0.40
1:N:96:ARG:NH2	3:P:61:VAL:HG22	2.35	0.40
1:N:310:MET:HE1	2:O:76:ILE:HB	2.02	0.40
1:N:467:LEU:O	1:N:471:ILE:HG13	2.21	0.40
2:B:14:SER:HB3	2:B:168:LEU:HD22	2.04	0.40
3:C:59:ARG:O	3:C:63:ARG:HG3	2.21	0.40
3:C:157:LYS:HE2	3:C:157:LYS:HB3	1.93	0.40
5:E:37:VAL:HG11	5:E:70:VAL:HG21	2.03	0.40
7:G:8:HIS:HA	7:G:11:TPO:O1P	2.21	0.40
26:G:269:CDL:C27	1:N:282:PHE:HE2	2.35	0.40
13:M:37:LEU:O	13:M:40:TYR:HB2	2.21	0.40
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	2.03	0.40
2:O:95:LEU:HD12	2:O:96:THR:H	1.86	0.40
2:O:104:TRP:NE1	2:O:203:ASN:H	2.19	0.40
2:O:191:LEU:HD23	2:O:191:LEU:HA	1.96	0.40
11:X:43:SER:HA	11:X:44:PRO:HD3	1.91	0.40
2:B:175:ILE:HA	2:B:176:PRO:HD2	1.85	0.40
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.21	0.40
5:E:52:LEU:HD22	5:E:64:ALA:HB1	2.03	0.40
26:G:269:CDL:H421	1:N:311:ILE:HG13	2.04	0.40
1:N:243:VAL:HB	17:N:516:HEA:CAC	2.51	0.40
1:N:288:TRP:O	1:N:291:HIS:HD2	2.04	0.40
1:N:390:MET:HE3	1:N:390:MET:HA	2.02	0.40
3:P:158:HIS:CE1	25:P:1265:PEK:H051	2.56	0.40
10:W:40:LEU:HD12	23:W:1060:CHD:H183	2.04	0.40
1:A:339:MET:HE2	18:A:523:TGL:HA52	2.03	0.40
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.57	0.40
3:C:57:TRP:O	3:C:57:TRP:HD1	2.04	0.40
2:O:32:PHE:HD2	2:O:32:PHE:HA	1.79	0.40
3:P:62:ILE:CD1	3:P:221:ARG:HD2	2.45	0.40
3:P:65:SER:HB3	3:P:71:HIS:CE1	2.56	0.40
3:P:109:THR:HA	27:P:4232:HOH:O	2.20	0.40
12:Y:9:LYS:HD3	12:Y:9:LYS:HA	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	466 (91%)	42 (8%)	4 (1%)	16	37
1	N	512/514 (100%)	469 (92%)	40 (8%)	3 (1%)	21	44
2	B	225/227 (99%)	202 (90%)	20 (9%)	3 (1%)	9	25
2	O	225/227 (99%)	198 (88%)	21 (9%)	6 (3%)	4	10
3	C	257/261 (98%)	247 (96%)	9 (4%)	1 (0%)	30	54
3	P	257/261 (98%)	246 (96%)	10 (4%)	1 (0%)	30	54
4	D	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	8 (6%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	80 (83%)	12 (12%)	4 (4%)	2	4
6	S	96/98 (98%)	83 (86%)	9 (9%)	4 (4%)	2	4
7	G	81/85 (95%)	60 (74%)	13 (16%)	8 (10%)	0	0
7	T	81/85 (95%)	61 (75%)	12 (15%)	8 (10%)	0	0
8	H	77/85 (91%)	66 (86%)	8 (10%)	3 (4%)	2	5
8	U	77/85 (91%)	66 (86%)	8 (10%)	3 (4%)	2	5
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	6	18
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	6	18
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	1 (2%)	1 (2%)	5	13
13	M	41/46 (89%)	36 (88%)	5 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	36 (88%)	5 (12%)	0	100	100
All	All	3504/3614 (97%)	3204 (91%)	249 (7%)	51 (2%)	8	22

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	93	PRO
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
8	H	8	ILE
2	O	60	GLU
6	S	93	PRO
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
2	B	89	GLU
6	F	95	GLN
7	G	3	ALA
7	G	40	GLY
8	H	10	ASN
1	N	9	SER
2	O	89	GLU
7	T	3	ALA
8	U	8	ILE
8	U	10	ASN
6	F	96	LEU
6	S	96	LEU
7	T	40	GLY
1	A	9	SER
7	G	54	ARG
1	N	91	ASP
3	P	38	ASN
10	W	15	ASP
1	A	91	ASP
1	A	369	ASP

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Mol	Chain	Res	Type
3	C	38	ASN
10	J	15	ASP
2	O	59	GLN
2	O	202	SER
2	B	92	ASN
2	O	92	ASN
7	T	6	GLY
12	Y	28	PHE
7	G	6	GLY
1	A	174	PRO
8	H	47	GLY
7	T	49	PRO
8	U	47	GLY
1	N	296	GLY
2	O	159	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/426 (32%)	132 (97%)	4 (3%)	37	67
1	N	426/426 (100%)	413 (97%)	13 (3%)	35	65
2	B	210/210 (100%)	192 (91%)	18 (9%)	10	25
2	O	210/210 (100%)	186 (89%)	24 (11%)	5	14
3	C	224/226 (99%)	211 (94%)	13 (6%)	18	42
3	P	224/226 (99%)	219 (98%)	5 (2%)	45	74
4	D	128/129 (99%)	122 (95%)	6 (5%)	23	51
4	Q	128/129 (99%)	120 (94%)	8 (6%)	16	39
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	63
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	63
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	59
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	31
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	23
8	H	71/75 (95%)	67 (94%)	4 (6%)	19	44
8	U	71/75 (95%)	68 (96%)	3 (4%)	26	55
9	I	57/57 (100%)	51 (90%)	6 (10%)	6	17
9	V	57/57 (100%)	55 (96%)	2 (4%)	32	61
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	76
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	76
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	48
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	48
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	48
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	48
13	M	37/38 (97%)	30 (81%)	7 (19%)	1	4
13	Z	37/38 (97%)	29 (78%)	8 (22%)	1	3
All	All	2750/3082 (89%)	2593 (94%)	157 (6%)	18	43

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	ASP
1	A	444	PRO
1	A	503	HIS
1	A	513	LEU
2	B	3	TYR
2	B	16	ILE
2	B	21	LEU
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	72	ILE
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	130	PRO
2	B	152	MET
2	B	167	SER
2	B	171	LYS

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Mol	Chain	Res	Type
2	B	183	THR
2	B	185	MET
2	B	187	SER
2	B	199	ILE
3	C	13	PRO
3	C	17	PRO
3	C	39	SER
3	C	73	PRO
3	C	77	LYS
3	C	110	PRO
3	C	127	LEU
3	C	144	ILE
3	C	179	SER
3	C	192	VAL
3	C	209	ILE
3	C	230	ASN
3	C	254	VAL
4	D	4	SER
4	D	30	VAL
4	D	51	LEU
4	D	74	SER
4	D	108	PRO
4	D	121	LYS
5	E	7	THR
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	92	VAL
6	F	95	GLN
7	G	17	ARG
7	G	26	PRO
7	G	36	TRP
7	G	43	GLU
7	G	84	LYS
8	H	8	ILE
8	H	29	CYS
8	H	60	TYR
8	H	62	SER
9	I	8	GLN
9	I	10	ARG
9	I	22	VAL
9	I	33	THR

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Mol	Chain	Res	Type
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU
11	K	32	MET
11	K	54	ARG
12	L	15	VAL
12	L	26	THR
13	M	5	PRO
13	M	13	LYS
13	M	34	LEU
13	M	37	LEU
13	M	39	ASN
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	46	THR
1	N	138	HIS
1	N	174	PRO
1	N	178	GLN
1	N	180	GLN
1	N	241	PRO
1	N	356	ILE
1	N	369	ASP
1	N	386	VAL
1	N	444	PRO
1	N	484	THR
1	N	498	CYS
2	O	16	ILE
2	O	33	LEU
2	O	42	ILE
2	O	43	SER
2	O	60	GLU
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	86	MET
2	O	91	ASN
2	O	107	SER
2	O	115	ASP
2	O	130	PRO
2	O	156	SER

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Mol	Chain	Res	Type
2	O	158	ASP
2	O	166	PRO
2	O	167	SER
2	O	171	LYS
2	O	183	THR
2	O	184	LEU
2	O	187	SER
2	O	217	LYS
2	O	223	SER
3	P	77	LYS
3	P	95	THR
3	P	110	PRO
3	P	150	SER
3	P	230	ASN
4	Q	6	VAL
4	Q	9	GLU
4	Q	30	VAL
4	Q	51	LEU
4	Q	110	THR
4	Q	121	LYS
4	Q	131	ILE
4	Q	143	ASN
5	R	80	GLU
5	R	87	GLN
5	R	90	ARG
6	S	48	LEU
6	S	50	PRO
6	S	53	THR
6	S	68	THR
6	S	80	GLN
6	S	94	HIS
7	T	17	ARG
7	T	27	SER
7	T	33	LEU
7	T	35	SER
7	T	55	ILE
7	T	84	LYS
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	33	THR

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Mol	Chain	Res	Type
10	W	50	LEU
11	X	38	ILE
11	X	54	ARG
12	Y	11	ILE
12	Y	26	THR
13	Z	9	PRO
13	Z	12	PRO
13	Z	13	LYS
13	Z	34	LEU
13	Z	37	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	512	ASN
2	B	10	GLN
2	B	52	HIS
2	B	91	ASN
2	B	140	ASN
3	C	50	ASN
3	C	68	GLN
3	C	70	HIS
3	C	122	HIS
3	C	204	HIS
3	C	226	HIS
4	D	32	ASN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
6	F	12	GLN
7	G	8	HIS
7	G	34	ASN
7	G	41	HIS
7	G	66	ASN
7	G	71	HIS
8	H	31	GLN
9	I	20	HIS
10	J	21	HIS
11	K	10	HIS

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Mol	Chain	Res	Type
11	K	35	GLN
1	N	55	ASN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	406	ASN
1	N	413	HIS
1	N	491	ASN
2	O	10	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
3	P	161	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	78	HIS
5	R	94	ASN
6	S	80	GLN
6	S	94	HIS
7	T	34	ASN
7	T	66	ASN
8	U	31	GLN
8	U	32	ASN
9	V	8	GLN
10	W	29	ASN
11	X	15	ASN
11	X	35	GLN

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$
1	FME	N	1	1	8,9,10	0.97	0	8,9,11	0.81	0
2	FME	O	1	2	8,9,10	0.64	0	8,9,11	1.45	2 (25%)
7	TPO	G	11	7	8,10,11	1.93	4 (50%)	10,14,16	1.08	1 (10%)
1	FME	A	1	1	8,9,10	0.75	0	8,9,11	1.01	0
7	TPO	T	11	7	8,10,11	1.97	4 (50%)	10,14,16	1.12	1 (10%)
2	FME	B	1	2	8,9,10	0.71	0	8,9,11	1.50	2 (25%)
9	SAC	V	1	9	7,8,9	3.02	2 (28%)	7,9,11	1.93	3 (42%)
9	SAC	I	1	9	7,8,9	2.76	2 (28%)	7,9,11	1.62	2 (28%)

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
1	FME	N	1	1	-	5/7/9/11	-
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
2	FME	B	1	2	-	2/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-
9	SAC	I	1	9	-	3/7/8/10	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	5.48	1.35	1.23
9	V	1	SAC	OAC-C1A	5.43	1.35	1.23
9	V	1	SAC	CA-N	5.27	1.54	1.46
9	I	1	SAC	CA-N	4.35	1.52	1.46
7	G	11	TPO	CB-CA	3.25	1.60	1.53
7	T	11	TPO	P-O1P	2.82	1.59	1.50
7	T	11	TPO	CG2-CB	2.78	1.58	1.51
7	G	11	TPO	CG2-CB	2.77	1.58	1.51
7	T	11	TPO	CB-CA	2.60	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-OG1	2.46	1.63	1.59
7	G	11	TPO	P-OG1	2.08	1.63	1.59
7	G	11	TPO	P-O1P	2.08	1.56	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-3.26	117.80	122.82
9	V	1	SAC	C2A-C1A-N	3.06	121.19	116.12
2	O	1	FME	C-CA-N	2.98	115.25	109.50
9	I	1	SAC	C2A-C1A-N	2.57	120.39	116.12
9	V	1	SAC	OAC-C1A-C2A	-2.55	117.52	122.05
9	V	1	SAC	C-CA-N	-2.48	104.70	109.50
7	T	11	TPO	O3P-P-OG1	2.38	115.11	105.85
2	O	1	FME	CA-N-CN	-2.35	119.21	122.82
9	I	1	SAC	C-CA-N	-2.31	105.04	109.50
2	B	1	FME	C-CA-N	2.15	113.65	109.50
7	G	11	TPO	O3P-P-OG1	2.03	113.78	105.85

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	CB-CA-N-C1A
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	O-C-CA-CB
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	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
2	B	1	FME	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
1	A	1	FME	CA-CB-CG-SD
1	N	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CA-N-CN
1	N	1	FME	CB-CG-SD-CE
1	A	1	FME	CB-CG-SD-CE
7	G	11	TPO	O-C-CA-CB
7	T	11	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 20 are monoatomic - leaving 44 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$
23	CHD	B	1086	-	32,32,32	0.95	0	51,51,51	2.45	20 (39%)
18	TGL	O	1521	-	62,62,62	1.06	5 (8%)	65,65,65	1.54	10 (15%)
26	CDL	P	1270	-	99,99,99	1.32	13 (13%)	105,111,111	1.07	8 (7%)
17	HEA	A	515	1	67,67,67	1.42	10 (14%)	81,103,103	1.45	12 (14%)
22	PSC	B	230	-	51,51,51	1.60	10 (19%)	57,59,59	1.11	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHD	P	1271	-	32,32,32	1.33	5 (15%)	51,51,51	3.79	26 (50%)
24	DMU	P	1272	-	34,34,34	2.81	14 (41%)	45,45,45	3.78	20 (44%)
18	TGL	Y	1522	-	62,62,62	1.43	5 (8%)	65,65,65	1.69	10 (15%)
24	DMU	C	272	-	34,34,34	2.75	14 (41%)	45,45,45	3.99	18 (40%)
17	HEA	N	515	1	67,67,67	1.56	11 (16%)	81,103,103	1.62	18 (22%)
18	TGL	N	1523	-	62,62,62	1.18	5 (8%)	65,65,65	1.44	9 (13%)
21	CUA	B	228	2	0,1,1	-	-	-	-	-
19	PGV	N	1266	-	50,50,50	1.25	6 (12%)	53,56,56	0.92	1 (1%)
23	CHD	J	60	-	32,32,32	1.56	3 (9%)	51,51,51	3.70	25 (49%)
18	TGL	L	522	-	62,62,62	1.39	5 (8%)	65,65,65	1.75	13 (20%)
23	CHD	C	525	-	32,32,32	1.32	2 (6%)	51,51,51	2.13	15 (29%)
23	CHD	C	271	-	32,32,32	1.30	4 (12%)	51,51,51	3.73	25 (49%)
19	PGV	N	1524	-	50,50,50	1.55	8 (16%)	53,56,56	1.07	5 (9%)
17	HEA	A	516	1	67,67,67	1.58	12 (17%)	81,103,103	1.73	21 (25%)
22	PSC	O	1230	-	51,51,51	1.65	10 (19%)	57,59,59	1.08	5 (8%)
19	PGV	A	524	-	50,50,50	1.55	8 (16%)	53,56,56	1.12	5 (9%)
23	CHD	G	86	-	32,32,32	1.22	3 (9%)	51,51,51	2.58	21 (41%)
23	CHD	W	1060	-	32,32,32	1.83	5 (15%)	51,51,51	3.62	25 (49%)
24	DMU	M	526	-	34,34,34	3.37	9 (26%)	45,45,45	3.56	21 (46%)
19	PGV	C	267	-	50,50,50	1.06	2 (4%)	53,56,56	1.08	6 (11%)
18	TGL	A	521	-	62,62,62	1.01	3 (4%)	65,65,65	1.52	11 (16%)
24	DMU	Z	1526	-	34,34,34	3.37	8 (23%)	45,45,45	3.47	21 (46%)
18	TGL	A	523	-	62,62,62	1.17	5 (8%)	65,65,65	1.42	10 (15%)
25	PEK	G	1263	-	52,52,52	2.36	15 (28%)	55,57,57	1.39	7 (12%)
26	CDL	C	270	-	99,99,99	1.26	13 (13%)	105,111,111	1.04	7 (6%)
19	PGV	P	1268	-	50,50,50	1.65	9 (18%)	53,56,56	0.89	2 (3%)
26	CDL	T	1269	-	99,99,99	1.48	15 (15%)	105,111,111	1.05	9 (8%)
25	PEK	T	1264	-	52,52,52	2.18	14 (26%)	55,57,57	1.54	10 (18%)
19	PGV	C	268	-	50,50,50	1.64	8 (16%)	53,56,56	0.93	2 (3%)
23	CHD	P	1525	-	32,32,32	1.53	5 (15%)	51,51,51	2.07	14 (27%)
21	CUA	O	228	2	0,1,1	-	-	-	-	-
25	PEK	P	1265	-	52,52,52	1.87	12 (23%)	55,57,57	1.09	5 (9%)
19	PGV	P	1267	-	50,50,50	1.12	4 (8%)	53,56,56	0.88	2 (3%)
25	PEK	C	265	-	52,52,52	1.93	12 (23%)	55,57,57	1.12	5 (9%)
25	PEK	T	263	-	52,52,52	2.38	14 (26%)	55,57,57	1.39	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	G	269	-	99,99,99	1.57	16 (16%)	105,111,111	1.04	7 (6%)
19	PGV	A	525	-	50,50,50	1.13	5 (10%)	53,56,56	0.99	2 (3%)
25	PEK	C	264	-	52,52,52	2.09	12 (23%)	55,57,57	1.55	11 (20%)
17	HEA	N	516	1	67,67,67	1.50	6 (8%)	81,103,103	1.92	25 (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
23	CHD	B	1086	-	-	2/9/74/74	0/4/4/4
18	TGL	O	1521	-	-	16/65/65/65	-
26	CDL	P	1270	-	-	71/110/110/110	-
17	HEA	A	515	1	-	11/36/76/76	-
22	PSC	B	230	-	-	34/55/55/55	-
23	CHD	P	1271	-	5/5/12/12	8/9/74/74	0/4/4/4
24	DMU	P	1272	-	6/6/10/10	11/19/59/59	0/2/2/2
18	TGL	Y	1522	-	-	17/65/65/65	-
24	DMU	C	272	-	6/6/10/10	10/19/59/59	0/2/2/2
17	HEA	N	515	1	-	11/36/76/76	-
18	TGL	N	1523	-	-	17/65/65/65	-
19	PGV	N	1266	-	-	11/55/55/55	-
23	CHD	J	60	-	5/5/12/12	8/9/74/74	0/4/4/4
18	TGL	L	522	-	-	15/65/65/65	-
23	CHD	C	525	-	-	2/9/74/74	0/4/4/4
23	CHD	C	271	-	5/5/12/12	8/9/74/74	0/4/4/4
19	PGV	N	1524	-	-	33/55/55/55	-
17	HEA	A	516	1	-	9/36/76/76	-
22	PSC	O	1230	-	-	34/55/55/55	-
19	PGV	A	524	-	-	33/55/55/55	-
23	CHD	W	1060	-	5/5/12/12	8/9/74/74	0/4/4/4
23	CHD	G	86	-	-	2/9/74/74	0/4/4/4
24	DMU	M	526	-	5/5/10/10	9/19/59/59	0/2/2/2
19	PGV	C	267	-	-	18/55/55/55	-
18	TGL	A	521	-	-	14/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DMU	Z	1526	-	5/5/10/10	9/19/59/59	0/2/2/2
18	TGL	A	523	-	-	17/65/65/65	-
25	PEK	G	1263	-	-	29/56/56/56	-
26	CDL	C	270	-	-	69/110/110/110	-
19	PGV	P	1268	-	-	35/55/55/55	-
26	CDL	T	1269	-	-	66/110/110/110	-
25	PEK	T	1264	-	-	22/56/56/56	-
19	PGV	C	268	-	-	34/55/55/55	-
23	CHD	P	1525	-	-	2/9/74/74	0/4/4/4
25	PEK	P	1265	-	-	17/56/56/56	-
19	PGV	P	1267	-	-	18/55/55/55	-
25	PEK	C	265	-	-	19/56/56/56	-
25	PEK	T	263	-	-	29/56/56/56	-
26	CDL	G	269	-	-	65/110/110/110	-
19	PGV	A	525	-	-	11/55/55/55	-
25	PEK	C	264	-	-	22/56/56/56	-
17	HEA	N	516	1	-	9/36/76/76	-

