



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 08:04 am BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

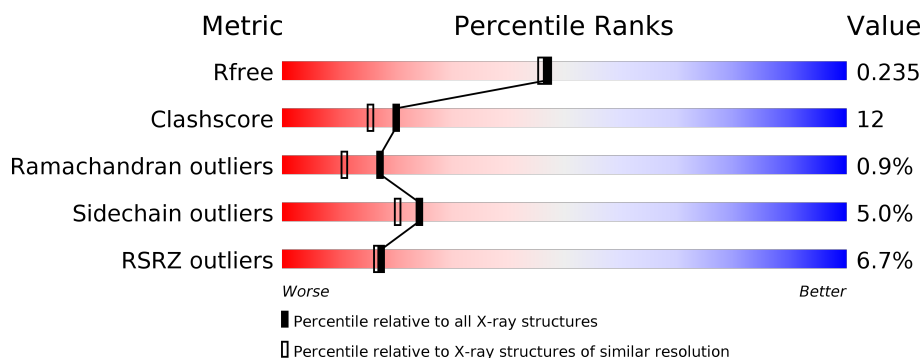
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>
1	N	514	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>
2	B	227	<div> <div></div> <div> <div></div> <div>77%</div> <div>20%</div> <div>••</div> </div> </div>
2	O	227	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>5%</div> </div> </div>
3	C	261	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>•••</div> </div> </div>
3	P	261	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>••</div> </div> </div>

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	516	X	-	-	-
19	PGV	U	1268	-	-	-	X
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	X
23	CHD	P	1271	X	-	-	-
23	CHD	P	1525	X	-	-	-
23	CHD	W	1059	X	-	-	X
24	UNX	C	262	-	-	-	X
24	UNX	P	262	-	-	-	X
25	PEK	G	1263	-	-	-	X
25	PEK	T	263	-	-	-	X
26	CDL	G	269	-	-	X	-
26	CDL	P	1270	-	-	X	-
26	CDL	T	1269	-	-	X	-
27	DMU	C	272	X	-	-	-
27	DMU	M	526	X	-	-	-
27	DMU	P	272	X	-	-	X
27	DMU	Z	1526	X	-	-	-
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32382 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	5	0
			4060	2712	628	684	36			
1	N	514	Total	C	N	O	S	0	5	0
			4060	2712	628	684	36			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

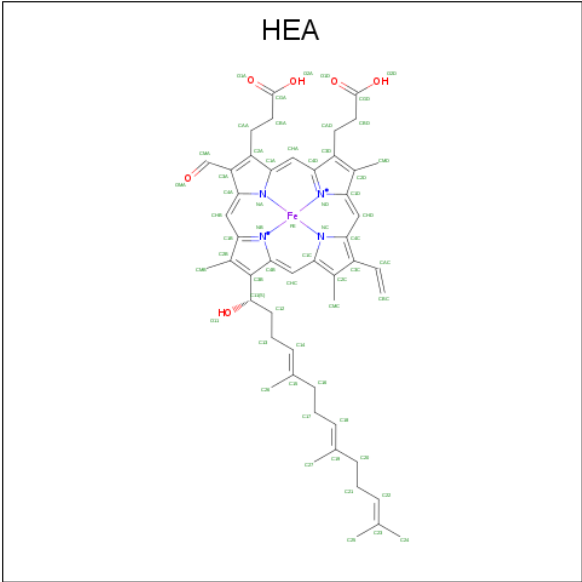
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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

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

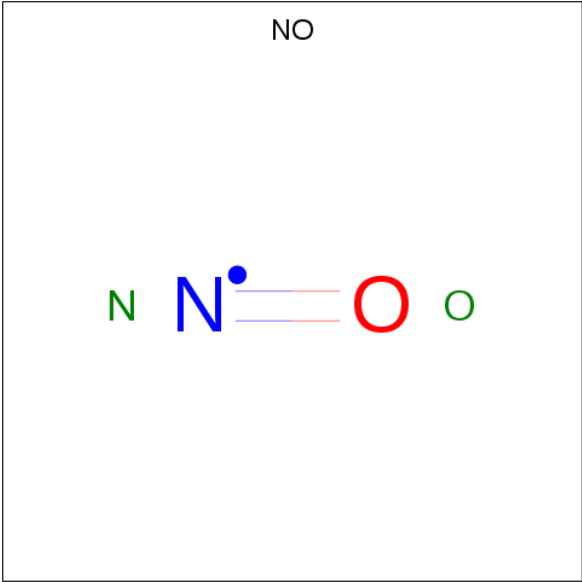
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 15 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



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

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

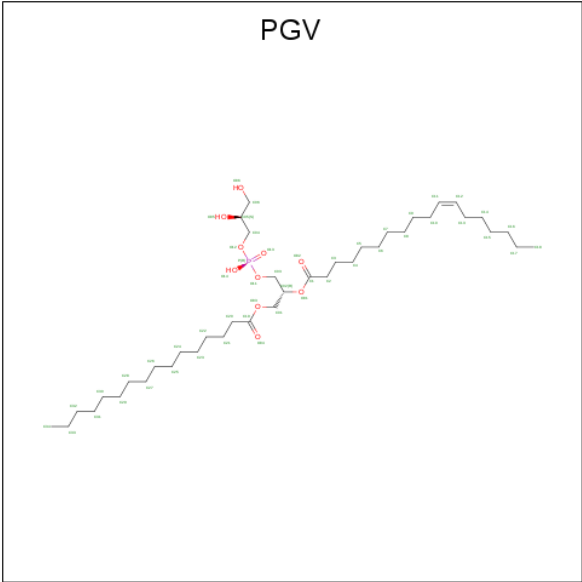
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

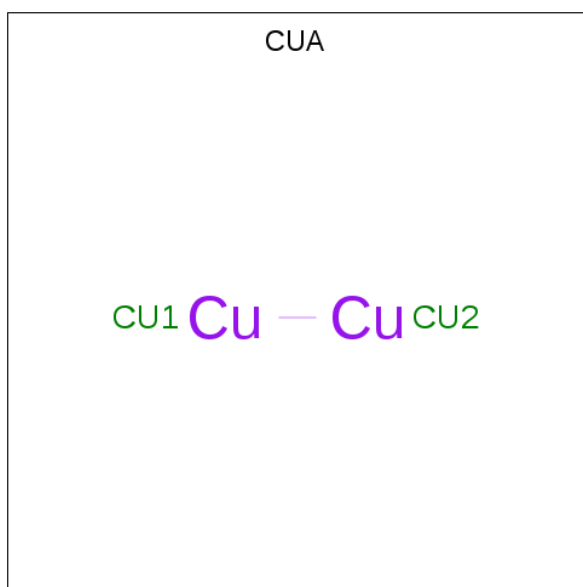
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

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



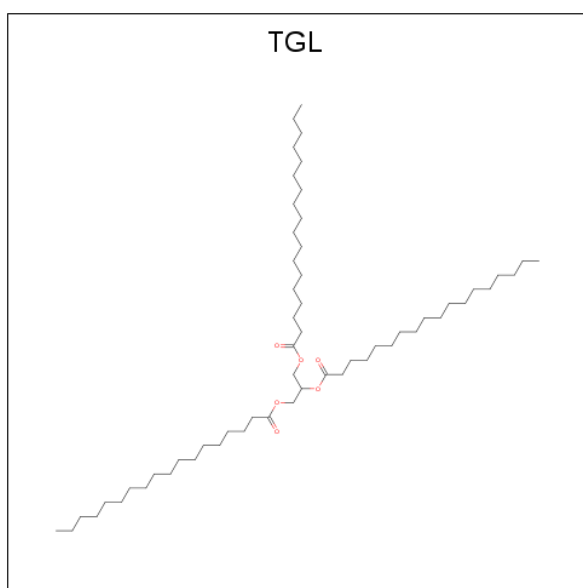
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



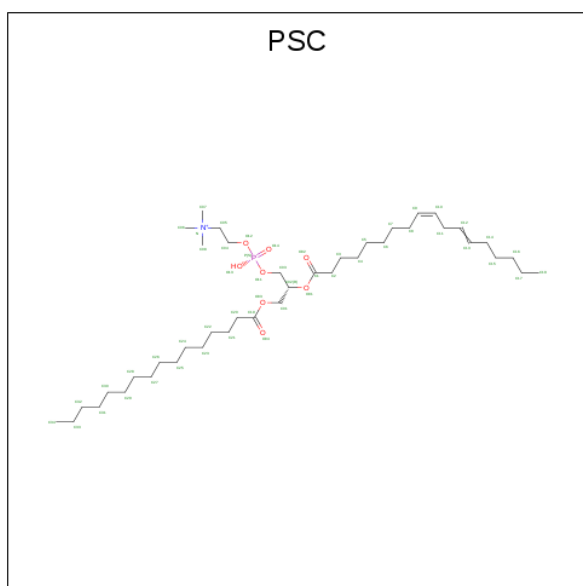
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		

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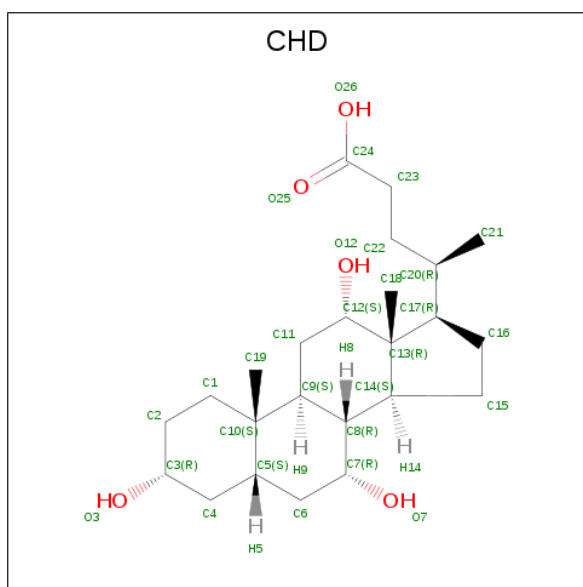
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

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

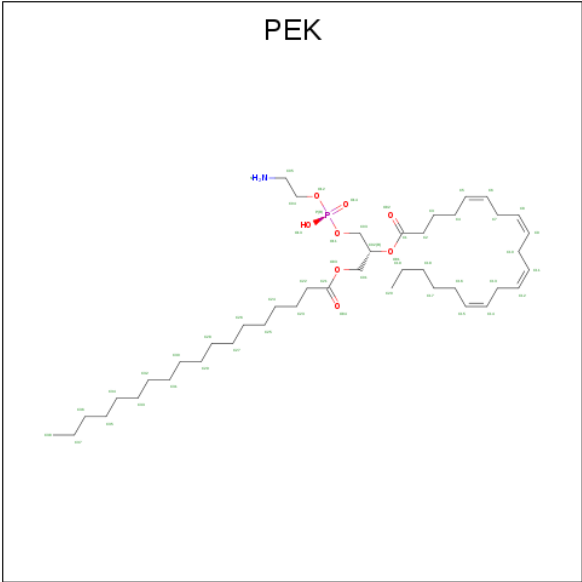


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	O	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

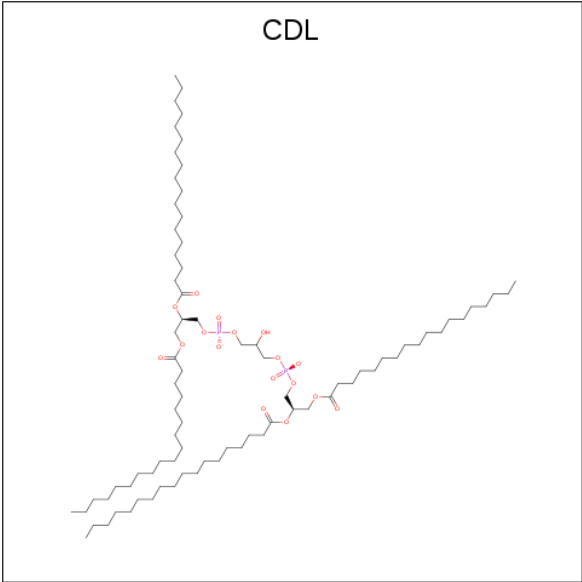
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total X 1 1	0	0
24	C	1	Total X 1 1	0	0

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



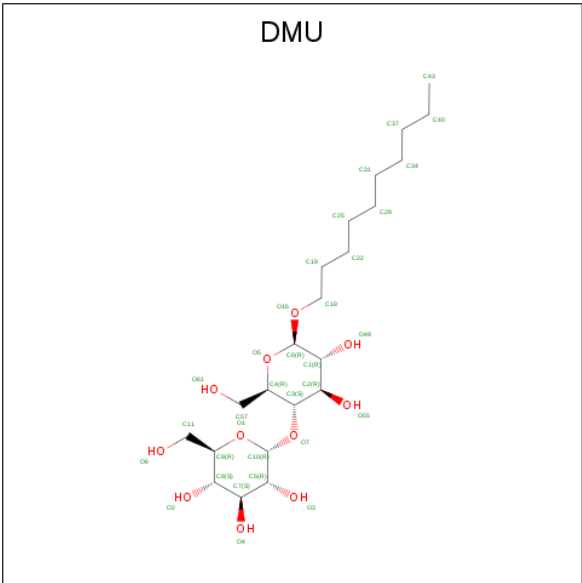
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is water.

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

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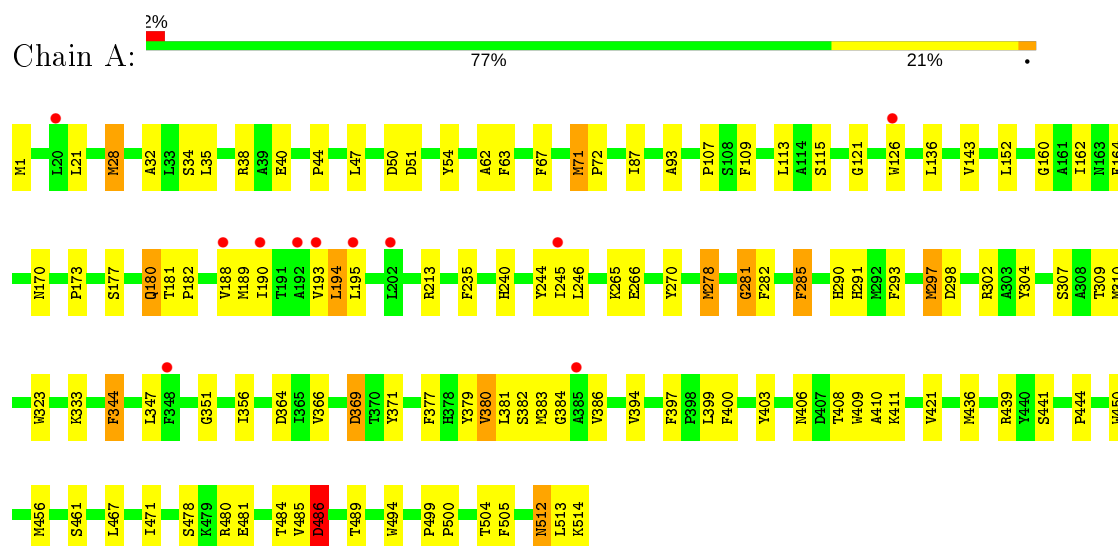
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	M	20	Total 20	O 20	0	0
29	N	207	Total 207	O 207	0	0
29	O	105	Total 105	O 105	0	0
29	P	96	Total 96	O 96	0	0
29	Q	57	Total 57	O 57	0	0
29	R	35	Total 35	O 35	0	0
29	S	63	Total 63	O 63	0	0
29	T	44	Total 44	O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

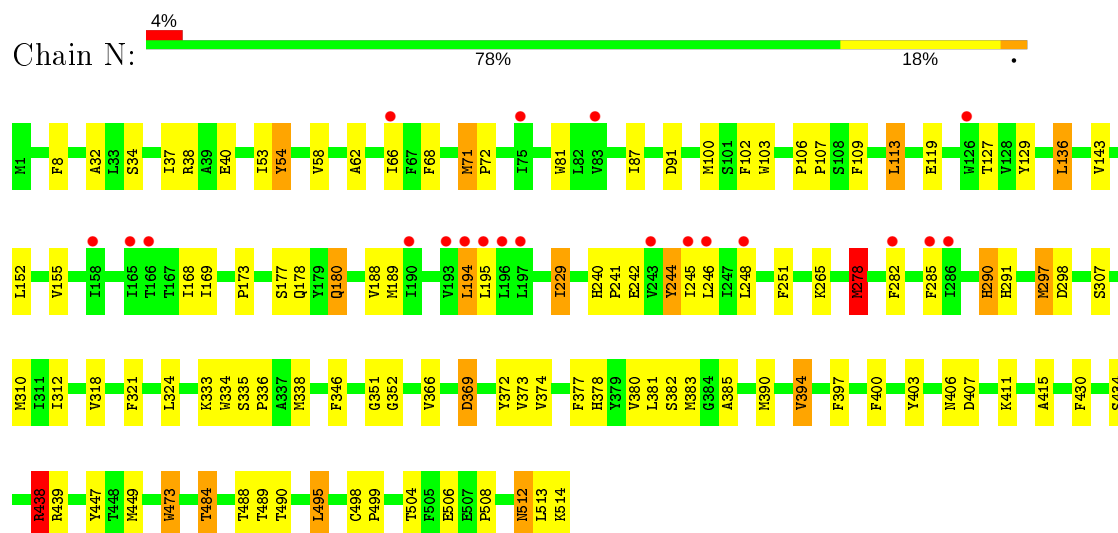
3 Residue-property plots [i](#)

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

• Molecule 1: Cytochrome c oxidase subunit 1

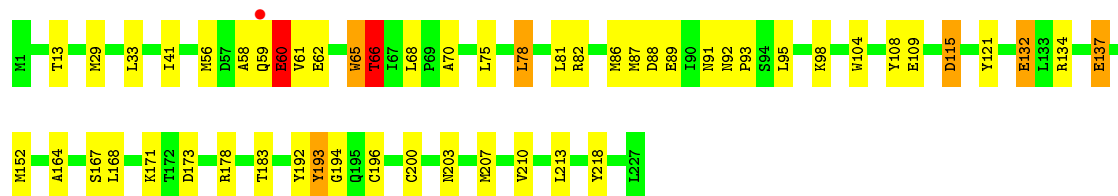


• Molecule 1: Cytochrome c oxidase subunit 1

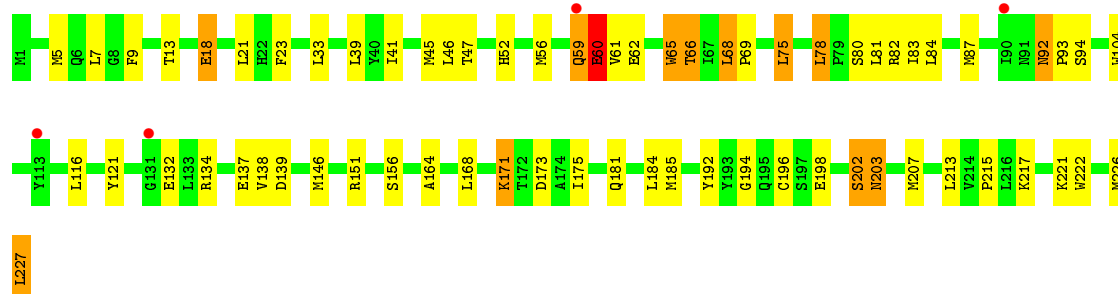


• Molecule 2: Cytochrome c oxidase subunit 2

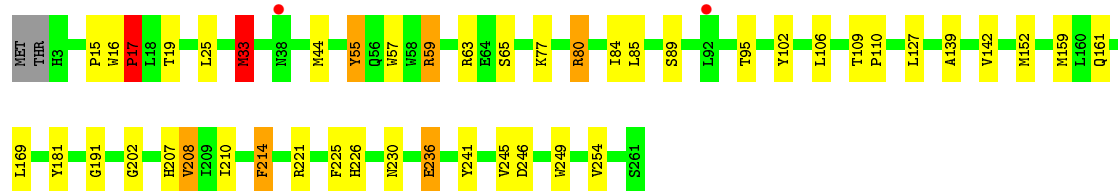
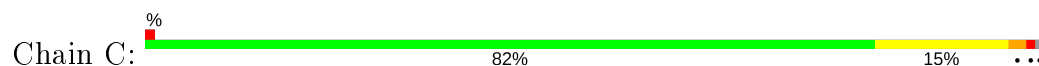




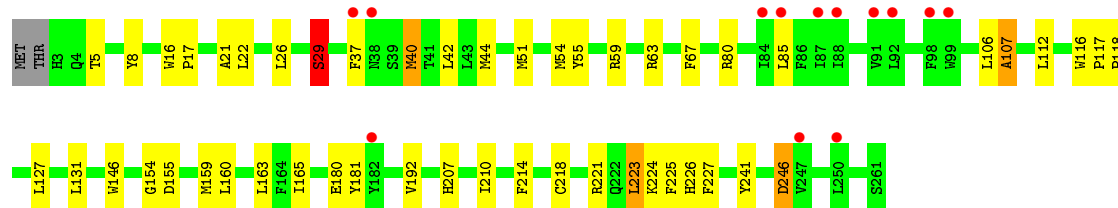
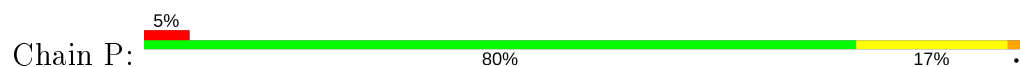
- Molecule 2: Cytochrome c oxidase subunit 2



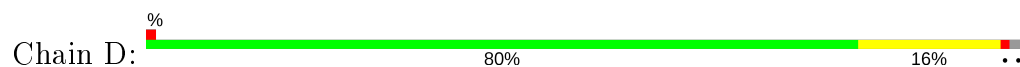
- Molecule 3: Cytochrome c oxidase subunit 3



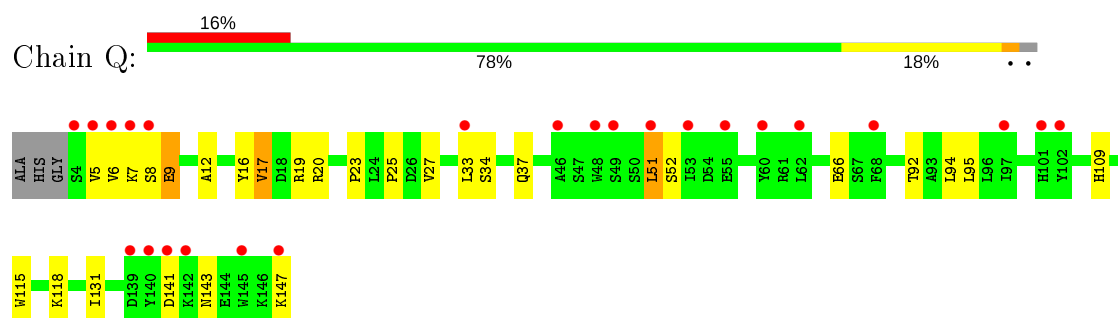
- Molecule 3: Cytochrome c oxidase subunit 3



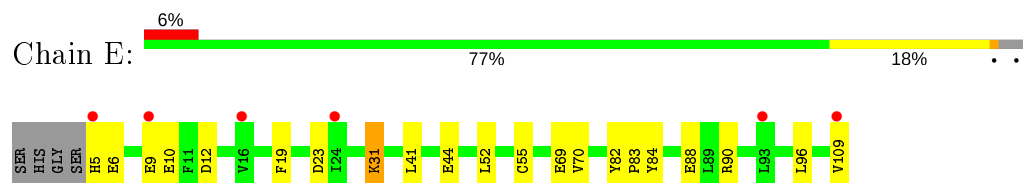
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



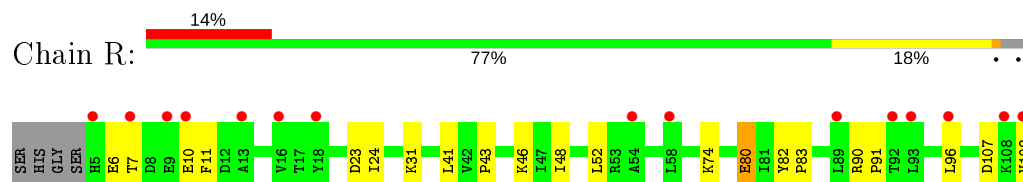
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



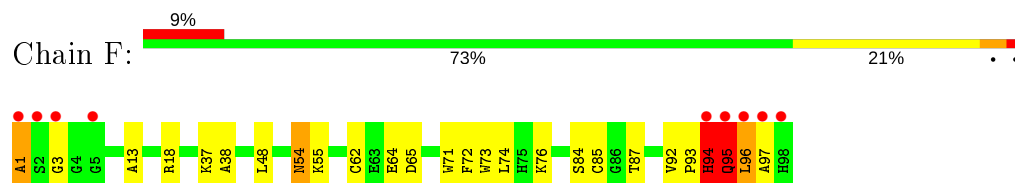
- Molecule 5: Cytochrome c oxidase subunit 5A



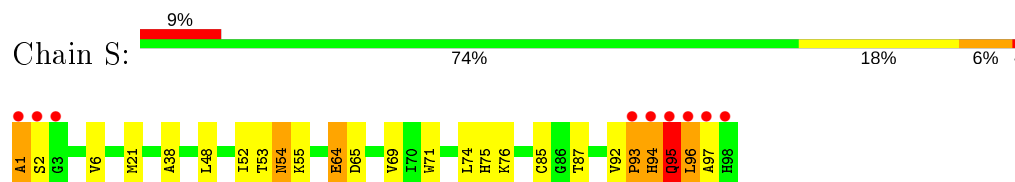
- Molecule 5: Cytochrome c oxidase subunit 5A



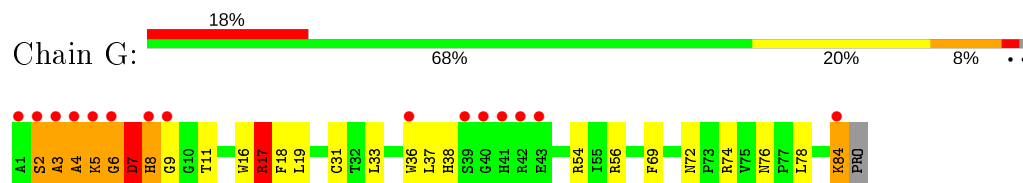
- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B

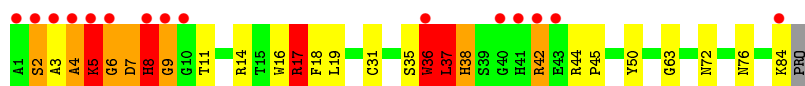


- Molecule 7: Cytochrome c oxidase subunit 6A2

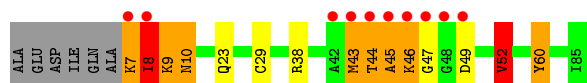
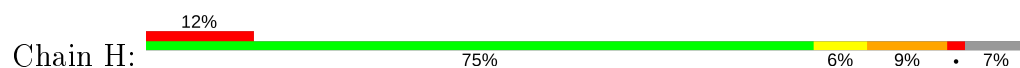


- Molecule 7: Cytochrome c oxidase subunit 6A2

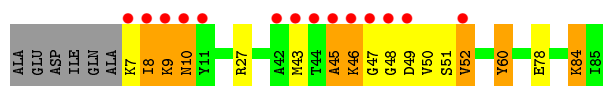
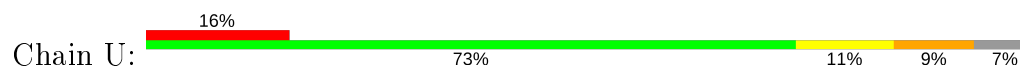




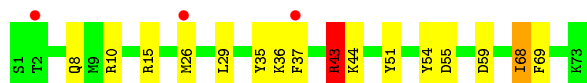
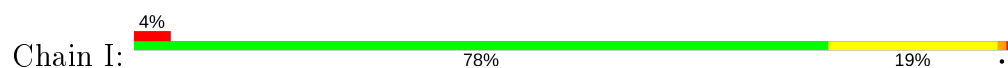
- Molecule 8: Cytochrome c oxidase subunit 6B1



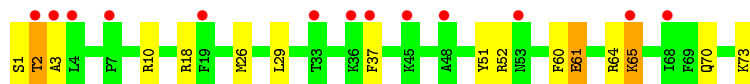
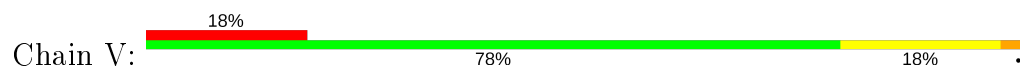
- Molecule 8: Cytochrome c oxidase subunit 6B1



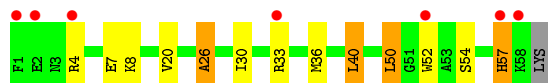
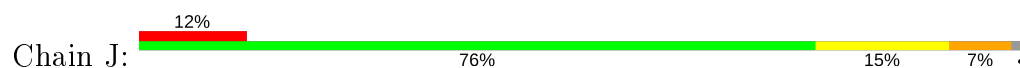
- Molecule 9: Cytochrome c oxidase subunit 6C



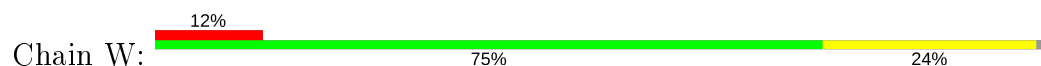
- Molecule 9: Cytochrome c oxidase subunit 6C



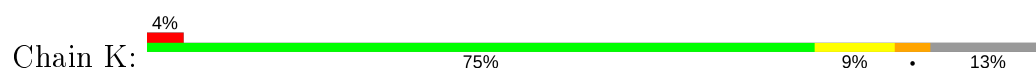
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



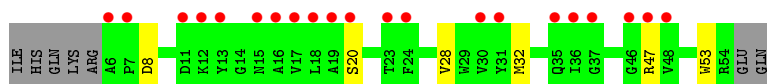
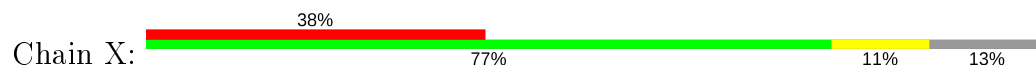
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



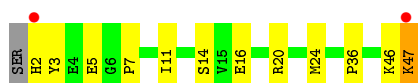
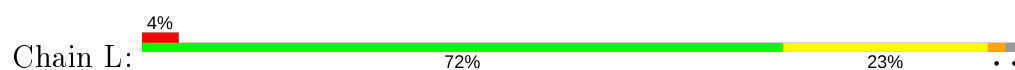
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



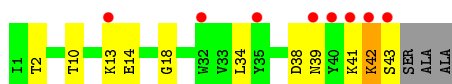
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.25Å 207.94Å 178.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 75.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.00) 98.7 (75.57-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.183 , 0.219 0.201 , 0.235	Depositor DCC
R_{free} test set	22073 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32382	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEK, ZN, CHD, HEA, SAC, CDL, PSC, NO, MG, TGL, PGV, TPO, UNX, CUA, NA, FME, CU, DMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.64	40/4189 (1.0%)	1.27	19/5722 (0.3%)
1	N	1.46	26/4189 (0.6%)	1.20	22/5722 (0.4%)
2	B	1.54	15/1860 (0.8%)	1.32	11/2534 (0.4%)
2	O	1.32	7/1860 (0.4%)	1.14	9/2534 (0.4%)
3	C	1.43	15/2197 (0.7%)	1.13	10/3005 (0.3%)
3	P	1.36	9/2197 (0.4%)	1.16	11/3005 (0.4%)
4	D	1.33	2/1229 (0.2%)	1.11	5/1658 (0.3%)
4	Q	1.24	5/1229 (0.4%)	1.04	5/1658 (0.3%)
5	E	1.32	4/871 (0.5%)	0.98	0/1182
5	R	1.15	0/871	0.98	1/1182 (0.1%)
6	F	1.44	6/765 (0.8%)	1.23	1/1038 (0.1%)
6	S	1.33	3/765 (0.4%)	1.17	1/1038 (0.1%)
7	G	1.38	3/690 (0.4%)	1.28	7/937 (0.7%)
7	T	1.36	3/690 (0.4%)	1.21	6/937 (0.6%)
8	H	1.34	0/682	1.12	2/921 (0.2%)
8	U	1.16	0/682	0.97	0/921
9	I	1.32	3/605 (0.5%)	1.20	5/802 (0.6%)
9	V	1.22	1/605 (0.2%)	0.97	1/802 (0.1%)
10	J	1.26	2/471 (0.4%)	1.09	2/636 (0.3%)
10	W	1.25	0/471	1.10	2/636 (0.3%)
11	K	1.36	0/398	1.19	4/546 (0.7%)
11	X	1.11	0/398	0.95	1/546 (0.2%)
12	L	1.42	2/393 (0.5%)	1.09	0/526
12	Y	1.35	1/393 (0.3%)	1.00	1/526 (0.2%)
13	M	1.41	1/345 (0.3%)	1.23	2/470 (0.4%)
13	Z	1.17	0/345	0.99	0/470
All	All	1.41	148/29390 (0.5%)	1.16	128/39954 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
6	F	0	1
6	S	0	2
12	Y	0	1
All	All	0	5

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	10.56	1.69	1.50
7	T	36	TRP	CB-CG	10.45	1.69	1.50
1	A	380[A]	VAL	CB-CG1	-9.14	1.33	1.52
1	A	380[B]	VAL	CB-CG1	-9.14	1.33	1.52
3	P	180	GLU	CD-OE1	8.86	1.35	1.25
2	O	198	GLU	C-O	8.77	1.40	1.23
2	B	59	GLN	CG-CD	8.68	1.71	1.51
1	A	371	TYR	CD1-CE1	8.39	1.51	1.39
1	N	54	TYR	CD1-CE1	8.15	1.51	1.39
1	A	394	VAL	CB-CG2	-8.09	1.35	1.52
1	A	371	TYR	CD2-CE2	8.00	1.51	1.39
1	A	189	MET	CG-SD	-7.71	1.61	1.81
1	A	285	PHE	CE1-CZ	7.71	1.51	1.37
3	C	57	TRP	CB-CG	7.58	1.63	1.50
2	B	200	CYS	CB-SG	7.56	1.95	1.82
3	C	181	TYR	CD1-CE1	7.56	1.50	1.39
2	B	132	GLU	CD-OE2	7.54	1.33	1.25
2	B	65	TRP	CB-CG	-7.53	1.36	1.50
3	P	218	CYS	CB-SG	7.53	1.95	1.82
3	C	142	VAL	CB-CG2	7.36	1.68	1.52
1	N	188	VAL	N-CA	7.05	1.60	1.46
3	C	102	TYR	CE1-CZ	7.03	1.47	1.38
12	L	16	GLU	CG-CD	7.03	1.62	1.51
1	A	512	ASN	CB-CG	-6.93	1.35	1.51
5	E	9	GLU	CG-CD	6.88	1.62	1.51
1	N	54	TYR	CD2-CE2	6.87	1.49	1.39
1	N	403	TYR	CD1-CE1	6.80	1.49	1.39
2	B	60	GLU	CG-CD	6.71	1.62	1.51
1	N	394	VAL	CB-CG2	-6.70	1.38	1.52
6	F	72	PHE	CE2-CZ	6.63	1.50	1.37
1	A	189	MET	CB-CG	6.62	1.72	1.51
1	N	434	SER	CB-OG	6.60	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	225	PHE	CE2-CZ	6.58	1.49	1.37
1	A	436	MET	N-CA	6.54	1.59	1.46
1	N	473	TRP	CE3-CZ3	6.51	1.49	1.38
1	A	113	LEU	CB-CG	6.48	1.71	1.52
2	B	115	ASP	CB-CG	6.45	1.65	1.51
3	C	57	TRP	CD1-NE1	6.43	1.48	1.38
2	B	218	TYR	CD1-CE1	6.41	1.49	1.39
1	N	102	PHE	CD2-CE2	-6.39	1.26	1.39
1	A	323	TRP	CB-CG	6.34	1.61	1.50
3	P	181	TYR	CD1-CE1	6.33	1.48	1.39
2	O	65	TRP	CB-CG	-6.33	1.38	1.50
1	A	439	ARG	C-O	6.30	1.35	1.23
2	B	108	TYR	CD2-CE2	6.22	1.48	1.39
2	B	59	GLN	CB-CG	6.17	1.69	1.52
2	O	192	TYR	CD1-CE1	6.16	1.48	1.39
7	G	17	ARG	CD-NE	-6.16	1.35	1.46
2	B	60	GLU	CB-CG	6.13	1.63	1.52
4	Q	9	GLU	CB-CG	6.12	1.63	1.52
1	A	297	MET	CB-CG	6.10	1.70	1.51
3	C	208	VAL	CB-CG2	6.10	1.65	1.52
3	C	254	VAL	CB-CG2	6.09	1.65	1.52
13	M	32	TRP	CG-CD1	6.03	1.45	1.36
3	C	55	TYR	CD2-CE2	6.02	1.48	1.39
10	J	20	VAL	CB-CG1	6.02	1.65	1.52
1	N	397	PHE	CE2-CZ	5.99	1.48	1.37
2	B	167	SER	CB-OG	-5.97	1.34	1.42
1	A	270	TYR	CB-CG	5.94	1.60	1.51
4	Q	17	VAL	CB-CG1	-5.94	1.40	1.52
1	A	397	PHE	CD2-CE2	5.84	1.50	1.39
9	I	69	PHE	CG-CD2	5.84	1.47	1.38
1	N	438	ARG	CB-CG	-5.83	1.36	1.52
1	A	93	ALA	CA-CB	5.80	1.64	1.52
1	N	372	TYR	CB-CG	5.79	1.60	1.51
3	C	214	PHE	CE2-CZ	5.78	1.48	1.37
1	N	297	MET	SD-CE	5.75	2.10	1.77
1	A	164	PHE	CE1-CZ	5.73	1.48	1.37
2	O	221	LYS	CD-CE	5.72	1.65	1.51
6	F	1	ALA	C-O	5.71	1.34	1.23
1	A	293	PHE	CE2-CZ	5.67	1.48	1.37
1	N	113	LEU	CB-CG	5.67	1.69	1.52
6	F	3	GLY	C-O	5.66	1.32	1.23
1	N	244	TYR	CD2-CE2	-5.66	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	VAL	CB-CG1	5.65	1.64	1.52
7	T	17	ARG	CD-NE	-5.62	1.36	1.46
3	P	16	TRP	CE3-CZ3	5.61	1.48	1.38
1	A	467	LEU	N-CA	-5.61	1.35	1.46
4	Q	115	TRP	CE3-CZ3	5.58	1.48	1.38
10	J	26	ALA	CA-CB	5.58	1.64	1.52
2	O	18	GLU	CB-CG	-5.58	1.41	1.52
5	E	84	TYR	CG-CD1	5.57	1.46	1.39
6	F	72	PHE	CE1-CZ	5.56	1.48	1.37
1	N	168	ILE	CB-CG2	5.55	1.70	1.52
4	Q	9	GLU	CG-CD	5.55	1.60	1.51
1	N	415	ALA	CA-CB	5.54	1.64	1.52
2	O	156	SER	CB-OG	5.54	1.49	1.42
3	P	246	ASP	CG-OD2	5.54	1.38	1.25
1	A	266	GLU	CB-CG	5.53	1.62	1.52
1	A	411	LYS	CE-NZ	5.53	1.62	1.49
1	N	189	MET	CB-CG	5.52	1.69	1.51
1	A	213	ARG	CG-CD	5.50	1.65	1.51
4	D	104	TYR	CD1-CE1	5.50	1.47	1.39
3	P	8	TYR	CD1-CE1	-5.46	1.31	1.39
1	N	372	TYR	CD2-CE2	5.46	1.47	1.39
1	N	8	PHE	CD2-CE2	5.45	1.50	1.39
1	A	281	GLY	C-O	5.43	1.32	1.23
3	C	249	TRP	CB-CG	5.42	1.60	1.50
12	L	5	GLU	CD-OE2	-5.42	1.19	1.25
12	Y	20	ARG	CG-CD	5.42	1.65	1.51
6	F	54	ASN	CB-CG	5.42	1.63	1.51
2	B	193	TYR	CD1-CE1	5.42	1.47	1.39
3	C	17	PRO	CG-CD	5.41	1.68	1.50
4	D	64	PHE	CE1-CZ	5.40	1.47	1.37
1	A	244	TYR	CD1-CE1	5.40	1.47	1.39
6	F	73	TRP	CE3-CZ3	5.40	1.47	1.38
5	E	88	GLU	CG-CD	5.37	1.60	1.51
1	A	379	TYR	CE2-CZ	5.36	1.45	1.38
2	B	137	GLU	C-O	5.35	1.33	1.23
7	G	5	LYS	CB-CG	5.33	1.67	1.52
3	C	89	SER	CB-OG	5.32	1.49	1.42
3	C	139	ALA	CA-CB	5.28	1.63	1.52
1	A	113	LEU	CG-CD1	5.27	1.71	1.51
9	I	69	PHE	CE2-CZ	5.27	1.47	1.37
1	A	126	TRP	CG-CD1	5.26	1.44	1.36
3	P	107	ALA	CA-CB	5.24	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	6	VAL	CA-CB	5.23	1.65	1.54
1	N	244	TYR	CE2-CZ	5.22	1.45	1.38
1	A	410	ALA	CA-CB	5.22	1.63	1.52
1	A	160	GLY	N-CA	5.22	1.53	1.46
1	A	304	TYR	CD2-CE2	5.22	1.47	1.39
1	A	505	PHE	CG-CD2	5.20	1.46	1.38
1	N	373	VAL	CB-CG2	5.20	1.63	1.52
2	B	121	TYR	CE1-CZ	-5.19	1.31	1.38
6	S	1	ALA	C-O	5.19	1.33	1.23
1	N	81	TRP	CD1-NE1	5.17	1.46	1.38
1	N	506	GLU	CB-CG	-5.16	1.42	1.52
6	S	2	SER	N-CA	5.14	1.56	1.46
1	A	193	VAL	CA-CB	5.13	1.65	1.54
1	A	63	PHE	CD1-CE1	5.12	1.49	1.39
1	N	447	TYR	CD2-CE2	5.12	1.47	1.39
1	A	67	PHE	CE2-CZ	5.12	1.47	1.37
1	A	494	TRP	CZ3-CH2	5.12	1.48	1.40
3	C	236	GLU	CG-CD	5.11	1.59	1.51
1	A	344	PHE	CD2-CE2	5.10	1.49	1.39
1	A	162	ILE	CA-CB	5.10	1.66	1.54
1	N	143	VAL	CB-CG2	5.10	1.63	1.52
7	T	50	TYR	CE1-CZ	5.09	1.45	1.38
5	E	19	PHE	CD1-CE1	5.07	1.49	1.39
9	V	51	TYR	CD1-CE1	5.07	1.47	1.39
3	P	181	TYR	CD2-CE2	5.07	1.47	1.39
1	A	235	PHE	CG-CD1	5.05	1.46	1.38
9	I	15	ARG	CG-CD	5.04	1.64	1.51
3	P	227	PHE	CE2-CZ	5.04	1.47	1.37
6	S	69	VAL	CA-CB	-5.04	1.44	1.54
2	B	192	TYR	CG-CD1	5.03	1.45	1.39
2	O	171	LYS	CB-CG	5.01	1.66	1.52
1	N	447	TYR	CD1-CE1	5.00	1.46	1.39

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	17	ARG	NE-CZ-NH2	-14.38	113.11	120.30
1	A	71	MET	CG-SD-CE	-14.02	77.77	100.20
7	G	17	ARG	NE-CZ-NH1	12.88	126.74	120.30
3	P	246	ASP	CB-CG-OD1	-12.27	107.26	118.30
1	N	278	MET	CG-SD-CE	-11.92	81.12	100.20
1	N	71	MET	CG-SD-CE	-11.66	81.54	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	221	ARG	NE-CZ-NH1	-10.62	114.99	120.30
1	A	136	LEU	CB-CG-CD1	-10.11	93.81	111.00
1	N	310	MET	CG-SD-CE	-9.35	85.24	100.20
9	I	43	ARG	NE-CZ-NH2	9.15	124.88	120.30
7	T	17	ARG	NE-CZ-NH2	-9.12	115.74	120.30
7	T	17	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	N	298	ASP	CB-CG-OD1	-8.56	110.59	118.30
4	D	20	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	N	298	ASP	CB-CG-OD2	8.40	125.86	118.30
8	H	38	ARG	NE-CZ-NH1	-8.36	116.12	120.30
1	A	298	ASP	CB-CG-OD2	8.29	125.76	118.30
1	N	113	LEU	CB-CG-CD2	8.07	124.71	111.00
2	B	173	ASP	CB-CG-OD1	7.96	125.47	118.30
2	B	65	TRP	CB-CA-C	7.75	125.90	110.40
4	D	51	LEU	CA-CB-CG	7.67	132.94	115.30
2	B	178	ARG	NE-CZ-NH1	-7.64	116.48	120.30
4	Q	20	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	278	MET	CG-SD-CE	-7.51	88.19	100.20
9	I	68	ILE	CG1-CB-CG2	7.30	127.45	111.40
4	Q	17	VAL	CB-CA-C	-7.20	97.72	111.40
1	A	512	ASN	CB-CA-C	-7.16	96.09	110.40
4	D	19	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	486	ASP	CB-CG-OD2	-7.04	111.97	118.30
3	P	29	SER	CB-CA-C	-6.96	96.88	110.10
2	B	152	MET	CG-SD-CE	6.95	111.31	100.20
13	M	34	LEU	CB-CG-CD1	6.86	122.66	111.00
1	N	136	LEU	CA-CB-CG	6.83	131.01	115.30
1	A	302	ARG	NE-CZ-NH2	-6.81	116.89	120.30
3	P	80	ARG	CG-CD-NE	-6.79	97.55	111.80
1	A	366	VAL	CG1-CB-CG2	-6.78	100.06	110.90
1	A	189	MET	CG-SD-CE	-6.77	89.37	100.20
1	N	438	ARG	NE-CZ-NH1	-6.76	116.92	120.30
8	H	52	VAL	CB-CA-C	-6.75	98.57	111.40
1	A	369	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	439	ARG	NE-CZ-NH1	-6.72	116.94	120.30
2	O	139	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	456	MET	CG-SD-CE	-6.65	89.56	100.20
10	W	44	LEU	CB-CG-CD1	-6.60	99.78	111.00
11	K	47	ARG	NE-CZ-NH1	-6.59	117.01	120.30
6	S	21	MET	CG-SD-CE	6.57	110.72	100.20
1	N	136	LEU	CB-CG-CD2	-6.50	99.95	111.00
4	Q	20	ARG	NE-CZ-NH2	-6.48	117.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	91	ASP	CB-CG-OD1	6.40	124.06	118.30
2	B	134	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	N	244	TYR	CG-CD2-CE2	6.29	126.33	121.30
1	A	35	LEU	CB-CG-CD1	-6.26	100.35	111.00
3	C	152	MET	CG-SD-CE	6.24	110.18	100.20
1	A	113	LEU	CB-CG-CD2	6.24	121.60	111.00
2	O	184	LEU	CA-CB-CG	6.22	129.60	115.30
4	D	20	ARG	NE-CZ-NH1	6.20	123.40	120.30
4	Q	51	LEU	CA-CB-CG	6.18	129.52	115.30
9	I	55	ASP	CB-CG-OD1	6.18	123.86	118.30
2	O	185	MET	CG-SD-CE	6.17	110.08	100.20
2	B	82	ARG	CG-CD-NE	-6.16	98.87	111.80
11	K	54	ARG	NE-CZ-NH2	-6.15	117.22	120.30
2	B	95	LEU	CB-CG-CD1	6.13	121.42	111.00
1	N	244	TYR	CZ-CE2-CD2	-6.11	114.30	119.80
1	A	188	VAL	CG1-CB-CG2	-6.03	101.26	110.90
3	P	163	LEU	CB-CG-CD2	-6.02	100.76	111.00
2	B	88	ASP	CB-CG-OD2	6.02	123.72	118.30
3	P	221	ARG	NE-CZ-NH2	6.01	123.31	120.30
7	G	78	LEU	CB-CG-CD1	-6.00	100.80	111.00
1	A	194	LEU	CB-CG-CD1	5.97	121.16	111.00
1	N	189	MET	CA-CB-CG	-5.95	103.18	113.30
3	C	59	ARG	NE-CZ-NH1	-5.95	117.33	120.30
10	J	40	LEU	CB-CG-CD2	5.94	121.10	111.00
3	P	180	GLU	OE1-CD-OE2	5.89	130.36	123.30
2	O	173	ASP	CB-CG-OD1	5.88	123.59	118.30
6	F	95	GLN	N-CA-C	5.87	126.85	111.00
1	N	438	ARG	CG-CD-NE	-5.81	99.61	111.80
1	A	189	MET	CA-CB-CG	-5.80	103.43	113.30
3	C	80	ARG	CG-CD-NE	-5.76	99.71	111.80
1	N	38	ARG	NE-CZ-NH1	5.73	123.17	120.30
11	X	32	MET	CG-SD-CE	5.68	109.30	100.20
7	T	44	ARG	NE-CZ-NH1	5.68	123.14	120.30
7	G	56	ARG	NE-CZ-NH2	-5.65	117.47	120.30
13	M	27	LEU	CB-CG-CD1	-5.63	101.44	111.00
2	O	202	SER	CB-CA-C	-5.62	99.42	110.10
3	P	192	VAL	CG1-CB-CG2	5.62	119.89	110.90
7	G	19	LEU	CB-CG-CD2	-5.62	101.45	111.00
1	N	369	ASP	CB-CG-OD2	5.62	123.36	118.30
1	N	438	ARG	CB-CA-C	-5.61	99.19	110.40
7	T	14	ARG	NE-CZ-NH1	-5.60	117.50	120.30
9	I	15	ARG	NE-CZ-NH2	5.59	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	43	ARG	NE-CZ-NH1	-5.59	117.50	120.30
12	Y	41	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	N	366	VAL	CG1-CB-CG2	-5.49	102.11	110.90
3	C	221	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	28	MET	CG-SD-CE	5.47	108.96	100.20
2	O	134	ARG	NE-CZ-NH1	-5.47	117.56	120.30
2	O	92	ASN	CB-CA-C	5.47	121.34	110.40
10	J	57	HIS	CB-CA-C	5.46	121.31	110.40
2	B	87	MET	CA-CB-CG	5.46	122.57	113.30
7	T	17	ARG	CB-CG-CD	-5.43	97.47	111.60
1	N	438	ARG	N-CA-CB	-5.39	100.89	110.60
4	D	137	LYS	CD-CE-NZ	-5.35	99.40	111.70
2	O	75	LEU	CB-CG-CD1	5.34	120.07	111.00
1	N	113	LEU	CB-CG-CD1	5.33	120.06	111.00
3	P	155	ASP	CB-CG-OD1	5.33	123.09	118.30
3	C	33	MET	CG-SD-CE	5.32	108.72	100.20
3	C	169	LEU	CB-CG-CD2	-5.31	101.97	111.00
2	O	82	ARG	NE-CZ-NH2	-5.28	117.66	120.30
7	G	7	ASP	N-CA-C	5.27	125.24	111.00
3	P	223	LEU	CB-CG-CD1	-5.22	102.12	111.00
2	B	66	THR	OG1-CB-CG2	5.22	122.01	110.00
4	Q	19	ARG	NE-CZ-NH1	-5.22	117.69	120.30
5	R	96	LEU	CA-CB-CG	5.21	127.29	115.30
3	C	33	MET	CB-CG-SD	5.18	127.93	112.40
3	C	44	MET	CG-SD-CE	5.18	108.48	100.20
7	G	17	ARG	CB-CG-CD	-5.17	98.16	111.60
1	A	152	LEU	CA-CB-CG	5.13	127.11	115.30
3	C	102	TYR	CB-CG-CD2	-5.12	117.92	121.00
11	K	39	GLU	OE1-CD-OE2	-5.12	117.15	123.30
1	N	229	ILE	CG1-CB-CG2	-5.12	100.13	111.40
7	T	19	LEU	CB-CG-CD2	-5.12	102.30	111.00
2	B	213	LEU	CB-CG-CD1	-5.10	102.32	111.00
3	C	85	LEU	CA-CB-CG	-5.10	103.56	115.30
3	P	40	MET	CB-CG-SD	-5.10	97.10	112.40
9	V	64	ARG	NE-CZ-NH1	5.09	122.85	120.30
11	K	47	ARG	CG-CD-NE	-5.09	101.12	111.80
1	N	194	LEU	CB-CG-CD1	5.07	119.61	111.00
10	W	44	LEU	CB-CG-CD2	5.02	119.54	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4060	0	4037	74	0
1	N	4060	0	4037	86	0
2	B	1824	0	1833	25	0
2	O	1824	0	1833	50	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	35	0
4	D	1195	0	1183	19	0
4	Q	1195	0	1183	20	0
5	E	852	0	845	10	0
5	R	852	0	845	19	0
6	F	748	0	728	22	0
6	S	748	0	728	40	0
7	G	675	0	643	45	0
7	T	675	0	643	43	0
8	H	662	0	623	19	0
8	U	662	0	623	20	0
9	I	601	0	613	8	0
9	V	601	0	613	9	0
10	J	460	0	459	13	0
10	W	460	0	459	12	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	16	0
12	Y	380	0	380	20	0
13	M	335	0	352	13	0
13	Z	335	0	352	6	0
14	A	120	0	108	16	0
14	N	120	0	108	9	0
15	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	2	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	102	0	152	16	0
19	C	102	0	152	10	0
19	N	102	0	152	7	0
19	P	51	0	76	3	0
19	U	51	0	76	4	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	63	0	110	4	0
21	D	63	0	110	10	0
21	L	63	0	110	15	0
21	N	63	0	110	14	0
21	O	63	0	110	5	0
21	Y	63	0	110	20	0
22	B	52	0	80	20	0
22	R	52	0	80	20	0
23	B	29	0	37	4	0
23	C	58	0	71	4	0
23	J	29	0	36	8	0
23	O	29	0	37	3	0
23	P	58	0	72	5	0
23	W	29	0	35	3	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	22	0
25	G	53	0	77	19	0
25	P	53	0	77	6	0
25	T	106	0	154	34	0
26	C	100	0	156	20	0
26	G	100	0	156	33	0
26	P	100	0	156	27	0
26	T	100	0	156	30	0
27	C	33	0	39	4	0
27	M	33	0	39	0	0
27	P	33	0	38	1	0
27	Z	33	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	217	0	0	5	0
29	B	127	0	0	3	0
29	C	93	0	0	4	0
29	D	86	0	0	6	0
29	E	52	0	0	0	0
29	F	72	0	0	3	0
29	G	42	0	0	7	0
29	H	46	0	0	1	0
29	I	31	0	0	3	0
29	J	28	0	0	4	0
29	K	27	0	0	2	0
29	L	16	0	0	1	0
29	M	20	0	0	0	0
29	N	207	0	0	6	0
29	O	105	0	0	2	0
29	P	96	0	0	3	0
29	Q	57	0	0	4	0
29	R	35	0	0	1	0
29	S	63	0	0	5	0
29	T	44	0	0	5	0
29	U	43	0	0	5	0
29	V	20	0	0	0	0
29	W	17	0	0	2	0
29	X	13	0	0	0	0
29	Y	12	0	0	1	0
29	Z	11	0	0	1	0
All	All	32382	0	31350	777	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 12.

