



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:45 am BST

PDB ID : 3AG4  
Title : Bovine Heart Cytochrome c Oxidase in the Cyanide Ion-bound Fully Reduced State at 100 K  
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2010-03-19  
Resolution : 2.05 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](mailto: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.

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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

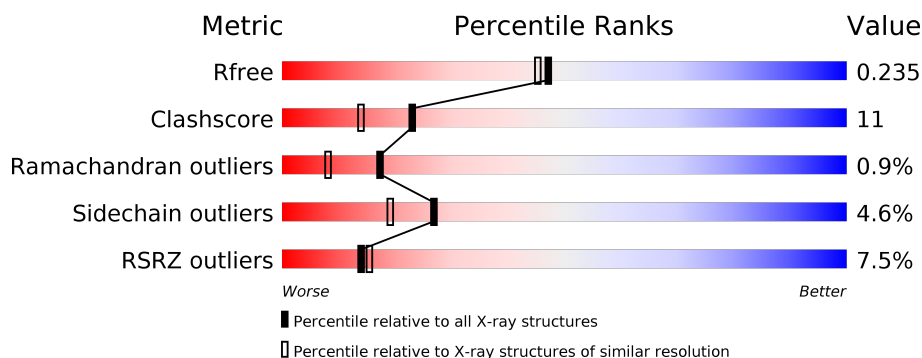
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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>9%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>.</div> </div> </div>
1	N	514	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>.</div> </div> </div>
2	B	227	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
2	O	227	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>
3	C	261	<div> <div></div> <div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div> </div>
3	P	261	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>22%</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	-	-	-
15	CYN	N	520	-	-	X	-
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1059	X	-	-	X
23	UNX	C	262	-	-	-	X
23	UNX	P	262	-	-	-	X
25	CDL	C	270	-	-	X	-
25	CDL	G	269	-	-	X	-
25	CDL	T	1269	-	-	X	-
28	DMU	G	272	X	-	-	-
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	-
28	DMU	Z	1526	X	-	-	-
9	SAC	V	1	-	-	-	X

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 32324 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called Cytochrome c oxidase 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			

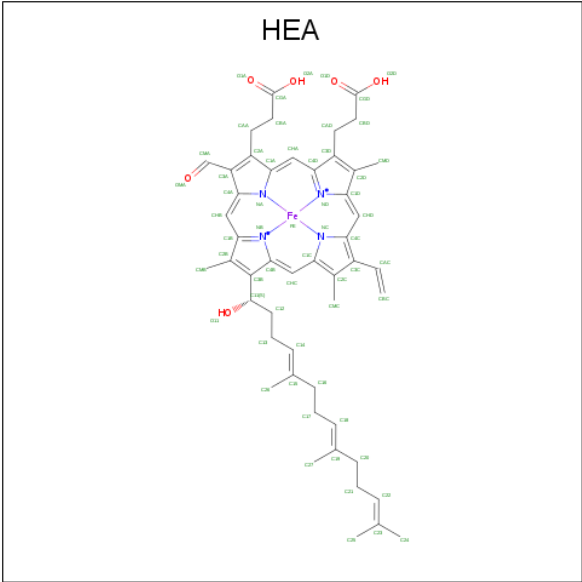
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

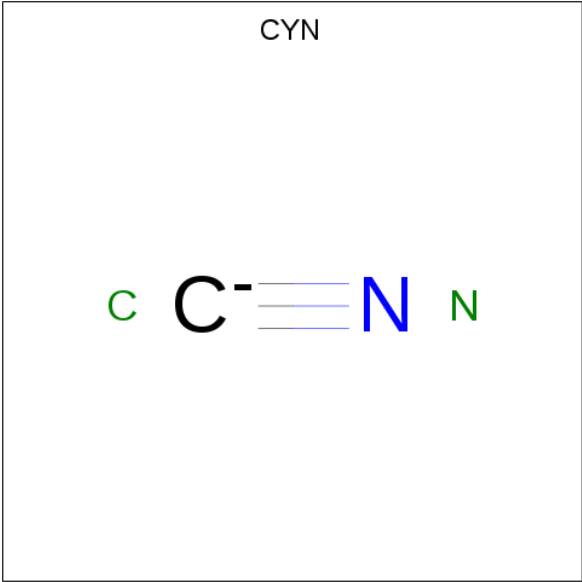
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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 CYANIDE ION (three-letter code: CYN) (formula: CN).



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

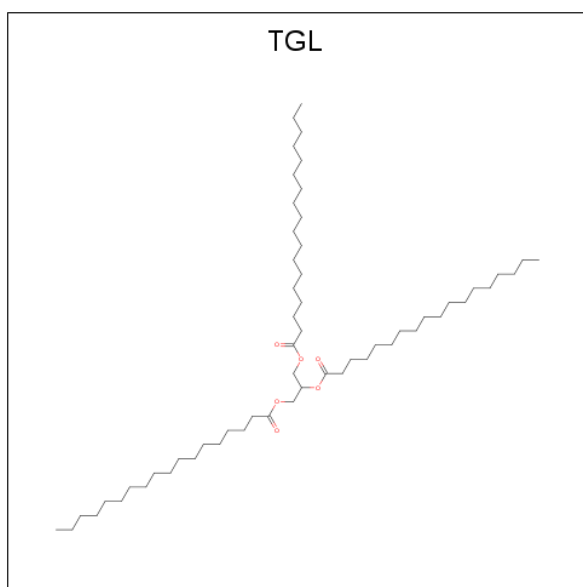
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

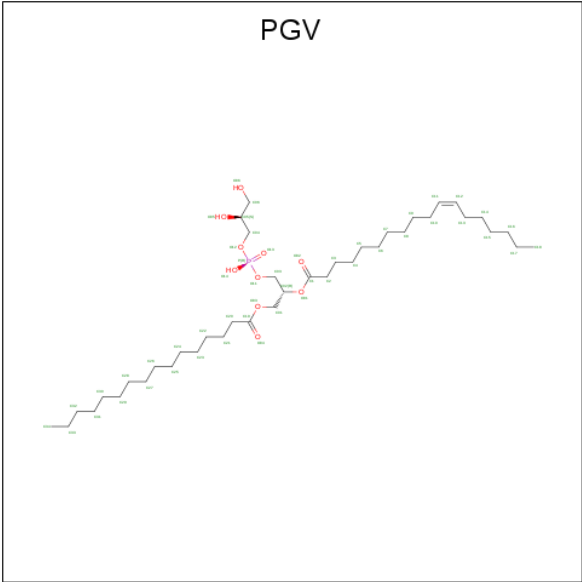
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



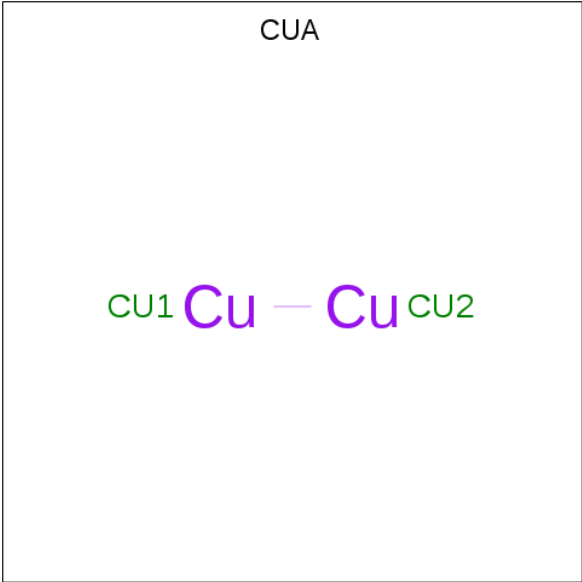
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



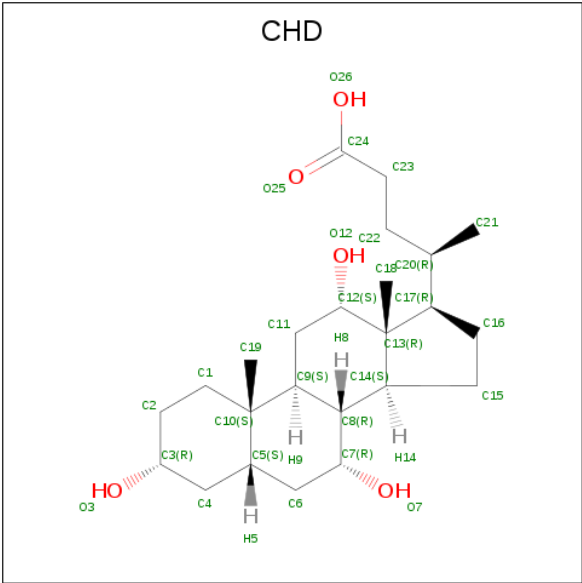
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



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

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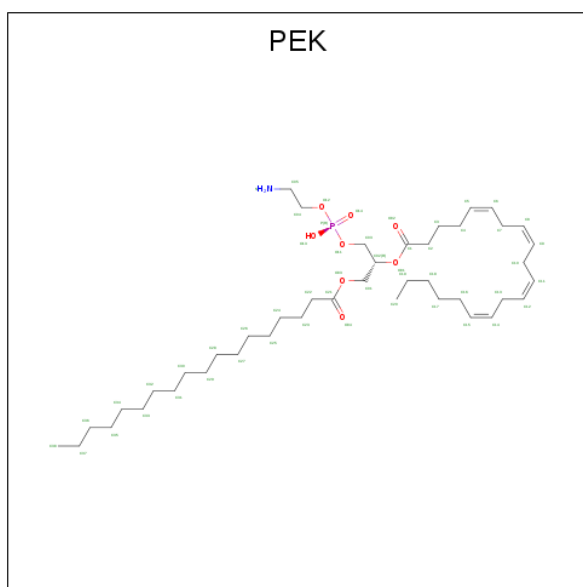
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

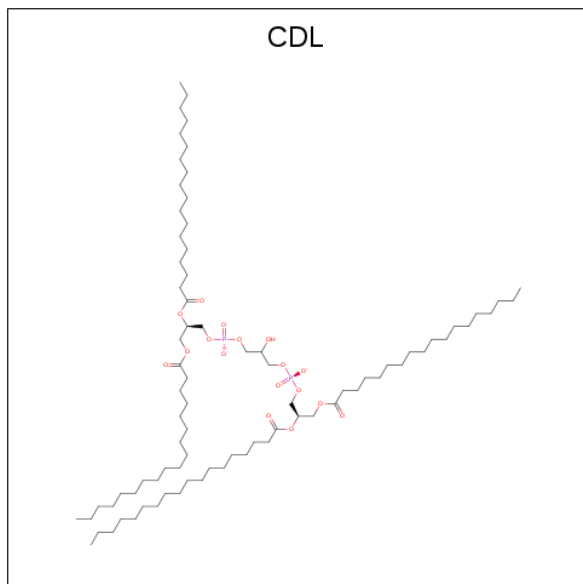
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total X 1 1	0	0
23	C	1	Total X 1 1	0	0

- Molecule 24 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: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



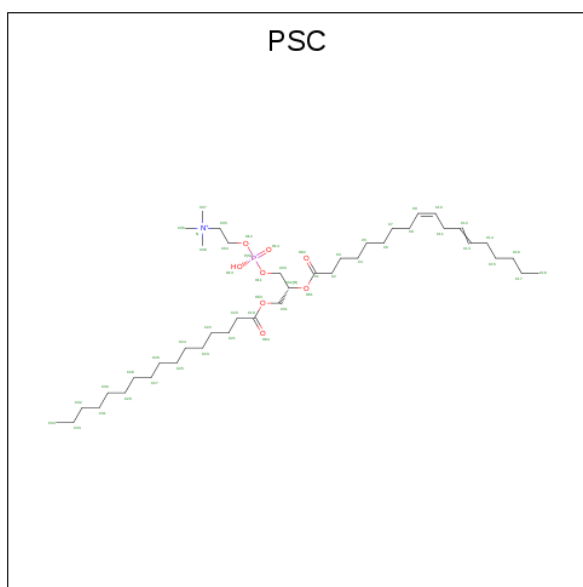
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	S	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula:  $C_{42}H_{81}NO_8P$ ).