All (345) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	1526	DMU	O16-C6	-8.64	1.25	1.40
24	M	526	DMU	O16-C6	-8.38	1.26	1.40
24	M	526	DMU	O7-C3	-7.89	1.23	1.43
24	Z	1526	DMU	O7-C3	-7.62	1.24	1.43
17	N	516	HEA	FE-ND	-7.61	1.71	1.94
24	Z	1526	DMU	O5-C4	-7.43	1.26	1.44
24	M	526	DMU	O1-C9	-7.24	1.26	1.44
24	Z	1526	DMU	O1-C9	-7.10	1.27	1.44
24	M	526	DMU	O5-C4	-7.10	1.27	1.44
24	Z	1526	DMU	O16-C18	-6.99	1.24	1.43
25	G	1263	PEK	O03-C21	6.99	1.53	1.33
18	Y	1522	TGL	OG2-CB1	6.98	1.54	1.34
24	M	526	DMU	O16-C18	-6.98	1.24	1.43
25	T	263	PEK	O03-C21	6.77	1.53	1.33
23	W	1060	CHD	C13-C17	6.66	1.66	1.55
25	C	264	PEK	O01-C1	6.65	1.53	1.34
23	J	60	CHD	C13-C17	6.38	1.66	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	1264	PEK	O01-C1	6.18	1.51	1.34
18	L	522	TGL	OG2-CB1	6.00	1.51	1.34
17	N	515	HEA	C11-C3B	-5.92	1.44	1.51
24	M	526	DMU	O7-C10	-5.91	1.25	1.41
24	P	1272	DMU	O16-C18	-5.89	1.27	1.43
24	Z	1526	DMU	O7-C10	-5.77	1.25	1.41
24	C	272	DMU	O16-C18	-5.75	1.27	1.43
25	T	1264	PEK	C15-C14	5.73	1.64	1.31
24	M	526	DMU	O1-C10	-5.47	1.27	1.41
19	N	1524	PGV	O03-C19	5.44	1.49	1.33
19	A	524	PGV	O03-C19	5.32	1.48	1.33
25	G	1263	PEK	C6-C5	5.25	1.61	1.31
25	C	264	PEK	C15-C14	5.22	1.61	1.31
19	C	268	PGV	O01-C1	5.15	1.48	1.34
25	C	264	PEK	C12-C11	5.15	1.60	1.31
25	T	263	PEK	C15-C14	5.09	1.60	1.31
24	P	1272	DMU	C8-C9	5.09	1.63	1.53
25	G	1263	PEK	C15-C14	5.06	1.60	1.31
25	T	263	PEK	C6-C5	5.00	1.60	1.31
25	T	263	PEK	C12-C11	4.99	1.60	1.31
25	G	1263	PEK	C03-C02	4.97	1.66	1.50
24	Z	1526	DMU	O1-C10	-4.97	1.29	1.41
24	P	1272	DMU	O7-C3	-4.96	1.31	1.43
22	O	1230	PSC	C10-C9	4.92	1.59	1.31
25	P	1265	PEK	C12-C11	4.89	1.59	1.31
26	G	269	CDL	OB6-CB5	4.87	1.48	1.34
25	C	265	PEK	C12-C11	4.85	1.59	1.31
19	C	268	PGV	C12-C11	4.85	1.59	1.31
25	T	1264	PEK	C6-C5	4.84	1.59	1.31
24	C	272	DMU	C8-C9	4.80	1.63	1.53
17	A	516	HEA	FE-ND	-4.77	1.80	1.94
25	G	1263	PEK	C12-C11	4.77	1.58	1.31
24	P	1272	DMU	C8-C7	4.77	1.64	1.52
24	P	1272	DMU	C6-C1	4.76	1.66	1.52
25	T	1264	PEK	C9-C8	4.75	1.58	1.31
19	P	1268	PGV	C12-C11	4.75	1.58	1.31
24	C	272	DMU	C3-C4	4.75	1.65	1.52
24	Z	1526	DMU	O5-C6	-4.74	1.29	1.41
24	C	272	DMU	C6-C1	4.72	1.66	1.52
19	P	1268	PGV	O01-C1	4.72	1.47	1.34
25	C	264	PEK	C6-C5	4.69	1.58	1.31
25	T	263	PEK	C01-C02	4.68	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	1525	CHD	C10-C9	-4.66	1.47	1.56
22	B	230	PSC	C10-C9	4.66	1.58	1.31
25	C	265	PEK	C15-C14	4.61	1.57	1.31
25	T	1264	PEK	C2-C1	4.57	1.64	1.50
25	T	263	PEK	C9-C8	4.56	1.57	1.31
25	P	1265	PEK	C15-C14	4.54	1.57	1.31
25	T	263	PEK	C03-C02	4.53	1.65	1.50
19	A	524	PGV	C12-C11	4.51	1.57	1.31
25	G	1263	PEK	C9-C8	4.51	1.57	1.31
24	P	1272	DMU	C3-C4	4.50	1.65	1.52
26	G	269	CDL	OA6-CA5	4.48	1.46	1.34
25	G	1263	PEK	C01-C02	4.48	1.64	1.50
25	P	1265	PEK	C9-C8	4.42	1.56	1.31
25	C	264	PEK	C9-C8	4.41	1.56	1.31
22	O	1230	PSC	C13-C12	4.41	1.56	1.31
19	N	1524	PGV	C12-C11	4.41	1.56	1.31
22	B	230	PSC	C13-C12	4.39	1.56	1.31
24	P	1272	DMU	C7-C5	4.37	1.63	1.52
24	P	1272	DMU	O16-C6	-4.37	1.32	1.40
25	T	1264	PEK	C12-C11	4.34	1.56	1.31
24	M	526	DMU	O5-C6	-4.30	1.30	1.41
25	T	1264	PEK	P-O11	4.28	1.76	1.59
25	C	265	PEK	C9-C8	4.24	1.55	1.31
26	G	269	CDL	C51-CB5	4.21	1.62	1.50
24	P	1272	DMU	C10-C5	4.19	1.64	1.52
24	C	272	DMU	C7-C5	4.19	1.63	1.52
23	C	525	CHD	C10-C9	-4.18	1.48	1.56
26	T	1269	CDL	OB6-CB5	4.17	1.46	1.34
25	C	265	PEK	O01-C1	4.11	1.45	1.34
24	C	272	DMU	C8-C7	4.09	1.62	1.52
25	P	1265	PEK	C6-C5	4.08	1.54	1.31
26	T	1269	CDL	C71-CB7	4.07	1.62	1.50
18	Y	1522	TGL	CB2-CB1	4.03	1.62	1.50
24	C	272	DMU	O5-C4	-4.01	1.34	1.44
26	T	1269	CDL	C51-CB5	3.99	1.62	1.50
19	N	1266	PGV	C12-C11	3.99	1.54	1.31
18	L	522	TGL	CB2-CB1	3.99	1.62	1.50
26	G	269	CDL	C71-CB7	3.98	1.62	1.50
25	C	265	PEK	C6-C5	3.95	1.54	1.31
25	C	265	PEK	P-O11	3.89	1.74	1.59
25	T	263	PEK	C22-C21	3.89	1.62	1.50
17	A	516	HEA	C1D-ND	-3.89	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	525	PGV	C12-C11	3.88	1.53	1.31
26	P	1270	CDL	PB2-OB2	3.87	1.74	1.59
22	B	230	PSC	P-O12	3.87	1.74	1.59
17	A	516	HEA	CHD-C4C	-3.87	1.30	1.39
26	G	269	CDL	CB2-C1	3.86	1.64	1.51
24	C	272	DMU	C2-C3	3.86	1.62	1.52
19	N	1266	PGV	O03-C19	3.84	1.44	1.33
25	G	1263	PEK	P-O11	3.83	1.74	1.59
23	P	1525	CHD	C13-C12	-3.82	1.48	1.54
23	W	1060	CHD	C20-C17	3.80	1.60	1.54
26	P	1270	CDL	OA8-CA7	3.78	1.44	1.33
24	C	272	DMU	O16-C6	-3.78	1.33	1.40
17	A	515	HEA	C11-C3B	-3.77	1.46	1.51
25	T	263	PEK	C2-C1	3.74	1.61	1.50
23	G	86	CHD	C1-C10	-3.74	1.47	1.54
25	C	265	PEK	O03-C21	3.71	1.44	1.33
19	P	1267	PGV	C12-C11	3.71	1.52	1.31
17	N	515	HEA	FE-NA	-3.71	1.82	1.95
18	N	1523	TGL	OG1-CA1	3.67	1.44	1.33
25	T	263	PEK	P-O11	3.65	1.73	1.59
26	C	270	CDL	PB2-OB2	3.65	1.73	1.59
24	C	272	DMU	C10-C5	3.65	1.63	1.52
19	C	267	PGV	C12-C11	3.65	1.52	1.31
24	C	272	DMU	O1-C9	-3.63	1.35	1.44
24	C	272	DMU	O7-C3	-3.63	1.34	1.43
26	C	270	CDL	OB8-CB7	3.61	1.43	1.33
25	P	1265	PEK	O03-C21	3.58	1.43	1.33
22	O	1230	PSC	C2-C1	3.57	1.61	1.50
19	P	1268	PGV	O03-C19	3.57	1.43	1.33
26	P	1270	CDL	OB8-CB7	3.57	1.43	1.33
26	T	1269	CDL	CB2-C1	3.54	1.63	1.51
19	A	524	PGV	C20-C19	3.54	1.61	1.50
17	N	516	HEA	CHD-C4C	-3.52	1.31	1.39
24	P	1272	DMU	C2-C1	3.50	1.61	1.52
22	O	1230	PSC	P-O12	3.50	1.73	1.59
18	A	523	TGL	CB2-CB1	3.50	1.60	1.50
26	G	269	CDL	CA6-CA4	3.48	1.61	1.50
26	G	269	CDL	CB6-CB4	3.47	1.61	1.50
25	C	265	PEK	P-O12	3.47	1.73	1.59
25	T	1264	PEK	C22-C21	3.45	1.60	1.50
17	A	515	HEA	CMA-C3A	-3.43	1.37	1.45
25	P	1265	PEK	C22-C21	3.43	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	O	1521	TGL	OG2-CB1	3.43	1.44	1.34
26	C	270	CDL	C71-CB7	3.41	1.60	1.50
19	C	268	PGV	O03-C19	3.39	1.43	1.33
25	C	265	PEK	C22-C21	3.36	1.60	1.50
19	C	268	PGV	C2-C1	3.36	1.60	1.50
25	T	263	PEK	O01-C1	3.34	1.43	1.34
19	N	1524	PGV	C20-C19	3.33	1.60	1.50
25	G	1263	PEK	C22-C21	3.33	1.60	1.50
25	P	1265	PEK	P-O11	3.32	1.72	1.59
25	T	1264	PEK	P-O12	3.31	1.72	1.59
17	A	515	HEA	C4B-NB	-3.30	1.34	1.40
17	N	515	HEA	C4B-NB	-3.26	1.34	1.40
18	A	523	TGL	OG2-CB1	3.26	1.43	1.34
23	C	271	CHD	C13-C17	3.26	1.61	1.55
26	T	1269	CDL	CB6-CB4	3.24	1.60	1.50
25	C	264	PEK	P-O12	3.23	1.72	1.59
19	N	1266	PGV	C2-C1	3.22	1.60	1.50
26	T	1269	CDL	OA6-CA5	3.19	1.43	1.34
17	A	516	HEA	C21-C22	3.18	1.60	1.50
26	P	1270	CDL	C71-CB7	3.17	1.59	1.50
19	P	1268	PGV	C2-C1	3.17	1.59	1.50
24	P	1272	DMU	O5-C4	-3.17	1.36	1.44
24	C	272	DMU	C2-C1	3.14	1.60	1.52
17	N	515	HEA	CMA-C3A	-3.14	1.38	1.45
18	L	522	TGL	CC2-CC1	3.13	1.59	1.50
26	G	269	CDL	OA8-CA7	3.13	1.42	1.33
18	A	521	TGL	CG3-CG2	3.11	1.60	1.50
25	G	1263	PEK	P-O12	3.11	1.71	1.59
26	P	1270	CDL	OB6-CB5	3.10	1.43	1.34
26	T	1269	CDL	OB8-CB7	3.06	1.42	1.33
22	B	230	PSC	O01-C1	3.05	1.42	1.34
25	P	1265	PEK	O01-C1	3.05	1.42	1.34
19	N	1524	PGV	P-O11	3.04	1.71	1.59
24	P	1272	DMU	C2-C3	3.03	1.60	1.52
19	P	1267	PGV	O03-C19	3.03	1.42	1.33
18	A	523	TGL	OG1-CA1	3.02	1.42	1.33
25	C	264	PEK	O03-C21	3.01	1.42	1.33
23	J	60	CHD	C20-C17	3.00	1.59	1.54
18	Y	1522	TGL	OG1-CA1	3.00	1.42	1.33
17	N	515	HEA	FE-ND	-3.00	1.85	1.94
18	N	1523	TGL	CA2-CA1	2.99	1.59	1.50
25	P	1265	PEK	P-O12	2.97	1.71	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	1268	PGV	C04-C05	2.96	1.61	1.51
18	N	1523	TGL	OG3-CC1	2.96	1.42	1.33
18	N	1523	TGL	CB2-CB1	2.95	1.59	1.50
25	G	1263	PEK	O03-C01	2.93	1.51	1.45
26	T	1269	CDL	CA6-CA4	2.92	1.59	1.50
23	W	1060	CHD	C13-C12	2.92	1.59	1.54
22	O	1230	PSC	O01-C1	2.91	1.42	1.34
26	T	1269	CDL	C11-CA5	2.91	1.59	1.50
23	P	1271	CHD	C13-C14	2.91	1.60	1.55
26	C	270	CDL	CA3-CA4	2.88	1.59	1.50
17	N	516	HEA	C11-C3B	-2.87	1.47	1.51
26	P	1270	CDL	C11-CA5	2.86	1.59	1.50
25	G	1263	PEK	C2-C1	2.84	1.59	1.50
22	B	230	PSC	C05-C04	2.84	1.59	1.51
17	A	515	HEA	C1A-C2A	-2.82	1.40	1.45
25	T	263	PEK	P-O12	2.81	1.70	1.59
19	A	524	PGV	P-O12	2.80	1.70	1.59
25	T	263	PEK	O03-C01	2.80	1.51	1.45
19	A	525	PGV	O01-C1	2.80	1.42	1.34
17	A	516	HEA	C1B-NB	-2.79	1.33	1.38
23	C	525	CHD	C13-C12	-2.78	1.50	1.54
19	A	525	PGV	O03-C19	2.78	1.41	1.33
22	B	230	PSC	C2-C1	2.78	1.58	1.50
19	C	268	PGV	P-O11	2.78	1.70	1.59
18	A	523	TGL	OG3-CC1	2.77	1.41	1.33
17	A	516	HEA	CHB-C1B	-2.77	1.32	1.39
17	A	515	HEA	C1B-NB	-2.77	1.33	1.38
26	C	270	CDL	C31-CA7	2.77	1.58	1.50
26	C	270	CDL	CA6-CA4	2.75	1.59	1.50
17	N	516	HEA	C21-C22	2.74	1.58	1.50
22	O	1230	PSC	O03-C19	2.73	1.41	1.33
26	T	1269	CDL	CB3-CB4	2.73	1.59	1.50
19	A	525	PGV	C03-C02	2.71	1.59	1.50
19	C	268	PGV	P-O12	2.71	1.70	1.59
23	P	1271	CHD	C13-C17	2.70	1.60	1.55
19	P	1268	PGV	P-O12	2.70	1.70	1.59
19	C	267	PGV	C01-C02	2.70	1.59	1.50
17	A	516	HEA	CHD-C1D	-2.69	1.33	1.38
25	C	264	PEK	C2-C1	2.68	1.58	1.50
17	N	515	HEA	C20-C19	2.67	1.56	1.51
19	N	1524	PGV	O01-C1	2.67	1.41	1.34
19	P	1268	PGV	C20-C19	2.66	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	O	1521	TGL	CG3-CG2	2.64	1.59	1.50
23	C	271	CHD	C13-C14	2.63	1.59	1.55
18	O	1521	TGL	OG3-CC1	2.62	1.41	1.33
17	A	516	HEA	FE-NB	-2.60	1.86	1.94
26	G	269	CDL	CB3-CB4	2.59	1.58	1.50
18	Y	1522	TGL	CG1-CG2	2.59	1.58	1.50
25	C	264	PEK	P-O11	2.59	1.69	1.59
23	P	1525	CHD	C10-C5	-2.58	1.51	1.55
19	P	1268	PGV	C06-C05	2.58	1.61	1.51
19	C	268	PGV	C04-C05	2.57	1.59	1.51
23	G	86	CHD	C8-C9	2.56	1.58	1.53
18	O	1521	TGL	CA2-CA1	2.56	1.58	1.50
17	A	515	HEA	CHC-C4B	-2.55	1.33	1.38
19	A	524	PGV	P-O11	2.55	1.69	1.59
22	O	1230	PSC	P-O11	2.54	1.69	1.59
25	P	1265	PEK	C03-C02	2.53	1.58	1.50
23	P	1271	CHD	C10-C5	2.52	1.59	1.55
18	A	521	TGL	OG2-CB1	2.52	1.41	1.34
25	G	1263	PEK	O01-C1	2.50	1.41	1.34
17	A	515	HEA	C4A-NA	-2.49	1.34	1.39
25	P	1265	PEK	C01-C02	2.49	1.58	1.50
23	C	271	CHD	C13-C12	2.48	1.58	1.54
26	C	270	CDL	OA8-CA7	2.48	1.40	1.33
23	P	1525	CHD	C18-C13	-2.48	1.50	1.54
26	P	1270	CDL	CB2-C1	2.48	1.59	1.51
26	T	1269	CDL	C85-C84	2.48	1.64	1.51
26	P	1270	CDL	C31-CA7	2.48	1.57	1.50
26	G	269	CDL	C31-CA7	2.48	1.57	1.50
22	B	230	PSC	O03-C19	2.48	1.40	1.33
18	L	522	TGL	CG1-CG2	2.47	1.58	1.50
17	N	515	HEA	CHC-C4B	-2.47	1.33	1.38
26	G	269	CDL	PA1-OA5	2.46	1.69	1.59
19	N	1266	PGV	C20-C19	2.46	1.57	1.50
26	C	270	CDL	OB6-CB5	2.45	1.41	1.34
26	G	269	CDL	OB8-CB7	2.43	1.40	1.33
25	C	264	PEK	C22-C21	2.43	1.57	1.50
23	P	1271	CHD	C8-C9	2.42	1.58	1.53
26	P	1270	CDL	PB2-OB5	2.42	1.68	1.59
26	T	1269	CDL	PA1-OA5	2.41	1.68	1.59
26	C	270	CDL	C11-CA5	2.41	1.57	1.50
19	A	524	PGV	C06-C05	2.41	1.61	1.51
19	A	524	PGV	O01-C1	2.40	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	1264	PEK	C16-C15	2.40	1.63	1.50
24	P	1272	DMU	O1-C9	-2.40	1.38	1.44
18	L	522	TGL	OG1-CA1	2.40	1.40	1.33
26	P	1270	CDL	CA3-CA4	2.38	1.58	1.50
23	G	86	CHD	C10-C5	-2.38	1.51	1.55
18	A	521	TGL	CA2-CA1	2.38	1.57	1.50
18	Y	1522	TGL	CC2-CC1	2.37	1.57	1.50
22	B	230	PSC	P-O11	2.37	1.68	1.59
26	T	1269	CDL	PA1-OA2	2.37	1.68	1.59
26	G	269	CDL	PA1-OA2	2.37	1.68	1.59
25	C	265	PEK	C2-C1	2.36	1.57	1.50
19	N	1524	PGV	C03-C02	2.36	1.58	1.50
26	P	1270	CDL	OA6-CA5	2.34	1.40	1.34
17	A	515	HEA	C4D-C3D	-2.34	1.41	1.45
17	N	516	HEA	C3A-C4A	2.34	1.50	1.46
19	C	268	PGV	C06-C05	2.33	1.60	1.51
22	O	1230	PSC	C05-C04	2.33	1.58	1.51
19	P	1268	PGV	P-O11	2.33	1.68	1.59
22	O	1230	PSC	C01-C02	2.32	1.58	1.50
23	P	1271	CHD	C13-C12	2.32	1.58	1.54
26	G	269	CDL	C11-CA5	2.32	1.57	1.50
19	N	1524	PGV	P-O12	2.30	1.68	1.59
25	C	264	PEK	P-O14	2.30	1.58	1.50
22	B	230	PSC	C03-C02	2.30	1.58	1.50
23	W	1060	CHD	C8-C7	2.30	1.57	1.53
25	C	265	PEK	C03-C02	2.29	1.58	1.50
26	C	270	CDL	OA6-CA5	2.29	1.40	1.34
24	C	272	DMU	O7-C10	-2.29	1.35	1.41
24	P	1272	DMU	O7-C10	-2.29	1.35	1.41
17	N	516	HEA	C22-C23	2.28	1.39	1.32
23	W	1060	CHD	C8-C14	2.28	1.58	1.53
19	N	1266	PGV	C01-C02	2.27	1.57	1.50
17	A	516	HEA	C4D-C3D	-2.27	1.41	1.45
19	A	524	PGV	C03-C02	2.26	1.57	1.50
26	P	1270	CDL	CA6-CA4	2.26	1.57	1.50
26	T	1269	CDL	OA8-CA7	2.25	1.39	1.33
25	C	264	PEK	C18-C17	2.25	1.63	1.51
25	T	1264	PEK	O03-C21	2.25	1.39	1.33
18	A	523	TGL	CA2-CA1	2.24	1.57	1.50
26	P	1270	CDL	PA1-OA5	2.23	1.68	1.59
26	G	269	CDL	C85-C84	2.22	1.62	1.51
19	P	1267	PGV	C20-C19	2.22	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	515	HEA	C4B-C3B	-2.22	1.40	1.44
19	A	525	PGV	C20-C19	2.22	1.57	1.50
26	G	269	CDL	PB2-OB2	2.20	1.68	1.59
17	N	515	HEA	C16-C15	2.20	1.55	1.51
26	C	270	CDL	PB2-OB5	2.20	1.68	1.59
25	G	1263	PEK	C23-C22	2.19	1.60	1.52
24	M	526	DMU	C8-C9	2.18	1.57	1.53
19	N	1266	PGV	C03-C02	2.17	1.57	1.50
19	N	1524	PGV	C06-C05	2.16	1.60	1.51
17	N	515	HEA	C1B-C2B	-2.16	1.40	1.44
26	C	270	CDL	CB2-C1	2.15	1.58	1.51
22	O	1230	PSC	C20-C19	2.15	1.56	1.50
25	G	1263	PEK	C4-C5	2.13	1.61	1.50
22	B	230	PSC	C01-C02	2.13	1.57	1.50
17	A	516	HEA	C4C-NC	-2.13	1.35	1.39
26	T	1269	CDL	PB2-OB2	2.11	1.67	1.59
18	O	1521	TGL	CC2-CC1	2.10	1.56	1.50
25	T	1264	PEK	C4-C5	2.09	1.61	1.50
19	P	1267	PGV	C01-C02	2.09	1.57	1.50
23	J	60	CHD	C8-C7	2.08	1.57	1.53
17	N	515	HEA	CHA-C4D	-2.07	1.34	1.39
26	C	270	CDL	PA1-OA5	2.07	1.67	1.59
25	T	263	PEK	C23-C22	2.06	1.59	1.52
25	T	1264	PEK	C01-C02	2.06	1.57	1.50
23	P	1525	CHD	C13-C17	-2.06	1.52	1.55
25	P	1265	PEK	C2-C1	2.06	1.56	1.50
17	A	515	HEA	C3A-C4A	-2.05	1.42	1.46
18	N	1523	TGL	OG2-CB1	2.05	1.40	1.34
17	A	515	HEA	CHC-C1C	-2.05	1.34	1.39
25	C	265	PEK	C01-C02	2.04	1.57	1.50
17	A	516	HEA	CMA-C3A	-2.04	1.40	1.45
23	C	271	CHD	C8-C14	2.04	1.57	1.53
17	A	516	HEA	C14-C15	2.02	1.37	1.33
25	T	1264	PEK	C18-C17	2.01	1.61	1.51