All (777) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:1265:PEK:H383	26:T:1269:CDL:C27	1.34	1.51
1:N:297:MET:CE	1:N:297:MET:SD	2.10	1.40
25:T:1265:PEK:C38	26:T:1269:CDL:H273	1.51	1.36
10:W:2:GLU:HB2	10:W:4:ARG:NH1	1.50	1.26
25:T:1265:PEK:C38	26:T:1269:CDL:C27	2.12	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:5:LYS:HD2	25:G:1263:PEK:C37	1.73	1.18
19:A:524:PGV:H311	13:M:19:LEU:HD23	1.24	1.16
19:U:1268:PGV:H032	29:U:4495:HOH:O	1.43	1.14
25:C:264:PEK:H162	25:C:264:PEK:H101	1.17	1.14
7:G:5:LYS:CD	25:G:1263:PEK:H371	1.78	1.13
26:C:270:CDL:HB22	10:J:8:LYS:NZ	1.62	1.13
29:B:2562:HOH:O	21:D:523:TGL:HC61	1.50	1.11
26:C:270:CDL:HB22	10:J:8:LYS:HZ2	1.09	1.10
7:G:84:LYS:HD2	7:G:84:LYS:H	1.03	1.10
12:L:20:ARG:NH2	21:L:522:TGL:HC32	1.64	1.10
25:T:1265:PEK:H383	26:T:1269:CDL:H271	1.23	1.10
26:G:269:CDL:H561	26:G:269:CDL:H762	1.33	1.09
8:H:52:VAL:HG12	8:U:46:LYS:HB2	1.17	1.09
21:N:1523:TGL:HC21	21:N:1523:TGL:HG11	1.31	1.08
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.26	1.06
26:G:269:CDL:H222	26:G:269:CDL:H522	1.39	1.04
1:N:513:LEU:O	1:N:514:LYS:HB2	1.55	1.04
7:G:5:LYS:CG	25:G:1263:PEK:H371	1.88	1.03
6:S:94:HIS:CD2	6:S:95:GLN:N	2.26	1.03
26:C:270:CDL:H212	26:C:270:CDL:H631	1.05	1.02
1:A:513:LEU:O	1:A:514:LYS:HB2	1.60	1.02
8:U:9:LYS:HG3	8:U:10:ASN:H	1.21	1.01
2:O:59:GLN:O	2:O:59:GLN:HG3	1.59	0.98
6:S:94:HIS:CD2	6:S:95:GLN:H	1.80	0.98
22:R:1229:PSC:C34	22:R:1229:PSC:H142	1.94	0.98
19:N:1524:PGV:H012	19:N:1524:PGV:H221	1.45	0.97
7:G:84:LYS:N	7:G:84:LYS:HD2	1.78	0.95
19:N:1524:PGV:H221	19:N:1524:PGV:C01	1.96	0.94
26:P:1270:CDL:HB21	26:P:1270:CDL:CB3	1.98	0.94
10:W:2:GLU:HB2	10:W:4:ARG:HH12	1.32	0.94
22:B:229:PSC:O01	22:B:229:PSC:H212	1.67	0.94
19:C:267:PGV:H181	26:C:270:CDL:H652	1.48	0.93
7:G:2:SER:OG	25:G:1263:PEK:H291	1.66	0.93
6:F:94:HIS:HB3	6:F:95:GLN:OE1	1.68	0.93
7:G:72:ASN:H	7:G:76:ASN:HD22	0.99	0.93
26:P:1270:CDL:HB21	26:P:1270:CDL:HB32	1.49	0.93
25:T:1265:PEK:H383	26:T:1269:CDL:H273	1.00	0.92
6:F:85:CYS:SG	6:F:87:THR:HG23	2.09	0.92
26:G:269:CDL:HA21	26:G:269:CDL:H112	1.52	0.92
25:T:1265:PEK:H381	26:T:1269:CDL:H273	1.48	0.92
10:W:2:GLU:HB2	10:W:4:ARG:HH11	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:229:PSC:H072	9:I:10:ARG:HH21	1.32	0.91
6:S:85:CYS:SG	6:S:87:THR:HG23	2.10	0.91
26:T:1269:CDL:H241	26:T:1269:CDL:H531	1.53	0.90
25:P:1264:PEK:H32	25:P:1264:PEK:H71	1.55	0.89
3:P:29:SER:HB2	3:P:42:LEU:HD13	1.53	0.89
25:T:1265:PEK:H71	29:T:4407:HOH:O	1.73	0.89
8:H:9:LYS:O	8:H:10:ASN:HB2	1.71	0.88
7:T:7:ASP:O	7:T:8:HIS:HB2	1.73	0.88
1:A:513:LEU:O	1:A:514:LYS:CB	2.22	0.87
7:G:84:LYS:H	7:G:84:LYS:CD	1.87	0.87
1:A:282:PHE:HA	7:T:4:ALA:CB	2.04	0.87
26:C:270:CDL:H212	26:C:270:CDL:C63	1.99	0.87
12:L:20:ARG:HH22	21:L:522:TGL:HC32	1.38	0.87
1:N:513:LEU:O	1:N:514:LYS:CB	2.23	0.86
7:G:2:SER:OG	25:G:1263:PEK:C29	2.22	0.86
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.41	0.86
12:Y:20:ARG:HH21	21:Y:1522:TGL:HC32	1.39	0.86
19:A:524:PGV:H011	19:A:524:PGV:H22	1.59	0.85
3:C:63:ARG:HH21	26:C:270:CDL:HA21	1.38	0.85
2:B:81:LEU:HD12	26:T:1269:CDL:H351	1.57	0.85
7:G:2:SER:O	25:G:1263:PEK:H331	1.77	0.84
9:I:44:LYS:HE2	29:I:4717:HOH:O	1.77	0.84
8:H:52:VAL:HG12	8:U:46:LYS:CB	2.06	0.83
19:A:524:PGV:H311	13:M:19:LEU:CD2	2.09	0.83
21:D:523:TGL:HG32	29:D:4105:HOH:O	1.76	0.83
6:F:97:ALA:CB	29:F:4782:HOH:O	2.26	0.83
7:G:5:LYS:HG3	25:G:1263:PEK:H371	1.60	0.82
7:G:3:ALA:HB1	25:G:1263:PEK:H383	1.61	0.82
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.60	0.82
12:Y:20:ARG:HH21	21:Y:1522:TGL:CC3	1.93	0.82
3:C:246:ASP:HB2	29:C:4124:HOH:O	1.81	0.81
7:G:72:ASN:H	7:G:76:ASN:ND2	1.78	0.81
8:U:9:LYS:HG3	8:U:10:ASN:N	1.94	0.81
6:S:76:LYS:HE2	29:S:4790:HOH:O	1.80	0.81
7:T:2:SER:OG	25:T:263:PEK:H301	1.79	0.81
5:R:7:THR:OG1	5:R:10:GLU:HG3	1.80	0.81
1:N:351:GLY:HA3	1:N:380[A]:VAL:HG13	1.62	0.81
22:B:229:PSC:C07	9:I:10:ARG:HH21	1.93	0.81
4:D:45:LYS:HB3	29:D:4504:HOH:O	1.81	0.81
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.63	0.80
22:B:229:PSC:H142	22:B:229:PSC:H343	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:45:ALA:O	8:U:47:GLY:N	2.14	0.80
6:S:94:HIS:HD2	6:S:95:GLN:N	1.80	0.80
26:C:270:CDL:C21	26:C:270:CDL:H631	2.01	0.80
21:N:1523:TGL:HC21	21:N:1523:TGL:CG1	2.12	0.80
25:C:264:PEK:H162	25:C:264:PEK:C10	2.07	0.79
26:T:1269:CDL:H111	26:T:1269:CDL:CA2	2.11	0.79
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.61	0.79
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.48	0.79
19:N:1524:PGV:H321	19:N:1524:PGV:H151	1.64	0.79
7:G:31:CYS:SG	26:G:269:CDL:H532	2.22	0.78
8:H:43:MET:HE3	8:H:49:ASP:H	1.47	0.78
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.63	0.78
22:R:1229:PSC:H142	22:R:1229:PSC:H343	1.63	0.78
12:L:20:ARG:HH21	21:L:522:TGL:HC32	1.48	0.78
8:U:9:LYS:O	8:U:10:ASN:HB2	1.82	0.77
10:W:33:ARG:HG2	23:W:1059:CHD:H152	1.66	0.77
6:F:97:ALA:HB3	29:F:4782:HOH:O	1.84	0.77
6:S:94:HIS:HD2	6:S:95:GLN:CA	1.97	0.77
3:P:107:ALA:HB2	19:U:1268:PGV:H031	1.66	0.77
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.67	0.77
1:A:351:GLY:HA3	1:A:380[A]:VAL:HG13	1.67	0.76
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.65	0.76
21:Y:1522:TGL:CA9	21:Y:1522:TGL:H231	2.14	0.76
7:T:72:ASN:H	7:T:76:ASN:HD22	1.33	0.76
25:C:264:PEK:H101	25:C:264:PEK:C16	2.08	0.76
2:O:227:LEU:OXT	2:O:227:LEU:HD13	1.86	0.76
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.21	0.75
26:G:269:CDL:H372	2:O:78:LEU:CD1	2.16	0.75
22:B:229:PSC:O02	22:B:229:PSC:H032	1.85	0.75
1:A:484:THR:HB	13:M:2:THR:OG1	1.87	0.75
22:B:229:PSC:H142	22:B:229:PSC:C34	2.17	0.75
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.84	0.74
6:F:1:ALA:HB3	6:S:65:ASP:OD1	1.87	0.74
4:D:20:ARG:HG3	29:D:4132:HOH:O	1.86	0.74
2:B:56:MET:HA	22:B:229:PSC:H201	1.68	0.74
19:A:521:PGV:H183	25:C:264:PEK:H332	1.68	0.74
26:T:1269:CDL:H111	26:T:1269:CDL:HA22	1.67	0.74
22:R:1229:PSC:H22	22:R:1229:PSC:H221	1.70	0.74
7:G:5:LYS:HD2	25:G:1263:PEK:H372	1.69	0.73
2:B:70:ALA:HB1	26:T:1269:CDL:H451	1.70	0.73
26:G:269:CDL:C22	26:G:269:CDL:H522	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:95:GLN:CG	29:S:4728:HOH:O	2.36	0.73
19:C:267:PGV:C18	26:C:270:CDL:H652	2.18	0.72
8:H:43:MET:HE3	8:H:49:ASP:N	2.04	0.72
21:N:1523:TGL:HA81	21:N:1523:TGL:H231	1.71	0.72
19:C:268:PGV:H061	29:C:4333:HOH:O	1.89	0.72
3:C:95:THR:HG21	19:C:268:PGV:H282	1.71	0.72
26:G:269:CDL:H171	29:G:4479:HOH:O	1.90	0.71
7:G:72:ASN:N	7:G:76:ASN:HD22	1.83	0.71
22:R:1229:PSC:H343	22:R:1229:PSC:C14	2.20	0.71
9:V:61:GLU:HG3	9:V:65:LYS:NZ	2.06	0.71
12:Y:20:ARG:NH2	21:Y:1522:TGL:HC32	2.05	0.71
6:S:52:ILE:O	6:S:94:HIS:ND1	2.25	0.70
12:Y:20:ARG:NH2	21:Y:1522:TGL:CC3	2.54	0.70
26:C:270:CDL:HA22	29:J:4496:HOH:O	1.92	0.70
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.27	0.70
7:G:3:ALA:CB	25:G:1263:PEK:H383	2.22	0.69
25:C:265:PEK:H041	7:G:17:ARG:HH22	1.57	0.69
19:N:1524:PGV:H012	19:N:1524:PGV:C22	2.22	0.69
1:N:351:GLY:CA	1:N:380[A]:VAL:HG13	2.21	0.69
6:S:94:HIS:HD2	6:S:95:GLN:HA	1.57	0.69
12:Y:12:PRO:HB2	21:Y:1522:TGL:HG11	1.72	0.69
22:B:229:PSC:H041	5:E:41:LEU:HD23	1.73	0.69
21:B:521:TGL:H252	21:B:521:TGL:HA91	1.75	0.69
7:T:3:ALA:CB	25:T:263:PEK:H383	2.22	0.69
21:D:523:TGL:H242	21:D:523:TGL:HA91	1.74	0.69
25:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.39	0.68
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.75	0.68
10:J:26:ALA:O	10:J:30:ILE:HD12	1.94	0.68
10:J:4:ARG:HD3	10:J:7:GLU:OE2	1.94	0.68
7:T:2:SER:O	25:T:263:PEK:H331	1.93	0.68
7:G:5:LYS:HB3	1:N:278:MET:SD	2.34	0.68
7:T:45:PRO:HD2	29:T:3099:HOH:O	1.94	0.68
26:C:270:CDL:H222	26:C:270:CDL:H661	1.76	0.68
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.76	0.67
6:S:94:HIS:CD2	6:S:95:GLN:CA	2.73	0.67
14:A:515:HEA:HMC1	14:A:515:HEA:HBC1	1.75	0.67
21:N:1523:TGL:HG11	21:N:1523:TGL:CC2	2.18	0.67
7:T:37:LEU:HD21	26:T:1269:CDL:H361	1.76	0.67
7:G:7:ASP:O	7:G:9:GLY:N	2.22	0.67
1:N:378:HIS:HA	1:N:382[A]:SER:OG	1.93	0.67
26:T:1269:CDL:OB4	26:T:1269:CDL:H1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:268:PGV:H102	29:C:4697:HOH:O	1.94	0.67
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.82	0.67
1:N:351:GLY:C	1:N:380[A]:VAL:CG1	2.62	0.66
29:A:4171:HOH:O	22:B:229:PSC:H32	1.96	0.66
2:O:52:HIS:CE1	22:R:1229:PSC:H202	2.31	0.66
21:Y:1522:TGL:OC1	21:Y:1522:TGL:HC51	1.96	0.66
2:B:183:THR:CG2	29:B:4424:HOH:O	2.43	0.66
25:C:265:PEK:H371	26:G:269:CDL:C27	2.26	0.66
2:O:227:LEU:HB2	29:O:4695:HOH:O	1.96	0.66
10:J:33:ARG:HG2	23:J:60:CHD:C15	2.25	0.66
1:A:282:PHE:HA	7:T:4:ALA:HB1	1.76	0.66
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.77	0.66
25:C:265:PEK:H042	6:F:1:ALA:H1	1.61	0.66
22:B:229:PSC:H31	22:B:229:PSC:H221	1.78	0.66
8:H:9:LYS:O	8:H:10:ASN:CB	2.43	0.65
29:N:4633:HOH:O	2:O:87:MET:SD	2.53	0.65
26:G:269:CDL:H752	1:N:282:PHE:HZ	1.62	0.65
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.79	0.65
26:T:1269:CDL:H111	26:T:1269:CDL:HA21	1.78	0.65
6:S:94:HIS:CG	6:S:95:GLN:H	2.12	0.65
6:F:87:THR:HG21	29:F:4730:HOH:O	1.97	0.65
19:P:1267:PGV:H181	26:P:1270:CDL:H651	1.79	0.65
4:D:86:MET:CE	29:K:4243:HOH:O	2.44	0.64
12:L:11:ILE:CG2	21:L:522:TGL:H272	2.27	0.64
1:N:407:ASP:O	1:N:411:LYS:HG3	1.97	0.64
12:Y:47:LYS:OXT	12:Y:47:LYS:HE2	1.97	0.64
25:C:265:PEK:H222	25:C:265:PEK:H6	1.80	0.64
26:T:1269:CDL:H241	26:T:1269:CDL:C53	2.27	0.64
7:T:7:ASP:CG	7:T:8:HIS:N	2.51	0.64
1:A:51:ASP:OD1	1:A:441:SER:OG	2.12	0.64
12:Y:22:LEU:O	12:Y:26:THR:HB	1.96	0.64
4:Q:94:LEU:HD23	11:X:28:VAL:HG21	1.79	0.64
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.63	0.63
1:N:87:ILE:O	1:N:173:PRO:HD3	1.99	0.63
8:H:43:MET:CE	8:H:49:ASP:H	2.11	0.63
1:N:113:LEU:HD12	21:Y:1522:TGL:C13	2.28	0.63
8:H:46:LYS:HE2	8:U:8:ILE:CG2	2.27	0.63
2:O:59:GLN:C	2:O:60:GLU:HG3	2.19	0.63
25:C:264:PEK:HN2	7:G:76:ASN:HD21	1.46	0.63
6:F:64:GLU:O	6:F:65:ASP:HB2	1.97	0.63
4:Q:92:THR:O	4:Q:95:LEU:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:2:GLU:HG2	29:W:4564:HOH:O	1.98	0.63
4:D:78:TRP:HB3	21:D:523:TGL:HB22	1.81	0.62
10:J:33:ARG:HG2	23:J:60:CHD:H151	1.80	0.62
1:A:485:VAL:HG22	13:M:1:ILE:HG13	1.82	0.62
25:P:1264:PEK:H12	25:P:1264:PEK:H242	1.80	0.62
6:S:94:HIS:CG	6:S:95:GLN:N	2.66	0.62
12:Y:2:HIS:CG	12:Y:3:TYR:H	2.17	0.62
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.82	0.62
13:M:10:THR:HA	13:M:14:GLU:OE2	2.00	0.62
26:P:1270:CDL:HB22	26:P:1270:CDL:PA1	2.40	0.62
22:R:1229:PSC:H071	9:V:10:ARG:HE	1.65	0.62
26:G:269:CDL:H351	2:O:78:LEU:HD12	1.80	0.61
3:P:29:SER:CB	3:P:42:LEU:HD13	2.28	0.61
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.83	0.61
1:N:488:THR:HB	1:N:495:LEU:HD13	1.82	0.61
23:P:1271:CHD:C16	23:P:1271:CHD:H232	2.31	0.61
14:A:516:HEA:HMC1	14:A:516:HEA:HBC1	1.81	0.61
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.15	0.61
1:N:351:GLY:C	1:N:380[A]:VAL:HG13	2.21	0.61
26:T:1269:CDL:H751	26:T:1269:CDL:H582	1.83	0.61
1:A:514:LYS:NZ	29:A:2645:HOH:O	2.34	0.61
19:A:524:PGV:H221	19:A:524:PGV:H012	1.82	0.61
3:C:63:ARG:NH2	26:C:270:CDL:HA21	2.15	0.61
2:O:62:GLU:O	2:O:66:THR:HB	2.01	0.61
3:C:33:MET:HE3	29:J:4237:HOH:O	2.01	0.60
10:W:2:GLU:CB	10:W:4:ARG:HH12	2.10	0.60
26:G:269:CDL:H362	2:O:81:LEU:HD12	1.83	0.60
8:U:48:GLY:HA2	29:U:4792:HOH:O	2.00	0.60
1:N:113:LEU:HD12	21:Y:1522:TGL:C14	2.31	0.60
1:N:484:THR:HB	13:Z:2:THR:OG1	2.02	0.60
4:Q:66:GLU:HG2	29:Q:4646:HOH:O	2.02	0.60
7:G:2:SER:OG	25:G:1263:PEK:H292	2.00	0.60
2:O:66:THR:HG21	23:O:229:CHD:H3	1.84	0.60
6:F:1:ALA:CB	6:S:65:ASP:OD1	2.49	0.60
12:L:2:HIS:CG	12:L:3:TYR:H	2.19	0.59
1:A:351:GLY:C	1:A:380[A]:VAL:CG1	2.70	0.59
7:G:6:GLY:O	25:G:1263:PEK:H311	2.03	0.59
29:A:2527:HOH:O	12:L:7:PRO:HG3	2.03	0.59
1:A:351:GLY:CA	1:A:380[A]:VAL:HG13	2.33	0.59
3:P:210:ILE:HG12	19:P:1267:PGV:H132	1.85	0.59
21:B:521:TGL:C28	21:B:521:TGL:H101	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.38	0.58
2:O:56:MET:HA	22:R:1229:PSC:H201	1.83	0.58
3:C:80:ARG:NH1	3:C:236:GLU:OE2	2.34	0.58
1:N:177:SER:H	1:N:180:GLN:NE2	2.00	0.58
1:N:377:PHE:O	1:N:381[A]:LEU:HB3	2.03	0.58
25:G:1263:PEK:H221	25:G:1263:PEK:HN1	1.68	0.58
21:N:1523:TGL:H231	21:N:1523:TGL:CA9	2.33	0.58
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.84	0.58
1:N:113:LEU:CD1	21:Y:1522:TGL:H292	2.33	0.58
21:N:1523:TGL:HC61	29:O:3562:HOH:O	2.03	0.58
4:Q:109:HIS:HD2	29:Q:3122:HOH:O	1.86	0.58
26:C:270:CDL:O1	26:C:270:CDL:OA3	2.11	0.58
1:N:377:PHE:O	1:N:381[B]:LEU:HB2	2.04	0.58
2:O:59:GLN:O	2:O:59:GLN:CG	2.40	0.58
1:A:400:PHE:HB3	21:L:522:TGL:H283	1.86	0.58
19:A:524:PGV:H142	19:A:524:PGV:C30	2.34	0.58
23:O:229:CHD:H212	23:O:229:CHD:H12	1.85	0.58
23:C:525:CHD:H152	19:C:268:PGV:H11	1.86	0.58
3:C:55:TYR:CE1	26:C:270:CDL:H512	2.38	0.58
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.39	0.58
9:V:10:ARG:HG3	9:V:10:ARG:HH11	1.68	0.58
9:V:61:GLU:HG3	9:V:65:LYS:HZ1	1.69	0.58
1:N:113:LEU:HD13	21:Y:1522:TGL:H292	1.85	0.57
25:C:265:PEK:H371	26:G:269:CDL:H273	1.86	0.57
26:C:270:CDL:CB2	10:J:8:LYS:HZ2	2.01	0.57
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.69	0.57
21:B:521:TGL:HC21	29:I:2606:HOH:O	2.04	0.57
25:C:265:PEK:H042	6:F:1:ALA:N	2.20	0.57
1:N:400:PHE:HB3	21:Y:1522:TGL:H283	1.87	0.57
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.87	0.57
1:N:449:MET:SD	2:O:5:MET:HG2	2.44	0.57
25:T:1265:PEK:C37	26:T:1269:CDL:C27	2.82	0.57
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.86	0.57
9:V:2:THR:HG22	9:V:3:ALA:H	1.69	0.57
7:G:7:ASP:HB3	29:N:4167:HOH:O	2.02	0.57
8:H:45:ALA:O	8:H:47:GLY:N	2.37	0.57
3:P:223:LEU:HD21	23:P:1271:CHD:H183	1.87	0.57
1:N:514:LYS:HA	6:S:38:ALA:CB	2.35	0.56
26:C:270:CDL:HB22	10:J:8:LYS:HZ1	1.65	0.56
1:A:307:SER:HB3	26:T:1269:CDL:H171	1.86	0.56
22:R:1229:PSC:H011	22:R:1229:PSC:C2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:TPO:CG2	7:G:11:TPO:O	2.53	0.56
29:N:4604:HOH:O	11:X:8:ASP:HB2	2.05	0.56
2:O:13:THR:HB	2:O:168:LEU:HD23	1.88	0.56
21:O:1521:TGL:H241	21:O:1521:TGL:H201	1.87	0.56
19:C:268:PGV:C06	29:C:4333:HOH:O	2.52	0.56
2:O:52:HIS:HE1	22:R:1229:PSC:H202	1.68	0.56
6:S:64:GLU:O	6:S:65:ASP:HB2	2.05	0.56
19:A:524:PGV:H312	13:M:16:ALA:HA	1.88	0.56
2:O:146:MET:HA	2:O:213:LEU:HD12	1.88	0.56
9:V:52:ARG:CZ	9:V:52:ARG:HB2	2.36	0.55
23:P:1271:CHD:H232	23:P:1271:CHD:H162	1.87	0.55
7:T:35:SER:HB3	7:T:36:TRP:CE3	2.42	0.55
6:S:54:ASN:HD22	6:S:54:ASN:C	2.09	0.55
7:T:5:LYS:CG	25:T:263:PEK:H371	2.36	0.55
7:G:2:SER:HG	25:G:1263:PEK:H291	1.71	0.55
12:L:14:SER:H	21:L:522:TGL:HC31	1.72	0.55
25:P:1264:PEK:C3	25:P:1264:PEK:H71	2.26	0.55
22:B:229:PSC:H42	29:I:2588:HOH:O	2.07	0.55
2:O:84:LEU:HA	2:O:87:MET:CE	2.36	0.55
3:P:40:MET:O	3:P:44:MET:HG2	2.07	0.55
6:S:92:VAL:HG23	6:S:92:VAL:O	2.06	0.55
1:A:382[A]:SER:O	1:A:386:VAL:HB	2.06	0.55
26:G:269:CDL:C11	26:G:269:CDL:HA21	2.33	0.55
2:O:164:ALA:O	2:O:194:GLY:HA3	2.07	0.55
21:D:523:TGL:HG31	21:D:523:TGL:OA1	2.07	0.55
14:A:516:HEA:HMC1	14:A:516:HEA:CBC	2.37	0.55
21:N:1523:TGL:CA8	21:N:1523:TGL:H231	2.36	0.55
25:T:1265:PEK:C38	26:T:1269:CDL:H271	2.11	0.55
4:D:34:SER:O	4:D:38:LYS:HG3	2.07	0.54
7:G:7:ASP:CB	29:N:4167:HOH:O	2.55	0.54
8:H:23:GLN:HG3	29:H:4128:HOH:O	2.07	0.54
5:R:48:ILE:O	5:R:52:LEU:HG	2.07	0.54
19:U:1268:PGV:C03	29:U:4495:HOH:O	2.22	0.54
6:S:1:ALA:N	25:T:1265:PEK:H041	2.22	0.54
7:T:5:LYS:HG3	25:T:263:PEK:H371	1.90	0.54
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.22	0.54
6:S:95:GLN:HG2	29:S:4728:HOH:O	2.05	0.54
23:W:1059:CHD:H41	29:W:4647:HOH:O	2.07	0.54
1:A:381[A]:LEU:HB2	14:A:516:HEA:CAC	2.38	0.54
6:S:95:GLN:HG3	29:S:4728:HOH:O	2.03	0.54
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.43	0.54
7:T:7:ASP:O	7:T:8:HIS:CB	2.53	0.54
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.43	0.53
3:C:59:ARG:HA	26:C:270:CDL:H522	1.90	0.53
9:V:1:SAC:OAC	9:V:1:SAC:HB3	2.09	0.53
21:D:523:TGL:CG3	29:D:4105:HOH:O	2.42	0.53
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.44	0.53
26:P:1270:CDL:H352	26:P:1270:CDL:H162	1.90	0.53
3:P:51:MET:HB3	26:P:1270:CDL:H392	1.90	0.53
1:N:297:MET:CE	1:N:297:MET:HB2	2.39	0.53
26:T:1269:CDL:C11	26:T:1269:CDL:HA22	2.36	0.53
8:U:43:MET:HE3	8:U:49:ASP:N	2.23	0.53
7:T:8:HIS:O	7:T:9:GLY:C	2.46	0.53
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.91	0.53
19:N:1524:PGV:H011	19:N:1524:PGV:H221	1.85	0.53
21:N:1523:TGL:HA92	21:N:1523:TGL:H231	1.91	0.53
3:C:106:LEU:HD13	19:C:268:PGV:H22	1.90	0.53
4:D:121:LYS:HD3	11:K:52:GLU:HA	1.91	0.53
1:A:47:LEU:O	13:M:41:LYS:HE3	2.09	0.53
7:T:42:ARG:HB2	29:T:4747:HOH:O	2.09	0.53
2:B:58:ALA:O	2:B:62:GLU:HG3	2.09	0.53
25:C:265:PEK:C37	26:G:269:CDL:C27	2.86	0.53
12:L:20:ARG:HH12	21:L:522:TGL:HC61	1.74	0.53
6:S:1:ALA:N	25:T:1265:PEK:C04	2.72	0.53
22:B:229:PSC:C07	9:I:10:ARG:NH2	2.69	0.52
26:G:269:CDL:H471	29:G:4791:HOH:O	2.08	0.52
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.56	0.52
1:A:28:MET:HE2	14:A:515:HEA:H271	1.92	0.52
19:A:524:PGV:C22	19:A:524:PGV:H012	2.39	0.52
2:B:183:THR:HG23	29:B:4424:HOH:O	2.04	0.52
1:N:352:GLY:N	1:N:380[A]:VAL:CG1	2.72	0.52
1:A:87:ILE:O	1:A:173:PRO:HD3	2.10	0.52
8:H:45:ALA:C	8:H:47:GLY:H	2.12	0.52
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.74	0.52
2:B:89:GLU:O	2:B:91:ASN:ND2	2.42	0.52
7:G:11:TPO:CG2	7:G:16:TRP:HE1	2.19	0.52
26:C:270:CDL:PA1	26:C:270:CDL:HB21	2.50	0.52
5:E:52:LEU:O	5:E:55:CYS:HB2	2.09	0.52
2:O:222:TRP:O	2:O:226:MET:HB2	2.10	0.52
6:F:55:LYS:HA	6:F:74:LEU:O	2.10	0.52
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:524:PGV:H142	19:A:524:PGV:H301	1.90	0.52
8:U:9:LYS:CG	8:U:10:ASN:H	2.09	0.52
2:O:84:LEU:HA	2:O:87:MET:HE3	1.92	0.51
25:C:264:PEK:H71	25:C:264:PEK:H32	1.93	0.51
4:D:61:ARG:HD2	29:D:2674:HOH:O	2.10	0.51
29:L:4557:HOH:O	13:M:32:TRP:HH2	1.94	0.51
6:S:76:LYS:HG3	6:S:93:PRO:HG2	1.92	0.51
6:S:94:HIS:O	6:S:95:GLN:HB2	2.09	0.51
5:R:23:ASP:O	5:R:24:ILE:C	2.49	0.51
6:S:95:GLN:O	6:S:97:ALA:N	2.43	0.51
7:G:3:ALA:HB3	25:G:1263:PEK:H362	1.91	0.51
1:N:290:HIS:HD2	1:N:291:HIS:CD2	2.26	0.51
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.98	0.51
12:L:20:ARG:HH22	21:L:522:TGL:CC3	2.19	0.51
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.92	0.51
8:H:7:LYS:O	8:H:8:ILE:HG22	2.10	0.51
1:N:381[A]:LEU:O	1:N:385:ALA:HB3	2.11	0.51
6:S:55:LYS:HA	6:S:74:LEU:O	2.11	0.51
3:P:131:LEU:HD21	26:T:1269:CDL:HB61	1.91	0.51
1:A:177:SER:H	1:A:180:GLN:NE2	2.08	0.51
2:B:62:GLU:O	2:B:66:THR:HB	2.11	0.51
3:P:59:ARG:HA	26:P:1270:CDL:H522	1.93	0.51
7:T:38:HIS:NE2	26:T:1269:CDL:HA21	2.26	0.51
8:U:43:MET:HG3	8:U:49:ASP:O	2.11	0.51
8:H:46:LYS:HE2	8:U:8:ILE:HG21	1.92	0.51
26:P:1270:CDL:OB7	26:P:1270:CDL:H112	2.10	0.51
25:C:265:PEK:C04	6:F:1:ALA:N	2.74	0.51
7:T:17:ARG:NH1	25:T:1265:PEK:O13	2.43	0.51
5:E:31:LYS:HE3	6:F:84:SER:O	2.12	0.50
2:O:83:ILE:O	2:O:87:MET:HG3	2.11	0.50
25:G:1263:PEK:H281	3:P:85:LEU:HD21	1.93	0.50
1:A:351:GLY:HA3	1:A:380[A]:VAL:CG1	2.39	0.50
26:G:269:CDL:C37	2:O:78:LEU:CD1	2.88	0.50
3:C:65:SER:HB2	19:C:267:PGV:H041	1.94	0.50
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.93	0.50
26:G:269:CDL:CA2	26:G:269:CDL:H112	2.33	0.50
8:U:27:ARG:HG2	29:U:4672:HOH:O	2.12	0.50
1:A:377:PHE:O	1:A:381[A]:LEU:HB3	2.11	0.50
1:N:381[A]:LEU:HD13	14:N:516:HEA:HBC2	1.94	0.50
6:S:1:ALA:H1	25:T:1265:PEK:C04	2.24	0.50
9:V:61:GLU:HG3	9:V:65:LYS:HZ2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:LEU:HD12	26:T:1269:CDL:H352	1.93	0.50
12:Y:2:HIS:N	29:Y:4665:HOH:O	2.44	0.50
7:T:8:HIS:O	7:T:9:GLY:O	2.30	0.49
12:Y:14:SER:H	21:Y:1522:TGL:HC31	1.77	0.49
3:P:59:ARG:HG3	26:P:1270:CDL:H511	1.93	0.49
1:A:347:LEU:HD22	1:A:383[B]:MET:SD	2.51	0.49
2:B:68:LEU:HB3	22:B:229:PSC:H182	1.92	0.49
7:G:5:LYS:HB2	25:G:1263:PEK:H351	1.95	0.49
10:J:36:MET:HG2	23:J:60:CHD:H221	1.95	0.49
21:N:1523:TGL:HG32	21:N:1523:TGL:OB1	2.11	0.49
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.49
26:G:269:CDL:H182	1:N:307:SER:CB	2.42	0.49
8:H:7:LYS:O	8:H:8:ILE:HB	2.12	0.49
1:A:21:LEU:CD2	21:L:522:TGL:HA81	2.43	0.49
7:T:5:LYS:HG3	25:T:263:PEK:C37	2.42	0.49
10:W:3:ASN:C	10:W:3:ASN:OD1	2.51	0.49
1:A:115:SER:O	1:A:121:GLY:HA2	2.12	0.49
6:F:54:ASN:OD1	6:F:76:LYS:HD2	2.12	0.49
1:N:489:THR:HA	6:S:71:TRP:O	2.12	0.49
29:N:4743:HOH:O	23:W:1059:CHD:H212	2.12	0.49
1:A:489:THR:HA	6:F:71:TRP:O	2.12	0.49
1:N:71:MET:HE3	1:N:195:LEU:HD21	1.94	0.49
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.77	0.49
3:C:191:GLY:HA3	29:G:2132:HOH:O	2.13	0.49
12:Y:20:ARG:NH2	21:Y:1522:TGL:HC31	2.25	0.49
1:A:310:MET:HE2	1:A:356:ILE:HG23	1.95	0.49
7:G:17:ARG:HD2	29:G:2446:HOH:O	2.12	0.49
3:C:84:ILE:HD13	25:T:263:PEK:H241	1.95	0.49
3:C:210:ILE:HG21	19:C:267:PGV:H282	1.95	0.49
4:D:86:MET:HE2	29:K:4243:HOH:O	2.10	0.49
25:C:265:PEK:C36	26:G:269:CDL:H271	2.42	0.49
4:D:60:TYR:OH	5:E:69:GLU:OE1	2.22	0.48
21:N:1523:TGL:HC81	2:O:47:THR:HA	1.95	0.48
5:R:41:LEU:HD22	22:R:1229:PSC:H072	1.95	0.48
1:N:53:ILE:HD12	12:Y:44:LEU:HD23	1.95	0.48
1:A:310:MET:CE	1:A:356:ILE:HG23	2.43	0.48
1:A:383[A]:MET:O	1:A:384[A]:GLY:C	2.48	0.48
1:N:381[A]:LEU:HB2	14:N:516:HEA:CAC	2.43	0.48
7:T:5:LYS:HG3	25:T:263:PEK:C38	2.42	0.48
7:T:72:ASN:H	7:T:76:ASN:ND2	2.06	0.48
7:G:11:TPO:HG23	7:G:11:TPO:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:1522:TGL:OC1	21:Y:1522:TGL:CC5	2.61	0.48
1:A:478:SER:O	13:M:6:ALA:HB1	2.13	0.48
22:B:229:PSC:H041	5:E:41:LEU:CD2	2.41	0.48
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.13	0.48
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.61	0.48
19:A:524:PGV:H011	19:A:524:PGV:C2	2.38	0.48
7:G:17:ARG:CD	29:G:2446:HOH:O	2.60	0.48
27:C:272:DMU:H1	7:G:69:PHE:HZ	1.79	0.48
1:N:248:LEU:O	1:N:251:PHE:HB2	2.13	0.48
7:G:4:ALA:CB	1:N:282:PHE:HA	2.39	0.48
7:T:38:HIS:HE1	26:T:1269:CDL:OA7	1.95	0.48
1:A:281:GLY:O	7:T:4:ALA:HB1	2.14	0.48
1:A:409:TRP:HB3	1:A:471:ILE:HG12	1.95	0.48
14:N:516:HEA:HBC1	14:N:516:HEA:HMC1	1.96	0.48
5:R:41:LEU:HD23	22:R:1229:PSC:H041	1.95	0.48
26:G:269:CDL:H762	26:G:269:CDL:C56	2.25	0.48
1:N:390:MET:O	1:N:394:VAL:HG13	2.13	0.48
1:N:155:VAL:CG2	25:P:1264:PEK:H382	2.44	0.48
4:Q:12:ALA:O	6:S:75:HIS:NE2	2.46	0.48
1:A:406:ASN:HD21	19:A:524:PGV:H21	1.78	0.47
25:C:265:PEK:H362	26:G:269:CDL:C27	2.44	0.47
7:G:5:LYS:HG3	25:G:1263:PEK:C37	2.40	0.47
3:P:22:LEU:O	3:P:26:LEU:HG	2.14	0.47
1:A:28:MET:CE	14:A:515:HEA:H271	2.45	0.47
21:O:1521:TGL:HA82	21:O:1521:TGL:H301	1.96	0.47
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.97	0.47
6:F:62:CYS:HB3	6:F:85:CYS:HB3	1.96	0.47
1:N:498:CYS:HA	1:N:499:PRO:HA	1.74	0.47
2:B:41:ILE:HD13	22:B:229:PSC:H342	1.97	0.47
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.97	0.47
14:N:515:HEA:HHC	14:N:515:HEA:H11	1.63	0.47
3:P:63:ARG:HE	26:P:1270:CDL:CA2	2.28	0.47
7:T:17:ARG:HD2	29:T:3446:HOH:O	2.13	0.47
27:C:272:DMU:O1	27:C:272:DMU:H29	2.15	0.47
8:U:45:ALA:C	8:U:47:GLY:H	2.13	0.47
2:B:13:THR:HB	2:B:168:LEU:HD23	1.97	0.47
25:C:265:PEK:C36	26:G:269:CDL:C27	2.93	0.47
10:J:40:LEU:HD12	23:J:60:CHD:H183	1.97	0.47
26:C:270:CDL:HA4	26:C:270:CDL:H131	1.97	0.47
4:D:109:HIS:HD2	29:D:2122:HOH:O	1.97	0.47
1:N:240:HIS:O	1:N:241:PRO:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:1229:PSC:O01	22:R:1229:PSC:H212	2.15	0.47
1:N:321:PHE:CD2	22:R:1229:PSC:H341	2.49	0.47
7:T:6:GLY:O	7:T:7:ASP:O	2.32	0.47
21:B:521:TGL:H211	21:B:521:TGL:H241	1.59	0.47
8:H:43:MET:O	8:H:44:THR:C	2.53	0.47
10:J:52:TRP:O	10:J:57:HIS:HE1	1.98	0.47
21:Y:1522:TGL:CC4	21:Y:1522:TGL:OC1	2.63	0.47
2:B:196:CYS:CB	2:B:207:MET:HG3	2.45	0.47
26:T:1269:CDL:H732	26:T:1269:CDL:H541	1.97	0.47
10:W:36:MET:HG3	10:W:40:LEU:HD12	1.97	0.47
7:G:38:HIS:CE1	26:G:269:CDL:H111	2.50	0.46
1:N:62:ALA:HB1	14:N:515:HEA:HMD3	1.96	0.46
21:Y:1522:TGL:H231	21:Y:1522:TGL:HA92	1.92	0.46
1:A:380[A]:VAL:HG23	1:A:381[A]:LEU:N	2.30	0.46
1:A:383[B]:MET:HG2	1:A:421:VAL:HG21	1.95	0.46
5:E:6:GLU:HB2	5:E:10:GLU:OE1	2.15	0.46
25:C:265:PEK:H362	26:G:269:CDL:H272	1.97	0.46
1:N:430:PHE:HE1	21:O:1521:TGL:HB21	1.79	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.97	0.46
23:O:229:CHD:H112	23:O:229:CHD:H12A	1.67	0.46
12:Y:47:LYS:HE3	13:Z:42:LYS:NZ	2.30	0.46
26:P:1270:CDL:H152	26:P:1270:CDL:H202	1.97	0.46
6:S:94:HIS:CD2	6:S:95:GLN:HA	2.44	0.46
1:A:309:THR:CG2	14:A:516:HEA:HMB2	2.45	0.46
2:B:66:THR:HG21	23:B:1085:CHD:H42	1.97	0.46
26:C:270:CDL:C13	26:C:270:CDL:HA4	2.45	0.46
27:C:272:DMU:H1	7:G:69:PHE:CZ	2.51	0.46
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.98	0.46
8:U:78:GLU:O	8:U:78:GLU:HG2	2.15	0.46
10:W:4:ARG:HD2	10:W:7:GLU:OE2	2.16	0.46
12:Y:2:HIS:NE2	12:Y:5:GLU:OE1	2.48	0.46
5:E:23:ASP:N	5:E:23:ASP:OD2	2.49	0.46
2:O:65:TRP:O	2:O:69:PRO:HG2	2.15	0.46
3:P:54:MET:HE3	26:P:1270:CDL:H601	1.97	0.46
4:Q:33:LEU:HA	4:Q:37:GLN:HE21	1.78	0.46
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.46	0.46
19:P:1267:PGV:C18	26:P:1270:CDL:H651	2.46	0.46
3:P:55:TYR:OH	26:P:1270:CDL:H121	2.15	0.46
2:B:92:ASN:HA	2:B:93:PRO:HD2	1.87	0.46
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.16	0.46
3:P:116:TRP:HA	3:P:117:PRO:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.15	0.46
1:N:346:PHE:CE2	21:O:1521:TGL:H271	2.50	0.46
7:T:2:SER:O	25:T:263:PEK:C33	2.62	0.46
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.98	0.46
1:A:309:THR:HG22	14:A:516:HEA:HMB2	1.99	0.45
26:P:1270:CDL:H181	26:P:1270:CDL:H632	1.97	0.45
4:Q:94:LEU:CD2	11:X:28:VAL:HG21	2.46	0.45
1:A:382[A]:SER:HB3	14:A:515:HEA:HMC2	1.98	0.45
1:A:399:LEU:O	1:A:499:PRO:HA	2.17	0.45
4:D:34:SER:H	4:D:37:GLN:NE2	2.14	0.45
23:J:60:CHD:H12A	23:J:60:CHD:H112	1.54	0.45
2:O:226:MET:O	2:O:227:LEU:C	2.55	0.45
4:Q:131:ILE:N	4:Q:131:ILE:HD12	2.32	0.45
5:R:23:ASP:N	5:R:23:ASP:OD2	2.34	0.45
1:A:170:ASN:OD1	3:C:77:LYS:HD2	2.17	0.45
5:R:11:PHE:CG	22:R:1229:PSC:H073	2.51	0.45
1:A:40:GLU:HG2	1:A:54:TYR:CD2	2.52	0.45
14:A:516:HEA:HHA	14:A:516:HEA:HAD2	1.79	0.45
25:C:265:PEK:C37	26:G:269:CDL:H271	2.45	0.45
5:R:31:LYS:O	5:R:31:LYS:HD2	2.16	0.45
1:A:240:HIS:C	1:A:240:HIS:CD2	2.89	0.45
7:G:84:LYS:NZ	29:G:4536:HOH:O	2.48	0.45
7:T:3:ALA:O	7:T:4:ALA:HB2	2.16	0.45
3:C:226:HIS:CE1	26:C:270:CDL:HB31	2.52	0.45
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.98	0.45
29:P:4419:HOH:O	25:T:1265:PEK:H41	2.17	0.45
7:T:17:ARG:CD	29:T:3446:HOH:O	2.65	0.45
1:A:71:MET:N	1:A:72:PRO:CD	2.80	0.45
26:G:269:CDL:C47	29:G:4791:HOH:O	2.64	0.45
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.79	0.45
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.99	0.45
1:A:461:SER:HB2	29:A:2700:HOH:O	2.16	0.45
2:B:66:THR:HG21	23:B:1085:CHD:H3	1.97	0.45
4:D:34:SER:H	4:D:37:GLN:HE21	1.65	0.45
21:L:522:TGL:H202	21:L:522:TGL:H231	1.27	0.45
26:P:1270:CDL:H652	26:P:1270:CDL:H612	1.98	0.45
3:P:51:MET:HG3	26:P:1270:CDL:H672	1.99	0.45
25:T:1265:PEK:H6	25:T:1265:PEK:H222	1.99	0.45
1:A:50:ASP:OD1	1:A:50:ASP:C	2.54	0.45
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.51	0.45
3:P:63:ARG:HE	26:P:1270:CDL:HA21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:3:ALA:O	7:G:4:ALA:HB2	2.16	0.44
13:Z:39:ASN:O	13:Z:43:SER:OG	2.27	0.44
1:N:100:MET:N	3:P:17:PRO:HB3	2.32	0.44
2:O:121:TYR:O	2:O:138:VAL:HA	2.17	0.44
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.00	0.44
19:A:524:PGV:H152	4:D:87:PHE:CZ	2.53	0.44
2:O:7:LEU:HD12	21:O:1521:TGL:HC31	1.98	0.44
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.98	0.44
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.18	0.44
1:N:113:LEU:HD12	21:Y:1522:TGL:H131	1.98	0.44
26:P:1270:CDL:H432	26:P:1270:CDL:H362	1.99	0.44
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.47	0.44
8:H:7:LYS:O	8:H:8:ILE:CB	2.65	0.44
3:C:16:TRP:N	3:C:17:PRO:CD	2.80	0.44
1:A:351:GLY:C	1:A:380[A]:VAL:HG13	2.38	0.44
2:B:56:MET:CA	22:B:229:PSC:H201	2.42	0.44
23:C:271:CHD:H232	23:C:271:CHD:H162	1.98	0.44
12:L:2:HIS:CG	12:L:3:TYR:N	2.85	0.44
21:N:1523:TGL:H181	2:O:47:THR:HB	2.00	0.44
26:P:1270:CDL:HB32	26:P:1270:CDL:CB2	2.36	0.44
5:R:80:GLU:CD	5:R:80:GLU:H	2.21	0.44
1:A:377:PHE:CD1	14:A:516:HEA:HAD1	2.52	0.44
22:B:229:PSC:C02	22:B:229:PSC:H212	2.46	0.44
8:H:49:ASP:O	8:H:52:VAL:HG22	2.18	0.44
9:I:54:TYR:OH	9:I:59:ASP:OD1	2.27	0.44
3:P:37:PHE:HD1	29:P:4771:HOH:O	2.00	0.44
1:A:486:ASP:HB2	29:A:2142:HOH:O	2.18	0.44
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.99	0.44
3:C:15:PRO:O	3:C:19:THR:HG23	2.18	0.44
26:G:269:CDL:CA2	26:G:269:CDL:C11	2.95	0.44
1:N:378:HIS:O	1:N:382[A]:SER:HB2	2.18	0.44
19:A:524:PGV:H12	4:D:87:PHE:CD2	2.53	0.43
9:I:43:ARG:HD3	9:I:43:ARG:HH11	1.62	0.43
11:K:6:ALA:HA	11:K:7:PRO:HD2	1.78	0.43
4:Q:12:ALA:CB	6:S:55:LYS:HE3	2.48	0.43
22:B:229:PSC:H062	22:B:229:PSC:H042	1.75	0.43
3:C:33:MET:CE	29:J:4237:HOH:O	2.61	0.43
26:G:269:CDL:H182	1:N:307:SER:HB2	2.00	0.43
25:P:1264:PEK:H32	25:P:1264:PEK:C7	2.38	0.43
1:A:181:THR:HA	1:A:182:PRO:HD3	1.78	0.43
1:A:34:SER:HB2	14:A:515:HEA:C2B	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:521:PGV:C18	25:C:264:PEK:H332	2.42	0.43
27:C:272:DMU:H29	27:C:272:DMU:C10	2.47	0.43
21:N:1523:TGL:H222	2:O:39:LEU:CD1	2.48	0.43
1:N:514:LYS:H	6:S:38:ALA:H	1.67	0.43
3:P:224:LYS:O	3:P:225:PHE:HB2	2.18	0.43
1:A:408:THR:HB	19:A:524:PGV:H32	2.01	0.43
3:C:109:THR:HB	3:C:110:PRO:CD	2.48	0.43
21:L:522:TGL:HC22	21:L:522:TGL:HC62	1.99	0.43
3:P:165:ILE:HG12	25:T:1265:PEK:H102	2.01	0.43
5:R:107:ASP:N	5:R:107:ASP:OD2	2.45	0.43
8:U:49:ASP:O	8:U:52:VAL:HG13	2.18	0.43
6:F:65:ASP:OD1	6:S:1:ALA:HB3	2.18	0.43
8:H:60:TYR:C	8:H:60:TYR:CD1	2.91	0.43
1:N:512:ASN:HB2	29:N:4003:HOH:O	2.18	0.43
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.53	0.43
21:Y:1522:TGL:C23	21:Y:1522:TGL:HA92	2.49	0.43
1:A:450:TRP:CE3	1:A:450:TRP:HA	2.54	0.43
12:L:46:LYS:O	12:L:47:LYS:HB2	2.18	0.43
26:P:1270:CDL:H222	26:P:1270:CDL:H191	1.77	0.43
12:Y:2:HIS:CG	12:Y:3:TYR:N	2.85	0.43
1:N:473:TRP:CZ3	13:Z:18:GLY:HA3	2.53	0.43
6:F:13:ALA:O	6:F:18:ARG:HD2	2.19	0.43
9:I:51:TYR:HA	9:I:54:TYR:HB2	2.00	0.43
1:N:312:ILE:HG22	1:N:312:ILE:O	2.17	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.19	0.43
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.76	0.43
27:P:272:DMU:H34	7:T:63:GLY:HA2	2.00	0.43
8:U:60:TYR:CD1	8:U:60:TYR:C	2.92	0.43
1:A:500:PRO:HB2	1:A:504:THR:HG21	2.00	0.43
26:G:269:CDL:H241	26:G:269:CDL:H531	1.99	0.43
5:R:41:LEU:CD2	22:R:1229:PSC:H041	2.48	0.43
5:R:74:LYS:HD2	5:R:74:LYS:HA	1.85	0.43
6:S:1:ALA:H2	25:T:1265:PEK:H041	1.83	0.43
6:S:1:ALA:N	25:T:1265:PEK:H042	2.33	0.43
1:A:344:PHE:CD2	1:A:384[B]:GLY:O	2.72	0.43
23:B:1085:CHD:H212	23:B:1085:CHD:H12	2.00	0.43
21:D:523:TGL:OG1	21:D:523:TGL:HB31	2.18	0.43
1:A:21:LEU:HD23	21:L:522:TGL:HA81	2.00	0.43
12:Y:11:ILE:CG2	21:Y:1522:TGL:H272	2.48	0.43
23:B:1085:CHD:H12A	23:B:1085:CHD:H112	1.69	0.42
1:N:382[A]:SER:O	1:N:383[A]:MET:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:109:HIS:CD2	29:Q:3122:HOH:O	2.68	0.42
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.01	0.42
23:J:60:CHD:H211	23:J:60:CHD:H232	1.74	0.42
2:O:68:LEU:HA	2:O:68:LEU:HD12	1.73	0.42
4:Q:33:LEU:HD22	4:Q:37:GLN:HB3	2.01	0.42
22:R:1229:PSC:H042	29:R:3664:HOH:O	2.19	0.42
5:R:11:PHE:CD1	22:R:1229:PSC:H073	2.54	0.42
1:A:246:LEU:HD13	1:A:381[A]:LEU:HD11	2.01	0.42
2:B:78:LEU:CD1	26:T:1269:CDL:H352	2.50	0.42
3:C:109:THR:HB	3:C:110:PRO:HD2	1.99	0.42
3:C:202:GLY:HA3	25:C:264:PEK:H21	2.01	0.42
2:O:202:SER:HB3	2:O:203:ASN:HD22	1.84	0.42
4:Q:7:LYS:HB3	4:Q:8:SER:H	1.68	0.42
5:R:80:GLU:N	5:R:80:GLU:CD	2.73	0.42
26:T:1269:CDL:H581	26:T:1269:CDL:H552	1.94	0.42
10:W:57:HIS:O	10:W:58:LYS:HB2	2.18	0.42
1:A:382[B]:SER:OG	14:A:515:HEA:H121	2.20	0.42
1:N:438:ARG:O	1:N:439:ARG:HB2	2.19	0.42
2:O:52:HIS:HE1	22:R:1229:PSC:H02	1.84	0.42
26:P:1270:CDL:CB2	26:P:1270:CDL:CB3	2.85	0.42
7:T:3:ALA:O	7:T:4:ALA:CB	2.67	0.42
12:L:20:ARG:HH22	21:L:522:TGL:CC5	2.33	0.42
3:P:106:LEU:HD13	19:U:1268:PGV:H21	2.01	0.42
7:G:3:ALA:O	7:G:4:ALA:CB	2.67	0.42
1:N:335:SER:HB2	1:N:336:PRO:HD2	2.00	0.42
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	2.02	0.42
5:R:90:ARG:HB3	5:R:91:PRO:CD	2.43	0.42
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.55	0.42
21:D:523:TGL:HA91	21:D:523:TGL:C24	2.47	0.42
1:A:1:FME:CE	12:L:3:TYR:HE1	2.33	0.42
13:M:13:LYS:HD2	13:M:13:LYS:C	2.40	0.42
4:D:101:HIS:CD2	4:D:102:TYR:CE2	3.08	0.42
1:N:127:THR:HB	1:N:129:TYR:CE2	2.55	0.42
1:N:514:LYS:HE2	29:S:3514:HOH:O	2.18	0.42
14:N:515:HEA:HMC1	14:N:515:HEA:CBC	2.46	0.42
6:F:92:VAL:O	6:F:92:VAL:HG23	2.18	0.41
26:G:269:CDL:OA7	26:G:269:CDL:H311	2.20	0.41
7:G:9:GLY:HA3	1:N:178:GLN:HE21	1.85	0.41
10:J:50:LEU:HD22	10:J:54:SER:OG	2.20	0.41
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.42	0.41
13:Z:41:LYS:NZ	29:Z:3672:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:OD2	14:A:516:HEA:O1A	2.38	0.41
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.02	0.41
21:D:523:TGL:HB71	21:D:523:TGL:HA52	2.01	0.41
12:L:24:MET:SD	21:L:522:TGL:H161	2.60	0.41
6:S:54:ASN:ND2	6:S:54:ASN:C	2.73	0.41
29:P:4425:HOH:O	7:T:11:TPO:CG2	2.68	0.41
7:T:7:ASP:CG	7:T:8:HIS:H	2.24	0.41
1:N:119:GLU:O	12:Y:46:LYS:HE2	2.21	0.41
1:N:377:PHE:HA	1:N:380[B]:VAL:HG22	2.02	0.41
8:U:84:LYS:HA	29:U:3538:HOH:O	2.21	0.41
10:W:31:LEU:HA	10:W:31:LEU:HD12	1.88	0.41
1:A:177:SER:H	1:A:180:GLN:HE21	1.68	0.41
23:C:525:CHD:H112	23:C:525:CHD:H12A	1.81	0.41
4:D:39:ALA:O	4:D:42:GLU:HB2	2.21	0.41
26:G:269:CDL:C24	26:G:269:CDL:H542	2.51	0.41
26:G:269:CDL:H571	26:G:269:CDL:H782	2.01	0.41
26:G:269:CDL:H821	26:G:269:CDL:H791	1.50	0.41
1:A:382[A]:SER:HB3	14:A:515:HEA:C2C	2.50	0.41
12:L:20:ARG:HH22	21:L:522:TGL:CC6	2.33	0.41
13:M:17:ILE:HD13	13:M:17:ILE:HG21	1.87	0.41
22:B:229:PSC:H242	22:B:229:PSC:H271	1.01	0.41
8:H:46:LYS:HE2	8:U:8:ILE:HG22	1.99	0.41
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.74	0.41
4:Q:52:SER:HB2	29:Q:4686:HOH:O	2.19	0.41
7:T:3:ALA:HB1	25:T:263:PEK:H383	2.00	0.41
8:U:50:VAL:O	8:U:51:SER:C	2.57	0.41
10:W:55:PHE:HA	10:W:56:PRO:HD3	1.83	0.41
1:A:195:LEU:HD23	1:A:245:ILE:HD13	2.02	0.41
1:N:334:TRP:CE3	21:N:1523:TGL:HA31	2.56	0.41
1:N:318:VAL:HG22	2:O:65:TRP:HD1	1.85	0.41
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.51	0.41
5:R:90:ARG:CB	5:R:91:PRO:HD3	2.44	0.41
6:F:92:VAL:O	6:F:92:VAL:CG2	2.69	0.41
21:N:1523:TGL:OB1	21:N:1523:TGL:CG3	2.68	0.41
22:R:1229:PSC:H063	22:R:1229:PSC:H042	1.76	0.41
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.02	0.41
1:A:190:ILE:CD1	1:A:278:MET:HG2	2.51	0.41
19:A:524:PGV:C21	19:A:524:PGV:H012	2.51	0.41
23:J:60:CHD:H161	29:J:4539:HOH:O	2.21	0.41
1:N:66:ILE:HG23	1:N:246:LEU:HD21	2.03	0.41
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HG3	6:F:38:ALA:HB2	2.02	0.41
2:O:226:MET:O	2:O:227:LEU:O	2.38	0.41
26:P:1270:CDL:HB21	26:P:1270:CDL:CB4	2.51	0.41
1:N:103:TRP:O	3:P:21:ALA:HB1	2.21	0.41
6:S:1:ALA:H1	25:T:1265:PEK:H042	1.86	0.41
25:T:1265:PEK:H311	25:T:1265:PEK:H282	1.84	0.41
7:T:3:ALA:CB	25:T:263:PEK:C38	2.95	0.41
25:C:264:PEK:C7	25:C:264:PEK:H32	2.51	0.40
22:R:1229:PSC:C02	22:R:1229:PSC:H212	2.51	0.40
26:T:1269:CDL:OA7	26:T:1269:CDL:H342	2.21	0.40
22:B:229:PSC:H341	22:B:229:PSC:H142	2.00	0.40
10:J:33:ARG:HG2	23:J:60:CHD:H152	2.01	0.40
19:N:1524:PGV:H22	19:N:1524:PGV:C01	2.52	0.40
3:P:226:HIS:CE1	26:P:1270:CDL:HB31	2.57	0.40
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.56	0.40
7:T:3:ALA:HB3	25:T:263:PEK:H383	2.01	0.40
4:D:92:THR:O	4:D:95:LEU:HB2	2.21	0.40
1:N:374:VAL:HG13	1:N:378:HIS:CE1	2.56	0.40
1:N:37:ILE:HD11	1:N:58:VAL:HA	2.03	0.40
1:N:68:PHE:HA	1:N:72:PRO:HG2	2.03	0.40
2:O:116:LEU:HD13	2:O:226:MET:HG3	2.03	0.40
2:B:98:LYS:HB2	2:B:109:GLU:HB2	2.02	0.40
2:B:164:ALA:O	2:B:194:GLY:HA3	2.21	0.40
21:D:523:TGL:H231	21:D:523:TGL:CA9	2.51	0.40
1:N:34:SER:HB2	14:N:515:HEA:C2B	2.51	0.40
23:P:1271:CHD:H12A	23:P:1271:CHD:H112	1.54	0.40
4:Q:16:TYR:HB2	4:Q:27:VAL:HG23	2.04	0.40
1:A:403:TYR:HA	1:A:480:ARG:O	2.21	0.40
3:C:207:HIS:HD2	3:C:241:TYR:OH	2.05	0.40
4:D:48:TRP:HB2	5:E:96:LEU:O	2.21	0.40
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.93	0.40
1:N:240:HIS:CE1	1:N:244:TYR:OH	2.74	0.40
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.85	0.40
3:P:131:LEU:CD2	26:T:1269:CDL:HB61	2.51	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	517/514 (101%)	502 (97%)	15 (3%)	0	100	100
1	N	517/514 (101%)	495 (96%)	22 (4%)	0	100	100
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	34	30
2	O	225/227 (99%)	219 (97%)	5 (2%)	1 (0%)	34	30
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	8 (6%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	100 (97%)	2 (2%)	1 (1%)	15	9
6	F	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	4	1
6	S	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	4	1
7	G	81/85 (95%)	68 (84%)	7 (9%)	6 (7%)	1	0
7	T	81/85 (95%)	67 (83%)	6 (7%)	8 (10%)	0	0
8	H	77/85 (91%)	68 (88%)	3 (4%)	6 (8%)	1	0
8	U	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	2	0
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3514/3614 (97%)	3356 (96%)	125 (4%)	33 (1%)	17	11