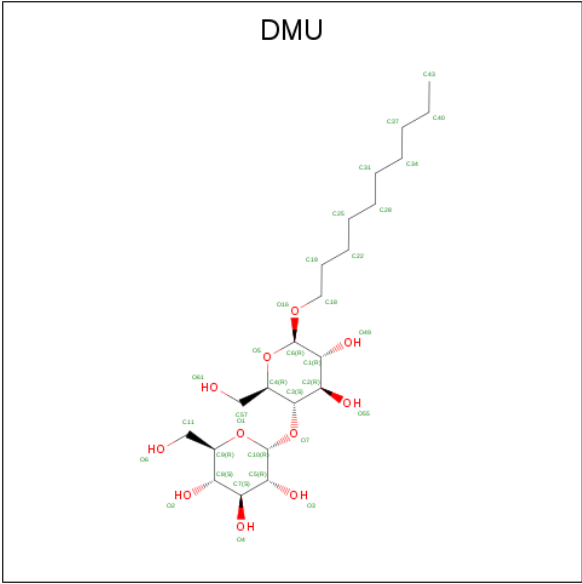


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	225	Total	O	0	0
			225	225		
29	B	125	Total	O	0	0
			125	125		
29	C	106	Total	O	0	0
			106	106		
29	D	91	Total	O	0	0
			91	91		
29	E	62	Total	O	0	0
			62	62		
29	F	75	Total	O	0	0
			75	75		
29	G	41	Total	O	0	0
			41	41		
29	H	47	Total	O	0	0
			47	47		

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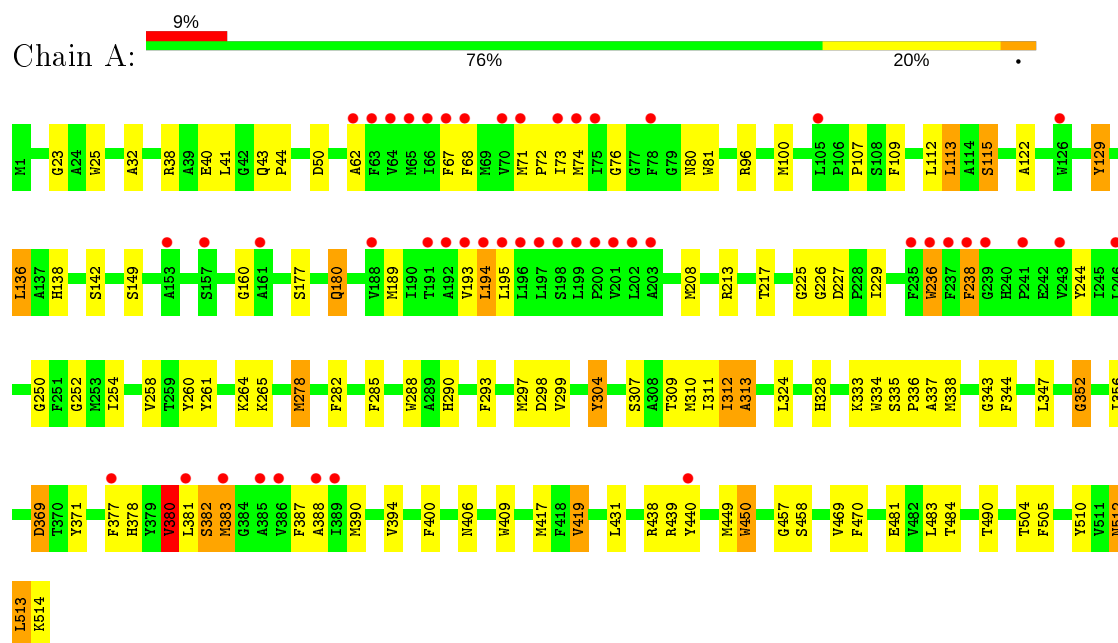
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	I	38	Total 38	O 38	0	0
29	J	20	Total 20	O 20	0	0
29	K	20	Total 20	O 20	0	0
29	L	22	Total 22	O 22	0	0
29	M	15	Total 15	O 15	0	0
29	N	199	Total 199	O 199	0	0
29	O	107	Total 107	O 107	0	0
29	P	100	Total 100	O 100	0	0
29	Q	55	Total 55	O 55	0	0
29	R	40	Total 40	O 40	0	0
29	S	56	Total 56	O 56	0	0
29	T	36	Total 36	O 36	0	0
29	U	41	Total 41	O 41	0	0
29	V	18	Total 18	O 18	0	0
29	W	12	Total 12	O 12	0	0
29	X	14	Total 14	O 14	0	0
29	Y	12	Total 12	O 12	0	0
29	Z	11	Total 11	O 11	0	0

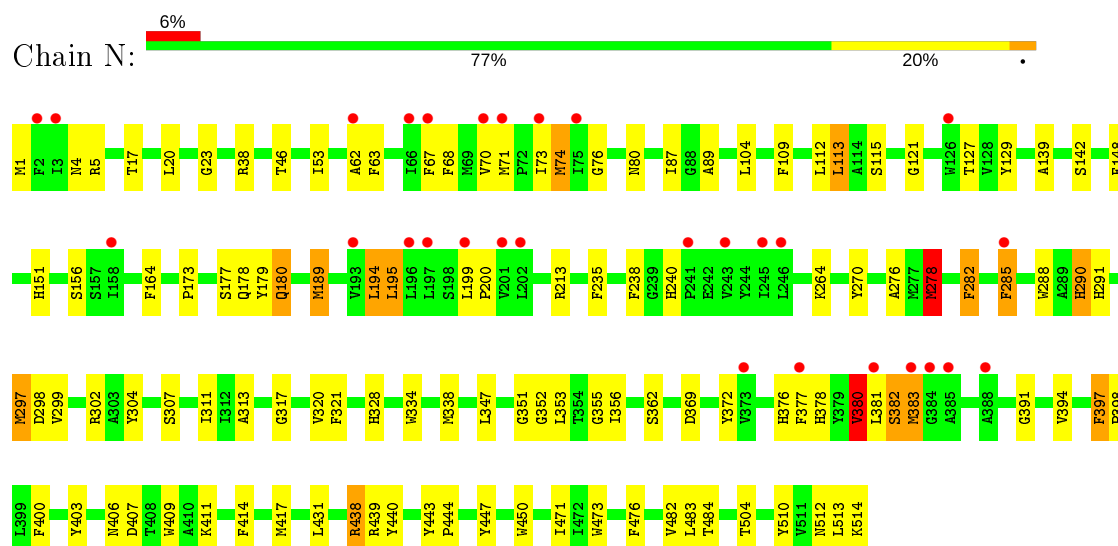
### 3 Residue-property plots [i](#)

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.

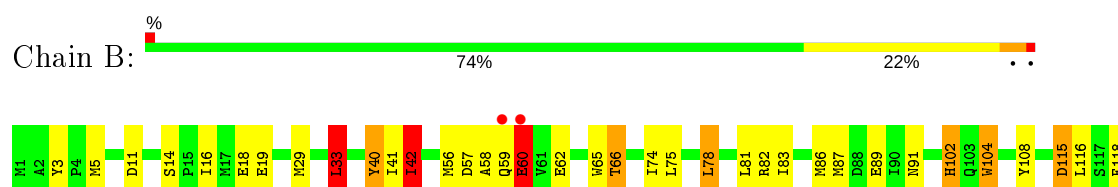
#### • Molecule 1: Cytochrome c oxidase subunit 1



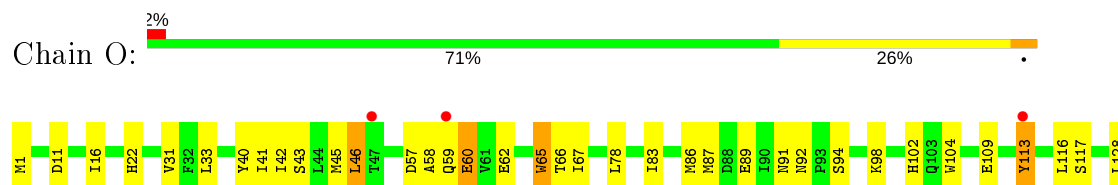
#### • Molecule 1: Cytochrome c oxidase subunit 1



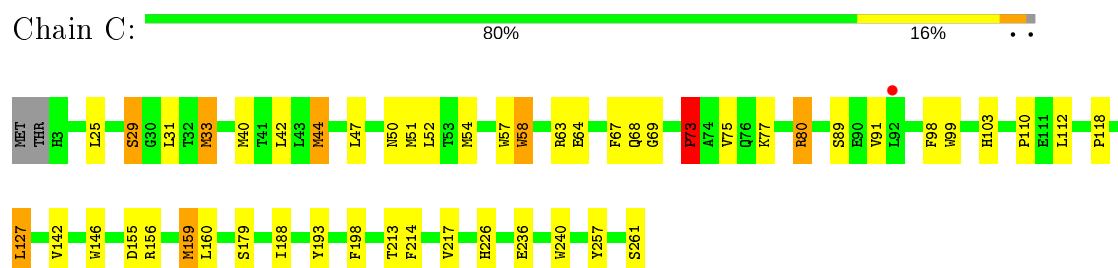
#### • Molecule 2: Cytochrome c oxidase subunit 2



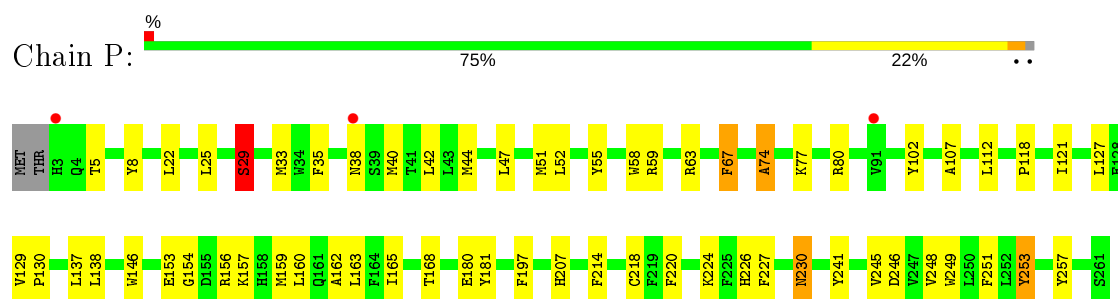
- Molecule 2: Cytochrome c oxidase subunit 2



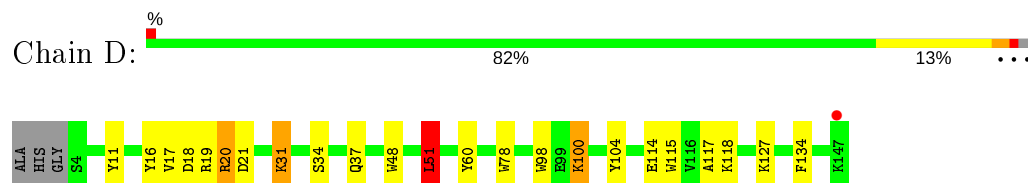
- Molecule 3: Cytochrome c oxidase subunit 3



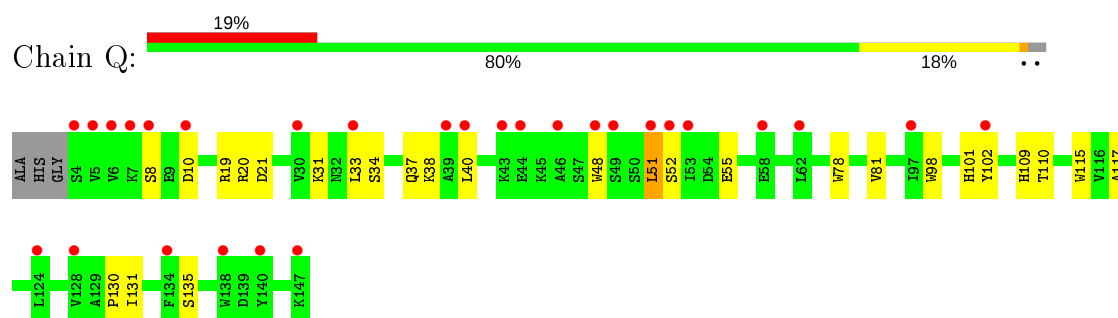
- Molecule 3: Cytochrome c oxidase subunit 3



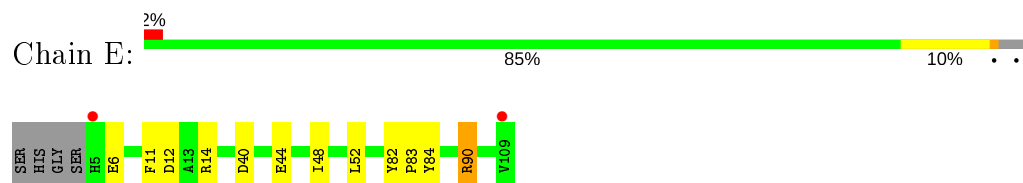
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