All (501) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	O16-C6-C1	11.48	125.71	108.27
23	P	1271	CHD	C10-C9-C8	11.40	124.55	111.84
23	C	271	CHD	C10-C9-C8	11.28	124.42	111.84
23	J	60	CHD	C13-C17-C20	9.89	131.46	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	272	DMU	O16-C6-C1	9.56	122.80	108.27
23	C	271	CHD	C17-C13-C14	9.51	109.65	100.11
23	J	60	CHD	C17-C13-C14	9.20	109.34	100.11
23	W	1060	CHD	C13-C17-C20	9.10	130.50	119.48
23	P	1271	CHD	C17-C13-C14	9.03	109.18	100.11
24	Z	1526	DMU	O1-C9-C11	8.94	128.59	106.44
24	M	526	DMU	O1-C9-C11	8.90	128.50	106.44
24	C	272	DMU	C1-C2-C3	8.78	129.60	109.68
23	W	1060	CHD	C17-C13-C14	8.51	108.65	100.11
24	P	1272	DMU	O1-C9-C11	8.25	126.89	106.44
23	J	60	CHD	C11-C12-C13	8.15	119.56	111.26
24	Z	1526	DMU	O5-C4-C3	7.99	126.24	109.72
23	C	271	CHD	C19-C10-C9	-7.92	100.53	111.18
23	P	1271	CHD	C19-C10-C9	-7.77	100.74	111.18
24	C	272	DMU	O1-C9-C11	7.65	125.40	106.44
23	P	1271	CHD	C17-C13-C12	-7.57	110.86	117.67
24	C	272	DMU	O5-C4-C3	7.55	125.34	109.72
23	W	1060	CHD	C10-C9-C8	7.49	120.18	111.84
23	W	1060	CHD	C11-C12-C13	7.35	118.74	111.26
24	C	272	DMU	C18-O16-C6	7.28	126.12	113.68
24	M	526	DMU	O5-C4-C3	7.13	124.45	109.72
23	G	86	CHD	C17-C13-C14	7.11	107.25	100.11
24	P	1272	DMU	O5-C4-C3	7.10	124.41	109.72
24	C	272	DMU	C6-O5-C4	7.00	127.39	113.72
23	J	60	CHD	C10-C9-C8	7.00	119.64	111.84
23	J	60	CHD	C6-C5-C10	6.94	120.05	112.66
24	C	272	DMU	O7-C3-C4	6.91	127.61	109.48
23	W	1060	CHD	C6-C5-C10	6.89	120.00	112.66
23	P	1271	CHD	C9-C8-C7	6.89	120.52	111.86
23	C	271	CHD	C19-C10-C1	-6.78	97.53	108.31
23	J	60	CHD	C18-C13-C14	-6.76	100.61	111.20
24	P	1272	DMU	C6-O5-C4	6.71	126.82	113.72
24	M	526	DMU	C6-O5-C4	6.70	126.80	113.72
24	M	526	DMU	O5-C6-O16	6.70	125.87	110.04
24	P	1272	DMU	O7-C3-C4	6.69	127.03	109.48
24	M	526	DMU	O5-C4-C57	6.61	122.83	106.44
23	W	1060	CHD	C18-C13-C14	-6.60	100.86	111.20
24	C	272	DMU	O7-C3-C2	6.58	123.96	107.23
24	M	526	DMU	C7-C8-C9	6.57	122.15	110.23
23	C	271	CHD	C9-C8-C7	6.44	119.96	111.86
23	P	1271	CHD	C1-C10-C5	6.44	116.99	107.75
24	Z	1526	DMU	C7-C8-C9	6.39	121.82	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	C13-C17-C20	6.38	127.21	119.48
23	W	1060	CHD	C4-C3-C2	6.35	118.36	110.62
23	B	1086	CHD	C17-C13-C14	6.34	106.48	100.11
23	C	271	CHD	C1-C10-C5	6.30	116.79	107.75
23	C	271	CHD	C17-C13-C12	-6.28	112.02	117.67
23	J	60	CHD	C4-C3-C2	6.26	118.26	110.62
24	C	272	DMU	O5-C6-C1	6.21	123.13	110.37
24	Z	1526	DMU	O5-C6-O16	6.17	124.63	110.04
23	P	1271	CHD	C19-C10-C1	-6.13	98.57	108.31
23	G	86	CHD	C9-C8-C7	-6.08	104.21	111.86
24	P	1272	DMU	O5-C4-C57	6.04	121.40	106.44
23	W	1060	CHD	C5-C6-C7	6.00	121.54	114.40
24	M	526	DMU	O7-C3-C2	6.00	122.47	107.23
24	Z	1526	DMU	C6-O5-C4	5.99	125.41	113.72
23	P	1271	CHD	C6-C5-C10	5.98	119.02	112.66
24	Z	1526	DMU	O5-C4-C57	5.97	121.23	106.44
24	C	272	DMU	O1-C9-C8	5.92	120.36	109.70
24	P	1272	DMU	C1-C2-C3	5.85	122.96	109.68
24	C	272	DMU	O7-C10-C5	5.83	122.42	108.09
17	N	516	HEA	C3C-C4C-NC	5.81	114.69	109.80
23	J	60	CHD	C5-C6-C7	5.72	121.20	114.40
23	B	1086	CHD	C16-C17-C13	-5.72	97.99	103.54
24	Z	1526	DMU	O5-C6-C1	5.65	121.97	110.37
23	C	271	CHD	C6-C5-C10	5.59	118.61	112.66
23	B	1086	CHD	C9-C8-C7	-5.58	104.83	111.86
24	P	1272	DMU	O5-C6-C1	5.55	121.77	110.37
23	C	525	CHD	C13-C17-C20	5.53	126.18	119.48
23	G	86	CHD	C16-C17-C13	-5.48	98.23	103.54
24	M	526	DMU	O5-C6-C1	5.29	121.23	110.37
23	P	1271	CHD	C15-C14-C8	-5.28	111.12	118.36
23	W	1060	CHD	C1-C10-C5	5.27	115.31	107.75
23	J	60	CHD	C9-C8-C7	5.25	118.47	111.86
23	J	60	CHD	C15-C14-C8	-5.24	111.18	118.36
24	Z	1526	DMU	O7-C3-C2	5.21	120.48	107.23
18	L	522	TGL	C12-C11-C10	-5.21	88.04	114.37
24	C	272	DMU	O5-C4-C57	5.21	119.34	106.44
24	P	1272	DMU	O7-C3-C2	5.19	120.42	107.23
23	C	525	CHD	C14-C8-C9	-5.15	102.55	109.75
23	J	60	CHD	C1-C10-C5	5.14	115.12	107.75
18	O	1521	TGL	CG2-OG2-CB1	5.13	130.07	117.80
24	P	1272	DMU	O1-C9-C8	5.07	118.84	109.70
23	W	1060	CHD	C9-C8-C7	5.02	118.18	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	1522	TGL	C12-C11-C10	-5.00	89.08	114.37
23	C	525	CHD	C2-C1-C10	4.93	121.05	112.74
23	P	1271	CHD	C4-C3-C2	4.93	116.63	110.62
24	C	272	DMU	C8-C7-C5	4.93	119.48	110.83
24	P	1272	DMU	C18-O16-C6	4.91	122.07	113.68
24	Z	1526	DMU	O7-C3-C4	4.89	122.31	109.48
23	C	271	CHD	C4-C3-C2	4.89	116.59	110.62
24	M	526	DMU	O7-C10-C5	4.89	120.11	108.09
23	G	86	CHD	C15-C14-C13	-4.88	98.81	103.54
23	W	1060	CHD	C15-C14-C8	-4.82	111.75	118.36
23	P	1271	CHD	C14-C13-C12	4.78	111.78	107.42
24	M	526	DMU	C10-C5-C7	4.77	120.05	110.01
18	A	521	TGL	CG2-OG2-CB1	4.74	129.14	117.80
17	A	516	HEA	C3C-C4C-NC	4.64	113.71	109.80
23	C	271	CHD	C15-C14-C8	-4.64	112.00	118.36
18	A	521	TGL	CG1-OG1-CA1	-4.60	100.30	117.12
24	M	526	DMU	O7-C3-C4	4.60	121.54	109.48
23	P	1525	CHD	C2-C1-C10	4.57	120.46	112.74
24	M	526	DMU	O1-C9-C8	4.54	117.88	109.70
23	G	86	CHD	C10-C9-C8	4.46	116.81	111.84
24	Z	1526	DMU	O1-C9-C8	4.46	117.73	109.70
23	C	271	CHD	C14-C8-C7	4.45	117.76	111.85
18	L	522	TGL	CB9-CB8-CB7	-4.45	91.88	114.37
18	O	1521	TGL	CG1-OG1-CA1	-4.43	100.94	117.12
24	Z	1526	DMU	C18-O16-C6	4.40	121.20	113.68
18	Y	1522	TGL	CB9-CB8-CB7	-4.40	92.13	114.37
23	C	271	CHD	C4-C5-C10	4.38	117.32	112.66
25	T	263	PEK	C02-O01-C1	4.33	128.16	117.80
24	Z	1526	DMU	C10-C5-C7	4.30	119.07	110.01
25	T	263	PEK	P-O11-C03	4.30	146.01	121.35
18	L	522	TGL	CG2-OG2-CB1	4.28	128.04	117.80
25	G	1263	PEK	P-O11-C03	4.28	145.85	121.35
23	C	525	CHD	O12-C12-C11	4.25	117.78	109.12
23	P	1271	CHD	C5-C6-C7	4.24	119.44	114.40
24	M	526	DMU	C10-O7-C3	4.24	128.02	117.98
23	P	1271	CHD	C14-C8-C7	4.22	117.45	111.85
18	L	522	TGL	C15-CC9-CC8	4.15	135.33	114.37
24	Z	1526	DMU	O7-C10-C5	4.14	118.28	108.09
24	P	1272	DMU	O7-C10-O1	4.12	121.52	110.69
17	N	516	HEA	CHA-C4D-C3D	-4.09	118.80	124.77
19	A	525	PGV	O01-C1-C2	-4.09	102.63	111.48
23	W	1060	CHD	C6-C5-C4	4.08	115.89	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	1522	TGL	C15-CC9-CC8	4.07	134.96	114.37
25	G	1263	PEK	C02-O01-C1	4.07	127.53	117.80
23	P	1525	CHD	C14-C8-C9	-4.06	104.08	109.75
24	M	526	DMU	C1-C2-C3	4.05	118.88	109.68
25	G	1263	PEK	O03-C01-C02	4.04	120.04	108.40
25	T	263	PEK	O03-C01-C02	4.03	120.01	108.40
17	N	515	HEA	C26-C15-C16	4.01	122.19	115.23
24	P	1272	DMU	C8-C7-C5	3.99	117.83	110.83
23	J	60	CHD	C13-C14-C8	3.99	119.77	114.72
24	Z	1526	DMU	C1-C2-C3	3.98	118.72	109.68
24	P	1272	DMU	O7-C10-C5	3.97	117.85	108.09
24	P	1272	DMU	O1-C10-C5	3.97	118.52	110.37
23	B	1086	CHD	C15-C14-C13	-3.96	99.70	103.54
17	N	516	HEA	C1D-ND-C4D	-3.96	100.52	105.21
23	J	60	CHD	C2-C1-C10	3.96	119.42	112.74
23	P	1525	CHD	C15-C14-C8	-3.95	112.94	118.36
18	Y	1522	TGL	C16-C15-CC9	3.95	134.31	114.37
23	P	1525	CHD	C1-C10-C5	3.94	113.40	107.75
23	B	1086	CHD	C5-C4-C3	3.94	118.64	112.71
23	B	1086	CHD	C15-C14-C8	-3.93	112.96	118.36
23	W	1060	CHD	C13-C14-C8	3.93	119.70	114.72
23	C	525	CHD	C15-C14-C8	-3.92	112.98	118.36
23	C	271	CHD	C1-C10-C9	3.92	117.43	111.34
23	W	1060	CHD	C2-C1-C10	3.91	119.34	112.74
23	C	525	CHD	C1-C10-C5	3.89	113.33	107.75
17	N	516	HEA	C2D-C1D-ND	3.87	114.29	109.84
23	C	271	CHD	C5-C6-C7	3.85	118.98	114.40
18	L	522	TGL	CC3-CC2-CC1	3.83	127.71	113.69
18	L	522	TGL	C16-C15-CC9	3.81	133.62	114.37
24	C	272	DMU	C10-O1-C9	3.80	121.15	113.72
23	G	86	CHD	C5-C4-C3	3.80	118.44	112.71
23	P	1271	CHD	C1-C10-C9	3.80	117.24	111.34
23	G	86	CHD	C15-C14-C8	-3.80	113.15	118.36
23	C	271	CHD	C18-C13-C12	-3.79	105.26	109.06
23	P	1271	CHD	C4-C5-C10	3.79	116.69	112.66
18	A	523	TGL	CG3-OG3-CC1	3.79	130.96	117.12
17	A	516	HEA	CHA-C4D-C3D	-3.79	119.25	124.77
17	A	516	HEA	CHA-C1A-NA	-3.78	120.33	124.45
18	L	522	TGL	C11-C10-CB9	3.77	133.40	114.37
23	G	86	CHD	C1-C2-C3	3.75	115.45	110.48
25	T	1264	PEK	C02-O01-C1	-3.73	108.88	117.80
25	C	264	PEK	C01-O03-C21	-3.73	103.50	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1086	CHD	C11-C12-C13	-3.71	107.49	111.26
17	N	515	HEA	C27-C19-C18	-3.68	114.17	123.63
26	C	270	CDL	PA1-OA5-CA3	3.62	142.09	121.35
23	C	271	CHD	C14-C13-C12	3.61	110.71	107.42
17	N	515	HEA	C3D-C4D-ND	3.60	113.83	110.35
24	C	272	DMU	O7-C10-O1	3.60	120.16	110.69
18	N	1523	TGL	CG3-OG3-CC1	3.59	130.24	117.12
23	P	1525	CHD	C1-C2-C3	3.59	115.24	110.48
23	J	60	CHD	C1-C2-C3	3.59	115.23	110.48
23	B	1086	CHD	C9-C11-C12	3.58	118.98	114.29
17	N	515	HEA	C3A-C2A-C1A	-3.58	103.66	107.05
22	B	230	PSC	C01-O03-C19	-3.56	104.09	117.12
18	Y	1522	TGL	CC3-CC2-CC1	3.56	126.75	113.69
17	A	515	HEA	C27-C19-C18	-3.56	114.50	123.63
18	Y	1522	TGL	C11-C10-CB9	3.55	132.32	114.37
23	P	1525	CHD	C6-C5-C10	3.52	116.41	112.66
23	G	86	CHD	O3-C3-C4	-3.51	102.85	109.84
18	Y	1522	TGL	CG2-OG2-CB1	3.51	126.20	117.80
18	N	1523	TGL	OG2-CB1-CB2	-3.50	103.91	111.48
23	B	1086	CHD	C10-C9-C8	3.49	115.73	111.84
26	P	1270	CDL	CB6-OB8-CB7	-3.46	104.47	117.12
23	G	86	CHD	C1-C10-C5	3.46	112.71	107.75
17	A	516	HEA	CMB-C2B-C3B	-3.45	123.60	130.28
19	N	1524	PGV	O01-C02-C03	3.45	120.72	108.34
17	N	516	HEA	CHB-C4A-NA	-3.45	120.70	124.45
26	P	1270	CDL	PA1-OA5-CA3	3.45	141.11	121.35
17	A	516	HEA	CHB-C4A-NA	-3.44	120.71	124.45
24	M	526	DMU	C18-O16-C6	3.43	119.55	113.68
23	P	1271	CHD	C18-C13-C12	-3.41	105.64	109.06
17	N	516	HEA	CHD-C1D-C2D	-3.41	117.25	126.95
23	W	1060	CHD	C9-C11-C12	3.41	118.76	114.29
25	T	1264	PEK	C01-O03-C21	-3.40	104.69	117.12
25	C	264	PEK	C2-C3-C4	-3.39	105.94	113.35
17	A	515	HEA	C2B-C1B-NB	3.37	113.80	109.90
24	P	1272	DMU	C10-O1-C9	3.34	120.25	113.72
23	B	1086	CHD	C1-C10-C5	3.33	112.53	107.75
19	A	524	PGV	C3-C2-C1	-3.32	101.52	113.69
18	N	1523	TGL	CG1-OG1-CA1	-3.32	104.97	117.12
25	C	264	PEK	P-O12-C04	-3.32	105.45	121.26
17	N	516	HEA	CHD-C1D-ND	3.31	128.46	124.37
23	J	60	CHD	C6-C5-C4	3.31	115.00	111.23
18	N	1523	TGL	CB3-CB2-CB1	3.31	125.81	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	523	TGL	CB3-CB2-CB1	3.30	125.80	113.69
25	C	265	PEK	P-O11-C03	3.30	140.28	121.35
23	B	1086	CHD	C1-C2-C3	3.29	114.84	110.48
18	N	1523	TGL	OG2-CG2-CG3	3.28	120.10	108.34
23	W	1060	CHD	C1-C2-C3	3.27	114.81	110.48
22	B	230	PSC	P-O12-C04	3.27	136.81	121.26
19	A	524	PGV	O01-C02-C03	3.25	119.99	108.34
23	P	1271	CHD	C5-C4-C3	3.24	117.60	112.71
24	Z	1526	DMU	O16-C6-C1	3.23	113.19	108.27
23	G	86	CHD	C19-C10-C5	-3.23	105.03	110.44
23	B	1086	CHD	C14-C8-C9	-3.23	105.24	109.75
17	N	516	HEA	C2A-C1A-NA	3.23	113.44	110.32
24	Z	1526	DMU	O7-C10-O1	3.23	119.18	110.69
17	A	515	HEA	C27-C19-C20	3.21	120.80	115.23
25	T	1264	PEK	P-O12-C04	-3.20	106.03	121.26
23	J	60	CHD	C16-C15-C14	3.18	111.38	105.14
23	W	1060	CHD	C16-C15-C14	3.18	111.38	105.14
17	A	515	HEA	C26-C15-C16	3.18	120.75	115.23
17	A	516	HEA	C2D-C1D-ND	3.17	113.49	109.84
23	G	86	CHD	C5-C6-C7	3.16	118.16	114.40
17	A	515	HEA	CMB-C2B-C1B	3.16	129.97	125.03
17	N	516	HEA	CHA-C1A-NA	-3.15	121.02	124.45
17	N	515	HEA	C2A-C1A-NA	3.14	113.35	110.32
23	W	1060	CHD	C19-C10-C5	-3.13	105.20	110.44
26	C	270	CDL	CB6-OB8-CB7	-3.13	105.67	117.12
17	N	516	HEA	C2B-C1B-NB	3.12	113.51	109.90
25	C	265	PEK	P-O12-C04	3.12	136.10	121.26
23	J	60	CHD	C15-C16-C17	3.11	111.24	105.14
17	N	516	HEA	C20-C19-C18	-3.11	114.19	121.17
17	N	516	HEA	C4A-C3A-C2A	-3.10	104.12	106.81
24	Z	1526	DMU	O1-C10-C5	3.10	116.74	110.37
24	M	526	DMU	O1-C10-C5	3.10	116.73	110.37
23	C	271	CHD	C5-C4-C3	3.08	117.35	112.71
24	Z	1526	DMU	C10-O7-C3	3.08	125.28	117.98
23	J	60	CHD	C19-C10-C9	-3.07	107.05	111.18
23	C	525	CHD	C1-C2-C3	3.07	114.55	110.48
23	W	1060	CHD	C15-C16-C17	3.06	111.14	105.14
23	W	1060	CHD	C18-C13-C12	-3.06	105.99	109.06
25	P	1265	PEK	P-O11-C03	3.06	138.89	121.35
23	C	271	CHD	C16-C15-C14	3.06	111.13	105.14
19	N	1266	PGV	O01-C1-C2	-3.06	104.87	111.48
23	P	1525	CHD	C11-C9-C10	-3.05	110.61	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	1264	PEK	C23-C22-C21	-3.05	102.53	113.69
26	T	1269	CDL	C22-C21-C20	3.05	129.77	114.37
23	C	525	CHD	C9-C11-C12	3.04	118.27	114.29
24	P	1272	DMU	C7-C8-C9	3.03	115.73	110.23
24	P	1272	DMU	C10-O7-C3	3.03	125.17	117.98
23	C	525	CHD	C5-C6-C7	3.03	118.00	114.40
25	C	265	PEK	C11-C10-C9	3.03	126.93	112.02
22	O	1230	PSC	C01-O03-C19	-3.02	106.08	117.12
25	G	1263	PEK	P-O12-C04	3.02	135.64	121.26
19	N	1524	PGV	C3-C2-C1	-3.01	102.68	113.69
23	G	86	CHD	C11-C12-C13	-3.00	108.21	111.26
19	C	268	PGV	C02-O01-C1	-3.00	110.62	117.80
25	C	264	PEK	O01-C1-C2	-2.99	105.01	111.48
26	G	269	CDL	C22-C21-C20	2.99	129.49	114.37
25	C	264	PEK	C3-C2-C1	-2.99	102.75	113.69
25	P	1265	PEK	C11-C10-C9	2.98	126.69	112.02
23	P	1525	CHD	C5-C6-C7	2.97	117.93	114.40
23	J	60	CHD	C19-C10-C5	-2.97	105.47	110.44
17	N	516	HEA	C3D-C4D-ND	2.96	113.21	110.35
18	A	523	TGL	OG1-CG1-CG2	2.96	116.92	108.40
22	O	1230	PSC	P-O12-C04	2.96	135.33	121.26
18	Y	1522	TGL	C13-C12-C11	2.95	129.26	114.37
23	P	1271	CHD	C15-C16-C17	2.94	110.91	105.14
23	C	271	CHD	C11-C12-C13	2.94	114.25	111.26
18	A	523	TGL	CG1-OG1-CA1	-2.93	106.39	117.12
17	N	515	HEA	C27-C19-C20	2.92	120.30	115.23
24	M	526	DMU	C10-O1-C9	2.92	119.42	113.72
26	P	1270	CDL	OB6-CB5-C51	-2.92	105.17	111.48
23	P	1525	CHD	O12-C12-C11	2.91	115.03	109.12
25	C	264	PEK	C23-C22-C21	-2.91	103.04	113.69
25	P	1265	PEK	C24-C23-C22	2.90	123.80	113.13
17	A	516	HEA	C2A-C1A-NA	2.90	113.12	110.32
23	C	271	CHD	C9-C11-C12	2.89	118.08	114.29
18	A	523	TGL	OG2-CB1-CB2	-2.89	105.23	111.48
25	C	264	PEK	C02-O01-C1	-2.88	110.89	117.80
18	A	521	TGL	CG3-CG2-CG1	2.88	118.50	111.78
17	N	515	HEA	OMA-CMA-C3A	-2.88	119.12	125.62
23	C	525	CHD	C19-C10-C9	-2.86	107.33	111.18
17	N	516	HEA	C4C-C3C-C2C	-2.85	103.75	107.30
23	P	1271	CHD	C16-C15-C14	2.85	110.72	105.14
23	G	86	CHD	C9-C11-C12	2.85	118.02	114.29
25	T	263	PEK	P-O12-C04	2.84	134.80	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	526	DMU	O16-C6-C1	2.84	112.59	108.27
23	C	525	CHD	C17-C13-C14	2.84	102.96	100.11
17	N	515	HEA	C26-C15-C14	-2.83	116.35	123.63
23	B	1086	CHD	C14-C8-C7	-2.82	108.10	111.85
25	T	1264	PEK	C3-C2-C1	-2.82	103.36	113.69
23	C	271	CHD	C15-C16-C17	2.81	110.64	105.14
24	M	526	DMU	C8-C7-C5	-2.79	105.94	110.83
17	N	516	HEA	CMB-C2B-C3B	-2.79	124.89	130.28
18	O	1521	TGL	CG3-CG2-CG1	2.78	118.28	111.78
19	A	524	PGV	C02-O01-C1	2.78	124.45	117.80
18	A	523	TGL	OG2-CG2-CG3	2.77	118.27	108.34
19	P	1268	PGV	C02-O01-C1	-2.76	111.18	117.80
23	P	1271	CHD	C11-C12-C13	2.76	114.07	111.26
17	A	516	HEA	C1D-ND-C4D	-2.75	101.95	105.21
25	C	265	PEK	C24-C23-C22	2.74	123.18	113.13
17	A	516	HEA	C3D-C4D-ND	2.73	112.99	110.35
18	A	523	TGL	OG3-CG3-CG2	-2.73	100.54	108.40
24	C	272	DMU	O1-C10-C5	2.71	115.94	110.37
18	O	1521	TGL	C12-C11-C10	-2.71	100.67	114.37
23	W	1060	CHD	C14-C8-C7	2.71	115.44	111.85
17	A	515	HEA	CMB-C2B-C3B	-2.71	125.04	130.28
18	L	522	TGL	C13-C12-C11	2.70	128.00	114.37
17	A	515	HEA	C21-C20-C19	-2.69	104.26	113.19
17	N	515	HEA	C21-C20-C19	-2.69	104.27	113.19
24	Z	1526	DMU	C10-O1-C9	2.69	118.97	113.72
17	A	516	HEA	CHD-C1D-C2D	-2.69	119.31	126.95
18	O	1521	TGL	CA8-CA7-CA6	-2.67	100.85	114.37
17	A	515	HEA	C12-C13-C14	-2.67	105.14	112.16
25	P	1265	PEK	P-O12-C04	2.67	133.98	121.26
25	G	1263	PEK	C03-C02-C01	2.65	117.96	111.78
17	N	515	HEA	C12-C13-C14	-2.64	105.22	112.16
17	N	516	HEA	C4B-NB-C1B	-2.64	102.08	105.21
23	G	86	CHD	O12-C12-C11	2.63	114.47	109.12
17	N	516	HEA	C20-C21-C22	2.63	125.03	112.02
25	C	264	PEK	O03-C21-C22	-2.63	103.82	111.83
23	G	86	CHD	C14-C8-C9	-2.63	106.08	109.75
26	P	1270	CDL	CB4-OB6-CB5	-2.63	111.51	117.80
17	A	516	HEA	CMB-C2B-C1B	2.62	129.13	125.03
26	P	1270	CDL	OA8-CA6-CA4	2.61	115.92	108.40
26	G	269	CDL	C23-C22-C21	2.61	127.55	114.37
18	O	1521	TGL	OG3-CC1-CC2	-2.59	103.95	111.83
23	C	271	CHD	C1-C2-C3	2.57	113.89	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	516	HEA	C20-C19-C18	-2.57	115.41	121.17
25	T	1264	PEK	C2-C3-C4	-2.56	107.75	113.35
23	P	1525	CHD	C17-C13-C12	2.56	119.97	117.67
25	C	264	PEK	C30-C29-C28	-2.56	101.44	114.37
23	P	1525	CHD	C9-C11-C12	2.55	117.63	114.29
17	A	516	HEA	C2B-C1B-NB	2.55	112.85	109.90
18	A	521	TGL	C12-C11-C10	-2.54	101.52	114.37
23	C	271	CHD	C2-C1-C10	2.54	117.03	112.74
23	C	525	CHD	C4-C3-C2	2.54	113.71	110.62
25	T	1264	PEK	C30-C29-C28	-2.54	101.55	114.37
24	M	526	DMU	C6-C1-C2	2.53	115.34	110.01
22	O	1230	PSC	O03-C19-C20	-2.53	104.12	111.83
25	T	1264	PEK	O03-C21-C22	-2.52	104.15	111.83
26	P	1270	CDL	OB6-CB5-OB7	2.52	129.59	123.70
26	T	1269	CDL	C23-C22-C21	2.52	127.10	114.37
23	B	1086	CHD	C2-C1-C10	2.52	116.99	112.74
23	B	1086	CHD	O12-C12-C11	2.51	114.22	109.12
23	J	60	CHD	C14-C8-C9	2.50	113.25	109.75
26	C	270	CDL	OB6-CB5-C51	-2.50	106.07	111.48
23	P	1525	CHD	C9-C10-C5	-2.50	105.04	108.51
18	A	523	TGL	OG2-CG2-CG1	2.49	117.29	108.34
25	C	264	PEK	O13-P-O14	2.49	124.01	112.44
23	P	1271	CHD	C2-C1-C10	2.47	116.91	112.74
18	A	521	TGL	OG3-CG3-CG2	2.47	115.50	108.40
17	N	516	HEA	C27-C19-C20	2.46	119.51	115.23
23	B	1086	CHD	C11-C9-C10	2.46	116.20	113.70
23	W	1060	CHD	C5-C4-C3	2.46	116.41	112.71
17	A	516	HEA	CAD-C3D-C4D	2.43	128.94	124.70
23	P	1271	CHD	C1-C2-C3	2.43	113.70	110.48
23	B	1086	CHD	C15-C16-C17	2.43	109.90	105.14
18	A	521	TGL	OG2-CG2-CG3	2.43	117.06	108.34
17	N	515	HEA	CMD-C2D-C1D	2.43	128.83	125.03
26	G	269	CDL	C83-C82-C81	2.43	126.63	114.37
23	W	1060	CHD	O12-C12-C13	2.42	115.11	111.02
25	G	1263	PEK	C14-C13-C12	2.42	123.92	112.02
26	G	269	CDL	OA6-CA4-CA6	2.41	117.01	108.34
17	N	515	HEA	C2B-C1B-NB	2.41	112.69	109.90
25	T	263	PEK	C2-C3-C4	2.41	118.62	113.35
17	A	516	HEA	C4A-C3A-C2A	-2.41	104.72	106.81
23	G	86	CHD	C2-C1-C10	2.41	116.81	112.74
23	W	1060	CHD	O7-C7-C6	2.41	115.84	109.86
26	G	269	CDL	C79-C78-C77	2.40	126.50	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	C4-C3-C2	2.40	113.54	110.62
26	C	270	CDL	C52-C51-CB5	-2.40	104.91	113.69
19	N	1524	PGV	C04-C05-C06	2.39	119.82	111.77
23	J	60	CHD	C5-C4-C3	2.39	116.31	112.71
17	A	516	HEA	C20-C21-C22	2.37	123.75	112.02
17	N	516	HEA	C4C-CHD-C1D	-2.37	120.67	126.25
18	L	522	TGL	C20-CA9-CA8	2.37	126.34	114.37
19	C	268	PGV	O03-C01-C02	2.36	115.20	108.40
23	J	60	CHD	C14-C8-C7	2.36	114.98	111.85
23	W	1060	CHD	C14-C8-C9	2.35	113.04	109.75
23	J	60	CHD	C18-C13-C12	-2.35	106.71	109.06
26	C	270	CDL	OA8-CA6-CA4	2.34	115.15	108.40
19	A	525	PGV	O01-C1-O02	2.34	129.18	123.70
25	T	263	PEK	O03-C21-C22	2.34	118.97	111.83
23	C	525	CHD	C6-C5-C10	2.34	115.15	112.66
18	L	522	TGL	CC7-CC6-CC5	2.33	126.16	114.37
26	T	1269	CDL	C19-C18-C17	2.33	126.16	114.37
26	G	269	CDL	C19-C18-C17	2.33	126.12	114.37
23	J	60	CHD	C9-C11-C12	2.33	117.34	114.29
18	A	521	TGL	CA8-CA7-CA6	-2.32	102.62	114.37
19	C	267	PGV	C03-C02-C01	2.32	117.20	111.78
18	A	523	TGL	CC3-CC2-CC1	-2.32	105.19	113.69
23	G	86	CHD	C11-C9-C10	2.32	116.06	113.70
24	M	526	DMU	O7-C10-O1	2.31	116.78	110.69
19	C	267	PGV	O01-C1-C2	-2.31	106.48	111.48
26	C	270	CDL	C80-C79-C78	2.30	126.02	114.37
17	A	515	HEA	C4B-NB-C1B	-2.30	102.48	105.21
24	Z	1526	DMU	C8-C7-C5	-2.30	106.80	110.83
25	T	1264	PEK	O03-C01-C02	-2.29	101.78	108.40
26	T	1269	CDL	C80-C79-C78	2.29	125.94	114.37
17	A	516	HEA	CHD-C1D-ND	2.29	127.19	124.37
19	P	1268	PGV	O03-C01-C02	2.28	114.96	108.40
24	Z	1526	DMU	C6-C1-C2	2.28	114.80	110.01
18	Y	1522	TGL	C10-CB9-CB8	2.28	125.88	114.37
26	T	1269	CDL	C83-C82-C81	2.27	125.86	114.37
17	N	515	HEA	C4B-NB-C1B	-2.27	102.52	105.21
18	N	1523	TGL	OG2-CG2-CG1	2.27	116.48	108.34
17	N	516	HEA	C1C-CHC-C4B	-2.26	120.93	126.25
26	G	269	CDL	C80-C79-C78	2.26	125.80	114.37
17	N	515	HEA	CHA-C4D-C3D	-2.26	121.48	124.77
18	A	521	TGL	CB7-CB6-CB5	-2.26	102.94	114.37
26	T	1269	CDL	OB8-CB7-C71	-2.26	104.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	524	PGV	O01-C1-C2	-2.25	106.61	111.48
17	A	516	HEA	CHC-C4B-NB	2.24	127.14	124.37
18	A	521	TGL	OG3-CC1-CC2	-2.24	105.01	111.83
23	G	86	CHD	C15-C16-C17	2.23	109.51	105.14
19	P	1267	PGV	C9-C10-C11	-2.22	100.16	112.60
17	A	515	HEA	C26-C15-C14	-2.22	117.93	123.63
23	P	1271	CHD	C9-C11-C12	2.21	117.18	114.29
26	T	1269	CDL	C79-C78-C77	2.21	125.53	114.37
23	G	86	CHD	C14-C8-C7	-2.21	108.92	111.85
18	A	521	TGL	C33-C19-C18	2.21	125.52	114.37
17	N	516	HEA	CMB-C2B-C1B	2.20	128.48	125.03
23	P	1271	CHD	O7-C7-C6	2.20	115.32	109.86
18	N	1523	TGL	OG1-CG1-CG2	2.20	114.73	108.40
19	N	1524	PGV	C02-O01-C1	2.19	123.05	117.80
23	C	525	CHD	C16-C17-C13	-2.19	101.41	103.54
17	A	516	HEA	C4C-C3C-C2C	-2.18	104.58	107.30
26	P	1270	CDL	C52-C51-CB5	-2.18	105.69	113.69
17	A	516	HEA	CHB-C1B-C2B	-2.18	121.58	125.03
24	P	1272	DMU	O55-C2-C1	2.18	115.51	110.38
17	A	515	HEA	C3B-C4B-NB	2.17	112.34	109.84
19	P	1267	PGV	C3-C2-C1	-2.17	105.73	113.69
24	C	272	DMU	O55-C2-C3	2.17	115.50	109.94
19	A	524	PGV	C04-C05-C06	2.17	119.07	111.77
25	T	263	PEK	C03-C02-C01	2.16	116.83	111.78
22	B	230	PSC	O01-C1-C2	-2.16	106.81	111.48
17	N	515	HEA	CMB-C2B-C3B	-2.15	126.11	130.28
24	C	272	DMU	C2-C3-C4	-2.15	106.16	110.93
18	N	1523	TGL	CG3-CG2-CG1	-2.15	106.76	111.78
23	G	86	CHD	C18-C13-C17	-2.14	107.85	111.20
17	A	515	HEA	OMA-CMA-C3A	-2.13	120.81	125.62
23	C	525	CHD	C14-C13-C12	-2.13	105.47	107.42
23	B	1086	CHD	O3-C3-C4	-2.13	105.61	109.84
19	C	267	PGV	C9-C10-C11	-2.12	100.73	112.60
25	T	263	PEK	C14-C13-C12	2.12	122.46	112.02
18	O	1521	TGL	C33-C19-C18	2.11	125.06	114.37
17	N	515	HEA	C1D-ND-C4D	-2.11	102.71	105.21
17	N	516	HEA	C4A-NA-C1A	-2.11	102.38	105.82
25	T	1264	PEK	C24-C23-C22	-2.11	105.38	113.13
17	A	516	HEA	CMD-C2D-C1D	2.10	128.32	125.03
18	O	1521	TGL	OG2-CG2-CG3	2.10	115.89	108.34
25	C	265	PEK	C2-C3-C4	2.10	117.95	113.35
18	L	522	TGL	CC4-CC3-CC2	2.10	120.84	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	1269	CDL	OB8-CB6-CB4	2.10	114.45	108.40
19	C	267	PGV	C02-O01-C1	-2.10	112.77	117.80
26	C	270	CDL	CB4-OB6-CB5	-2.10	112.77	117.80
23	C	271	CHD	C6-C5-C4	-2.10	108.83	111.23
23	B	1086	CHD	C18-C13-C17	-2.09	107.92	111.20
18	A	523	TGL	CA3-CA2-CA1	-2.07	106.10	113.69
23	J	60	CHD	O7-C7-C6	2.07	115.00	109.86
22	O	1230	PSC	C07-N-C06	-2.06	103.56	108.98
18	O	1521	TGL	CB9-CB8-CB7	-2.06	103.94	114.37
25	C	264	PEK	O03-C21-O04	2.06	128.79	123.63
26	P	1270	CDL	C80-C79-C78	2.06	124.79	114.37
17	N	515	HEA	C4A-C3A-C2A	2.06	108.60	106.81
17	N	516	HEA	C1A-CHA-C4D	-2.06	121.64	126.02
26	T	1269	CDL	C20-C19-C18	2.06	124.77	114.37
25	P	1265	PEK	C2-C3-C4	2.06	117.84	113.35
23	C	271	CHD	O7-C7-C6	2.05	114.96	109.86
23	P	1271	CHD	O12-C12-C13	2.05	114.49	111.02
18	L	522	TGL	C14-C13-C12	-2.05	104.00	114.37
18	O	1521	TGL	CA3-CA2-CA1	-2.05	106.18	113.69
19	C	267	PGV	C3-C2-C1	-2.04	106.20	113.69
18	A	521	TGL	CA3-CA2-CA1	-2.04	106.20	113.69
19	N	1524	PGV	O01-C1-C2	-2.04	107.06	111.48
23	B	1086	CHD	C4-C3-C2	2.04	113.11	110.62
18	L	522	TGL	CA9-CA8-CA7	2.04	124.69	114.37
18	Y	1522	TGL	C20-CA9-CA8	2.04	124.68	114.37
19	C	267	PGV	O12-P-O13	-2.04	100.86	108.94
17	N	516	HEA	C4C-NC-C1C	-2.03	102.51	105.82
22	O	1230	PSC	P-O11-C03	2.03	132.98	121.35
22	B	230	PSC	O03-C19-C20	-2.03	105.66	111.83
23	P	1271	CHD	C6-C5-C4	-2.02	108.92	111.23
18	N	1523	TGL	CC3-CC2-CC1	-2.02	106.30	113.69
17	N	515	HEA	CMB-C2B-C1B	2.01	128.18	125.03
17	N	516	HEA	CHC-C4B-NB	2.01	126.86	124.37
25	G	1263	PEK	C2-C3-C4	2.01	117.75	113.35
24	P	1272	DMU	O55-C2-C3	2.01	115.08	109.94

All (42) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	C	271	CHD	C8
23	C	271	CHD	C3
23	C	271	CHD	C12

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Mol	Chain	Res	Type	Atom
23	C	271	CHD	C14
23	C	271	CHD	C9
23	J	60	CHD	C17
23	J	60	CHD	C8
23	J	60	CHD	C12
23	J	60	CHD	C14
23	J	60	CHD	C9
23	P	1271	CHD	C8
23	P	1271	CHD	C3
23	P	1271	CHD	C12
23	P	1271	CHD	C14
23	P	1271	CHD	C9
23	W	1060	CHD	C17
23	W	1060	CHD	C8
23	W	1060	CHD	C12
23	W	1060	CHD	C14
23	W	1060	CHD	C9
24	C	272	DMU	C2
24	C	272	DMU	C9
24	C	272	DMU	C4
24	C	272	DMU	C10
24	C	272	DMU	C5
24	C	272	DMU	C6
24	M	526	DMU	C2
24	M	526	DMU	C9
24	M	526	DMU	C4
24	M	526	DMU	C5
24	M	526	DMU	C6
24	P	1272	DMU	C2
24	P	1272	DMU	C9
24	P	1272	DMU	C4
24	P	1272	DMU	C10
24	P	1272	DMU	C5
24	P	1272	DMU	C6
24	Z	1526	DMU	C2
24	Z	1526	DMU	C9
24	Z	1526	DMU	C4
24	Z	1526	DMU	C5
24	Z	1526	DMU	C6

All (885) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	515	HEA	C2A-C3A-CMA-OMA
17	A	515	HEA	C4A-C3A-CMA-OMA
17	N	515	HEA	C2A-C3A-CMA-OMA
17	N	515	HEA	C4A-C3A-CMA-OMA
18	A	521	TGL	CB2-CB1-OG2-CG2
18	O	1521	TGL	CB2-CB1-OG2-CG2
19	A	524	PGV	C04-O12-P-O11
19	A	524	PGV	C04-O12-P-O13
19	A	524	PGV	C04-O12-P-O14
19	A	524	PGV	C02-C03-O11-P
19	A	524	PGV	C05-C04-O12-P
19	A	524	PGV	C04-C05-C06-O06
19	A	524	PGV	O05-C05-C06-O06
19	A	524	PGV	O02-C1-O01-C02
19	C	268	PGV	C04-O12-P-O11
19	C	268	PGV	C04-O12-P-O13
19	C	268	PGV	C04-O12-P-O14
19	C	268	PGV	C04-C05-C06-O06
19	N	1524	PGV	C04-O12-P-O11
19	N	1524	PGV	C04-O12-P-O13
19	N	1524	PGV	C04-O12-P-O14
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	C05-C04-O12-P
19	N	1524	PGV	C04-C05-C06-O06
19	N	1524	PGV	O05-C05-C06-O06
19	N	1524	PGV	O02-C1-O01-C02
19	P	1268	PGV	C04-O12-P-O11
19	P	1268	PGV	C04-O12-P-O13
19	P	1268	PGV	C04-O12-P-O14
23	J	60	CHD	C16-C17-C20-C21
23	J	60	CHD	C16-C17-C20-C22
23	W	1060	CHD	C16-C17-C20-C21
23	W	1060	CHD	C16-C17-C20-C22
24	M	526	DMU	O5-C6-O16-C18
24	Z	1526	DMU	O5-C6-O16-C18
25	C	265	PEK	C03-O11-P-O13
25	C	265	PEK	C04-O12-P-O11
25	C	265	PEK	C04-O12-P-O13
25	C	265	PEK	C04-O12-P-O14
25	G	1263	PEK	C03-O11-P-O12
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	O12-C04-C05-N
25	P	1265	PEK	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
25	P	1265	PEK	C04-O12-P-O11
25	P	1265	PEK	C04-O12-P-O13
25	T	263	PEK	C03-O11-P-O12
25	T	263	PEK	C03-O11-P-O14
25	T	263	PEK	O12-C04-C05-N
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	CA4-CA3-OA5-PA1
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB3
26	C	270	CDL	CB2-OB2-PB2-OB4
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	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CA4-CA3-OA5-PA1
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	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CB3-OB5-PB2-OB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
26	T	1269	CDL	OB6-CB4-CB6-OB8
19	A	524	PGV	O04-C19-O03-C01
19	N	1524	PGV	O04-C19-O03-C01
17	A	515	HEA	C21-C22-C23-C25
17	N	515	HEA	C21-C22-C23-C25
19	A	524	PGV	C20-C19-O03-C01
19	N	1524	PGV	C20-C19-O03-C01
18	A	523	TGL	OC1-CC1-OG3-CG3
18	N	1523	TGL	OC1-CC1-OG3-CG3
18	A	521	TGL	OB1-CB1-OG2-CG2
22	B	230	PSC	O02-C1-O01-C02
22	O	1230	PSC	O02-C1-O01-C02
26	C	270	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	OA7-CA5-OA6-CA4
18	N	1523	TGL	CC2-CC1-OG3-CG3
19	A	524	PGV	C2-C1-O01-C02
19	N	1524	PGV	C2-C1-O01-C02
17	A	515	HEA	C26-C15-C16-C17
17	N	515	HEA	C26-C15-C16-C17
17	A	515	HEA	C14-C15-C16-C17
17	N	515	HEA	C14-C15-C16-C17
18	A	521	TGL	CA2-CA1-OG1-CG1
18	A	523	TGL	CC2-CC1-OG3-CG3
18	O	1521	TGL	CA2-CA1-OG1-CG1
26	G	269	CDL	C31-CA7-OA8-CA6
26	T	1269	CDL	C31-CA7-OA8-CA6
26	P	1270	CDL	C57-C58-C59-C60
26	G	269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C40-C41-C42-C43
18	A	521	TGL	OA1-CA1-OG1-CG1
18	L	522	TGL	OA1-CA1-OG1-CG1
18	O	1521	TGL	OA1-CA1-OG1-CG1
18	O	1521	TGL	OB1-CB1-OG2-CG2
18	Y	1522	TGL	C21-C20-CA9-CA8
26	C	270	CDL	C57-C58-C59-C60
26	G	269	CDL	C17-C18-C19-C20
26	P	1270	CDL	C80-C81-C82-C83
17	A	516	HEA	C21-C22-C23-C25
17	N	516	HEA	C21-C22-C23-C25
18	A	521	TGL	C16-C15-CC9-CC8
18	L	522	TGL	C21-C20-CA9-CA8
18	O	1521	TGL	C16-C15-CC9-CC8
26	C	270	CDL	C20-C21-C22-C23
26	C	270	CDL	C77-C78-C79-C80
26	C	270	CDL	C80-C81-C82-C83
26	G	269	CDL	C37-C38-C39-C40
26	G	269	CDL	C40-C41-C42-C43
26	G	269	CDL	C57-C58-C59-C60
26	G	269	CDL	C77-C78-C79-C80
26	G	269	CDL	C80-C81-C82-C83
26	P	1270	CDL	C20-C21-C22-C23
26	T	1269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C57-C58-C59-C60
26	T	1269	CDL	C60-C61-C62-C63
26	T	1269	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C80-C81-C82-C83
26	G	269	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	O1-C1-CA2-OA2
18	Y	1522	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	OA9-CA7-OA8-CA6
26	C	270	CDL	C60-C61-C62-C63
26	T	1269	CDL	C17-C18-C19-C20
22	B	230	PSC	C2-C1-O01-C02
22	O	1230	PSC	C2-C1-O01-C02
26	G	269	CDL	C11-CA5-OA6-CA4
26	T	1269	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	C40-C41-C42-C43
26	G	269	CDL	C60-C61-C62-C63
26	P	1270	CDL	C60-C61-C62-C63
26	P	1270	CDL	C40-C41-C42-C43
26	P	1270	CDL	C77-C78-C79-C80
23	J	60	CHD	C17-C20-C22-C23
23	W	1060	CHD	C17-C20-C22-C23
26	P	1270	CDL	C17-C18-C19-C20
26	C	270	CDL	C17-C18-C19-C20
26	T	1269	CDL	C37-C38-C39-C40
26	T	1269	CDL	OA7-CA5-OA6-CA4
23	J	60	CHD	C21-C20-C22-C23
23	W	1060	CHD	C21-C20-C22-C23
26	P	1270	CDL	C37-C38-C39-C40
26	C	270	CDL	C37-C38-C39-C40
18	L	522	TGL	CA2-CA1-OG1-CG1
18	Y	1522	TGL	CA2-CA1-OG1-CG1
18	A	523	TGL	C21-C20-CA9-CA8
18	N	1523	TGL	C21-C20-CA9-CA8
24	P	1272	DMU	O6-C11-C9-O1
18	N	1523	TGL	C11-C10-CB9-CB8
17	N	515	HEA	C17-C18-C19-C27
18	L	522	TGL	C16-C15-CC9-CC8
18	O	1521	TGL	C11-C10-CB9-CB8
18	A	521	TGL	C21-C20-CA9-CA8
18	A	521	TGL	C11-C10-CB9-CB8
18	A	523	TGL	C11-C10-CB9-CB8
18	O	1521	TGL	C21-C20-CA9-CA8
18	Y	1522	TGL	C16-C15-CC9-CC8
18	N	1523	TGL	C16-C15-CC9-CC8

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Mol	Chain	Res	Type	Atoms
24	P	1272	DMU	C3-C4-C57-O61
18	A	523	TGL	C16-C15-CC9-CC8
19	A	524	PGV	O12-C04-C05-C06
19	N	1524	PGV	O12-C04-C05-C06
26	C	270	CDL	CA2-C1-CB2-OB2
26	G	269	CDL	CB2-C1-CA2-OA2
26	P	1270	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CB2-C1-CA2-OA2
18	A	523	TGL	CA2-CA1-OG1-CG1
18	N	1523	TGL	CA2-CA1-OG1-CG1
22	B	230	PSC	C20-C19-O03-C01
22	O	1230	PSC	C20-C19-O03-C01
18	Y	1522	TGL	C11-C10-CB9-CB8
18	L	522	TGL	C11-C10-CB9-CB8
24	M	526	DMU	O6-C11-C9-C8
24	Z	1526	DMU	C3-C4-C57-O61
24	Z	1526	DMU	O6-C11-C9-C8
19	A	524	PGV	C19-C20-C21-C22
19	A	524	PGV	O12-C04-C05-O05
19	N	1524	PGV	O12-C04-C05-O05
23	J	60	CHD	C13-C17-C20-C21
23	W	1060	CHD	C13-C17-C20-C21
19	N	1524	PGV	C19-C20-C21-C22
23	C	271	CHD	C13-C17-C20-C22
23	J	60	CHD	C13-C17-C20-C22
23	P	1271	CHD	C13-C17-C20-C22
23	W	1060	CHD	C13-C17-C20-C22
22	B	230	PSC	O04-C19-O03-C01
22	O	1230	PSC	O04-C19-O03-C01
24	C	272	DMU	C3-C4-C57-O61
25	G	1263	PEK	O03-C01-C02-O01
25	T	263	PEK	O03-C01-C02-O01
17	A	515	HEA	C21-C22-C23-C24
17	N	515	HEA	C21-C22-C23-C24
17	N	516	HEA	C21-C22-C23-C24
24	M	526	DMU	C3-C4-C57-O61
25	C	264	PEK	C22-C21-O03-C01
25	T	263	PEK	C1-C2-C3-C4
17	A	516	HEA	C21-C22-C23-C24
26	G	269	CDL	OA7-CA5-OA6-CA4
25	G	1263	PEK	C28-C29-C30-C31
25	G	1263	PEK	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
18	A	523	TGL	OA1-CA1-OG1-CG1
18	N	1523	TGL	OA1-CA1-OG1-CG1
25	C	264	PEK	O04-C21-O03-C01
25	T	263	PEK	C28-C29-C30-C31
26	T	1269	CDL	C73-C74-C75-C76
19	C	268	PGV	O12-C04-C05-O05
19	P	1268	PGV	O12-C04-C05-O05
26	C	270	CDL	O1-C1-CB2-OB2
26	G	269	CDL	O1-C1-CB2-OB2
26	P	1270	CDL	O1-C1-CB2-OB2
26	T	1269	CDL	O1-C1-CB2-OB2
24	C	272	DMU	O6-C11-C9-C8
26	C	270	CDL	CB7-C71-C72-C73
22	B	230	PSC	C20-C21-C22-C23
26	G	269	CDL	C73-C74-C75-C76
25	T	1264	PEK	O04-C21-O03-C01
24	C	272	DMU	O6-C11-C9-O1
25	T	1264	PEK	C22-C21-O03-C01
19	C	268	PGV	C2-C1-O01-C02
19	P	1268	PGV	C2-C1-O01-C02
22	O	1230	PSC	C20-C21-C22-C23
26	C	270	CDL	CA5-C11-C12-C13
26	P	1270	CDL	CB7-C71-C72-C73
19	C	268	PGV	O12-C04-C05-C06
19	P	1268	PGV	O12-C04-C05-C06
26	G	269	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CA2-C1-CB2-OB2
26	P	1270	CDL	CA5-C11-C12-C13
17	A	515	HEA	C17-C18-C19-C27
19	C	268	PGV	O02-C1-O01-C02
19	P	1268	PGV	O02-C1-O01-C02
24	C	272	DMU	C1-C6-O16-C18
24	P	1272	DMU	C1-C6-O16-C18
22	B	230	PSC	C1-C2-C3-C4
22	O	1230	PSC	C1-C2-C3-C4
19	P	1268	PGV	C04-C05-C06-O06
18	Y	1522	TGL	CC2-CC3-CC4-CC5
26	G	269	CDL	C15-C16-C17-C18
24	P	1272	DMU	O5-C6-O16-C18
18	L	522	TGL	CC2-CC3-CC4-CC5
22	O	1230	PSC	C22-C23-C24-C25
18	L	522	TGL	CC3-CC4-CC5-CC6