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
8	H	8	ILE
8	H	44	THR
8	H	46	LYS
2	O	60	GLU
5	R	6	GLU
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	37	LEU
7	T	38	HIS
8	U	10	ASN
8	U	45	ALA
8	U	46	LYS
7	G	3	ALA
7	G	37	LEU
7	T	9	GLY
8	U	8	ILE
2	B	60	GLU
6	F	96	LEU
8	H	10	ASN
8	H	43	MET
7	T	5	LYS
7	G	6	GLY
8	H	45	ALA
7	T	6	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/426 (101%)	419 (97%)	11 (3%)	46	48
1	N	430/426 (101%)	414 (96%)	16 (4%)	34	32
2	B	210/210 (100%)	200 (95%)	10 (5%)	25	22
2	O	210/210 (100%)	196 (93%)	14 (7%)	16	11
3	C	224/226 (99%)	217 (97%)	7 (3%)	40	40
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	55
4	D	128/129 (99%)	124 (97%)	4 (3%)	40	40
4	Q	128/129 (99%)	121 (94%)	7 (6%)	21	17
5	E	92/95 (97%)	88 (96%)	4 (4%)	29	26
5	R	92/95 (97%)	89 (97%)	3 (3%)	38	37
6	F	81/81 (100%)	76 (94%)	5 (6%)	18	13
6	S	81/81 (100%)	77 (95%)	4 (5%)	25	21
7	G	67/68 (98%)	59 (88%)	8 (12%)	5	3
7	T	67/68 (98%)	58 (87%)	9 (13%)	4	2
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	6
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	10
9	I	57/57 (100%)	50 (88%)	7 (12%)	4	2
9	V	57/57 (100%)	48 (84%)	9 (16%)	2	1
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	58
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	58
11	K	39/46 (85%)	36 (92%)	3 (8%)	13	8
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	19
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	48
12	Y	39/40 (98%)	36 (92%)	3 (8%)	13	8
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	3
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3048/3082 (99%)	2895 (95%)	153 (5%)	24	20

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	44	PRO
1	A	109	PHE
1	A	180	GLN
1	A	265	LYS
1	A	297	MET
1	A	333	LYS
1	A	369	ASP
1	A	444	PRO
1	A	486	ASP
1	A	512	ASN
2	B	33	LEU
2	B	60	GLU
2	B	61	VAL
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	115	ASP
2	B	171	LYS
3	C	17	PRO
3	C	33	MET
3	C	127	LEU
3	C	159	MET
3	C	161	GLN
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	20	ARG
4	D	31	LYS
4	D	51	LEU
5	E	31	LYS
5	E	70	VAL
5	E	90	ARG
5	E	109	VAL
6	F	37	LYS

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Mol	Chain	Res	Type
6	F	48	LEU
6	F	94	HIS
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	8	HIS
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	29	CYS
8	H	52	VAL
8	H	60	TYR
9	I	8	GLN
9	I	26	MET
9	I	29	LEU
9	I	36	LYS
9	I	37	PHE
9	I	43	ARG
9	I	68	ILE
10	J	50	LEU
11	K	20	SER
11	K	47	ARG
11	K	54	ARG
12	L	47	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
1	N	109	PHE
1	N	136	LEU
1	N	152	LEU
1	N	169	ILE
1	N	180	GLN
1	N	278	MET
1	N	290	HIS
1	N	333	LYS

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Mol	Chain	Res	Type
1	N	338	MET
1	N	369	ASP
1	N	438	ARG
1	N	484	THR
1	N	495	LEU
1	N	504	THR
1	N	508	PRO
1	N	512	ASN
2	O	18	GLU
2	O	33	LEU
2	O	59	GLN
2	O	60	GLU
2	O	61	VAL
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	171	LYS
2	O	203	ASN
2	O	217	LYS
2	O	227	LEU
3	P	29	SER
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	246	ASP
4	Q	5	VAL
4	Q	9	GLU
4	Q	17	VAL
4	Q	51	LEU
4	Q	141	ASP
4	Q	143	ASN
4	Q	147	LYS
5	R	46	LYS
5	R	80	GLU
5	R	109	VAL
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	64	GLU
7	T	2	SER

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Mol	Chain	Res	Type
7	T	5	LYS
7	T	8	HIS
7	T	17	ARG
7	T	18	PHE
7	T	36	TRP
7	T	37	LEU
7	T	42	ARG
7	T	84	LYS
8	U	7	LYS
8	U	9	LYS
8	U	52	VAL
8	U	60	TYR
8	U	84	LYS
9	V	2	THR
9	V	18	ARG
9	V	26	MET
9	V	29	LEU
9	V	37	PHE
9	V	61	GLU
9	V	65	LYS
9	V	70	GLN
9	V	73	LYS
10	W	50	LEU
11	X	20	SER
11	X	47	ARG
12	Y	20	ARG
12	Y	26	THR
12	Y	47	LYS
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN

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Mol	Chain	Res	Type
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	68	GLN
3	C	70	HIS
3	C	207	HIS
4	D	29	HIS
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
5	E	78	HIS
5	E	94	ASN
7	G	76	ASN
8	H	23	GLN
9	I	8	GLN
10	J	29	ASN
10	J	57	HIS
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	328	HIS
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	52	HIS
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
2	O	203	ASN
3	P	50	ASN
3	P	68	GLN
3	P	70	HIS
3	P	207	HIS
4	Q	37	GLN
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
6	S	94	HIS
6	S	95	GLN

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Mol	Chain	Res	Type
6	S	98	HIS
7	T	8	HIS
7	T	76	ASN
8	U	12	GLN
9	V	8	GLN
13	Z	36	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	TPO	T	11	7	8,10,11	3.02	4 (50%)	10,14,16	1.81	3 (30%)
2	FME	B	1	2	8,9,10	2.26	3 (37%)	7,9,11	8.18	5 (71%)
9	SAC	I	1	9	7,8,9	2.69	2 (28%)	8,9,11	2.30	3 (37%)
7	TPO	G	11	7	8,10,11	2.83	4 (50%)	10,14,16	1.44	2 (20%)
9	SAC	V	1	9	7,8,9	3.44	2 (28%)	8,9,11	2.29	3 (37%)
1	FME	N	1	1	8,9,10	0.67	0	7,9,11	6.10	1 (14%)
1	FME	A	1	1	8,9,10	0.70	0	7,9,11	5.41	2 (28%)
2	FME	O	1	2	8,9,10	1.21	1 (12%)	7,9,11	5.21	3 (42%)

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

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-OG1	6.58	1.71	1.59
9	V	1	SAC	CA-N	6.41	1.55	1.46
9	V	1	SAC	OAC-C1A	5.79	1.36	1.23
7	G	11	TPO	P-OG1	5.37	1.69	1.59
9	I	1	SAC	OAC-C1A	5.33	1.35	1.23
2	B	1	FME	O1-CN	-4.75	1.08	1.22
9	I	1	SAC	CA-N	4.22	1.52	1.46
7	G	11	TPO	P-O1P	4.17	1.64	1.50
7	T	11	TPO	P-O1P	3.63	1.62	1.50
2	B	1	FME	CA-N	2.78	1.50	1.46
7	G	11	TPO	P-O2P	2.50	1.64	1.54
2	B	1	FME	CG-SD	-2.36	1.68	1.81
2	O	1	FME	O1-CN	-2.29	1.15	1.22
7	T	11	TPO	P-O3P	2.26	1.63	1.54
7	T	11	TPO	P-O2P	2.05	1.62	1.54
7	G	11	TPO	CG2-CB	2.01	1.56	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.70	90.98	122.82
1	N	1	FME	CA-N-CN	-15.77	98.57	122.82
1	A	1	FME	CA-N-CN	-13.36	102.27	122.82
2	O	1	FME	CA-N-CN	-13.30	102.36	122.82
1	A	1	FME	CE-SD-CG	4.61	116.22	100.40
2	B	1	FME	CG-CB-CA	-4.12	101.51	112.95
9	V	1	SAC	CA-N-C1A	4.11	130.73	123.15
9	V	1	SAC	C-CA-N	4.05	117.05	109.73
9	I	1	SAC	C-CA-N	3.66	116.34	109.73
7	T	11	TPO	O3P-P-OG1	3.32	120.87	105.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	SAC	OG-CB-CA	-3.19	102.83	110.97
9	I	1	SAC	CA-N-C1A	3.09	128.84	123.15
7	T	11	TPO	P-OG1-CB	3.06	132.46	123.21
2	B	1	FME	C-CA-N	3.04	115.22	109.73
7	G	11	TPO	O2P-P-OG1	2.54	117.36	105.99
2	B	1	FME	CB-CG-SD	-2.52	99.92	113.48
7	G	11	TPO	O-C-CA	-2.30	118.74	124.78
2	B	1	FME	O-C-CA	-2.28	118.80	124.78
7	T	11	TPO	O-C-CA	-2.19	119.03	124.78
2	O	1	FME	CG-CB-CA	-2.13	107.04	112.95
2	O	1	FME	O1-CN-N	-2.12	119.68	125.27
9	V	1	SAC	O-C-CA	-2.06	119.37	124.78

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
2	B	1	FME	O1-CN-N-CA
9	I	1	SAC	O-C-CA-CB
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	V	1	SAC	CB-CA-N-C1A
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	O	1	FME	O1-CN-N-CA
9	V	1	SAC	N-CA-CB-OG
1	A	1	FME	CB-CG-SD-CE
9	V	1	SAC	C-CA-CB-OG
9	I	1	SAC	C-CA-N-C1A
1	A	1	FME	C-CA-CB-CG
7	T	11	TPO	CB-OG1-P-O3P
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	2	0
7	G	11	TPO	4	0
9	V	1	SAC	1	0
1	A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSC	R	1229	-	51,51,51	1.34	3 (5%)	57,59,59	1.30	3 (5%)
14	HEA	N	515	1	44,67,67	1.06	3 (6%)	37,103,103	1.87	10 (27%)
27	DMU	Z	1526	-	34,34,34	1.12	2 (5%)	45,45,45	3.14	26 (57%)
14	HEA	A	515	1	44,67,67	1.38	8 (18%)	37,103,103	2.10	13 (35%)
21	TGL	B	521	-	62,62,62	1.30	6 (9%)	65,65,65	1.89	14 (21%)
19	PGV	P	1267	-	50,50,50	0.93	3 (6%)	53,56,56	1.53	8 (15%)
19	PGV	U	1268	-	50,50,50	1.58	4 (8%)	53,56,56	1.85	8 (15%)
25	PEK	T	263	-	52,52,52	1.46	3 (5%)	55,57,57	1.33	6 (10%)
21	TGL	D	523	-	62,62,62	1.61	7 (11%)	65,65,65	1.54	13 (20%)
22	PSC	B	229	-	51,51,51	1.21	3 (5%)	57,59,59	1.35	7 (12%)
19	PGV	C	268	-	50,50,50	1.42	4 (8%)	53,56,56	1.64	7 (13%)
15	NO	A	520	16	0,1,1	0.00	-	-		
20	CUA	B	228	2	0,1,1	0.00	-	-		
14	HEA	N	516	1,15	44,67,67	1.23	6 (13%)	37,103,103	2.44	14 (37%)
23	CHD	J	60	-	29,32,32	0.96	0	48,51,51	5.36	35 (72%)
25	PEK	P	1264	-	52,52,52	0.92	3 (5%)	55,57,57	1.78	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	TGL	O	1521	-	62,62,62	1.37	6 (9%)	65,65,65	1.59	11 (16%)
23	CHD	O	229	-	29,32,32	1.65	5 (17%)	48,51,51	5.72	32 (66%)
25	PEK	C	264	-	52,52,52	0.91	2 (3%)	55,57,57	1.77	15 (27%)
25	PEK	C	265	-	52,52,52	1.61	6 (11%)	55,57,57	1.62	8 (14%)
15	NO	N	520	14,16	0,1,1	0.00	-	-		
26	CDL	G	269	-	99,99,99	1.44	12 (12%)	105,111,111	1.53	20 (19%)
19	PGV	C	267	-	50,50,50	0.88	3 (6%)	53,56,56	1.36	8 (15%)
21	TGL	Y	1522	-	62,62,62	1.70	10 (16%)	65,65,65	2.18	18 (27%)
26	CDL	P	1270	-	99,99,99	1.46	12 (12%)	105,111,111	1.69	21 (20%)
26	CDL	T	1269	-	99,99,99	1.43	12 (12%)	105,111,111	1.53	15 (14%)
21	TGL	L	522	-	62,62,62	1.58	7 (11%)	65,65,65	2.11	16 (24%)
20	CUA	O	228	2	0,1,1	0.00	-	-		
23	CHD	C	525	-	29,32,32	1.60	6 (20%)	48,51,51	5.59	38 (79%)
19	PGV	A	524	-	50,50,50	1.35	3 (6%)	53,56,56	1.64	9 (16%)
26	CDL	C	270	-	99,99,99	1.49	13 (13%)	105,111,111	1.46	18 (17%)
19	PGV	A	521	-	50,50,50	1.27	6 (12%)	53,56,56	1.72	13 (24%)
21	TGL	N	1523	-	62,62,62	1.41	7 (11%)	65,65,65	1.40	10 (15%)
25	PEK	T	1265	-	52,52,52	1.43	6 (11%)	55,57,57	1.52	7 (12%)
23	CHD	P	1271	-	29,32,32	0.81	1 (3%)	48,51,51	5.14	33 (68%)
23	CHD	B	1085	-	29,32,32	1.89	6 (20%)	48,51,51	5.76	34 (70%)
27	DMU	P	272	-	34,34,34	1.67	6 (17%)	45,45,45	3.36	25 (55%)
19	PGV	N	1524	-	50,50,50	1.09	2 (4%)	53,56,56	1.30	6 (11%)
27	DMU	C	272	-	34,34,34	1.51	4 (11%)	45,45,45	3.41	25 (55%)
19	PGV	N	1266	-	50,50,50	0.99	2 (4%)	53,56,56	1.55	11 (20%)
23	CHD	W	1059	-	29,32,32	1.27	3 (10%)	48,51,51	5.45	32 (66%)
23	CHD	C	271	-	29,32,32	0.75	0	48,51,51	5.08	34 (70%)
23	CHD	P	1525	-	29,32,32	1.72	6 (20%)	48,51,51	5.63	38 (79%)
25	PEK	G	1263	-	52,52,52	1.33	3 (5%)	55,57,57	1.41	6 (10%)
27	DMU	M	526	-	34,34,34	1.12	4 (11%)	45,45,45	3.36	25 (55%)
14	HEA	A	516	1	44,67,67	1.54	7 (15%)	37,103,103	2.24	11 (29%)

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
22	PSC	R	1229	-	-	34/55/55/55	-
27	DMU	P	272	-	6/6/10/10	7/19/59/59	0/2/2/2
14	HEA	A	515	1	3/3/7/16	2/24/76/76	-
25	PEK	C	264	-	-	25/56/56/56	-
19	PGV	P	1267	-	-	15/55/55/55	-
19	PGV	U	1268	-	-	31/55/55/55	-
21	TGL	D	523	-	-	34/65/65/65	-
22	PSC	B	229	-	-	37/55/55/55	-
19	PGV	C	268	-	-	31/55/55/55	-
26	CDL	P	1270	-	-	68/110/110/110	-
14	HEA	N	516	1,15	3/3/7/16	2/24/76/76	-
23	CHD	J	60	-	2/2/12/12	5/7/74/74	0/4/4/4
25	PEK	P	1264	-	-	28/56/56/56	-
21	TGL	O	1521	-	-	36/65/65/65	-
23	CHD	O	229	-	-	1/7/74/74	0/4/4/4
19	PGV	A	521	-	-	11/55/55/55	-
25	PEK	T	263	-	-	26/56/56/56	-
25	PEK	C	265	-	-	25/56/56/56	-
26	CDL	G	269	-	-	64/110/110/110	-
19	PGV	C	267	-	-	13/55/55/55	-
21	TGL	Y	1522	-	-	37/65/65/65	-
27	DMU	M	526	-	4/4/10/10	8/19/59/59	0/2/2/2
26	CDL	T	1269	-	-	64/110/110/110	-
21	TGL	L	522	-	-	37/65/65/65	-
23	CHD	C	525	-	-	2/7/74/74	0/4/4/4
19	PGV	A	524	-	-	36/55/55/55	-
26	CDL	C	270	-	-	59/110/110/110	-
27	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
21	TGL	N	1523	-	-	36/65/65/65	-
25	PEK	T	1265	-	-	25/56/56/56	-
23	CHD	P	1271	-	1/1/12/12	4/7/74/74	0/4/4/4
21	TGL	B	521	-	-	34/65/65/65	-
14	HEA	N	515	1	3/3/7/16	2/24/76/76	-
19	PGV	N	1524	-	-	31/55/55/55	-
27	DMU	C	272	-	6/6/10/10	12/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
19	PGV	N	1266	-	-	14/55/55/55	-
23	CHD	W	1059	-	1/1/12/12	4/7/74/74	0/4/4/4
23	CHD	C	271	-	1/1/12/12	4/7/74/74	0/4/4/4
14	HEA	A	516	1	3/3/7/16	4/24/76/76	-
25	PEK	G	1263	-	-	26/56/56/56	-
23	CHD	P	1525	-	1/1/12/12	2/7/74/74	0/4/4/4

All (215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	1522	TGL	OG2-CB1	7.89	1.56	1.34
19	U	1268	PGV	O01-C1	7.27	1.54	1.34
21	L	522	TGL	OG2-CB1	7.26	1.54	1.34
27	P	272	DMU	O16-C6	7.00	1.52	1.40
19	C	268	PGV	O01-C1	6.57	1.52	1.34
25	C	265	PEK	O03-C21	6.45	1.52	1.33
27	C	272	DMU	O16-C6	6.02	1.50	1.40
25	C	265	PEK	O01-C1	5.80	1.50	1.34
25	T	1265	PEK	O01-C1	5.73	1.50	1.34
23	B	1085	CHD	C18-C13	5.72	1.63	1.54
26	P	1270	CDL	OA6-CA5	5.65	1.50	1.34
26	G	269	CDL	OA6-CA5	5.64	1.50	1.34
26	C	270	CDL	OA8-CA7	5.62	1.49	1.33
19	A	524	PGV	O03-C19	5.60	1.49	1.33
26	T	1269	CDL	OA6-CA5	5.59	1.50	1.34
22	R	1229	PSC	O01-C1	5.58	1.50	1.34
25	G	1263	PEK	O03-C21	5.56	1.49	1.33
25	G	1263	PEK	O01-C1	5.55	1.49	1.34
25	T	1265	PEK	O03-C21	5.50	1.49	1.33
21	D	523	TGL	OG2-CB1	5.46	1.49	1.34
21	N	1523	TGL	OG2-CB1	5.42	1.49	1.34
25	T	263	PEK	O03-C21	5.41	1.49	1.33
21	D	523	TGL	OG1-CA1	5.37	1.49	1.33
26	P	1270	CDL	OA8-CA7	5.30	1.48	1.33
25	T	263	PEK	C05-C04	5.28	1.71	1.50
21	O	1521	TGL	OG1-CA1	5.24	1.48	1.33
21	Y	1522	TGL	OG3-CC1	5.22	1.48	1.33
21	D	523	TGL	OB1-CB1	5.22	1.38	1.22
19	N	1524	PGV	O03-C19	5.19	1.48	1.33
19	U	1268	PGV	O03-C19	5.15	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	269	CDL	OB6-CB5	5.11	1.48	1.34
26	C	270	CDL	OB8-CB7	5.05	1.48	1.33
26	P	1270	CDL	OB8-CB7	5.00	1.47	1.33
14	A	516	HEA	C3B-C11	4.97	1.56	1.52
21	B	521	TGL	OG1-CA1	4.96	1.47	1.33
26	G	269	CDL	OA8-CA7	4.95	1.47	1.33
21	O	1521	TGL	OG2-CB1	4.95	1.48	1.34
26	P	1270	CDL	OB6-CB5	4.94	1.48	1.34
23	B	1085	CHD	C10-C5	-4.91	1.47	1.55
21	L	522	TGL	OG1-CA1	4.85	1.47	1.33
26	T	1269	CDL	OB6-CB5	4.84	1.47	1.34
21	N	1523	TGL	OG1-CA1	4.75	1.47	1.33
21	D	523	TGL	OG3-CC1	4.72	1.47	1.33
21	B	521	TGL	OG2-CB1	4.71	1.47	1.34
25	T	263	PEK	O01-C1	4.70	1.47	1.34
26	T	1269	CDL	OB8-CB7	4.67	1.47	1.33
22	B	229	PSC	O03-C19	4.61	1.46	1.33
23	P	1525	CHD	C13-C12	-4.60	1.47	1.54
26	C	270	CDL	OB6-CB5	4.54	1.47	1.34
22	B	229	PSC	O01-C1	4.48	1.46	1.34
26	T	1269	CDL	OA8-CA7	4.45	1.46	1.33
19	A	524	PGV	O01-C1	4.41	1.46	1.34
26	C	270	CDL	OA6-CA5	4.37	1.46	1.34
19	A	521	PGV	O01-C1	4.30	1.46	1.34
21	N	1523	TGL	OG3-CC1	4.27	1.45	1.33
22	R	1229	PSC	O03-C19	4.22	1.45	1.33
19	C	268	PGV	O03-C19	4.22	1.45	1.33
23	O	229	CHD	C18-C13	4.15	1.61	1.54
19	A	521	PGV	O03-C19	4.13	1.45	1.33
23	W	1059	CHD	C20-C17	4.13	1.61	1.54
22	R	1229	PSC	C13-C12	4.10	1.55	1.31
23	O	229	CHD	C13-C14	-4.07	1.48	1.55
26	G	269	CDL	OB8-CB7	4.04	1.45	1.33
21	O	1521	TGL	OG3-CC1	4.00	1.45	1.33
21	Y	1522	TGL	OG1-CA1	3.94	1.44	1.33
21	L	522	TGL	OG3-CC1	3.82	1.44	1.33
14	N	516	HEA	C3B-C11	-3.80	1.49	1.52
23	C	525	CHD	O12-C12	3.66	1.49	1.43
19	N	1266	PGV	O01-C1	3.65	1.44	1.34
25	C	265	PEK	O03-C01	3.59	1.53	1.45
22	B	229	PSC	C13-C12	3.59	1.52	1.31
21	L	522	TGL	C20-CA9	-3.58	1.31	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1085	CHD	C13-C14	-3.55	1.49	1.55
27	Z	1526	DMU	C3-C4	-3.50	1.43	1.52
25	C	264	PEK	O01-C1	3.47	1.44	1.34
26	G	269	CDL	C59-C58	-3.46	1.32	1.51
26	C	270	CDL	C18-C17	3.44	1.70	1.51
19	N	1524	PGV	O01-C1	3.44	1.44	1.34
21	B	521	TGL	OG3-CC1	3.44	1.43	1.33
23	C	525	CHD	C18-C13	3.42	1.60	1.54
19	C	268	PGV	P-O11	3.40	1.73	1.59
21	Y	1522	TGL	C20-CA9	-3.40	1.32	1.51
25	P	1264	PEK	O01-C1	3.39	1.43	1.34
19	N	1266	PGV	O03-C19	3.33	1.43	1.33
23	O	229	CHD	C10-C5	-3.33	1.50	1.55
27	Z	1526	DMU	O16-C6	3.32	1.45	1.40
26	C	270	CDL	C59-C58	-3.30	1.33	1.51
25	C	265	PEK	P-O12	3.23	1.72	1.59
26	T	1269	CDL	C62-C61	-3.17	1.33	1.51
21	O	1521	TGL	C10-CB9	-3.17	1.33	1.51
21	O	1521	TGL	C20-CA9	-3.17	1.33	1.51
26	P	1270	CDL	C59-C58	-3.14	1.33	1.51
21	B	521	TGL	C10-CB9	-3.14	1.33	1.51
27	M	526	DMU	C3-C4	-3.11	1.44	1.52
26	T	1269	CDL	C59-C58	-3.10	1.34	1.51
25	C	265	PEK	P-O11	3.08	1.71	1.59
26	C	270	CDL	C79-C78	-3.06	1.34	1.51
23	P	1525	CHD	C6-C5	-3.03	1.48	1.53
26	G	269	CDL	C42-C41	-3.03	1.34	1.51
26	P	1270	CDL	C22-C21	-3.01	1.34	1.51
26	G	269	CDL	C62-C61	-2.99	1.34	1.51
26	T	1269	CDL	C79-C78	-2.99	1.34	1.51
25	T	1265	PEK	P-O12	2.98	1.71	1.59
26	P	1270	CDL	C19-C18	-2.97	1.34	1.51
23	P	1271	CHD	C20-C17	2.97	1.59	1.54
21	L	522	TGL	C10-CB9	-2.97	1.34	1.51
14	A	516	HEA	CMD-C2D	2.95	1.58	1.51
21	N	1523	TGL	C10-CB9	-2.95	1.35	1.51
26	C	270	CDL	C39-C38	-2.94	1.35	1.51
26	C	270	CDL	C62-C61	-2.93	1.35	1.51
19	A	521	PGV	C03-C02	2.93	1.59	1.50
21	N	1523	TGL	C20-CA9	-2.92	1.35	1.51
23	W	1059	CHD	C11-C9	2.91	1.58	1.53
21	Y	1522	TGL	C10-CB9	-2.91	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	270	CDL	C82-C81	-2.90	1.35	1.51
23	B	1085	CHD	C11-C12	2.89	1.58	1.53
26	P	1270	CDL	C82-C81	-2.89	1.35	1.51
19	P	1267	PGV	O01-C1	2.88	1.42	1.34
26	G	269	CDL	C39-C38	-2.87	1.35	1.51
26	P	1270	CDL	C39-C38	-2.86	1.35	1.51
21	Y	1522	TGL	OG2-CG2	2.86	1.53	1.46
26	G	269	CDL	C22-C21	-2.85	1.35	1.51
26	T	1269	CDL	C82-C81	-2.85	1.35	1.51
26	G	269	CDL	C19-C18	-2.83	1.35	1.51
26	C	270	CDL	C22-C21	-2.83	1.35	1.51
26	G	269	CDL	C79-C78	-2.83	1.35	1.51
21	D	523	TGL	C15-CC9	-2.82	1.35	1.51
26	P	1270	CDL	C62-C61	-2.81	1.35	1.51
26	T	1269	CDL	C42-C41	-2.81	1.35	1.51
14	A	516	HEA	CAD-C3D	2.81	1.56	1.52
25	T	1265	PEK	P-O11	2.80	1.70	1.59
21	N	1523	TGL	C15-CC9	-2.79	1.35	1.51
27	P	272	DMU	O5-C6	2.78	1.48	1.41
27	C	272	DMU	O5-C6	2.76	1.48	1.41
26	T	1269	CDL	C39-C38	-2.75	1.36	1.51
21	Y	1522	TGL	CG1-CG2	2.72	1.59	1.50
19	P	1267	PGV	O03-C19	2.69	1.41	1.33
26	T	1269	CDL	C19-C18	-2.69	1.36	1.51
14	N	515	HEA	C4D-CHA	2.69	1.48	1.41
26	C	270	CDL	C19-C18	-2.68	1.36	1.51
14	N	516	HEA	CAD-C3D	2.68	1.56	1.52
21	D	523	TGL	C20-CA9	-2.67	1.36	1.51
26	T	1269	CDL	C22-C21	-2.65	1.36	1.51
21	B	521	TGL	C20-CA9	-2.64	1.36	1.51
21	Y	1522	TGL	CG3-CG2	2.64	1.58	1.50
14	A	515	HEA	C1C-CHC	2.63	1.48	1.41
14	A	516	HEA	C3C-C2C	-2.63	1.36	1.40
19	C	267	PGV	O03-C19	2.60	1.40	1.33
26	P	1270	CDL	C79-C78	-2.60	1.37	1.51
23	W	1059	CHD	C13-C17	2.60	1.60	1.55
23	P	1525	CHD	C11-C9	2.60	1.58	1.53
23	O	229	CHD	C1-C2	-2.60	1.47	1.53
21	O	1521	TGL	C15-CC9	-2.59	1.37	1.51
26	P	1270	CDL	C42-C41	-2.58	1.37	1.51
26	C	270	CDL	C42-C41	-2.56	1.37	1.51
21	L	522	TGL	C15-CC9	-2.52	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	1522	TGL	C15-CC9	-2.52	1.37	1.51
23	C	525	CHD	C13-C12	-2.51	1.50	1.54
19	A	521	PGV	P-O14	-2.51	1.43	1.55
19	A	521	PGV	C01-C02	2.51	1.58	1.50
26	G	269	CDL	C82-C81	-2.51	1.37	1.51
25	P	1264	PEK	O03-C21	2.48	1.40	1.33
23	P	1525	CHD	C10-C5	-2.46	1.51	1.55
23	O	229	CHD	C6-C7	-2.46	1.48	1.52
23	C	525	CHD	C4-C3	2.44	1.56	1.51
14	A	516	HEA	C20-C19	2.44	1.56	1.51
14	A	515	HEA	C4B-C3B	-2.44	1.37	1.42
14	A	516	HEA	C3C-CAC	2.40	1.52	1.47
27	P	272	DMU	O5-C4	2.39	1.50	1.44
27	M	526	DMU	C6-C1	-2.39	1.45	1.52
27	C	272	DMU	O1-C10	2.38	1.47	1.41
19	A	521	PGV	O01-C02	-2.37	1.40	1.46
21	D	523	TGL	C10-CB9	-2.36	1.38	1.51
21	L	522	TGL	CC2-CC1	2.36	1.57	1.50
27	P	272	DMU	O1-C10	2.35	1.47	1.41
14	N	516	HEA	C1C-CHC	2.32	1.47	1.41
23	B	1085	CHD	C8-C7	-2.32	1.49	1.53
19	C	267	PGV	C03-C02	2.31	1.57	1.50
14	A	515	HEA	C12-C13	2.31	1.61	1.53
21	B	521	TGL	C15-CC9	-2.30	1.38	1.51
25	C	265	PEK	C22-C21	2.28	1.57	1.50
14	A	515	HEA	CMC-C2C	2.27	1.56	1.51
19	C	268	PGV	O04-C19	-2.22	1.15	1.22
14	N	516	HEA	OMA-CMA	2.22	1.29	1.21
23	C	525	CHD	C1-C2	-2.22	1.48	1.53
14	N	516	HEA	C4C-CHD	2.22	1.47	1.41
23	C	525	CHD	C1-C10	-2.22	1.50	1.54
14	A	515	HEA	C3A-C2A	-2.20	1.37	1.40
27	P	272	DMU	O7-C10	2.20	1.47	1.41
27	M	526	DMU	O49-C1	-2.19	1.37	1.43
19	A	524	PGV	C20-C19	2.17	1.57	1.50
23	P	1525	CHD	C16-C17	2.17	1.58	1.54
21	Y	1522	TGL	CB2-CB1	2.16	1.57	1.50
23	P	1525	CHD	C13-C14	-2.15	1.51	1.55
25	G	1263	PEK	P-O11	2.11	1.67	1.59
19	U	1268	PGV	C04-C05	2.11	1.58	1.51
14	N	515	HEA	OMA-CMA	2.10	1.28	1.21
14	N	516	HEA	C14-C15	2.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	1265	PEK	C03-C02	2.07	1.57	1.50
25	P	1264	PEK	C2-C1	2.07	1.56	1.50
19	U	1268	PGV	P-O11	2.06	1.67	1.59
19	P	1267	PGV	P-O14	-2.06	1.45	1.55
21	N	1523	TGL	OB1-CB1	2.06	1.28	1.22
27	C	272	DMU	C3-C4	-2.06	1.47	1.52
25	C	264	PEK	C2-C1	2.05	1.56	1.50
14	A	515	HEA	O11-C11	2.05	1.47	1.42
19	C	267	PGV	O01-C1	2.05	1.40	1.34
23	B	1085	CHD	O12-C12	2.03	1.47	1.43
27	P	272	DMU	C3-C4	-2.03	1.47	1.52
14	A	516	HEA	C3A-C2A	-2.02	1.37	1.40
27	M	526	DMU	C8-C9	-2.02	1.48	1.53
14	N	515	HEA	C4C-CHD	2.02	1.46	1.41
14	A	515	HEA	C1B-CHB	2.01	1.46	1.41
25	T	1265	PEK	C22-C21	2.01	1.56	1.50
14	A	515	HEA	C1A-C2A	-2.00	1.38	1.42