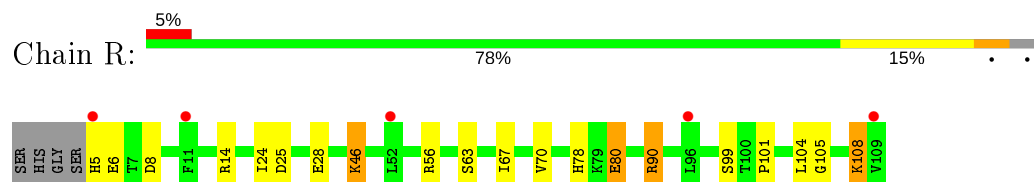
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



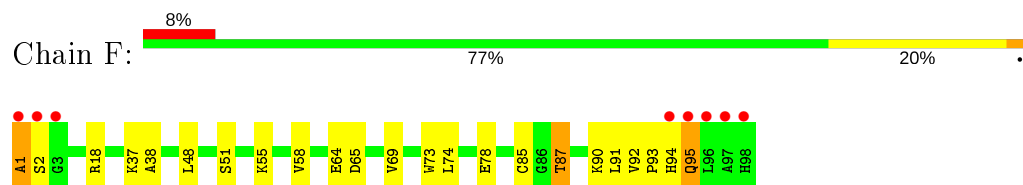
- Molecule 5: Cytochrome c oxidase subunit 5A



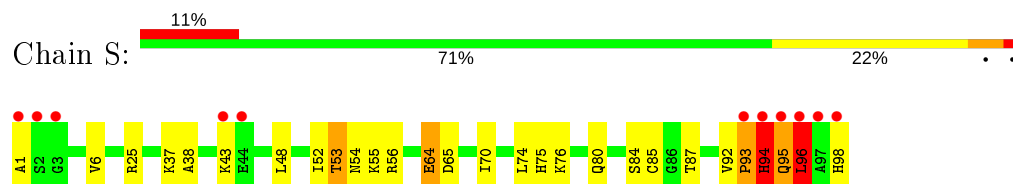
- Molecule 5: Cytochrome c oxidase subunit 5A



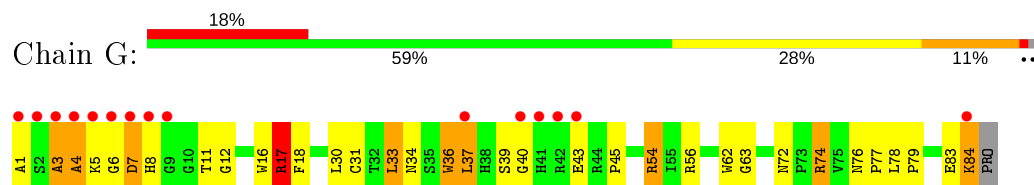
- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B

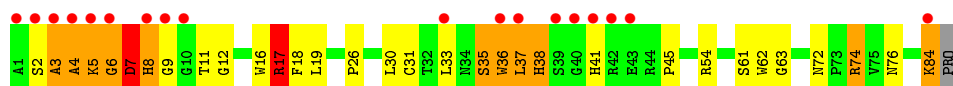


- Molecule 7: Cytochrome c oxidase subunit 6A2

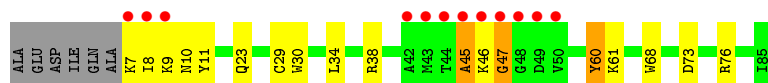
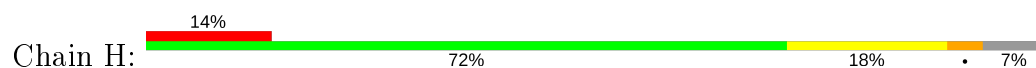


- Molecule 7: Cytochrome c oxidase subunit 6A2

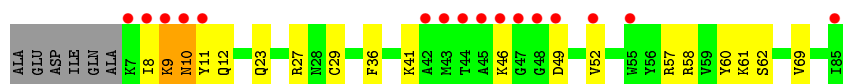




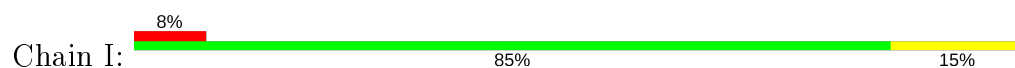
- Molecule 8: Cytochrome c oxidase subunit 6B1



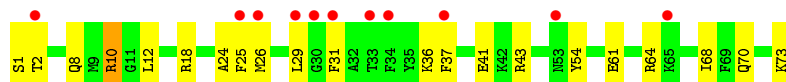
- Molecule 8: Cytochrome c oxidase subunit 6B1



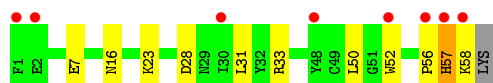
- Molecule 9: Cytochrome c oxidase subunit 6C



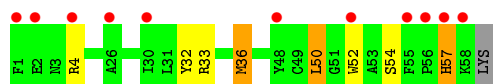
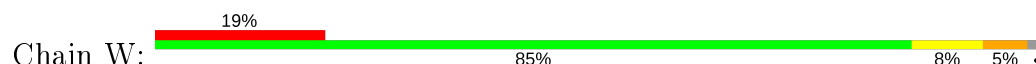
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 10: Cytochrome c oxidase polypeptide 7A1




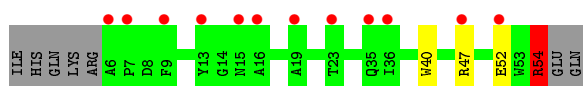
- Molecule 11: Cytochrome c oxidase subunit 7B

Chain K:  75% 11% 13%




- Molecule 11: Cytochrome c oxidase subunit 7B

Chain X:  21% 80% 5% 13%



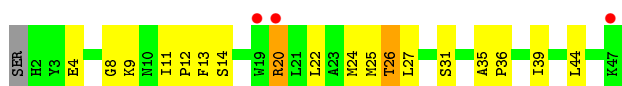
- Molecule 12: Cytochrome c oxidase subunit 7C

Chain L:  2% 72% 21% 5%



- Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:  6% 60% 34% 10%



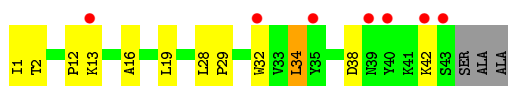
- Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:  7% 70% 13% 11% 7%



- Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:  15% 67% 24% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.36Å 206.65Å 178.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.05 52.61 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.05) 99.8 (52.61-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, $R_{free}$	0.186 , 0.219 0.204 , 0.235	Depositor DCC
$R_{free}$ test set	21002 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 63.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32324	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, PGV, TPO, UNX, CUA, NA, FME, CYN, 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	1.69	52/4156 (1.3%)	1.27	32/5678 (0.6%)
1	N	1.51	31/4156 (0.7%)	1.11	14/5678 (0.2%)
2	B	1.53	13/1860 (0.7%)	1.21	11/2534 (0.4%)
2	O	1.24	3/1860 (0.2%)	1.08	5/2534 (0.2%)
3	C	1.52	14/2197 (0.6%)	1.07	6/3005 (0.2%)
3	P	1.51	16/2197 (0.7%)	1.05	3/3005 (0.1%)
4	D	1.55	12/1229 (1.0%)	1.22	7/1658 (0.4%)
4	Q	1.12	2/1229 (0.2%)	0.95	3/1658 (0.2%)
5	E	1.45	1/871 (0.1%)	1.04	2/1182 (0.2%)
5	R	1.20	2/871 (0.2%)	0.96	1/1182 (0.1%)
6	F	1.46	4/765 (0.5%)	1.17	2/1038 (0.2%)
6	S	1.28	1/765 (0.1%)	1.16	4/1038 (0.4%)
7	G	1.35	1/690 (0.1%)	1.10	5/937 (0.5%)
7	T	1.36	3/690 (0.4%)	1.23	5/937 (0.5%)
8	H	1.35	1/682 (0.1%)	1.12	5/921 (0.5%)
8	U	1.13	1/682 (0.1%)	0.95	0/921
9	I	1.34	3/605 (0.5%)	1.03	0/802
9	V	1.18	0/605	0.95	1/802 (0.1%)
10	J	1.25	0/471	1.04	1/636 (0.2%)
10	W	1.16	0/471	1.00	0/636
11	K	1.44	3/398 (0.8%)	1.08	1/546 (0.2%)
11	X	1.18	2/398 (0.5%)	0.96	2/546 (0.4%)
12	L	1.64	4/393 (1.0%)	1.11	2/526 (0.4%)
12	Y	1.42	0/393	1.04	0/526
13	M	1.49	1/345 (0.3%)	1.18	1/470 (0.2%)
13	Z	1.22	0/345	0.97	1/470 (0.2%)
All	All	1.45	170/29324 (0.6%)	1.12	114/39866 (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
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
12	L	0	1
All	All	0	5