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Mol	Chain	Res	Type	Atoms
19	A	524	PGV	C4-C5-C6-C7
19	C	268	PGV	C24-C25-C26-C27
19	N	1524	PGV	C4-C5-C6-C7
19	P	1267	PGV	C22-C23-C24-C25
22	B	230	PSC	C29-C30-C31-C32
19	P	1268	PGV	C24-C25-C26-C27
26	P	1270	CDL	C51-C52-C53-C54
26	P	1270	CDL	C59-C60-C61-C62
26	T	1269	CDL	C58-C59-C60-C61
19	C	268	PGV	C13-C14-C15-C16
22	B	230	PSC	C22-C23-C24-C25
25	C	265	PEK	C25-C26-C27-C28
25	P	1265	PEK	C25-C26-C27-C28
25	T	263	PEK	C29-C30-C31-C32
26	C	270	CDL	C51-C52-C53-C54
19	C	268	PGV	O05-C05-C06-O06
19	P	1268	PGV	O05-C05-C06-O06
19	C	267	PGV	C7-C8-C9-C10
19	P	1267	PGV	C7-C8-C9-C10
22	O	1230	PSC	C29-C30-C31-C32
25	G	1263	PEK	C29-C30-C31-C32
26	C	270	CDL	C59-C60-C61-C62
26	G	269	CDL	C58-C59-C60-C61
26	T	1269	CDL	C56-C57-C58-C59
19	C	267	PGV	C22-C23-C24-C25
19	N	1266	PGV	C29-C30-C31-C32
19	P	1268	PGV	C13-C14-C15-C16
26	G	269	CDL	C56-C57-C58-C59
26	T	1269	CDL	C15-C16-C17-C18
24	M	526	DMU	C25-C28-C31-C34
26	T	1269	CDL	C72-C73-C74-C75
24	P	1272	DMU	O6-C11-C9-C8
26	G	269	CDL	C72-C73-C74-C75
26	P	1270	CDL	C16-C17-C18-C19
26	G	269	CDL	CA5-C11-C12-C13
19	C	268	PGV	C22-C23-C24-C25
25	G	1263	PEK	C27-C28-C29-C30
26	C	270	CDL	C73-C74-C75-C76
19	N	1266	PGV	C6-C7-C8-C9
25	T	263	PEK	C27-C28-C29-C30
26	C	270	CDL	C16-C17-C18-C19
26	C	270	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
25	T	1264	PEK	C1-C2-C3-C4
26	T	1269	CDL	CA5-C11-C12-C13
19	A	525	PGV	C29-C30-C31-C32
24	Z	1526	DMU	C25-C28-C31-C34
19	P	1268	PGV	C22-C23-C24-C25
26	P	1270	CDL	C73-C74-C75-C76
18	L	522	TGL	CB4-CB5-CB6-CB7
18	Y	1522	TGL	CB4-CB5-CB6-CB7
23	P	1271	CHD	C13-C17-C20-C21
18	Y	1522	TGL	CC3-CC4-CC5-CC6
19	A	525	PGV	C6-C7-C8-C9
22	B	230	PSC	C2-C3-C4-C5
22	O	1230	PSC	C2-C3-C4-C5
25	P	1265	PEK	C16-C17-C18-C19
26	P	1270	CDL	C55-C56-C57-C58
25	C	264	PEK	C31-C32-C33-C34
19	P	1268	PGV	O04-C19-O03-C01
19	A	524	PGV	C22-C23-C24-C25
19	A	525	PGV	C7-C8-C9-C10
19	N	1266	PGV	C7-C8-C9-C10
24	P	1272	DMU	C25-C28-C31-C34
17	N	515	HEA	C17-C18-C19-C20
19	A	524	PGV	C24-C25-C26-C27
19	N	1524	PGV	C24-C25-C26-C27
19	P	1268	PGV	C27-C28-C29-C30
25	C	265	PEK	C16-C17-C18-C19
26	G	269	CDL	C13-C14-C15-C16
26	P	1270	CDL	C36-C37-C38-C39
25	P	1265	PEK	C21-C22-C23-C24
19	P	1268	PGV	C20-C19-O03-C01
19	N	1524	PGV	C22-C23-C24-C25
25	T	1264	PEK	C23-C24-C25-C26
26	C	270	CDL	C74-C75-C76-C77
24	C	272	DMU	O5-C6-O16-C18
19	A	524	PGV	C20-C21-C22-C23
19	A	524	PGV	C28-C29-C30-C31
19	N	1524	PGV	C28-C29-C30-C31
26	P	1270	CDL	C75-C76-C77-C78
19	C	268	PGV	C27-C28-C29-C30
19	N	1266	PGV	C23-C24-C25-C26
26	C	270	CDL	C55-C56-C57-C58
26	C	270	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C13-C14-C15-C16
19	N	1266	PGV	C5-C6-C7-C8
19	A	525	PGV	C23-C24-C25-C26
26	P	1270	CDL	C72-C73-C74-C75
23	C	271	CHD	C13-C17-C20-C21
26	P	1270	CDL	C51-CB5-OB6-CB4
25	C	265	PEK	C21-C22-C23-C24
26	C	270	CDL	C13-C14-C15-C16
26	P	1270	CDL	C74-C75-C76-C77
25	C	264	PEK	C23-C24-C25-C26
26	G	269	CDL	C79-C80-C81-C82
19	N	1524	PGV	C20-C21-C22-C23
26	T	1269	CDL	C79-C80-C81-C82
25	T	1264	PEK	C31-C32-C33-C34
23	P	1271	CHD	C16-C17-C20-C21
26	C	270	CDL	C32-C33-C34-C35
26	P	1270	CDL	C13-C14-C15-C16
19	A	525	PGV	C5-C6-C7-C8
26	P	1270	CDL	C32-C33-C34-C35
26	C	270	CDL	C72-C73-C74-C75
25	G	1263	PEK	C25-C26-C27-C28
26	C	270	CDL	C51-CB5-OB6-CB4
19	C	268	PGV	O04-C19-O03-C01
26	P	1270	CDL	C18-C19-C20-C21
25	C	264	PEK	C1-C2-C3-C4
19	C	267	PGV	C13-C14-C15-C16
25	C	264	PEK	C16-C17-C18-C19
18	A	523	TGL	OG2-CG2-CG3-OG3
18	N	1523	TGL	OG2-CG2-CG3-OG3
19	P	1267	PGV	C11-C10-C9-C8
22	B	230	PSC	C13-C14-C15-C16
22	O	1230	PSC	C13-C14-C15-C16
19	C	268	PGV	C20-C19-O03-C01
19	C	268	PGV	C3-C4-C5-C6
19	P	1267	PGV	C13-C14-C15-C16
19	P	1268	PGV	C3-C4-C5-C6
24	C	272	DMU	C25-C28-C31-C34
25	T	263	PEK	C25-C26-C27-C28
25	T	1264	PEK	C22-C23-C24-C25
19	P	1268	PGV	C28-C29-C30-C31
25	C	265	PEK	C29-C30-C31-C32
25	P	1265	PEK	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C18-C19-C20-C21
26	G	269	CDL	C43-C44-C45-C46
19	C	268	PGV	C28-C29-C30-C31
19	C	268	PGV	C30-C31-C32-C33
25	T	1264	PEK	C16-C17-C18-C19
25	T	1264	PEK	C25-C26-C27-C28
26	C	270	CDL	C71-C72-C73-C74
26	P	1270	CDL	C71-C72-C73-C74
26	G	269	CDL	CB5-C51-C52-C53
19	P	1268	PGV	C30-C31-C32-C33
19	P	1268	PGV	C1-C2-C3-C4
25	C	264	PEK	C25-C26-C27-C28
26	T	1269	CDL	C43-C44-C45-C46
23	C	271	CHD	C16-C17-C20-C22
19	C	268	PGV	C11-C10-C9-C8
19	P	1268	PGV	C11-C10-C9-C8
26	T	1269	CDL	C82-C83-C84-C85
26	G	269	CDL	OA5-CA3-CA4-CA6
26	T	1269	CDL	OA5-CA3-CA4-CA6
18	L	522	TGL	OB1-CB1-OG2-CG2
25	T	1264	PEK	C35-C36-C37-C38
23	C	271	CHD	C16-C17-C20-C21
22	O	1230	PSC	C27-C28-C29-C30
26	C	270	CDL	C38-C39-C40-C41
25	C	265	PEK	C31-C32-C33-C34
25	C	264	PEK	C22-C23-C24-C25
25	T	263	PEK	C16-C17-C18-C19
26	G	269	CDL	C82-C83-C84-C85
19	C	268	PGV	C25-C26-C27-C28
26	C	270	CDL	OB7-CB5-OB6-CB4
22	B	230	PSC	O03-C01-C02-C03
22	O	1230	PSC	O03-C01-C02-C03
25	G	1263	PEK	O03-C01-C02-C03
25	T	263	PEK	O03-C01-C02-C03
25	T	1264	PEK	O03-C01-C02-C03
26	C	270	CDL	CB3-CB4-CB6-OB8
26	G	269	CDL	CB3-CB4-CB6-OB8
26	P	1270	CDL	CB3-CB4-CB6-OB8
26	T	1269	CDL	CB3-CB4-CB6-OB8
26	C	270	CDL	C64-C65-C66-C67
22	B	230	PSC	C27-C28-C29-C30
26	P	1270	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
25	T	263	PEK	C34-C35-C36-C37
25	G	1263	PEK	C16-C17-C18-C19
26	C	270	CDL	C63-C64-C65-C66
26	P	1270	CDL	C63-C64-C65-C66
19	P	1267	PGV	C25-C26-C27-C28
19	C	268	PGV	C1-C2-C3-C4
26	C	270	CDL	C42-C43-C44-C45
26	G	269	CDL	C21-C22-C23-C24
23	P	1271	CHD	C16-C17-C20-C22
26	P	1270	CDL	C64-C65-C66-C67
18	Y	1522	TGL	OB1-CB1-OG2-CG2
26	P	1270	CDL	OB7-CB5-OB6-CB4
26	P	1270	CDL	C34-C35-C36-C37
26	T	1269	CDL	C31-C32-C33-C34
19	C	267	PGV	C23-C24-C25-C26
26	C	270	CDL	C34-C35-C36-C37
26	T	1269	CDL	C21-C22-C23-C24
19	P	1268	PGV	C25-C26-C27-C28
25	T	263	PEK	C26-C27-C28-C29
26	G	269	CDL	C31-C32-C33-C34
18	Y	1522	TGL	CC2-CC1-OG3-CG3
19	A	524	PGV	C03-C02-O01-C1
19	N	1524	PGV	C03-C02-O01-C1
19	C	267	PGV	C25-C26-C27-C28
25	P	1265	PEK	C31-C32-C33-C34
19	C	267	PGV	C11-C10-C9-C8
19	N	1524	PGV	C5-C6-C7-C8
25	G	1263	PEK	C26-C27-C28-C29
25	G	1263	PEK	C34-C35-C36-C37
26	P	1270	CDL	C61-C62-C63-C64
22	O	1230	PSC	C23-C24-C25-C26
26	P	1270	CDL	C44-C45-C46-C47
19	A	525	PGV	C25-C26-C27-C28
19	P	1267	PGV	C23-C24-C25-C26
26	C	270	CDL	C61-C62-C63-C64
19	P	1267	PGV	C15-C16-C17-C18
26	T	1269	CDL	CB5-C51-C52-C53
22	B	230	PSC	C23-C24-C25-C26
26	G	269	CDL	C14-C15-C16-C17
26	P	1270	CDL	C42-C43-C44-C45
25	T	1264	PEK	O03-C01-C02-O01
19	C	267	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	B	230	PSC	C14-C15-C16-C17
26	C	270	CDL	C84-C85-C86-C87
19	C	268	PGV	C5-C6-C7-C8
22	O	1230	PSC	C3-C4-C5-C6
25	G	1263	PEK	C15-C16-C17-C18
26	C	270	CDL	C44-C45-C46-C47
19	N	1266	PGV	C25-C26-C27-C28
25	T	1264	PEK	C32-C33-C34-C35
26	T	1269	CDL	C14-C15-C16-C17
22	O	1230	PSC	C14-C15-C16-C17
22	B	230	PSC	C11-C12-C13-C14
22	O	1230	PSC	C11-C12-C13-C14
19	C	267	PGV	C24-C25-C26-C27
19	P	1268	PGV	C5-C6-C7-C8
24	Z	1526	DMU	C22-C25-C28-C31
26	T	1269	CDL	C35-C36-C37-C38
26	T	1269	CDL	C71-C72-C73-C74
19	P	1267	PGV	C24-C25-C26-C27
25	C	264	PEK	C24-C25-C26-C27
26	G	269	CDL	C33-C34-C35-C36
26	T	1269	CDL	C33-C34-C35-C36
18	A	521	TGL	OC1-CC1-OG3-CG3
17	A	515	HEA	C4C-C3C-CAC-CBC
17	A	516	HEA	C4C-C3C-CAC-CBC
19	A	524	PGV	C5-C6-C7-C8
25	C	264	PEK	C32-C33-C34-C35
25	T	1264	PEK	C27-C28-C29-C30
26	G	269	CDL	C53-C54-C55-C56
26	P	1270	CDL	C84-C85-C86-C87
26	G	269	CDL	C44-C45-C46-C47
25	T	1264	PEK	C24-C25-C26-C27
26	G	269	CDL	C71-C72-C73-C74
26	T	1269	CDL	C41-C42-C43-C44
26	T	1269	CDL	C53-C54-C55-C56
26	C	270	CDL	OB5-CB3-CB4-CB6
26	P	1270	CDL	OB5-CB3-CB4-CB6
26	G	269	CDL	C41-C42-C43-C44
26	T	1269	CDL	C44-C45-C46-C47
19	C	268	PGV	C31-C32-C33-C34
25	C	264	PEK	C35-C36-C37-C38
26	G	269	CDL	C35-C36-C37-C38
18	A	521	TGL	CB6-CB7-CB8-CB9

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Mol	Chain	Res	Type	Atoms
19	P	1268	PGV	C31-C32-C33-C34
18	Y	1522	TGL	CC5-CC6-CC7-CC8
18	L	522	TGL	CC5-CC6-CC7-CC8
18	O	1521	TGL	OC1-CC1-OG3-CG3
25	T	263	PEK	C30-C31-C32-C33
24	M	526	DMU	C22-C25-C28-C31
19	A	524	PGV	O03-C01-C02-C03
19	N	1524	PGV	O03-C01-C02-C03
25	C	264	PEK	O03-C01-C02-C03
22	B	230	PSC	C3-C4-C5-C6
24	C	272	DMU	C22-C25-C28-C31
24	M	526	DMU	O5-C4-C57-O61
25	C	264	PEK	C27-C28-C29-C30
19	C	268	PGV	O01-C02-C03-O11
26	C	270	CDL	OB5-CB3-CB4-OB6
26	P	1270	CDL	OA5-CA3-CA4-OA6
26	P	1270	CDL	OB5-CB3-CB4-OB6
25	T	1264	PEK	C2-C1-O01-C02
25	T	263	PEK	C15-C16-C17-C18
19	P	1268	PGV	C14-C15-C16-C17
26	G	269	CDL	C19-C20-C21-C22
25	C	264	PEK	O03-C01-C02-O01
26	C	270	CDL	OB6-CB4-CB6-OB8
26	P	1270	CDL	OB6-CB4-CB6-OB8
25	C	264	PEK	C5-C6-C7-C8
25	C	264	PEK	C9-C10-C11-C12
25	C	265	PEK	C11-C12-C13-C14
25	G	1263	PEK	C6-C7-C8-C9
25	P	1265	PEK	C11-C12-C13-C14
25	T	263	PEK	C6-C7-C8-C9
25	T	1264	PEK	C5-C6-C7-C8
25	T	1264	PEK	C9-C10-C11-C12
26	C	270	CDL	C39-C40-C41-C42
26	T	1269	CDL	C19-C20-C21-C22
19	P	1267	PGV	C20-C21-C22-C23
25	T	1264	PEK	C26-C27-C28-C29
26	C	270	CDL	C24-C25-C26-C27
19	N	1266	PGV	C30-C31-C32-C33
25	G	1263	PEK	C30-C31-C32-C33
26	P	1270	CDL	C43-C44-C45-C46
19	A	525	PGV	C30-C31-C32-C33
26	P	1270	CDL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C14-C15-C16-C17
24	P	1272	DMU	O5-C4-C57-O61
26	P	1270	CDL	C23-C24-C25-C26
19	N	1524	PGV	C12-C13-C14-C15
19	P	1268	PGV	C12-C13-C14-C15
19	C	267	PGV	C20-C21-C22-C23
19	C	268	PGV	C23-C24-C25-C26
26	P	1270	CDL	C39-C40-C41-C42
17	N	515	HEA	C15-C16-C17-C18
19	C	268	PGV	C15-C16-C17-C18
25	G	1263	PEK	C22-C21-O03-C01
18	L	522	TGL	CC7-CC8-CC9-C15
19	P	1268	PGV	C23-C24-C25-C26
19	C	268	PGV	C12-C13-C14-C15
25	C	265	PEK	C35-C36-C37-C38
18	L	522	TGL	CC2-CC1-OG3-CG3
25	T	263	PEK	C22-C21-O03-C01
25	C	264	PEK	C17-C18-C19-C20
25	T	1264	PEK	C17-C18-C19-C20
22	B	230	PSC	C01-C02-C03-O11
25	G	1263	PEK	C01-C02-C03-O11
25	T	263	PEK	C01-C02-C03-O11
26	P	1270	CDL	OA5-CA3-CA4-CA6
24	P	1272	DMU	C22-C25-C28-C31
26	G	269	CDL	CA7-C31-C32-C33
26	P	1270	CDL	C76-C77-C78-C79
19	P	1268	PGV	C15-C16-C17-C18
24	P	1272	DMU	C34-C37-C40-C43
25	C	264	PEK	C26-C27-C28-C29
25	G	1263	PEK	O04-C21-O03-C01
18	O	1521	TGL	CB6-CB7-CB8-CB9
26	C	270	CDL	C76-C77-C78-C79
26	C	270	CDL	C43-C44-C45-C46
25	T	263	PEK	O04-C21-O03-C01
22	O	1230	PSC	C31-C32-C33-C34
19	A	524	PGV	C12-C13-C14-C15
26	P	1270	CDL	C52-C53-C54-C55
25	P	1265	PEK	C34-C35-C36-C37
26	G	269	CDL	OB9-CB7-OB8-CB6
26	C	270	CDL	C52-C53-C54-C55
18	A	521	TGL	CC2-CC1-OG3-CG3
22	B	230	PSC	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
22	O	1230	PSC	C24-C25-C26-C27
26	C	270	CDL	OA5-CA3-CA4-OA6
26	G	269	CDL	OA5-CA3-CA4-OA6
26	T	1269	CDL	OA5-CA3-CA4-OA6
26	G	269	CDL	CA3-CA4-CA6-OA8
24	Z	1526	DMU	O16-C18-C19-C22
26	T	1269	CDL	CA7-C31-C32-C33
19	A	524	PGV	O03-C01-C02-O01
26	G	269	CDL	OA6-CA4-CA6-OA8
26	T	1269	CDL	OA6-CA4-CA6-OA8
26	G	269	CDL	C54-C55-C56-C57
22	B	230	PSC	C04-C05-N-C08
26	T	1269	CDL	OB9-CB7-OB8-CB6
25	P	1265	PEK	C35-C36-C37-C38
18	Y	1522	TGL	CC7-CC8-CC9-C15
25	T	263	PEK	C02-C03-O11-P
26	C	270	CDL	C23-C24-C25-C26
26	T	1269	CDL	C54-C55-C56-C57
18	O	1521	TGL	CC2-CC1-OG3-CG3
18	N	1523	TGL	CA9-C20-C21-C22
26	G	269	CDL	C24-C25-C26-C27
24	Z	1526	DMU	O5-C4-C57-O61
22	B	230	PSC	C31-C32-C33-C34
19	N	1524	PGV	C01-C02-C03-O11
22	O	1230	PSC	C01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-CA6
25	C	265	PEK	C32-C33-C34-C35
23	C	271	CHD	C17-C20-C22-C23
25	T	263	PEK	C21-C22-C23-C24
25	G	1263	PEK	C02-C03-O11-P
18	A	523	TGL	OB1-CB1-OG2-CG2
25	G	1263	PEK	O01-C02-C03-O11
25	T	263	PEK	C2-C3-C4-C5
25	C	265	PEK	C34-C35-C36-C37
22	O	1230	PSC	C04-C05-N-C07
22	O	1230	PSC	C04-C05-N-C08
18	A	521	TGL	C12-C13-C14-C29
19	P	1267	PGV	C31-C32-C33-C34
17	A	516	HEA	C4A-C3A-CMA-OMA
17	N	516	HEA	C4A-C3A-CMA-OMA
25	P	1265	PEK	C3-C4-C5-C6
19	C	267	PGV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	O03-C01-C02-O01
22	B	230	PSC	O03-C01-C02-O01
22	O	1230	PSC	O03-C01-C02-O01
26	T	1269	CDL	CA3-CA4-CA6-OA8
19	P	1268	PGV	C4-C5-C6-C7
25	C	265	PEK	C3-C4-C5-C6
26	C	270	CDL	C78-C79-C80-C81
25	G	1263	PEK	C21-C22-C23-C24
19	A	524	PGV	C26-C27-C28-C29
18	A	523	TGL	CA9-C20-C21-C22
25	P	1265	PEK	C32-C33-C34-C35
25	C	265	PEK	C03-O11-P-O12
25	C	265	PEK	C03-O11-P-O14
25	G	1263	PEK	C03-O11-P-O13
25	P	1265	PEK	C03-O11-P-O12
25	P	1265	PEK	C03-O11-P-O14
25	T	263	PEK	C03-O11-P-O13
26	C	270	CDL	CA3-OA5-PA1-OA3
26	C	270	CDL	CB2-OB2-PB2-OB5
26	G	269	CDL	CA2-OA2-PA1-OA3
26	G	269	CDL	CB2-OB2-PB2-OB5
26	P	1270	CDL	CA3-OA5-PA1-OA3
26	P	1270	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CA2-OA2-PA1-OA3
26	G	269	CDL	C78-C79-C80-C81
26	P	1270	CDL	C78-C79-C80-C81
26	T	1269	CDL	C64-C65-C66-C67
17	A	516	HEA	C2C-C3C-CAC-CBC
25	G	1263	PEK	C2-C3-C4-C5
19	P	1267	PGV	C05-C04-O12-P
26	G	269	CDL	CB4-CB3-OB5-PB2
26	T	1269	CDL	CB4-CB3-OB5-PB2
19	C	268	PGV	C4-C5-C6-C7
19	N	1266	PGV	C9-C10-C11-C12
22	B	230	PSC	C04-C05-N-C07
19	A	524	PGV	C01-C02-C03-O11
19	C	268	PGV	C01-C02-C03-O11
19	P	1268	PGV	C01-C02-C03-O11
26	T	1269	CDL	C24-C25-C26-C27
19	A	525	PGV	C9-C10-C11-C12
19	P	1268	PGV	O01-C02-C03-O11
25	T	263	PEK	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
25	G	1263	PEK	C32-C33-C34-C35
26	T	1269	CDL	CB7-C71-C72-C73
26	C	270	CDL	C11-C12-C13-C14
25	G	1263	PEK	C31-C32-C33-C34
26	T	1269	CDL	C12-C13-C14-C15
26	T	1269	CDL	C36-C37-C38-C39
19	N	1524	PGV	C26-C27-C28-C29
19	C	267	PGV	C05-C04-O12-P
17	A	515	HEA	C17-C18-C19-C20
24	M	526	DMU	C19-C22-C25-C28
26	P	1270	CDL	C11-C12-C13-C14
25	T	263	PEK	C32-C33-C34-C35
25	T	263	PEK	C31-C32-C33-C34
26	G	269	CDL	C36-C37-C38-C39
26	G	269	CDL	C64-C65-C66-C67
25	C	264	PEK	C29-C30-C31-C32
18	A	521	TGL	CG2-CG3-OG3-CC1
26	G	269	CDL	C12-C13-C14-C15
19	N	1524	PGV	C11-C10-C9-C8
24	M	526	DMU	O16-C18-C19-C22
23	C	271	CHD	C21-C20-C22-C23
17	N	515	HEA	C4C-C3C-CAC-CBC
25	T	263	PEK	C24-C25-C26-C27
26	C	270	CDL	C82-C83-C84-C85
26	T	1269	CDL	C78-C79-C80-C81
26	G	269	CDL	C38-C39-C40-C41
18	O	1521	TGL	C12-C13-C14-C29
18	N	1523	TGL	OB1-CB1-OG2-CG2
19	A	525	PGV	C26-C27-C28-C29
25	G	1263	PEK	C24-C25-C26-C27
19	C	268	PGV	C02-C03-O11-P
19	P	1268	PGV	C02-C03-O11-P
19	P	1268	PGV	C05-C04-O12-P
23	P	1271	CHD	C17-C20-C22-C23
24	P	1272	DMU	C18-C19-C22-C25
25	C	265	PEK	C17-C18-C19-C20
17	A	515	HEA	C15-C16-C17-C18
26	G	269	CDL	C22-C23-C24-C25
26	P	1270	CDL	C41-C42-C43-C44
19	N	1266	PGV	C26-C27-C28-C29
26	T	1269	CDL	C59-C60-C61-C62
17	A	516	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	P	1265	PEK	C30-C31-C32-C33
25	P	1265	PEK	C17-C18-C19-C20
18	Y	1522	TGL	CB5-CB6-CB7-CB8
26	T	1269	CDL	C22-C23-C24-C25
22	O	1230	PSC	C21-C22-C23-C24
18	A	521	TGL	CG1-CG2-OG2-CB1
18	O	1521	TGL	CG1-CG2-OG2-CB1
22	B	230	PSC	C03-C02-O01-C1
22	O	1230	PSC	C03-C02-O01-C1
19	A	524	PGV	C11-C10-C9-C8
17	A	516	HEA	CAD-CBD-CGD-O1D
24	P	1272	DMU	C4-C3-O7-C10
26	G	269	CDL	CB7-C71-C72-C73
17	A	515	HEA	C2C-C3C-CAC-CBC
17	N	515	HEA	C2C-C3C-CAC-CBC
17	N	516	HEA	C2C-C3C-CAC-CBC
17	N	516	HEA	CAD-CBD-CGD-O1D
17	N	516	HEA	CAD-CBD-CGD-O2D
19	C	267	PGV	C29-C30-C31-C32
19	P	1267	PGV	C02-C03-O11-P
22	B	230	PSC	C21-C22-C23-C24
23	B	1086	CHD	C22-C23-C24-O25
22	O	1230	PSC	C4-C5-C6-C7
19	P	1267	PGV	C1-C2-C3-C4
26	G	269	CDL	C18-C19-C20-C21
22	B	230	PSC	C9-C10-C11-C12
22	O	1230	PSC	C9-C10-C11-C12
23	G	86	CHD	C22-C23-C24-O25
26	T	1269	CDL	C38-C39-C40-C41
19	C	268	PGV	C05-C04-O12-P
26	C	270	CDL	C1-CA2-OA2-PA1
26	P	1270	CDL	C1-CA2-OA2-PA1
18	L	522	TGL	CB5-CB6-CB7-CB8
18	L	522	TGL	OG2-CB1-CB2-CB3
24	C	272	DMU	C34-C37-C40-C43
23	B	1086	CHD	C22-C23-C24-O26
23	C	525	CHD	C22-C23-C24-O26
26	C	270	CDL	CA3-CA4-CA6-OA8
19	C	267	PGV	C14-C15-C16-C17
17	A	516	HEA	CAA-CBA-CGA-O1A
25	C	265	PEK	C30-C31-C32-C33
18	Y	1522	TGL	OG2-CB1-CB2-CB3