All (718) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C6-C5-C10	15.31	128.91	112.66
23	C	271	CHD	C10-C9-C8	14.65	127.55	111.82
23	O	229	CHD	C18-C13-C12	-13.90	94.92	109.07
23	J	60	CHD	C10-C9-C8	13.01	125.79	111.82
23	O	229	CHD	C14-C13-C12	12.96	119.47	107.40
23	P	1525	CHD	C1-C10-C5	12.96	126.94	107.77
23	O	229	CHD	C6-C5-C10	12.92	126.37	112.66
23	P	1525	CHD	C6-C5-C10	12.84	126.30	112.66
23	P	1271	CHD	C10-C9-C8	12.73	125.48	111.82
23	C	525	CHD	C6-C5-C10	12.57	126.01	112.66
23	B	1085	CHD	C1-C10-C5	12.49	126.24	107.77
23	P	1525	CHD	C18-C13-C12	-11.98	96.87	109.07
23	C	525	CHD	C1-C10-C5	11.91	125.38	107.77
23	P	1525	CHD	C4-C3-C2	11.56	124.35	110.55
23	B	1085	CHD	C10-C9-C8	11.42	124.08	111.82
23	O	229	CHD	C1-C10-C5	11.22	124.36	107.77
23	B	1085	CHD	C18-C13-C12	-11.17	97.70	109.07
23	P	1525	CHD	C14-C13-C12	10.68	117.34	107.40
23	W	1059	CHD	C13-C17-C20	10.58	132.12	119.50
23	P	1525	CHD	C17-C13-C12	10.36	127.12	117.67
23	W	1059	CHD	C10-C9-C8	10.35	122.93	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C23-C22-C20	-10.23	100.94	114.72
23	W	1059	CHD	C14-C8-C7	10.15	125.27	111.81
23	J	60	CHD	C13-C17-C20	10.07	131.51	119.50
23	B	1085	CHD	C17-C13-C12	9.90	126.70	117.67
23	W	1059	CHD	C6-C5-C4	-9.74	99.98	111.19
23	C	525	CHD	C4-C3-C2	9.67	122.10	110.55
23	C	525	CHD	C10-C9-C8	9.45	121.97	111.82
23	O	229	CHD	C19-C10-C9	-9.18	98.53	111.18
23	C	525	CHD	C19-C10-C9	-9.11	98.63	111.18
23	P	1271	CHD	C6-C7-C8	8.97	121.06	111.48
23	B	1085	CHD	C14-C13-C12	8.97	115.75	107.40
23	C	525	CHD	C11-C12-C13	8.92	120.41	111.24
23	O	229	CHD	C10-C9-C8	8.86	121.34	111.82
23	P	1525	CHD	C19-C10-C9	-8.85	98.98	111.18
23	P	1271	CHD	C18-C13-C12	-8.81	100.09	109.07
23	B	1085	CHD	C4-C3-C2	8.72	120.97	110.55
23	P	1525	CHD	C15-C14-C13	8.68	112.07	103.55
23	W	1059	CHD	C15-C14-C13	8.58	111.97	103.55
23	W	1059	CHD	C11-C12-C13	8.56	120.03	111.24
23	W	1059	CHD	C16-C17-C13	8.56	111.95	103.55
23	P	1525	CHD	C10-C9-C8	8.50	120.95	111.82
23	J	60	CHD	C17-C13-C12	8.44	125.37	117.67
23	C	525	CHD	C17-C13-C12	8.43	125.36	117.67
23	J	60	CHD	C18-C13-C12	-8.42	100.49	109.07
23	C	271	CHD	C15-C14-C8	8.26	129.88	118.33
23	C	271	CHD	C6-C5-C10	8.23	121.40	112.66
23	W	1059	CHD	C1-C10-C9	-8.17	98.51	111.35
23	O	229	CHD	C17-C13-C12	8.16	125.11	117.67
23	J	60	CHD	C1-C10-C5	8.13	119.79	107.77
23	W	1059	CHD	C15-C14-C8	8.06	129.59	118.33
23	C	525	CHD	C18-C13-C17	-8.06	98.60	111.21
23	P	1271	CHD	C14-C13-C12	8.03	114.88	107.40
21	Y	1522	TGL	OG2-CB1-CB2	7.99	128.72	111.50
23	J	60	CHD	C16-C17-C13	7.99	111.39	103.55
23	J	60	CHD	C4-C3-C2	7.97	120.06	110.55
23	B	1085	CHD	C5-C4-C3	7.94	124.42	112.76
23	C	525	CHD	C13-C17-C20	7.93	128.97	119.50
23	O	229	CHD	C1-C2-C3	7.88	120.58	110.47
23	C	271	CHD	C5-C6-C7	7.86	123.14	114.46
27	M	526	DMU	O1-C9-C8	7.80	123.87	109.69
23	B	1085	CHD	C19-C10-C9	-7.80	100.44	111.18
23	W	1059	CHD	C5-C6-C7	7.79	123.06	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	229	CHD	C11-C12-C13	7.79	119.24	111.24
23	C	271	CHD	C16-C17-C13	7.74	111.15	103.55
23	C	525	CHD	C17-C13-C14	7.70	107.85	100.09
23	J	60	CHD	C6-C5-C10	7.68	120.81	112.66
23	C	271	CHD	C18-C13-C12	-7.66	101.27	109.07
26	P	1270	CDL	OA6-CA5-C11	7.63	127.95	111.50
27	P	272	DMU	O1-C9-C8	7.60	123.50	109.69
23	P	1271	CHD	C1-C10-C5	7.56	118.96	107.77
23	P	1271	CHD	C6-C5-C10	7.55	120.68	112.66
27	Z	1526	DMU	O1-C9-C8	7.52	123.35	109.69
23	B	1085	CHD	C6-C7-C8	7.45	119.43	111.48
23	W	1059	CHD	C5-C4-C3	7.43	123.67	112.76
27	C	272	DMU	O1-C9-C8	7.43	123.18	109.69
23	P	1271	CHD	C16-C17-C20	7.40	123.60	112.15
27	C	272	DMU	O5-C4-C57	7.38	124.79	106.44
27	Z	1526	DMU	O1-C10-C5	7.36	125.93	110.35
23	P	1271	CHD	C15-C14-C8	7.33	128.58	118.33
23	J	60	CHD	C5-C6-C7	7.31	122.53	114.46
23	J	60	CHD	C11-C12-C13	7.26	118.70	111.24
23	B	1085	CHD	C18-C13-C17	-7.22	99.91	111.21
27	M	526	DMU	O1-C10-C5	7.19	125.56	110.35
21	L	522	TGL	OG3-CC1-OC1	-7.14	105.58	123.59
27	C	272	DMU	O16-C6-C1	7.12	119.42	108.30
14	N	516	HEA	C27-C19-C20	7.07	127.16	115.27
21	B	521	TGL	OG2-CB1-CB2	7.06	126.72	111.50
23	W	1059	CHD	C6-C7-C8	7.05	119.01	111.48
23	J	60	CHD	C6-C7-C8	7.05	119.01	111.48
27	M	526	DMU	O5-C4-C57	7.02	123.89	106.44
23	C	271	CHD	C1-C2-C3	6.99	119.44	110.47
23	C	271	CHD	C14-C13-C12	6.95	113.87	107.40
19	U	1268	PGV	O01-C1-C2	6.91	126.40	111.50
23	O	229	CHD	O12-C12-C13	-6.91	99.35	111.03
23	O	229	CHD	C14-C8-C9	6.90	119.19	109.71
23	P	1271	CHD	C4-C3-C2	6.84	118.72	110.55
23	C	271	CHD	C16-C17-C20	6.81	122.69	112.15
23	P	1271	CHD	C11-C9-C8	6.80	120.83	110.88
23	P	1271	CHD	C1-C2-C3	6.78	119.17	110.47
19	U	1268	PGV	O03-C19-C20	6.77	133.16	111.91
27	P	272	DMU	C18-O16-C6	6.70	124.95	113.84
19	C	268	PGV	O03-C19-C20	6.67	132.85	111.91
23	J	60	CHD	C14-C8-C7	6.67	120.65	111.81
23	W	1059	CHD	C1-C2-C3	6.66	119.01	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C5-C4-C3	6.65	122.53	112.76
23	P	1271	CHD	C14-C8-C7	6.64	120.62	111.81
23	P	1271	CHD	C16-C17-C13	6.62	110.05	103.55
23	C	271	CHD	C15-C14-C13	6.61	110.03	103.55
23	C	271	CHD	C6-C7-C8	6.60	118.53	111.48
23	C	525	CHD	C14-C13-C12	6.60	113.55	107.40
23	P	1271	CHD	C5-C4-C3	6.60	122.45	112.76
27	Z	1526	DMU	O5-C6-C1	6.60	124.31	110.35
23	J	60	CHD	C5-C4-C3	6.60	122.44	112.76
23	C	271	CHD	C1-C10-C5	6.59	117.51	107.77
23	W	1059	CHD	C2-C1-C10	6.56	124.03	112.78
23	W	1059	CHD	C9-C10-C5	6.53	117.75	108.58
23	B	1085	CHD	C15-C14-C13	6.52	109.95	103.55
23	C	271	CHD	C4-C5-C10	6.49	119.55	112.66
26	T	1269	CDL	OA6-CA5-C11	6.48	125.47	111.50
23	C	271	CHD	C4-C3-C2	6.47	118.28	110.55
23	J	60	CHD	C9-C11-C12	6.39	122.73	114.30
23	J	60	CHD	C6-C5-C4	-6.39	103.84	111.19
23	B	1085	CHD	C14-C8-C9	6.36	118.44	109.71
23	O	229	CHD	C6-C5-C4	-6.35	103.88	111.19
23	B	1085	CHD	O12-C12-C13	-6.27	100.43	111.03
23	J	60	CHD	C14-C13-C12	6.23	113.20	107.40
23	W	1059	CHD	C4-C3-C2	6.19	117.95	110.55
23	B	1085	CHD	C17-C13-C14	6.19	106.34	100.09
23	O	229	CHD	C15-C14-C8	6.19	126.99	118.33
23	C	271	CHD	C11-C9-C8	6.19	119.93	110.88
23	O	229	CHD	C5-C4-C3	6.17	121.81	112.76
25	C	265	PEK	O03-C21-C22	6.14	131.19	111.91
23	O	229	CHD	C9-C8-C7	6.11	119.19	111.88
23	W	1059	CHD	C6-C5-C10	6.10	119.13	112.66
21	Y	1522	TGL	OG1-CG1-CG2	6.10	126.18	108.43
14	A	516	HEA	C3C-C4C-NC	6.09	117.09	109.21
23	J	60	CHD	C1-C10-C9	-6.08	101.80	111.35
23	W	1059	CHD	C1-C10-C5	6.08	116.76	107.77
27	C	272	DMU	O1-C10-C5	6.07	123.21	110.35
23	J	60	CHD	C1-C2-C3	6.06	118.24	110.47
21	O	1521	TGL	OG2-CB1-CB2	6.04	124.52	111.50
27	P	272	DMU	O1-C10-C5	6.03	123.12	110.35
27	Z	1526	DMU	C2-C3-C4	6.02	124.74	110.93
25	G	1263	PEK	O01-C1-C2	6.00	124.43	111.50
23	P	1525	CHD	C6-C5-C4	-5.95	104.34	111.19
22	R	1229	PSC	O01-C1-C2	5.92	124.26	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	1265	PEK	O03-C21-C22	5.91	130.44	111.91
23	C	525	CHD	C18-C13-C12	-5.90	103.06	109.07
23	P	1525	CHD	C11-C9-C10	5.89	119.80	113.73
23	W	1059	CHD	C14-C13-C12	5.89	112.88	107.40
26	C	270	CDL	OA6-CA5-C11	5.82	124.05	111.50
27	P	272	DMU	O5-C4-C3	5.82	122.02	109.75
23	P	1271	CHD	C17-C13-C12	5.81	122.97	117.67
23	B	1085	CHD	C6-C5-C4	-5.79	104.52	111.19
23	J	60	CHD	C15-C14-C13	5.78	109.22	103.55
23	B	1085	CHD	C4-C5-C10	-5.74	106.56	112.66
23	P	1271	CHD	C2-C1-C10	5.73	122.60	112.78
27	P	272	DMU	C6-C1-C2	5.72	121.91	110.00
27	P	272	DMU	O5-C4-C57	5.71	120.64	106.44
23	C	525	CHD	C6-C5-C4	-5.71	104.62	111.19
23	C	525	CHD	O3-C3-C4	5.69	121.18	109.85
23	O	229	CHD	C11-C9-C8	5.68	119.19	110.88
23	J	60	CHD	C2-C1-C10	5.68	122.52	112.78
23	C	525	CHD	C15-C14-C13	5.64	109.08	103.55
21	L	522	TGL	CA4-CA3-CA2	-5.63	92.94	113.19
23	P	1271	CHD	C5-C6-C7	5.59	120.63	114.46
23	B	1085	CHD	C11-C12-C13	5.59	116.98	111.24
26	G	269	CDL	OB6-CB5-C51	5.55	123.46	111.50
27	Z	1526	DMU	O5-C4-C57	5.55	120.22	106.44
23	C	525	CHD	O12-C12-C13	-5.54	101.66	111.03
14	N	515	HEA	C13-C12-C11	-5.54	106.03	114.35
23	J	60	CHD	C15-C14-C8	5.52	126.05	118.33
23	W	1059	CHD	C4-C5-C10	5.51	118.51	112.66
23	O	229	CHD	C4-C3-C2	5.49	117.11	110.55
27	C	272	DMU	C18-O16-C6	5.49	122.94	113.84
23	C	271	CHD	C2-C1-C10	5.47	122.16	112.78
27	M	526	DMU	C2-C3-C4	5.47	123.46	110.93
14	A	516	HEA	C27-C19-C20	5.45	124.43	115.27
21	Y	1522	TGL	CG2-OG2-CB1	5.41	131.12	117.79
23	P	1525	CHD	O12-C12-C13	-5.39	101.91	111.03
23	P	1271	CHD	C9-C11-C12	5.39	121.42	114.30
27	C	272	DMU	C6-O5-C4	5.36	124.21	113.69
27	P	272	DMU	O16-C6-C1	5.34	116.65	108.30
26	G	269	CDL	OA6-CA5-C11	5.34	123.01	111.50
25	C	265	PEK	O01-C1-C2	5.29	122.90	111.50
27	C	272	DMU	C8-C7-C5	5.25	119.98	110.82
23	O	229	CHD	O12-C12-C11	-5.19	98.55	109.12
14	A	515	HEA	C13-C12-C11	-5.19	106.56	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C15-C14-C13	5.18	108.64	103.55
23	P	1525	CHD	C18-C13-C14	-5.18	103.11	111.21
27	P	272	DMU	C8-C7-C5	5.17	119.85	110.82
27	M	526	DMU	O16-C6-C1	5.17	116.37	108.30
23	C	271	CHD	C19-C10-C9	-5.15	104.09	111.18
23	O	229	CHD	C17-C13-C14	5.11	105.24	100.09
27	M	526	DMU	C8-C7-C5	5.09	119.72	110.82
26	T	1269	CDL	OB6-CB5-C51	5.04	122.36	111.50
25	C	264	PEK	O01-C1-O02	-5.03	111.55	123.70
23	O	229	CHD	C15-C14-C13	5.03	108.49	103.55
21	L	522	TGL	OG3-CC1-CC2	5.01	127.64	111.91
23	O	229	CHD	C18-C13-C17	-4.97	103.44	111.21
14	N	516	HEA	C13-C12-C11	-4.97	106.89	114.35
27	C	272	DMU	C2-C3-C4	4.94	122.25	110.93
27	M	526	DMU	C6-O5-C4	4.93	123.36	113.69
19	A	524	PGV	C4-C3-C2	-4.91	95.54	113.19
23	W	1059	CHD	C9-C8-C7	4.91	117.74	111.88
23	C	525	CHD	C14-C8-C9	4.90	116.44	109.71
23	P	1271	CHD	C4-C5-C10	4.90	117.86	112.66
23	B	1085	CHD	O7-C7-C6	-4.89	97.82	109.94
23	P	1271	CHD	O7-C7-C6	-4.89	97.82	109.94
27	C	272	DMU	O1-C9-C11	4.88	118.58	106.44
23	J	60	CHD	C13-C14-C8	4.88	120.97	114.74
19	C	268	PGV	O01-C1-C2	4.85	121.96	111.50
23	C	525	CHD	C19-C10-C5	-4.85	102.14	110.36
23	W	1059	CHD	C17-C13-C12	4.84	122.09	117.67
14	A	516	HEA	C20-C19-C18	-4.83	111.34	121.12
23	P	1525	CHD	C11-C9-C8	4.79	117.89	110.88
26	C	270	CDL	OB8-CB7-C71	4.78	126.91	111.91
21	L	522	TGL	CG2-OG2-CB1	4.77	129.53	117.79
23	C	271	CHD	C22-C23-C24	-4.76	103.35	113.59
23	P	1271	CHD	C19-C10-C9	-4.76	104.62	111.18
23	B	1085	CHD	C15-C14-C8	4.76	124.98	118.33
21	B	521	TGL	OG3-CC1-CC2	4.75	126.81	111.91
25	T	1265	PEK	O03-C21-O04	-4.73	111.66	123.59
23	C	525	CHD	C11-C9-C10	4.73	118.60	113.73
23	O	229	CHD	O7-C7-C6	-4.69	98.30	109.94
25	P	1264	PEK	C2-C3-C4	4.69	121.59	113.23
19	A	524	PGV	O03-C19-C20	4.68	126.60	111.91
23	P	1525	CHD	C9-C8-C7	4.65	117.44	111.88
27	M	526	DMU	O5-C6-C1	4.63	120.16	110.35
21	D	523	TGL	CB3-CB2-CB1	4.59	130.31	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	C1-C10-C9	-4.57	104.17	111.35
27	Z	1526	DMU	C8-C7-C5	4.57	118.80	110.82
23	C	271	CHD	C9-C11-C12	4.56	120.32	114.30
21	B	521	TGL	OG3-CC1-OC1	-4.50	112.23	123.59
23	C	525	CHD	O7-C7-C6	-4.48	98.83	109.94
19	P	1267	PGV	O12-P-O13	-4.47	91.61	109.07
23	P	1525	CHD	O7-C7-C6	-4.45	98.91	109.94
19	N	1266	PGV	O01-C1-O02	-4.39	113.08	123.70
23	W	1059	CHD	C22-C20-C17	4.38	119.34	110.28
21	Y	1522	TGL	OG1-CA1-CA2	4.38	125.65	111.91
27	P	272	DMU	O1-C9-C11	4.37	117.30	106.44
27	P	272	DMU	O5-C6-O16	4.37	120.31	109.97
27	M	526	DMU	C6-C1-C2	4.37	119.09	110.00
23	P	1271	CHD	C21-C20-C17	4.36	119.60	112.92
19	A	521	PGV	C8-C9-C10	-4.32	94.96	113.79
21	D	523	TGL	CG2-OG2-CB1	4.32	128.42	117.79
26	P	1270	CDL	OA8-CA7-C31	4.31	125.44	111.91
21	Y	1522	TGL	OG1-CA1-OA1	-4.31	112.71	123.59
23	P	1525	CHD	C9-C11-C12	4.30	119.98	114.30
23	J	60	CHD	C22-C20-C17	4.30	119.16	110.28
23	P	1271	CHD	C18-C13-C17	-4.29	104.49	111.21
23	O	229	CHD	C18-C13-C14	-4.27	104.53	111.21
27	C	272	DMU	O7-C3-C2	4.27	118.64	107.28
23	J	60	CHD	C19-C10-C5	-4.27	103.12	110.36
19	P	1267	PGV	O14-P-O13	4.26	133.32	112.24
23	C	525	CHD	C9-C8-C7	4.25	116.96	111.88
21	B	521	TGL	OG2-CG2-CG3	4.24	123.75	108.40
21	O	1521	TGL	OG3-CC1-CC2	4.23	125.19	111.91
25	T	263	PEK	O01-C1-C2	4.23	120.62	111.50
27	M	526	DMU	O55-C2-C3	4.21	121.10	109.94
23	P	1525	CHD	C18-C13-C17	-4.21	104.62	111.21
27	Z	1526	DMU	O16-C6-C1	4.21	114.87	108.30
27	Z	1526	DMU	O1-C9-C11	4.20	116.87	106.44
21	L	522	TGL	CC3-CC2-CC1	4.19	128.87	113.62
14	N	516	HEA	CAD-CBD-CGD	-4.19	105.64	112.67
26	P	1270	CDL	OB8-CB7-C71	4.19	125.06	111.91
27	P	272	DMU	O7-C10-C5	4.18	118.94	108.10
26	T	1269	CDL	OA8-CA7-C31	4.17	124.98	111.91
21	N	1523	TGL	OG3-CC1-CC2	4.16	124.97	111.91
27	C	272	DMU	C6-C1-C2	4.16	118.66	110.00
27	P	272	DMU	C6-O5-C4	4.16	121.85	113.69
23	C	525	CHD	C6-C7-C8	4.15	115.91	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	1264	PEK	O01-C1-O02	-4.15	113.67	123.70
19	U	1268	PGV	O04-C19-C20	-4.15	107.54	123.73
23	B	1085	CHD	C2-C1-C10	4.14	119.88	112.78
19	N	1524	PGV	C4-C3-C2	-4.13	98.33	113.19
23	P	1525	CHD	C5-C4-C3	4.13	118.83	112.76
23	W	1059	CHD	C11-C9-C10	4.13	117.98	113.73
23	P	1271	CHD	C17-C13-C14	4.13	104.25	100.09
26	P	1270	CDL	CB4-OB6-CB5	-4.12	107.64	117.79
27	M	526	DMU	O1-C9-C11	4.11	116.66	106.44
19	A	521	PGV	O03-C19-C20	4.10	124.79	111.91
14	A	515	HEA	C26-C15-C16	4.10	122.17	115.27
21	B	521	TGL	CG3-OG3-CC1	4.10	132.29	117.12
27	C	272	DMU	C7-C8-C9	4.08	117.52	110.24
25	P	1264	PEK	O03-C01-C02	-4.07	96.58	108.43
14	A	516	HEA	C4B-C3B-C2B	-4.07	104.03	106.87
23	W	1059	CHD	C11-C9-C8	4.06	116.82	110.88
19	P	1267	PGV	O03-C19-O04	-4.05	113.37	123.59
27	P	272	DMU	C1-C2-C3	4.04	118.91	109.68
27	M	526	DMU	O7-C3-C2	4.04	118.02	107.28
21	L	522	TGL	OG2-CB1-CB2	4.04	120.20	111.50
27	Z	1526	DMU	O5-C4-C3	4.02	118.23	109.75
21	N	1523	TGL	CG3-CG2-CG1	-4.02	102.28	111.79
23	P	1525	CHD	C5-C6-C7	4.02	118.90	114.46
27	C	272	DMU	O5-C6-C1	4.02	118.85	110.35
23	C	525	CHD	C11-C9-C8	4.01	116.74	110.88
27	Z	1526	DMU	C7-C8-C9	4.00	117.37	110.24
27	M	526	DMU	C7-C8-C9	4.00	117.37	110.24
23	W	1059	CHD	C21-C20-C17	3.97	119.00	112.92
23	P	1271	CHD	C13-C17-C20	3.96	124.22	119.50
23	C	271	CHD	C11-C12-C13	3.94	115.28	111.24
23	J	60	CHD	C4-C5-C10	3.93	116.83	112.66
23	O	229	CHD	O3-C3-C4	3.93	117.67	109.85
23	P	1271	CHD	C9-C10-C5	3.92	114.08	108.58
23	C	271	CHD	C23-C22-C20	-3.91	109.45	114.72
23	C	271	CHD	C17-C13-C12	3.90	121.22	117.67
23	C	525	CHD	O12-C12-C11	-3.89	101.20	109.12
21	Y	1522	TGL	OG3-CC1-CC2	3.89	124.10	111.91
23	J	60	CHD	C11-C9-C8	3.88	116.56	110.88
23	P	1525	CHD	C17-C13-C14	3.88	104.01	100.09
21	N	1523	TGL	OG3-CC1-OC1	-3.88	113.80	123.59
23	W	1059	CHD	C9-C11-C12	3.86	119.40	114.30
25	C	265	PEK	O03-C21-O04	-3.86	113.85	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	C21-C20-C22	-3.85	104.32	110.36
21	L	522	TGL	CA8-CA7-CA6	-3.85	94.88	114.42
27	C	272	DMU	O61-C57-C4	3.83	124.44	111.29
23	O	229	CHD	C5-C6-C7	3.82	118.67	114.46
27	C	272	DMU	O5-C4-C3	3.81	117.79	109.75
23	P	1525	CHD	C21-C20-C17	3.81	118.75	112.92
23	C	525	CHD	C18-C13-C14	-3.80	105.27	111.21
25	T	1265	PEK	O01-C1-C2	3.79	119.68	111.50
27	M	526	DMU	O7-C10-C5	-3.78	98.30	108.10
27	P	272	DMU	C7-C8-C9	3.78	116.99	110.24
23	P	1525	CHD	O3-C3-C4	3.74	117.30	109.85
27	C	272	DMU	C1-C2-C3	3.73	118.20	109.68
26	P	1270	CDL	CA4-OA6-CA5	3.71	126.93	117.79
14	A	515	HEA	CMB-C2B-C1B	-3.70	122.77	128.46
14	N	516	HEA	C13-C14-C15	-3.70	118.75	127.66
21	O	1521	TGL	OG1-CA1-CA2	3.70	123.52	111.91
23	B	1085	CHD	C9-C11-C12	3.68	119.15	114.30
19	N	1524	PGV	O03-C19-C20	3.67	123.43	111.91
23	C	271	CHD	C21-C20-C17	3.67	118.53	112.92
21	Y	1522	TGL	OG2-CG2-CG1	3.65	121.61	108.40
23	P	1271	CHD	C23-C22-C20	-3.65	109.81	114.72
21	O	1521	TGL	CG2-OG2-CB1	3.65	126.77	117.79
25	P	1264	PEK	O13-P-O14	3.63	130.21	112.24
22	B	229	PSC	O01-C1-C2	3.63	119.33	111.50
23	C	525	CHD	C5-C4-C3	3.63	118.09	112.76
25	C	264	PEK	C2-C3-C4	3.63	119.70	113.23
23	C	525	CHD	C22-C20-C17	-3.63	102.79	110.28
26	T	1269	CDL	CB6-CB4-CB3	-3.63	103.21	111.79
27	Z	1526	DMU	C6-O5-C4	3.62	120.80	113.69
14	N	515	HEA	C1B-C2B-C3B	-3.62	104.47	107.00
23	C	525	CHD	C1-C2-C3	3.62	115.11	110.47
27	C	272	DMU	O5-C6-O16	3.61	118.53	109.97
23	J	60	CHD	O12-C12-C11	-3.61	101.78	109.12
21	N	1523	TGL	OG1-CG1-CG2	3.61	118.93	108.43
23	P	1525	CHD	C13-C17-C20	3.59	123.78	119.50
19	N	1266	PGV	O01-C1-C2	3.59	119.24	111.50
19	N	1266	PGV	O03-C19-C20	3.59	123.16	111.91
19	C	268	PGV	O04-C19-C20	-3.59	109.74	123.73
27	M	526	DMU	O5-C4-C3	3.58	117.30	109.75
23	B	1085	CHD	O12-C12-C11	-3.57	101.84	109.12
19	A	521	PGV	O01-C1-C2	3.57	119.19	111.50
27	P	272	DMU	O7-C3-C4	3.56	119.21	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	1264	PEK	O01-C1-C2	3.54	119.13	111.50
19	A	524	PGV	C8-C9-C10	-3.54	98.37	113.79
27	P	272	DMU	C2-C3-C4	3.53	119.03	110.93
14	A	516	HEA	CBD-CAD-C3D	3.53	118.99	112.49
23	O	229	CHD	C16-C17-C20	3.52	117.60	112.15
23	J	60	CHD	C9-C10-C5	3.51	113.50	108.58
19	P	1267	PGV	O03-C19-C20	3.50	122.89	111.91
26	P	1270	CDL	C53-C52-C51	-3.48	100.67	113.19
21	Y	1522	TGL	CB3-CB2-CB1	3.48	126.28	113.62
23	B	1085	CHD	C11-C9-C8	3.48	115.97	110.88
23	C	271	CHD	O7-C7-C6	-3.48	101.32	109.94
23	P	1525	CHD	C11-C12-C13	3.47	114.80	111.24
23	P	1271	CHD	O12-C12-C11	-3.46	102.07	109.12
23	P	1525	CHD	C16-C17-C20	3.46	117.50	112.15
19	A	524	PGV	O03-C19-O04	-3.44	114.90	123.59
14	N	516	HEA	C4B-C3B-C2B	-3.43	104.47	106.87
25	G	1263	PEK	O03-C01-C02	3.41	118.36	108.43
23	P	1525	CHD	C14-C8-C9	3.39	114.37	109.71
27	P	272	DMU	C10-C5-C7	3.38	117.04	110.00
23	B	1085	CHD	C14-C8-C7	3.38	116.29	111.81
23	P	1271	CHD	C19-C10-C5	-3.38	104.62	110.36
25	P	1264	PEK	C03-C02-C01	-3.37	103.82	111.79
25	T	263	PEK	C2-C3-C4	3.37	119.23	113.23
26	G	269	CDL	OB8-CB7-OB9	-3.37	115.10	123.59
23	P	1271	CHD	C11-C12-C13	3.36	114.69	111.24
19	N	1524	PGV	O01-C1-C2	3.35	118.73	111.50
19	A	524	PGV	O01-C02-C01	3.35	120.54	108.40
21	B	521	TGL	OG1-CA1-CA2	3.35	122.42	111.91
14	A	515	HEA	CAA-CBA-CGA	-3.35	107.05	112.67
27	M	526	DMU	O3-C5-C7	3.35	118.09	110.35
25	P	1264	PEK	O01-C02-C01	-3.34	96.31	108.40
21	O	1521	TGL	OG3-CC1-OC1	-3.34	115.17	123.59
27	Z	1526	DMU	O7-C10-C5	-3.33	99.47	108.10
21	D	523	TGL	OG1-CA1-CA2	3.33	122.35	111.91
27	C	272	DMU	C10-C5-C7	3.32	116.92	110.00
19	C	268	PGV	P-O11-C03	3.31	141.11	121.68
23	P	1525	CHD	C6-C7-C8	3.31	115.02	111.48
22	B	229	PSC	C30-C29-C28	-3.30	97.65	114.42
23	B	1085	CHD	C23-C22-C20	-3.30	110.27	114.72
25	C	264	PEK	O03-C01-C02	-3.30	98.83	108.43
25	T	263	PEK	O03-C21-O04	-3.29	115.28	123.59
21	D	523	TGL	C10-CB9-CB8	3.29	131.11	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	O12-C12-C11	-3.28	102.43	109.12
19	U	1268	PGV	O02-C1-C2	-3.28	110.95	123.73
23	O	229	CHD	C11-C9-C10	3.27	117.10	113.73
14	N	515	HEA	C21-C20-C19	-3.27	102.22	112.98
25	T	263	PEK	O03-C21-C22	3.27	122.17	111.91
14	N	516	HEA	C1B-C2B-C3B	-3.27	104.72	107.00
23	P	1525	CHD	C16-C17-C13	3.24	106.73	103.55
23	C	271	CHD	C17-C13-C14	3.24	103.36	100.09
23	C	525	CHD	C19-C10-C1	3.24	113.48	108.26
19	C	267	PGV	O12-P-O13	-3.23	96.46	109.07
23	C	525	CHD	C5-C6-C7	3.22	118.02	114.46
14	A	516	HEA	CAA-CBA-CGA	-3.22	107.27	112.67
25	C	264	PEK	C3-C2-C1	-3.21	101.95	113.62
26	T	1269	CDL	OA6-CA5-OA7	-3.20	115.96	123.70
22	R	1229	PSC	O03-C19-C20	3.20	121.94	111.91
27	Z	1526	DMU	C1-C2-C3	3.18	116.94	109.68
26	C	270	CDL	OB8-CB7-OB9	-3.17	115.59	123.59
19	A	521	PGV	O01-C1-O02	-3.17	116.05	123.70
27	P	272	DMU	O16-C18-C19	3.16	120.64	109.56
23	C	271	CHD	O3-C3-C4	-3.16	103.56	109.85
23	B	1085	CHD	C11-C9-C10	3.16	116.98	113.73
25	C	264	PEK	C03-C02-C01	-3.15	104.34	111.79
19	A	521	PGV	C7-C6-C5	-3.15	98.44	114.42
14	A	515	HEA	C16-C17-C18	3.15	122.22	111.88
23	O	229	CHD	C16-C17-C13	3.15	106.64	103.55
21	B	521	TGL	C15-CC9-CC8	3.14	130.34	114.42
14	N	516	HEA	CMB-C2B-C3B	3.13	130.81	124.69
14	A	516	HEA	C12-C13-C14	-3.13	103.97	112.23
26	P	1270	CDL	OA8-CA7-OA9	-3.12	115.72	123.59
23	O	229	CHD	C6-C7-C8	3.12	114.81	111.48
23	C	271	CHD	C6-C5-C4	-3.11	107.61	111.19
23	C	271	CHD	C19-C10-C1	-3.11	103.26	108.26
25	C	264	PEK	C25-C24-C23	-3.09	98.72	114.42
19	N	1524	PGV	O03-C01-C02	3.06	117.35	108.43
21	L	522	TGL	OG1-CG1-CG2	3.06	117.34	108.43
14	A	515	HEA	C17-C18-C19	-3.06	120.30	127.66
27	C	272	DMU	O7-C3-C4	3.05	117.81	109.45
23	J	60	CHD	C11-C9-C10	3.05	116.87	113.73
23	B	1085	CHD	C16-C17-C13	3.04	106.53	103.55
27	M	526	DMU	O55-C2-C1	3.03	117.36	110.35
14	N	516	HEA	CAD-C3D-C2D	-3.02	118.58	127.25
21	B	521	TGL	CG2-OG2-CB1	3.02	125.22	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C16-C17-C20	3.01	116.81	112.15
23	C	525	CHD	C15-C14-C8	3.01	122.54	118.33
25	G	1263	PEK	O03-C21-C22	3.00	121.32	111.91
26	P	1270	CDL	OA6-CA5-OA7	-3.00	116.45	123.70
27	Z	1526	DMU	C10-C5-C7	3.00	116.24	110.00
22	B	229	PSC	O03-C19-C20	3.00	121.31	111.91
27	M	526	DMU	C31-C28-C25	-3.00	99.21	114.42
23	O	229	CHD	C1-C10-C9	-2.96	106.69	111.35
19	A	521	PGV	O03-C19-O04	-2.96	116.12	123.59
14	N	515	HEA	OMA-CMA-C3A	-2.95	118.48	124.91
14	N	516	HEA	C27-C19-C18	-2.95	116.11	123.68
22	B	229	PSC	C32-C31-C30	-2.94	99.49	114.42
26	G	269	CDL	C80-C79-C78	2.94	129.35	114.42
26	C	270	CDL	C42-C41-C40	2.93	129.31	114.42
23	C	271	CHD	C14-C8-C7	2.92	115.68	111.81
23	C	271	CHD	O12-C12-C11	-2.92	103.17	109.12
23	W	1059	CHD	C18-C13-C14	-2.92	106.64	111.21
23	B	1085	CHD	C19-C10-C5	-2.92	105.41	110.36
26	G	269	CDL	C83-C82-C81	2.91	129.22	114.42
27	Z	1526	DMU	O7-C3-C2	2.91	115.03	107.28
23	P	1525	CHD	C22-C20-C17	-2.91	104.28	110.28
25	G	1263	PEK	O01-C1-O02	-2.89	116.71	123.70
25	T	263	PEK	C01-O03-C21	2.89	127.83	117.12
27	P	272	DMU	C10-O1-C9	2.89	119.36	113.69
23	J	60	CHD	C18-C13-C14	-2.89	106.69	111.21
25	C	264	PEK	O01-C1-C2	2.87	117.70	111.50
14	A	516	HEA	CBA-CAA-C2A	-2.87	107.19	112.48
23	W	1059	CHD	C18-C13-C12	-2.87	106.14	109.07
23	B	1085	CHD	C16-C17-C20	2.87	116.58	112.15
26	P	1270	CDL	C79-C78-C77	2.86	128.95	114.42
23	B	1085	CHD	C1-C10-C9	-2.86	106.86	111.35
27	Z	1526	DMU	C11-C9-C8	2.86	119.70	113.00
23	P	1525	CHD	C13-C14-C8	2.85	118.38	114.74
26	G	269	CDL	OB6-CB5-OB7	-2.85	116.81	123.70
19	N	1266	PGV	C23-C22-C21	-2.85	99.96	114.42
14	N	516	HEA	CBD-CAD-C3D	2.85	117.74	112.49
14	N	515	HEA	C13-C14-C15	-2.84	120.81	127.66
26	T	1269	CDL	OA8-CA7-OA9	-2.84	116.42	123.59
19	C	267	PGV	C30-C29-C28	-2.84	100.01	114.42
21	L	522	TGL	CB4-CB3-CB2	-2.83	103.00	113.19
26	C	270	CDL	OA8-CA7-C31	2.83	120.78	111.91
19	A	521	PGV	C8-C7-C6	2.83	128.77	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	521	PGV	C23-C22-C21	-2.82	100.09	114.42
27	Z	1526	DMU	C57-C4-C3	2.82	121.54	113.33
19	C	267	PGV	O03-C19-O04	-2.82	116.48	123.59
21	D	523	TGL	OG1-CA1-OA1	-2.82	116.48	123.59
26	T	1269	CDL	OB5-PB2-OB3	-2.81	98.08	109.07
22	R	1229	PSC	O01-C1-O02	-2.81	116.92	123.70
26	T	1269	CDL	C43-C42-C41	2.80	128.66	114.42
14	A	515	HEA	CMB-C2B-C3B	2.78	130.13	124.69
27	P	272	DMU	O5-C6-C1	2.78	116.23	110.35
23	B	1085	CHD	C18-C13-C14	-2.76	106.89	111.21
19	N	1524	PGV	O01-C1-O02	-2.75	117.05	123.70
14	A	516	HEA	O11-C11-C3B	-2.75	104.07	112.00
14	A	515	HEA	CAD-CBD-CGD	-2.75	108.06	112.67
21	L	522	TGL	C22-C21-C20	-2.74	100.49	114.42
14	N	515	HEA	C26-C15-C16	2.74	119.89	115.27
25	P	1264	PEK	O11-P-O14	-2.74	98.36	109.07
27	C	272	DMU	C10-O1-C9	2.74	119.06	113.69
23	C	525	CHD	C15-C16-C17	2.73	110.55	105.13
14	A	515	HEA	O11-C11-C3B	-2.72	104.15	112.00
27	M	526	DMU	C11-C9-C8	2.72	119.37	113.00
19	C	267	PGV	O14-P-O12	2.71	120.35	107.75
26	P	1270	CDL	OB8-CB7-OB9	-2.71	116.75	123.59
25	G	1263	PEK	C01-O03-C21	2.71	127.15	117.12
19	A	521	PGV	C9-C8-C7	2.70	128.15	114.42
21	Y	1522	TGL	OG2-CG2-CG3	2.70	118.18	108.40
25	C	264	PEK	C01-O03-C21	2.69	127.09	117.12
27	M	526	DMU	O4-C7-C5	-2.69	104.13	110.35
27	M	526	DMU	O49-C1-C2	2.68	116.54	110.35
27	M	526	DMU	C10-C5-C7	2.67	115.56	110.00
25	C	264	PEK	C32-C31-C30	-2.67	100.85	114.42
26	G	269	CDL	CA6-OA8-CA7	2.67	127.02	117.12
23	P	1525	CHD	C1-C2-C3	2.67	113.89	110.47
27	Z	1526	DMU	O3-C5-C7	2.66	116.51	110.35
23	J	60	CHD	O7-C7-C6	-2.65	103.37	109.94
23	C	525	CHD	C1-C10-C9	-2.65	107.19	111.35
14	A	515	HEA	C26-C15-C14	-2.64	116.90	123.68
27	P	272	DMU	O55-C2-C3	-2.64	102.94	109.94
27	P	272	DMU	C11-C9-C8	2.64	119.19	113.00
21	O	1521	TGL	CG3-OG3-CC1	2.64	126.89	117.12
21	B	521	TGL	CG1-OG1-CA1	2.64	126.89	117.12
26	C	270	CDL	C18-C17-C16	-2.64	101.04	114.42
21	O	1521	TGL	CG1-OG1-CA1	2.63	126.86	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	OA6-CA4-CA6	2.63	117.92	108.40
21	N	1523	TGL	CG3-OG3-CC1	2.63	126.85	117.12
27	M	526	DMU	C1-C2-C3	2.63	115.68	109.68
14	A	515	HEA	C21-C20-C19	-2.63	104.34	112.98
19	N	1524	PGV	O03-C19-O04	-2.62	116.97	123.59
21	Y	1522	TGL	OG3-CC1-OC1	-2.62	116.98	123.59
19	A	524	PGV	O03-C01-C02	2.62	116.06	108.43
14	N	516	HEA	CMB-C2B-C1B	-2.62	124.44	128.46
23	O	229	CHD	C19-C10-C5	-2.61	105.94	110.36
27	C	272	DMU	O16-C18-C19	2.61	118.70	109.56
27	M	526	DMU	C22-C19-C18	-2.61	101.94	113.49
26	C	270	CDL	OA6-CA5-OA7	-2.59	117.45	123.70
21	L	522	TGL	C26-C25-C24	-2.58	101.31	114.42
21	B	521	TGL	CC3-CC2-CC1	2.58	123.01	113.62
19	A	521	PGV	C6-C5-C4	-2.58	101.33	114.42
27	M	526	DMU	O7-C10-O1	-2.58	103.47	110.67
21	Y	1522	TGL	OG2-CB1-OB1	-2.58	117.48	123.70
27	Z	1526	DMU	O5-C6-O16	2.56	116.05	109.97
23	P	1271	CHD	C6-C5-C4	-2.56	108.25	111.19
25	T	1265	PEK	O03-C01-C02	2.55	115.87	108.43
27	P	272	DMU	O7-C10-O1	2.55	117.80	110.67
21	Y	1522	TGL	OB1-CB1-CB2	-2.55	113.80	123.73
25	T	263	PEK	O01-C1-O02	-2.55	117.55	123.70
25	C	265	PEK	C24-C23-C22	2.53	122.30	113.19
23	P	1525	CHD	C2-C1-C10	2.53	117.12	112.78
25	P	1264	PEK	O04-C21-C22	2.53	133.59	123.73
19	N	1266	PGV	C15-C14-C13	-2.52	102.82	113.79
21	D	523	TGL	OG2-CB1-CB2	-2.52	106.07	111.50
14	A	515	HEA	C3C-C4C-NC	2.52	112.47	109.21
21	L	522	TGL	OG1-CA1-CA2	2.51	119.78	111.91
26	G	269	CDL	OA8-CA7-C31	2.50	119.75	111.91
25	C	265	PEK	O12-C04-C05	2.50	118.44	109.10
21	L	522	TGL	CA9-CA8-CA7	-2.50	101.75	114.42
23	C	271	CHD	C18-C13-C17	-2.50	107.30	111.21
23	J	60	CHD	C9-C8-C7	2.49	114.85	111.88
21	O	1521	TGL	OG2-CB1-OB1	-2.49	117.69	123.70
19	C	268	PGV	O03-C19-O04	-2.48	117.34	123.59
23	W	1059	CHD	C23-C22-C20	-2.47	111.39	114.72
25	T	1265	PEK	C2-C3-C4	-2.47	108.82	113.23
21	L	522	TGL	C15-CC9-CC8	2.47	126.97	114.42
21	N	1523	TGL	OG1-CA1-CA2	2.47	119.65	111.91
26	P	1270	CDL	OB6-CB5-C51	2.47	116.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	1269	CDL	C82-C81-C80	2.46	126.93	114.42
19	A	521	PGV	C15-C14-C13	-2.46	103.06	113.79
23	W	1059	CHD	C19-C10-C1	-2.46	104.30	108.26
26	G	269	CDL	CB2-C1-CA2	-2.45	105.57	112.79
21	O	1521	TGL	C15-CC9-CC8	2.45	126.88	114.42
21	L	522	TGL	OG2-CG2-CG1	2.43	117.21	108.40
21	D	523	TGL	C11-C10-CB9	2.43	126.76	114.42
27	Z	1526	DMU	O16-C18-C19	2.43	118.07	109.56
26	G	269	CDL	C82-C81-C80	2.42	126.72	114.42
21	D	523	TGL	CC4-CC3-CC2	-2.42	104.49	113.19
19	P	1267	PGV	C7-C6-C5	-2.40	102.23	114.42
26	P	1270	CDL	OA8-CA6-CA4	2.40	115.43	108.43
26	C	270	CDL	O1-C1-CB2	2.40	117.97	109.56
19	A	524	PGV	O14-P-O13	2.40	124.09	112.24
22	B	229	PSC	O01-C1-O02	-2.40	117.91	123.70
22	B	229	PSC	C27-C26-C25	-2.39	102.30	114.42
26	G	269	CDL	OA6-CA5-OA7	-2.38	117.95	123.70
26	P	1270	CDL	C42-C41-C40	2.36	126.42	114.42
23	W	1059	CHD	C19-C10-C5	-2.36	106.36	110.36
26	C	270	CDL	O1-C1-CA2	-2.36	101.28	109.56
19	U	1268	PGV	O01-C02-C01	2.36	116.94	108.40
21	Y	1522	TGL	C15-CC9-CC8	2.36	126.39	114.42
21	Y	1522	TGL	CG3-OG3-CC1	2.36	125.85	117.12
14	N	515	HEA	CAD-C3D-C2D	2.35	134.01	127.25
21	Y	1522	TGL	C26-C25-C24	-2.35	102.49	114.42
25	C	264	PEK	C26-C25-C24	-2.35	102.50	114.42
14	N	516	HEA	C16-C15-C14	2.35	125.87	121.12
26	C	270	CDL	CA6-OA8-CA7	2.35	125.81	117.12
26	P	1270	CDL	OB4-PB2-OB3	2.34	123.83	112.24
23	C	525	CHD	C9-C11-C12	2.34	117.39	114.30
26	T	1269	CDL	OB8-CB7-OB9	-2.34	117.68	123.59
26	G	269	CDL	OB8-CB7-C71	2.34	119.25	111.91
26	C	270	CDL	C53-C52-C51	-2.34	104.79	113.19
21	B	521	TGL	OB1-CB1-CB2	-2.34	114.62	123.73
19	C	268	PGV	O01-C02-C03	2.34	116.86	108.40
25	P	1264	PEK	C24-C23-C22	-2.33	104.80	113.19
21	L	522	TGL	OB1-CB1-CB2	-2.33	114.63	123.73
19	A	524	PGV	C8-C7-C6	-2.32	102.65	114.42
19	N	1266	PGV	C6-C5-C4	-2.32	102.66	114.42
14	N	515	HEA	C3C-C4C-NC	2.31	112.20	109.21
14	A	516	HEA	C13-C14-C15	-2.31	122.09	127.66
27	Z	1526	DMU	O7-C10-O1	-2.29	104.26	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	1264	PEK	C33-C32-C31	-2.29	102.80	114.42
19	N	1266	PGV	O14-P-O12	-2.29	97.12	107.75
19	P	1267	PGV	C03-C02-C01	-2.28	106.39	111.79
26	G	269	CDL	O1-C1-CB2	2.28	117.57	109.56
23	O	229	CHD	C2-C1-C10	2.27	116.68	112.78
21	N	1523	TGL	OG1-CA1-OA1	-2.27	117.86	123.59
19	C	268	PGV	O02-C1-C2	-2.26	114.90	123.73
25	C	265	PEK	O13-P-O11	2.26	118.25	107.75
21	D	523	TGL	OG2-CG2-CG3	2.26	116.58	108.40
21	B	521	TGL	OG1-CG1-CG2	-2.26	101.86	108.43
26	P	1270	CDL	C54-C53-C52	-2.26	102.97	114.42
26	C	270	CDL	C83-C82-C81	2.25	125.86	114.42
26	C	270	CDL	C39-C38-C37	2.25	125.85	114.42
19	U	1268	PGV	C15-C14-C13	2.25	123.59	113.79
19	N	1266	PGV	O01-C02-C01	-2.25	100.26	108.40
25	C	265	PEK	O04-C21-C22	-2.25	114.96	123.73
21	D	523	TGL	C20-CA9-CA8	2.25	125.83	114.42
27	Z	1526	DMU	C6-C1-C2	2.25	114.67	110.00
19	N	1266	PGV	O03-C19-O04	-2.24	117.93	123.59
21	N	1523	TGL	OG2-CB1-CB2	2.24	116.33	111.50
21	N	1523	TGL	OG2-CG2-CG3	2.24	116.51	108.40
14	N	516	HEA	O11-C11-C3B	-2.23	105.56	112.00
19	C	267	PGV	O14-P-O13	2.23	123.29	112.24
26	P	1270	CDL	C56-C55-C54	-2.23	103.08	114.42
25	C	264	PEK	O13-P-O14	2.23	123.28	112.24
14	N	516	HEA	C20-C19-C18	-2.23	116.61	121.12
19	P	1267	PGV	C4-C3-C2	-2.22	105.20	113.19
26	T	1269	CDL	C39-C38-C37	2.21	125.66	114.42
27	C	272	DMU	C11-C9-C8	2.21	118.19	113.00
25	C	264	PEK	O03-C21-O04	-2.21	118.01	123.59
19	A	524	PGV	C02-O01-C1	2.21	123.23	117.79
25	C	265	PEK	P-O11-C03	2.20	134.60	121.68
23	C	525	CHD	O7-C7-C8	-2.20	104.51	109.43
21	Y	1522	TGL	C10-CB9-CB8	2.20	125.58	114.42
14	A	516	HEA	OMA-CMA-C3A	-2.20	120.12	124.91
26	G	269	CDL	C23-C22-C21	2.20	125.57	114.42
21	D	523	TGL	C13-C12-C11	2.19	125.56	114.42
26	T	1269	CDL	CB6-OB8-CB7	2.19	125.24	117.12
23	P	1525	CHD	C4-C5-C10	-2.19	110.33	112.66
14	N	515	HEA	CMB-C2B-C3B	2.19	128.98	124.69
19	C	267	PGV	O03-C19-C20	2.19	118.78	111.91
21	D	523	TGL	CB5-CB4-CB3	2.19	125.53	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	1269	CDL	C20-C19-C18	2.19	125.53	114.42
26	C	270	CDL	OB4-PB2-OB3	2.18	123.04	112.24
23	J	60	CHD	C14-C8-C9	2.18	112.71	109.71
21	D	523	TGL	C21-C20-CA9	2.18	125.50	114.42
25	G	1263	PEK	C2-C3-C4	2.18	117.11	113.23
23	C	525	CHD	C22-C23-C24	-2.18	108.91	113.59
26	T	1269	CDL	CA4-OA6-CA5	2.18	123.15	117.79
25	C	264	PEK	C35-C34-C33	-2.18	103.38	114.42
25	P	1264	PEK	C3-C2-C1	-2.17	105.71	113.62
23	C	525	CHD	C2-C1-C10	2.17	116.50	112.78
23	P	1525	CHD	C19-C10-C5	-2.17	106.69	110.36
27	Z	1526	DMU	O55-C2-C3	2.16	115.67	109.94
23	B	1085	CHD	C13-C14-C8	2.16	117.50	114.74
21	B	521	TGL	OG2-CB1-OB1	-2.16	118.49	123.70
23	J	60	CHD	O12-C12-C13	-2.15	107.39	111.03
26	P	1270	CDL	C40-C39-C38	2.15	125.36	114.42
21	N	1523	TGL	C21-C20-CA9	2.15	125.36	114.42
27	P	272	DMU	O49-C1-C2	-2.15	105.37	110.35
26	C	270	CDL	C22-C21-C20	2.15	125.35	114.42
26	G	269	CDL	CB6-CB4-CB3	-2.15	106.70	111.79
25	C	264	PEK	C24-C23-C22	-2.15	105.48	113.19
14	N	515	HEA	C12-C11-C3B	2.14	118.19	112.56
27	Z	1526	DMU	O7-C3-C4	2.13	115.29	109.45
27	Z	1526	DMU	O61-C57-C4	2.13	118.61	111.29
27	C	272	DMU	O2-C8-C7	-2.13	105.42	110.35
26	C	270	CDL	C57-C56-C55	-2.13	103.62	114.42
25	T	1265	PEK	C24-C23-C22	2.13	120.84	113.19
19	P	1267	PGV	C22-C21-C20	-2.13	105.55	113.19
26	G	269	CDL	OA8-CA6-CA4	2.13	114.62	108.43
19	U	1268	PGV	C29-C28-C27	2.12	125.21	114.42
22	B	229	PSC	C16-C15-C14	2.12	123.03	113.79
23	P	1271	CHD	C1-C10-C9	-2.12	108.03	111.35
25	C	264	PEK	C11-C10-C9	2.11	122.44	112.02
23	C	271	CHD	C22-C20-C17	-2.11	105.93	110.28
19	A	521	PGV	C5-C4-C3	-2.11	103.74	114.42
19	C	267	PGV	O03-C01-C02	-2.10	102.32	108.43
25	T	1265	PEK	C35-C34-C33	-2.09	103.80	114.42
26	P	1270	CDL	OA7-CA5-C11	-2.09	115.59	123.73
19	N	1266	PGV	C26-C25-C24	2.08	124.97	114.42
26	G	269	CDL	C85-C84-C83	2.08	124.97	114.42
26	P	1270	CDL	CA6-CA4-CA3	-2.08	106.88	111.79
26	T	1269	CDL	C83-C82-C81	2.08	124.96	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	521	PGV	C25-C24-C23	-2.07	103.91	114.42
27	C	272	DMU	O55-C2-C3	2.07	115.43	109.94
26	P	1270	CDL	C55-C54-C53	-2.07	103.92	114.42
21	O	1521	TGL	OG2-CG2-CG3	2.06	115.88	108.40
27	C	272	DMU	O7-C10-C5	2.06	113.44	108.10
23	C	271	CHD	C19-C10-C5	-2.06	106.87	110.36
27	P	272	DMU	O7-C3-C2	2.05	112.73	107.28
26	P	1270	CDL	C20-C19-C18	2.05	124.82	114.42
25	P	1264	PEK	C35-C34-C33	-2.05	104.03	114.42
19	C	267	PGV	C21-C20-C19	-2.05	106.18	113.62
25	P	1264	PEK	O03-C21-C22	-2.04	105.49	111.91
19	U	1268	PGV	C24-C23-C22	2.04	124.77	114.42
21	O	1521	TGL	OG2-CG2-CG1	2.04	115.77	108.40
21	B	521	TGL	C16-C15-CC9	2.03	124.75	114.42
21	Y	1522	TGL	C16-C15-CC9	2.02	124.68	114.42
25	P	1264	PEK	C37-C36-C35	-2.02	96.58	115.30
26	C	270	CDL	C80-C79-C78	2.02	124.66	114.42
21	Y	1522	TGL	CG3-CG2-CG1	-2.01	107.04	111.79
23	B	1085	CHD	C1-C2-C3	2.01	113.04	110.47
19	N	1266	PGV	C04-C05-C06	-2.01	104.53	111.67
14	A	515	HEA	OMA-CMA-C3A	-2.01	120.54	124.91
26	G	269	CDL	C62-C61-C60	2.01	124.60	114.42
26	G	269	CDL	CB6-OB8-CB7	2.00	124.55	117.12
27	Z	1526	DMU	O55-C2-C1	2.00	114.98	110.35
26	C	270	CDL	C16-C15-C14	-2.00	104.27	114.42

All (39) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
27	Z	1526	DMU	C2
27	Z	1526	DMU	C4
27	Z	1526	DMU	C9
27	Z	1526	DMU	C6
27	Z	1526	DMU	C5
27	P	272	DMU	C5
27	P	272	DMU	C6
27	P	272	DMU	C9
27	P	272	DMU	C4
27	P	272	DMU	C2

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Mol	Chain	Res	Type	Atom
27	P	272	DMU	C10
14	A	515	HEA	ND
14	A	515	HEA	NA
14	A	515	HEA	NB
14	N	516	HEA	ND
14	N	516	HEA	NA
14	N	516	HEA	NB
23	J	60	CHD	C17
23	J	60	CHD	C9
23	P	1271	CHD	C9
27	C	272	DMU	C5
27	C	272	DMU	C6
27	C	272	DMU	C9
27	C	272	DMU	C4
27	C	272	DMU	C2
27	C	272	DMU	C3
23	W	1059	CHD	C17
23	C	271	CHD	C9
23	P	1525	CHD	C9
27	M	526	DMU	C2
27	M	526	DMU	C4
27	M	526	DMU	C9
27	M	526	DMU	C5
14	A	516	HEA	ND
14	A	516	HEA	NA
14	A	516	HEA	NB

All (946) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	1229	PSC	C03-O11-P-O12
22	R	1229	PSC	C04-O12-P-O14
22	R	1229	PSC	O12-C04-C05-N
22	R	1229	PSC	C2-C1-O01-C02
14	N	515	HEA	C14-C15-C16-C17
14	N	515	HEA	C26-C15-C16-C17
27	Z	1526	DMU	C19-C18-O16-C6
27	P	272	DMU	C1-C6-O16-C18
19	U	1268	PGV	O12-C04-C05-C06
19	U	1268	PGV	C2-C1-O01-C02
25	T	263	PEK	C03-O11-P-O13
25	T	263	PEK	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	D	523	TGL	CB2-CB1-OG2-CG2
21	D	523	TGL	CC2-CC1-OG3-CG3
21	D	523	TGL	OC1-CC1-OG3-CG3
22	B	229	PSC	C03-O11-P-O12
22	B	229	PSC	O12-C04-C05-N
19	C	268	PGV	O01-C02-C03-O11
19	C	268	PGV	C02-C03-O11-P
19	C	268	PGV	C2-C1-O01-C02
25	C	264	PEK	O12-C04-C05-N
25	C	264	PEK	C10-C11-C12-C13
25	C	264	PEK	C11-C12-C13-C14
25	C	264	PEK	C12-C13-C14-C15
14	N	516	HEA	O11-C11-C12-C13
23	J	60	CHD	C16-C17-C20-C21
25	P	1264	PEK	C7-C8-C9-C10
21	Y	1522	TGL	CB2-CB1-OG2-CG2
21	Y	1522	TGL	OB1-CB1-OG2-CG2
25	C	265	PEK	C04-O12-P-O13
25	C	265	PEK	C7-C8-C9-C10
25	C	265	PEK	C13-C14-C15-C16
26	G	269	CDL	CA2-C1-CB2-OB2
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4
26	G	269	CDL	OB6-CB4-CB6-OB8
19	A	524	PGV	C02-C03-O11-P
19	A	524	PGV	C04-C05-C06-O06
19	A	524	PGV	O02-C1-O01-C02
19	A	524	PGV	O04-C19-O03-C01
19	A	524	PGV	C20-C19-O03-C01
26	P	1270	CDL	CB2-C1-CA2-OA2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA3-OA5-PA1-OA3
26	P	1270	CDL	CA3-OA5-PA1-OA4
26	P	1270	CDL	OA7-CA5-OA6-CA4
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CB2-OB2-PB2-OB4
26	P	1270	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CB2-C1-CA2-OA2
26	T	1269	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	C11-CA5-OA6-CA4
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB2-OB2-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
26	C	270	CDL	C1-CA2-OA2-PA1
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB4
19	A	521	PGV	C04-O12-P-O13
21	N	1523	TGL	CC2-CC1-OG3-CG3
21	N	1523	TGL	OC1-CC1-OG3-CG3
25	T	1265	PEK	C03-O11-P-O13
19	N	1524	PGV	C03-O11-P-O12
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	O02-C1-O01-C02
27	C	272	DMU	O5-C6-O16-C18
23	W	1059	CHD	C13-C17-C20-C22
23	W	1059	CHD	C16-C17-C20-C21
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	C13-C14-C15-C16
14	A	516	HEA	C3B-C11-C12-C13
14	A	516	HEA	O11-C11-C12-C13
26	P	1270	CDL	OA9-CA7-OA8-CA6
19	N	1524	PGV	O04-C19-O03-C01
26	P	1270	CDL	C31-CA7-OA8-CA6
22	R	1229	PSC	O04-C19-O03-C01
25	T	263	PEK	O04-C21-O03-C01
22	B	229	PSC	O04-C19-O03-C01
25	G	1263	PEK	O04-C21-O03-C01
23	J	60	CHD	C16-C17-C20-C22
22	R	1229	PSC	O02-C1-O01-C02
19	U	1268	PGV	O02-C1-O01-C02
21	D	523	TGL	OB1-CB1-OG2-CG2
19	C	268	PGV	O02-C1-O01-C02
25	C	265	PEK	O02-C1-O01-C02
25	T	1265	PEK	O02-C1-O01-C02
22	R	1229	PSC	C20-C19-O03-C01
22	B	229	PSC	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C20-C19-O03-C01
25	G	1263	PEK	C22-C21-O03-C01
27	P	272	DMU	O6-C11-C9-O1
19	A	524	PGV	C2-C1-O01-C02
19	N	1524	PGV	C2-C1-O01-C02
21	Y	1522	TGL	C20-C21-C22-C23
26	G	269	CDL	C79-C80-C81-C82
26	P	1270	CDL	C61-C62-C63-C64
25	T	263	PEK	C22-C21-O03-C01
21	L	522	TGL	CA2-CA1-OG1-CG1
19	P	1267	PGV	C10-C11-C12-C13
25	T	263	PEK	C13-C14-C15-C16
19	C	268	PGV	C10-C11-C12-C13
25	C	264	PEK	C13-C14-C15-C16
25	P	1264	PEK	C13-C14-C15-C16
19	C	267	PGV	C10-C11-C12-C13
19	A	521	PGV	C10-C11-C12-C13
19	N	1524	PGV	C10-C11-C12-C13
25	G	1263	PEK	C4-C5-C6-C7
26	C	270	CDL	OA7-CA5-OA6-CA4
27	Z	1526	DMU	O5-C4-C57-O61
27	M	526	DMU	O5-C4-C57-O61
19	C	268	PGV	O12-C04-C05-O05
26	G	269	CDL	O1-C1-CB2-OB2
26	T	1269	CDL	O1-C1-CA2-OA2
21	B	521	TGL	C12-C13-C14-C29
27	M	526	DMU	O6-C11-C9-C8
25	C	265	PEK	C2-C1-O01-C02
25	T	1265	PEK	C2-C1-O01-C02
26	P	1270	CDL	C19-C20-C21-C22
21	B	521	TGL	C21-C22-C23-C24
21	L	522	TGL	C20-C21-C22-C23
19	A	521	PGV	C6-C7-C8-C9
23	P	1271	CHD	C13-C17-C20-C21
23	W	1059	CHD	C16-C17-C20-C22
19	A	524	PGV	C20-C21-C22-C23
21	N	1523	TGL	C16-C15-CC9-CC8
23	C	271	CHD	C17-C20-C22-C23
19	A	524	PGV	C05-C04-O12-P
21	L	522	TGL	OA1-CA1-OG1-CG1
27	Z	1526	DMU	O5-C6-O16-C18
21	Y	1522	TGL	CC3-CC4-CC5-CC6

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Mol	Chain	Res	Type	Atoms
21	Y	1522	TGL	CC1-CC2-CC3-CC4
22	B	229	PSC	C24-C25-C26-C27
21	Y	1522	TGL	C16-C15-CC9-CC8
21	L	522	TGL	CC1-CC2-CC3-CC4
19	N	1524	PGV	C19-C20-C21-C22
26	T	1269	CDL	CA2-C1-CB2-OB2
27	C	272	DMU	O6-C11-C9-C8
26	T	1269	CDL	C40-C41-C42-C43
19	U	1268	PGV	C20-C19-O03-C01
21	O	1521	TGL	CC2-CC1-OG3-CG3
27	P	272	DMU	C3-C4-C57-O61
25	T	1265	PEK	C28-C29-C30-C31
21	D	523	TGL	CB9-C10-C11-C12
19	U	1268	PGV	O12-C04-C05-O05
26	T	1269	CDL	CB7-C71-C72-C73
23	J	60	CHD	C13-C17-C20-C21
26	G	269	CDL	C11-CA5-OA6-CA4
19	U	1268	PGV	C20-C21-C22-C23
26	G	269	CDL	C40-C41-C42-C43
21	Y	1522	TGL	CA2-CA1-OG1-CG1
23	C	271	CHD	C21-C20-C22-C23
19	C	268	PGV	C1-C2-C3-C4
25	P	1264	PEK	C1-C2-C3-C4
26	C	270	CDL	CB5-C51-C52-C53
22	R	1229	PSC	C11-C12-C13-C14
25	P	1264	PEK	C10-C11-C12-C13
25	C	265	PEK	C10-C11-C12-C13
25	T	1265	PEK	C13-C14-C15-C16
27	C	272	DMU	O5-C4-C57-O61
19	N	1524	PGV	O05-C05-C06-O06
19	A	524	PGV	C12-C13-C14-C15
22	R	1229	PSC	C1-C2-C3-C4
21	B	521	TGL	CB1-CB2-CB3-CB4
21	O	1521	TGL	CA1-CA2-CA3-CA4
26	G	269	CDL	CA5-C11-C12-C13
26	G	269	CDL	CB7-C71-C72-C73
26	P	1270	CDL	CB5-C51-C52-C53
21	N	1523	TGL	CB1-CB2-CB3-CB4
26	T	1269	CDL	C60-C61-C62-C63
27	Z	1526	DMU	O6-C11-C9-O1
26	G	269	CDL	OA7-CA5-OA6-CA4
21	L	522	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
25	C	264	PEK	C1-C2-C3-C4
25	G	1263	PEK	C21-C22-C23-C24
23	W	1059	CHD	C13-C17-C20-C21
23	J	60	CHD	C13-C17-C20-C22
26	G	269	CDL	C31-CA7-OA8-CA6
21	O	1521	TGL	C12-C13-C14-C29
21	O	1521	TGL	OC1-CC1-OG3-CG3
21	Y	1522	TGL	C25-C26-C27-C28
26	G	269	CDL	C60-C61-C62-C63
26	P	1270	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	O1-C1-CB2-OB2
19	U	1268	PGV	O04-C19-O03-C01
21	B	521	TGL	CA1-CA2-CA3-CA4
27	C	272	DMU	O16-C18-C19-C22
19	U	1268	PGV	C10-C11-C12-C13
25	T	1265	PEK	C4-C5-C6-C7
25	T	1265	PEK	C10-C11-C12-C13
23	P	1271	CHD	C21-C20-C22-C23
26	G	269	CDL	OA9-CA7-OA8-CA6
26	G	269	CDL	C51-CB5-OB6-CB4
21	L	522	TGL	CB2-CB1-OG2-CG2
25	T	263	PEK	C03-O11-P-O12
25	C	265	PEK	C04-O12-P-O11
26	G	269	CDL	CB3-OB5-PB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	T	1269	CDL	CB3-OB5-PB2-OB2
25	G	1263	PEK	C03-O11-P-O12
27	Z	1526	DMU	O16-C18-C19-C22
22	B	229	PSC	O02-C1-O01-C02
26	G	269	CDL	OB7-CB5-OB6-CB4
26	G	269	CDL	C55-C56-C57-C58
22	B	229	PSC	C04-C05-N-C06
22	B	229	PSC	C04-C05-N-C07
26	C	270	CDL	C38-C39-C40-C41
21	Y	1522	TGL	C22-C23-C24-C25
22	B	229	PSC	C2-C1-O01-C02
22	R	1229	PSC	C20-C21-C22-C23
21	B	521	TGL	CC7-CC8-CC9-C15
25	T	263	PEK	C31-C32-C33-C34
21	D	523	TGL	C10-C11-C12-C13
21	D	523	TGL	CC2-CC3-CC4-CC5
22	B	229	PSC	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
21	O	1521	TGL	C11-C10-CB9-CB8
21	Y	1522	TGL	C10-C11-C12-C13
26	G	269	CDL	C58-C59-C60-C61
26	G	269	CDL	C80-C81-C82-C83
19	C	267	PGV	C24-C25-C26-C27
26	P	1270	CDL	C74-C75-C76-C77
21	L	522	TGL	CA3-CA4-CA5-CA6
26	C	270	CDL	C77-C78-C79-C80
19	N	1266	PGV	C5-C6-C7-C8
25	G	1263	PEK	C27-C28-C29-C30
21	D	523	TGL	CA6-CA7-CA8-CA9
22	B	229	PSC	C3-C4-C5-C6
22	B	229	PSC	C25-C26-C27-C28
25	P	1264	PEK	C30-C31-C32-C33
21	O	1521	TGL	C14-C29-C30-C31
21	Y	1522	TGL	C21-C22-C23-C24
26	G	269	CDL	C43-C44-C45-C46
26	C	270	CDL	C23-C24-C25-C26
19	N	1524	PGV	C7-C8-C9-C10
25	G	1263	PEK	C23-C24-C25-C26
22	B	229	PSC	C03-C02-O01-C1
21	B	521	TGL	CC5-CC6-CC7-CC8
19	C	268	PGV	C3-C4-C5-C6
25	C	265	PEK	C32-C33-C34-C35
26	P	1270	CDL	C16-C17-C18-C19
26	P	1270	CDL	C37-C38-C39-C40
26	T	1269	CDL	C23-C24-C25-C26
26	T	1269	CDL	C82-C83-C84-C85
25	C	264	PEK	C7-C8-C9-C10
26	P	1270	CDL	C71-C72-C73-C74
26	T	1269	CDL	C36-C37-C38-C39
26	T	1269	CDL	C76-C77-C78-C79
26	C	270	CDL	C57-C58-C59-C60
21	N	1523	TGL	C20-C21-C22-C23
26	P	1270	CDL	O1-C1-CB2-OB2
22	R	1229	PSC	C25-C26-C27-C28
19	U	1268	PGV	C26-C27-C28-C29
26	P	1270	CDL	C59-C60-C61-C62
26	T	1269	CDL	C12-C13-C14-C15
21	N	1523	TGL	CC5-CC6-CC7-CC8
27	Z	1526	DMU	C22-C25-C28-C31
22	B	229	PSC	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	O	1521	TGL	CA6-CA7-CA8-CA9
26	G	269	CDL	C59-C60-C61-C62
26	P	1270	CDL	C43-C44-C45-C46
26	T	1269	CDL	C32-C33-C34-C35
21	L	522	TGL	CA7-CA8-CA9-C20
21	L	522	TGL	C11-C12-C13-C14
21	L	522	TGL	C17-C18-C19-C33
26	C	270	CDL	C19-C20-C21-C22
26	C	270	CDL	C76-C77-C78-C79
21	Y	1522	TGL	OA1-CA1-OG1-CG1
22	R	1229	PSC	C22-C23-C24-C25
19	U	1268	PGV	C29-C30-C31-C32
25	P	1264	PEK	C23-C24-C25-C26
21	O	1521	TGL	CC7-CC8-CC9-C15
21	Y	1522	TGL	CB4-CB5-CB6-CB7
26	G	269	CDL	C22-C23-C24-C25
26	G	269	CDL	C61-C62-C63-C64
19	C	267	PGV	C7-C8-C9-C10
26	P	1270	CDL	C42-C43-C44-C45
26	C	270	CDL	C41-C42-C43-C44
25	T	1265	PEK	C29-C30-C31-C32
19	N	1266	PGV	C26-C27-C28-C29
21	Y	1522	TGL	CB1-CB2-CB3-CB4
21	B	521	TGL	CA2-CA3-CA4-CA5
25	T	263	PEK	C30-C31-C32-C33
19	C	268	PGV	C28-C29-C30-C31
25	C	264	PEK	C23-C24-C25-C26
26	G	269	CDL	C37-C38-C39-C40
19	C	267	PGV	C14-C15-C16-C17
26	P	1270	CDL	C21-C22-C23-C24
26	P	1270	CDL	C72-C73-C74-C75
21	N	1523	TGL	C21-C20-CA9-CA8
19	P	1267	PGV	C7-C8-C9-C10
25	P	1264	PEK	C16-C17-C18-C19
21	O	1521	TGL	CC5-CC6-CC7-CC8
26	G	269	CDL	C41-C42-C43-C44
26	P	1270	CDL	C81-C82-C83-C84
19	U	1268	PGV	C04-C05-C06-O06
19	C	268	PGV	C04-C05-C06-O06
19	N	1524	PGV	C04-C05-C06-O06
21	O	1521	TGL	OB1-CB1-OG2-CG2
21	D	523	TGL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C58-C59-C60-C61
26	C	270	CDL	C78-C79-C80-C81
21	N	1523	TGL	CC2-CC3-CC4-CC5
19	N	1266	PGV	C6-C7-C8-C9
21	B	521	TGL	CA5-CA6-CA7-CA8
21	B	521	TGL	CC6-CC7-CC8-CC9
19	U	1268	PGV	C27-C28-C29-C30
21	D	523	TGL	C18-C19-C33-C34
22	B	229	PSC	C21-C22-C23-C24
25	C	264	PEK	C34-C35-C36-C37
25	C	265	PEK	C25-C26-C27-C28
26	G	269	CDL	C11-C12-C13-C14
26	G	269	CDL	C81-C82-C83-C84
26	P	1270	CDL	C12-C13-C14-C15
26	P	1270	CDL	C14-C15-C16-C17
26	P	1270	CDL	C20-C21-C22-C23
26	T	1269	CDL	C11-C12-C13-C14
21	L	522	TGL	CC3-CC4-CC5-CC6
21	L	522	TGL	C22-C23-C24-C25
26	C	270	CDL	C36-C37-C38-C39
26	C	270	CDL	C40-C41-C42-C43
27	Z	1526	DMU	C25-C28-C31-C34
21	B	521	TGL	CB3-CB4-CB5-CB6
19	U	1268	PGV	C24-C25-C26-C27
22	B	229	PSC	C5-C6-C7-C8
21	O	1521	TGL	CC2-CC3-CC4-CC5
26	G	269	CDL	C57-C58-C59-C60
26	C	270	CDL	C39-C40-C41-C42
19	N	1266	PGV	C25-C26-C27-C28
25	T	1265	PEK	O12-C04-C05-N
21	B	521	TGL	C13-C14-C29-C30
21	B	521	TGL	C22-C23-C24-C25
26	G	269	CDL	C33-C34-C35-C36
26	G	269	CDL	C52-C53-C54-C55
26	G	269	CDL	C82-C83-C84-C85
26	T	1269	CDL	C80-C81-C82-C83
26	G	269	CDL	C63-C64-C65-C66
26	C	270	CDL	C43-C44-C45-C46
25	G	1263	PEK	C31-C32-C33-C34
21	D	523	TGL	CA2-CA1-OG1-CG1
22	B	229	PSC	C4-C5-C6-C7
21	Y	1522	TGL	CC7-CC8-CC9-C15

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Mol	Chain	Res	Type	Atoms
21	L	522	TGL	C21-C22-C23-C24
19	N	1524	PGV	C3-C4-C5-C6
21	D	523	TGL	CA4-CA5-CA6-CA7
26	P	1270	CDL	C53-C54-C55-C56
26	C	270	CDL	C12-C13-C14-C15
21	B	521	TGL	CA7-CA8-CA9-C20
25	C	264	PEK	C28-C29-C30-C31
25	P	1264	PEK	C32-C33-C34-C35
21	Y	1522	TGL	C15-C16-C17-C18
26	P	1270	CDL	C36-C37-C38-C39
26	C	270	CDL	C63-C64-C65-C66
19	N	1524	PGV	C26-C27-C28-C29
25	G	1263	PEK	O03-C01-C02-C03
22	R	1229	PSC	C11-C10-C9-C8
25	T	263	PEK	C10-C11-C12-C13
21	O	1521	TGL	CA2-CA3-CA4-CA5
25	G	1263	PEK	C25-C26-C27-C28
26	T	1269	CDL	C59-C60-C61-C62
21	O	1521	TGL	CB2-CB1-OG2-CG2
19	U	1268	PGV	O05-C05-C06-O06
19	A	524	PGV	O05-C05-C06-O06
19	A	524	PGV	C13-C14-C15-C16
22	B	229	PSC	C13-C14-C15-C16
19	C	268	PGV	C11-C10-C9-C8
25	P	1264	PEK	C15-C16-C17-C18
19	C	268	PGV	C24-C25-C26-C27
25	T	263	PEK	C24-C25-C26-C27
21	D	523	TGL	CB2-CB3-CB4-CB5
26	T	1269	CDL	CB5-C51-C52-C53
25	T	263	PEK	C34-C35-C36-C37
26	T	1269	CDL	C13-C14-C15-C16
21	L	522	TGL	C16-C17-C18-C19
21	N	1523	TGL	C19-C33-C34-C35
21	O	1521	TGL	CB5-CB6-CB7-CB8
21	O	1521	TGL	CB6-CB7-CB8-CB9
21	L	522	TGL	CC4-CC5-CC6-CC7
26	C	270	CDL	C11-C12-C13-C14
21	N	1523	TGL	CB9-C10-C11-C12
19	N	1266	PGV	C7-C8-C9-C10
25	T	263	PEK	C25-C26-C27-C28
21	D	523	TGL	C20-C21-C22-C23
25	P	1264	PEK	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
22	B	229	PSC	C04-C05-N-C08
19	A	524	PGV	C19-C20-C21-C22
22	R	1229	PSC	C2-C3-C4-C5
26	P	1270	CDL	C40-C41-C42-C43
26	T	1269	CDL	C72-C73-C74-C75
19	N	1266	PGV	C4-C5-C6-C7
26	G	269	CDL	C71-CB7-OB8-CB6
27	Z	1526	DMU	C28-C31-C34-C37
19	A	521	PGV	C26-C27-C28-C29
26	P	1270	CDL	C77-C78-C79-C80
21	N	1523	TGL	C16-C17-C18-C19
21	D	523	TGL	C12-C13-C14-C29
21	D	523	TGL	CC5-CC6-CC7-CC8
21	D	523	TGL	C16-C17-C18-C19
19	C	267	PGV	C13-C14-C15-C16
19	A	524	PGV	C5-C6-C7-C8
21	L	522	TGL	C25-C26-C27-C28
21	N	1523	TGL	C10-C11-C12-C13
22	B	229	PSC	C11-C12-C13-C14
21	D	523	TGL	OA1-CA1-OG1-CG1
21	B	521	TGL	CC4-CC5-CC6-CC7
19	U	1268	PGV	C30-C31-C32-C33
25	C	264	PEK	C15-C16-C17-C18
19	A	521	PGV	C11-C10-C9-C8
25	T	1265	PEK	C2-C3-C4-C5
21	B	521	TGL	OB1-CB1-OG2-CG2
19	C	268	PGV	C20-C19-O03-C01
21	N	1523	TGL	CA2-CA1-OG1-CG1
19	U	1268	PGV	C22-C23-C24-C25
26	C	270	CDL	C73-C74-C75-C76
25	T	1265	PEK	C16-C17-C18-C19
27	M	526	DMU	C19-C22-C25-C28
26	C	270	CDL	C34-C35-C36-C37
21	O	1521	TGL	CC1-CC2-CC3-CC4
21	B	521	TGL	CA3-CA4-CA5-CA6
21	O	1521	TGL	CA3-CA4-CA5-CA6
21	O	1521	TGL	C20-C21-C22-C23
26	T	1269	CDL	C78-C79-C80-C81
26	C	270	CDL	C83-C84-C85-C86
21	N	1523	TGL	C21-C22-C23-C24
26	T	1269	CDL	C81-C82-C83-C84
21	D	523	TGL	C21-C20-CA9-CA8