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	181	TYR	CD1-CE1	9.79	1.54	1.39
1	A	438	ARG	CB-CG	-9.36	1.27	1.52
1	A	388	ALA	CA-CB	8.80	1.71	1.52
3	P	29	SER	CB-OG	-8.78	1.30	1.42
1	N	139	ALA	CA-CB	8.50	1.70	1.52
1	A	81	TRP	CE3-CZ3	8.43	1.52	1.38
7	T	36	TRP	CB-CG	8.38	1.65	1.50
1	N	270	TYR	CD2-CE2	8.23	1.51	1.39
1	A	288	TRP	CE3-CZ3	8.19	1.52	1.38
4	D	100	LYS	CE-NZ	7.99	1.69	1.49
1	N	74	MET	CB-CG	7.90	1.76	1.51
1	A	469	VAL	CB-CG2	7.73	1.69	1.52
1	A	68	PHE	CD2-CE2	7.69	1.54	1.39
2	O	198	GLU	C-O	7.62	1.37	1.23
4	D	11	TYR	CB-CG	7.41	1.62	1.51
1	A	470	PHE	CE2-CZ	7.40	1.51	1.37
3	P	180	GLU	CD-OE1	7.21	1.33	1.25
2	B	198	GLU	C-O	7.18	1.37	1.23
4	D	104	TYR	CD2-CE2	6.99	1.49	1.39
1	A	74	MET	CB-CG	6.90	1.73	1.51
3	C	57	TRP	CB-CG	6.88	1.62	1.50
1	A	244	TYR	CD2-CE2	6.81	1.49	1.39
1	N	414	PHE	CE1-CZ	6.80	1.50	1.37
1	A	261	TYR	CE2-CZ	6.78	1.47	1.38
7	G	36	TRP	CB-CG	6.71	1.62	1.50
11	K	29	TRP	CB-CG	6.69	1.62	1.50
4	D	100	LYS	CD-CE	6.65	1.67	1.51
1	A	238	PHE	CE2-CZ	6.64	1.50	1.37
12	L	16	GLU	CG-CD	6.57	1.61	1.51
11	K	20	SER	CB-OG	-6.53	1.33	1.42
1	N	63	PHE	CG-CD1	6.50	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	253	TYR	CD2-CE2	6.48	1.49	1.39
9	I	47	TYR	CE2-CZ	6.46	1.47	1.38
12	L	4	GLU	CG-CD	6.46	1.61	1.51
3	P	74	ALA	CA-CB	6.37	1.65	1.52
1	A	371	TYR	CD1-CE1	6.33	1.48	1.39
1	A	193	VAL	CB-CG2	6.29	1.66	1.52
1	A	352	GLY	N-CA	6.28	1.55	1.46
1	N	299	VAL	CB-CG1	6.22	1.66	1.52
1	N	372	TYR	CD1-CE1	6.21	1.48	1.39
1	A	236	TRP	CB-CG	6.14	1.61	1.50
1	A	244	TYR	CE1-CZ	6.14	1.46	1.38
2	B	18	GLU	CG-CD	6.14	1.61	1.51
3	C	29	SER	CB-OG	-6.13	1.34	1.42
4	D	127	LYS	CB-CG	6.11	1.69	1.52
1	N	288	TRP	CB-CG	6.09	1.61	1.50
3	C	193	TYR	CD1-CE1	6.08	1.48	1.39
1	A	261	TYR	CZ-OH	6.06	1.48	1.37
7	T	5	LYS	CB-CG	6.04	1.68	1.52
3	P	227	PHE	CE2-CZ	6.03	1.48	1.37
12	L	16	GLU	CB-CG	6.02	1.63	1.52
1	N	195	LEU	C-O	6.01	1.34	1.23
1	A	458	SER	CB-OG	6.01	1.50	1.42
1	N	397	PHE	CE2-CZ	6.00	1.48	1.37
1	A	129	TYR	CD2-CE2	5.98	1.48	1.39
2	B	132	GLU	CD-OE1	-5.97	1.19	1.25
9	I	54	TYR	CD2-CE2	5.96	1.48	1.39
1	N	473	TRP	CB-CG	5.96	1.60	1.50
3	C	240	TRP	CG-CD1	5.94	1.45	1.36
1	A	112	LEU	CG-CD1	5.92	1.73	1.51
1	A	244	TYR	CD1-CE1	5.91	1.48	1.39
5	E	84	TYR	CE2-CZ	5.90	1.46	1.38
5	R	70	VAL	CB-CG2	5.90	1.65	1.52
3	C	58	TRP	CB-CG	5.89	1.60	1.50
1	N	164	PHE	CD1-CE1	5.88	1.51	1.39
3	C	75	VAL	CB-CG2	5.88	1.65	1.52
1	N	447	TYR	CD1-CE1	5.85	1.48	1.39
1	N	476	PHE	CD1-CE1	5.84	1.50	1.39
2	B	115	ASP	CB-CG	5.82	1.64	1.51
3	P	257	TYR	CD1-CE1	5.82	1.48	1.39
1	A	304	TYR	CD1-CE1	5.79	1.48	1.39
2	B	159	VAL	CB-CG2	5.78	1.65	1.52
6	F	58	VAL	CB-CG2	5.77	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	TYR	CD1-CE1	5.77	1.48	1.39
2	O	198	GLU	CG-CD	5.77	1.60	1.51
3	C	198	PHE	CE2-CZ	5.75	1.48	1.37
1	A	113	LEU	CG-CD1	5.74	1.73	1.51
1	N	89	ALA	C-O	5.74	1.34	1.23
3	C	142	VAL	CB-CG1	5.74	1.65	1.52
1	A	457	GLY	N-CA	5.74	1.54	1.46
4	D	134	PHE	CG-CD2	5.73	1.47	1.38
6	S	54	ASN	CB-CG	-5.71	1.38	1.51
1	N	320	VAL	CB-CG2	5.69	1.64	1.52
1	A	113	LEU	CB-CG	5.69	1.69	1.52
1	N	473	TRP	CE3-CZ3	5.69	1.48	1.38
3	C	99	TRP	CE3-CZ3	5.68	1.48	1.38
3	P	35	PHE	CG-CD2	5.66	1.47	1.38
1	A	40	GLU	CB-CG	5.66	1.62	1.52
1	A	419	VAL	CB-CG1	5.64	1.64	1.52
3	P	153	GLU	CG-CD	5.63	1.60	1.51
2	B	121	TYR	CG-CD1	5.62	1.46	1.39
1	A	149	SER	CA-CB	5.62	1.61	1.52
8	U	69	VAL	CB-CG1	5.61	1.64	1.52
2	B	40	TYR	N-CA	-5.58	1.35	1.46
1	A	122	ALA	CA-CB	5.55	1.64	1.52
1	A	409	TRP	CB-CG	5.54	1.60	1.50
4	D	19	ARG	CZ-NH2	5.52	1.40	1.33
3	P	245	VAL	CB-CG2	5.52	1.64	1.52
3	C	80	ARG	CZ-NH1	5.50	1.40	1.33
2	B	121	TYR	CE2-CZ	5.50	1.45	1.38
2	B	104	TRP	CZ3-CH2	5.49	1.48	1.40
1	N	179	TYR	CB-CG	5.49	1.59	1.51
1	A	67	PHE	CE2-CZ	5.49	1.47	1.37
1	N	113	LEU	CG-CD1	5.48	1.72	1.51
11	K	39	GLU	CB-CG	5.45	1.62	1.52
1	N	297	MET	CG-SD	5.45	1.95	1.81
4	D	60	TYR	CE1-CZ	5.44	1.45	1.38
1	A	505	PHE	CE1-CZ	5.43	1.47	1.37
1	A	264	LYS	CG-CD	-5.41	1.34	1.52
4	D	117	ALA	CA-CB	5.39	1.63	1.52
1	A	313	ALA	CA-CB	5.39	1.63	1.52
1	A	293	PHE	CG-CD1	5.38	1.46	1.38
2	B	60	GLU	CB-CG	5.38	1.62	1.52
1	A	258	VAL	CB-CG2	5.37	1.64	1.52
3	C	89	SER	CB-OG	5.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	235	PHE	CD2-CE2	5.37	1.50	1.39
6	F	69	VAL	CB-CG1	5.36	1.64	1.52
4	Q	117	ALA	CA-CB	5.33	1.63	1.52
1	A	469	VAL	CB-CG1	5.33	1.64	1.52
9	I	54	TYR	CD1-CE1	5.33	1.47	1.39
1	N	447	TYR	CD2-CE2	5.31	1.47	1.39
1	A	260	TYR	CD1-CE1	5.30	1.47	1.39
1	A	419	VAL	CA-CB	5.27	1.65	1.54
1	N	70	VAL	CB-CG1	5.27	1.64	1.52
2	B	118	PHE	CE2-CZ	5.26	1.47	1.37
1	A	252	GLY	N-CA	5.26	1.53	1.46
3	P	218	CYS	CB-SG	5.25	1.91	1.82
8	H	68	TRP	CB-CG	5.25	1.59	1.50
1	A	382	SER	CB-OG	5.24	1.49	1.42
4	D	118	LYS	CD-CE	5.23	1.64	1.51
2	O	198	GLU	CD-OE1	-5.23	1.19	1.25
1	A	115	SER	CB-OG	-5.23	1.35	1.42
3	P	251	PHE	CE2-CZ	5.22	1.47	1.37
1	N	276	ALA	CA-CB	5.22	1.63	1.52
3	P	257	TYR	CE2-CZ	5.20	1.45	1.38
4	D	60	TYR	CD2-CE2	5.20	1.47	1.39
1	A	297	MET	CG-SD	5.19	1.94	1.81
3	C	58	TRP	CE3-CZ3	5.19	1.47	1.38
13	M	3	ALA	CA-CB	5.18	1.63	1.52
3	C	73	PRO	CB-CG	5.17	1.75	1.50
1	N	394	VAL	CB-CG2	-5.17	1.42	1.52
1	A	438	ARG	CG-CD	5.17	1.64	1.51
1	A	450	TRP	CB-CG	5.15	1.59	1.50
1	N	282	PHE	CB-CG	-5.14	1.42	1.51
3	P	102	TYR	CD1-CE1	5.14	1.47	1.39
1	A	299	VAL	CB-CG2	-5.13	1.42	1.52
4	D	115	TRP	CZ3-CH2	5.13	1.48	1.40
3	P	197	PHE	CE1-CZ	5.13	1.47	1.37
1	N	391	GLY	N-CA	5.13	1.53	1.46
2	B	108	TYR	CE2-CZ	5.12	1.45	1.38
1	N	148	PHE	CD1-CE1	5.12	1.49	1.39
6	F	73	TRP	CE3-CZ3	5.12	1.47	1.38
4	Q	81	VAL	CB-CG1	5.10	1.63	1.52
1	N	285	PHE	CD2-CE2	5.10	1.49	1.39
1	A	67	PHE	CD2-CE2	5.07	1.49	1.39
5	R	70	VAL	CB-CG1	-5.06	1.42	1.52
6	F	1	ALA	C-O	5.06	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	TRP	CE2-CZ2	5.05	1.48	1.39
3	P	67	PHE	CE1-CZ	5.05	1.47	1.37
1	A	226	GLY	N-CA	5.05	1.53	1.46
3	C	69	GLY	CA-C	5.04	1.59	1.51
1	A	38	ARG	CD-NE	5.04	1.55	1.46
1	N	67	PHE	CE2-CZ	5.03	1.47	1.37
1	A	40	GLU	CD-OE2	-5.03	1.20	1.25
12	L	21	LEU	CG-CD1	5.03	1.70	1.51
7	T	26	PRO	CG-CD	5.03	1.67	1.50
11	X	52	GLU	CG-CD	5.03	1.59	1.51
11	X	40	TRP	CG-CD1	5.02	1.43	1.36
1	A	387	PHE	CD2-CE2	5.01	1.49	1.39
1	N	443	TYR	CD1-CE1	5.01	1.46	1.39