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Mol	Chain	Res	Type	Atoms
23	G	86	CHD	C22-C23-C24-O26
23	P	1271	CHD	C22-C23-C24-O26
19	A	524	PGV	C21-C22-C23-C24
26	P	1270	CDL	C15-C16-C17-C18
22	O	1230	PSC	C7-C8-C9-C10
19	C	267	PGV	C02-C03-O11-P
23	C	271	CHD	C22-C23-C24-O25
23	P	1271	CHD	C22-C23-C24-O25
19	A	524	PGV	C2-C3-C4-C5
23	C	271	CHD	C22-C23-C24-O26
22	B	230	PSC	C7-C8-C9-C10
25	G	1263	PEK	C3-C4-C5-C6
25	T	263	PEK	C3-C4-C5-C6
25	T	1264	PEK	C3-C4-C5-C6
23	P	1271	CHD	C21-C20-C22-C23
22	B	230	PSC	C04-C05-N-C06
22	O	1230	PSC	C04-C05-N-C06
19	P	1268	PGV	C26-C27-C28-C29
19	P	1267	PGV	C14-C15-C16-C17
24	Z	1526	DMU	C34-C37-C40-C43
19	C	267	PGV	C9-C10-C11-C12
19	P	1267	PGV	C9-C10-C11-C12
19	P	1267	PGV	C11-C12-C13-C14
26	T	1269	CDL	C18-C19-C20-C21
19	N	1266	PGV	O03-C19-C20-C21
23	P	1525	CHD	C22-C23-C24-O26
19	C	267	PGV	C11-C12-C13-C14
25	G	1263	PEK	C14-C15-C16-C17
25	T	263	PEK	C14-C15-C16-C17
23	C	525	CHD	C22-C23-C24-O25
19	P	1267	PGV	C21-C22-C23-C24
19	N	1524	PGV	C25-C26-C27-C28
26	P	1270	CDL	CA3-CA4-CA6-OA8
26	P	1270	CDL	C54-C55-C56-C57
18	Y	1522	TGL	OG3-CC1-CC2-CC3
17	N	516	HEA	CAA-CBA-CGA-O1A
19	C	268	PGV	C26-C27-C28-C29
22	B	230	PSC	C4-C5-C6-C7
26	C	270	CDL	C15-C16-C17-C18
19	N	1524	PGV	O01-C1-C2-C3
22	O	1230	PSC	O03-C19-C20-C21
19	C	267	PGV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C83-C84-C85-C86
19	C	268	PGV	O03-C01-C02-O01
23	P	1525	CHD	C22-C23-C24-O25
19	N	1266	PGV	C11-C12-C13-C14
22	B	230	PSC	C12-C13-C14-C15
22	B	230	PSC	O03-C19-C20-C21
25	T	1264	PEK	O01-C1-C2-C3
26	C	270	CDL	C52-C51-CB5-OB6
18	O	1521	TGL	CG2-CG3-OG3-CC1
19	N	1524	PGV	C21-C22-C23-C24
18	A	523	TGL	OG2-CB1-CB2-CB3
18	L	522	TGL	OG3-CC1-CC2-CC3
24	C	272	DMU	C4-C3-O7-C10
18	N	1523	TGL	C21-C22-C23-C24
26	C	270	CDL	C54-C55-C56-C57
25	C	264	PEK	O01-C1-C2-C3
26	P	1270	CDL	C52-C51-CB5-OB6
19	N	1524	PGV	C9-C10-C11-C12
22	O	1230	PSC	C12-C13-C14-C15
18	A	523	TGL	CB2-CB3-CB4-CB5
19	A	524	PGV	O01-C1-C2-C3
26	T	1269	CDL	C62-C63-C64-C65
17	A	516	HEA	CAA-CBA-CGA-O2A
19	A	525	PGV	C11-C12-C13-C14
26	G	269	CDL	C59-C60-C61-C62
19	C	267	PGV	C1-C2-C3-C4
26	P	1270	CDL	C32-C31-CA7-OA8
19	N	1524	PGV	C2-C3-C4-C5
18	O	1521	TGL	C13-C14-C29-C30
18	N	1523	TGL	OG2-CB1-CB2-CB3
26	C	270	CDL	C32-C31-CA7-OA8
24	M	526	DMU	C19-C18-O16-C6
23	W	1060	CHD	C22-C23-C24-O25
23	W	1060	CHD	C22-C23-C24-O26
22	O	1230	PSC	O01-C1-C2-C3
26	P	1270	CDL	C12-C11-CA5-OA6
17	N	516	HEA	C4C-C3C-CAC-CBC
18	A	523	TGL	C21-C22-C23-C24
18	A	523	TGL	OG1-CG1-CG2-OG2
18	N	1523	TGL	OG1-CG1-CG2-OG2
19	P	1268	PGV	O03-C01-C02-O01
19	A	524	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
18	N	1523	TGL	CB2-CB3-CB4-CB5
18	A	523	TGL	OG3-CC1-CC2-CC3
26	P	1270	CDL	C82-C83-C84-C85
22	B	230	PSC	O01-C1-C2-C3
19	P	1267	PGV	C29-C30-C31-C32
18	A	523	TGL	CG3-CG2-OG2-CB1
18	N	1523	TGL	CG3-CG2-OG2-CB1
24	Z	1526	DMU	C19-C22-C25-C28
17	N	516	HEA	CAA-CBA-CGA-O2A
26	C	270	CDL	C12-C11-CA5-OA6
26	T	1269	CDL	C76-C77-C78-C79
22	B	230	PSC	O04-C19-C20-C21
23	J	60	CHD	C22-C23-C24-O25
19	A	525	PGV	O03-C19-C20-C21
22	O	1230	PSC	O02-C1-C2-C3
18	Y	1522	TGL	C12-C13-C14-C29
24	C	272	DMU	O5-C4-C57-O61
18	Y	1522	TGL	CC6-CC7-CC8-CC9
18	A	521	TGL	CB7-CB8-CB9-C10
26	T	1269	CDL	C55-C56-C57-C58
22	B	230	PSC	O01-C02-C03-O11
22	O	1230	PSC	O01-C02-C03-O11
26	G	269	CDL	C55-C56-C57-C58
19	A	524	PGV	C9-C10-C11-C12
25	C	264	PEK	O02-C1-C2-C3
22	B	230	PSC	O02-C1-C2-C3
25	T	1264	PEK	O02-C1-C2-C3
18	O	1521	TGL	C10-C11-C12-C13
19	N	1524	PGV	O02-C1-C2-C3
19	P	1268	PGV	C7-C8-C9-C10
18	A	523	TGL	OC1-CC1-CC2-CC3
19	A	524	PGV	O02-C1-C2-C3
26	P	1270	CDL	C52-C51-CB5-OB7
18	N	1523	TGL	OG3-CC1-CC2-CC3
26	C	270	CDL	C52-C51-CB5-OB7
26	P	1270	CDL	C32-C31-CA7-OA9
25	C	265	PEK	C26-C27-C28-C29
26	G	269	CDL	C62-C63-C64-C65
18	N	1523	TGL	OC1-CC1-CC2-CC3
22	O	1230	PSC	O04-C19-C20-C21
26	C	270	CDL	C32-C31-CA7-OA9
18	O	1521	TGL	OG1-CA1-CA2-CA3

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Mol	Chain	Res	Type	Atoms
23	J	60	CHD	C22-C23-C24-O26
25	C	264	PEK	C3-C4-C5-C6

There are no ring outliers.

42 monomers are involved in 347 short contacts:

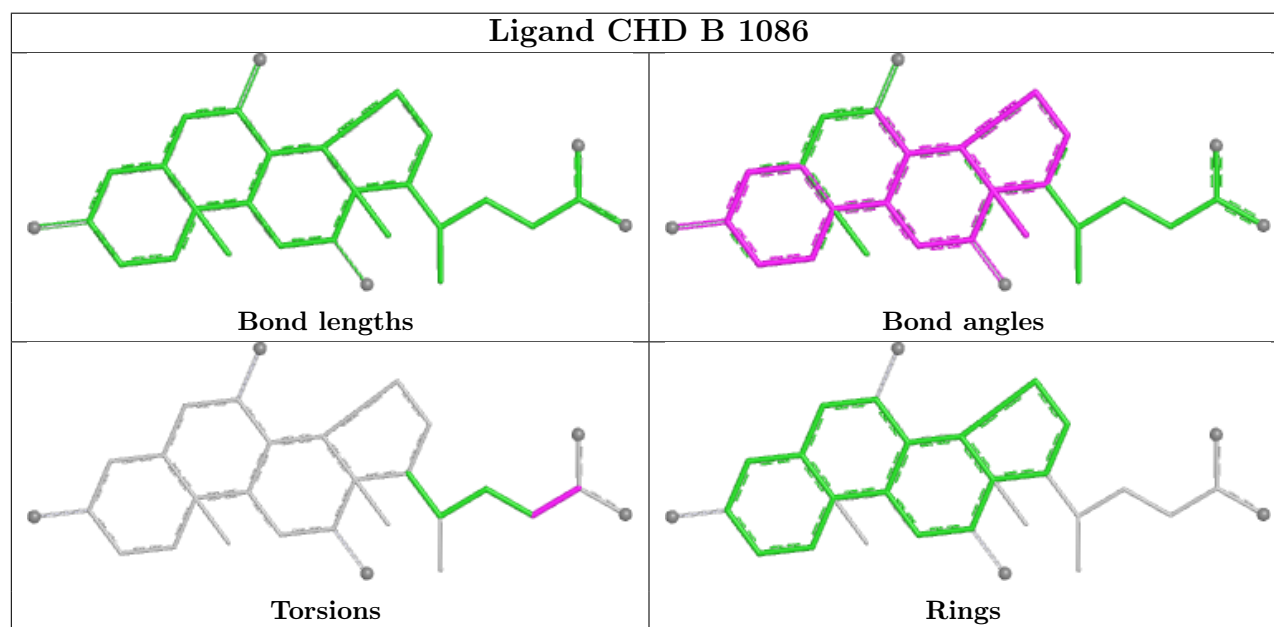
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	1086	CHD	5	0
18	O	1521	TGL	8	0
26	P	1270	CDL	17	0
17	A	515	HEA	15	0
22	B	230	PSC	21	0
23	P	1271	CHD	5	0
24	P	1272	DMU	4	0
18	Y	1522	TGL	16	0
24	C	272	DMU	3	0
17	N	515	HEA	12	0
18	N	1523	TGL	9	0
19	N	1266	PGV	3	0
23	J	60	CHD	4	0
18	L	522	TGL	20	0
23	C	525	CHD	1	0
23	C	271	CHD	4	0
19	N	1524	PGV	7	0
17	A	516	HEA	2	0
22	O	1230	PSC	20	0
19	A	524	PGV	5	0
23	G	86	CHD	1	0
23	W	1060	CHD	3	0
24	M	526	DMU	2	0
19	C	267	PGV	6	0
18	A	521	TGL	8	0
24	Z	1526	DMU	1	0
18	A	523	TGL	4	0
25	G	1263	PEK	10	0
26	C	270	CDL	17	0
19	P	1268	PGV	2	0
26	T	1269	CDL	32	0
25	T	1264	PEK	12	0
19	C	268	PGV	1	0
23	P	1525	CHD	1	0
25	P	1265	PEK	10	0

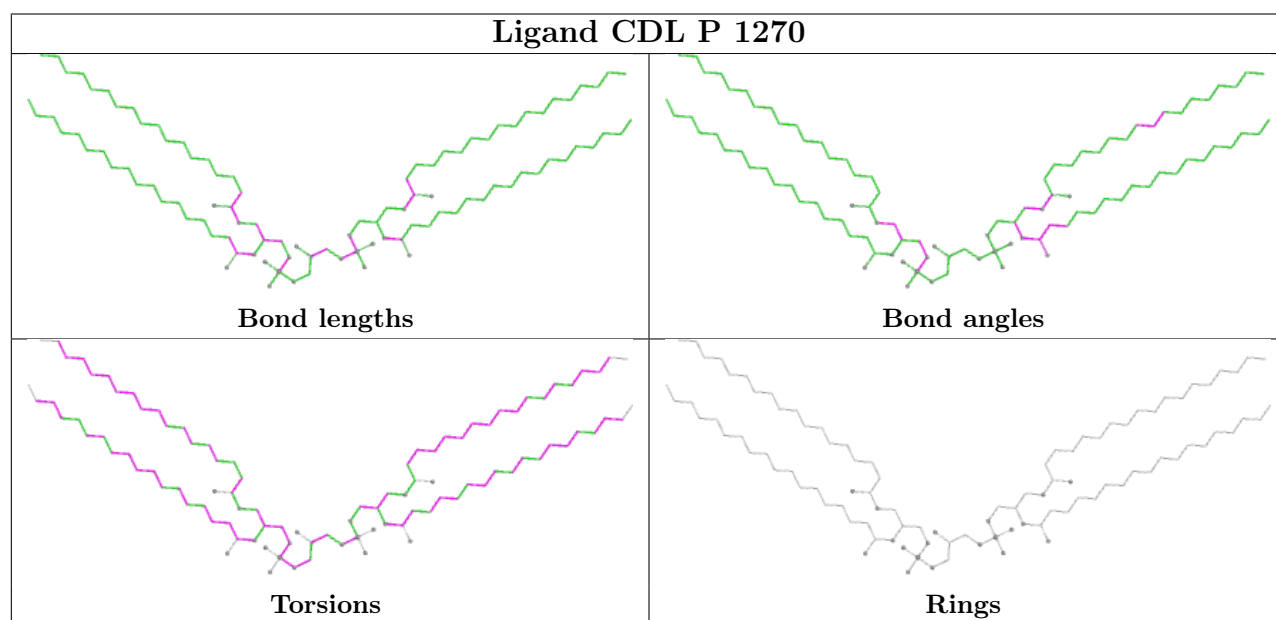
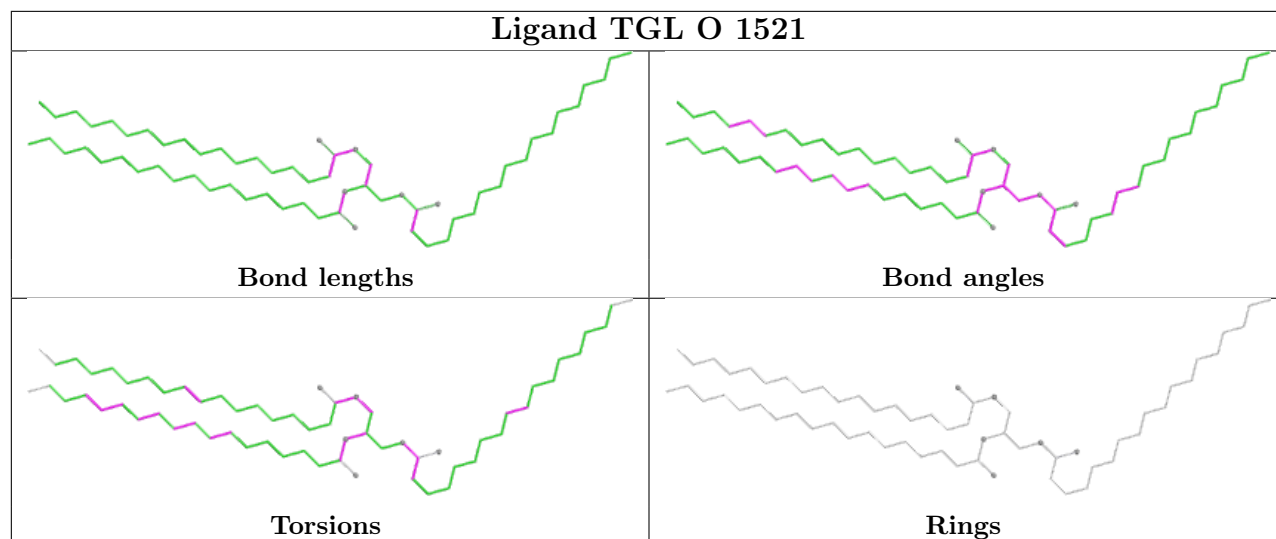
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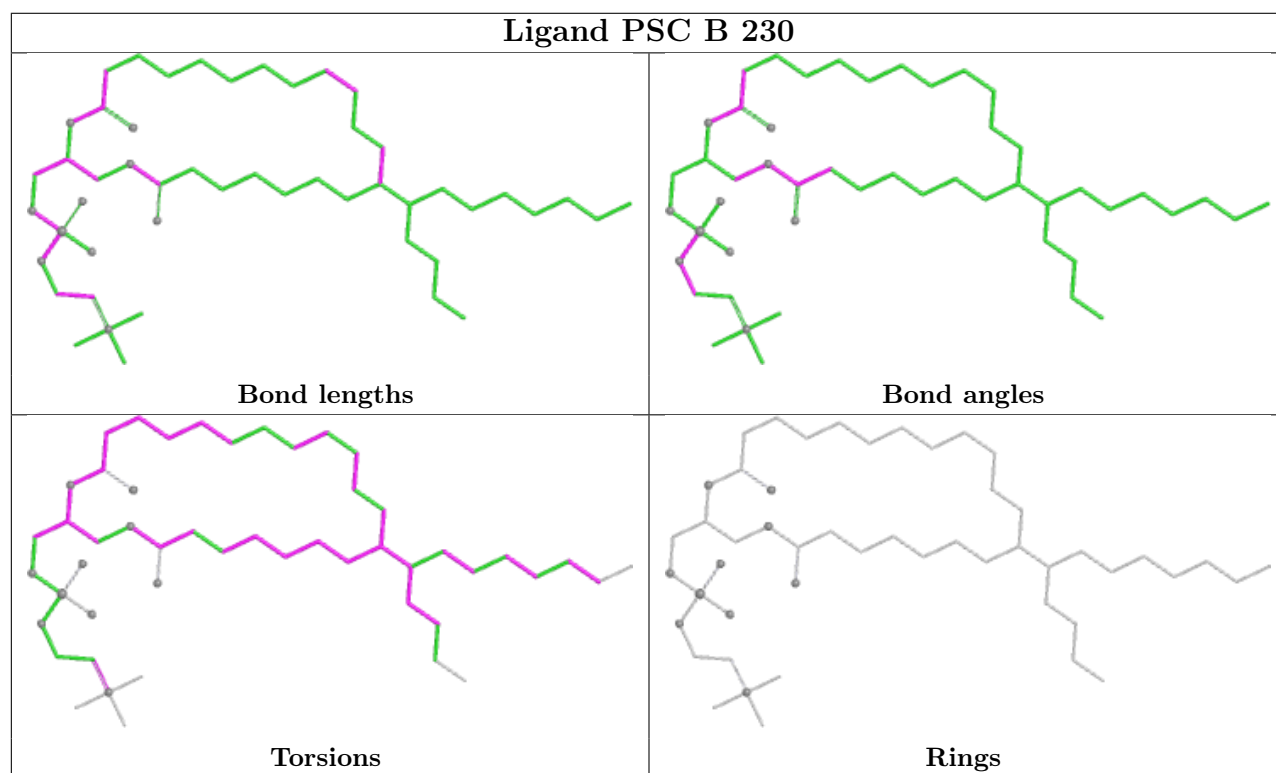
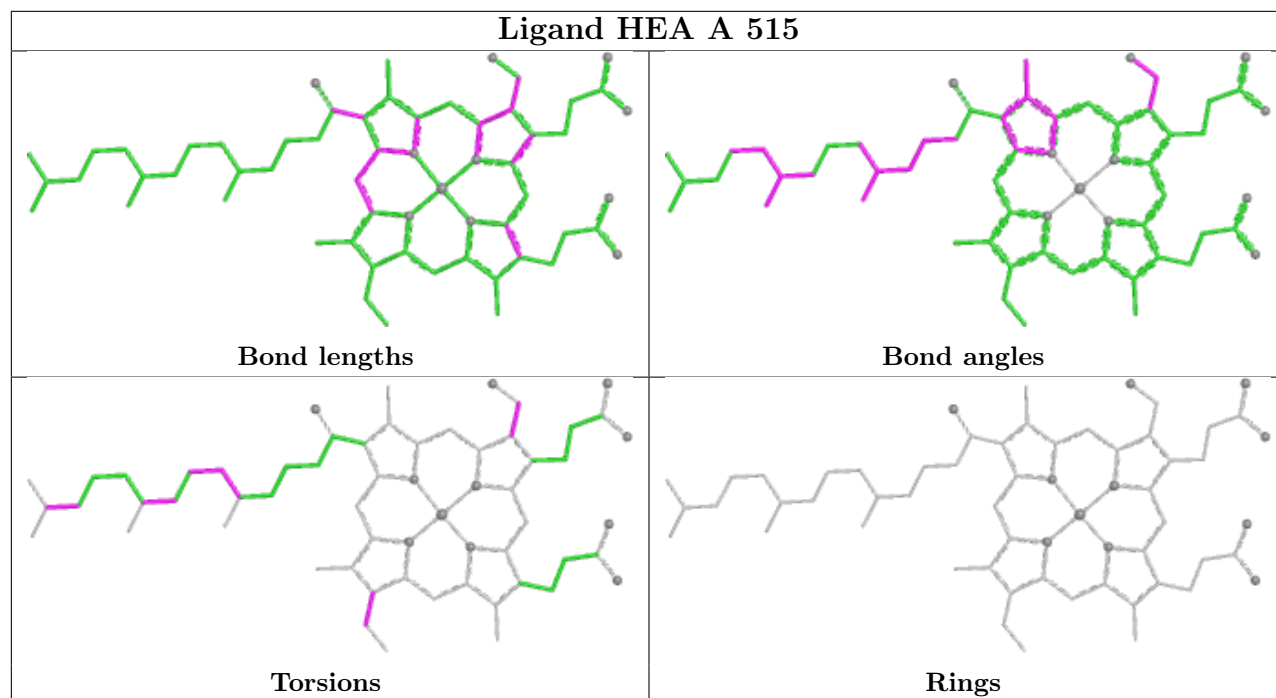
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	P	1267	PGV	10	0
25	C	265	PEK	11	0
25	T	263	PEK	11	0
26	G	269	CDL	23	0
19	A	525	PGV	4	0
25	C	264	PEK	9	0
17	N	516	HEA	6	0

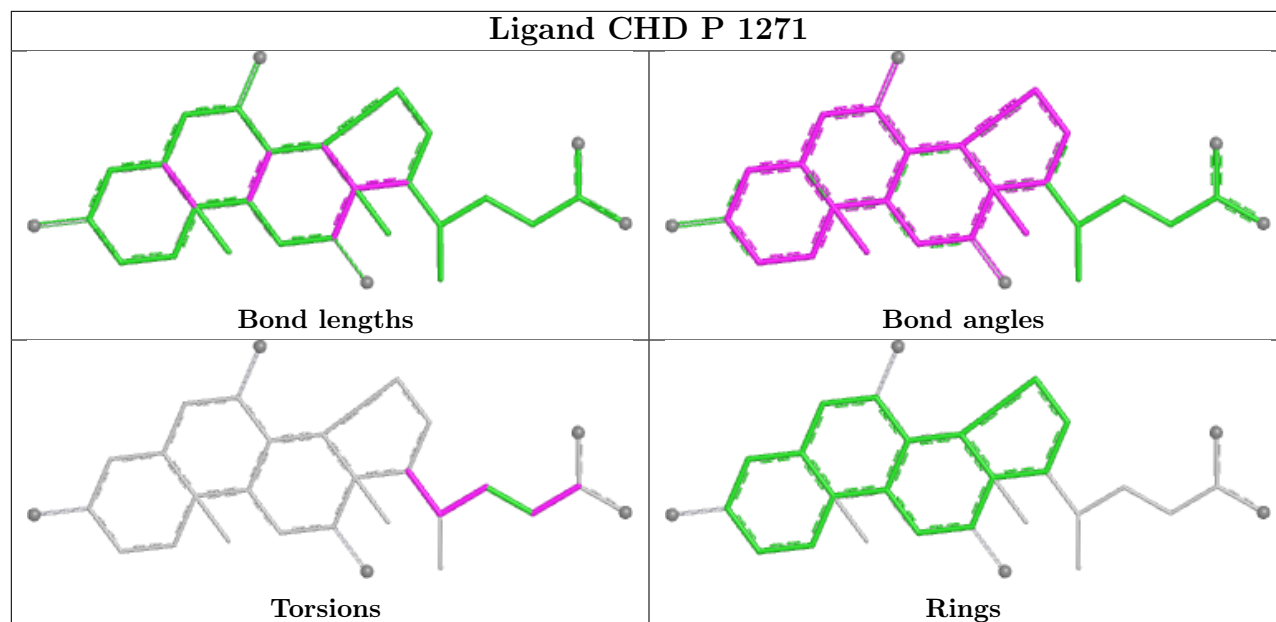
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



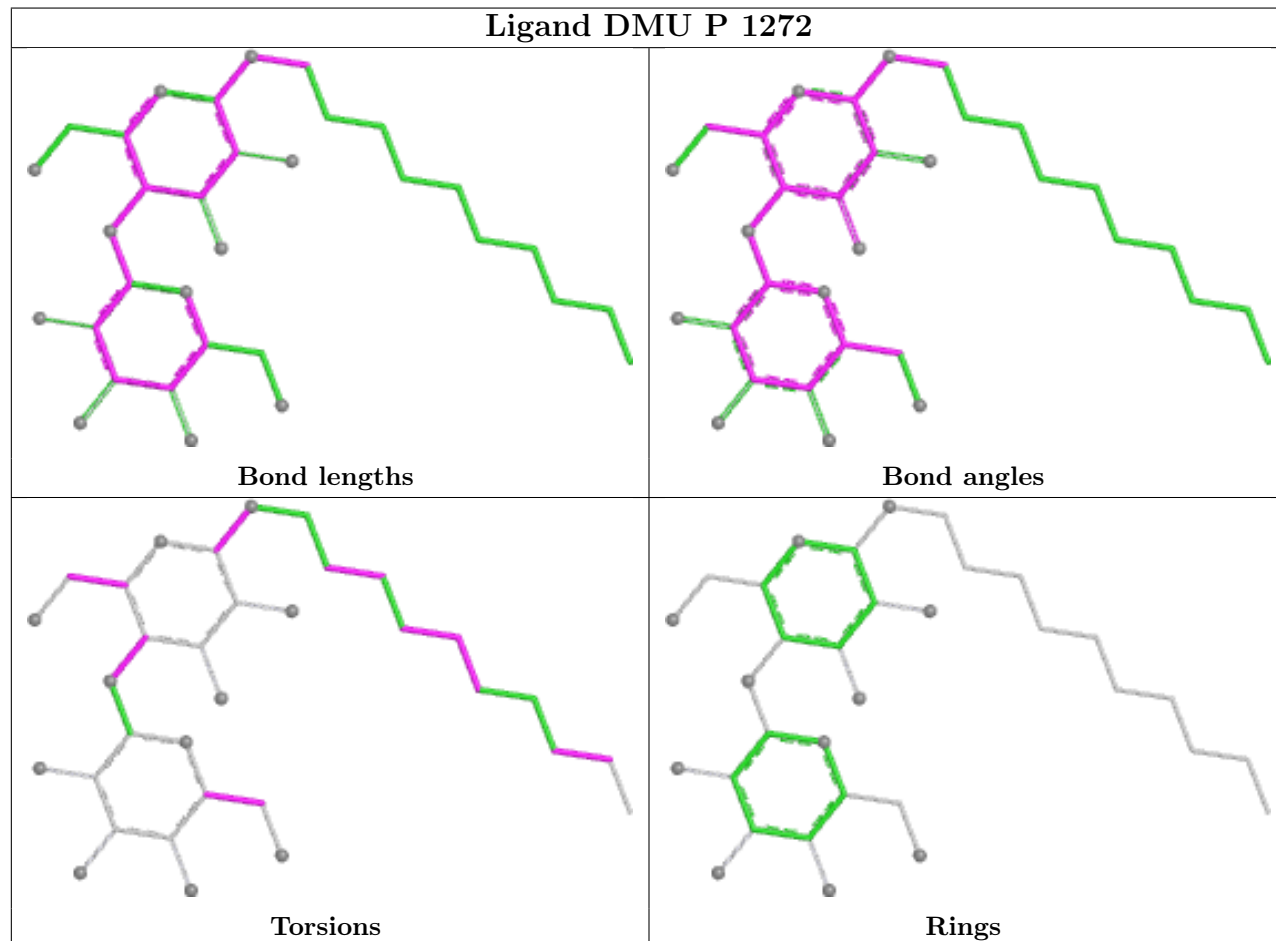


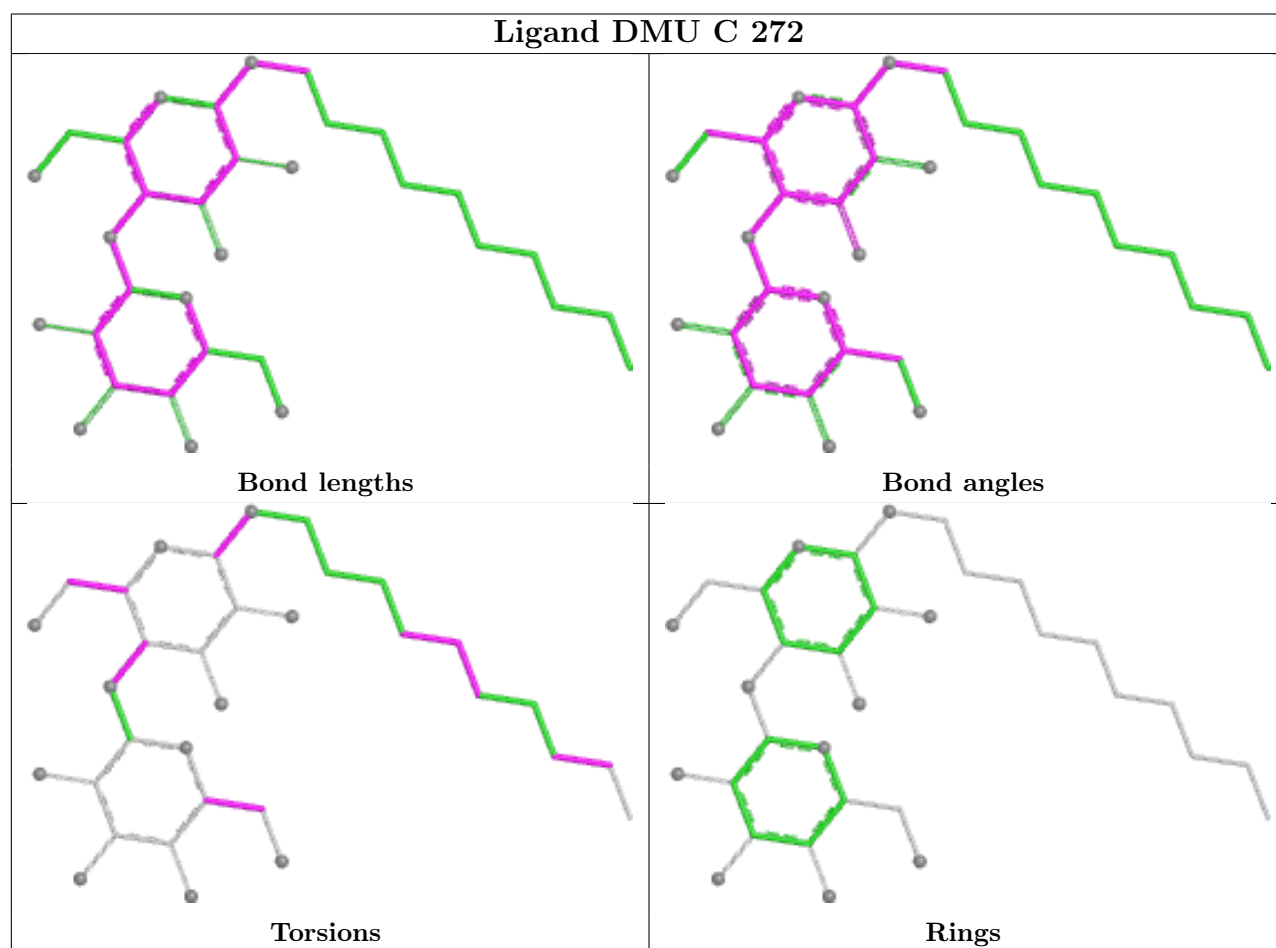
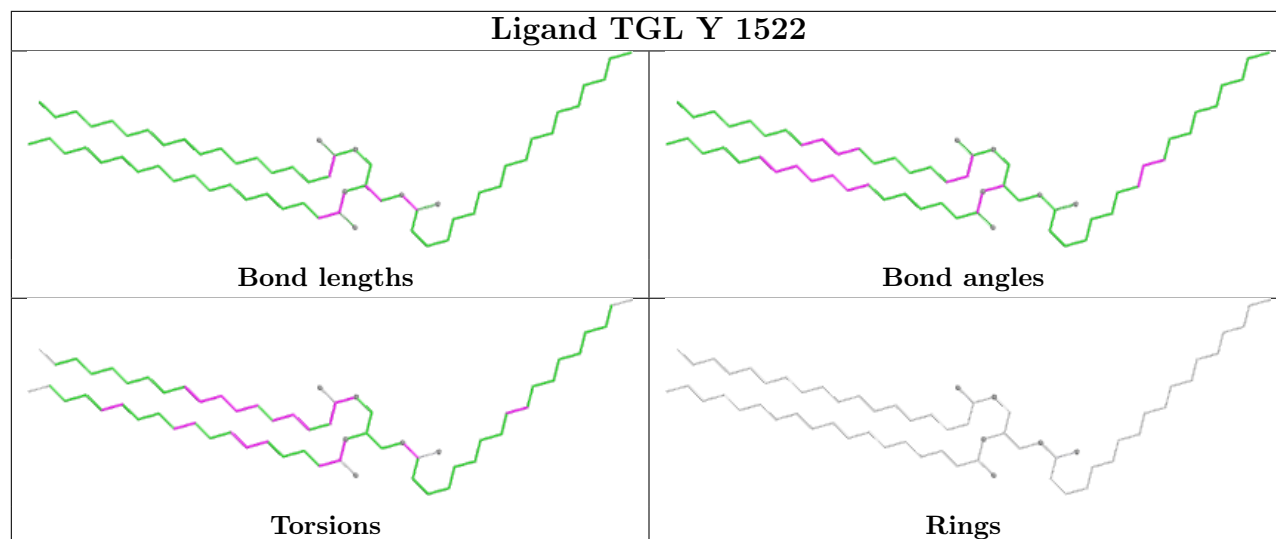