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Mol	Chain	Res	Type	Atoms
22	B	229	PSC	C20-C21-C22-C23
25	C	265	PEK	C26-C27-C28-C29
26	P	1270	CDL	C34-C35-C36-C37
19	N	1266	PGV	C29-C30-C31-C32
21	B	521	TGL	CB2-CB1-OG2-CG2
26	P	1270	CDL	C51-CB5-OB6-CB4
26	T	1269	CDL	C51-CB5-OB6-CB4
26	C	270	CDL	C51-CB5-OB6-CB4
22	B	229	PSC	C26-C27-C28-C29
25	C	264	PEK	C25-C26-C27-C28
26	P	1270	CDL	C13-C14-C15-C16
26	P	1270	CDL	C23-C24-C25-C26
26	T	1269	CDL	C39-C40-C41-C42
26	C	270	CDL	OB7-CB5-OB6-CB4
21	D	523	TGL	CA5-CA6-CA7-CA8
27	C	272	DMU	C19-C22-C25-C28
26	T	1269	CDL	OA6-CA4-CA6-OA8
25	G	1263	PEK	O03-C01-C02-O01
25	P	1264	PEK	C28-C29-C30-C31
26	P	1270	CDL	C11-C12-C13-C14
21	N	1523	TGL	C15-C16-C17-C18
21	N	1523	TGL	C22-C23-C24-C25
25	P	1264	PEK	C27-C28-C29-C30
26	G	269	CDL	C78-C79-C80-C81
26	C	270	CDL	C17-C18-C19-C20
25	C	265	PEK	C2-C3-C4-C5
19	A	524	PGV	C11-C10-C9-C8
21	Y	1522	TGL	C18-C19-C33-C34
19	C	268	PGV	C23-C24-C25-C26
26	C	270	CDL	C21-C22-C23-C24
27	C	272	DMU	C31-C34-C37-C40
26	P	1270	CDL	C57-C58-C59-C60
21	O	1521	TGL	C16-C17-C18-C19
26	G	269	CDL	OB9-CB7-OB8-CB6
26	T	1269	CDL	OB7-CB5-OB6-CB4
19	C	268	PGV	C30-C31-C32-C33
26	P	1270	CDL	CA3-OA5-PA1-OA2
26	T	1269	CDL	CA2-OA2-PA1-OA5
27	C	272	DMU	C3-C4-C57-O61
22	B	229	PSC	C01-C02-C03-O11
19	C	268	PGV	C01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C01-C02-C03-O11
26	C	270	CDL	CB7-C71-C72-C73
22	R	1229	PSC	C24-C25-C26-C27
21	B	521	TGL	C11-C12-C13-C14
21	O	1521	TGL	CC3-CC4-CC5-CC6
26	G	269	CDL	C32-C33-C34-C35
21	O	1521	TGL	C15-C16-C17-C18
26	G	269	CDL	C20-C21-C22-C23
19	A	521	PGV	C25-C26-C27-C28
21	Y	1522	TGL	C12-C13-C14-C29
19	C	268	PGV	O12-C04-C05-C06
27	Z	1526	DMU	O6-C11-C9-C8
21	B	521	TGL	CB4-CB5-CB6-CB7
26	T	1269	CDL	C53-C54-C55-C56
26	C	270	CDL	C84-C85-C86-C87
21	B	521	TGL	CA9-C20-C21-C22
25	T	263	PEK	O03-C01-C02-C03
26	P	1270	CDL	CB3-CB4-CB6-OB8
26	T	1269	CDL	CA3-CA4-CA6-OA8
19	N	1524	PGV	O03-C01-C02-C03
19	C	268	PGV	C6-C7-C8-C9
21	Y	1522	TGL	C29-C30-C31-C32
26	P	1270	CDL	C73-C74-C75-C76
25	T	1265	PEK	C25-C26-C27-C28
26	P	1270	CDL	C24-C25-C26-C27
26	P	1270	CDL	CA7-C31-C32-C33
19	U	1268	PGV	C23-C24-C25-C26
21	Y	1522	TGL	C21-C20-CA9-CA8
26	T	1269	CDL	C71-CB7-OB8-CB6
19	A	521	PGV	C31-C32-C33-C34
25	C	264	PEK	C30-C31-C32-C33
25	C	265	PEK	C35-C36-C37-C38
21	D	523	TGL	C33-C34-C35-C36
21	O	1521	TGL	CA5-CA6-CA7-CA8
19	C	268	PGV	C31-C32-C33-C34
25	C	264	PEK	C24-C25-C26-C27
26	T	1269	CDL	C44-C45-C46-C47
19	N	1524	PGV	C15-C16-C17-C18
21	Y	1522	TGL	CG1-CG2-OG2-CB1
19	A	524	PGV	C01-C02-O01-C1
21	N	1523	TGL	CG3-CG2-OG2-CB1
27	P	272	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
21	L	522	TGL	CA5-CA6-CA7-CA8
21	B	521	TGL	C23-C24-C25-C26
19	U	1268	PGV	C6-C7-C8-C9
25	T	263	PEK	O01-C02-C03-O11
22	B	229	PSC	C11-C10-C9-C8
21	O	1521	TGL	CB1-CB2-CB3-CB4
19	A	524	PGV	C15-C16-C17-C18
21	N	1523	TGL	OA1-CA1-OG1-CG1
27	C	272	DMU	C1-C6-O16-C18
25	T	263	PEK	O03-C01-C02-O01
21	B	521	TGL	C24-C25-C26-C27
19	P	1267	PGV	C25-C26-C27-C28
21	N	1523	TGL	CA6-CA7-CA8-CA9
19	C	268	PGV	C13-C14-C15-C16
26	P	1270	CDL	C64-C65-C66-C67
19	N	1524	PGV	C31-C32-C33-C34
25	P	1264	PEK	C34-C35-C36-C37
21	Y	1522	TGL	CA5-CA6-CA7-CA8
26	P	1270	CDL	C52-C53-C54-C55
23	C	271	CHD	C16-C17-C20-C22
21	D	523	TGL	CC4-CC5-CC6-CC7
19	A	524	PGV	C14-C15-C16-C17
26	T	1269	CDL	C21-C22-C23-C24
26	C	270	CDL	C42-C43-C44-C45
19	P	1267	PGV	C31-C32-C33-C34
25	T	1265	PEK	C22-C23-C24-C25
25	G	1263	PEK	C17-C18-C19-C20
26	T	1269	CDL	OB9-CB7-OB8-CB6
21	O	1521	TGL	C13-C14-C29-C30
25	T	1265	PEK	C30-C31-C32-C33
26	T	1269	CDL	C75-C76-C77-C78
19	N	1524	PGV	C30-C31-C32-C33
19	N	1266	PGV	C23-C24-C25-C26
19	P	1267	PGV	C20-C21-C22-C23
26	G	269	CDL	C36-C37-C38-C39
19	C	267	PGV	C31-C32-C33-C34
26	C	270	CDL	C59-C60-C61-C62
25	C	264	PEK	C4-C5-C6-C7
25	C	265	PEK	C4-C5-C6-C7
21	Y	1522	TGL	C17-C18-C19-C33
19	N	1524	PGV	C25-C26-C27-C28
26	C	270	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
19	N	1266	PGV	C31-C32-C33-C34
27	M	526	DMU	O5-C6-O16-C18
26	P	1270	CDL	OA5-CA3-CA4-CA6
26	P	1270	CDL	OB5-CB3-CB4-CB6
26	C	270	CDL	OB5-CB3-CB4-CB6
22	R	1229	PSC	C21-C22-C23-C24
21	Y	1522	TGL	CC4-CC5-CC6-CC7
26	P	1270	CDL	OB7-CB5-OB6-CB4
27	P	272	DMU	C5-C10-O7-C3
26	G	269	CDL	C21-C22-C23-C24
26	T	1269	CDL	C38-C39-C40-C41
25	C	264	PEK	C35-C36-C37-C38
19	A	524	PGV	C31-C32-C33-C34
27	M	526	DMU	C25-C28-C31-C34
19	C	267	PGV	C15-C16-C17-C18
26	G	269	CDL	CA4-CA3-OA5-PA1
26	P	1270	CDL	C1-CA2-OA2-PA1
26	C	270	CDL	C56-C57-C58-C59
26	G	269	CDL	C34-C35-C36-C37
21	L	522	TGL	C16-C15-CC9-CC8
21	D	523	TGL	CG1-CG2-CG3-OG3
21	Y	1522	TGL	OG1-CG1-CG2-CG3
26	G	269	CDL	CB3-CB4-CB6-OB8
26	C	270	CDL	CB3-CB4-CB6-OB8
22	R	1229	PSC	C23-C24-C25-C26
26	G	269	CDL	C53-C54-C55-C56
26	G	269	CDL	C62-C63-C64-C65
26	T	1269	CDL	C43-C44-C45-C46
26	T	1269	CDL	C52-C53-C54-C55
19	C	268	PGV	O04-C19-O03-C01
19	P	1267	PGV	C13-C14-C15-C16
21	B	521	TGL	CC2-CC3-CC4-CC5
25	P	1264	PEK	C26-C27-C28-C29
19	N	1524	PGV	C21-C22-C23-C24
21	B	521	TGL	C29-C30-C31-C32
21	L	522	TGL	CC2-CC3-CC4-CC5
26	C	270	CDL	C15-C16-C17-C18
22	R	1229	PSC	C9-C10-C11-C12
25	T	263	PEK	C11-C10-C9-C8
22	B	229	PSC	C9-C10-C11-C12
25	C	264	PEK	C9-C10-C11-C12
25	P	1264	PEK	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	P	1264	PEK	C11-C10-C9-C8
25	P	1264	PEK	C12-C13-C14-C15
25	C	265	PEK	C5-C6-C7-C8
25	C	265	PEK	C11-C10-C9-C8
25	T	1265	PEK	C03-O11-P-O12
25	T	1265	PEK	C6-C7-C8-C9
25	T	1265	PEK	C11-C10-C9-C8
25	G	1263	PEK	C6-C7-C8-C9
25	G	1263	PEK	C11-C10-C9-C8
25	G	1263	PEK	C11-C12-C13-C14
21	Y	1522	TGL	CB5-CB6-CB7-CB8
25	C	265	PEK	C28-C29-C30-C31
19	A	521	PGV	C23-C24-C25-C26
25	C	265	PEK	O01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-OA6
25	P	1264	PEK	C22-C23-C24-C25
21	Y	1522	TGL	CC5-CC6-CC7-CC8
21	L	522	TGL	OG1-CA1-CA2-CA3
21	B	521	TGL	CC9-C15-C16-C17
21	L	522	TGL	CB4-CB5-CB6-CB7
25	G	1263	PEK	C16-C17-C18-C19
19	C	268	PGV	C14-C15-C16-C17
26	C	270	CDL	C80-C81-C82-C83
19	U	1268	PGV	O03-C01-C02-O01
22	B	229	PSC	O03-C01-C02-O01
26	P	1270	CDL	OB6-CB4-CB6-OB8
26	C	270	CDL	OA6-CA4-CA6-OA8
26	T	1269	CDL	C18-C19-C20-C21
21	L	522	TGL	CB6-CB7-CB8-CB9
21	B	521	TGL	C21-C20-CA9-CA8
19	N	1266	PGV	C24-C25-C26-C27
19	C	268	PGV	C25-C26-C27-C28
26	P	1270	CDL	C22-C23-C24-C25
26	T	1269	CDL	C83-C84-C85-C86
25	T	263	PEK	C02-C03-O11-P
25	T	1265	PEK	C23-C24-C25-C26
21	B	521	TGL	C15-C16-C17-C18
19	C	268	PGV	C15-C16-C17-C18
25	P	1264	PEK	C3-C4-C5-C6
21	L	522	TGL	C12-C13-C14-C29
26	C	270	CDL	C58-C59-C60-C61
26	G	269	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
21	N	1523	TGL	C12-C13-C14-C29
27	M	526	DMU	C22-C25-C28-C31
25	C	265	PEK	C01-C02-C03-O11
26	G	269	CDL	C35-C36-C37-C38
27	Z	1526	DMU	C34-C37-C40-C43
19	U	1268	PGV	C3-C4-C5-C6
23	P	1525	CHD	C13-C17-C20-C22
25	C	265	PEK	C33-C34-C35-C36
26	G	269	CDL	C19-C20-C21-C22
21	L	522	TGL	CC7-CC8-CC9-C15
25	C	264	PEK	C32-C33-C34-C35
21	B	521	TGL	C16-C17-C18-C19
21	N	1523	TGL	CC4-CC5-CC6-CC7
22	R	1229	PSC	C28-C29-C30-C31
25	P	1264	PEK	C24-C25-C26-C27
21	L	522	TGL	CA2-CA3-CA4-CA5
21	N	1523	TGL	CC9-C15-C16-C17
22	R	1229	PSC	C01-C02-O01-C1
21	B	521	TGL	CG1-CG2-OG2-CB1
21	O	1521	TGL	CG1-CG2-OG2-CB1
19	N	1524	PGV	C03-C02-O01-C1
25	T	263	PEK	C23-C24-C25-C26
21	Y	1522	TGL	C19-C33-C34-C35
25	C	264	PEK	C17-C18-C19-C20
26	P	1270	CDL	C15-C16-C17-C18
21	O	1521	TGL	C10-C11-C12-C13
22	R	1229	PSC	O03-C01-C02-C03
22	B	229	PSC	O03-C01-C02-C03
22	B	229	PSC	C02-C03-O11-P
26	G	269	CDL	C44-C45-C46-C47
26	C	270	CDL	OB5-CB3-CB4-OB6
25	G	1263	PEK	O01-C02-C03-O11
19	A	524	PGV	C7-C8-C9-C10
21	O	1521	TGL	C29-C30-C31-C32
21	N	1523	TGL	C24-C25-C26-C27
26	P	1270	CDL	OA6-CA4-CA6-OA8
21	N	1523	TGL	OG2-CG2-CG3-OG3
21	D	523	TGL	C22-C23-C24-C25
19	C	268	PGV	C27-C28-C29-C30
19	C	267	PGV	C12-C13-C14-C15
26	G	269	CDL	C77-C78-C79-C80
26	T	1269	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C32-C31-CA7-OA8
19	U	1268	PGV	C31-C32-C33-C34
21	L	522	TGL	C33-C34-C35-C36
27	M	526	DMU	C34-C37-C40-C43
27	C	272	DMU	C5-C10-O7-C3
22	R	1229	PSC	C04-O12-P-O11
19	C	268	PGV	C04-O12-P-O11
26	G	269	CDL	CB2-OB2-PB2-OB5
19	A	524	PGV	C04-O12-P-O11
22	R	1229	PSC	C02-C03-O11-P
19	P	1267	PGV	C02-C03-O11-P
19	C	267	PGV	C02-C03-O11-P
14	A	515	HEA	C14-C15-C16-C17
19	C	267	PGV	C20-C21-C22-C23
19	A	524	PGV	C2-C3-C4-C5
22	R	1229	PSC	C03-O11-P-O13
22	R	1229	PSC	C04-O12-P-O13
22	B	229	PSC	C03-O11-P-O13
25	C	265	PEK	C04-O12-P-O14
19	A	524	PGV	C04-O12-P-O14
26	T	1269	CDL	CA2-OA2-PA1-OA3
26	T	1269	CDL	CA2-OA2-PA1-OA4
26	T	1269	CDL	CA3-OA5-PA1-OA4
25	T	1265	PEK	C03-O11-P-O14
19	N	1524	PGV	C03-O11-P-O14
25	G	1263	PEK	C03-O11-P-O13
19	U	1268	PGV	C01-C02-C03-O11
25	T	263	PEK	C01-C02-C03-O11
25	G	1263	PEK	C01-C02-C03-O11
21	L	522	TGL	C13-C14-C29-C30
25	T	263	PEK	O12-C04-C05-N
26	T	1269	CDL	C74-C75-C76-C77
23	C	271	CHD	C16-C17-C20-C21
26	G	269	CDL	C15-C16-C17-C18
19	U	1268	PGV	C12-C13-C14-C15
19	U	1268	PGV	C14-C15-C16-C17
19	A	524	PGV	C22-C23-C24-C25
21	N	1523	TGL	CA3-CA4-CA5-CA6
22	B	229	PSC	O01-C02-C03-O11
26	P	1270	CDL	OB5-CB3-CB4-OB6
25	C	264	PEK	C3-C4-C5-C6
25	G	1263	PEK	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
21	O	1521	TGL	C21-C20-CA9-CA8
25	G	1263	PEK	C29-C30-C31-C32
25	P	1264	PEK	C21-C22-C23-C24
21	D	523	TGL	CB5-CB6-CB7-CB8
22	R	1229	PSC	C04-C05-N-C06
21	B	521	TGL	C14-C29-C30-C31
21	Y	1522	TGL	C11-C12-C13-C14
19	P	1267	PGV	C1-C2-C3-C4
26	P	1270	CDL	CA5-C11-C12-C13
22	B	229	PSC	C22-C23-C24-C25
21	Y	1522	TGL	CG1-CG2-CG3-OG3
26	P	1270	CDL	CA3-CA4-CA6-OA8
26	C	270	CDL	CA3-CA4-CA6-OA8
19	A	521	PGV	C29-C30-C31-C32
21	N	1523	TGL	CG1-CG2-CG3-OG3
14	A	516	HEA	C4D-C3D-CAD-CBD
22	R	1229	PSC	O03-C01-C02-O01
21	D	523	TGL	OG2-CG2-CG3-OG3
19	A	524	PGV	O03-C01-C02-O01
26	C	270	CDL	OB6-CB4-CB6-OB8
19	N	1524	PGV	O03-C01-C02-O01
27	P	272	DMU	C22-C25-C28-C31
21	Y	1522	TGL	C23-C24-C25-C26
26	T	1269	CDL	C33-C34-C35-C36
26	T	1269	CDL	C63-C64-C65-C66
26	C	270	CDL	CA4-CA3-OA5-PA1
19	A	524	PGV	C1-C2-C3-C4
21	D	523	TGL	OG1-CA1-CA2-CA3
21	D	523	TGL	C29-C30-C31-C32
19	A	524	PGV	C29-C30-C31-C32
26	G	269	CDL	C71-C72-C73-C74
26	C	270	CDL	C52-C51-CB5-OB6
23	C	525	CHD	C13-C17-C20-C22
21	B	521	TGL	CC3-CC4-CC5-CC6
21	D	523	TGL	CB4-CB5-CB6-CB7
25	T	263	PEK	C32-C33-C34-C35
25	C	265	PEK	C31-C32-C33-C34
21	O	1521	TGL	OG3-CC1-CC2-CC3
26	T	1269	CDL	C61-C62-C63-C64
26	G	269	CDL	C75-C76-C77-C78
26	C	270	CDL	C18-C19-C20-C21
26	C	270	CDL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
23	P	1271	CHD	C20-C22-C23-C24
21	D	523	TGL	CG3-CG2-OG2-CB1
25	C	265	PEK	C34-C35-C36-C37
25	G	1263	PEK	C22-C23-C24-C25
19	P	1267	PGV	C9-C10-C11-C12
26	P	1270	CDL	CA4-CA3-OA5-PA1
25	T	1265	PEK	C33-C34-C35-C36
14	A	515	HEA	C26-C15-C16-C17
21	D	523	TGL	OG2-CB1-CB2-CB3
26	P	1270	CDL	C38-C39-C40-C41
19	N	1524	PGV	C9-C10-C11-C12
25	P	1264	PEK	O03-C01-C02-O01
21	Y	1522	TGL	CB2-CB3-CB4-CB5
19	U	1268	PGV	C04-O12-P-O11
19	A	524	PGV	C03-O11-P-O12
26	T	1269	CDL	CB2-OB2-PB2-OB5
19	A	521	PGV	C04-O12-P-O11
25	T	1265	PEK	C04-O12-P-O11
21	Y	1522	TGL	CA6-CA7-CA8-CA9
26	C	270	CDL	C20-C21-C22-C23
26	C	270	CDL	C31-C32-C33-C34
26	C	270	CDL	C79-C80-C81-C82
26	T	1269	CDL	C34-C35-C36-C37
19	N	1524	PGV	C28-C29-C30-C31
25	G	1263	PEK	C30-C31-C32-C33
25	G	1263	PEK	C02-C03-O11-P
22	B	229	PSC	C12-C13-C14-C15
23	P	1525	CHD	C13-C17-C20-C21
26	C	270	CDL	CA7-C31-C32-C33
21	O	1521	TGL	CA7-CA8-CA9-C20
26	P	1270	CDL	C78-C79-C80-C81
25	T	1265	PEK	C22-C21-O03-C01
19	U	1268	PGV	C11-C10-C9-C8
25	T	263	PEK	C15-C16-C17-C18
25	C	264	PEK	C2-C3-C4-C5
19	C	267	PGV	C1-C2-C3-C4
26	G	269	CDL	C74-C75-C76-C77
27	C	272	DMU	C34-C37-C40-C43
26	T	1269	CDL	CA5-C11-C12-C13
25	C	265	PEK	C14-C15-C16-C17
19	N	1524	PGV	O01-C02-C03-O11
19	N	1524	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
25	T	1265	PEK	O04-C21-O03-C01
19	P	1267	PGV	C29-C30-C31-C32
19	C	268	PGV	O03-C01-C02-O01
21	N	1523	TGL	CA2-CA3-CA4-CA5
19	U	1268	PGV	C02-C03-O11-P
26	G	269	CDL	C1-CA2-OA2-PA1
19	N	1524	PGV	C05-C04-O12-P
21	L	522	TGL	OG2-CB1-CB2-CB3
25	P	1264	PEK	C2-C3-C4-C5
21	D	523	TGL	CB7-CB8-CB9-C10
26	G	269	CDL	C64-C65-C66-C67
19	P	1267	PGV	C15-C16-C17-C18
25	C	265	PEK	C29-C30-C31-C32
21	O	1521	TGL	CB7-CB8-CB9-C10
21	N	1523	TGL	CA7-CA8-CA9-C20
23	J	60	CHD	C21-C20-C22-C23
22	R	1229	PSC	C15-C16-C17-C18
19	C	267	PGV	C9-C10-C11-C12
21	B	521	TGL	OC1-CC1-OG3-CG3
26	T	1269	CDL	C62-C63-C64-C65
23	P	1271	CHD	C16-C17-C20-C22
22	R	1229	PSC	C10-C11-C12-C13
22	B	229	PSC	C10-C11-C12-C13
21	D	523	TGL	CC9-C15-C16-C17
25	T	263	PEK	C26-C27-C28-C29
27	M	526	DMU	C28-C31-C34-C37
26	P	1270	CDL	OA5-CA3-CA4-OA6
25	T	1265	PEK	C31-C32-C33-C34
19	N	1524	PGV	C20-C21-C22-C23
19	N	1266	PGV	C11-C10-C9-C8
25	T	1265	PEK	C27-C28-C29-C30
19	P	1267	PGV	C28-C29-C30-C31
21	L	522	TGL	CA9-C20-C21-C22
26	P	1270	CDL	C39-C40-C41-C42
26	T	1269	CDL	C56-C57-C58-C59
27	C	272	DMU	C4-C3-O7-C10
25	T	263	PEK	C21-C22-C23-C24
26	G	269	CDL	OA6-CA4-CA6-OA8
19	P	1267	PGV	C14-C15-C16-C17
25	T	263	PEK	C4-C5-C6-C7
21	Y	1522	TGL	CB7-CB8-CB9-C10
19	A	524	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C17-C18-C19-C20
19	A	524	PGV	C26-C27-C28-C29
26	P	1270	CDL	C44-C45-C46-C47
21	N	1523	TGL	CA5-CA6-CA7-CA8
23	C	525	CHD	C13-C17-C20-C21
19	C	268	PGV	C22-C23-C24-C25
21	N	1523	TGL	C13-C14-C29-C30
19	A	521	PGV	C4-C5-C6-C7
26	P	1270	CDL	C55-C56-C57-C58
19	N	1266	PGV	C9-C10-C11-C12
19	U	1268	PGV	O01-C02-C03-O11
25	P	1264	PEK	C17-C18-C19-C20
21	O	1521	TGL	OG1-CA1-CA2-CA3
21	O	1521	TGL	CC4-CC5-CC6-CC7
26	T	1269	CDL	OB5-CB3-CB4-CB6
25	C	264	PEK	C14-C15-C16-C17
21	B	521	TGL	C20-C21-C22-C23
21	L	522	TGL	OG3-CC1-CC2-CC3
26	C	270	CDL	C12-C11-CA5-OA6
19	C	267	PGV	C05-C04-O12-P
26	T	1269	CDL	CB4-CB3-OB5-PB2
21	N	1523	TGL	OG1-CG1-CG2-OG2
19	A	524	PGV	C3-C4-C5-C6
21	N	1523	TGL	C14-C29-C30-C31
25	P	1264	PEK	O01-C1-C2-C3
27	P	272	DMU	C34-C37-C40-C43
27	C	272	DMU	C25-C28-C31-C34
26	G	269	CDL	C32-C31-CA7-OA8
14	N	516	HEA	C26-C15-C16-C17
25	C	264	PEK	C16-C17-C18-C19
22	R	1229	PSC	C04-C05-N-C07
22	R	1229	PSC	C04-C05-N-C08
25	T	263	PEK	C3-C4-C5-C6
25	C	264	PEK	O01-C1-C2-C3
19	N	1524	PGV	O01-C1-C2-C3
19	A	524	PGV	C23-C24-C25-C26
21	N	1523	TGL	CA9-C20-C21-C22
22	R	1229	PSC	C12-C13-C14-C15
25	P	1264	PEK	C14-C15-C16-C17
23	O	229	CHD	C17-C20-C22-C23
22	R	1229	PSC	C26-C27-C28-C29
21	Y	1522	TGL	CC6-CC7-CC8-CC9

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Mol	Chain	Res	Type	Atoms
21	L	522	TGL	C21-C20-CA9-CA8
19	U	1268	PGV	O01-C1-C2-C3
26	G	269	CDL	C52-C51-CB5-OB6
21	Y	1522	TGL	C13-C14-C29-C30
21	O	1521	TGL	OG1-CG1-CG2-OG2
21	Y	1522	TGL	OG1-CG1-CG2-OG2
21	L	522	TGL	C23-C24-C25-C26
19	C	268	PGV	O05-C05-C06-O06
21	D	523	TGL	CB6-CB7-CB8-CB9
19	A	524	PGV	C4-C5-C6-C7
21	B	521	TGL	CB6-CB7-CB8-CB9
19	N	1266	PGV	O03-C19-C20-C21
21	N	1523	TGL	C17-C18-C19-C33
26	G	269	CDL	C32-C31-CA7-OA9
21	N	1523	TGL	CC6-CC7-CC8-CC9
19	A	524	PGV	O12-C04-C05-C06
26	P	1270	CDL	CA2-C1-CB2-OB2
26	C	270	CDL	C12-C11-CA5-OA7
19	N	1524	PGV	O02-C1-C2-C3
22	B	229	PSC	C7-C8-C9-C10
26	P	1270	CDL	C79-C80-C81-C82
25	P	1264	PEK	O03-C01-C02-C03
26	C	270	CDL	O1-C1-CA2-OA2
19	U	1268	PGV	C05-C04-O12-P
19	C	268	PGV	C05-C04-O12-P
21	L	522	TGL	C11-C10-CB9-CB8
19	C	268	PGV	C04-O12-P-O13
26	G	269	CDL	CA3-OA5-PA1-OA3
26	G	269	CDL	CA3-OA5-PA1-OA4
19	A	524	PGV	C03-O11-P-O13
26	C	270	CDL	CB2-OB2-PB2-OB3
19	N	1266	PGV	C04-O12-P-O13
19	P	1267	PGV	O03-C01-C02-O01
19	P	1267	PGV	C27-C28-C29-C30
21	L	522	TGL	C29-C30-C31-C32
19	U	1268	PGV	O02-C1-C2-C3
25	C	264	PEK	O02-C1-C2-C3
21	O	1521	TGL	C18-C19-C33-C34
19	A	524	PGV	C9-C10-C11-C12
22	B	229	PSC	C05-C04-O12-P
25	P	1264	PEK	O02-C1-C2-C3
22	R	1229	PSC	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
21	L	522	TGL	CB5-CB6-CB7-CB8
22	B	229	PSC	C6-C7-C8-C9
14	A	516	HEA	C26-C15-C16-C17
21	L	522	TGL	OA1-CA1-CA2-CA3
25	C	265	PEK	C24-C25-C26-C27
22	B	229	PSC	C19-C20-C21-C22
21	O	1521	TGL	C25-C26-C27-C28
21	N	1523	TGL	CB5-CB6-CB7-CB8
19	A	524	PGV	O03-C19-C20-C21
21	L	522	TGL	OC1-CC1-CC2-CC3

There are no ring outliers.

38 monomers are involved in 373 short contacts:

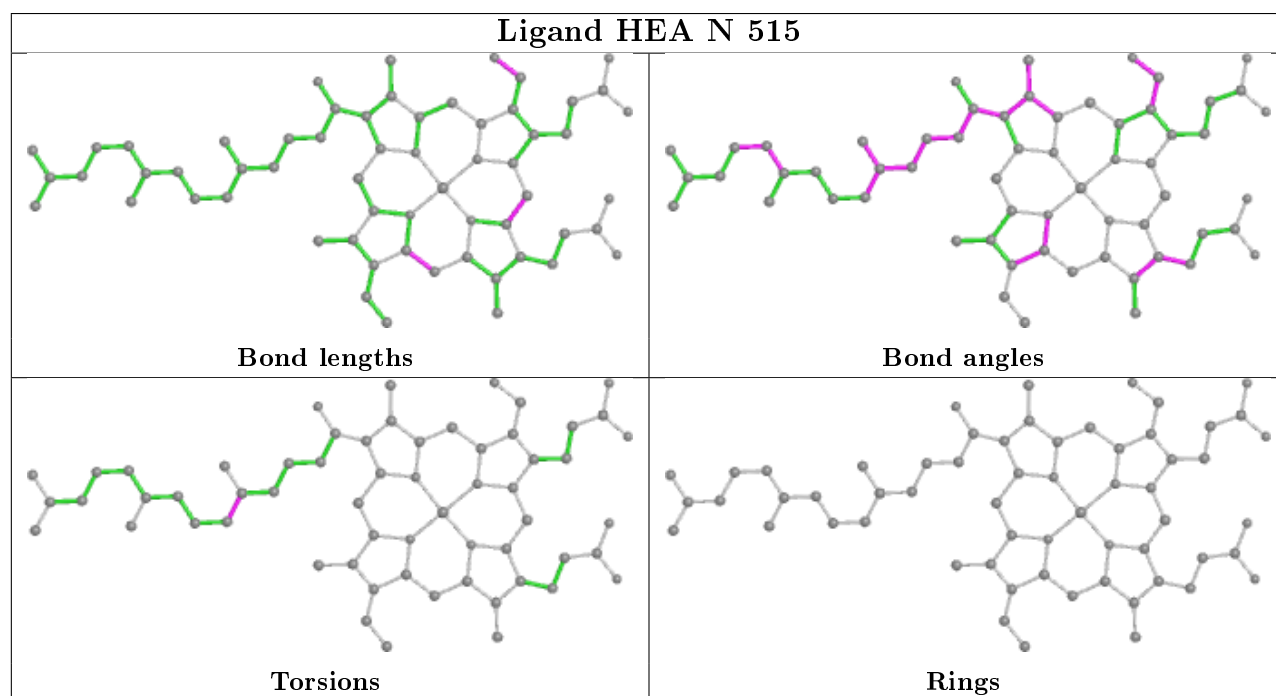
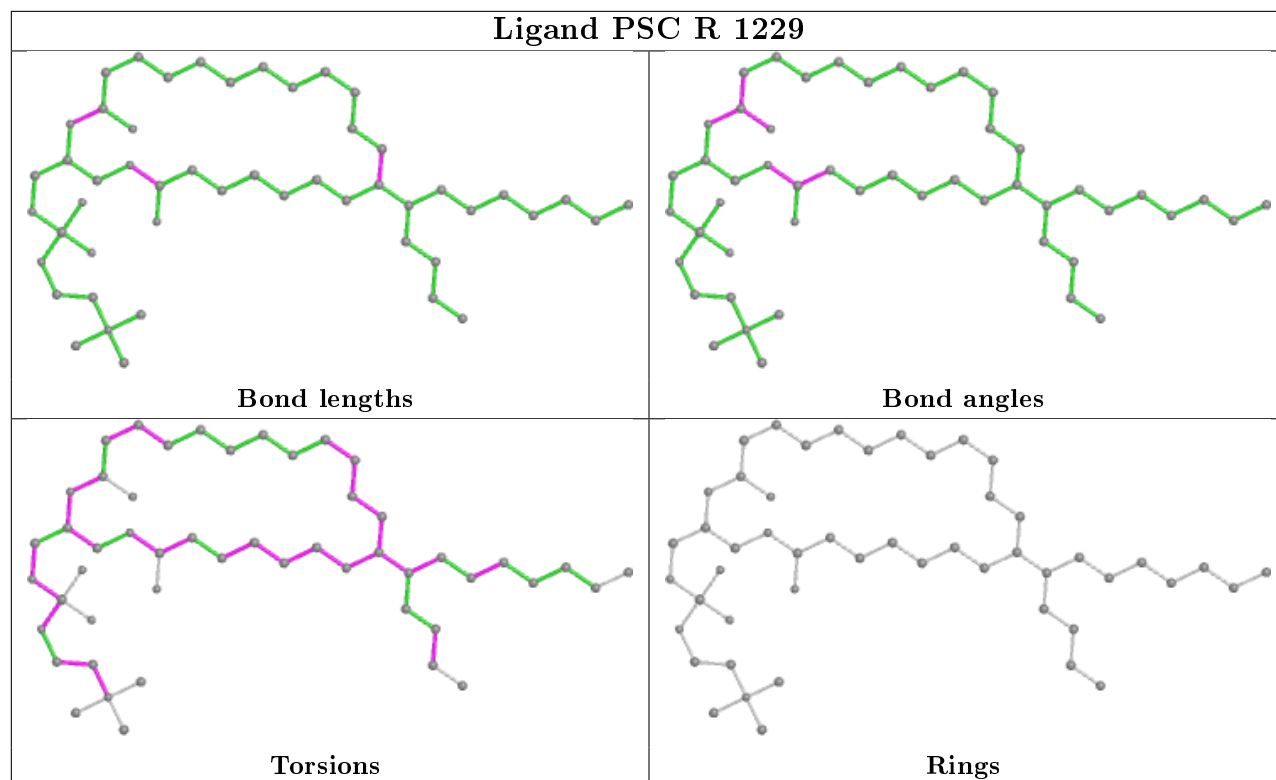
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	R	1229	PSC	20	0
14	N	515	HEA	6	0
14	A	515	HEA	8	0
21	B	521	TGL	4	0
19	P	1267	PGV	3	0
19	U	1268	PGV	4	0
25	T	263	PEK	14	0
21	D	523	TGL	10	0
22	B	229	PSC	20	0
19	C	268	PGV	6	0
14	N	516	HEA	3	0
23	J	60	CHD	8	0
25	P	1264	PEK	6	0
21	O	1521	TGL	5	0
23	O	229	CHD	3	0
25	C	264	PEK	9	0
25	C	265	PEK	13	0
26	G	269	CDL	33	0
19	C	267	PGV	4	0
21	Y	1522	TGL	20	0
26	P	1270	CDL	27	0
26	T	1269	CDL	30	0
21	L	522	TGL	15	0
23	C	525	CHD	2	0
19	A	524	PGV	14	0
26	C	270	CDL	20	0
19	A	521	PGV	2	0

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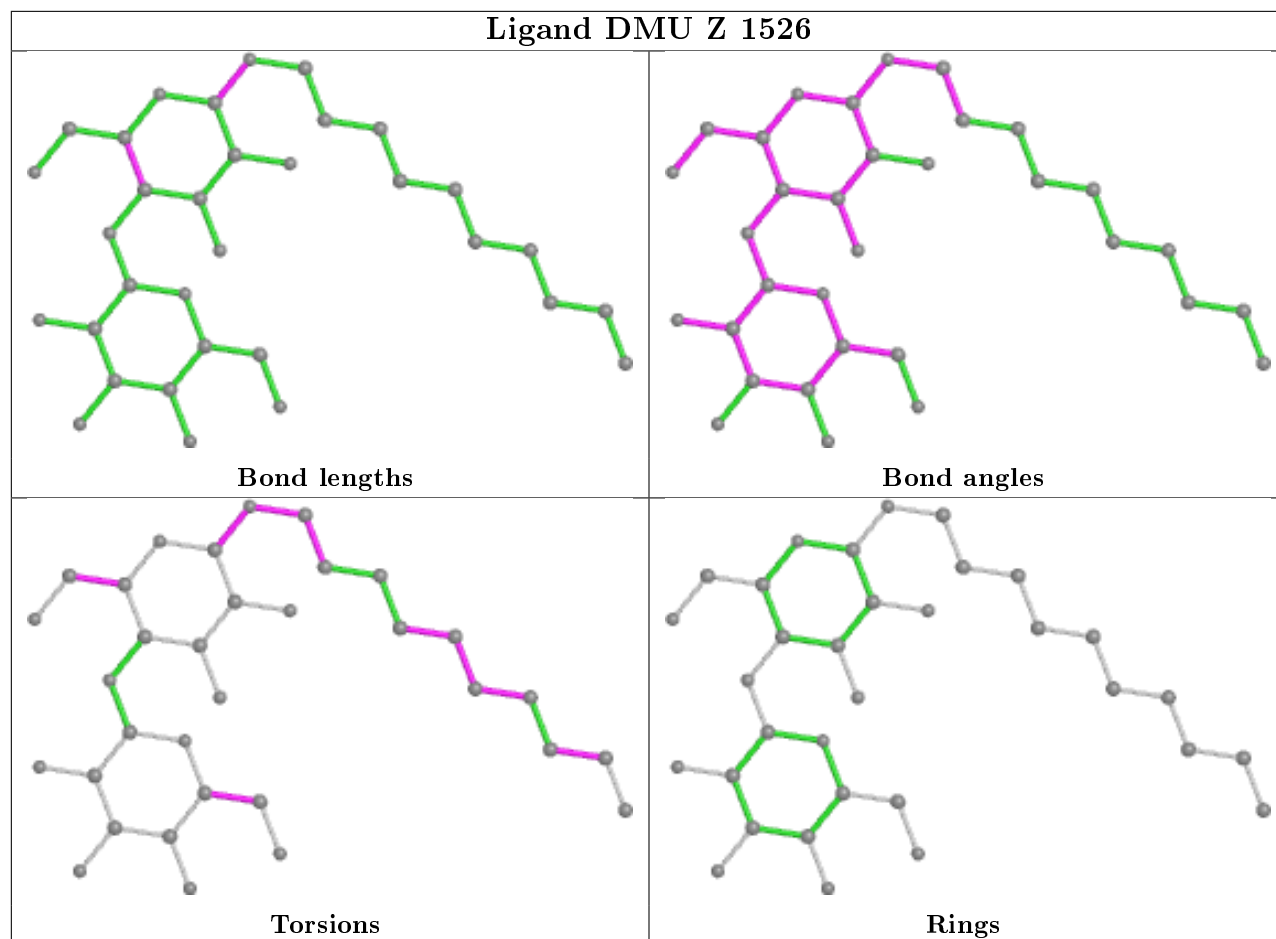
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	1523	TGL	14	0
25	T	1265	PEK	20	0
23	P	1271	CHD	5	0
23	B	1085	CHD	4	0
27	P	272	DMU	1	0
19	N	1524	PGV	7	0
27	C	272	DMU	4	0
23	W	1059	CHD	3	0
23	C	271	CHD	2	0
25	G	1263	PEK	19	0
14	A	516	HEA	8	0

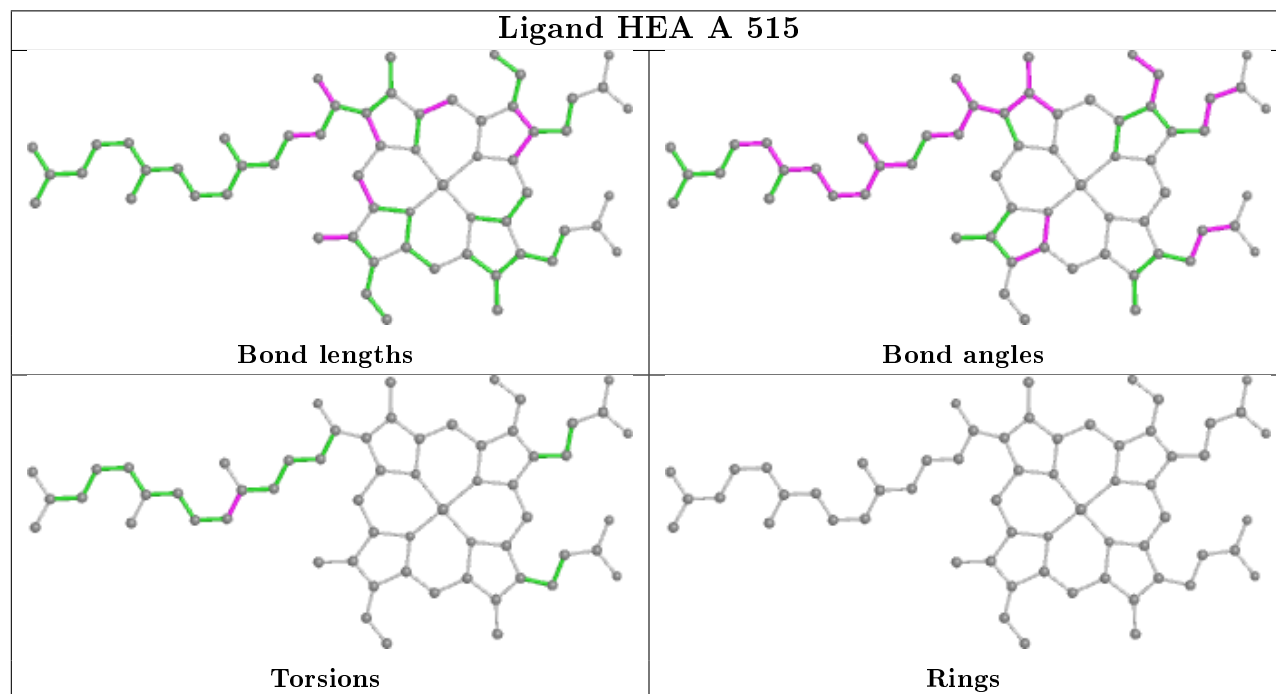
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

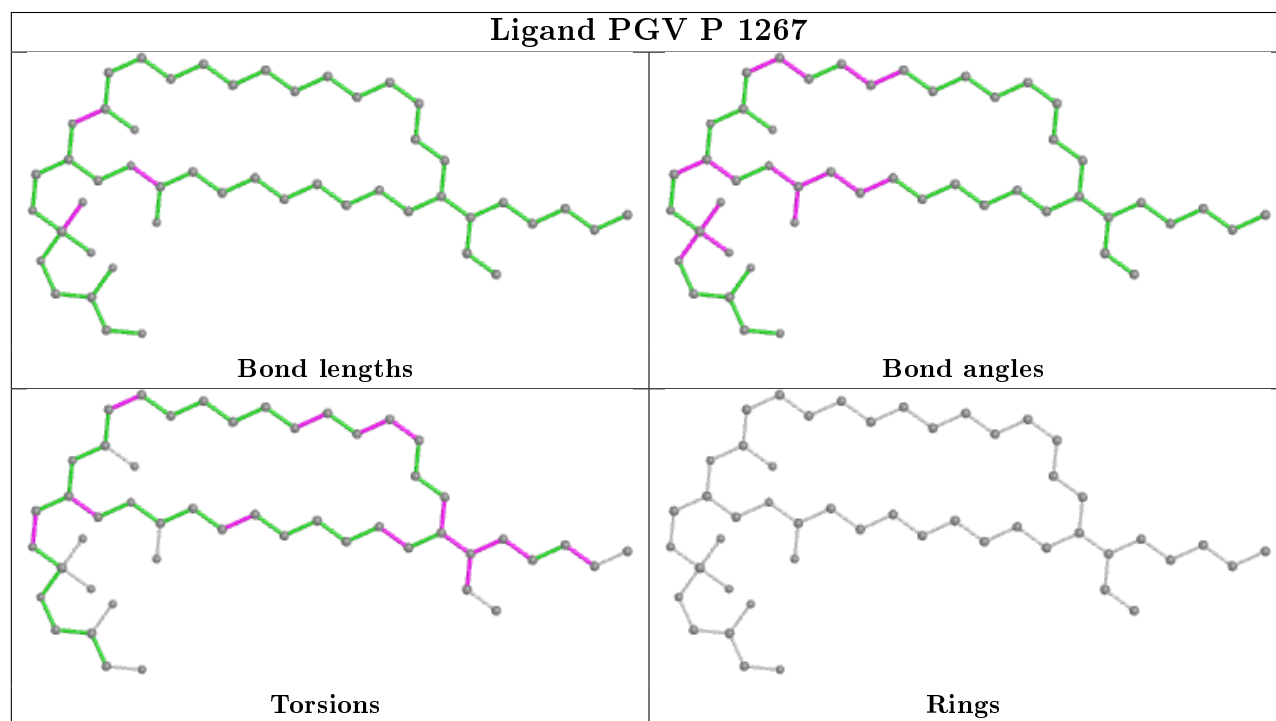
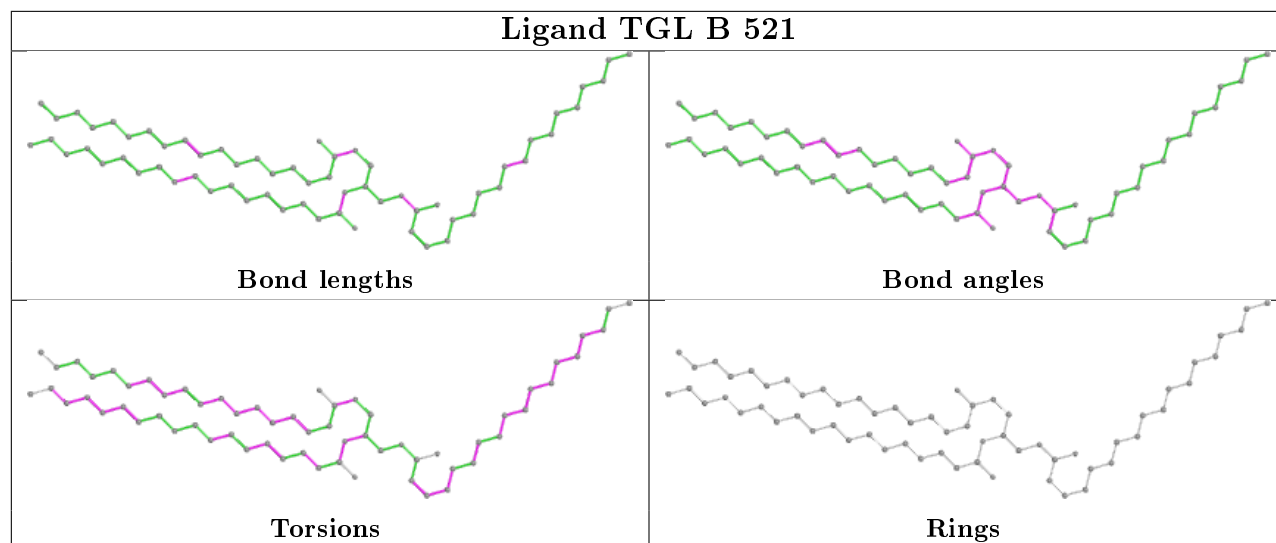


Ligand DMU Z 1526

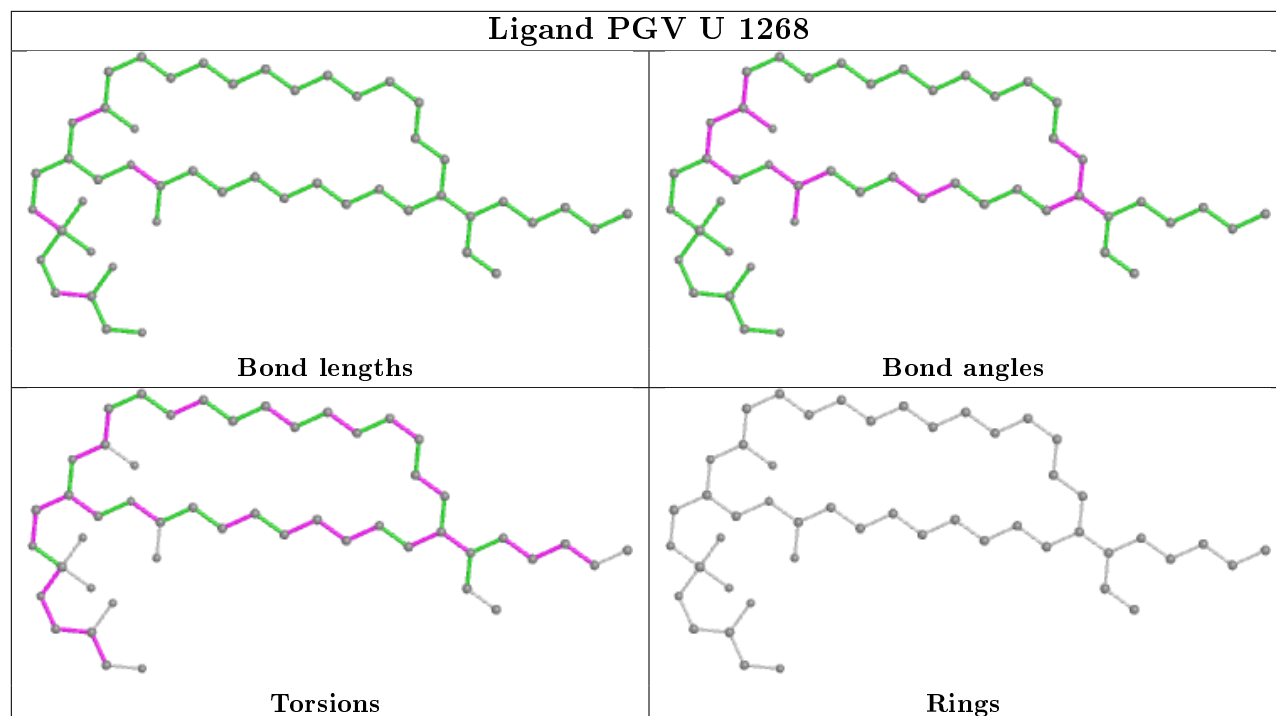


Ligand HEA A 515

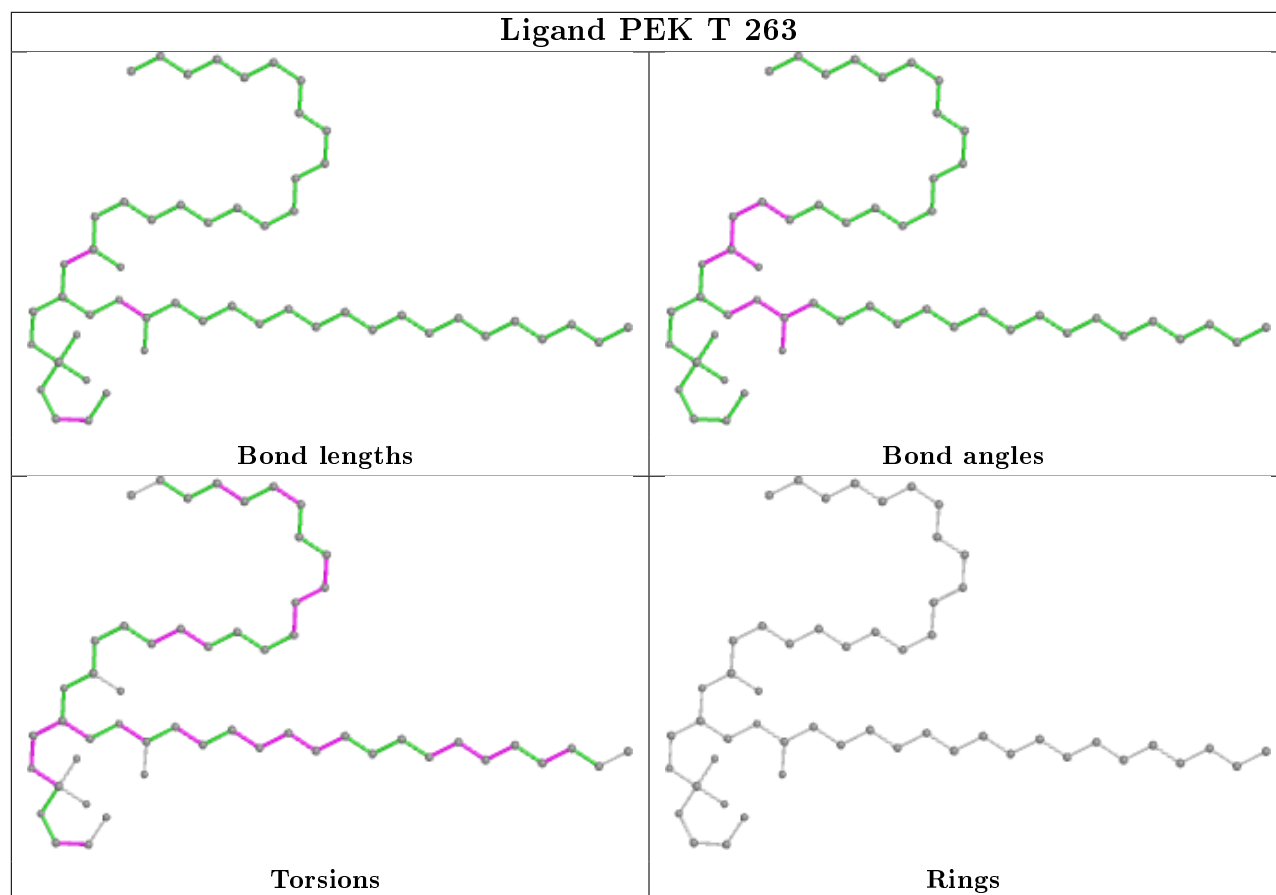


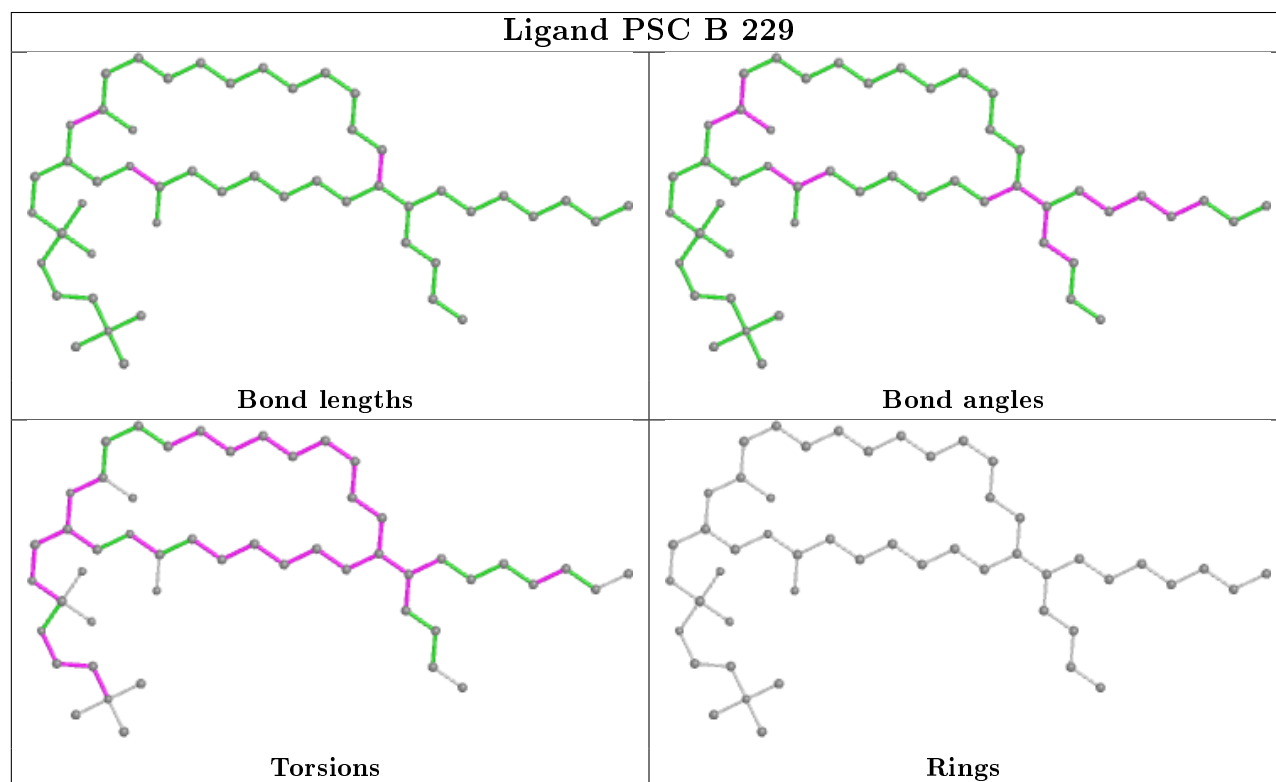
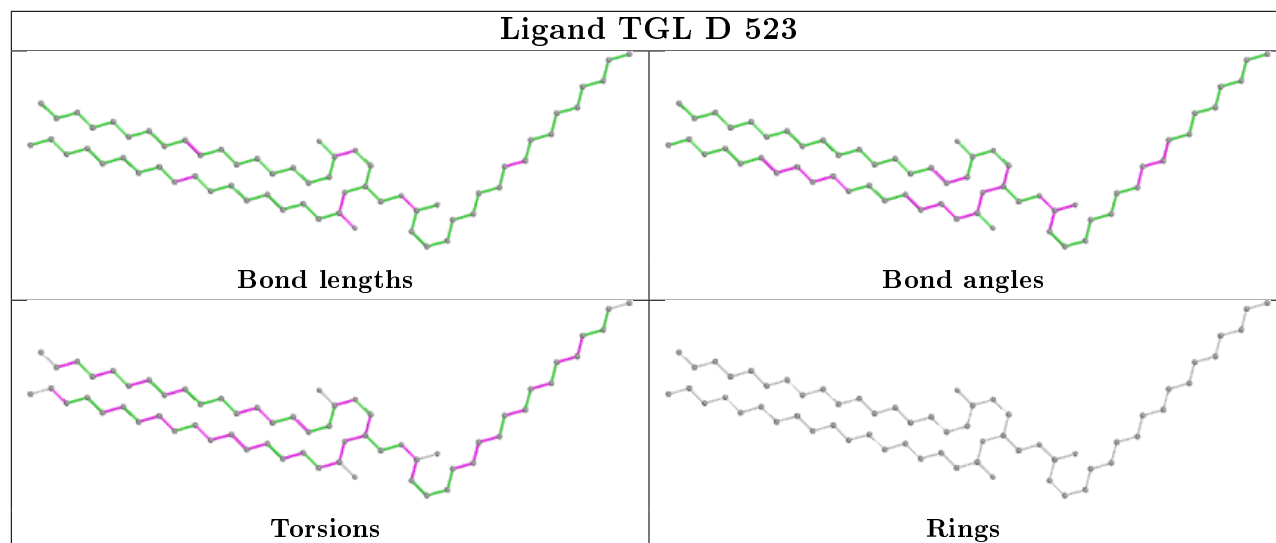