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	-16.98	111.81	120.30
1	A	310	MET	CG-SD-CE	-14.80	76.53	100.20
1	A	278	MET	CG-SD-CE	-14.00	77.80	100.20
1	N	278	MET	CG-SD-CE	-12.95	79.47	100.20
4	D	20	ARG	NE-CZ-NH1	12.84	126.72	120.30
7	T	17	ARG	NE-CZ-NH1	10.76	125.68	120.30
7	T	17	ARG	NE-CZ-NH2	-10.38	115.11	120.30
3	C	80	ARG	NE-CZ-NH2	-10.14	115.23	120.30
6	F	18	ARG	NE-CZ-NH2	-9.52	115.54	120.30
4	Q	20	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	A	297	MET	CG-SD-CE	-8.89	85.98	100.20
6	F	18	ARG	NE-CZ-NH1	8.66	124.63	120.30
13	M	34	LEU	CB-CG-CD1	8.47	125.39	111.00
1	A	227	ASP	CB-CG-OD2	8.34	125.81	118.30
2	O	11	ASP	CB-CG-OD2	8.34	125.81	118.30
3	C	80	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	96	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	189	MET	CG-SD-CE	-8.12	87.22	100.20
4	Q	20	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	449	MET	CA-CB-CG	-7.50	100.54	113.30
11	K	54	ARG	NE-CZ-NH1	-7.49	116.55	120.30
1	A	194	LEU	CB-CG-CD2	7.43	123.63	111.00
8	H	38	ARG	NE-CZ-NH1	-7.37	116.61	120.30
7	T	33	LEU	CA-CB-CG	7.25	131.98	115.30
1	A	380	VAL	CG1-CB-CG2	7.13	122.30	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	54	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	438	ARG	CB-CA-C	-6.98	96.44	110.40
1	A	380	VAL	CB-CA-C	-6.90	98.28	111.40
6	S	56	ARG	NE-CZ-NH1	-6.82	116.89	120.30
11	X	54	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	N	113	LEU	CB-CG-CD1	6.70	122.38	111.00
1	A	383	MET	CB-CA-C	-6.67	97.06	110.40
1	A	113	LEU	CB-CG-CD2	6.65	122.31	111.00
5	E	40	ASP	CB-CG-OD2	6.54	124.19	118.30
1	N	383	MET	CA-CB-CG	6.50	124.35	113.30
2	B	29	MET	CG-SD-CE	6.47	110.55	100.20
1	A	213	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	P	80	ARG	CG-CD-NE	-6.37	98.43	111.80
3	P	80	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	136	LEU	CA-CB-CG	6.25	129.69	115.30
8	H	38	ARG	NE-CZ-NH2	6.25	123.43	120.30
3	P	163	LEU	CB-CG-CD1	6.25	121.63	111.00
1	A	298	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	278	MET	CA-CB-CG	-6.22	102.73	113.30
2	B	42	ILE	CG1-CB-CG2	-6.16	97.85	111.40
1	A	512	ASN	CB-CA-C	-6.15	98.10	110.40
1	A	213	ARG	NE-CZ-NH1	6.12	123.36	120.30
3	C	31	LEU	CB-CG-CD2	-6.10	100.63	111.00
1	N	240	HIS	N-CA-CB	6.10	121.58	110.60
3	C	44	MET	CG-SD-CE	6.05	109.89	100.20
4	Q	10	ASP	CB-CG-OD1	6.01	123.71	118.30
6	S	94	HIS	N-CA-C	6.01	127.22	111.00
2	B	158	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	74	MET	CB-CG-SD	-5.97	94.50	112.40
3	C	33	MET	CG-SD-CE	5.96	109.74	100.20
6	S	54	ASN	CB-CA-C	-5.94	98.52	110.40
1	A	380	VAL	CA-CB-CG2	5.93	119.80	110.90
1	N	298	ASP	CB-CG-OD2	5.92	123.63	118.30
1	N	438	ARG	NE-CZ-NH1	5.90	123.25	120.30
5	E	90	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	96	ARG	NE-CZ-NH1	5.89	123.24	120.30
7	G	33	LEU	CA-CB-CG	5.89	128.84	115.30
1	A	417	MET	CG-SD-CE	-5.88	90.78	100.20
2	O	202	SER	CB-CA-C	-5.85	98.99	110.10
2	B	178	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	208	MET	CG-SD-CE	5.76	109.42	100.20
5	R	90	ARG	NE-CZ-NH2	-5.75	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	LEU	CA-CB-CG	-5.74	102.10	115.30
8	H	34	LEU	CB-CG-CD1	-5.74	101.25	111.00
2	B	11	ASP	CB-CG-OD2	5.69	123.42	118.30
8	H	61	LYS	CB-CG-CD	-5.68	96.84	111.60
2	O	46	LEU	CB-CG-CD1	-5.68	101.35	111.00
1	A	439	ARG	NE-CZ-NH1	-5.64	117.48	120.30
11	X	54	ARG	NE-CZ-NH1	-5.61	117.50	120.30
2	B	178	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	438	ARG	CA-CB-CG	5.59	125.70	113.40
12	L	41	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	369	ASP	CB-CG-OD2	5.55	123.30	118.30
2	O	158	ASP	CB-CG-OD1	5.54	123.29	118.30
4	D	31	LYS	CD-CE-NZ	-5.54	98.96	111.70
1	N	380	VAL	CB-CA-C	-5.53	100.89	111.40
7	T	19	LEU	CB-CG-CD2	-5.50	101.66	111.00
3	C	236	GLU	CA-CB-CG	-5.49	101.33	113.40
2	B	173	ASP	CB-CG-OD1	5.48	123.23	118.30
1	N	302	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	50	ASP	CB-CG-OD2	5.47	123.22	118.30
2	B	5	MET	CG-SD-CE	-5.44	91.49	100.20
8	H	73	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	N	5	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	B	136	LEU	CB-CG-CD1	-5.39	101.84	111.00
7	T	7	ASP	N-CA-C	5.38	125.52	111.00
1	N	383	MET	CB-CA-C	-5.36	99.68	110.40
6	S	53	THR	C-N-CA	5.34	135.04	121.70
1	A	194	LEU	CB-CG-CD1	5.33	120.07	111.00
2	B	102	HIS	CB-CA-C	-5.32	99.76	110.40
7	G	17	ARG	CB-CG-CD	-5.32	97.78	111.60
1	N	194	LEU	CB-CG-CD2	5.31	120.02	111.00
12	L	20	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	100	MET	CG-SD-CE	5.29	108.66	100.20
1	N	213	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	N	74	MET	CB-CG-SD	-5.24	96.69	112.40
1	N	189	MET	CA-CB-CG	-5.21	104.45	113.30
7	G	54	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	113	LEU	CB-CG-CD1	5.19	119.83	111.00
4	D	21	ASP	CB-CG-OD2	5.18	122.97	118.30
10	J	28	ASP	CB-CG-OD1	5.17	122.95	118.30
4	D	19	ARG	NE-CZ-NH1	-5.17	117.72	120.30
2	O	134	ARG	NE-CZ-NH2	-5.15	117.72	120.30
9	V	10	ARG	NE-CZ-NH2	-5.14	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	ARG	NE-CZ-NH2	-5.14	117.73	120.30
4	D	51	LEU	CA-CB-CG	5.05	126.91	115.30
4	D	20	ARG	CG-CD-NE	-5.04	101.21	111.80
7	G	56	ARG	NE-CZ-NH2	-5.04	117.78	120.30
13	Z	34	LEU	CB-CG-CD1	5.04	119.56	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
12	L	2	HIS	Peptide
6	S	93	PRO	Peptide
10	W	57	HIS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	74	0
1	N	4027	0	4001	84	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	58	0
3	C	2110	0	2027	36	0
3	P	2110	0	2027	46	0
4	D	1195	0	1183	17	0
4	Q	1195	0	1183	21	0
5	E	852	0	845	5	0
5	R	852	0	845	11	0
6	F	748	0	728	16	0
6	S	748	0	728	25	0
7	G	675	0	643	37	0
7	T	675	0	643	49	0
8	H	662	0	623	6	0
8	U	662	0	623	11	0
9	I	601	0	613	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	601	0	613	17	0
10	J	460	0	459	7	0
10	W	460	0	459	9	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	11	0
12	Y	380	0	380	15	0
13	M	335	0	352	9	0
13	Z	335	0	352	8	0
14	A	120	0	108	13	0
14	N	120	0	108	13	0
15	A	2	0	0	0	0
15	N	2	0	0	2	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	63	0	110	7	0
19	D	63	0	110	13	0
19	L	63	0	110	15	0
19	N	126	0	220	22	0
19	Q	63	0	110	10	0
20	A	102	0	152	10	0
20	C	102	0	152	6	0
20	N	102	0	152	7	0
20	P	102	0	152	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	3	0
22	C	58	0	70	4	0
22	J	29	0	36	2	0
22	O	29	0	36	1	0
22	P	58	0	73	5	0
22	W	29	0	35	6	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	3	0
24	G	106	0	154	24	0
24	S	53	0	77	16	0
24	T	106	0	154	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	100	0	156	21	0
25	G	100	0	156	28	0
25	P	100	0	156	19	0
25	T	100	0	156	34	0
26	E	52	0	80	16	0
26	R	52	0	80	14	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	3	0
28	M	33	0	38	1	0
28	P	33	0	38	5	0
28	Z	33	0	39	2	0
29	A	225	0	0	8	0
29	B	125	0	0	4	0
29	C	106	0	0	2	0
29	D	91	0	0	1	0
29	E	62	0	0	0	0
29	F	75	0	0	2	0
29	G	41	0	0	3	0
29	H	47	0	0	2	0
29	I	38	0	0	1	0
29	J	20	0	0	1	0
29	K	20	0	0	1	0
29	L	22	0	0	1	0
29	M	15	0	0	1	0
29	N	199	0	0	4	0
29	O	107	0	0	4	0
29	P	100	0	0	3	0
29	Q	55	0	0	2	0
29	R	40	0	0	1	0
29	S	56	0	0	5	0
29	T	36	0	0	4	0
29	U	41	0	0	4	0
29	V	18	0	0	1	0
29	W	12	0	0	0	0
29	X	14	0	0	0	0
29	Y	12	0	0	1	0
29	Z	11	0	0	0	0
All	All	32324	0	31275	705	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (705) 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)
1:N:74:MET:CB	1:N:74:MET:CG	1.76	1.56
1:A:312:ILE:CG1	1:A:312:ILE:CD1	1.78	1.54
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.69	1.51
3:C:73:PRO:CB	3:C:73:PRO:CG	1.75	1.48
14:A:516:HEA:O11	14:A:516:HEA:C11	1.64	1.45
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.58	1.17
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.07	1.16
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.11	1.15
10:W:33:ARG:HG2	22:W:1059:CHD:H152	1.24	1.14
25:G:269:CDL:H241	25:G:269:CDL:H541	1.29	1.13
26:E:229:PSC:H072	9:I:10:ARG:HH21	1.13	1.09
6:S:52:ILE:O	6:S:94:HIS:CE1	2.07	1.08
2:B:41:ILE:HD13	26:E:229:PSC:H342	1.36	1.07
7:T:5:LYS:HD2	24:T:263:PEK:H383	1.37	1.07
6:F:1:ALA:HB2	29:G:4415:HOH:O	1.54	1.06
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.19	1.06
26:E:229:PSC:C07	9:I:10:ARG:HH21	1.67	1.06
7:T:84:LYS:H	7:T:84:LYS:HD2	0.94	1.05
6:S:94:HIS:CD2	6:S:95:GLN:H	1.75	1.05
24:S:1265:PEK:C38	25:T:1269:CDL:H272	1.86	1.04
25:T:1269:CDL:C11	25:T:1269:CDL:HA21	1.87	1.04
6:F:85:CYS:SG	6:F:87:THR:HG23	1.97	1.03
25:G:269:CDL:C24	25:G:269:CDL:H541	1.89	1.02
25:G:269:CDL:C11	25:G:269:CDL:HA21	1.92	0.99
12:L:20:ARG:HH22	19:L:522:TGL:HC32	0.84	0.98
7:T:84:LYS:H	7:T:84:LYS:CD	1.76	0.98
6:F:1:ALA:N	24:G:265:PEK:H041	1.77	0.98