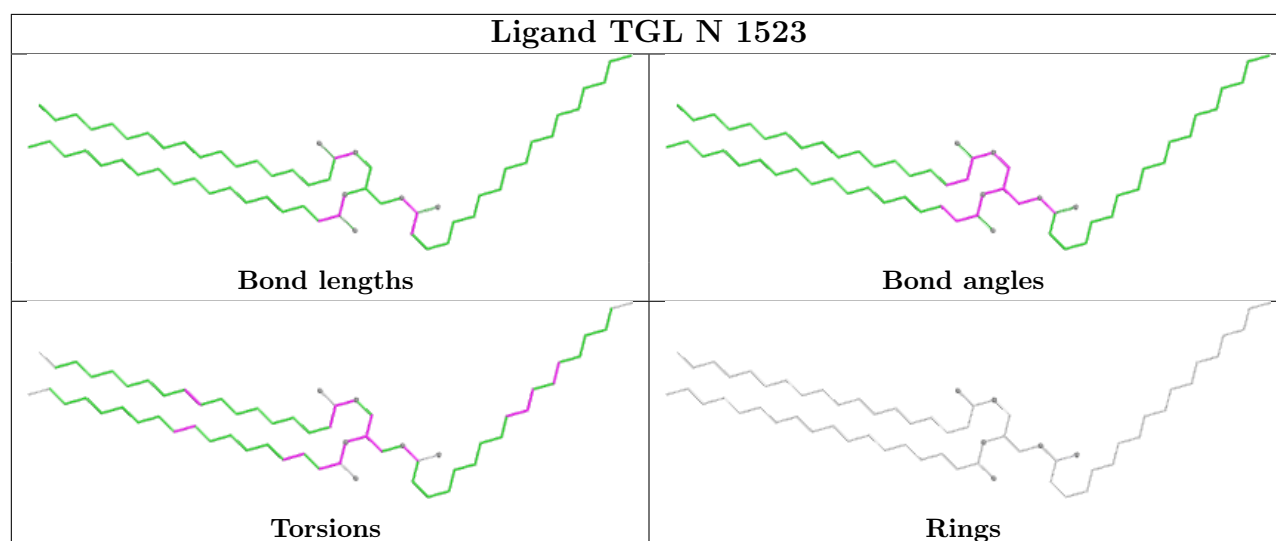
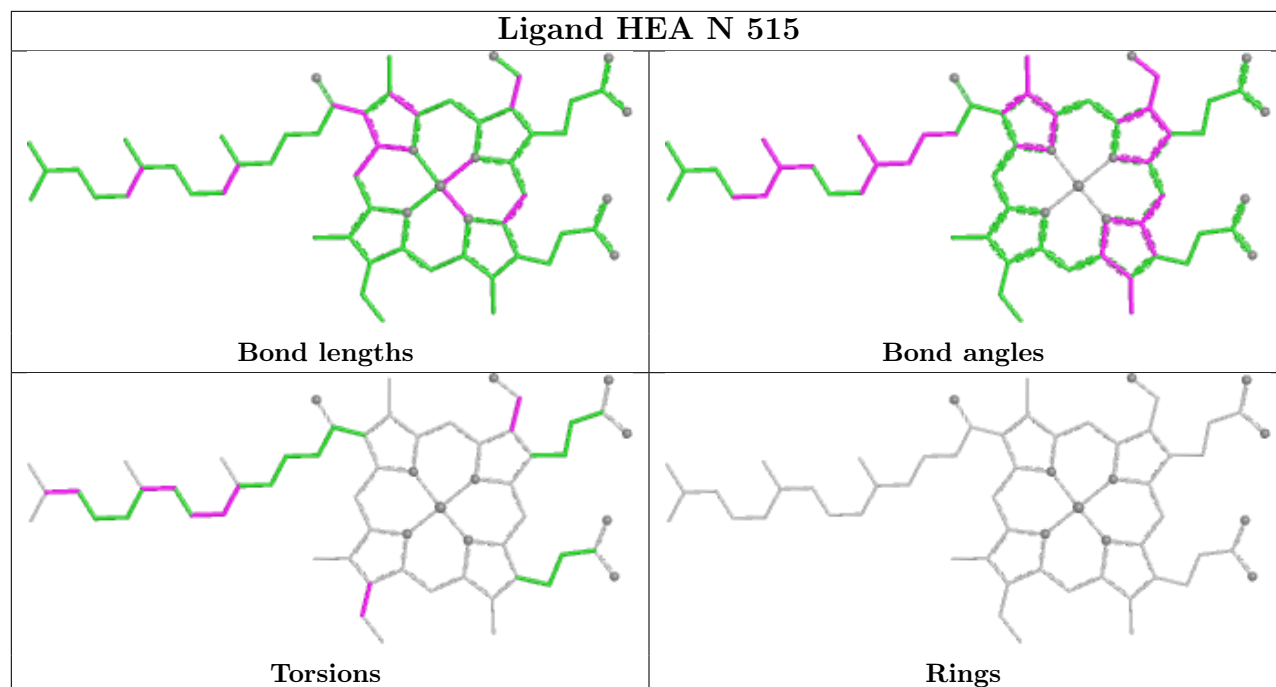
Ligand CHD P 1271



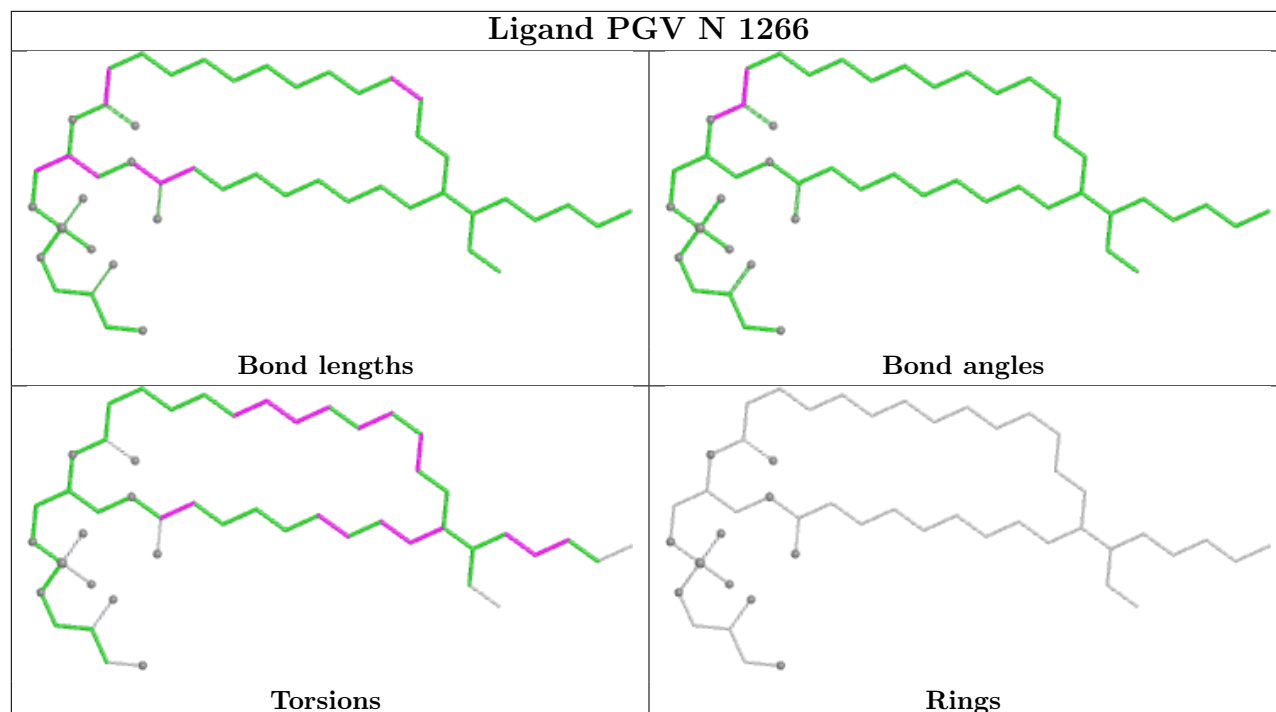
Ligand DMU P 1272



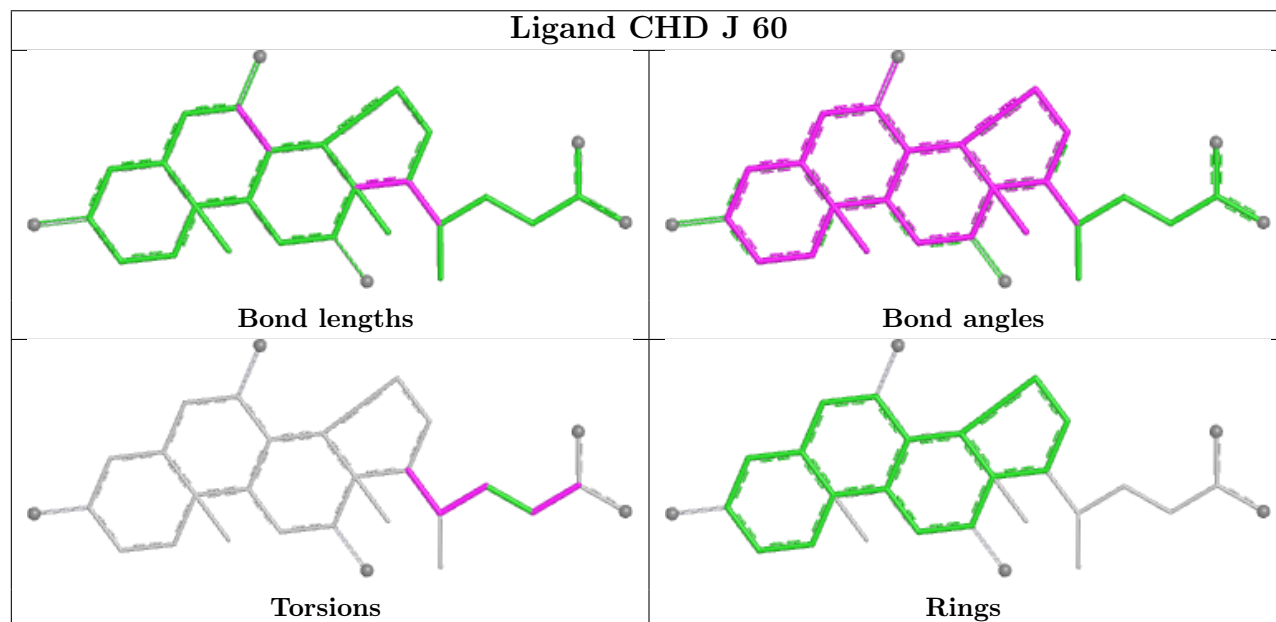




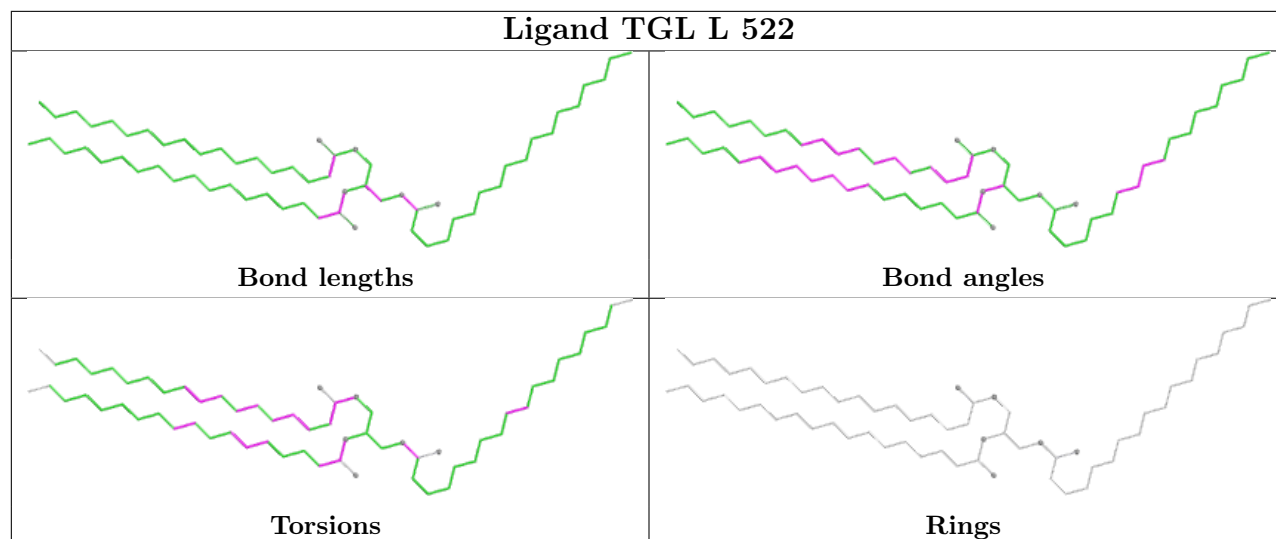
Ligand PGV N 1266



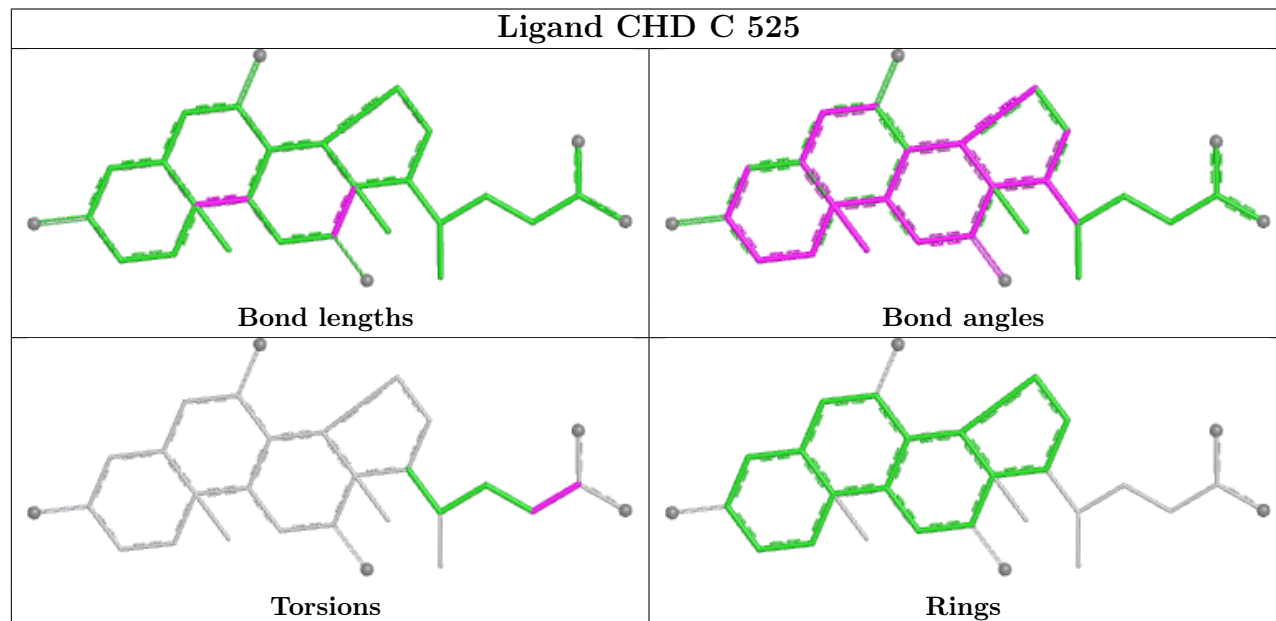
Ligand CHD J 60

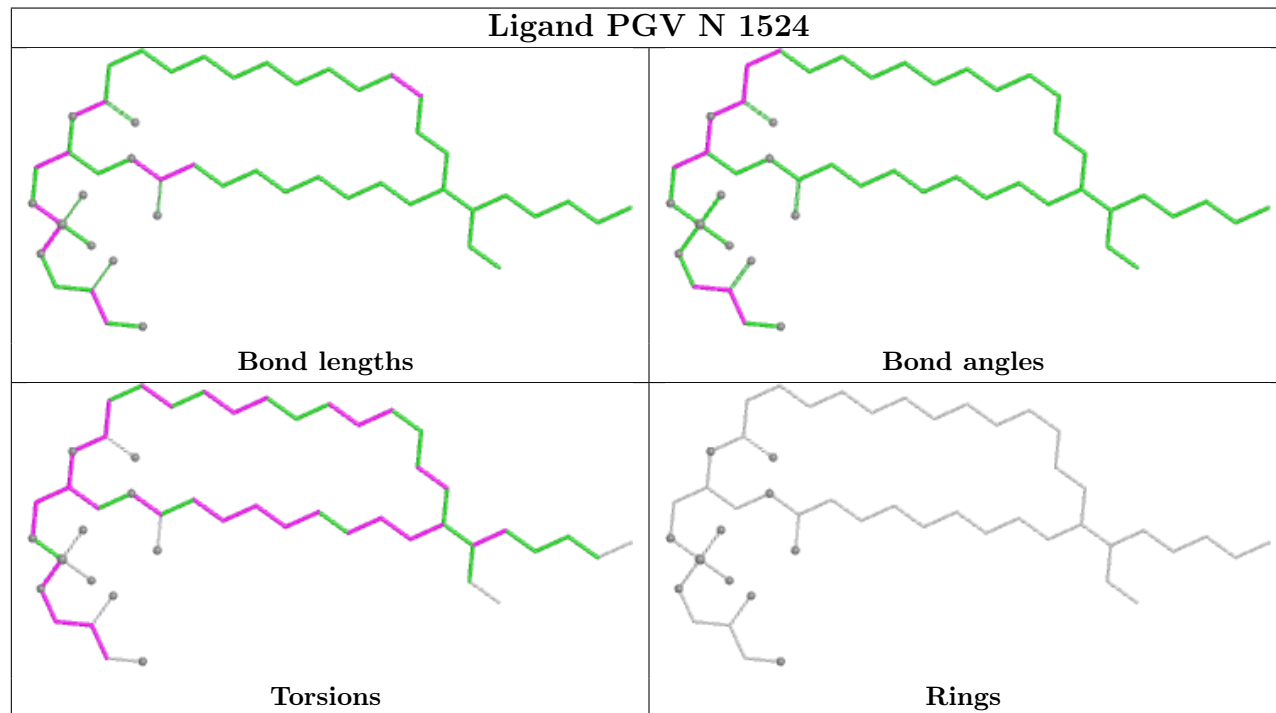
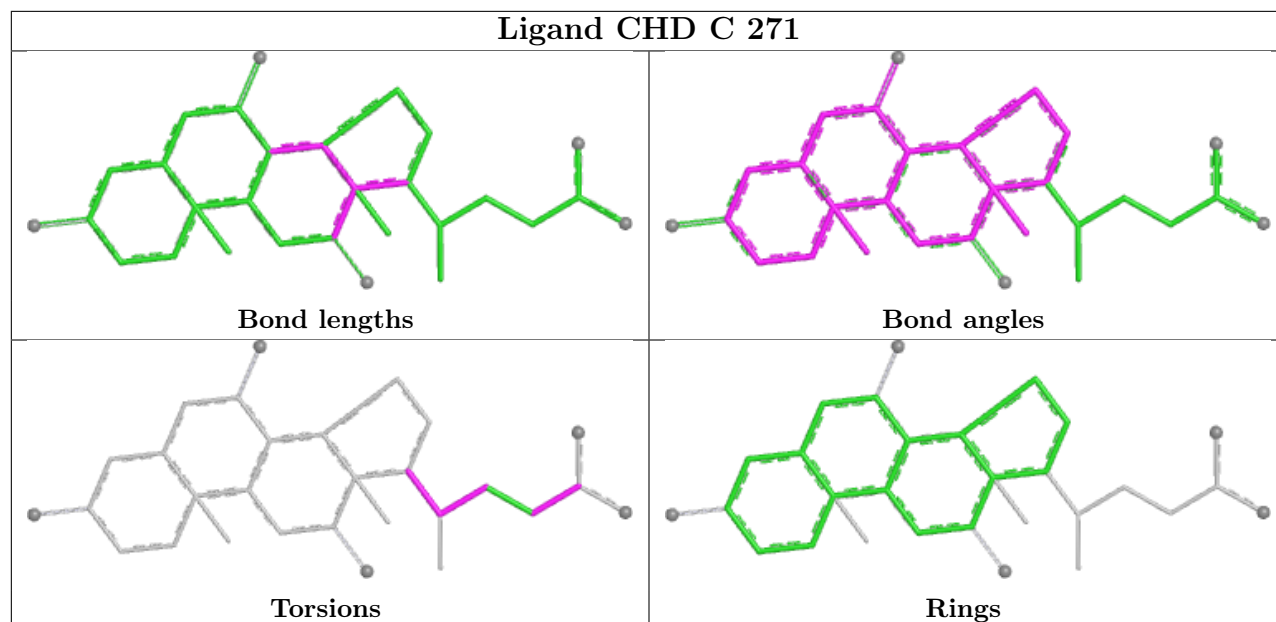


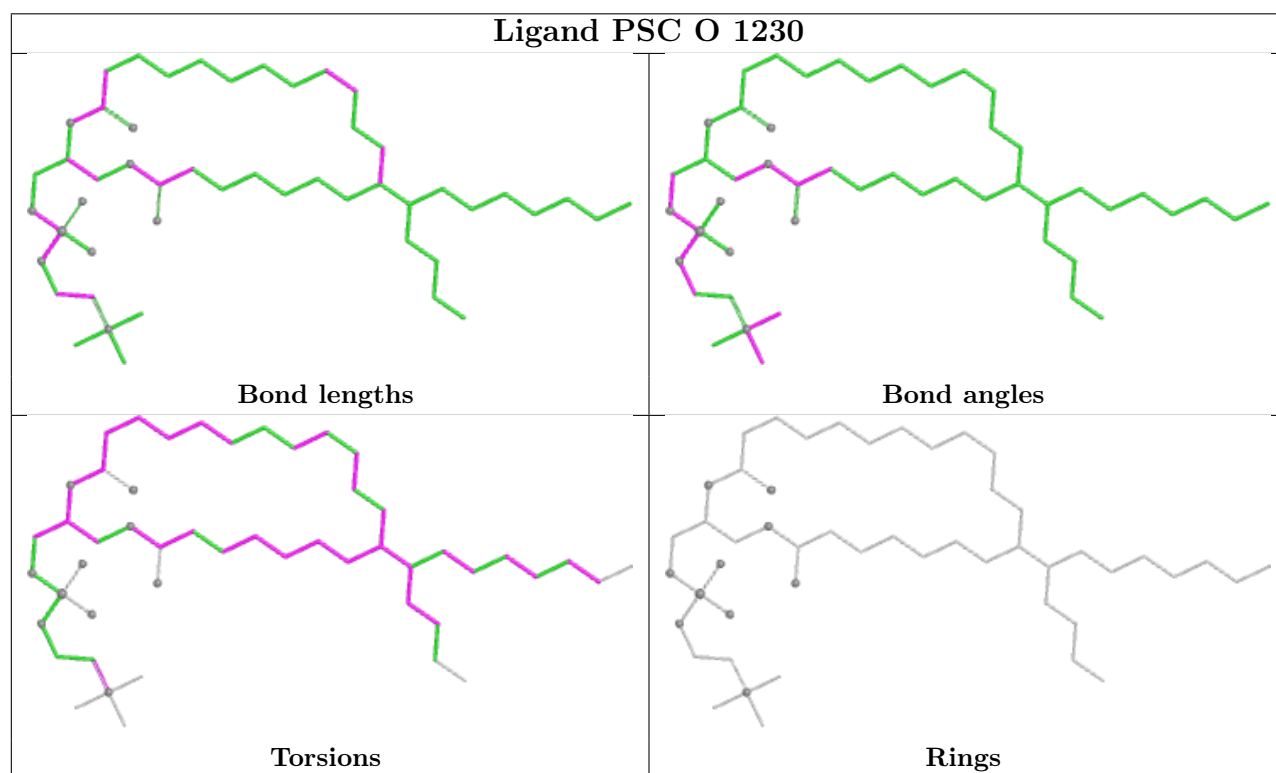
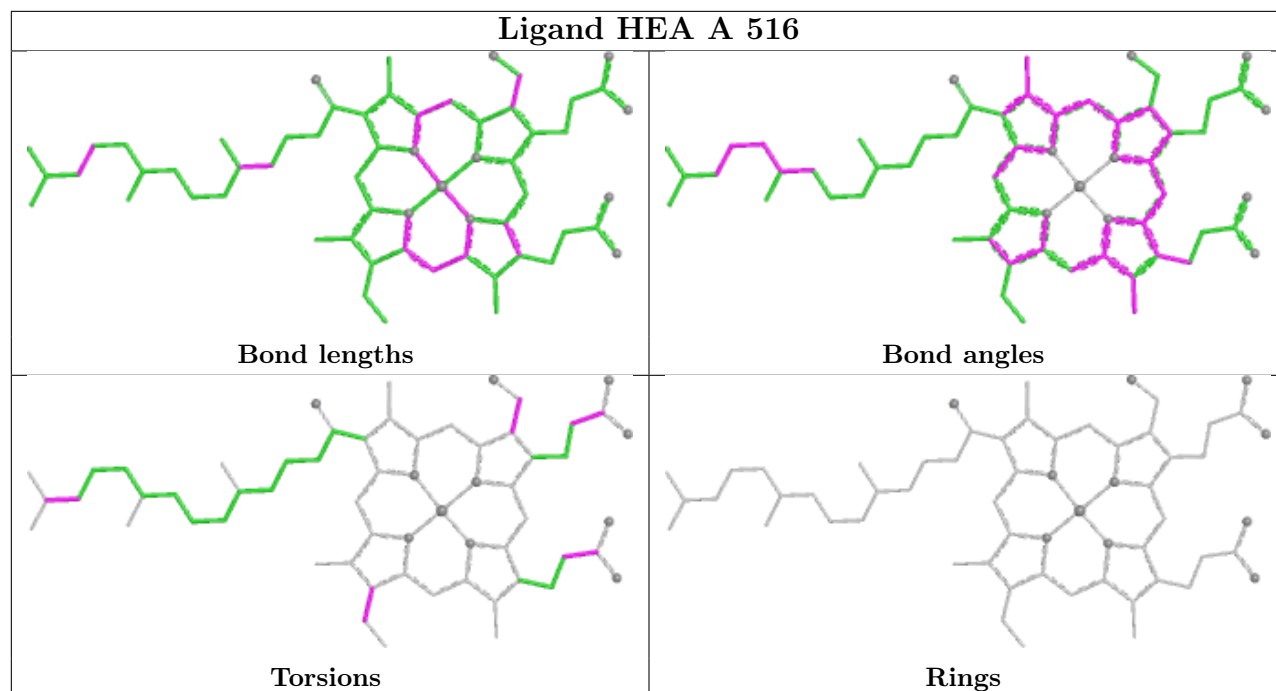
Ligand TGL L 522

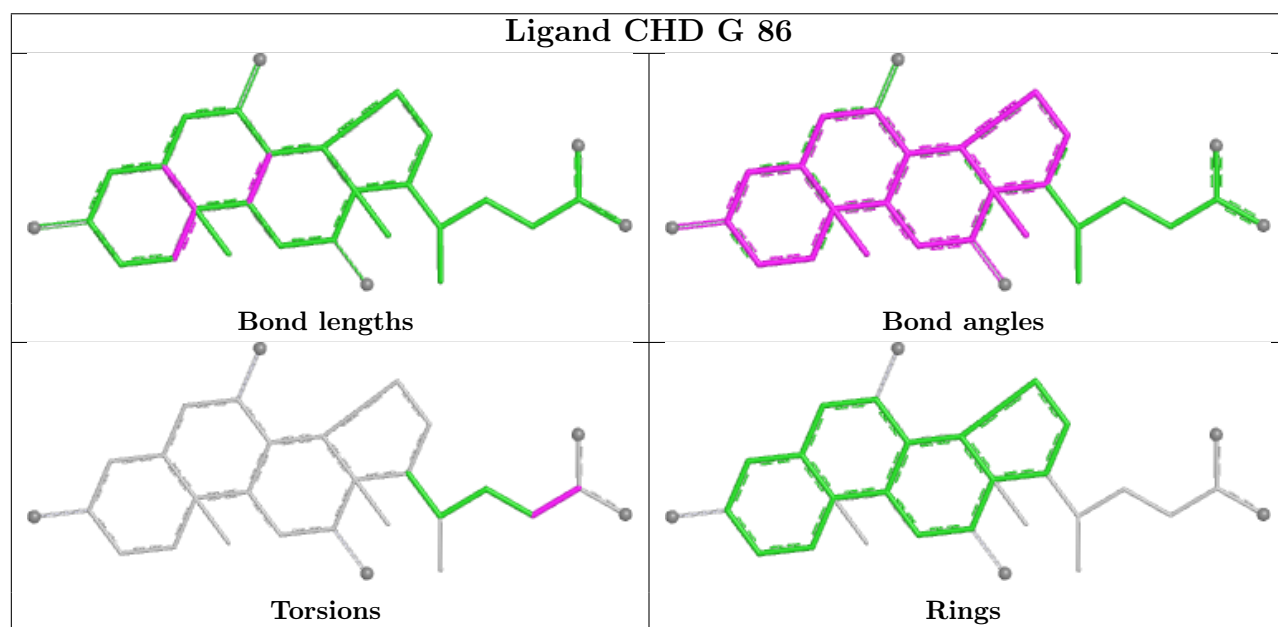
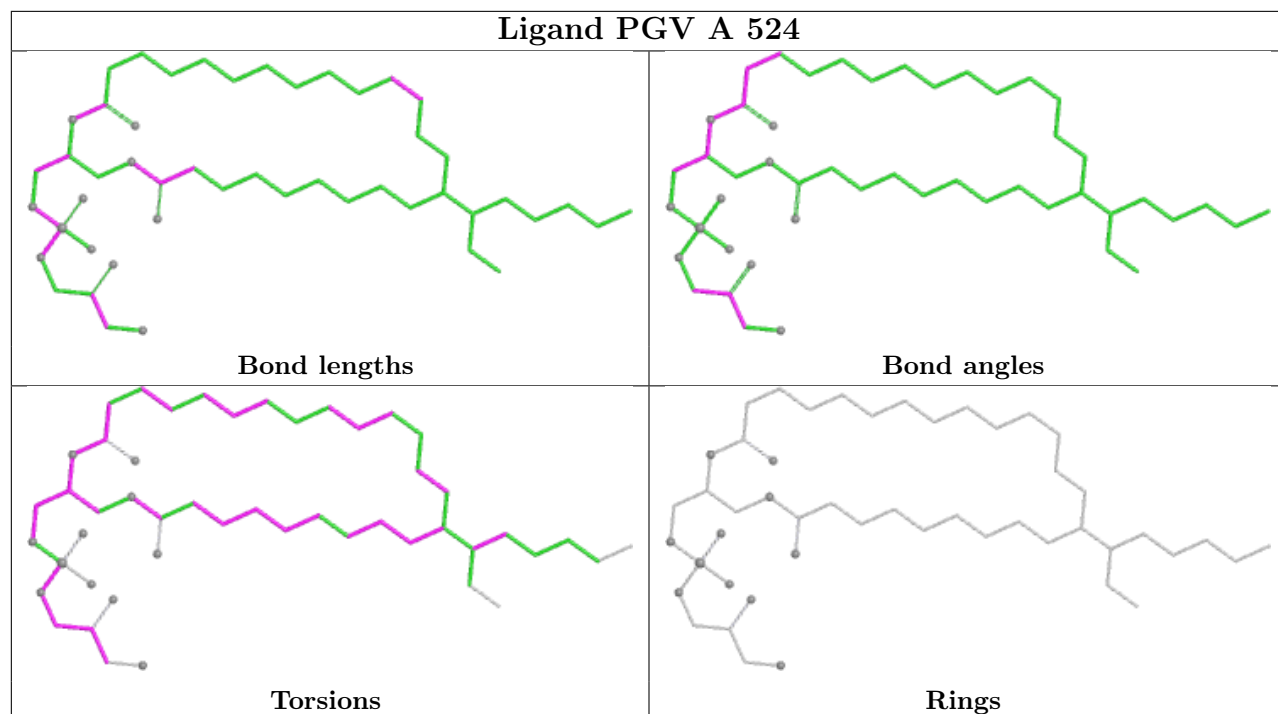