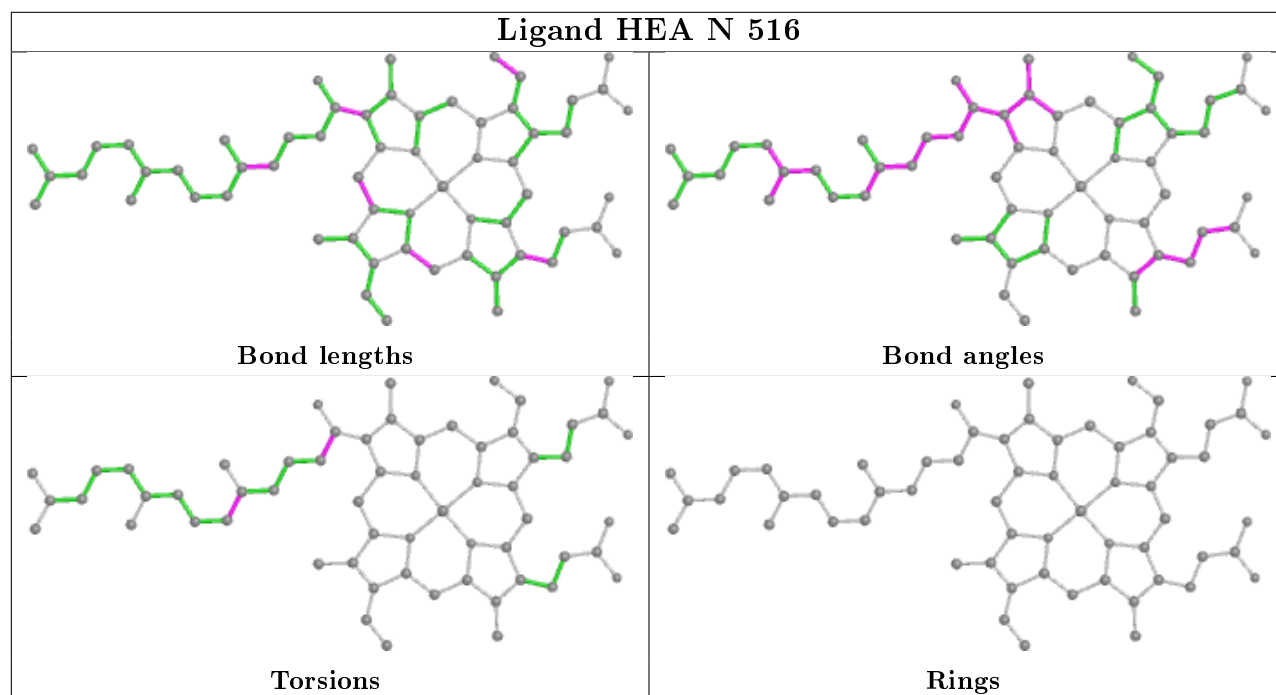
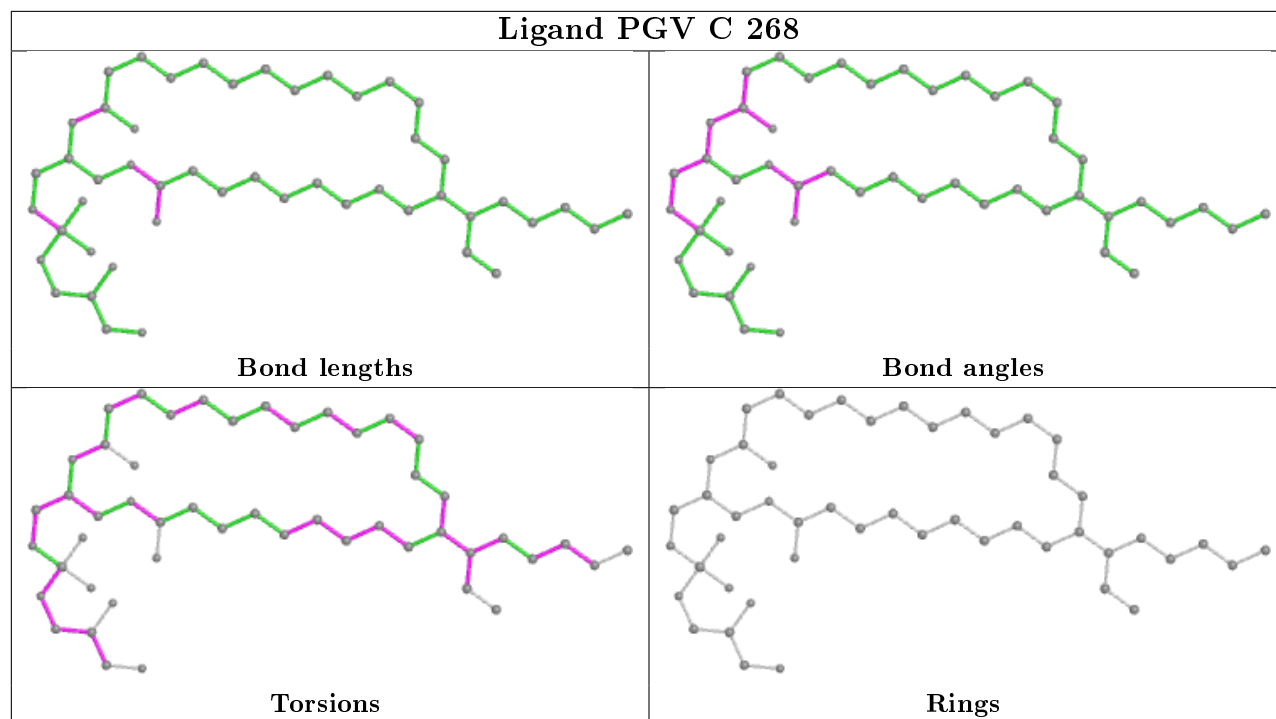
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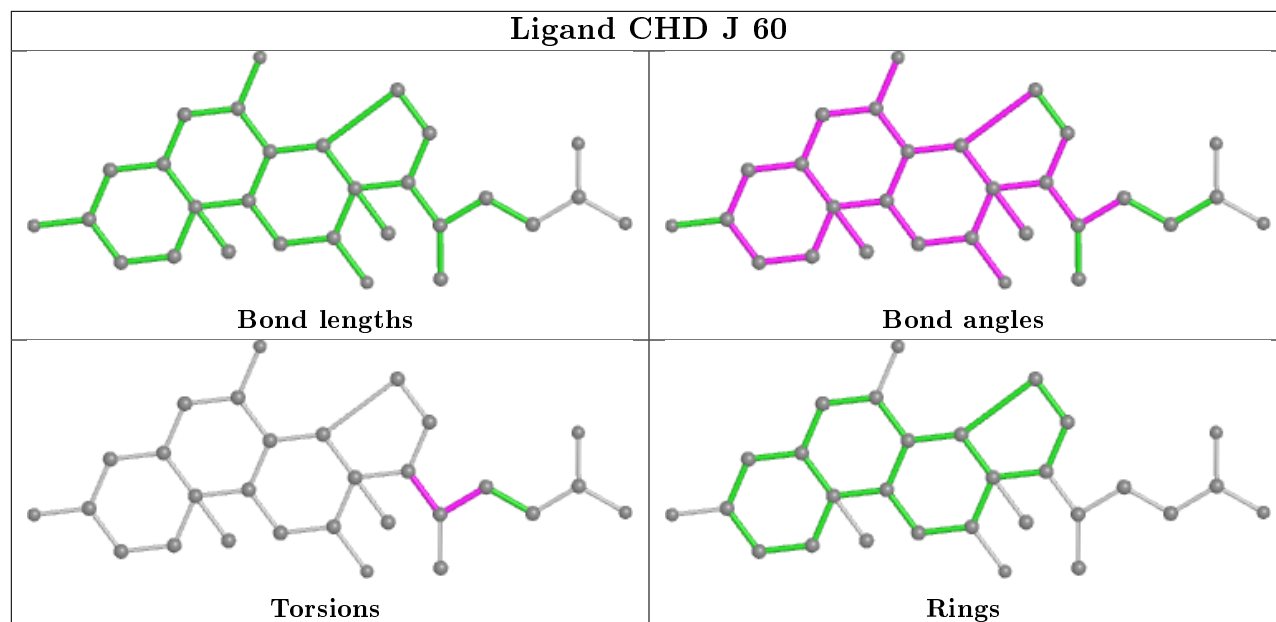
Ligand PEK T 263



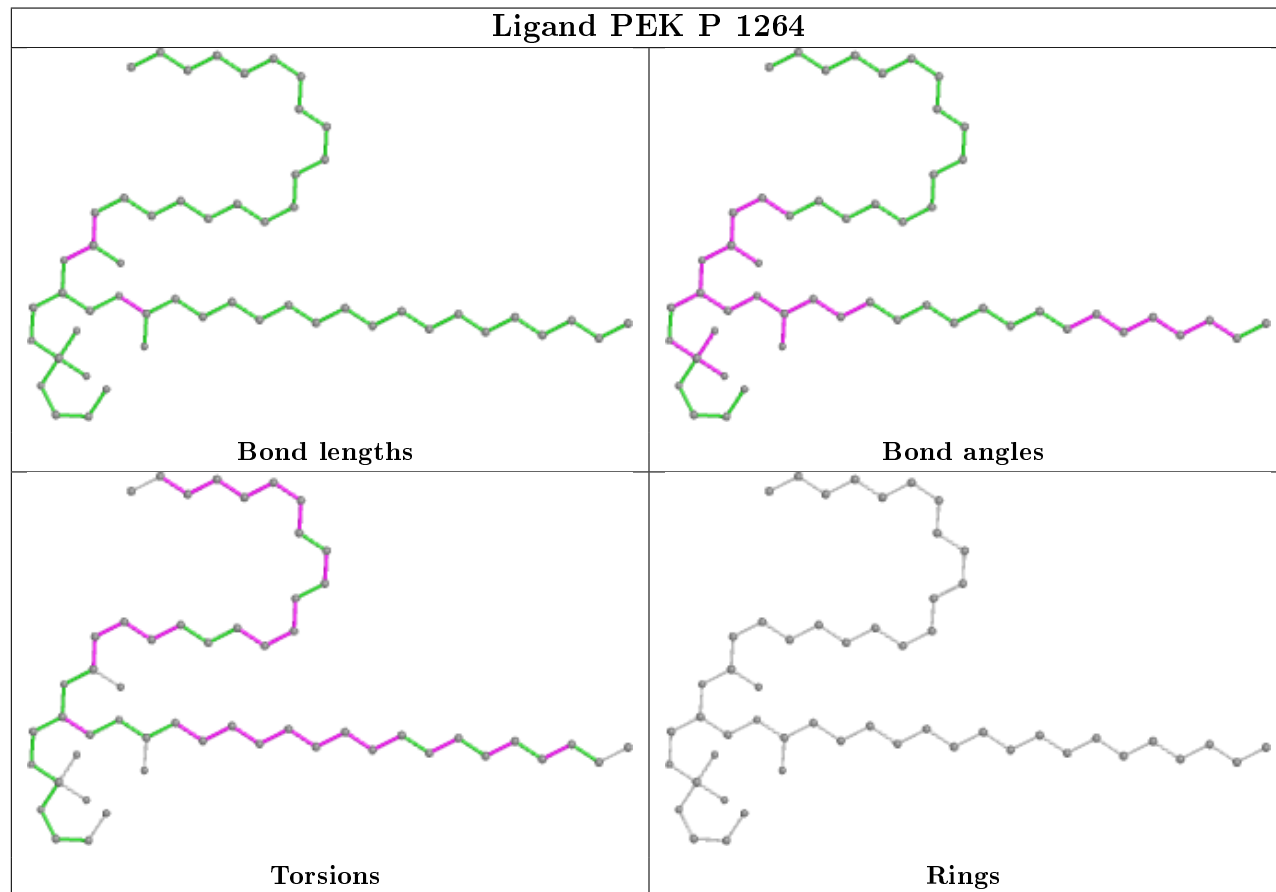


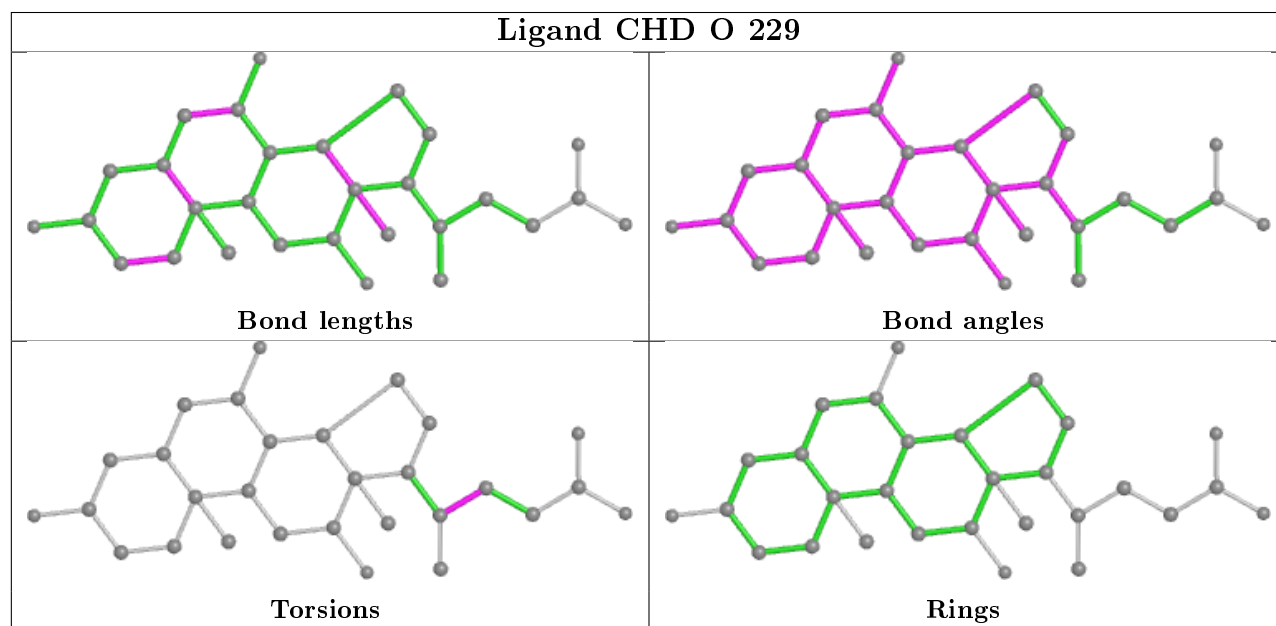
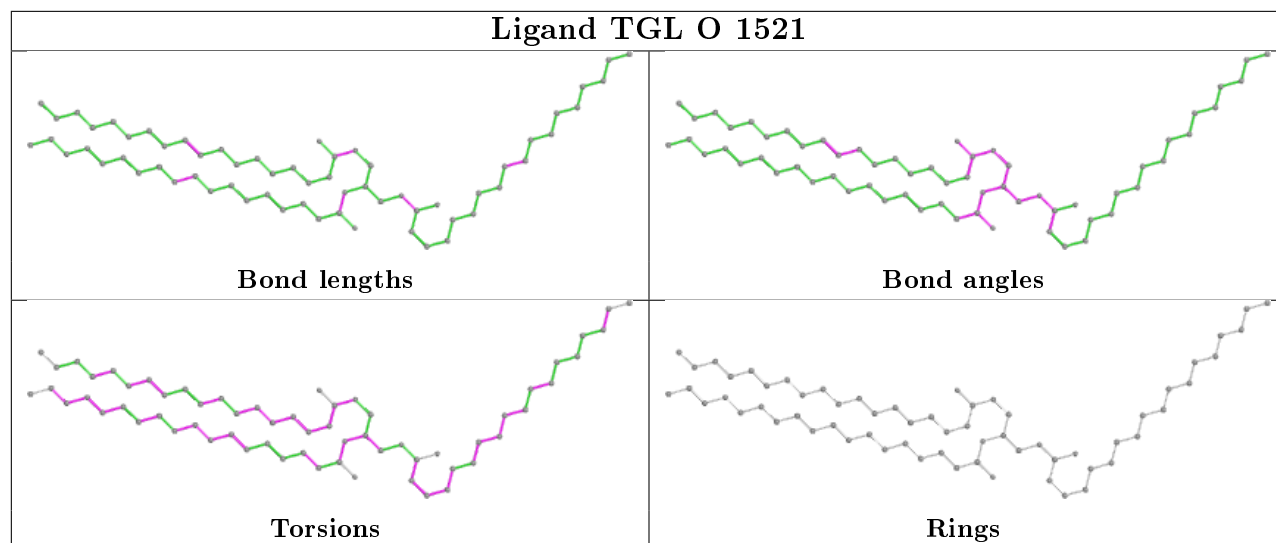


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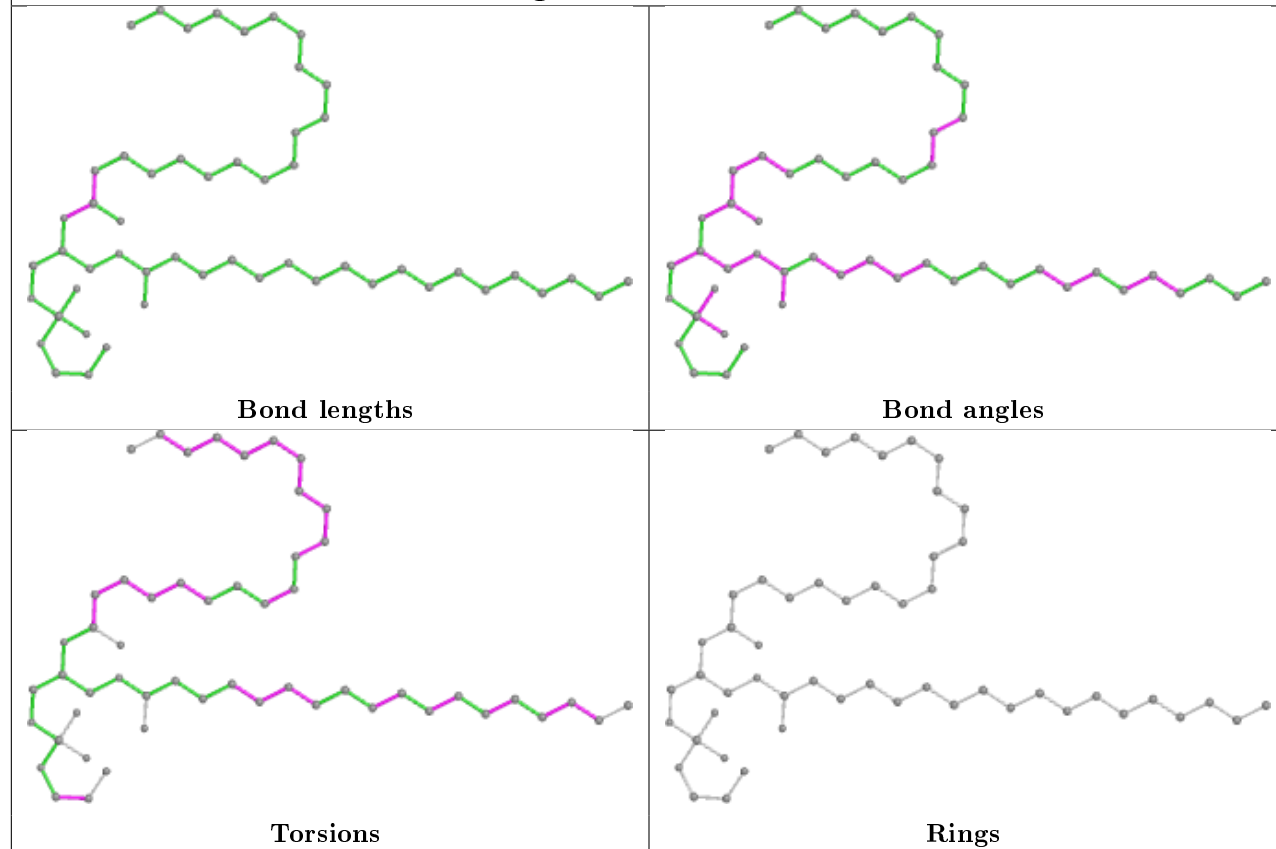


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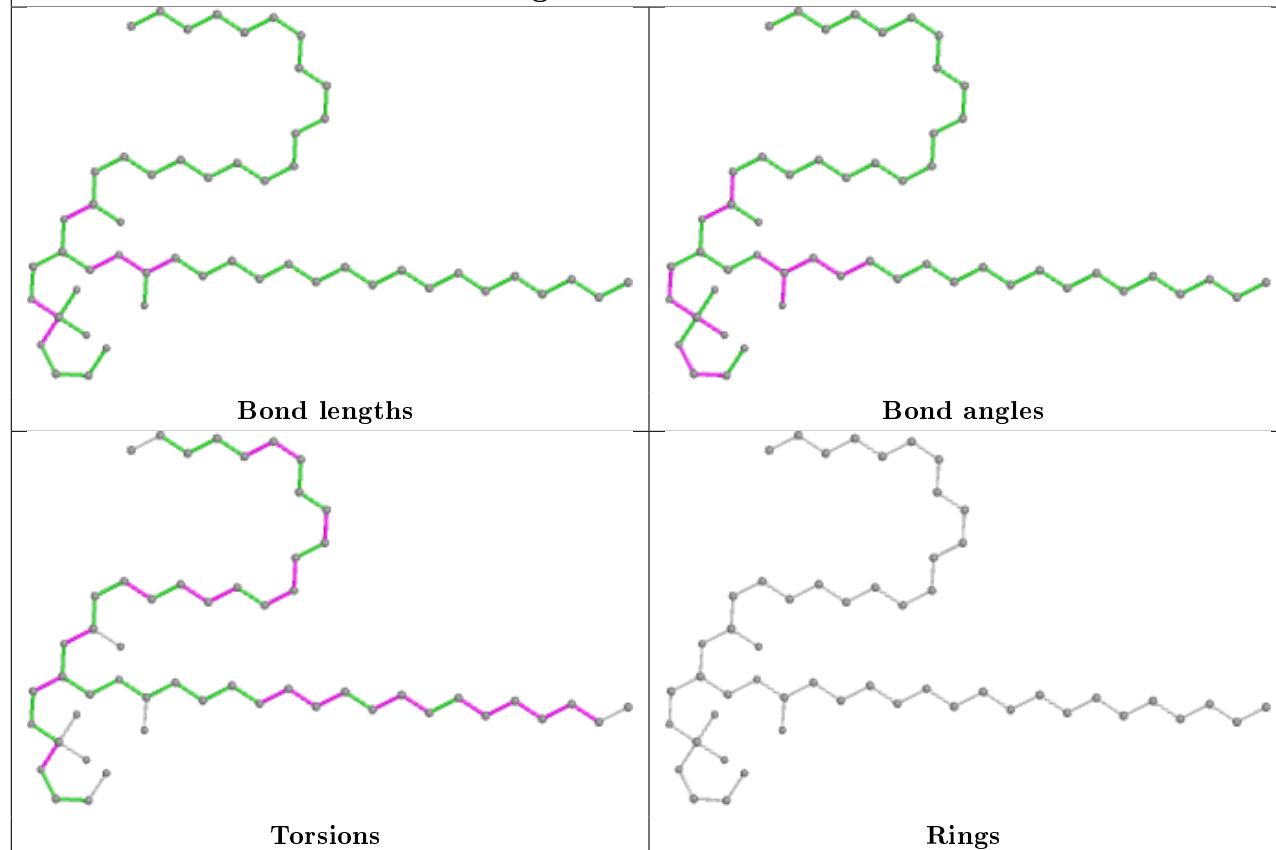


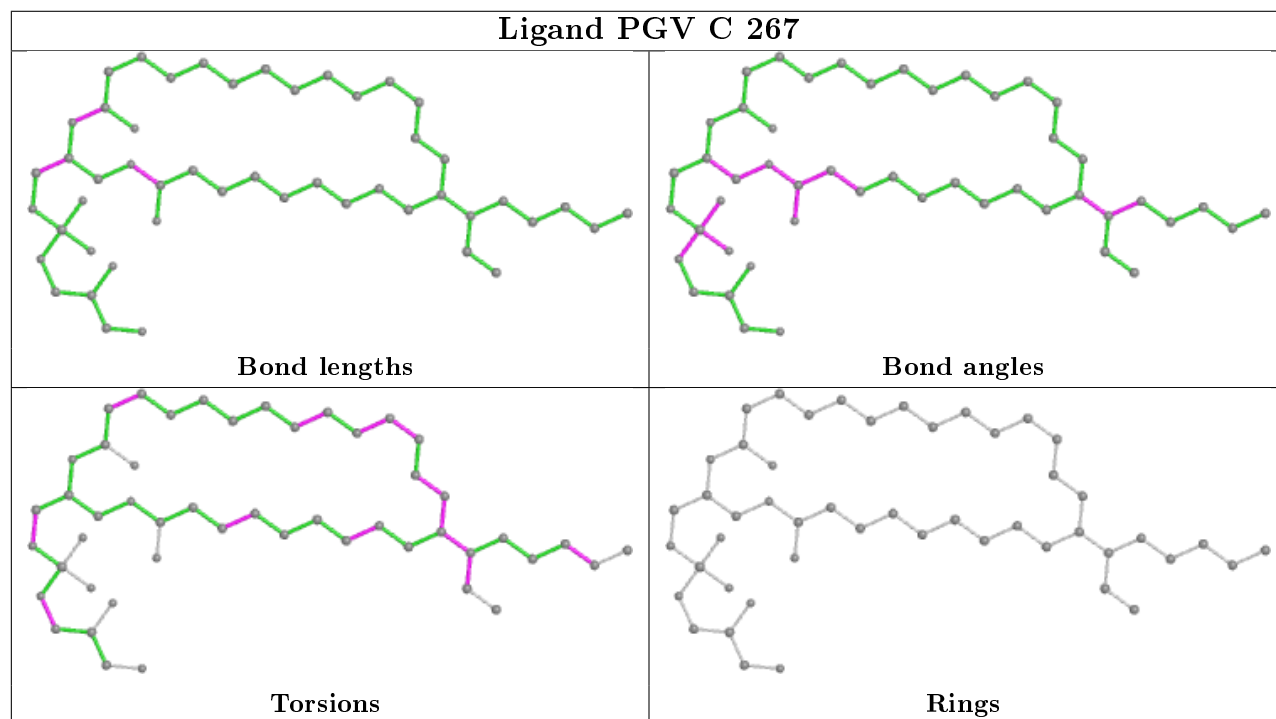
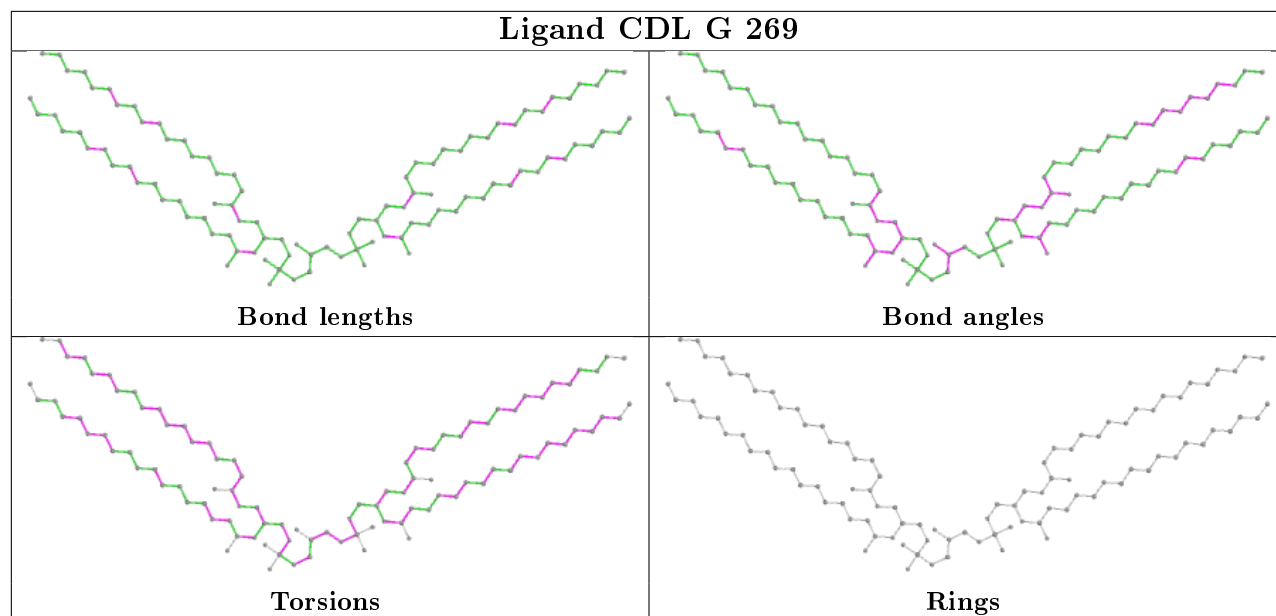


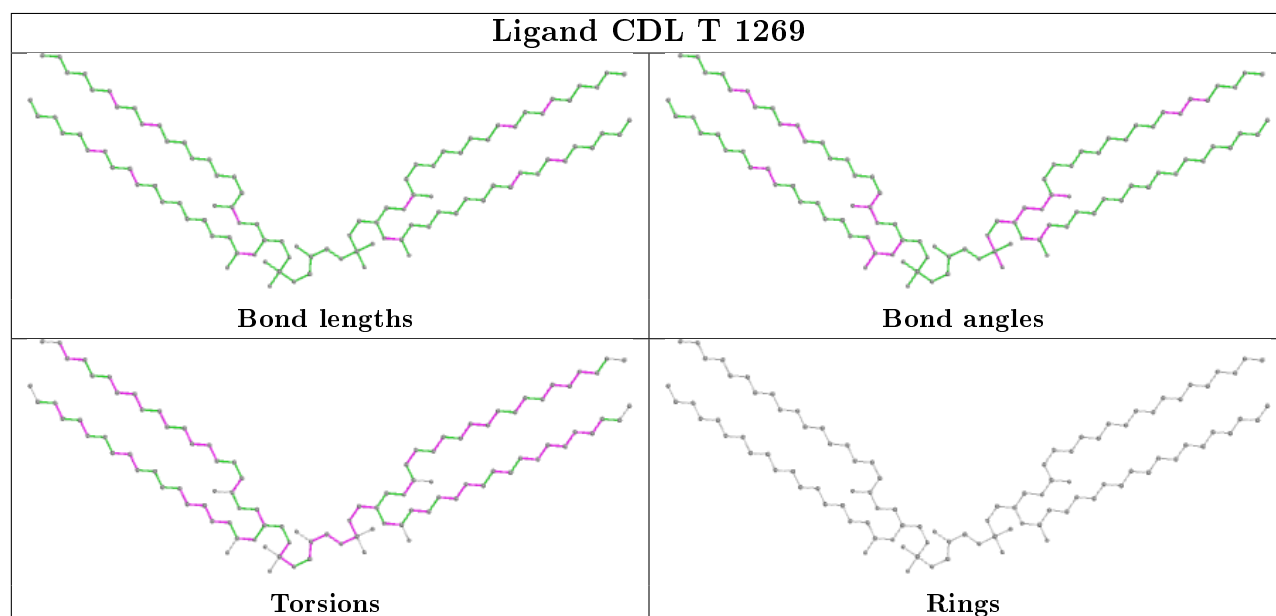
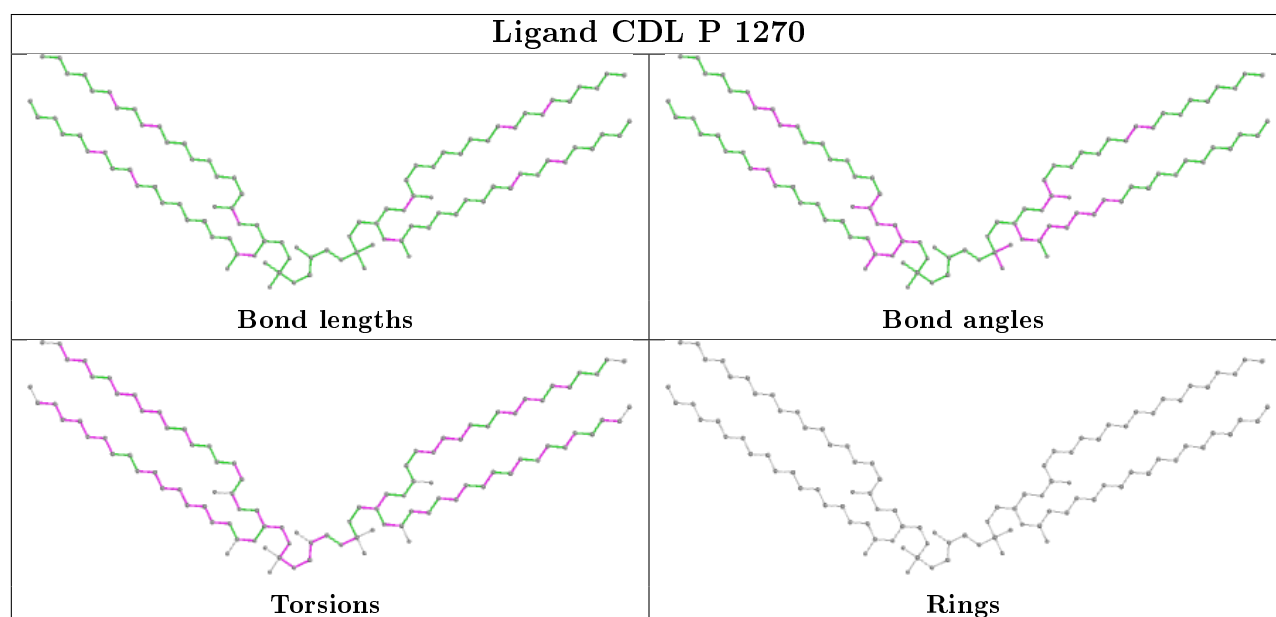
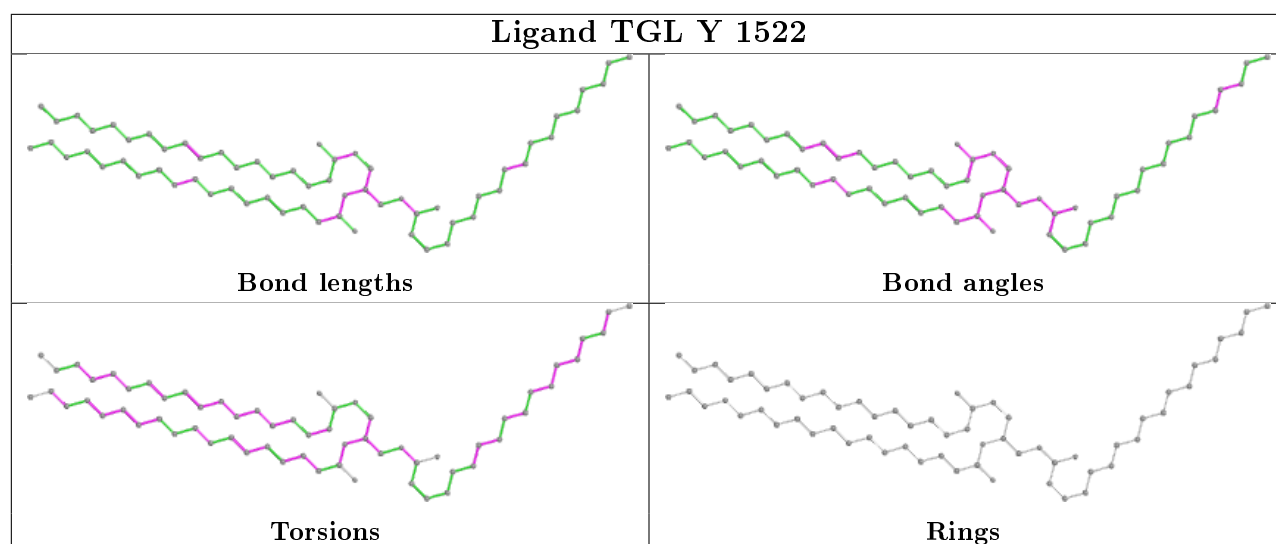
Ligand PEK C 264