25:G:269:CDL:HA21	25:G:269:CDL:H112	1.45	0.97
7:T:5:LYS:CD	24:T:263:PEK:H383	1.94	0.96
7:T:84:LYS:N	7:T:84:LYS:HD2	1.79	0.96
20:C:267:PGV:H181	29:C:4710:HOH:O	1.62	0.96
20:N:1524:PGV:H011	20:N:1524:PGV:H22	1.46	0.96
19:L:522:TGL:H231	19:L:522:TGL:HA92	1.49	0.95
7:G:84:LYS:HD2	7:G:84:LYS:H	1.30	0.95
25:T:1269:CDL:H111	25:T:1269:CDL:HA21	1.49	0.95
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	1.82	0.94
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.32	0.93
7:G:5:LYS:HB3	1:N:278:MET:SD	2.07	0.93
14:N:516:HEA:HMD1	14:N:516:HEA:HBD2	1.47	0.93
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:CG	24:T:263:PEK:H383	2.01	0.91
7:T:31:CYS:SG	25:T:1269:CDL:H532	2.10	0.91
24:C:264:PEK:H32	24:C:264:PEK:H71	1.54	0.89
1:N:400:PHE:HB3	19:N:1522:TGL:H283	1.55	0.88
1:A:311:ILE:HD12	25:T:1269:CDL:H212	1.56	0.88
7:G:72:ASN:H	7:G:76:ASN:HD22	1.13	0.88
24:S:1265:PEK:H383	25:T:1269:CDL:H272	1.56	0.87
25:T:1269:CDL:H112	25:T:1269:CDL:HA21	1.53	0.87
1:N:74:MET:CB	1:N:74:MET:SD	2.62	0.87
7:G:84:LYS:H	7:G:84:LYS:CD	1.88	0.86
12:L:20:ARG:HH22	19:L:522:TGL:CC3	1.81	0.86
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.40	0.85
4:D:34:SER:H	4:D:37:GLN:HE21	1.25	0.85
3:P:157:LYS:NZ	24:S:1265:PEK:H051	1.91	0.85
25:G:269:CDL:H601	25:G:269:CDL:H751	1.59	0.84
9:V:1:SAC:OAC	9:V:1:SAC:HB3	1.77	0.84
6:S:94:HIS:HD2	6:S:95:GLN:H	1.22	0.84
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.43	0.84
7:G:5:LYS:HG3	24:G:1263:PEK:H383	1.59	0.84
28:P:1272:DMU:O1	28:P:1272:DMU:H30	1.78	0.83
1:N:347:LEU:HD13	1:N:383:MET:SD	2.18	0.83
2:O:227:LEU:CB	29:O:4762:HOH:O	2.27	0.82
6:S:75:HIS:H	6:S:80:GLN:HE22	1.27	0.82
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.61	0.82
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.62	0.81
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.43	0.81
2:O:227:LEU:HB3	29:O:4762:HOH:O	1.78	0.81
14:A:516:HEA:HMD1	14:A:516:HEA:HBD2	1.62	0.81
8:U:9:LYS:O	8:U:10:ASN:HB2	1.79	0.81
3:C:80:ARG:NH1	24:T:263:PEK:H032	1.97	0.80
7:T:76:ASN:HD21	24:T:1264:PEK:HN2	1.26	0.80
6:F:1:ALA:H2	24:G:265:PEK:H041	1.44	0.80
24:S:1265:PEK:H381	25:T:1269:CDL:H272	1.62	0.80
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.22	0.80
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.64	0.79
7:T:37:LEU:HD23	25:T:1269:CDL:H352	1.63	0.79
6:F:1:ALA:H1	24:G:265:PEK:H041	1.47	0.79
25:G:269:CDL:C54	25:G:269:CDL:H241	2.12	0.79
8:H:23:GLN:HG3	29:H:4165:HOH:O	1.83	0.79
24:T:1264:PEK:H31	24:T:1264:PEK:H71	1.65	0.79
26:E:229:PSC:C07	9:I:10:ARG:NH2	2.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:PHE:CE1	25:C:270:CDL:H1	2.12	0.79
3:C:63:ARG:HE	25:C:270:CDL:CA2	1.97	0.77
7:G:84:LYS:N	7:G:84:LYS:HD2	2.00	0.77
6:S:52:ILE:O	6:S:94:HIS:HE1	1.65	0.77
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.20	0.76
28:P:1272:DMU:H34	7:T:63:GLY:H	1.49	0.76
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.49	0.76
1:A:312:ILE:CG2	1:A:312:ILE:CD1	2.64	0.76
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.67	0.76
7:T:5:LYS:HG3	24:T:263:PEK:H383	1.69	0.75
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.75
7:T:72:ASN:H	7:T:76:ASN:HD22	1.35	0.74
6:S:1:ALA:H1	24:S:1265:PEK:C04	2.00	0.74
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.23	0.74
7:G:72:ASN:H	7:G:76:ASN:ND2	1.84	0.74
6:S:85:CYS:SG	6:S:87:THR:HG23	2.28	0.74
1:A:484:THR:HB	13:M:2:THR:OG1	1.88	0.74
20:A:524:PGV:H311	13:M:19:LEU:HD23	1.69	0.73
24:S:1265:PEK:H381	25:T:1269:CDL:C27	2.18	0.73
3:C:80:ARG:HH11	24:T:263:PEK:H032	1.52	0.73
11:K:52:GLU:HG3	29:K:4738:HOH:O	1.87	0.73
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.71	0.73
7:T:5:LYS:HB2	24:T:263:PEK:H362	1.71	0.73
10:W:36:MET:HB3	22:W:1059:CHD:C18	2.19	0.73
2:B:41:ILE:HD13	26:E:229:PSC:C34	2.17	0.72
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG12	1.70	0.72
12:L:20:ARG:NH2	19:L:522:TGL:CC3	2.47	0.72
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.70	0.72
1:N:381:LEU:HB2	14:N:516:HEA:CAC	2.20	0.72
3:P:63:ARG:HE	25:P:1270:CDL:CA2	2.02	0.72
26:E:229:PSC:O01	26:E:229:PSC:H212	1.88	0.72
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.72	0.72
24:G:265:PEK:H383	25:G:269:CDL:H272	1.72	0.72
19:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.70	0.72
1:A:347:LEU:HD13	1:A:383:MET:HB3	1.72	0.71
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.20	0.71
4:D:78:TRP:CA	19:D:523:TGL:HB22	2.20	0.71
10:J:52:TRP:O	10:J:57:HIS:HE1	1.72	0.71
7:T:5:LYS:HD2	24:T:263:PEK:C38	2.15	0.71
11:X:54:ARG:NH2	11:X:54:ARG:HG3	1.84	0.71
1:A:278:MET:SD	7:T:5:LYS:HB3	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.72	0.71
6:S:1:ALA:N	24:S:1265:PEK:C04	2.53	0.71
20:C:268:PGV:H31	29:C:4316:HOH:O	1.91	0.71
24:C:264:PEK:HN2	7:G:76:ASN:HD21	1.36	0.71
26:E:229:PSC:H32	26:E:229:PSC:H011	1.72	0.71
7:T:31:CYS:SG	25:T:1269:CDL:C55	2.79	0.71
25:T:1269:CDL:H522	25:T:1269:CDL:H222	1.73	0.70
6:F:1:ALA:N	24:G:265:PEK:C04	2.55	0.70
1:N:317:GLY:HA3	14:N:516:HEA:H202	1.72	0.70
1:A:324:LEU:HD22	2:B:42:ILE:HG13	1.74	0.69
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	1.92	0.69
1:A:312:ILE:CD1	1:A:312:ILE:CB	2.69	0.69
14:N:516:HEA:NB	15:N:520:CYN:C	2.55	0.69
24:G:265:PEK:C38	25:G:269:CDL:H272	2.23	0.69
4:Q:78:TRP:HA	19:Q:1523:TGL:HB22	1.75	0.69
25:G:269:CDL:H181	25:G:269:CDL:H511	1.75	0.69
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.75	0.69
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.56	0.68
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.27	0.68
7:G:5:LYS:HB2	24:G:1263:PEK:H362	1.76	0.68
6:S:1:ALA:N	24:S:1265:PEK:H041	2.09	0.68
25:T:1269:CDL:H541	25:T:1269:CDL:H241	1.76	0.68
26:E:229:PSC:H072	9:I:10:ARG:NH2	1.99	0.68
3:P:157:LYS:HZ1	24:S:1265:PEK:H051	1.59	0.68
2:O:67:ILE:HD11	29:O:4812:HOH:O	1.92	0.67
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.93	0.67
3:P:52:LEU:HD21	25:P:1270:CDL:H412	1.77	0.67
25:G:269:CDL:H201	1:N:311:ILE:HD12	1.77	0.66
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.77	0.66
8:H:45:ALA:O	8:H:47:GLY:N	2.28	0.66
7:T:5:LYS:HB2	24:T:263:PEK:C36	2.24	0.66
3:P:246:ASP:HB2	29:P:4260:HOH:O	1.95	0.66
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.76	0.66
1:N:151:HIS:CD2	24:T:1264:PEK:H382	2.30	0.66
1:N:113:LEU:CD1	19:N:1522:TGL:H292	2.25	0.66
11:X:54:ARG:HH21	11:X:54:ARG:CG	1.96	0.66
8:U:49:ASP:O	8:U:52:VAL:HG22	1.95	0.66
3:P:157:LYS:HZ2	24:S:1265:PEK:H051	1.57	0.66
3:P:224:LYS:HD3	25:P:1270:CDL:HB31	1.76	0.66
4:Q:52:SER:OG	4:Q:55:GLU:HG3	1.96	0.65
25:C:270:CDL:H661	25:C:270:CDL:H242	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:227:LEU:HB2	29:O:4762:HOH:O	1.94	0.65
25:C:270:CDL:H661	25:C:270:CDL:C24	2.26	0.65
25:T:1269:CDL:H562	25:T:1269:CDL:H762	1.77	0.65
1:N:113:LEU:HD12	19:N:1522:TGL:H292	1.79	0.64
26:E:229:PSC:H241	26:E:229:PSC:H62	1.79	0.64
7:T:38:HIS:HD1	7:T:38:HIS:N	1.95	0.64
7:T:3:ALA:HB3	24:T:263:PEK:H382	1.78	0.64
24:S:1265:PEK:C38	25:T:1269:CDL:C27	2.69	0.64
19:A:521:TGL:H281	19:A:521:TGL:H102	1.80	0.64
10:W:33:ARG:CG	22:W:1059:CHD:H152	2.14	0.64
7:G:3:ALA:HB1	24:G:1263:PEK:H382	1.80	0.64
6:S:64:GLU:O	6:S:65:ASP:HB2	1.96	0.64
2:O:42:ILE:HG22	19:Q:1523:TGL:H251	1.80	0.64
6:S:1:ALA:H2	24:S:1265:PEK:H041	1.62	0.64
20:N:1524:PGV:H22	20:N:1524:PGV:C01	2.24	0.63
6:S:94:HIS:CD2	6:S:95:GLN:N	2.59	0.63
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.81	0.63
2:B:81:LEU:HD12	25:T:1269:CDL:H362	1.81	0.63
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.64	0.63
1:N:514:LYS:HE2	29:S:3514:HOH:O	1.99	0.63
7:G:5:LYS:CG	24:G:1263:PEK:H383	2.27	0.63
9:I:31:PHE:CD1	9:I:31:PHE:C	2.72	0.63
2:O:141:ARG:H	9:V:70:GLN:HE22	1.47	0.63
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.80	0.63
3:P:55:TYR:CE1	25:P:1270:CDL:H521	2.34	0.63
2:B:83:ILE:O	2:B:87:MET:HG3	1.99	0.63
19:N:1522:TGL:HA22	12:Y:13:PHE:HB3	1.81	0.63
1:A:400:PHE:HB3	19:L:522:TGL:H283	1.81	0.62
25:G:269:CDL:HA21	25:G:269:CDL:H111	1.81	0.62
24:G:265:PEK:H381	25:G:269:CDL:C27	2.28	0.62
26:R:1229:PSC:C07	9:V:10:ARG:HH21	2.13	0.62
1:N:20:LEU:HB3	19:N:1522:TGL:H221	1.80	0.62
2:O:42:ILE:HG21	19:Q:1523:TGL:H232	1.82	0.62
4:D:78:TRP:HA	19:D:523:TGL:HB22	1.79	0.61
24:G:265:PEK:C38	25:G:269:CDL:C27	2.78	0.61
1:N:177:SER:H	1:N:180:GLN:NE2	1.99	0.61
1:N:53:ILE:HG12	29:N:3704:HOH:O	1.99	0.61
1:A:324:LEU:CD2	2:B:42:ILE:HG13	2.29	0.61
2:O:57:ASP:H	26:R:1229:PSC:H202	1.65	0.61
6:S:95:GLN:HB2	29:S:4526:HOH:O	2.01	0.61
7:T:8:HIS:ND1	24:T:263:PEK:H312	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ALA:HB2	1:A:356:ILE:HD11	1.81	0.61
6:F:1:ALA:H1	24:G:265:PEK:C04	2.13	0.61
2:O:41:ILE:HD13	26:R:1229:PSC:H342	1.81	0.61
22:P:1271:CHD:H151	29:P:4657:HOH:O	2.00	0.61