Ligand CHD C 525

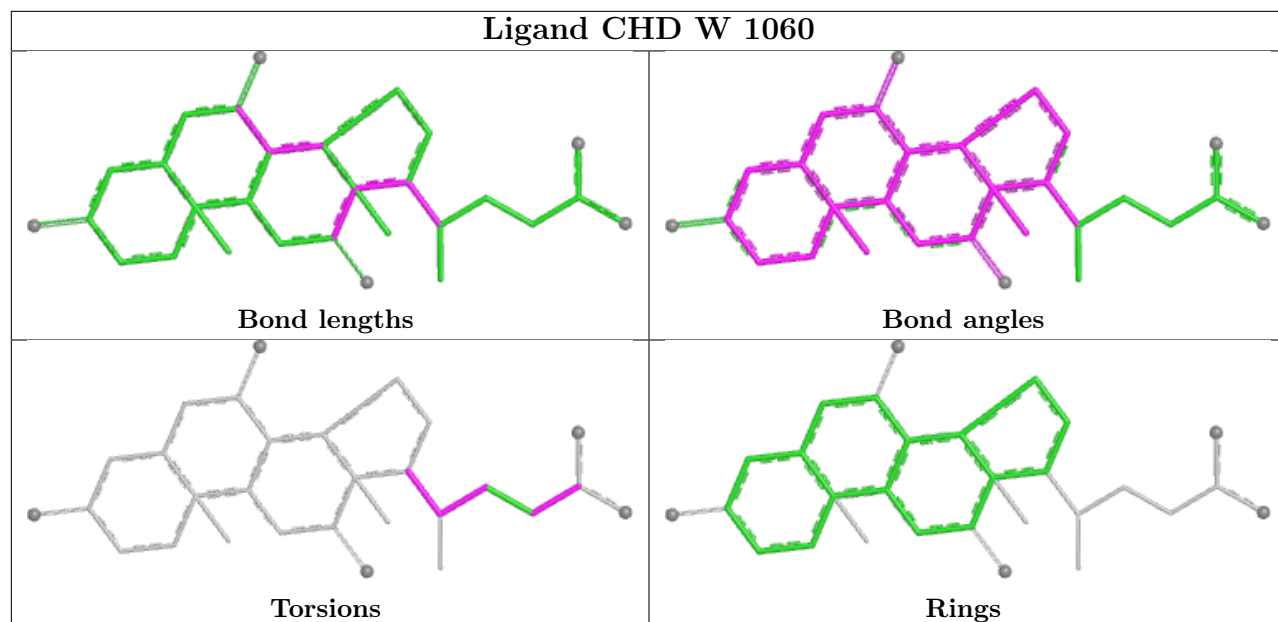




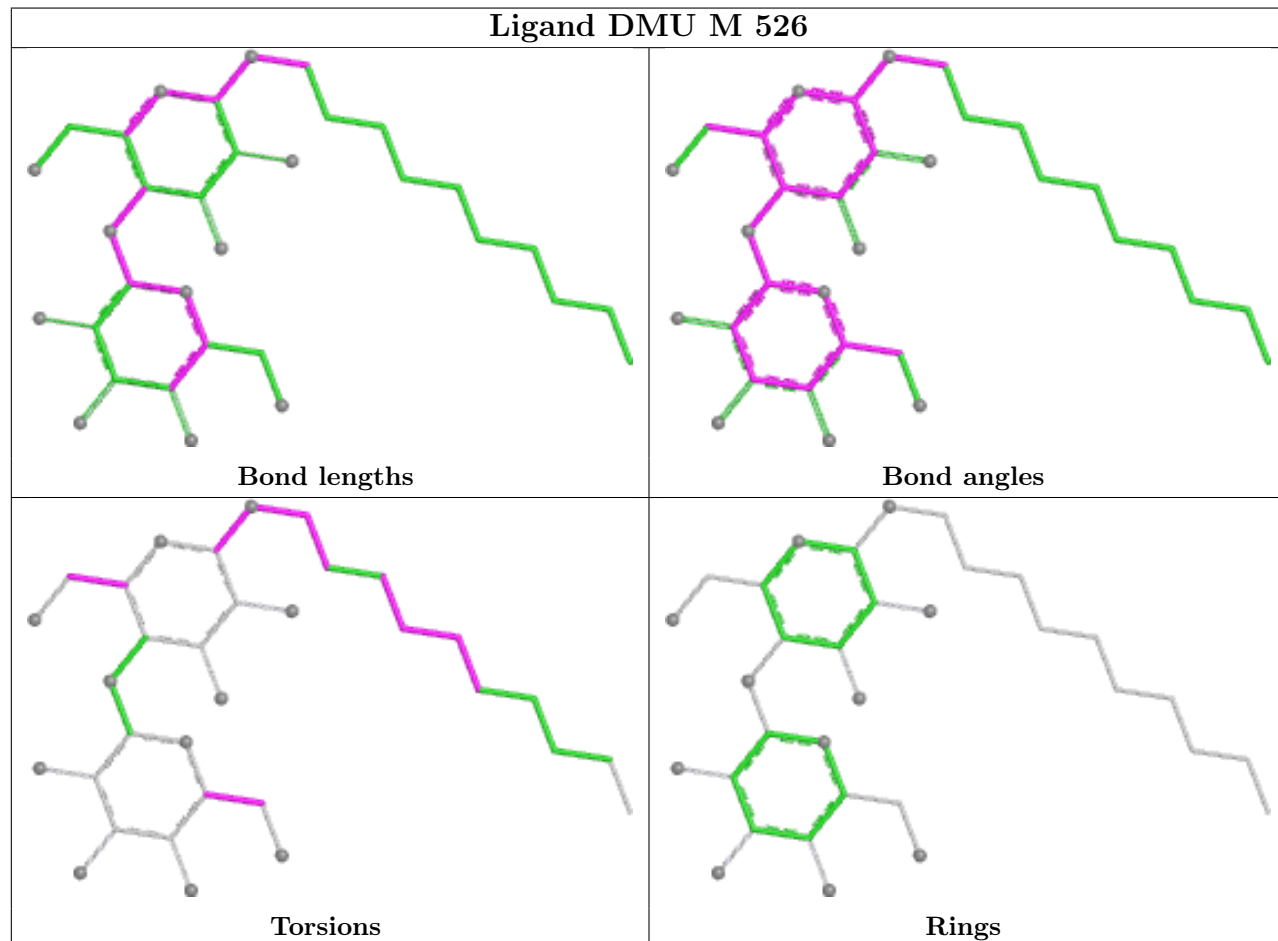


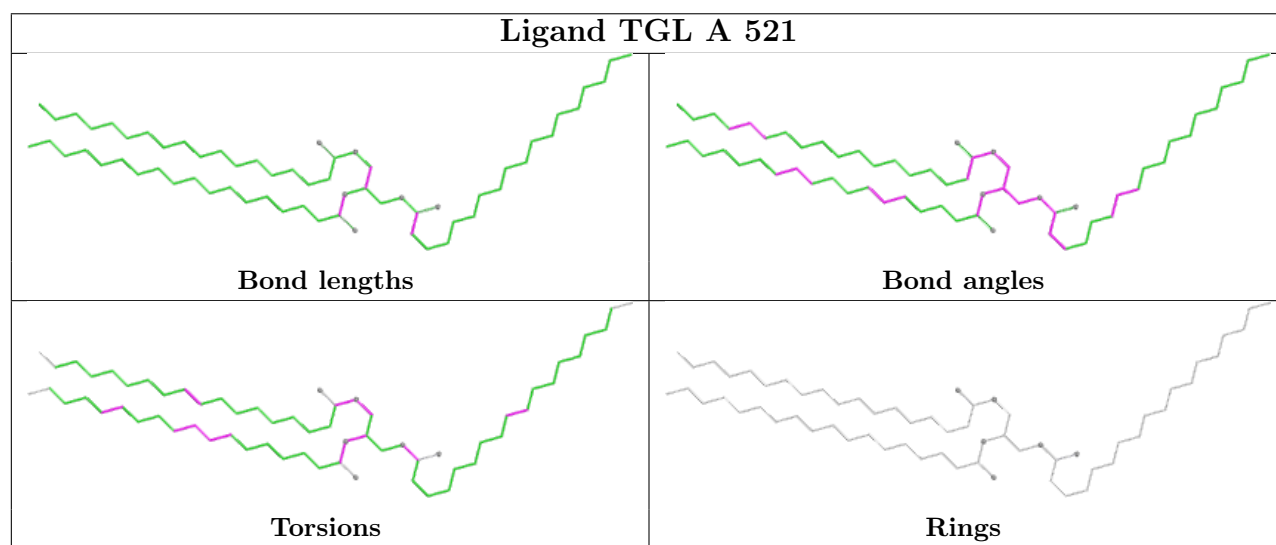
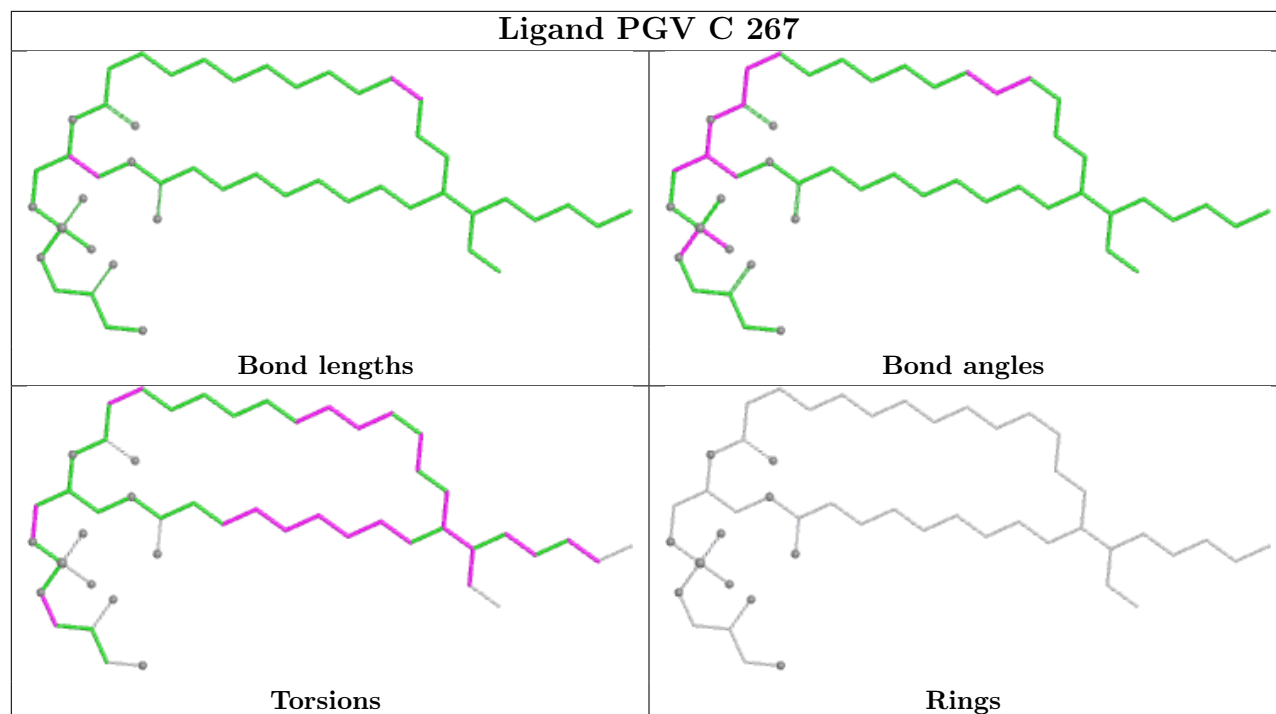


Ligand CHD W 1060

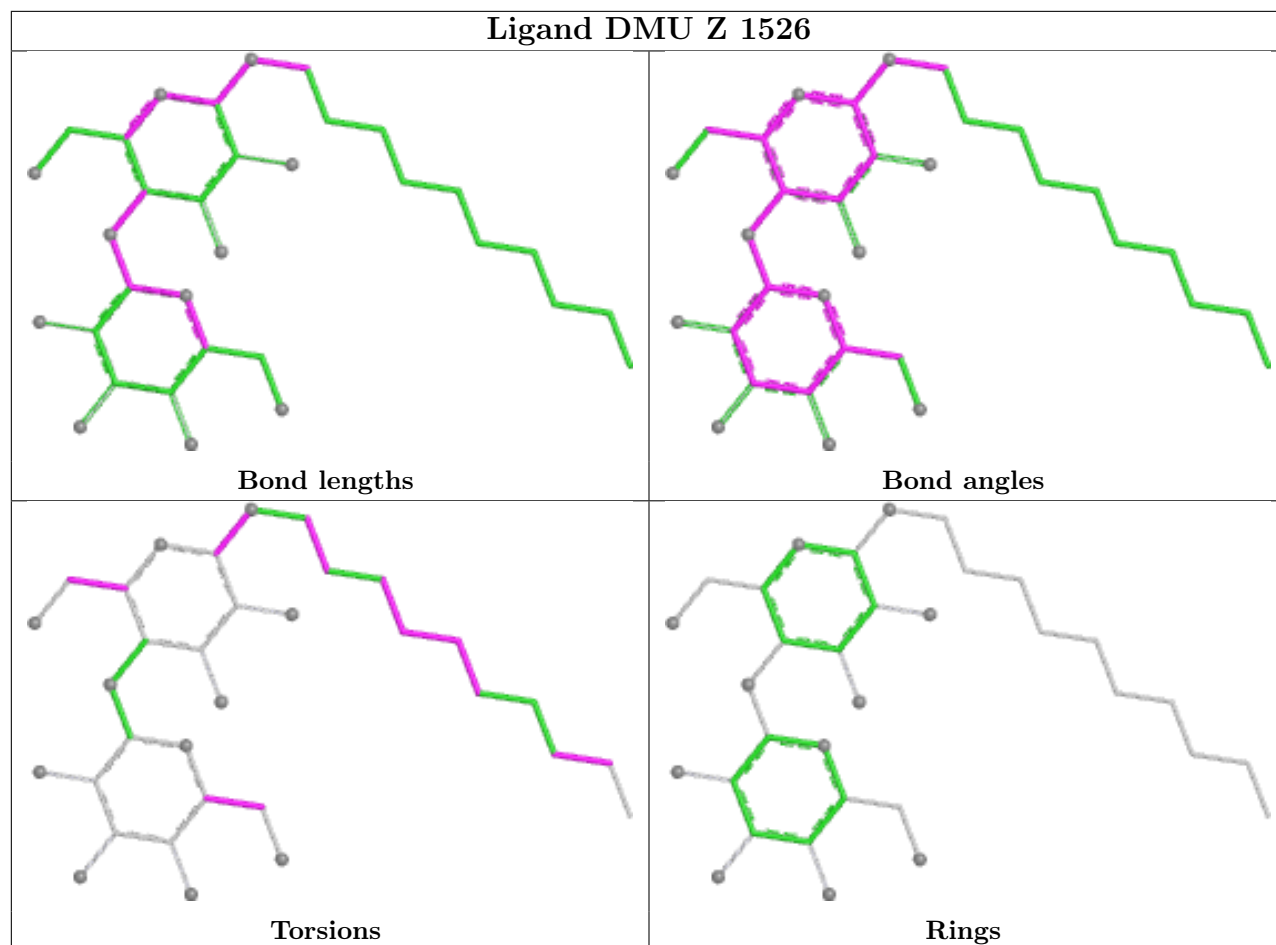


Ligand DMU M 526

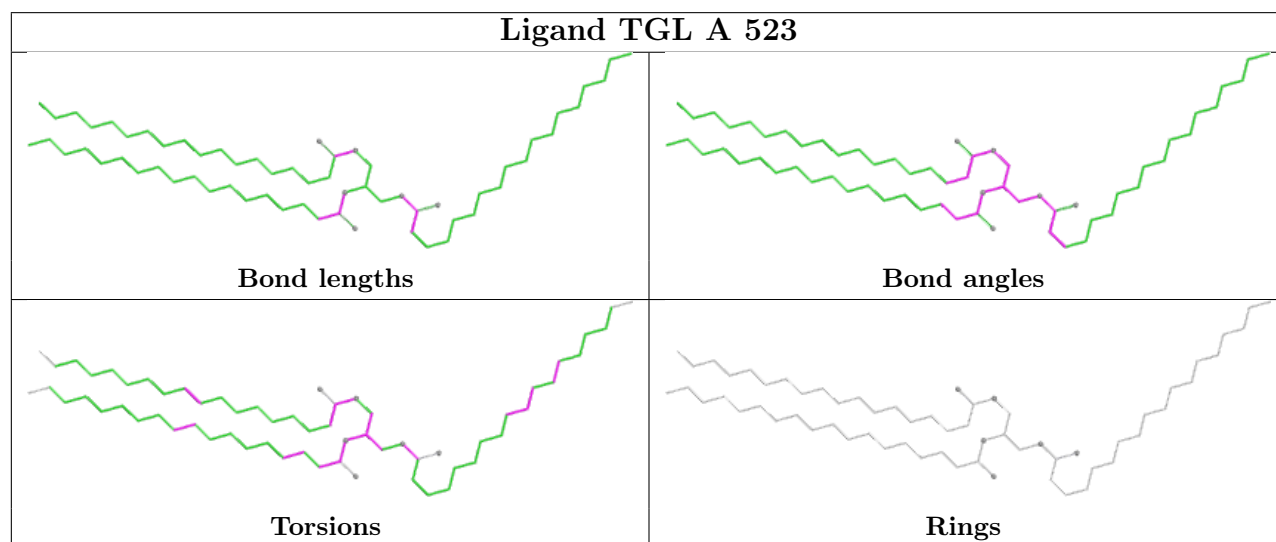




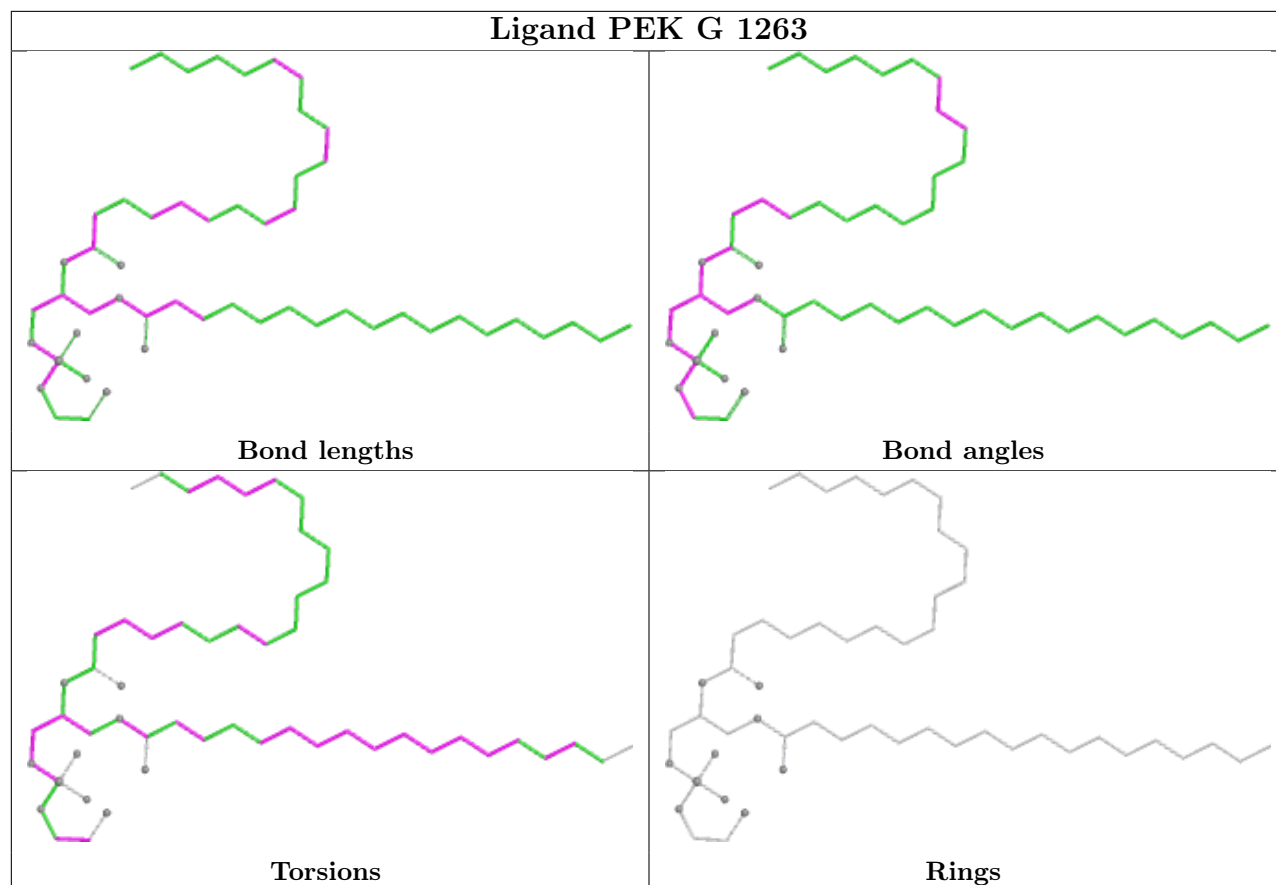
Ligand DMU Z 1526



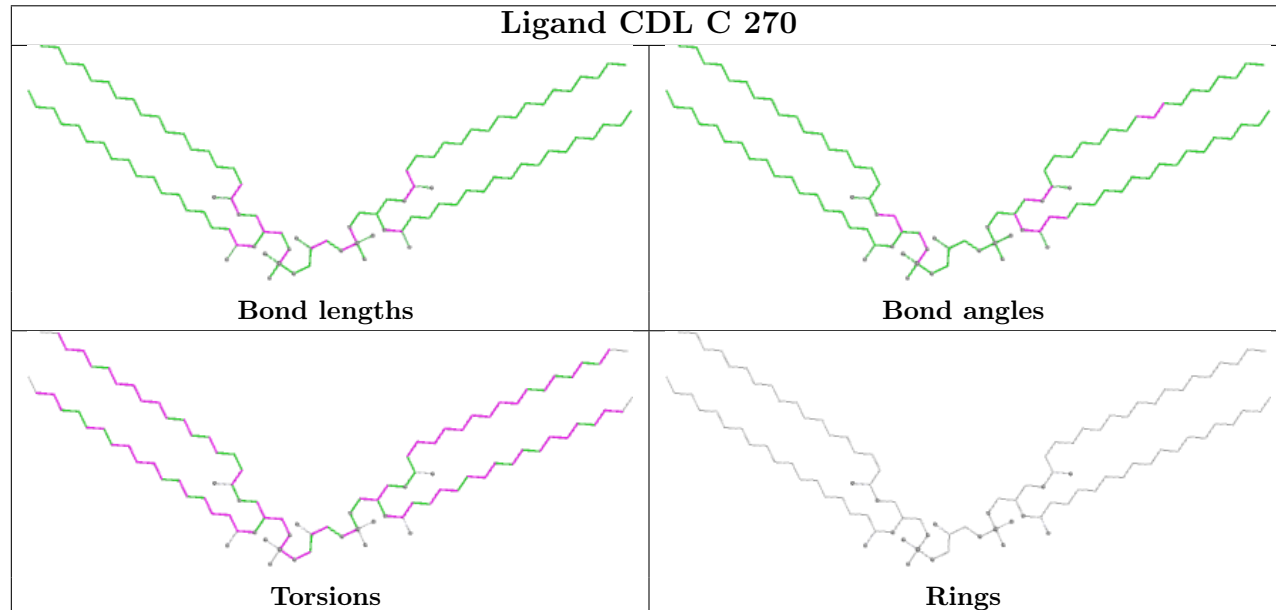
Ligand TGL A 523

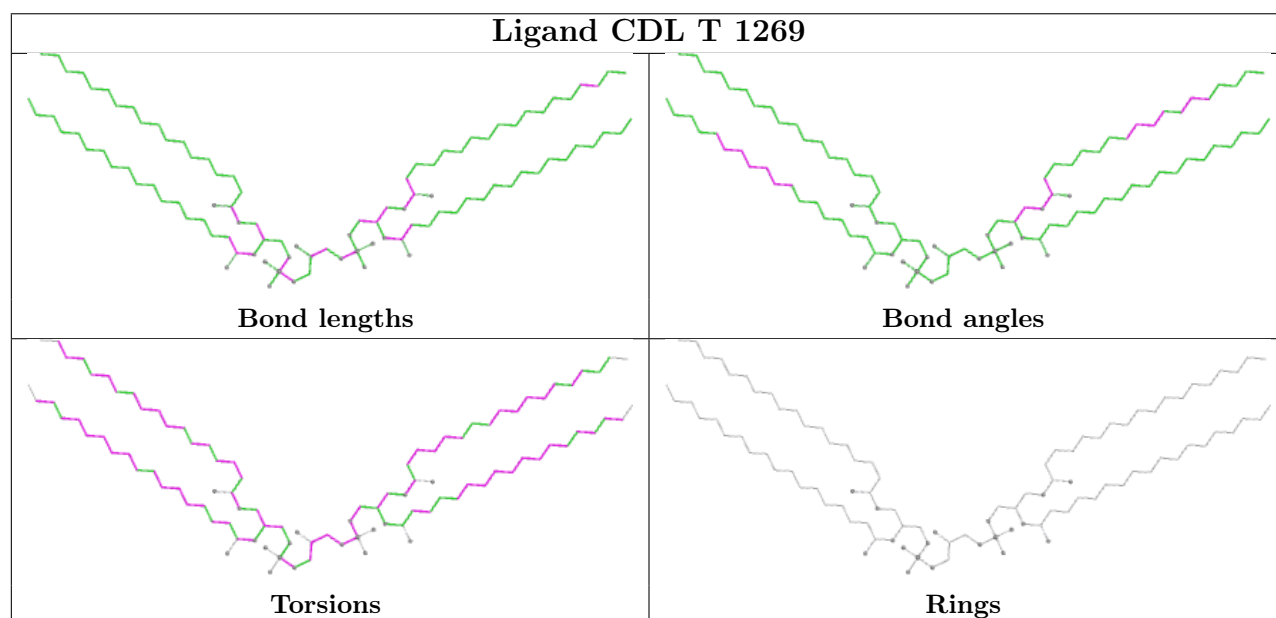
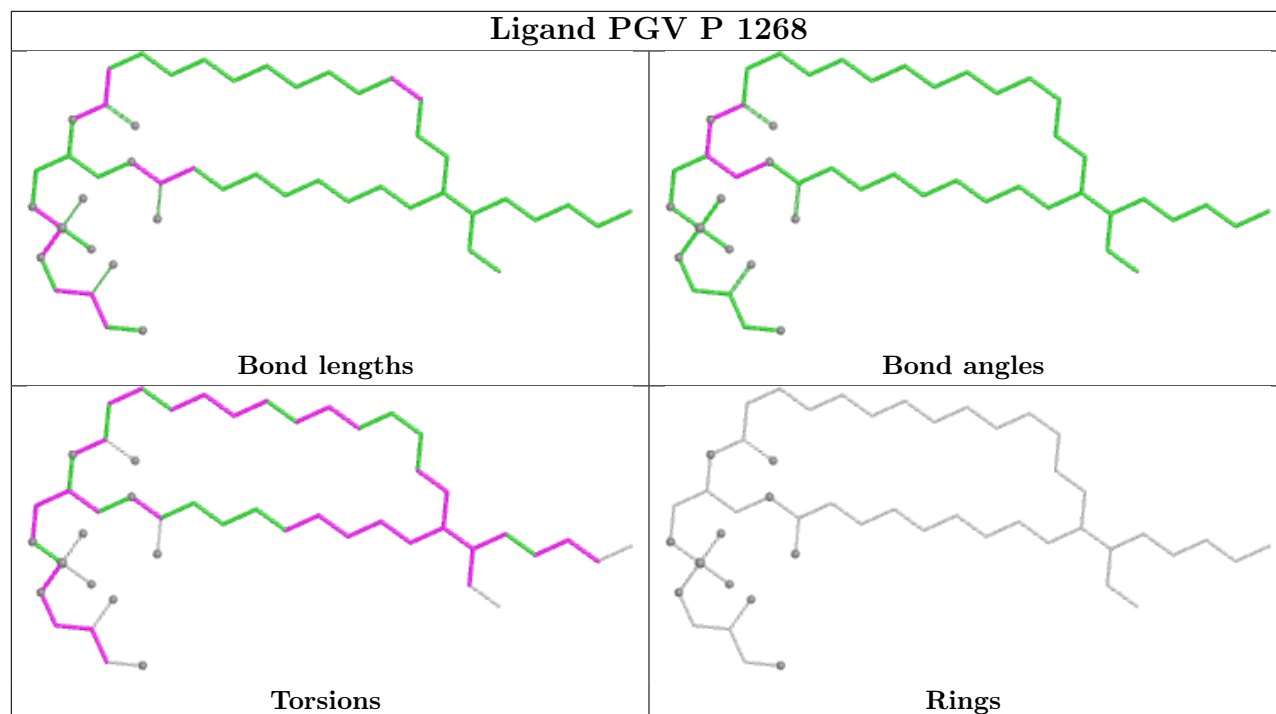