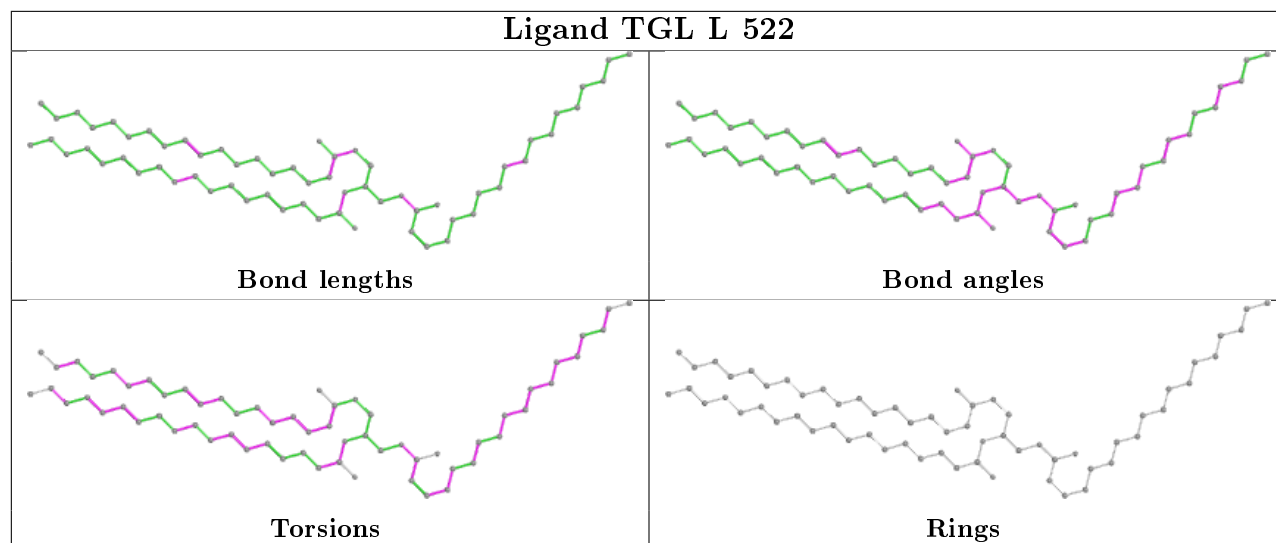
Ligand PEK C 265



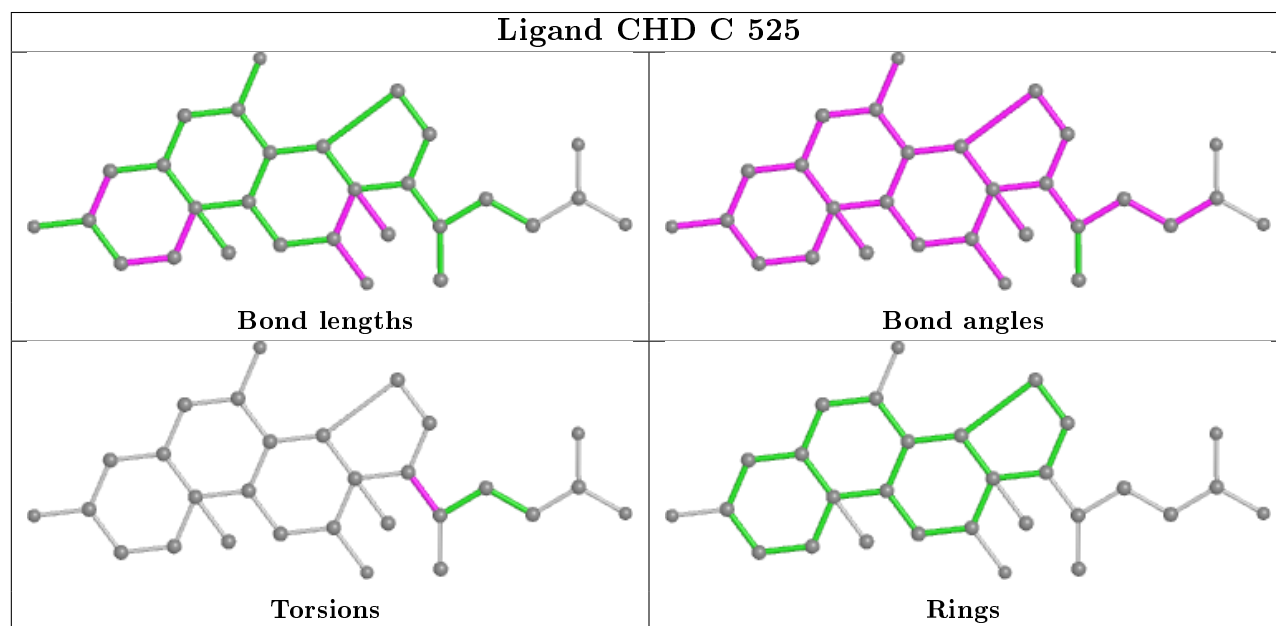


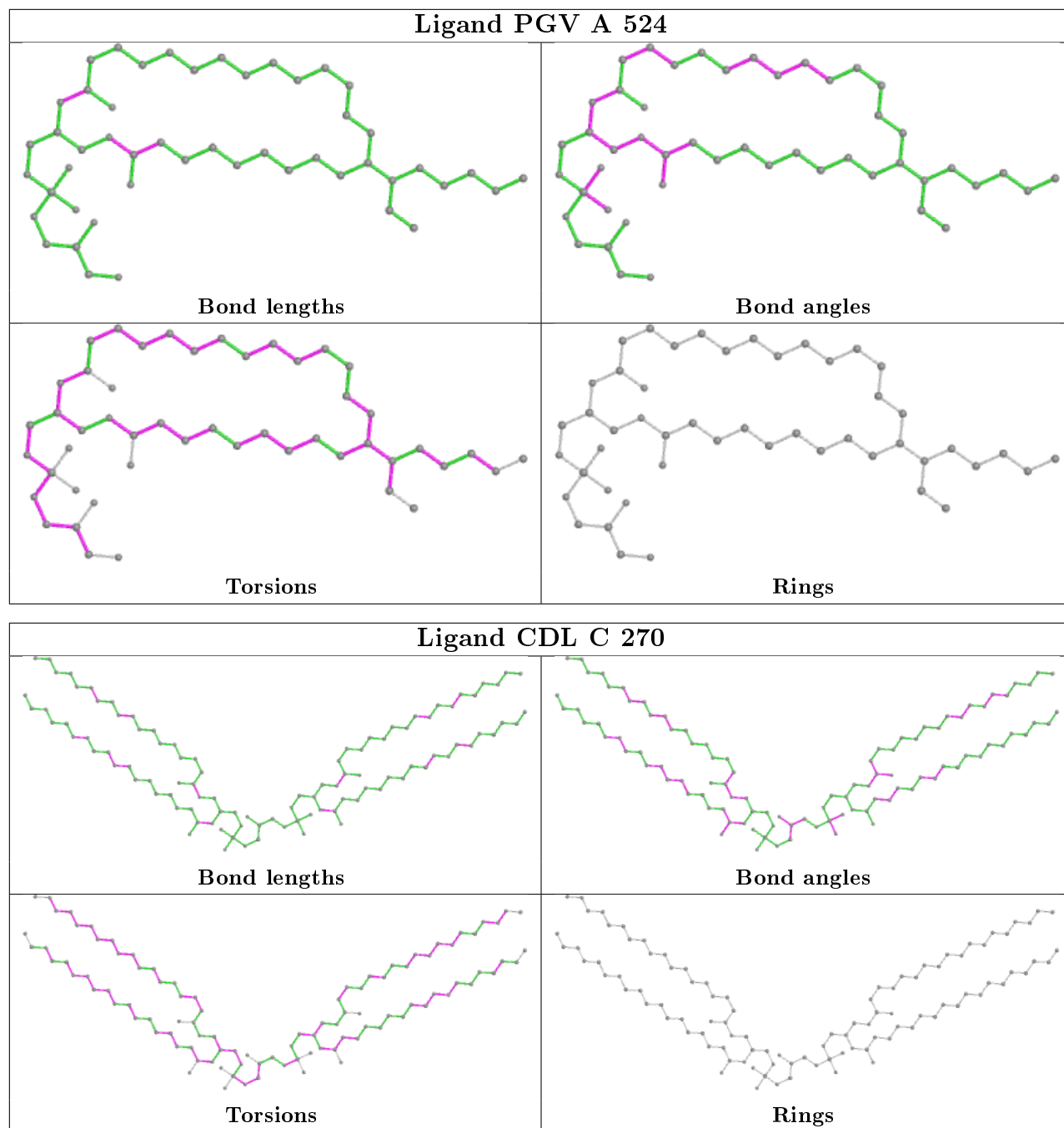


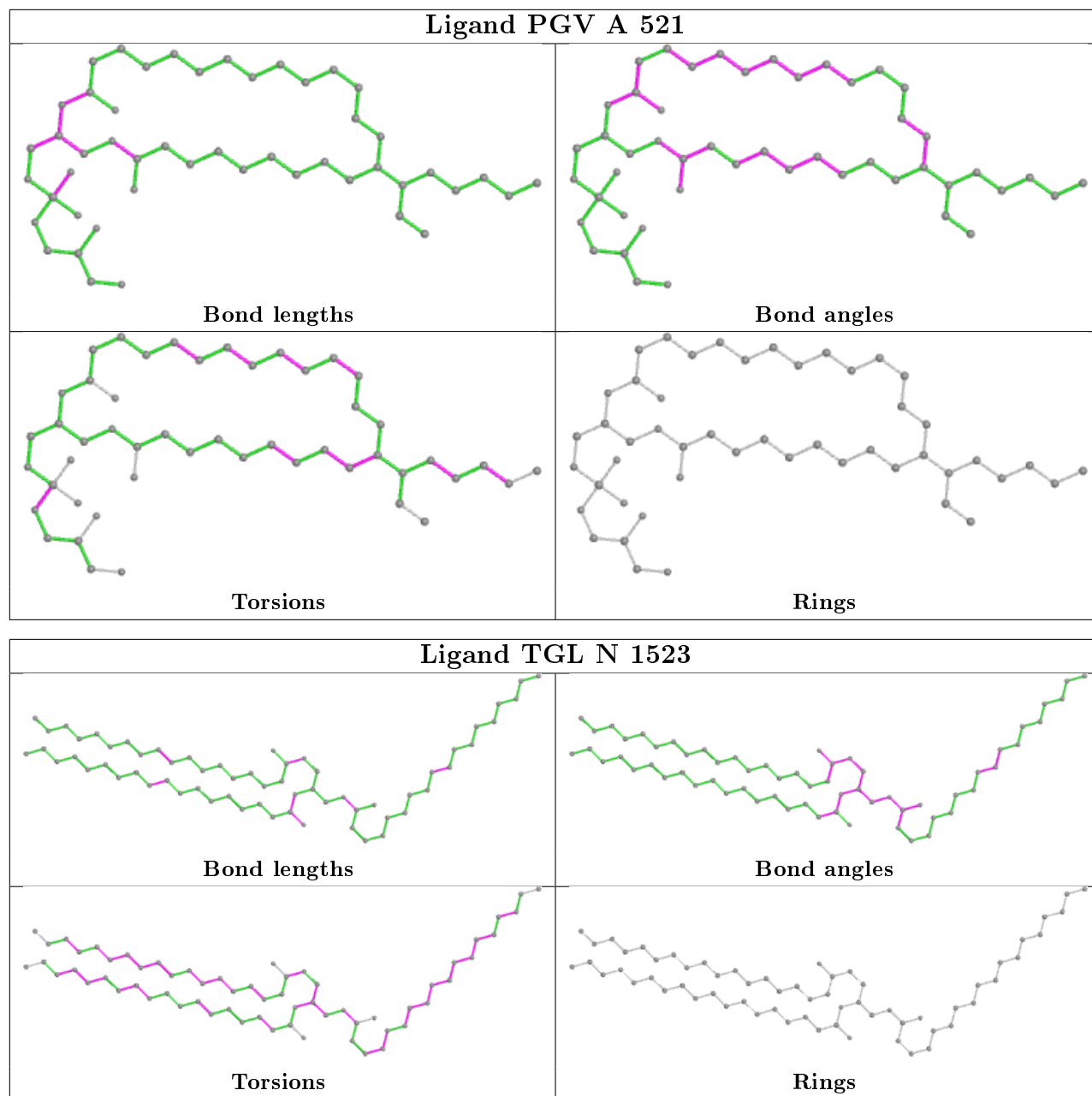
Ligand TGL L 522



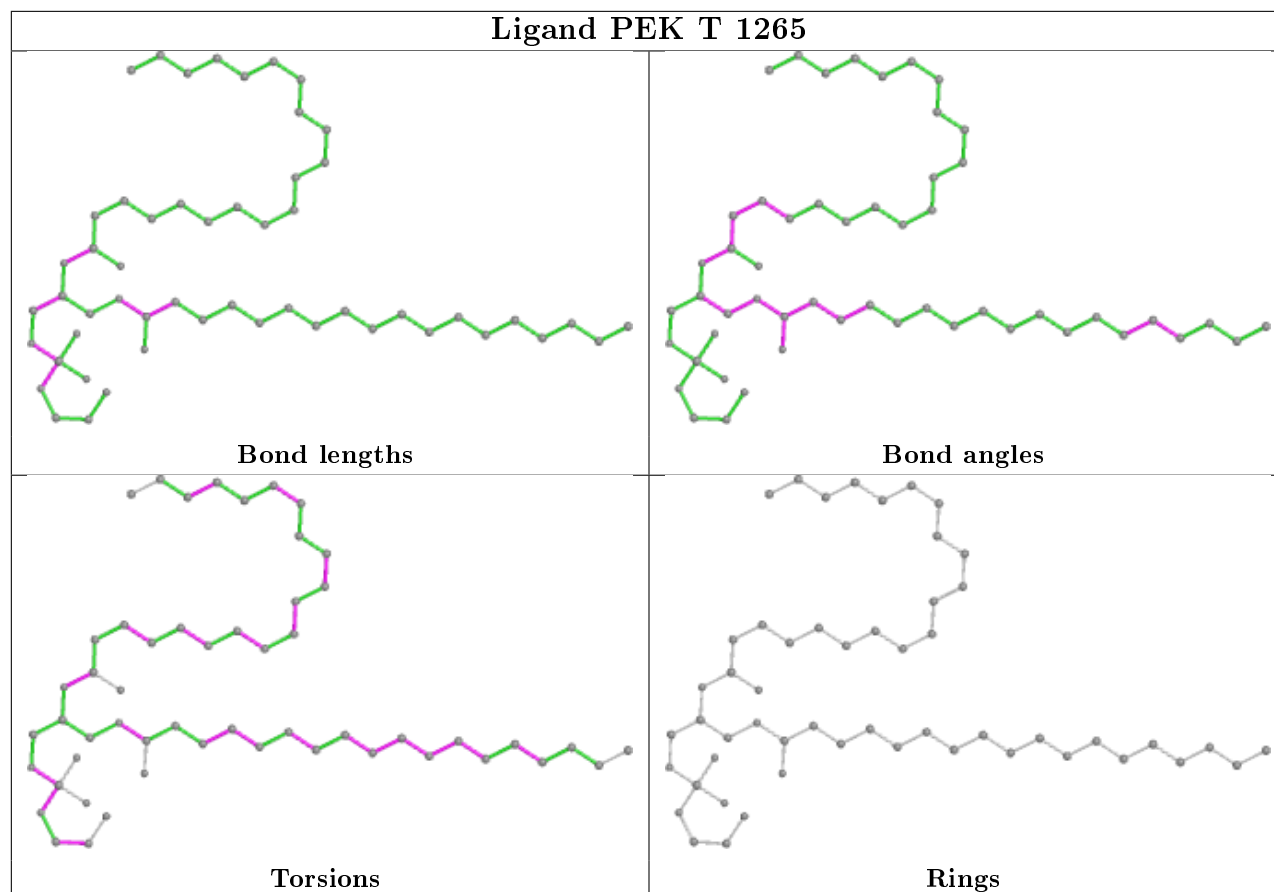
Ligand CHD C 525



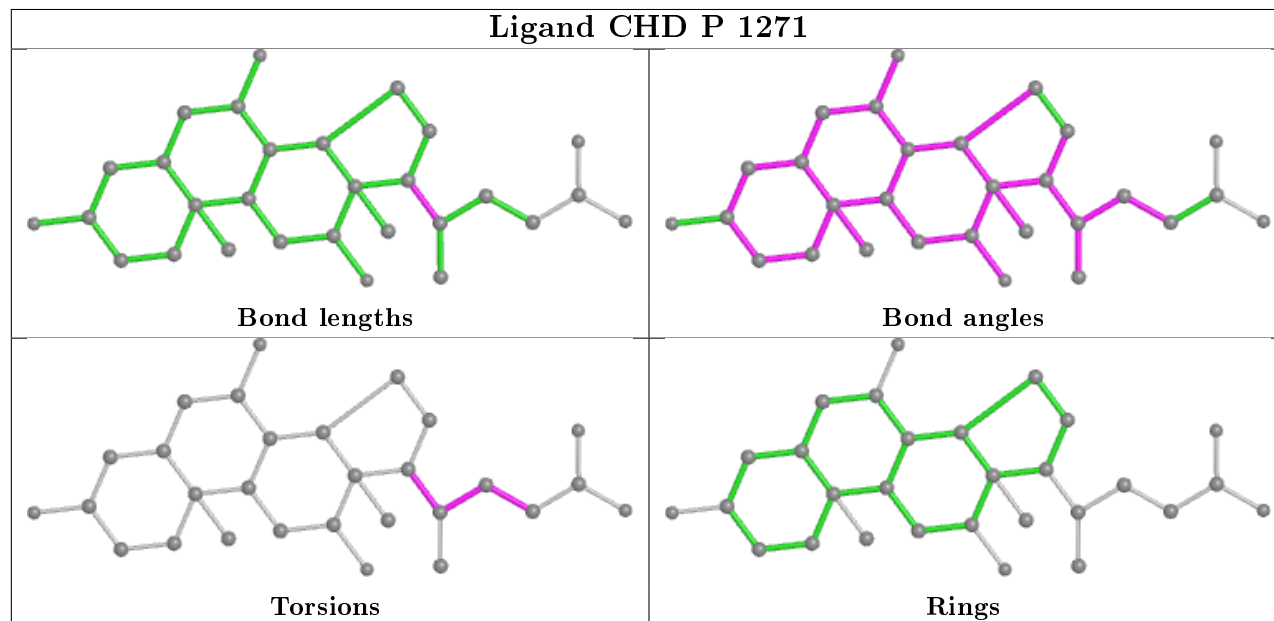




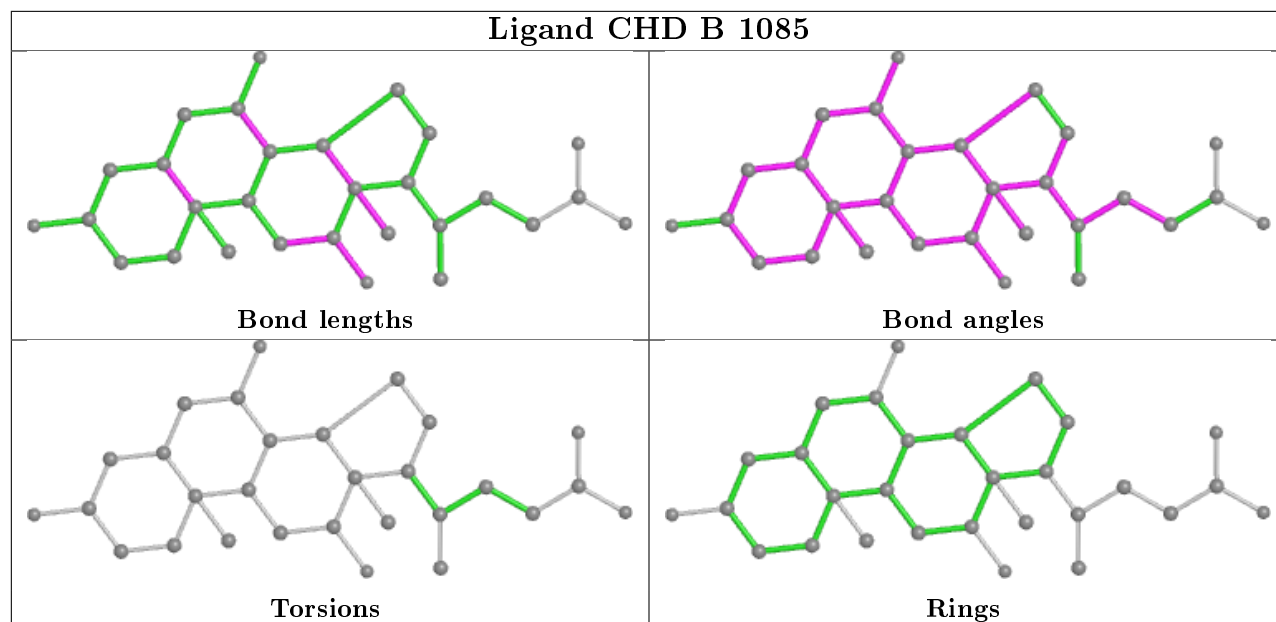
Ligand PEK T 1265



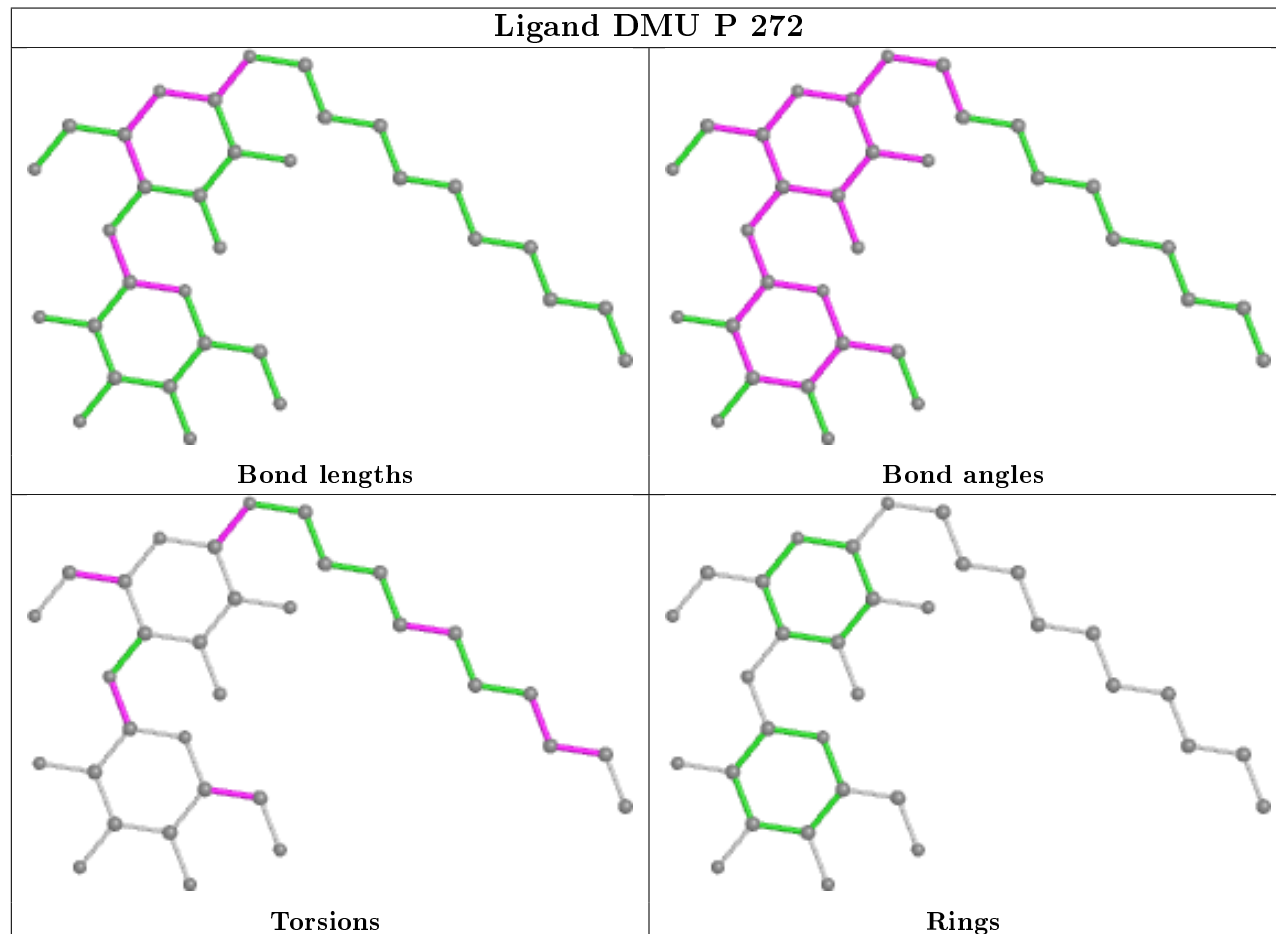
Ligand CHD P 1271



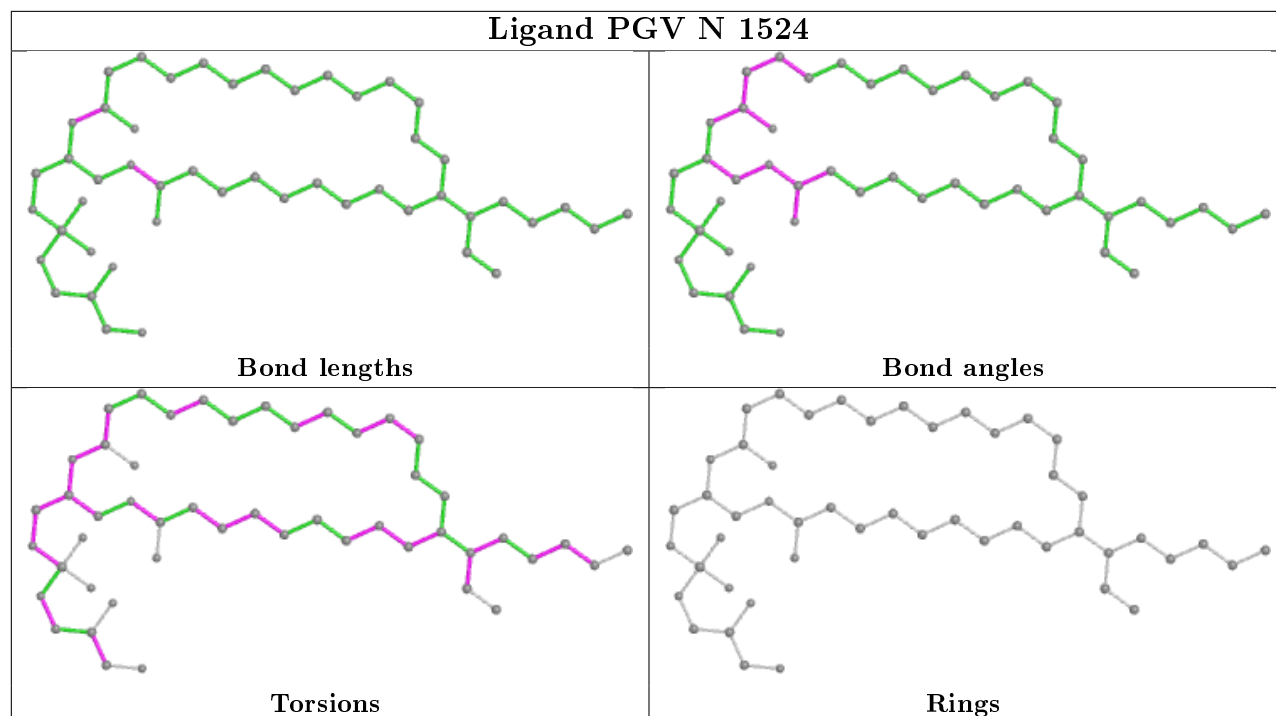
Ligand CHD B 1085



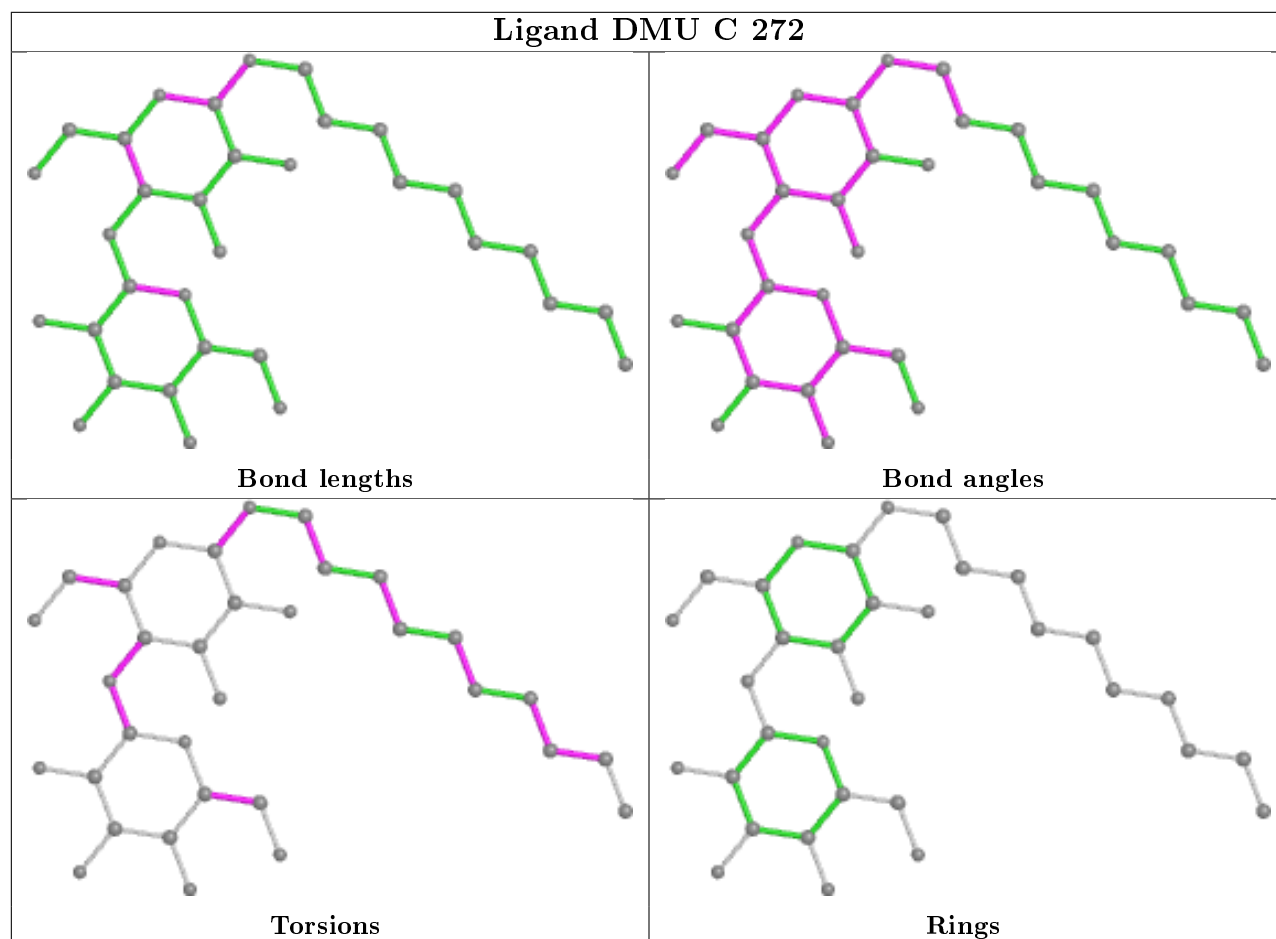
Ligand DMU P 272



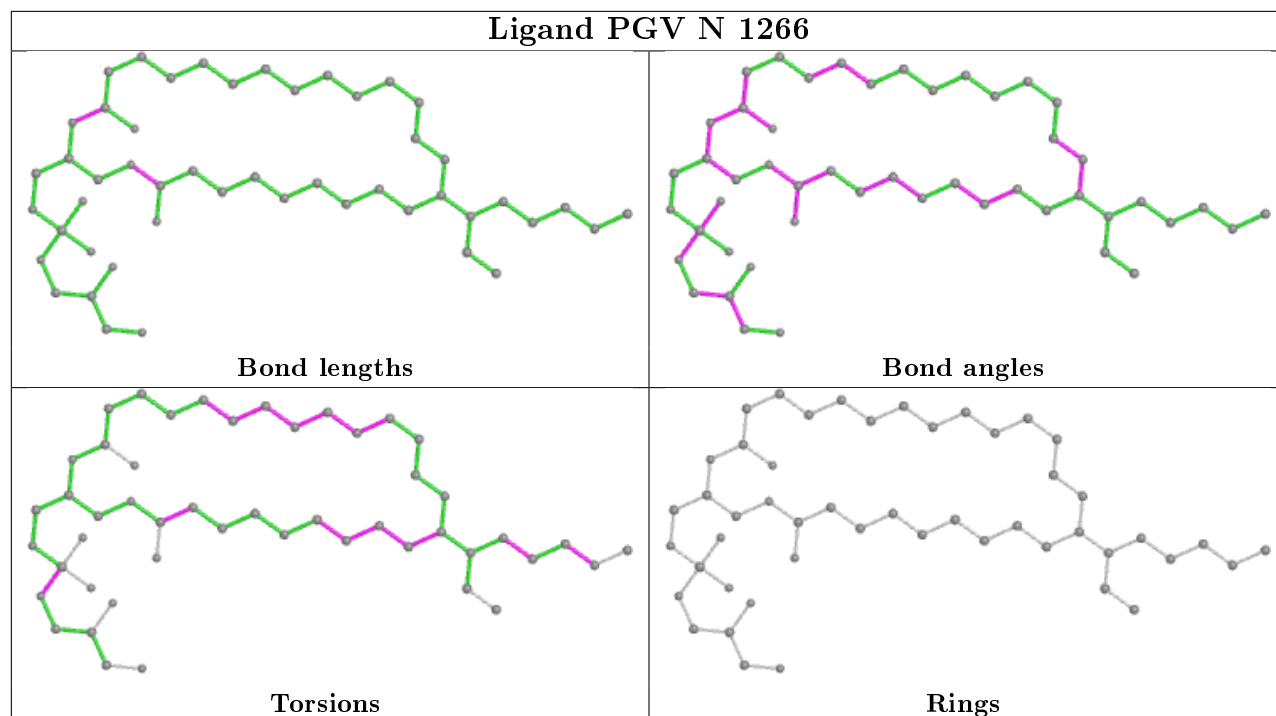
Ligand PGV N 1524



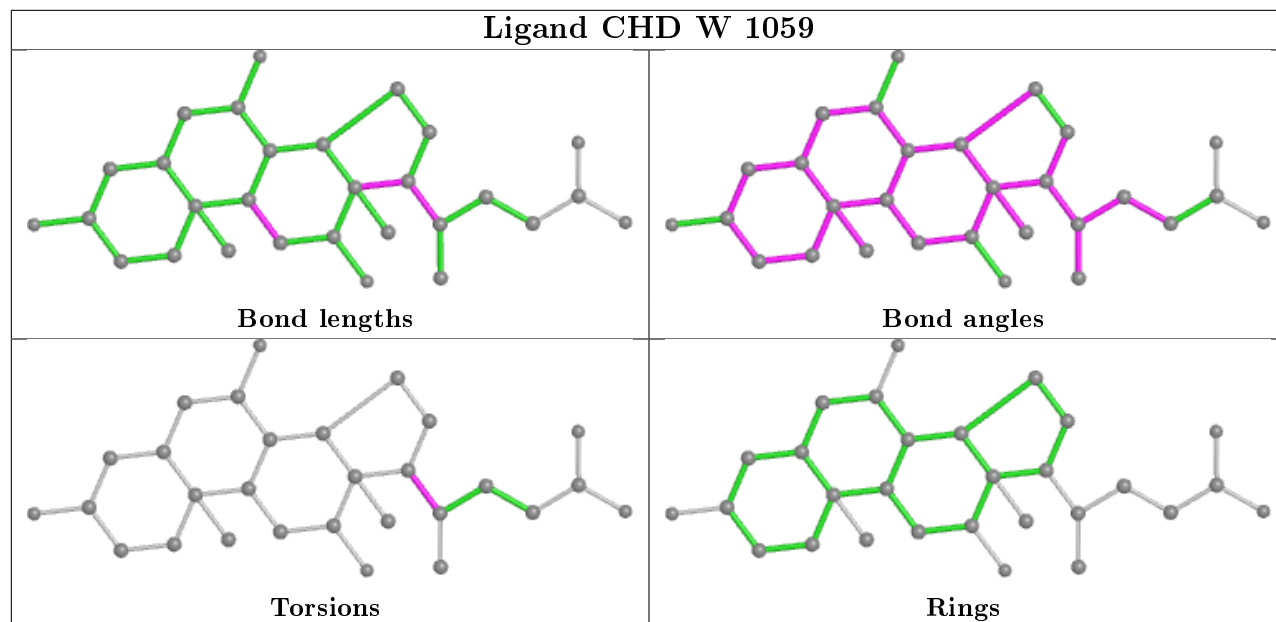
Ligand DMU C 272

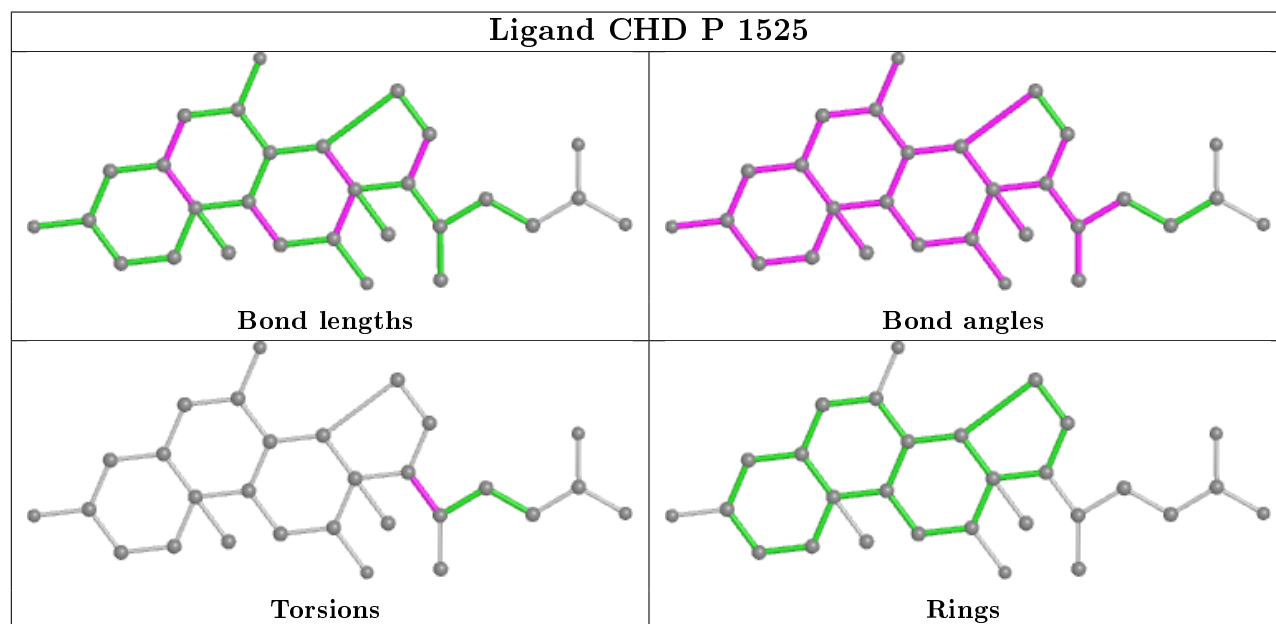
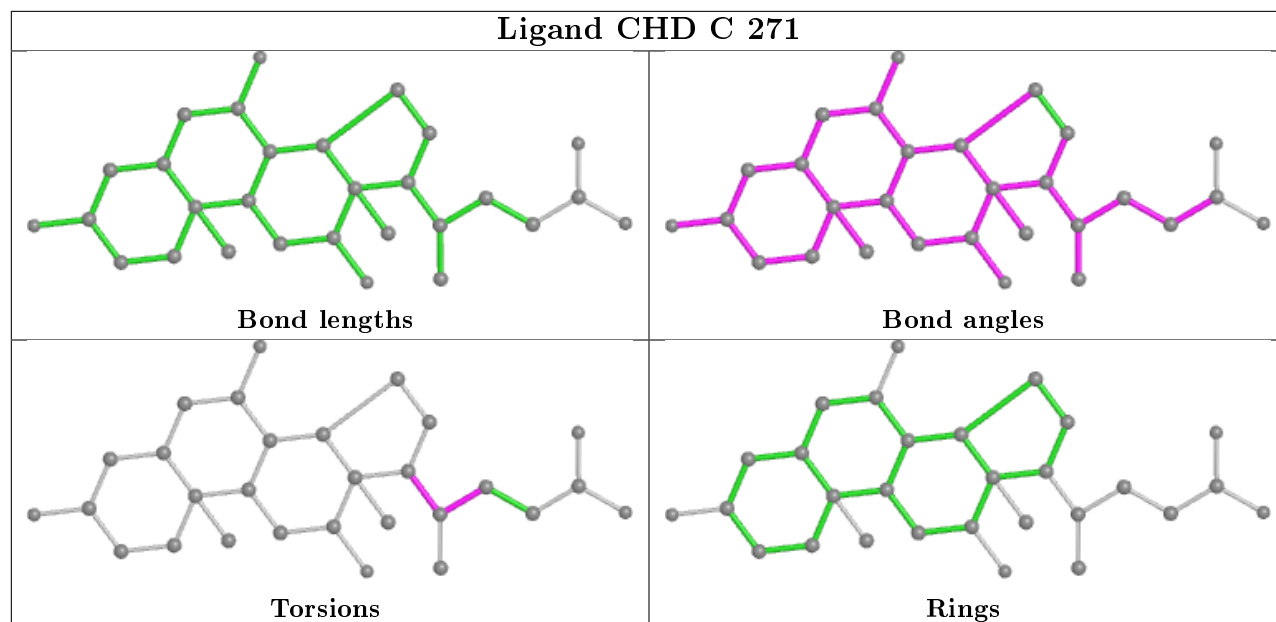


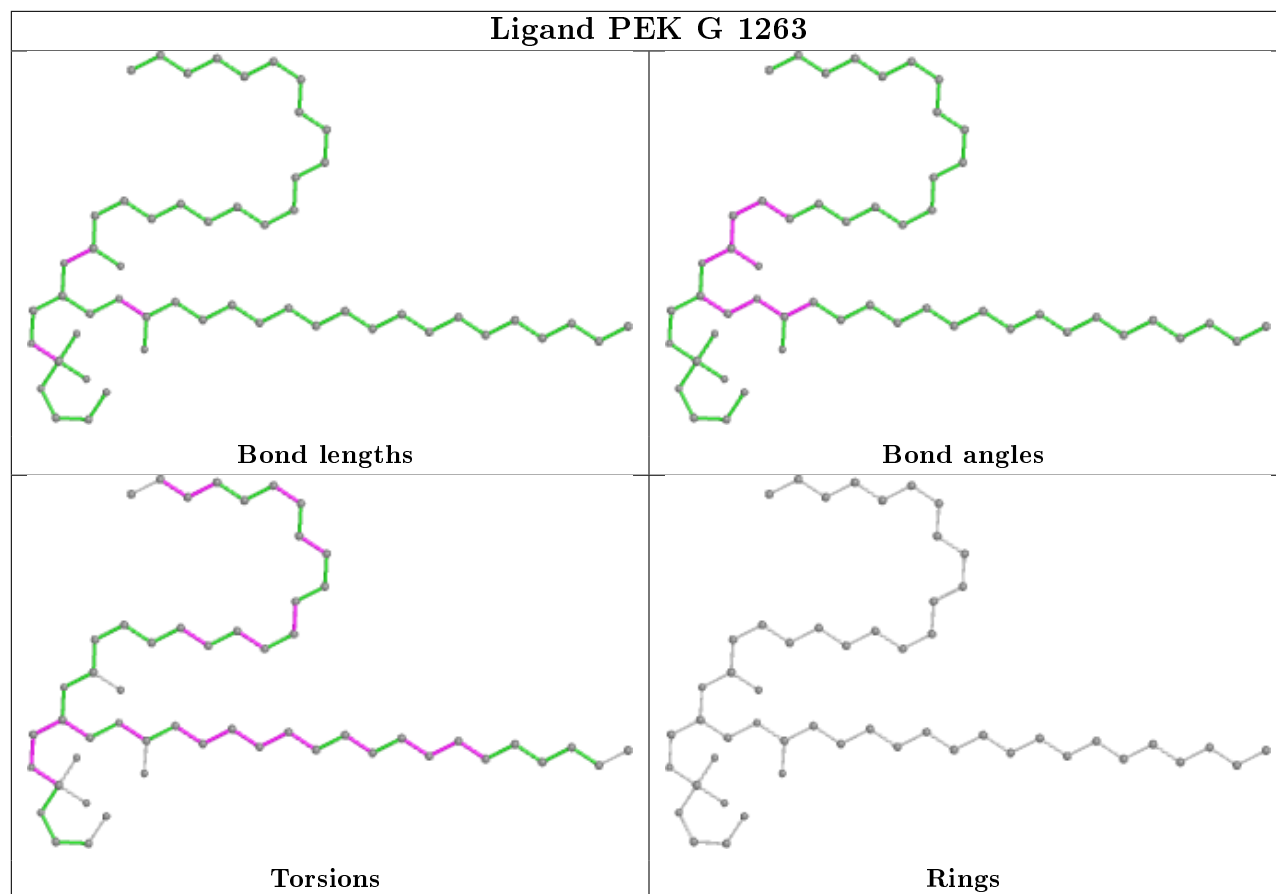
Ligand PGV N 1266



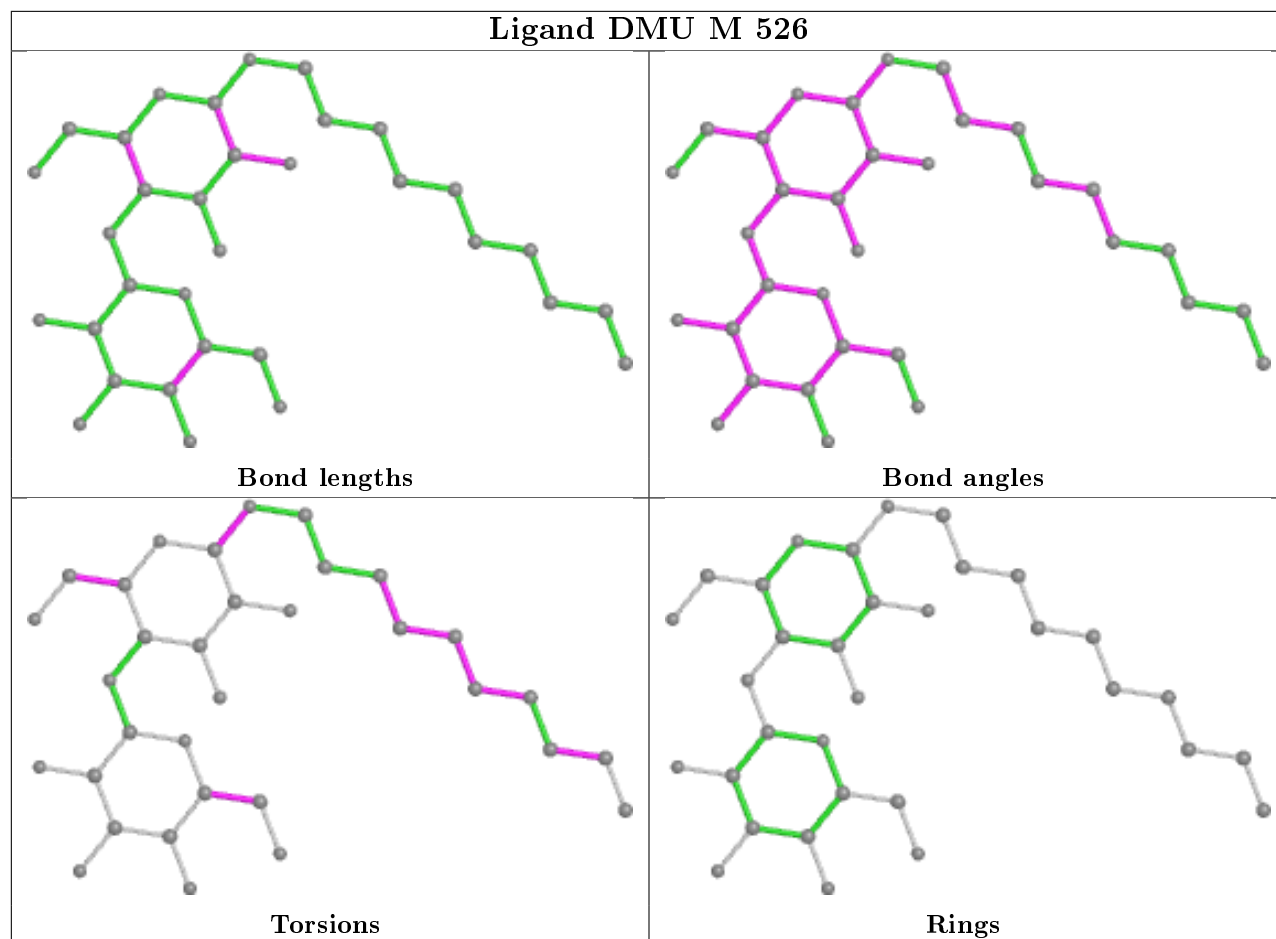
Ligand CHD W 1059



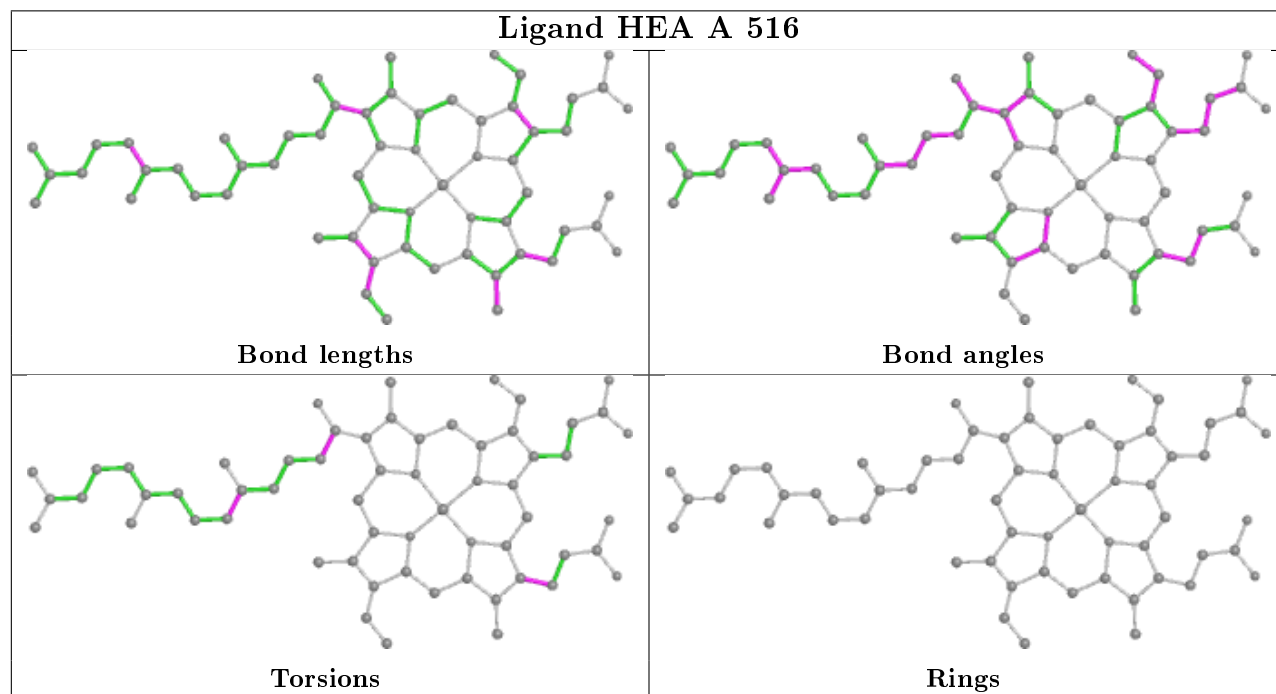




Ligand DMU M 526



Ligand HEA A 516



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	0.30	11 (2%) 63 62	23, 29, 38, 65	0
1	N	513/514 (99%)	0.23	20 (3%) 39 38	29, 35, 44, 71	0
2	B	226/227 (99%)	-0.25	1 (0%) 92 92	24, 33, 53, 72	0
2	O	226/227 (99%)	-0.14	4 (1%) 68 66	31, 42, 64, 81	0
3	C	259/261 (99%)	-0.17	2 (0%) 86 85	26, 32, 43, 66	0
3	P	259/261 (99%)	0.05	13 (5%) 28 28	30, 36, 48, 67	0
4	D	144/147 (97%)	-0.17	1 (0%) 87 87	30, 40, 53, 66	0
4	Q	144/147 (97%)	1.06	24 (16%) 1 1	39, 50, 71, 105	0
5	E	105/109 (96%)	0.36	6 (5%) 23 23	33, 40, 64, 97	0
5	R	105/109 (96%)	0.97	15 (14%) 2 2	36, 46, 70, 97	0
6	F	98/98 (100%)	0.44	9 (9%) 9 8	30, 41, 80, 117	0
6	S	98/98 (100%)	0.30	9 (9%) 9 8	34, 46, 80, 113	0
7	G	83/85 (97%)	0.83	15 (18%) 1 1	29, 38, 90, 106	0
7	T	83/85 (97%)	1.00	15 (18%) 1 1	32, 41, 91, 106	0
8	H	79/85 (92%)	0.27	10 (12%) 3 3	29, 41, 81, 101	0
8	U	79/85 (92%)	0.62	14 (17%) 1 1	37, 47, 85, 106	0
9	I	72/73 (98%)	0.25	3 (4%) 36 35	31, 46, 65, 70	0
9	V	72/73 (98%)	0.96	13 (18%) 1 1	36, 52, 67, 77	0
10	J	58/59 (98%)	0.52	7 (12%) 4 3	32, 41, 66, 95	0
10	W	58/59 (98%)	0.54	7 (12%) 4 3	36, 45, 67, 97	0
11	K	49/56 (87%)	0.03	2 (4%) 37 36	31, 39, 54, 64	0
11	X	49/56 (87%)	1.79	21 (42%) 0 0	42, 50, 66, 78	0
12	L	46/47 (97%)	-0.24	2 (4%) 35 34	29, 34, 51, 77	0
12	Y	46/47 (97%)	-0.06	1 (2%) 62 60	35, 43, 60, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.04	4 (9%) 8 8	31, 34, 72, 96	0
13	Z	43/46 (93%)	0.74	8 (18%) 1 1	39, 44, 81, 104	0
All	All	3550/3614 (98%)	0.27	237 (6%) 17 17	23, 38, 64, 117	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	14.9
6	F	1	ALA	10.4
6	S	98	HIS	9.8
6	S	1	ALA	9.6
6	S	97	ALA	9.1
7	G	1	ALA	8.9
4	Q	4	SER	8.5
6	F	97	ALA	8.2
7	T	1	ALA	7.4
6	F	96	LEU	7.2
6	S	2	SER	6.5
5	R	109	VAL	6.5
13	Z	42	LYS	6.3
6	F	98	HIS	6.3
5	E	5	HIS	6.3
8	U	7	LYS	5.9
4	Q	51	LEU	5.8
10	J	1	PHE	5.6
6	S	94	HIS	5.6
7	T	3	ALA	5.6
7	G	36	TRP	5.5
7	T	36	TRP	5.4
4	Q	48	TRP	5.4
9	I	37	PHE	5.3
6	S	96	LEU	5.3
7	T	84	LYS	5.2
8	U	8	ILE	5.2
4	Q	5	VAL	5.1
13	Z	43	SER	4.9
7	G	40	GLY	4.9
9	V	37	PHE	4.9
11	X	7	PRO	4.9
8	U	44	THR	4.9
10	J	58	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
7	G	8	HIS	4.8
13	Z	41	LYS	4.8
9	V	2	THR	4.7
7	G	2	SER	4.7
7	T	42	ARG	4.6
11	X	19	ALA	4.6
6	F	94	HIS	4.6
8	H	45	ALA	4.5
8	H	48	GLY	4.5
5	R	5	HIS	4.5
13	M	43	SER	4.5
13	M	42	LYS	4.4
7	G	41	HIS	4.3
7	G	42	ARG	4.3
2	O	113	TYR	4.3
10	W	57	HIS	4.2
7	T	41	HIS	4.2
7	T	5	LYS	4.2
10	W	58	LYS	4.2
4	Q	33	LEU	4.1
7	G	84	LYS	4.1
7	G	6	GLY	4.1
11	X	16	ALA	4.1
4	Q	46	ALA	4.0
2	O	90	ILE	4.0
8	U	10	ASN	4.0
7	T	4	ALA	3.9
10	W	55	PHE	3.9
8	H	8	ILE	3.9
7	T	40	GLY	3.9
13	Z	40	TYR	3.9
5	R	96	LEU	3.8
4	Q	145	TRP	3.8
13	Z	35	TYR	3.8
5	R	7	THR	3.7
8	H	44	THR	3.7
12	L	47	LYS	3.7
4	Q	49	SER	3.7
6	F	2	SER	3.7
12	Y	47	LYS	3.7
10	J	57	HIS	3.7
13	Z	39	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	59	GLN	3.5
3	P	88	ILE	3.5
11	X	13	TYR	3.4
7	T	10	GLY	3.4
8	U	49	ASP	3.4
13	M	39	ASN	3.4
11	X	47	ARG	3.4
5	R	108	LYS	3.4
3	P	91	VAL	3.4
8	U	48	GLY	3.4
13	M	40	TYR	3.3
7	G	5	LYS	3.3
11	X	24	PHE	3.3
4	Q	141	ASP	3.3
4	Q	102	TYR	3.3
10	W	52	TRP	3.3
7	G	3	ALA	3.3
11	X	6	ALA	3.3
8	U	52	VAL	3.2
11	X	17	VAL	3.2
8	U	11	TYR	3.2
7	T	8	HIS	3.2
6	F	95	GLN	3.1
6	S	93	PRO	3.1
7	G	43	GLU	3.1
5	E	109	VAL	3.1
10	W	1	PHE	3.0
11	X	46	GLY	3.0
4	Q	7	LYS	3.0
9	V	36	LYS	3.0
7	T	9	GLY	3.0
5	R	58	LEU	3.0
10	J	2	GLU	3.0
8	U	9	LYS	3.0
7	G	4	ALA	3.0
1	N	193	VAL	2.9
12	L	2	HIS	2.9
8	H	7	LYS	2.9
10	J	52	TRP	2.9
7	T	6	GLY	2.9
4	Q	139	ASP	2.9
9	I	2	THR	2.8

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Mol	Chain	Res	Type	RSRZ
3	P	37	PHE	2.8
11	K	7	PRO	2.8
9	V	68	ILE	2.8
11	X	23	THR	2.8
9	V	3	ALA	2.7
7	T	43	GLU	2.7
13	Z	32	TRP	2.7
4	Q	53	ILE	2.7
7	G	39	SER	2.7
4	Q	147	LYS	2.7
9	V	7	PRO	2.7
8	H	47	GLY	2.7
5	R	93	LEU	2.7
7	T	2	SER	2.7
11	K	19	ALA	2.7
4	Q	142	LYS	2.7
11	X	18	LEU	2.7
9	V	53	ASN	2.7
5	R	54	ALA	2.7
1	N	195	LEU	2.6
8	H	46	LYS	2.6
11	X	11	ASP	2.6
1	N	190	ILE	2.6
3	C	92	LEU	2.6
3	P	182	TYR	2.6
10	W	2	GLU	2.6
1	N	165	ILE	2.6
3	P	99	TRP	2.6
9	I	26	MET	2.5
5	R	9	GLU	2.5
13	Z	13	LYS	2.5
8	U	43	MET	2.5
5	R	89	LEU	2.5
4	D	147	LYS	2.5
4	Q	140	TYR	2.5
8	U	45	ALA	2.5
3	P	84	ILE	2.5
3	P	92	LEU	2.4
3	P	38	ASN	2.4
11	X	20	SER	2.4
5	R	92	THR	2.4
2	O	59	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	196	LEU	2.4
1	N	282	PHE	2.4
1	N	245	ILE	2.4
8	U	47	GLY	2.4
1	A	193	VAL	2.4
10	J	4	ARG	2.4
3	P	247	VAL	2.3
4	Q	101	HIS	2.3
8	H	43	MET	2.3
11	X	15	ASN	2.3
11	X	36	ILE	2.3
4	Q	60	TYR	2.3
8	U	42	ALA	2.3
1	A	126	TRP	2.3
11	X	30	VAL	2.3
5	R	10	GLU	2.3
1	N	126	TRP	2.3
9	V	45	LYS	2.3
10	W	4	ARG	2.3
1	N	286	ILE	2.3
1	N	246	LEU	2.2
11	X	12	LYS	2.2
10	J	33	ARG	2.2
11	X	35	GLN	2.2
1	N	66	ILE	2.2
1	A	20	LEU	2.2
1	A	195	LEU	2.2
5	R	13	ALA	2.2
9	V	48	ALA	2.2
7	G	9	GLY	2.2
8	H	49	ASP	2.2
3	P	250	LEU	2.2
4	Q	62	LEU	2.2
1	N	285	PHE	2.2
1	A	192	ALA	2.2
4	Q	97	ILE	2.2
8	H	42	ALA	2.2
4	Q	55	GLU	2.2
2	O	131	GLY	2.2
3	P	87	ILE	2.2
6	S	3	GLY	2.2
4	Q	8	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	2.1
1	N	248	LEU	2.1
3	P	85	LEU	2.1
1	N	83	VAL	2.1
3	P	98	PHE	2.1
5	R	16	VAL	2.1
6	F	5	GLY	2.1
1	A	245	ILE	2.1
11	X	48	VAL	2.1
5	R	18	TYR	2.1
6	F	3	GLY	2.1
8	U	46	LYS	2.1
5	E	9	GLU	2.1
1	N	166	THR	2.1
9	V	33	THR	2.1
1	A	190	ILE	2.1
1	N	75	ILE	2.1
1	N	158	ILE	2.1
1	N	197	LEU	2.1
5	E	93	LEU	2.1
1	A	188	VAL	2.1
5	E	16	VAL	2.1
11	X	31	TYR	2.1
6	S	95	GLN	2.1
9	V	65	LYS	2.1
1	N	194	LEU	2.1
9	V	19	PHE	2.1
11	X	37	GLY	2.1
1	A	348	PHE	2.0
9	V	4	LEU	2.0
1	A	385	ALA	2.0
1	N	243	VAL	2.0
4	Q	68	PHE	2.0
3	C	38	ASN	2.0
5	E	24	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	SAC	V	1	9/10	0.44	0.47	83,84,85,86	0
7	TPO	T	11	11/12	0.61	0.28	75,82,102,103	0
9	SAC	I	1	9/10	0.67	0.28	73,76,78,80	0
7	TPO	G	11	11/12	0.68	0.27	69,76,102,102	0
1	FME	A	1	10/11	0.91	0.18	44,51,71,75	0
1	FME	N	1	10/11	0.93	0.18	46,53,78,82	0
2	FME	O	1	10/11	0.96	0.11	40,42,47,55	0
2	FME	B	1	10/11	0.97	0.12	33,33,41,48	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	UNX	C	262	1/1	0.08	0.56	80,80,80,80	0
27	DMU	P	272	33/33	0.33	0.44	77,107,124,124	0
27	DMU	C	272	33/33	0.35	0.39	68,100,115,116	0
25	PEK	T	1265	53/53	0.52	0.32	49,79,110,118	0
24	UNX	P	262	1/1	0.55	0.53	79,79,79,79	0
25	PEK	C	265	53/53	0.58	0.31	49,83,106,107	0
26	CDL	G	269	100/100	0.58	0.31	62,86,116,120	0
25	PEK	G	1263	53/53	0.62	0.51	52,103,133,134	0
22	PSC	R	1229	52/52	0.63	0.33	48,99,136,139	0
21	TGL	Y	1522	63/63	0.64	0.30	51,73,89,92	0
26	CDL	T	1269	100/100	0.65	0.30	58,86,114,118	0
23	CHD	W	1059	29/29	0.65	0.45	101,109,113,115	0
25	PEK	T	263	53/53	0.65	0.42	52,103,125,127	0
22	PSC	B	229	52/52	0.68	0.34	43,92,139,143	0
19	PGV	U	1268	51/51	0.69	0.41	60,84,103,105	0
21	TGL	N	1523	63/63	0.72	0.24	61,79,97,99	0
19	PGV	C	268	51/51	0.72	0.38	53,81,98,102	0
19	PGV	N	1524	51/51	0.72	0.28	54,74,103,105	0
26	CDL	P	1270	100/100	0.74	0.30	36,94,119,119	0
23	CHD	J	60	29/29	0.74	0.46	99,105,108,110	0
21	TGL	L	522	63/63	0.76	0.26	43,66,82,89	0

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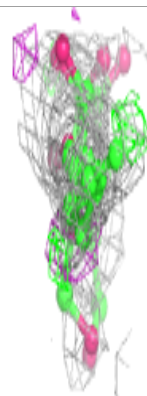
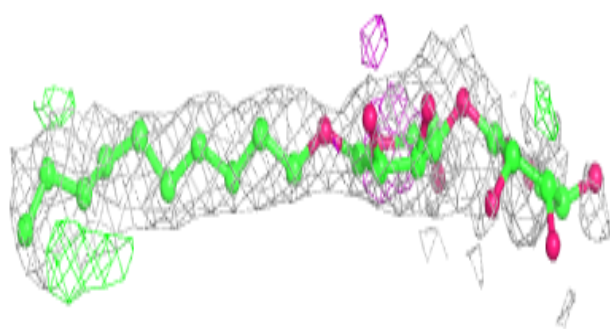
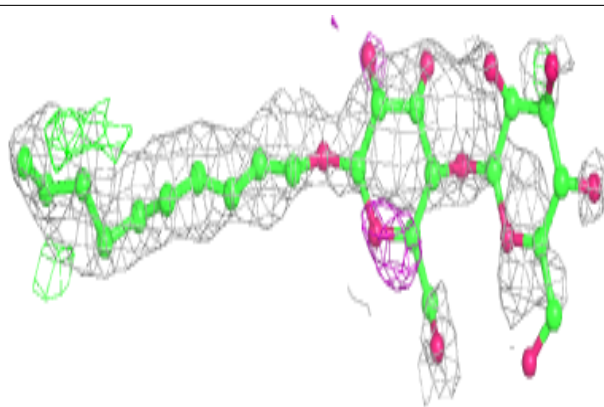
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	TGL	D	523	63/63	0.76	0.22	48,69,91,91	0
19	PGV	A	524	51/51	0.76	0.23	44,72,112,114	0
27	DMU	Z	1526	33/33	0.79	0.28	49,57,70,70	0
26	CDL	C	270	100/100	0.79	0.33	41,91,129,130	0
21	TGL	O	1521	63/63	0.80	0.21	58,80,95,96	0
23	CHD	C	271	29/29	0.86	0.25	79,83,85,85	0
21	TGL	B	521	63/63	0.86	0.22	53,74,88,90	0
23	CHD	P	1271	29/29	0.87	0.29	78,92,94,95	0
27	DMU	M	526	33/33	0.90	0.15	33,47,65,71	0
25	PEK	P	1264	53/53	0.92	0.16	35,50,86,88	0
17	MG	N	518	1/1	0.93	0.17	34,34,34,34	0
19	PGV	P	1267	51/51	0.93	0.17	29,40,82,87	0
25	PEK	C	264	53/53	0.94	0.14	30,46,78,80	0
18	NA	N	519	1/1	0.95	0.11	39,39,39,39	0
19	PGV	C	267	51/51	0.95	0.14	28,40,73,76	0
15	NO	N	520	2/2	0.95	0.14	39,39,39,42	0
19	PGV	N	1266	51/51	0.95	0.20	30,42,65,69	0
23	CHD	C	525	29/29	0.96	0.19	26,33,39,41	0
23	CHD	P	1525	29/29	0.96	0.18	32,37,43,47	0
18	NA	A	519	1/1	0.97	0.08	32,32,32,32	0
19	PGV	A	521	51/51	0.97	0.14	23,35,63,67	0
20	CUA	O	228	2/2	0.97	0.09	34,34,34,36	0
15	NO	A	520	2/2	0.97	0.10	32,32,32,36	0
23	CHD	O	229	29/29	0.97	0.10	27,32,38,40	0
23	CHD	B	1085	29/29	0.97	0.10	27,31,36,42	0
14	HEA	N	515	60/60	0.97	0.14	28,36,45,49	0
17	MG	A	518	1/1	0.98	0.18	23,23,23,23	0
14	HEA	N	516	60/60	0.98	0.18	27,33,37,40	0
14	HEA	A	515	60/60	0.98	0.15	22,28,41,42	0
28	ZN	F	99	1/1	0.99	0.08	37,37,37,37	0
20	CUA	B	228	2/2	0.99	0.13	27,27,27,28	0
16	CU	N	517	1/1	0.99	0.15	35,35,35,35	0
28	ZN	S	99	1/1	0.99	0.08	43,43,43,43	0
14	HEA	A	516	60/60	0.99	0.17	18,26,31,36	0
16	CU	A	517	1/1	1.00	0.15	29,29,29,29	0

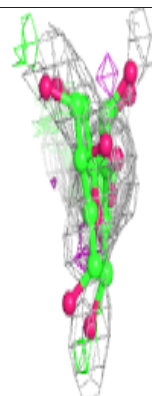
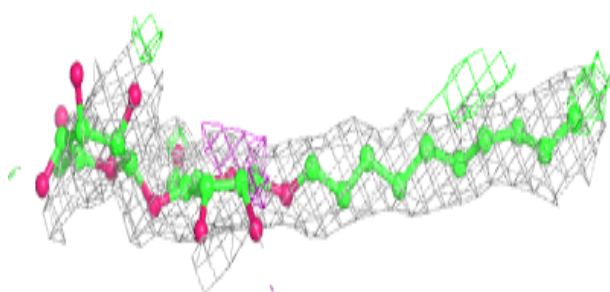
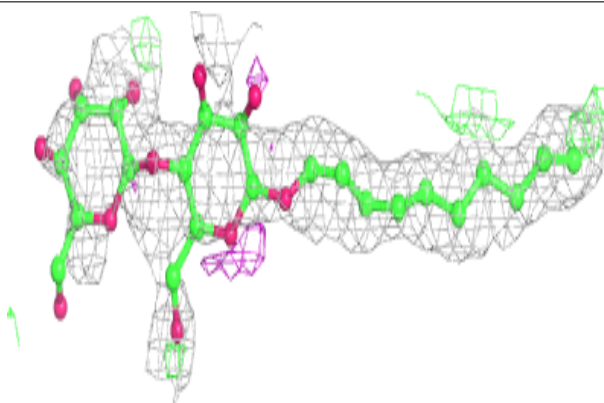
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DMU P 272:

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

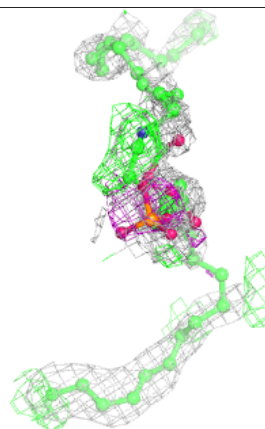
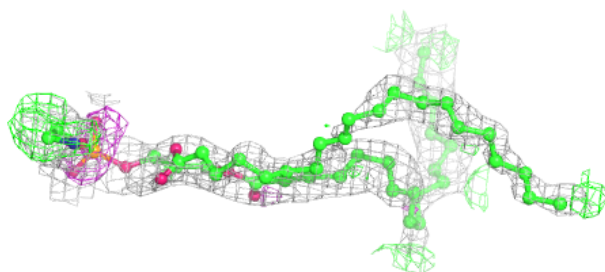
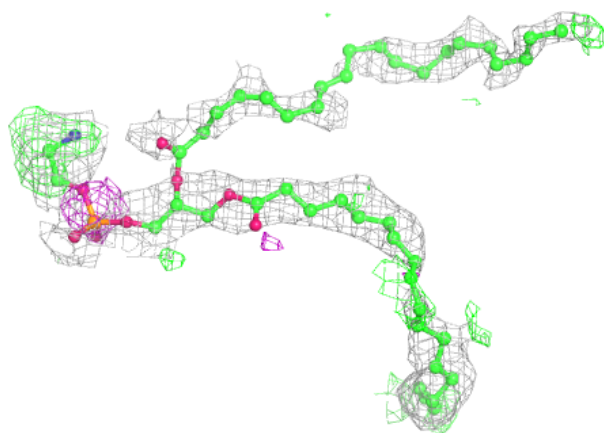
**Electron density around DMU C 272:**

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



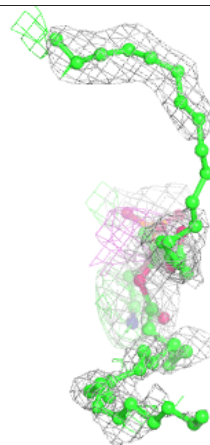
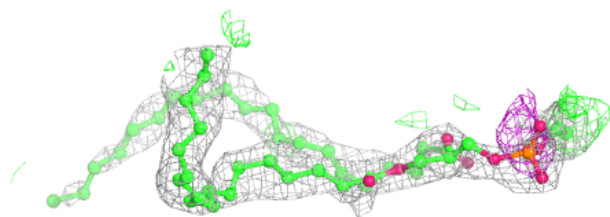
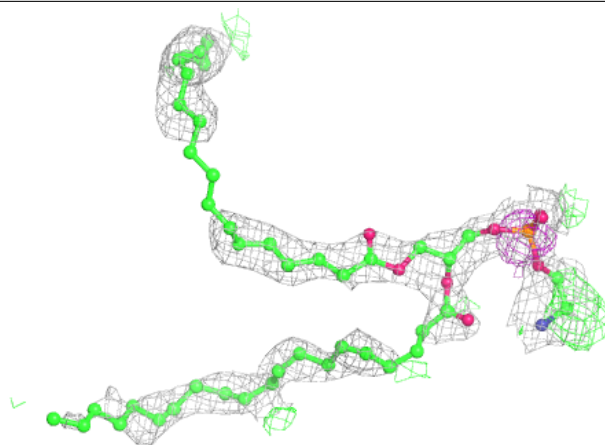
Electron density around PEK T 1265:

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

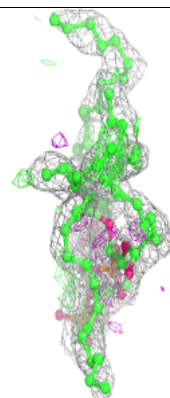
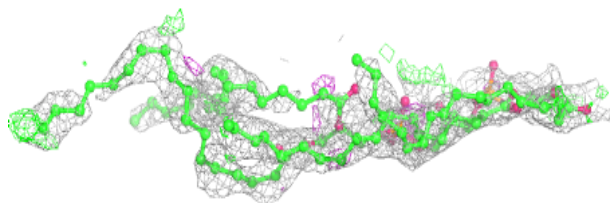
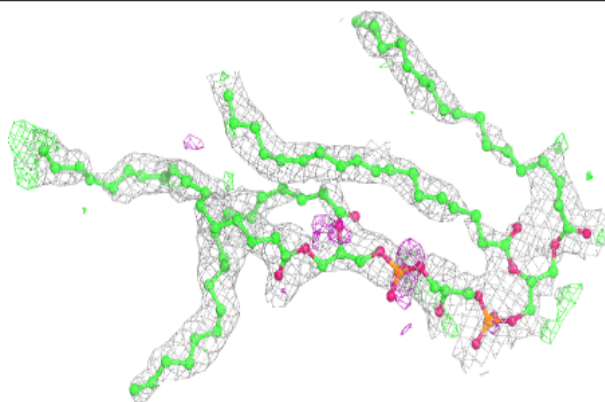


Electron density around PEK C 265:

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

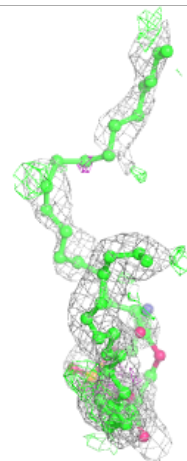
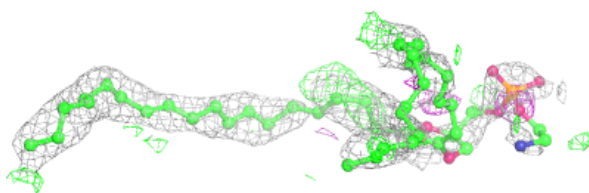
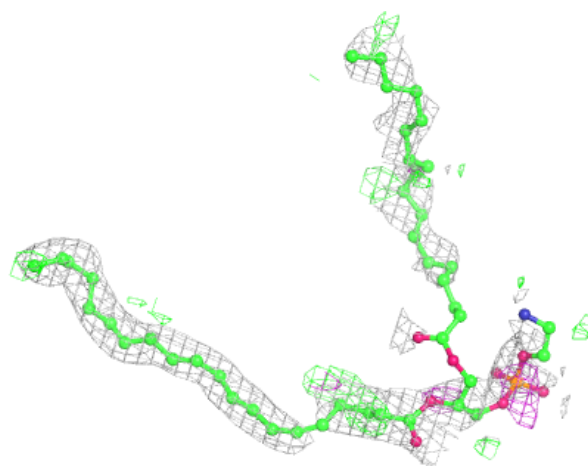
**Electron density around CDL G 269:**

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



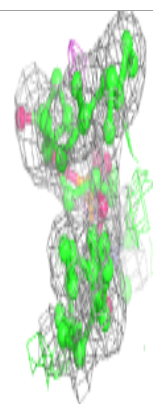
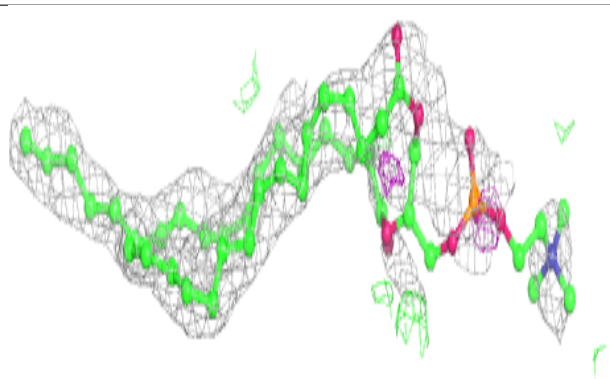
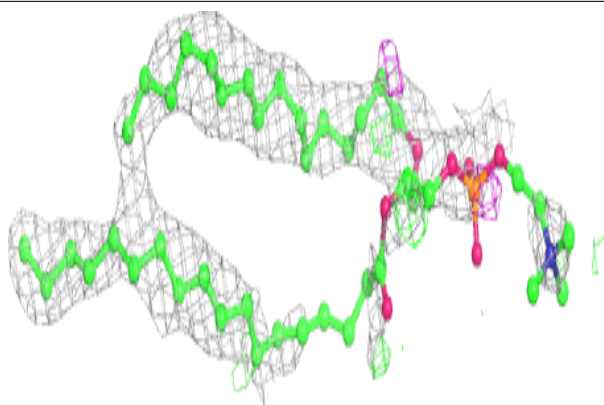
Electron density around PEK G 1263:

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



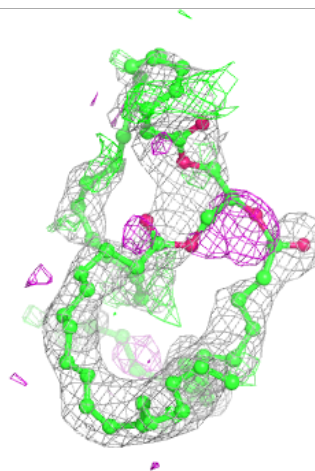
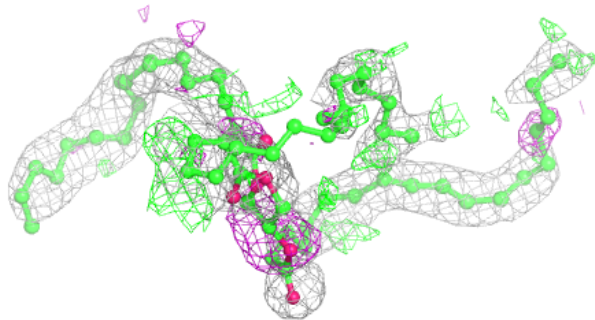
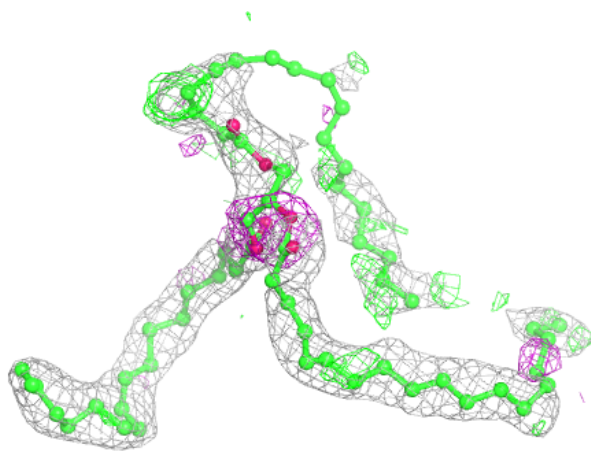
Electron density around PSC R 1229:

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



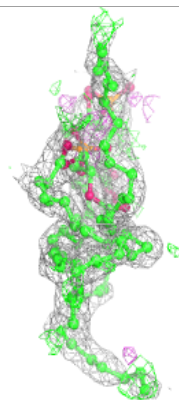
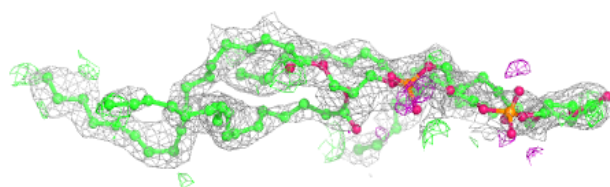
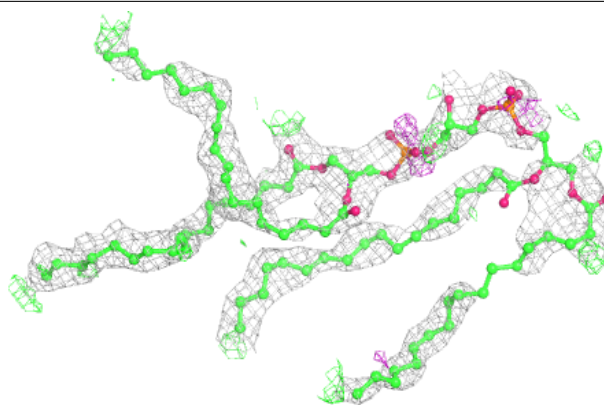
Electron density around TGL Y 1522:

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

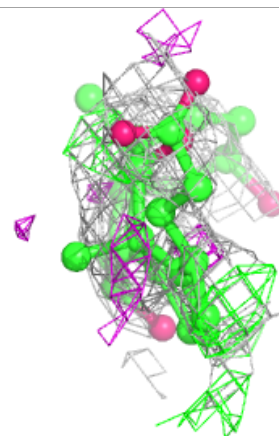
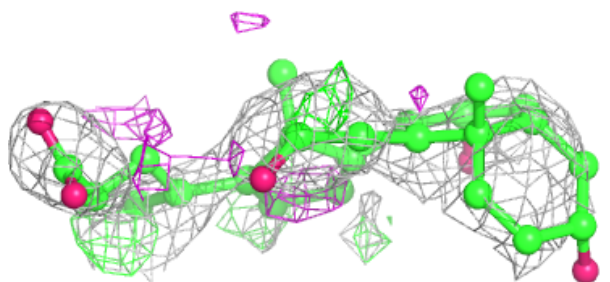
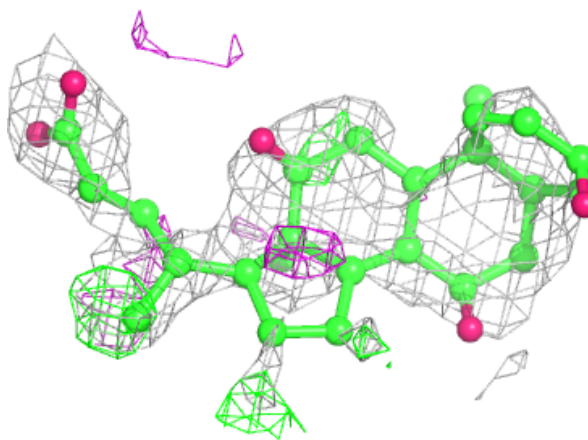