5:R:6:GLU:OE1	5:R:14:ARG:NH2	2.32	0.61
1:A:513:LEU:O	1:A:514:LYS:HB2	2.01	0.60
4:Q:130:PRO:HD2	4:Q:131:ILE:HD12	1.84	0.60
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.34	0.60
1:A:265:LYS:HE3	29:F:4709:HOH:O	2.01	0.60
14:A:516:HEA:HO1	14:A:516:HEA:C11	2.07	0.60
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.48	0.60
1:A:136:LEU:HB2	29:A:4376:HOH:O	2.02	0.60
10:W:36:MET:HG3	22:W:1059:CHD:H183	1.84	0.60
13:M:42:LYS:HA	13:M:42:LYS:CE	2.27	0.60
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.20	0.60
7:T:30:LEU:HD12	25:T:1269:CDL:H261	1.84	0.60
7:T:12:GLY:HA3	29:T:3372:HOH:O	2.02	0.60
1:N:87:ILE:O	1:N:173:PRO:HD3	2.02	0.59
1:N:74:MET:CA	1:N:74:MET:CG	2.75	0.59
7:T:3:ALA:CB	24:T:263:PEK:H382	2.33	0.59
1:A:312:ILE:CD1	1:A:312:ILE:HG23	2.31	0.59
7:T:37:LEU:CD2	25:T:1269:CDL:H352	2.31	0.59
20:A:524:PGV:H062	29:M:2126:HOH:O	2.02	0.59
24:G:265:PEK:H381	25:G:269:CDL:H273	1.84	0.59
3:P:226:HIS:CE1	25:P:1270:CDL:HB32	2.38	0.59
20:N:1524:PGV:H312	13:Z:16:ALA:HA	1.84	0.59
29:B:2562:HOH:O	19:D:523:TGL:HC72	2.02	0.59
1:A:378:HIS:HA	1:A:382:SER:HB2	1.85	0.58
26:E:229:PSC:H071	9:I:10:ARG:NH2	2.17	0.58
29:A:4410:HOH:O	4:D:100:LYS:HD3	2.01	0.58
1:N:381:LEU:HB2	14:N:516:HEA:HAC	1.83	0.58
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.42	0.58
20:A:522:PGV:H183	24:C:264:PEK:H332	1.85	0.58
1:N:53:ILE:HD12	12:Y:44:LEU:HD23	1.86	0.58
20:A:522:PGV:H343	29:A:4723:HOH:O	2.03	0.58
3:P:226:HIS:HE1	25:P:1270:CDL:HB32	1.69	0.58
6:F:90:LYS:HD2	29:F:4397:HOH:O	2.03	0.58
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.04	0.58
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.39	0.58
7:G:31:CYS:SG	25:G:269:CDL:H532	2.44	0.58
7:G:3:ALA:O	7:G:4:ALA:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:36:MET:HB3	22:W:1059:CHD:H183	1.86	0.58
7:G:7:ASP:HA	1:N:178:GLN:HG2	1.86	0.58
2:O:224:ALA:O	2:O:227:LEU:HG	2.03	0.57
12:L:12:PRO:HB2	19:L:522:TGL:HG2	1.85	0.57
26:R:1229:PSC:H212	26:R:1229:PSC:C02	2.34	0.57
2:B:86:MET:O	2:B:89:GLU:HB2	2.04	0.57
3:C:127:LEU:HG	25:G:269:CDL:OB3	2.04	0.57
1:A:335:SER:HB2	1:A:336:PRO:HD2	1.87	0.57
25:G:269:CDL:CA2	25:G:269:CDL:H112	2.28	0.57
19:A:521:TGL:H201	19:A:521:TGL:H241	1.86	0.57
4:Q:130:PRO:HA	4:Q:135:SER:HB2	1.86	0.57
6:S:94:HIS:HD2	6:S:95:GLN:N	1.98	0.57
10:J:7:GLU:HG3	29:J:4595:HOH:O	2.04	0.57
12:L:14:SER:H	19:L:522:TGL:HC31	1.69	0.56
8:U:61:LYS:HD3	29:U:4240:HOH:O	2.05	0.56
19:N:1522:TGL:HC31	12:Y:14:SER:H	1.71	0.56
20:A:524:PGV:H02	20:A:524:PGV:O14	2.04	0.56
19:N:1521:TGL:C28	19:N:1521:TGL:H111	2.36	0.56
3:P:40:MET:O	3:P:44:MET:HG2	2.05	0.56
2:O:116:LEU:HD12	2:O:117:SER:N	2.20	0.56
3:C:217:VAL:HG22	25:C:270:CDL:H732	1.86	0.56
25:G:269:CDL:H201	1:N:311:ILE:CD1	2.36	0.56
12:L:25:MET:HG2	19:L:522:TGL:HA62	1.87	0.56
7:G:45:PRO:HD2	29:G:2099:HOH:O	2.05	0.55
19:N:1522:TGL:H362	29:Y:4623:HOH:O	2.06	0.55
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.71	0.55
20:C:267:PGV:H182	25:C:270:CDL:H662	1.86	0.55
7:G:5:LYS:CD	24:G:1263:PEK:H383	2.36	0.55
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.88	0.55
7:G:37:LEU:HD21	25:G:269:CDL:H361	1.88	0.55
26:R:1229:PSC:H142	26:R:1229:PSC:H343	1.87	0.55
2:B:14:SER:HB3	2:B:168:LEU:CD2	2.35	0.55
4:Q:78:TRP:CA	19:Q:1523:TGL:HB22	2.37	0.55
1:A:311:ILE:CD1	25:T:1269:CDL:H212	2.35	0.55
10:J:56:PRO:HB2	10:J:58:LYS:HD3	1.89	0.55
19:N:1521:TGL:H102	19:N:1521:TGL:H281	1.89	0.55
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.88	0.55
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.89	0.54
7:G:30:LEU:CD2	25:G:269:CDL:H471	2.37	0.54
24:T:1264:PEK:H242	24:T:1264:PEK:H12	1.88	0.54
7:G:62:TRP:HB3	28:G:272:DMU:H29	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:1270:CDL:H781	25:P:1270:CDL:H231	1.89	0.54
3:C:91:VAL:HG13	24:T:263:PEK:H15	1.90	0.54
7:T:3:ALA:O	7:T:4:ALA:HB2	2.08	0.54
9:V:61:GLU:HG3	9:V:64:ARG:HH21	1.72	0.54
14:A:515:HEA:HMC1	14:A:515:HEA:HBC1	1.90	0.54
3:C:47:LEU:O	3:C:51:MET:HG2	2.07	0.54
8:U:36:PHE:CD1	8:U:57:ARG:HB2	2.43	0.54
1:A:312:ILE:HD12	1:A:312:ILE:CG2	2.39	0.53
2:B:217:LYS:HG2	29:B:4225:HOH:O	2.06	0.53
13:M:39:ASN:O	13:M:43:SER:HB2	2.07	0.53
1:N:362:SER:HA	2:O:87:MET:HE1	1.91	0.53
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.41	0.53
1:A:343:GLY:O	1:A:347:LEU:HG	2.08	0.53
7:G:30:LEU:HD23	25:G:269:CDL:H471	1.90	0.53
7:T:6:GLY:O	24:T:263:PEK:H311	2.08	0.53
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.90	0.53
1:A:347:LEU:HD22	1:A:383:MET:SD	2.48	0.53
1:N:76:GLY:O	1:N:80:ASN:HB2	2.08	0.53
26:R:1229:PSC:O01	26:R:1229:PSC:H212	2.09	0.53
1:A:483:LEU:HD21	13:M:4:LYS:HD3	1.91	0.53
2:O:164:ALA:O	2:O:194:GLY:HA3	2.08	0.53
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.90	0.53
19:D:523:TGL:H363	9:I:16:ARG:HH21	1.74	0.53
2:B:164:ALA:O	2:B:194:GLY:HA3	2.07	0.53
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.91	0.53
2:O:141:ARG:HG3	9:V:70:GLN:NE2	2.24	0.53
20:N:1524:PGV:H311	13:Z:19:LEU:HD23	1.90	0.53
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.45	0.52
14:N:516:HEA:HMD1	14:N:516:HEA:CBD	2.27	0.52
1:A:73:ILE:CD1	14:A:515:HEA:H22	2.39	0.52
13:Z:28:LEU:N	13:Z:29:PRO:CD	2.73	0.52
2:B:59:GLN:C	2:B:60:GLU:HG3	2.30	0.52
2:O:191:LEU:HG	9:V:68:ILE:HD12	1.91	0.52
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.09	0.52
4:D:78:TRP:HA	19:D:523:TGL:CB2	2.39	0.52
9:V:18:ARG:HG3	29:V:3588:HOH:O	2.09	0.52
1:N:317:GLY:CA	14:N:516:HEA:H202	2.39	0.52
24:T:1264:PEK:H42	24:T:1264:PEK:H222	1.90	0.52
12:Y:22:LEU:O	12:Y:26:THR:HB	2.09	0.52
4:D:34:SER:H	4:D:37:GLN:NE2	2.01	0.52
7:G:12:GLY:HA3	29:G:4330:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:33:LEU:O	4:Q:38:LYS:HE2	2.09	0.52
7:T:38:HIS:ND1	7:T:38:HIS:N	2.55	0.52
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.92	0.52
5:E:48:ILE:O	5:E:52:LEU:HG	2.10	0.52
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.90	0.51
1:N:151:HIS:HD2	24:T:1264:PEK:H382	1.72	0.51
1:A:304:TYR:HD1	25:T:1269:CDL:HB32	1.74	0.51
3:C:226:HIS:CE1	25:C:270:CDL:HB31	2.45	0.51
1:N:378:HIS:HA	1:N:382:SER:HB2	1.93	0.51
2:B:58:ALA:O	2:B:62:GLU:HG3	2.11	0.51
2:O:83:ILE:O	2:O:87:MET:HG3	2.10	0.51
7:G:4:ALA:CB	1:N:282:PHE:HA	2.39	0.51
25:C:270:CDL:H311	25:C:270:CDL:H151	1.93	0.51
25:T:1269:CDL:H171	29:T:4401:HOH:O	2.10	0.51
7:T:12:GLY:CA	29:T:3372:HOH:O	2.58	0.51
12:Y:35:ALA:O	12:Y:39:ILE:HG13	2.11	0.51
20:A:524:PGV:H212	29:A:4691:HOH:O	2.12	0.50
7:T:30:LEU:CD1	25:T:1269:CDL:H261	2.40	0.50
4:D:98:TRP:CE3	28:M:526:DMU:H12	2.46	0.50
7:T:37:LEU:HB3	7:T:38:HIS:HD1	1.75	0.50
20:N:1524:PGV:H252	13:Z:12:PRO:HG3	1.93	0.50
2:O:134:ARG:HB2	4:Q:110:THR:HG21	1.92	0.50
7:T:5:LYS:HG3	24:T:263:PEK:C38	2.39	0.50
1:N:406:ASN:ND2	20:N:1524:PGV:H032	2.26	0.50
20:P:1267:PGV:H172	25:P:1270:CDL:H662	1.94	0.50
7:G:5:LYS:HD2	24:G:1263:PEK:H383	1.94	0.50
3:P:59:ARG:HB2	25:P:1270:CDL:H512	1.93	0.50
1:A:309:THR:HG22	14:A:516:HEA:HMB2	1.93	0.50
3:C:213:THR:HG23	25:C:270:CDL:H771	1.94	0.50
10:J:33:ARG:HG2	22:J:60:CHD:H151	1.92	0.50
1:N:307:SER:O	1:N:311:ILE:HG13	2.12	0.50
1:A:25:TRP:CE3	19:L:522:TGL:HB91	2.47	0.49
1:N:417:MET:HE3	29:N:3166:HOH:O	2.12	0.49
2:O:89:GLU:O	2:O:91:ASN:ND2	2.46	0.49
2:B:19:GLU:HA	2:B:19:GLU:OE2	2.12	0.49
4:D:78:TRP:CA	19:D:523:TGL:CB2	2.89	0.49
3:P:168:THR:HG22	24:S:1265:PEK:H14	1.94	0.49
7:T:38:HIS:NE2	25:T:1269:CDL:H131	2.28	0.49
19:A:521:TGL:H281	19:A:521:TGL:C10	2.43	0.49
2:B:57:ASP:H	26:E:229:PSC:H201	1.78	0.49
28:P:1272:DMU:C10	28:P:1272:DMU:H30	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:40:TYR:CE2	9:V:24:ALA:HB2	2.48	0.49
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.43	0.49
1:A:347:LEU:HD13	1:A:383:MET:SD	2.52	0.49
10:J:52:TRP:O	10:J:57:HIS:CE1	2.61	0.49
3:P:107:ALA:HB2	20:P:1268:PGV:H031	1.94	0.49
7:T:2:SER:O	24:T:263:PEK:H331	2.12	0.49
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.44	0.49
7:G:63:GLY:H	28:G:272:DMU:H40	1.77	0.49
1:N:351:GLY:C	1:N:380:VAL:HG13	2.33	0.49
2:O:168:LEU:HD13	2:O:184:LEU:HG	1.95	0.49
2:B:66:THR:HG21	22:B:1085:CHD:H42	1.95	0.49
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.11	0.49
10:W:50:LEU:HD22	10:W:54:SER:HG	1.77	0.49
2:O:57:ASP:N	26:R:1229:PSC:H202	2.27	0.48
13:Z:32:TRP:N	28:Z:1526:DMU:H1	2.28	0.48
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.49	0.48
3:P:165:ILE:HG12	24:S:1265:PEK:H102	1.96	0.48
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.79	0.48
2:O:113:TYR:HD1	8:U:58:ARG:NH2	2.11	0.48
19:A:521:TGL:H122	19:A:521:TGL:H283	1.95	0.48
1:N:189:MET:O	1:N:189:MET:HG3	2.13	0.48
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.97	0.48
4:Q:101:HIS:CD2	4:Q:102:TYR:CD2	3.02	0.48
3:C:103:HIS:HA	20:C:268:PGV:H012	1.95	0.48