Ligand PEK G 1263

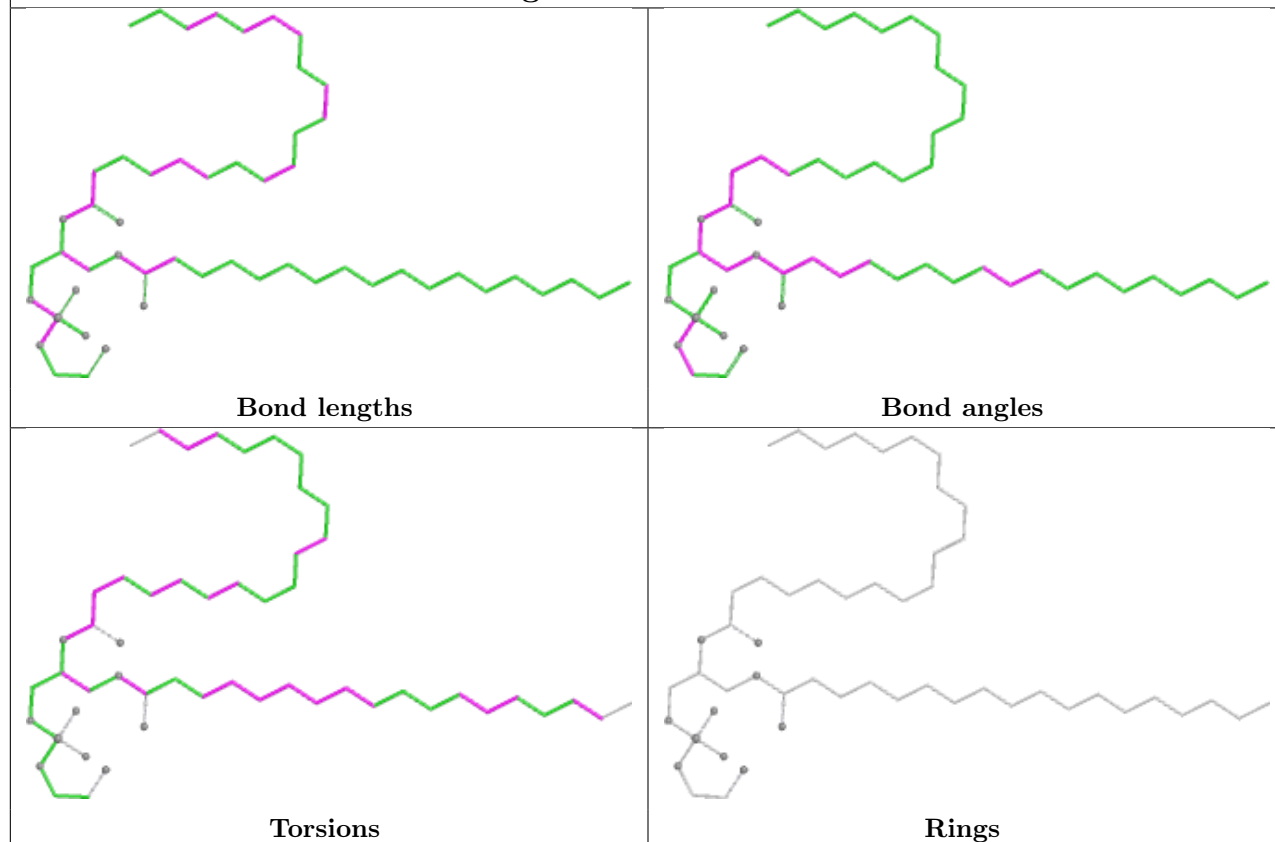


Ligand CDL C 270

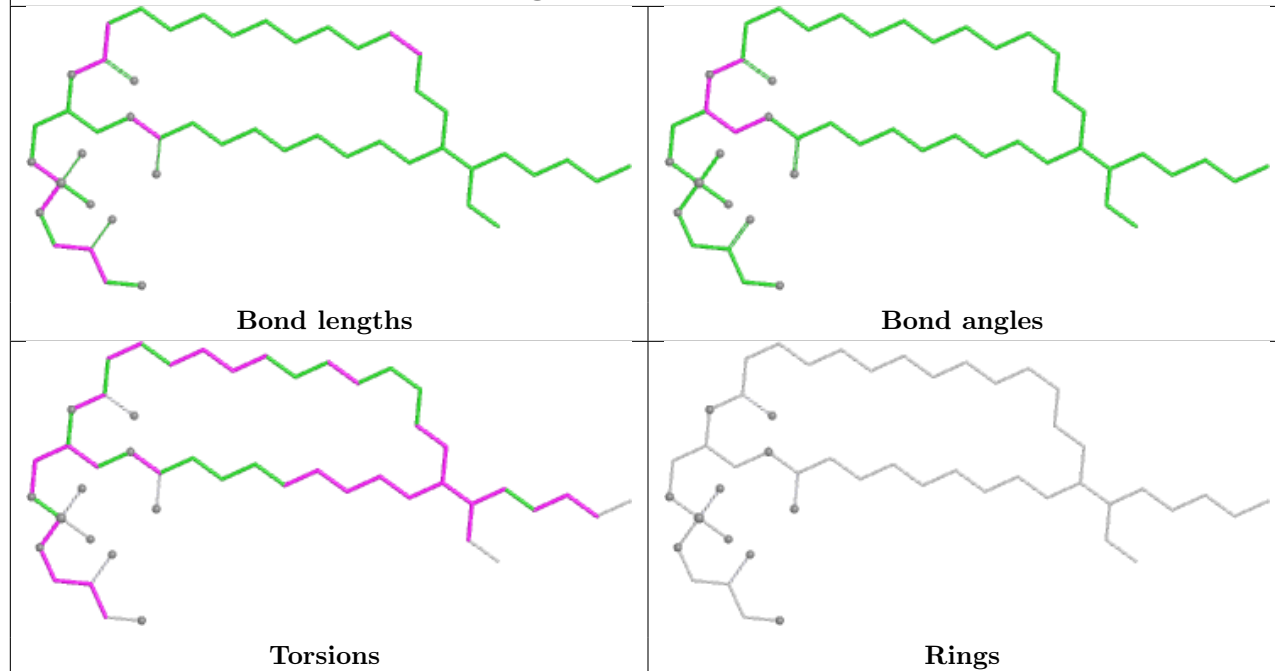




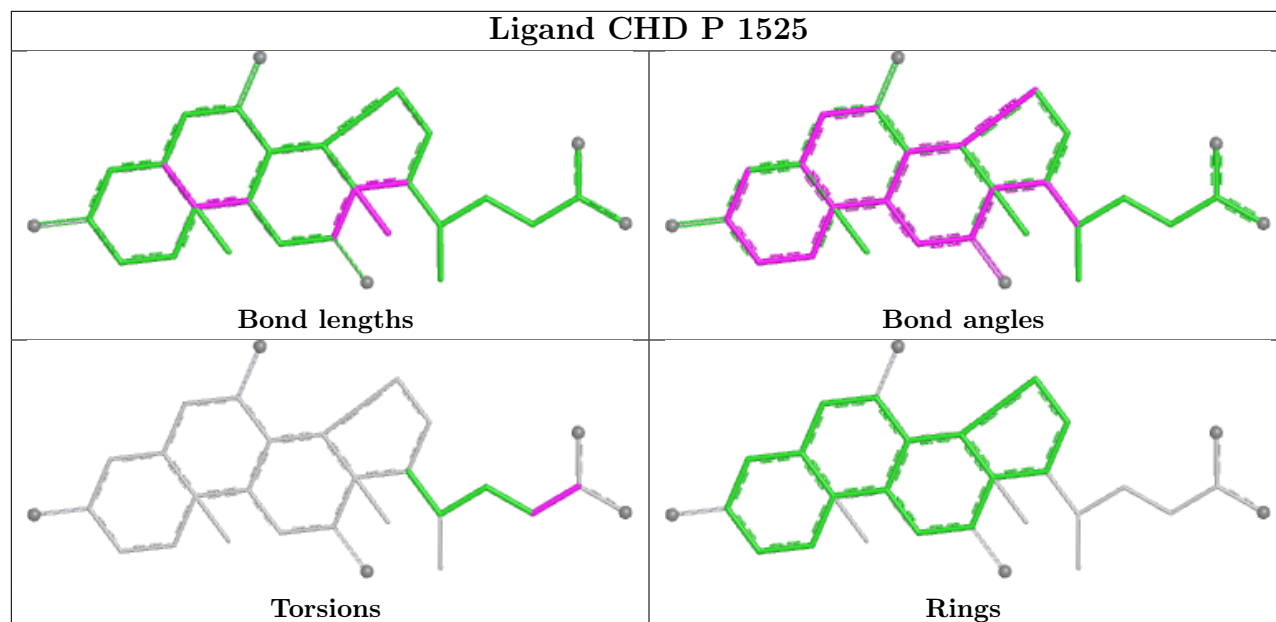
Ligand PEK T 1264



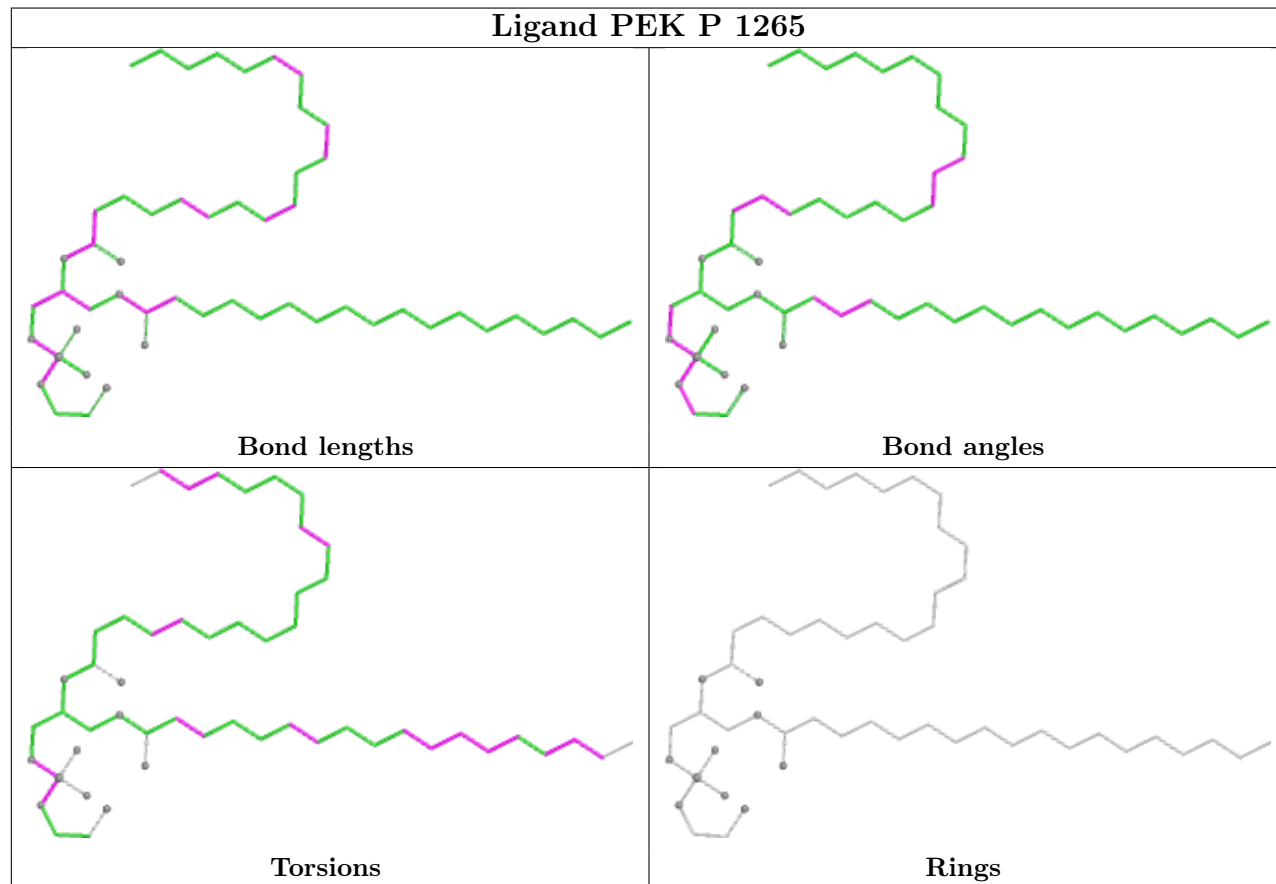
Ligand PGV C 268

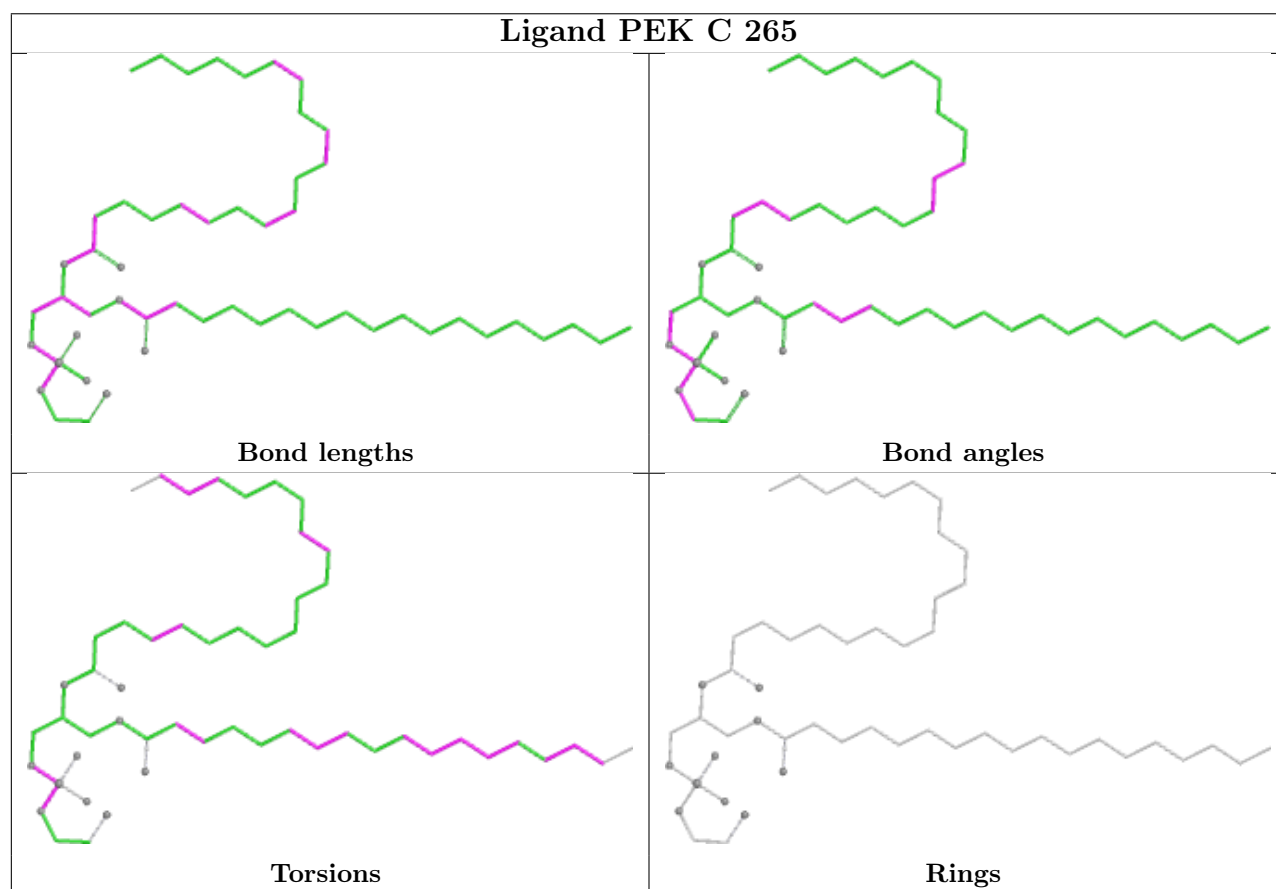
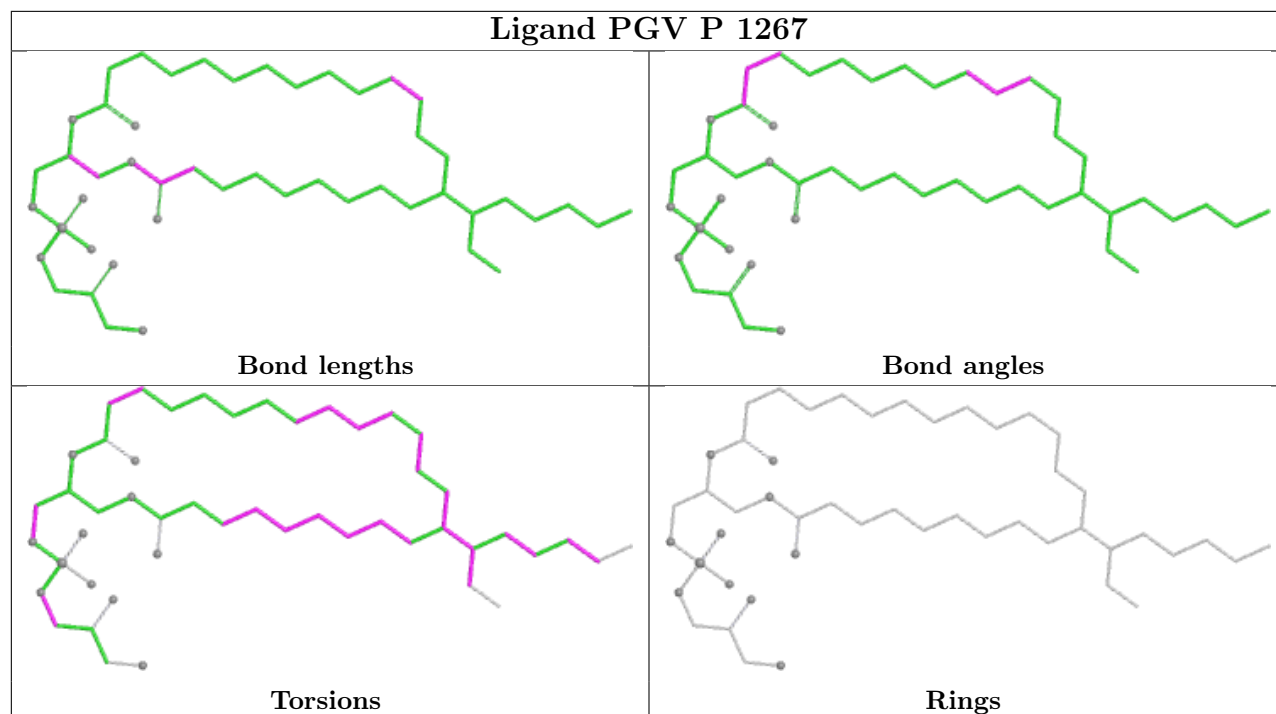


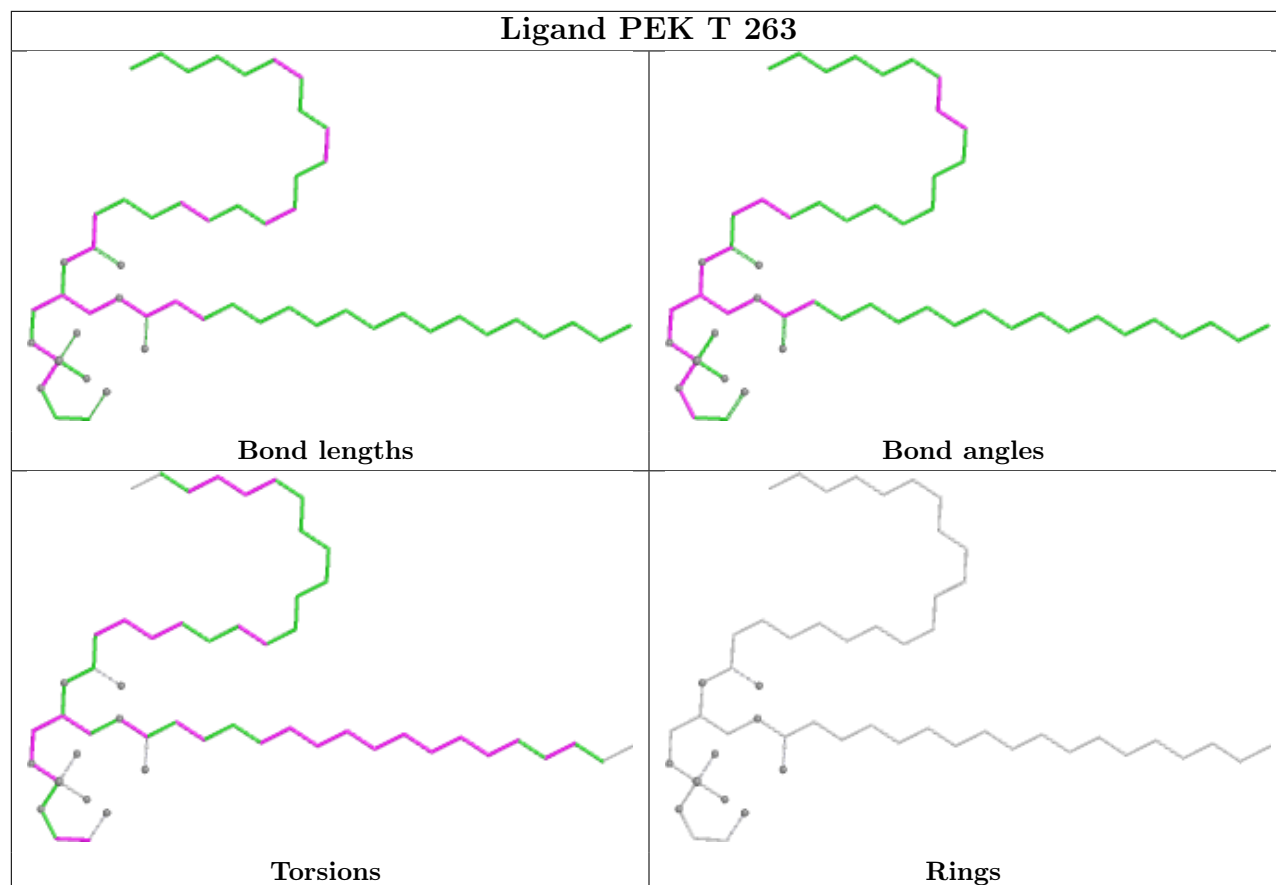
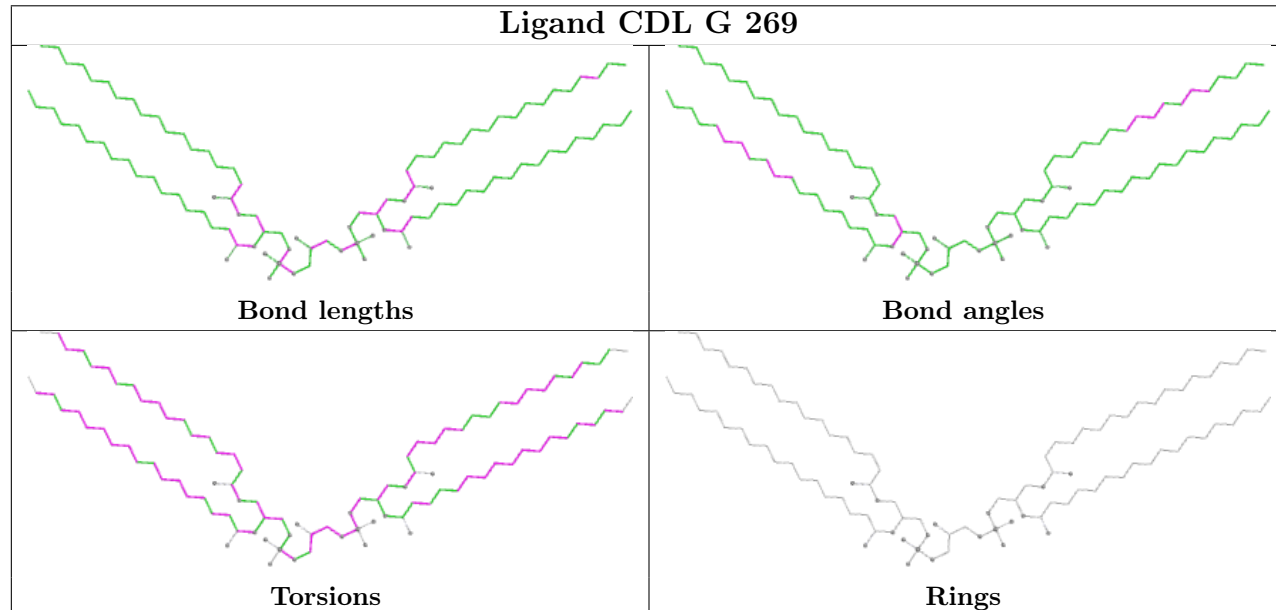
Ligand CHD P 1525

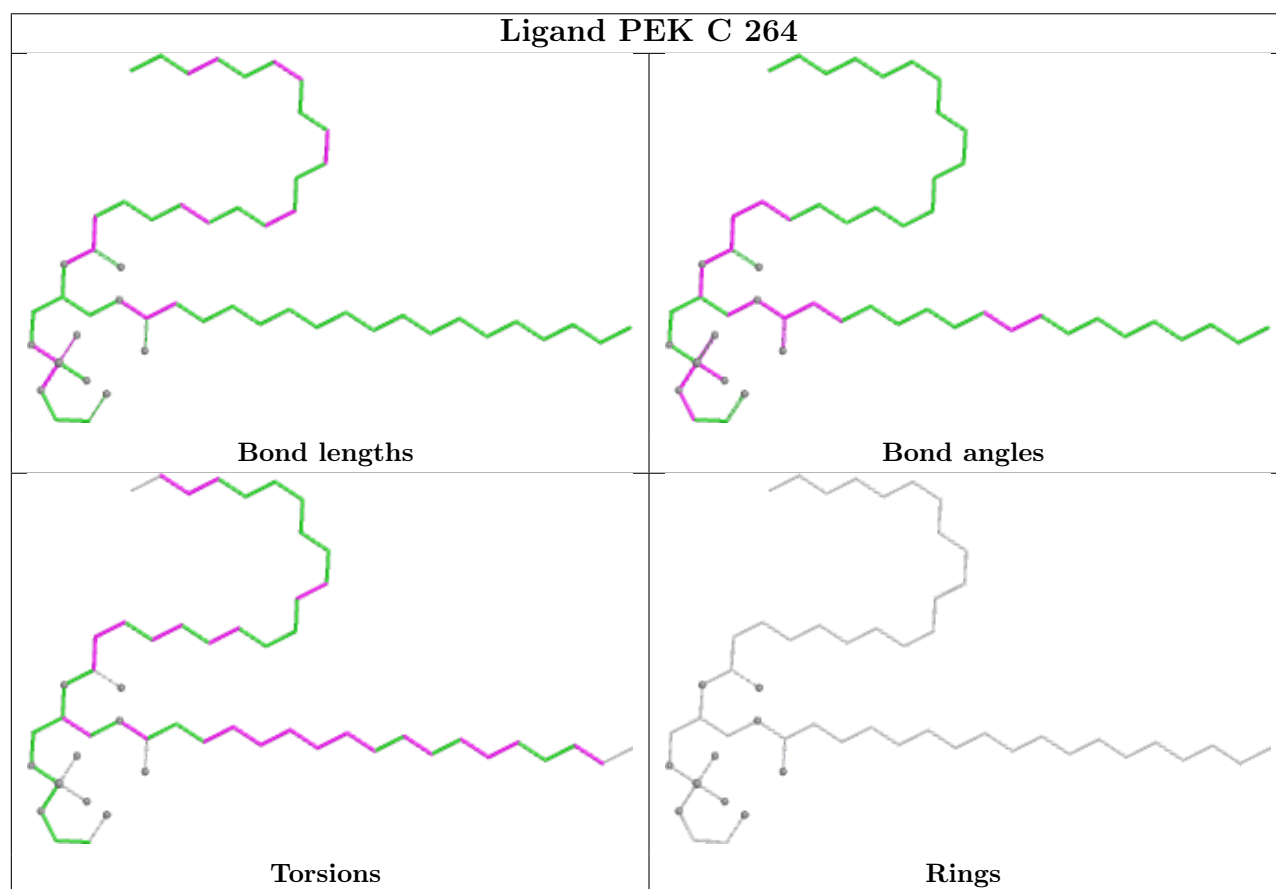
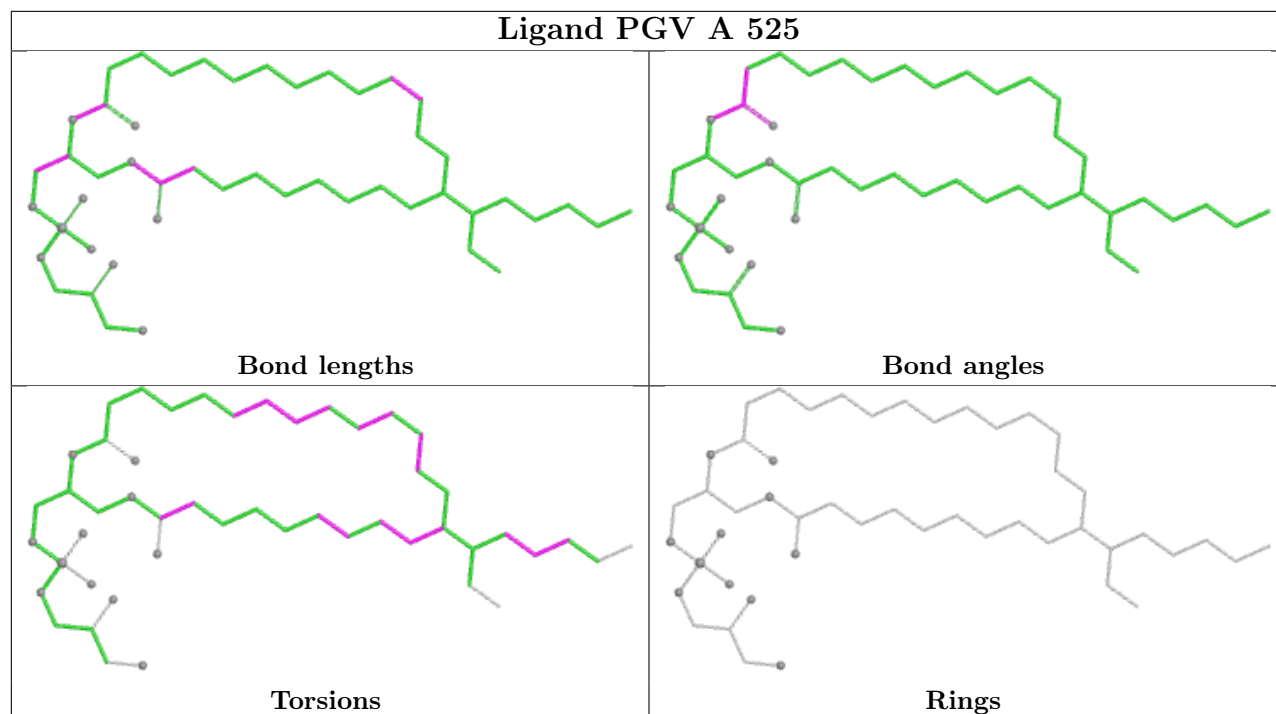


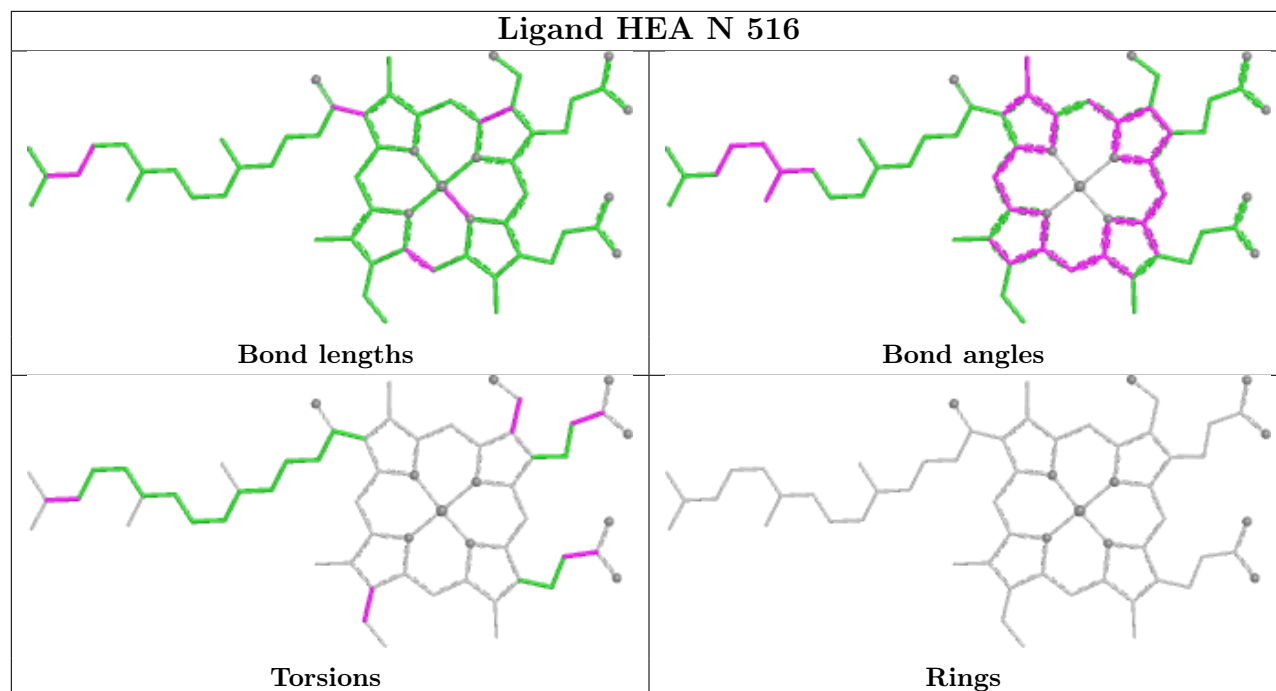
Ligand PEK P 1265





Ligand PEK T 263**Ligand CDL G 269**





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.