Electron density around CDL T 1269:

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

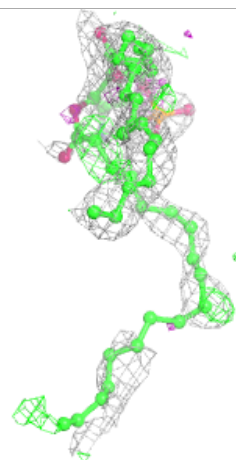
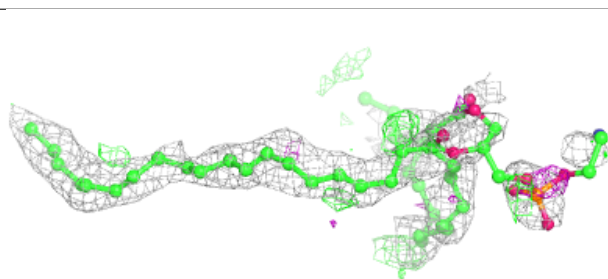
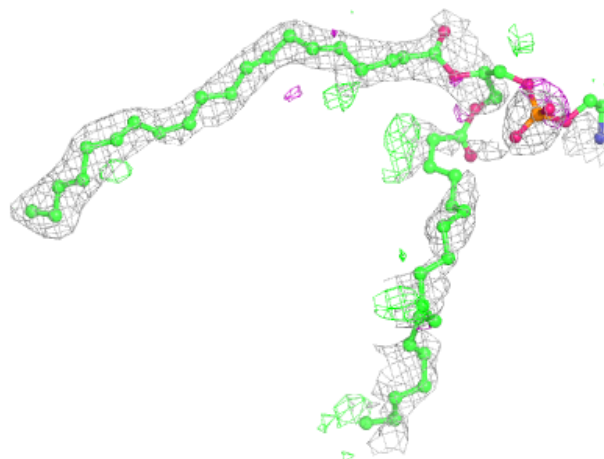
**Electron density around CHD W 1059:**

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



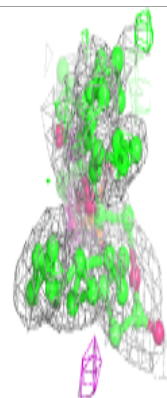
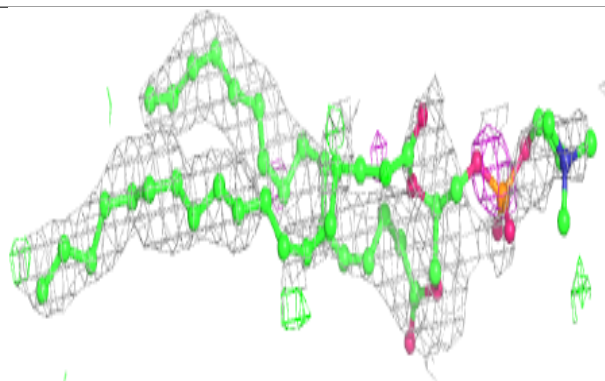
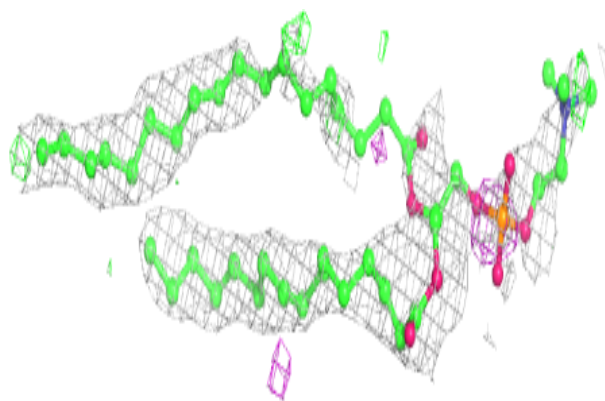
Electron density around PEK T 263:

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

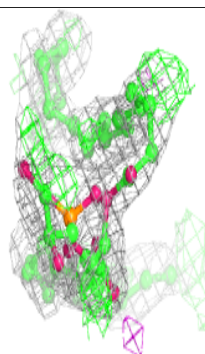
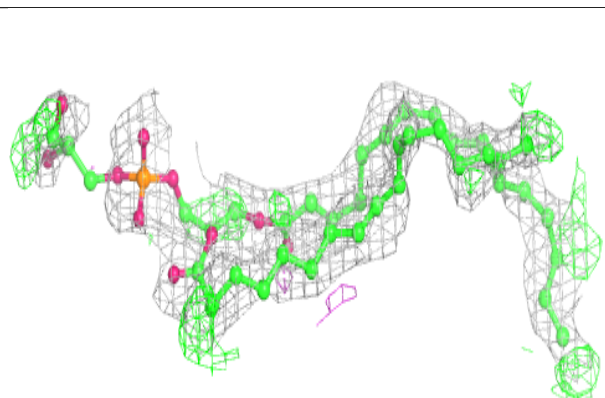
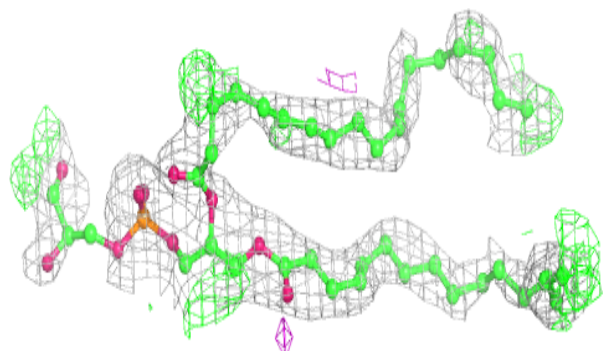


Electron density around PSC B 229:

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

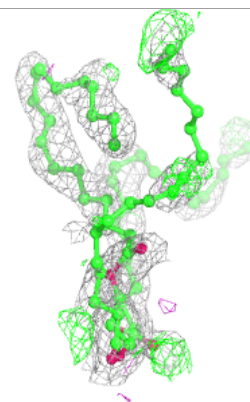
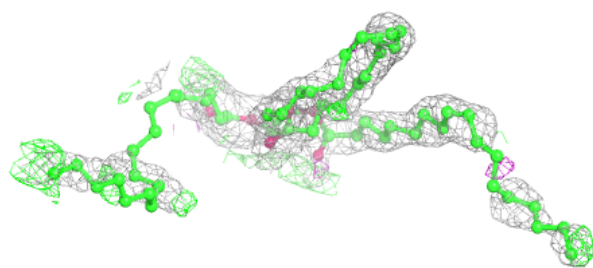
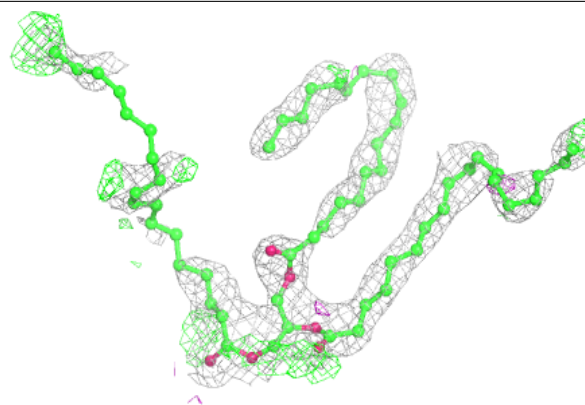
**Electron density around PGV U 1268:**

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

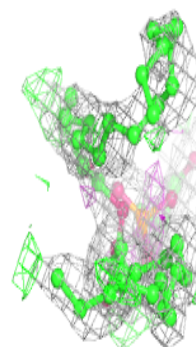
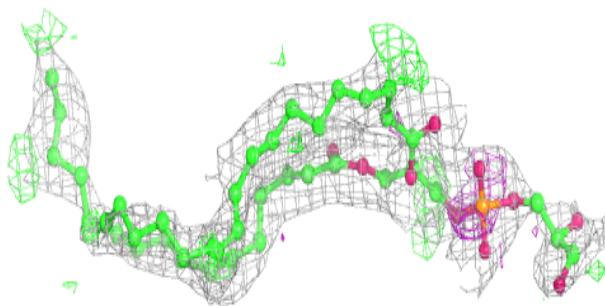
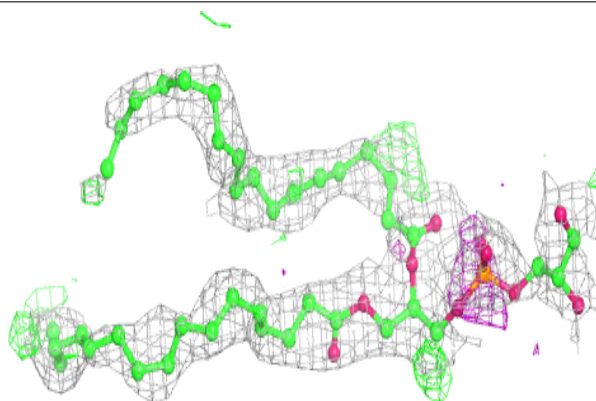


Electron density around TGL N 1523:

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

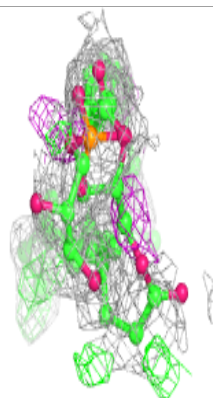
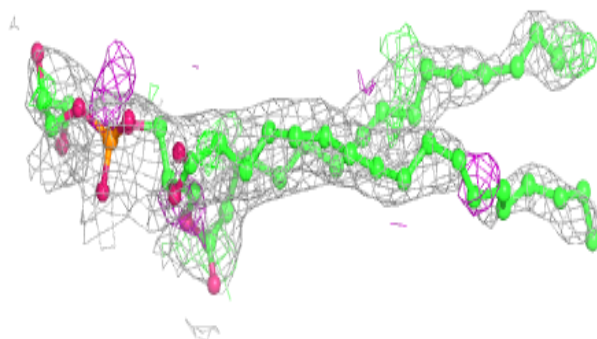
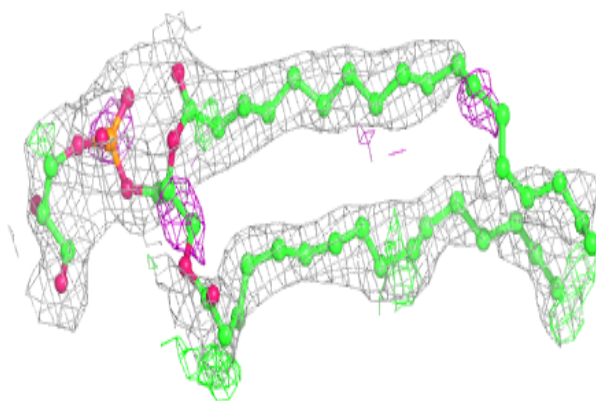
**Electron density around PGV C 268:**

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

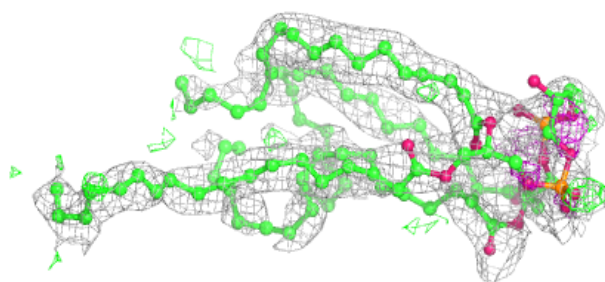
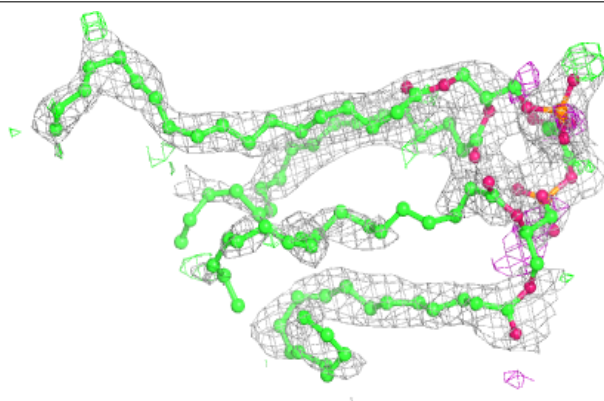


Electron density around PGL N 1524:

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

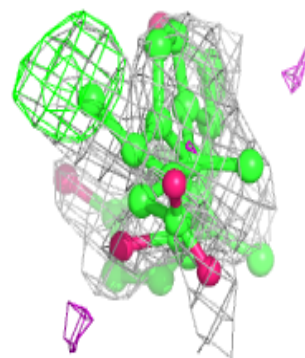
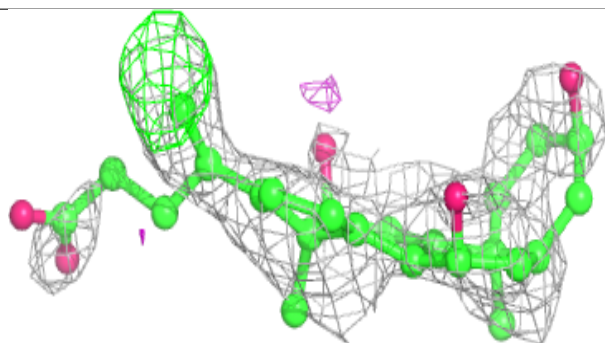
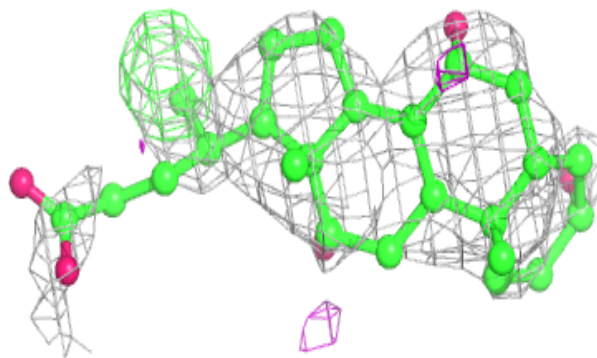
**Electron density around CDL P 1270:**

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

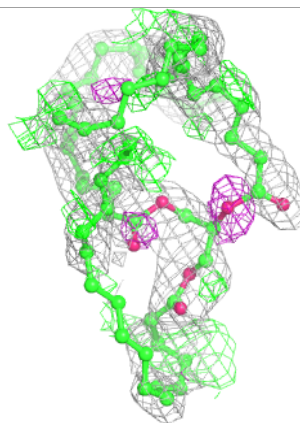
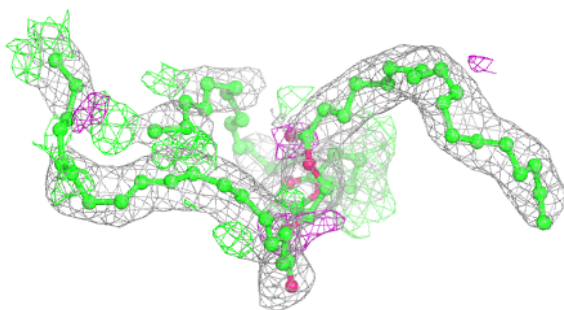
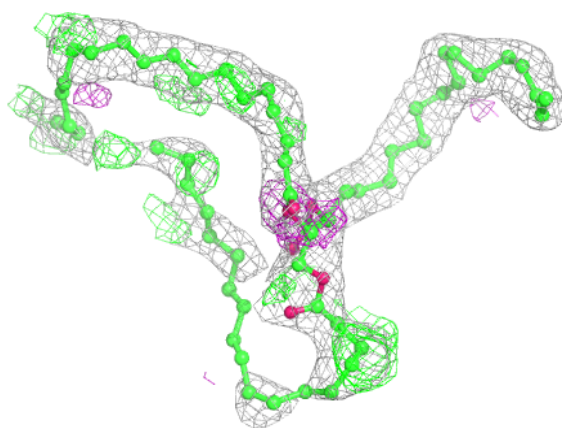


Electron density around CHD J 60:

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

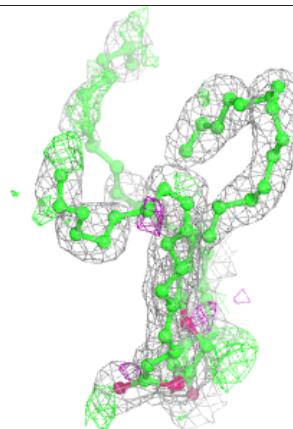
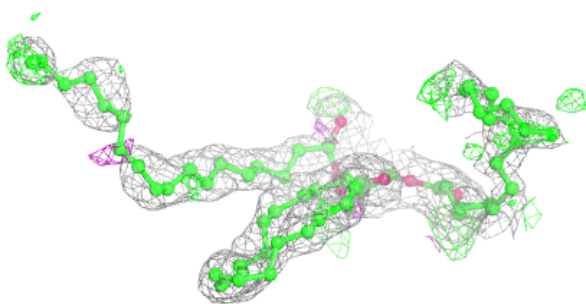
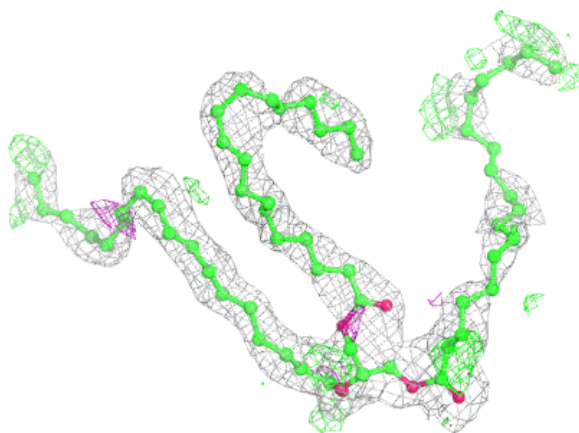
**Electron density around TGL L 522:**

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

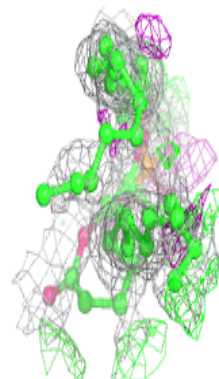
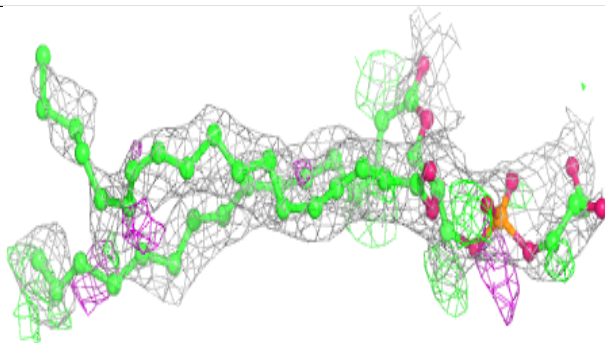
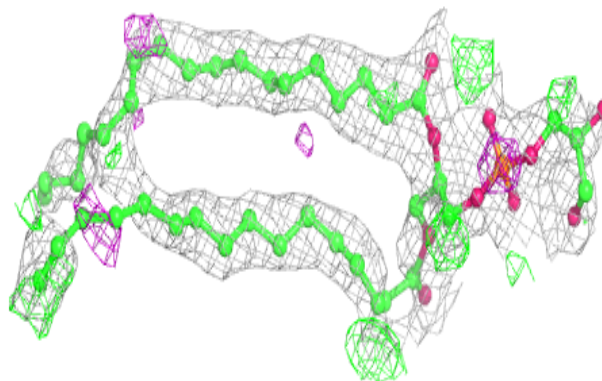


Electron density around TGL D 523:

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

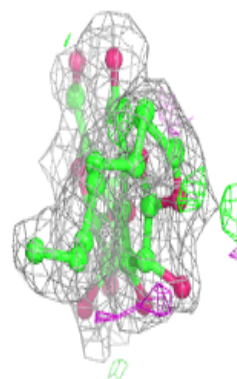
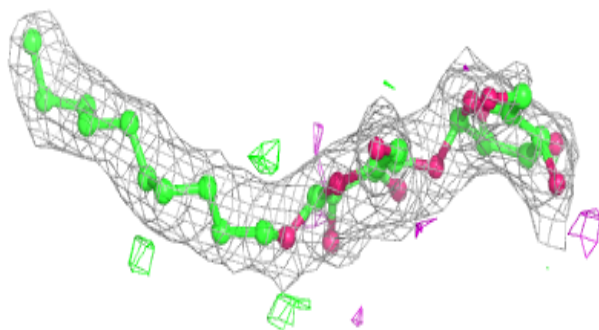
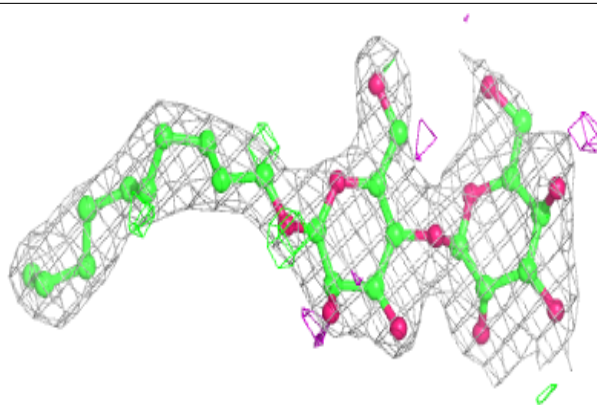
**Electron density around PGV A 524:**

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



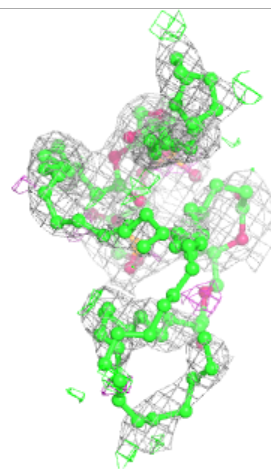
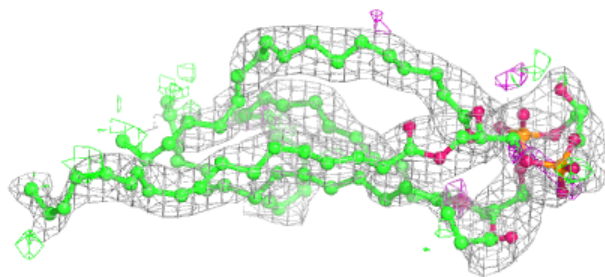
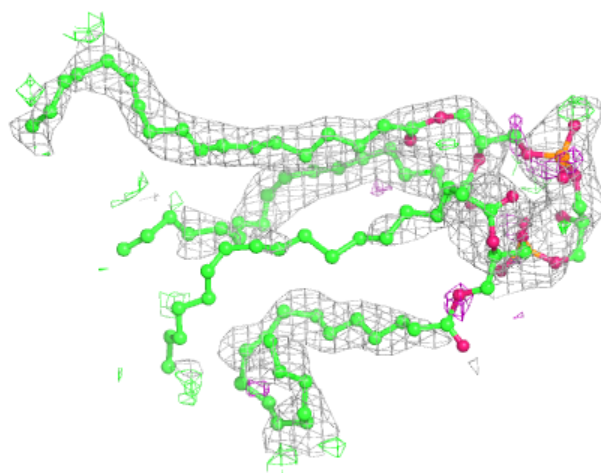
Electron density around DMU Z 1526:

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



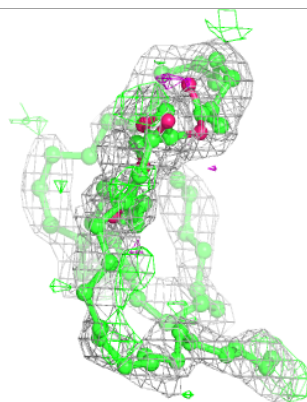
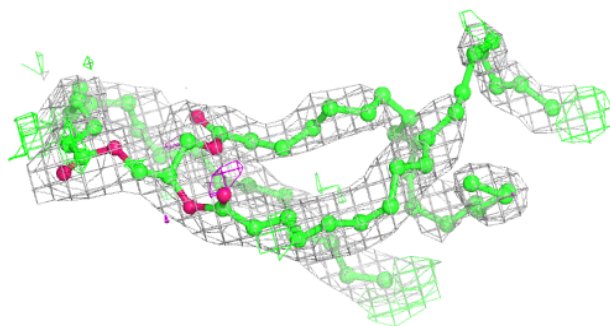
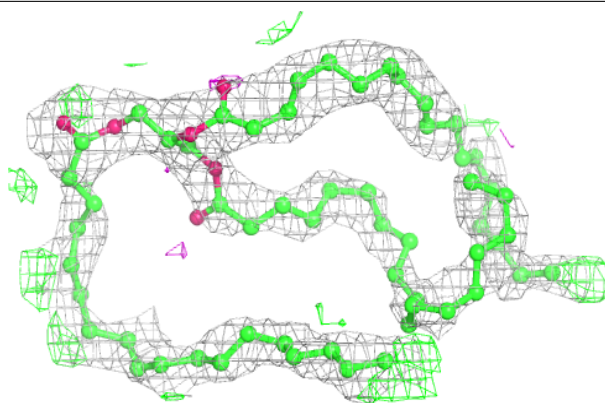
Electron density around CDL C 270:

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

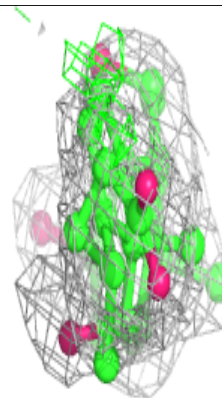
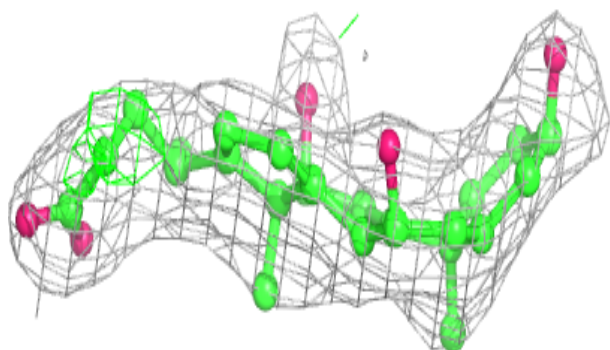
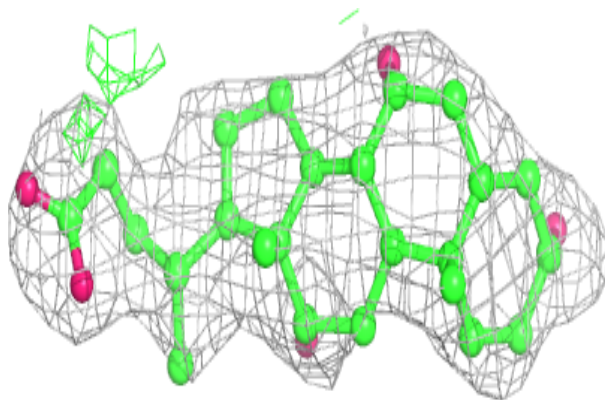


Electron density around TGL O 1521:

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

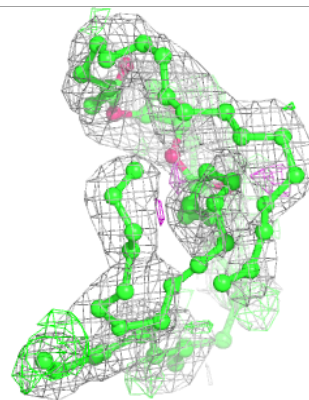
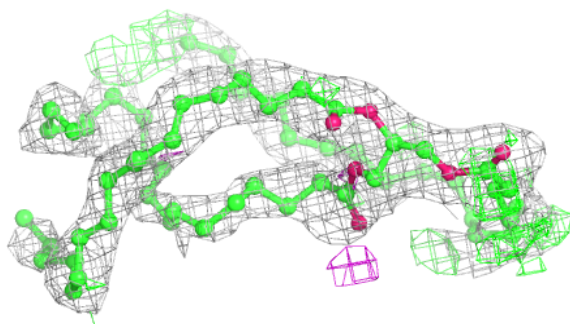
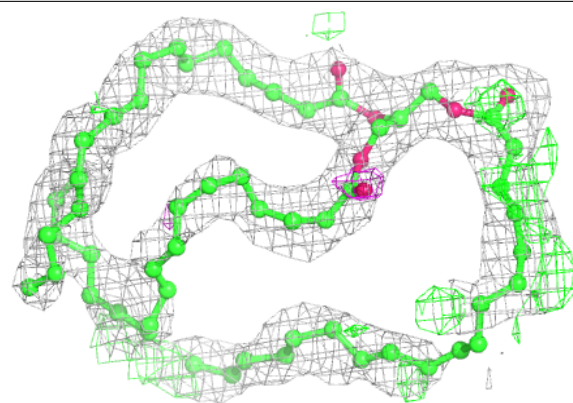
**Electron density around CHD C 271:**

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

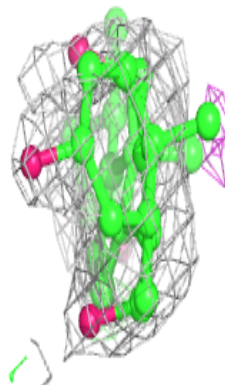
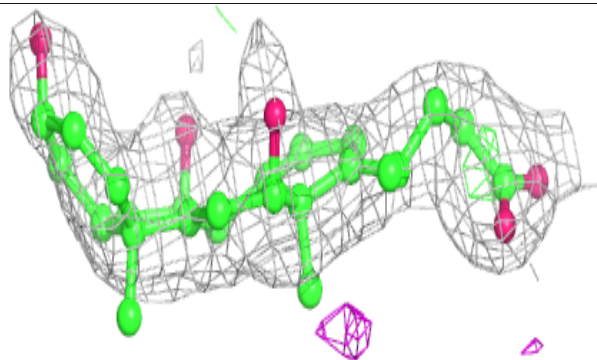
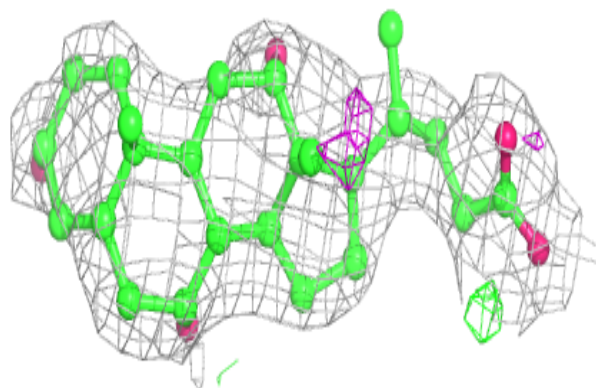


Electron density around TGL B 521:

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

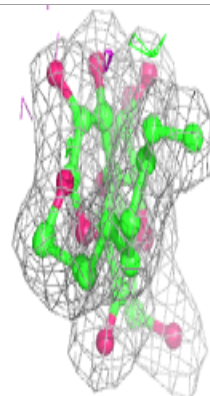
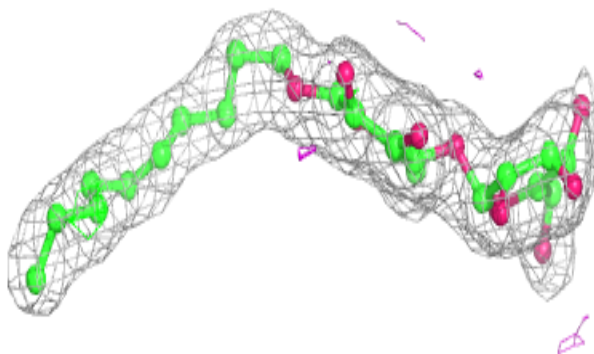
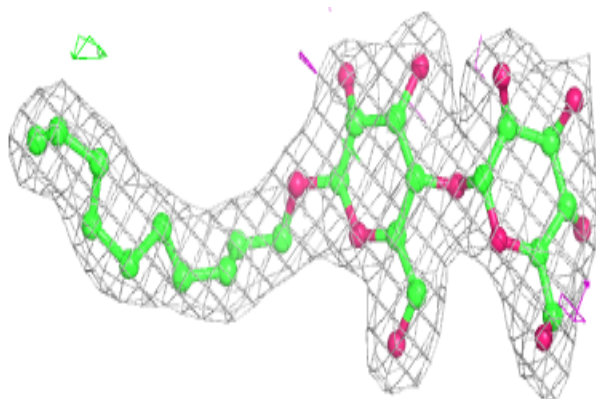
**Electron density around CHD P 1271:**

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

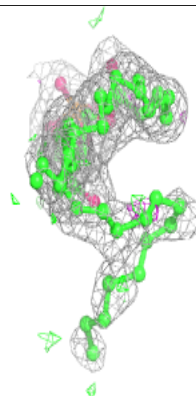
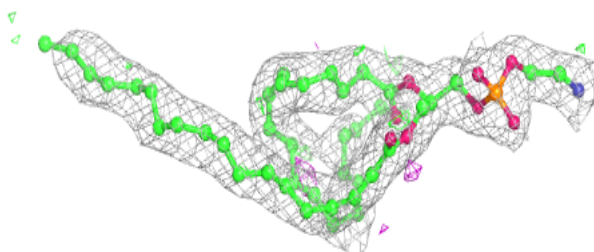
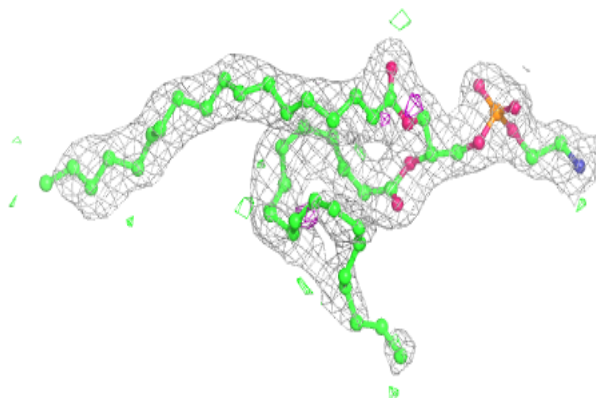


Electron density around DMU M 526:

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

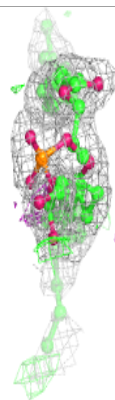
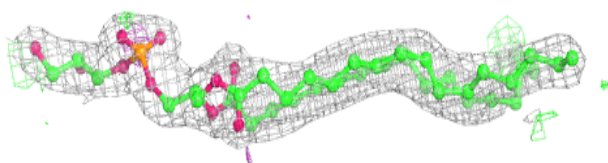
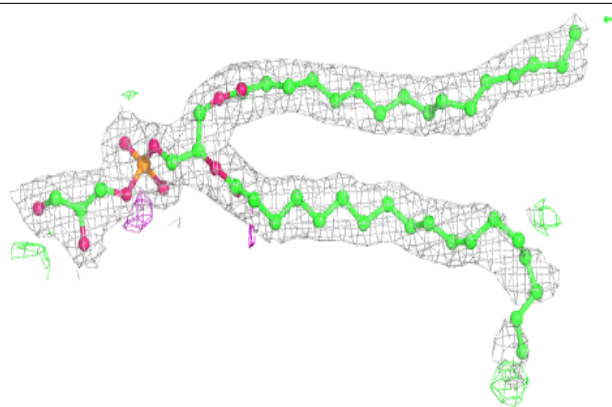
**Electron density around PEK P 1264:**

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

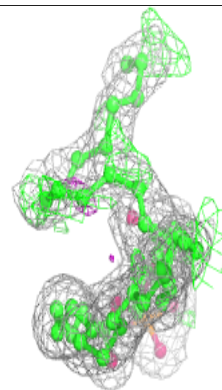
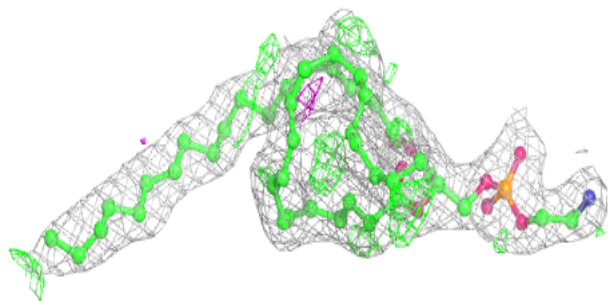
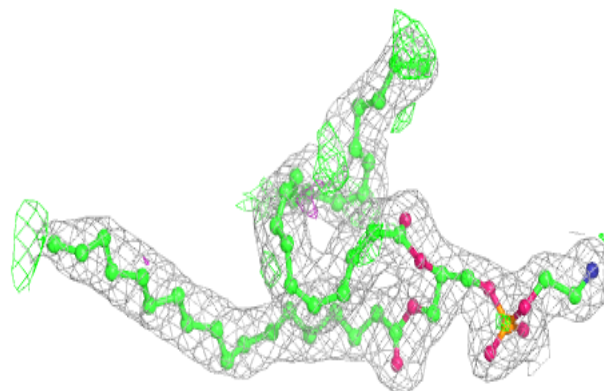


Electron density around PGV P 1267:

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

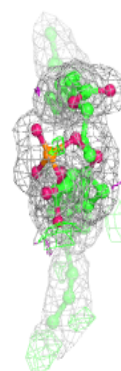
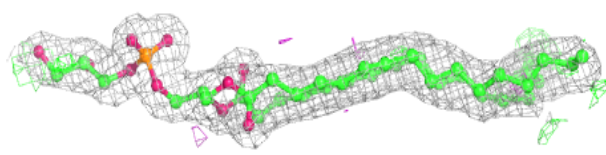
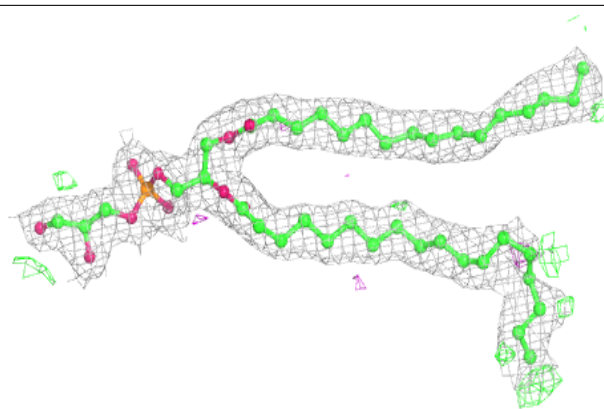
**Electron density around PEK C 264:**

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

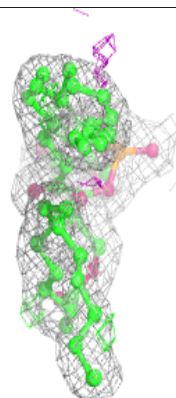
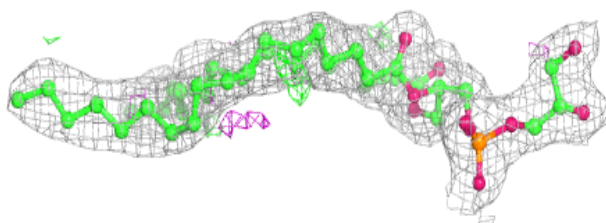
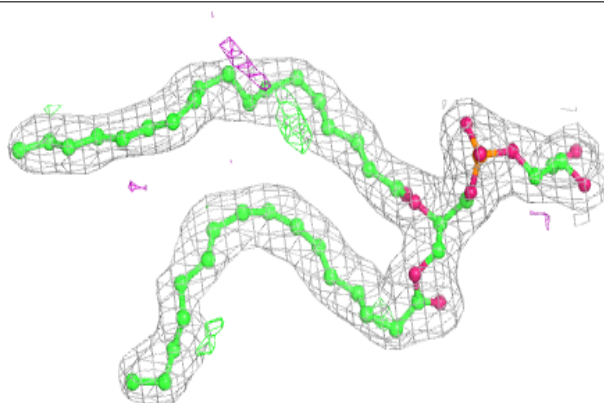


Electron density around PGV C 267:

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

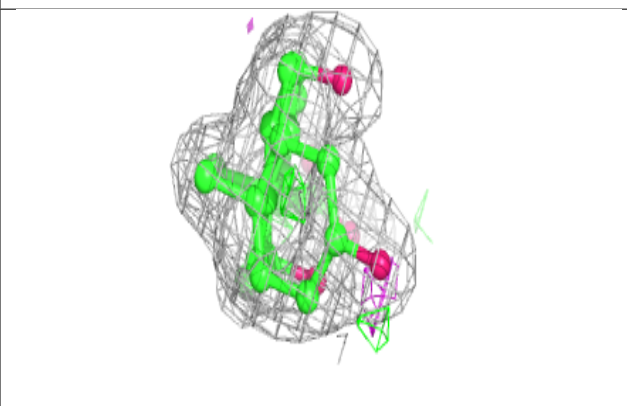
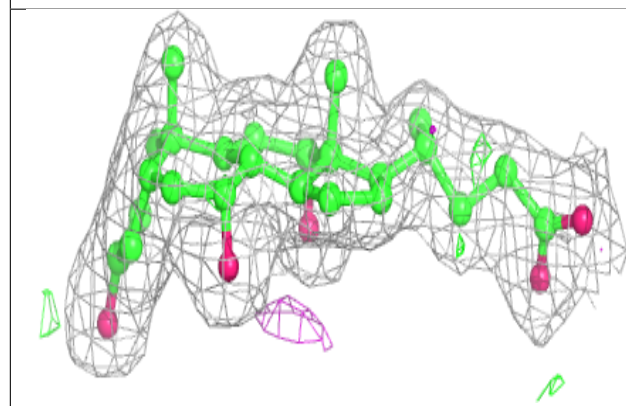
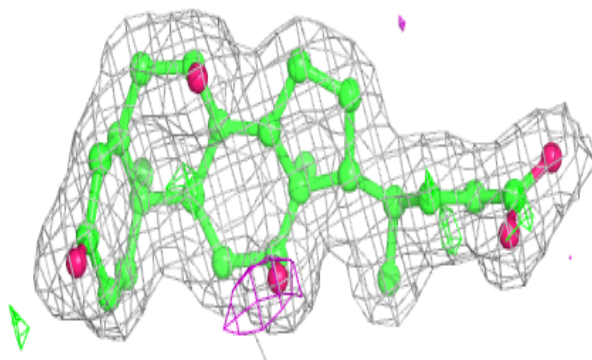
**Electron density around PGV N 1266:**

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

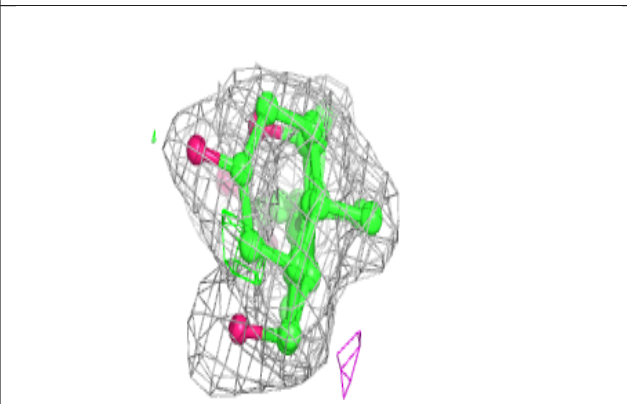
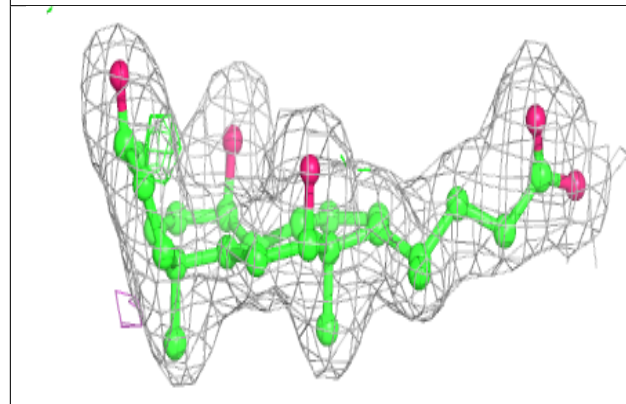
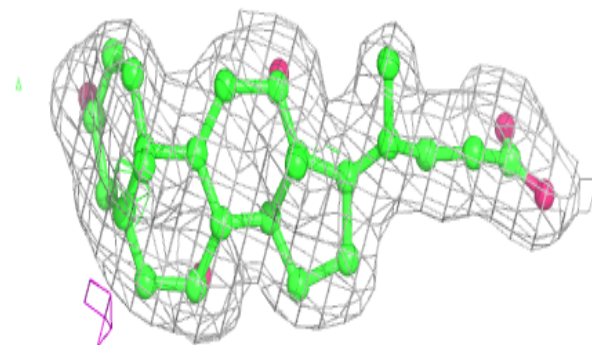


Electron density around CHD C 525:

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

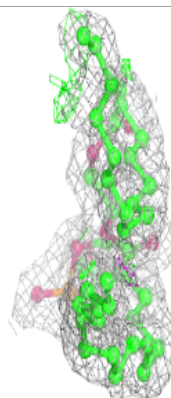
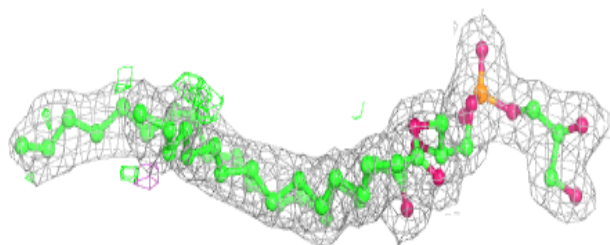
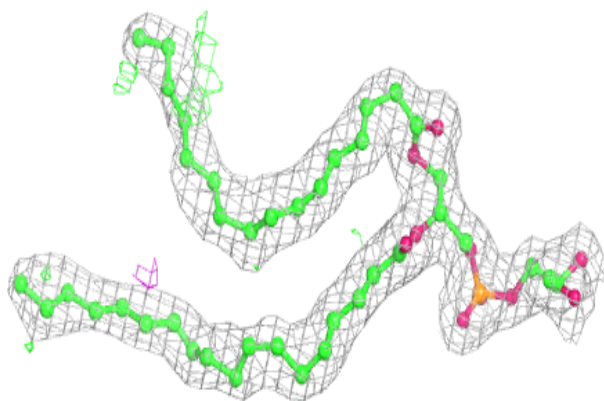
**Electron density around CHD P 1525:**

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

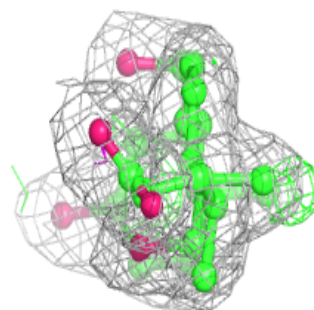
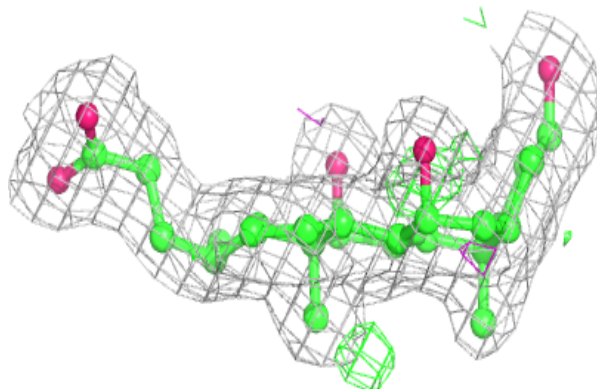
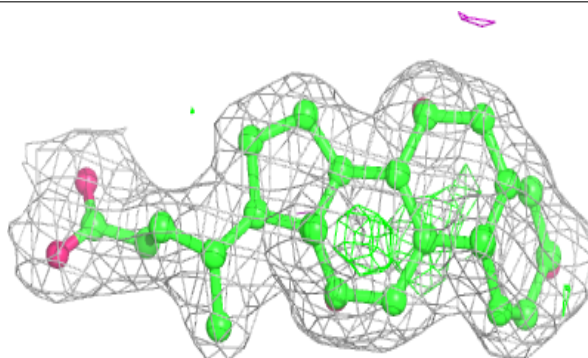


Electron density around PGV A 521:

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

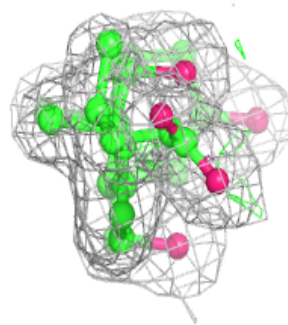
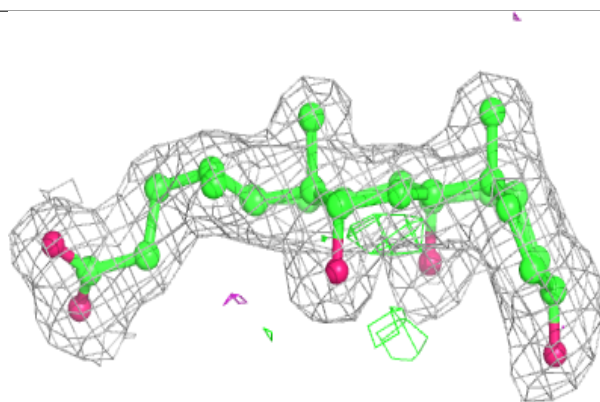
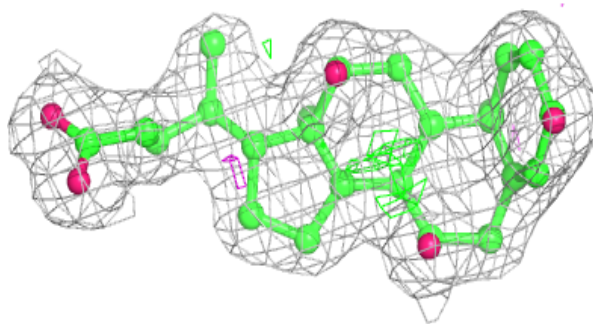
**Electron density around CHD O 229:**

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

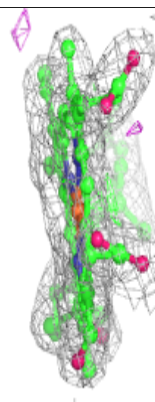
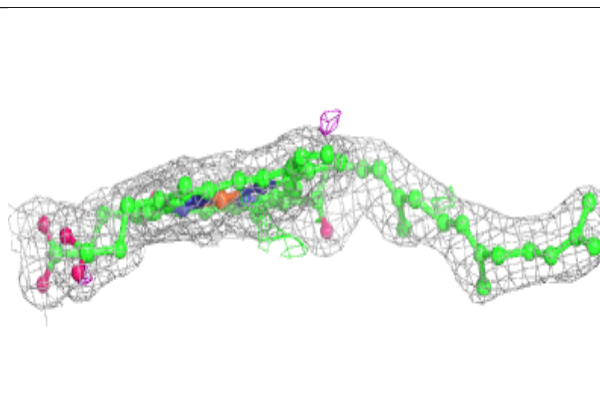
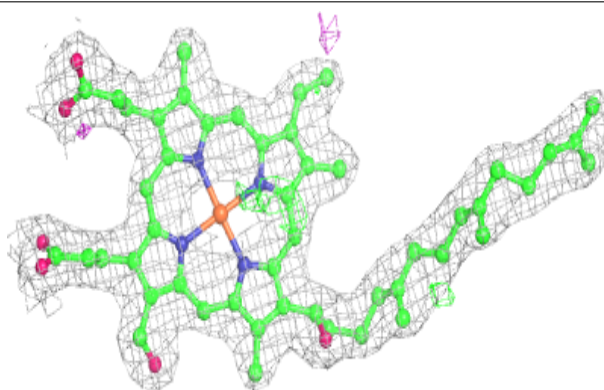


Electron density around CHD B 1085:

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

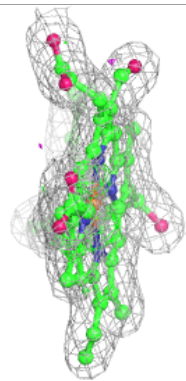
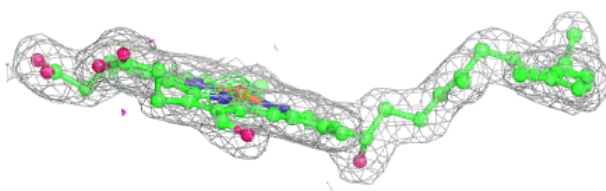
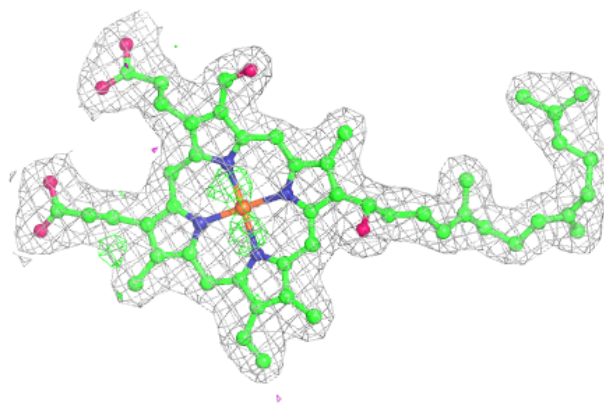
**Electron density around HEA N 515:**

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

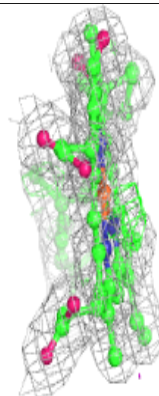
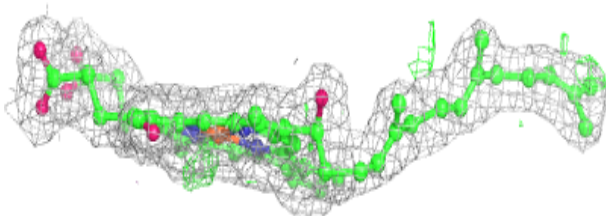
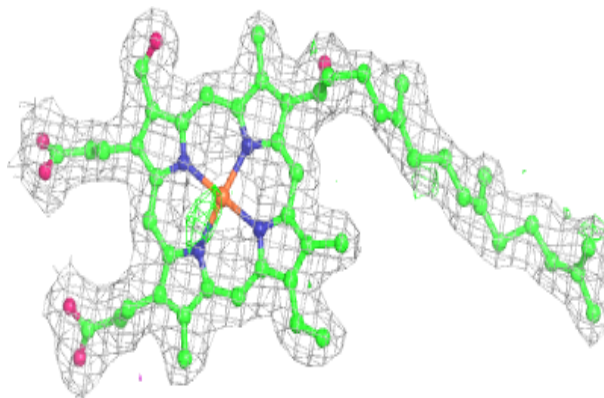


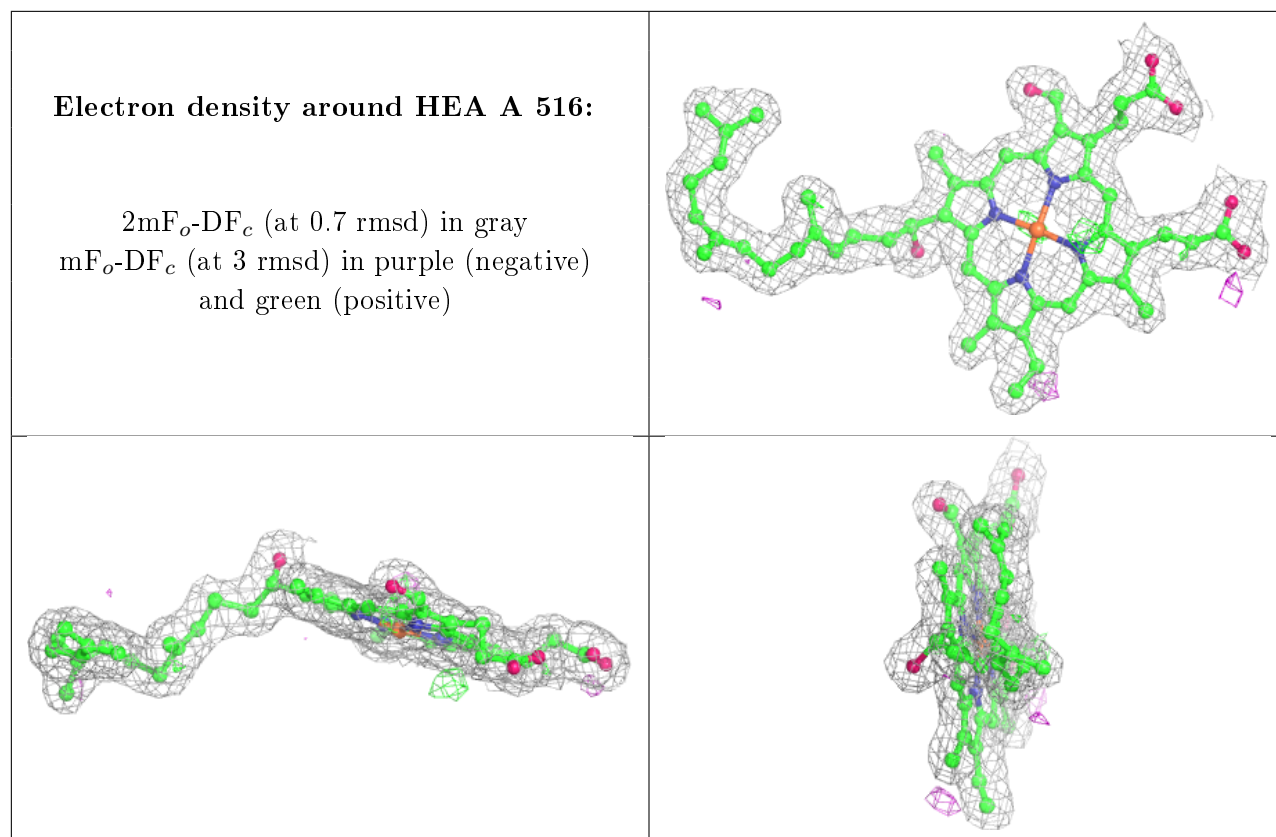
Electron density around HEA N 516:

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

**Electron density around HEA A 515:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.