1:N:377:PHE:CD1	14:N:516:HEA:HAD1	2.49	0.48
5:R:63:SER:O	5:R:67:ILE:HG13	2.13	0.48
1:N:113:LEU:HD13	19:N:1522:TGL:H292	1.95	0.48
14:N:516:HEA:NA	15:N:520:CYN:C	2.76	0.48
7:T:72:ASN:H	7:T:76:ASN:ND2	2.07	0.48
22:O:229:CHD:H212	22:O:229:CHD:H12	1.95	0.48
3:C:52:LEU:HD23	25:C:270:CDL:H362	1.96	0.48
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.79	0.48
25:G:269:CDL:HB32	1:N:304:TYR:HD1	1.79	0.48
1:N:1:FME:HCN	1:N:4:ASN:H	1.79	0.48
12:Y:20:ARG:NH2	12:Y:24:MET:CG	2.66	0.48
6:S:87:THR:HG22	29:S:4655:HOH:O	2.14	0.47
1:N:353:LEU:HB3	2:O:31:VAL:HG13	1.96	0.47
3:P:129:VAL:N	3:P:130:PRO:CD	2.76	0.47
1:A:347:LEU:HD13	1:A:383:MET:CB	2.42	0.47
26:E:229:PSC:C02	26:E:229:PSC:H212	2.43	0.47
1:N:438:ARG:O	1:N:439:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:334:TRP:HB2	19:Q:1523:TGL:HG11	1.94	0.47
24:T:1264:PEK:H11	24:T:1264:PEK:C15	2.44	0.47
26:E:229:PSC:H21	29:I:4186:HOH:O	2.15	0.47
4:Q:109:HIS:HD2	29:Q:3122:HOH:O	1.97	0.47
19:Q:1523:TGL:HG12	19:Q:1523:TGL:CC2	2.43	0.47
4:Q:40:LEU:HD11	4:Q:55:GLU:HB3	1.95	0.47
1:N:53:ILE:CD1	12:Y:44:LEU:HD23	2.45	0.47
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.97	0.47
26:R:1229:PSC:H222	26:R:1229:PSC:H32	1.97	0.47
6:S:55:LYS:HA	6:S:74:LEU:O	2.13	0.47
7:T:30:LEU:HD12	25:T:1269:CDL:C26	2.45	0.47
12:Y:8:GLY:HA2	12:Y:11:ILE:HD11	1.95	0.47
1:A:328:HIS:CE1	9:I:17:LEU:HD22	2.49	0.47
2:B:57:ASP:H	26:E:229:PSC:C20	2.28	0.47
5:R:78:HIS:CD2	9:V:12:LEU:HD13	2.49	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.47
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.77	0.47
3:C:63:ARG:NE	25:C:270:CDL:HA22	2.21	0.47
25:G:269:CDL:H541	25:G:269:CDL:H242	1.87	0.47
7:G:3:ALA:O	7:G:4:ALA:CB	2.61	0.47
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.30	0.47
8:U:9:LYS:HB2	8:U:9:LYS:HE2	1.68	0.47
2:O:40:TYR:HE2	9:V:24:ALA:HB2	1.79	0.47
24:G:1263:PEK:H042	3:P:77:LYS:NZ	2.29	0.47
2:B:74:ILE:HG13	25:T:1269:CDL:H441	1.97	0.47
8:U:27:ARG:NH1	29:U:3431:HOH:O	2.46	0.47
19:N:1521:TGL:H281	19:N:1521:TGL:H111	1.96	0.47
19:L:522:TGL:H231	19:L:522:TGL:CA9	2.29	0.47
2:O:163:TRP:NE1	2:O:209:ILE:HG12	2.30	0.47
28:P:1272:DMU:H29	7:T:62:TRP:HB3	1.97	0.47
1:A:73:ILE:HD11	14:A:515:HEA:H22	1.97	0.46
25:C:270:CDL:H652	25:C:270:CDL:H621	1.33	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.96	0.46
11:X:54:ARG:NH2	11:X:54:ARG:CG	2.64	0.46
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.97	0.46
14:A:516:HEA:HMC1	14:A:516:HEA:CBC	2.46	0.46
28:P:1272:DMU:H34	7:T:63:GLY:N	2.24	0.46
3:P:47:LEU:O	3:P:51:MET:HG2	2.15	0.46
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.98	0.46
1:A:41:LEU:HD21	1:A:440:TYR:O	2.15	0.46
26:R:1229:PSC:H343	26:R:1229:PSC:C13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:98:TRP:CD2	28:Z:1526:DMU:H10	2.49	0.46
19:A:521:TGL:C30	19:A:521:TGL:H122	2.45	0.46
2:O:42:ILE:HG21	19:Q:1523:TGL:C23	2.45	0.46
1:N:407:ASP:O	1:N:411:LYS:HG3	2.16	0.46
3:C:257:TYR:O	3:C:261:SER:HB3	2.16	0.46
3:P:230:ASN:HB2	29:S:3400:HOH:O	2.16	0.46
3:P:25:LEU:O	3:P:29:SER:HB2	2.15	0.46
20:A:524:PGV:H232	20:A:524:PGV:H41	1.98	0.46
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.98	0.46
7:G:83:GLU:HG2	7:G:84:LYS:HZ2	1.79	0.46
1:N:115:SER:HB2	1:N:142:SER:O	2.14	0.46
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.97	0.46
28:G:272:DMU:O1	28:G:272:DMU:H30	2.16	0.46
2:O:98:LYS:HB2	2:O:109:GLU:HB2	1.98	0.46
7:T:45:PRO:HD2	29:T:3099:HOH:O	2.16	0.46
7:T:8:HIS:O	7:T:9:GLY:C	2.54	0.46
4:D:114:GLU:OE1	11:K:51:LYS:NZ	2.40	0.46
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.16	0.46
5:R:46:LYS:HG2	29:R:4450:HOH:O	2.15	0.46
1:N:178:GLN:HB2	29:N:3430:HOH:O	2.16	0.45
19:N:1522:TGL:HG11	12:Y:12:PRO:HG2	1.97	0.45
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.51	0.45
1:N:313:ALA:HB2	1:N:356:ILE:HD11	1.97	0.45
7:T:7:ASP:O	7:T:9:GLY:N	2.47	0.45
1:A:177:SER:H	1:A:180:GLN:HE21	1.65	0.45
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.81	0.45
1:A:307:SER:O	1:A:311:ILE:HG13	2.17	0.45
1:N:112:LEU:HD23	1:N:112:LEU:C	2.36	0.45
29:A:4735:HOH:O	4:D:17:VAL:CG1	2.65	0.45
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.98	0.45
22:C:525:CHD:H112	22:C:525:CHD:H12A	1.69	0.45
2:O:116:LEU:CD1	2:O:226:MET:HG3	2.46	0.45
24:T:1264:PEK:H71	24:T:1264:PEK:C3	2.40	0.45
8:U:23:GLN:HG3	29:U:4336:HOH:O	2.15	0.45
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.98	0.45
1:N:53:ILE:HD12	12:Y:44:LEU:CD2	2.46	0.45
2:O:58:ALA:O	2:O:62:GLU:HG3	2.16	0.45
26:R:1229:PSC:H251	26:R:1229:PSC:H221	1.72	0.45
29:B:3446:HOH:O	7:T:17:ARG:HD2	2.16	0.45
9:V:25:PHE:CE2	9:V:29:LEU:HD22	2.51	0.45
12:Y:27:LEU:O	12:Y:31:SER:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HE3	29:A:2645:HOH:O	2.17	0.45
19:D:523:TGL:H332	19:D:523:TGL:H172	1.76	0.45
7:G:1:ALA:HB2	20:P:1268:PGV:H321	1.98	0.45
1:N:127:THR:HB	1:N:129:TYR:CE2	2.51	0.45
1:N:352:GLY:N	1:N:380:VAL:HG13	2.32	0.45
22:P:1525:CHD:H12A	22:P:1525:CHD:H112	1.55	0.45
6:F:1:ALA:H2	24:G:265:PEK:C04	2.20	0.44
2:B:56:MET:HG2	26:E:229:PSC:H211	1.99	0.44
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.98	0.44
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.99	0.44
25:G:269:CDL:H152	25:G:269:CDL:H182	1.33	0.44
1:N:355:GLY:C	14:N:516:HEA:HMB3	2.38	0.44
25:P:1270:CDL:H232	25:P:1270:CDL:H262	1.79	0.44
1:A:390:MET:O	1:A:394:VAL:HG22	2.17	0.44
2:B:102:HIS:O	2:B:104:TRP:HA	2.17	0.44
1:N:17:THR:OG1	19:N:1522:TGL:H281	2.18	0.44
1:N:482:VAL:HG22	13:Z:1:ILE:HD11	1.98	0.44
25:G:269:CDL:H181	25:G:269:CDL:C51	2.46	0.44
20:P:1267:PGV:H12	20:P:1267:PGV:H152	1.20	0.44
29:B:3446:HOH:O	7:T:17:ARG:CD	2.66	0.44
19:D:523:TGL:H302	19:D:523:TGL:H132	1.69	0.44
1:N:113:LEU:HD12	19:N:1522:TGL:C29	2.46	0.44
22:P:1271:CHD:H112	22:P:1271:CHD:H12A	1.52	0.44
3:P:253:TYR:CE2	25:T:1269:CDL:H641	2.52	0.44
9:V:36:LYS:O	9:V:41:GLU:CG	2.65	0.44
1:A:250:GLY:O	1:A:254:ILE:HG12	2.17	0.44
3:C:63:ARG:HE	25:C:270:CDL:HA21	1.81	0.44
7:G:34:ASN:HB2	25:G:269:CDL:H162	2.00	0.44
2:O:1:FME:SD	2:O:133:LEU:HD11	2.57	0.44
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.17	0.44
6:S:92:VAL:HG23	6:S:92:VAL:O	2.18	0.44
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.45	0.44
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.00	0.44
19:N:1522:TGL:HC62	19:N:1522:TGL:HC32	1.43	0.44
1:N:199:LEU:N	1:N:200:PRO:CD	2.81	0.44
1:N:483:LEU:HD23	1:N:483:LEU:HA	1.90	0.44
2:O:41:ILE:O	2:O:42:ILE:C	2.56	0.44
3:P:224:LYS:CD	25:P:1270:CDL:HB31	2.44	0.44
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.71	0.44
25:C:270:CDL:H241	25:C:270:CDL:H661	1.97	0.43
5:E:11:PHE:CG	26:E:229:PSC:H073	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:TYR:CE2	9:I:24:ALA:HB2	2.53	0.43
19:Q:1523:TGL:H122	19:Q:1523:TGL:HB92	1.76	0.43
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.00	0.43
14:A:516:HEA:CBD	14:A:516:HEA:HMD1	2.41	0.43
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.99	0.43
2:O:139:ASP:OD2	2:O:140:ASN:N	2.50	0.43
6:S:70:ILE:HG13	6:S:84:SER:HB3	2.00	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.17	0.43
6:F:64:GLU:O	6:F:65:ASP:HB2	2.18	0.43
7:G:72:ASN:OD1	7:G:74:ARG:HB2	2.18	0.43
22:J:60:CHD:H12A	22:J:60:CHD:H112	1.81	0.43
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.43
3:P:118:PRO:HD2	3:P:121:ILE:HG13	2.01	0.43
3:P:156:ARG:HE	22:P:1271:CHD:C24	2.31	0.43
1:A:115:SER:HB2	1:A:142:SER:O	2.18	0.43
1:A:309:THR:CG2	14:A:516:HEA:HMB2	2.48	0.43
1:A:113:LEU:CD1	19:L:522:TGL:H292	2.49	0.43
1:A:113:LEU:HD12	19:L:522:TGL:H292	2.00	0.43
19:N:1522:TGL:HC22	19:N:1522:TGL:HC82	2.00	0.43
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.06	0.43
1:N:484:THR:HB	13:Z:2:THR:OG1	2.18	0.43
1:A:347:LEU:CD1	1:A:383:MET:HB3	2.45	0.43
25:C:270:CDL:CB2	25:C:270:CDL:PA1	3.07	0.43
7:G:76:ASN:HA	7:G:77:PRO:HD2	1.93	0.43
1:N:104:LEU:HB2	1:N:156:SER:HB2	2.00	0.43
5:R:105:GLY:O	5:R:108:LYS:HG3	2.18	0.43
2:O:113:TYR:HD1	8:U:58:ARG:HH22	1.67	0.43
1:A:334:TRP:HB2	19:D:523:TGL:HG11	2.00	0.43
29:A:4735:HOH:O	4:D:17:VAL:HG11	2.19	0.43
12:L:41:ARG:HG3	13:M:40:TYR:CE1	2.54	0.43
1:N:46:THR:O	1:N:46:THR:HG23	2.18	0.43
26:R:1229:PSC:H232	26:R:1229:PSC:H201	1.28	0.43
12:Y:4:GLU:HB3	12:Y:9:LYS:HB3	2.01	0.43
3:C:50:ASN:ND2	3:C:54:MET:CE	2.82	0.43
24:G:1263:PEK:H042	3:P:77:LYS:HZ1	1.82	0.43
12:L:11:ILE:CG2	19:L:522:TGL:H272	2.48	0.43
19:N:1521:TGL:H283	19:N:1521:TGL:H111	2.00	0.43
19:N:1522:TGL:H251	19:N:1522:TGL:H282	1.41	0.43
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.18	0.43
1:N:440:TYR:CZ	2:O:205:SER:HA	2.53	0.43
1:A:307:SER:CB	25:T:1269:CDL:H182	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:60:TYR:C	8:H:60:TYR:CD1	2.92	0.43
2:O:226:MET:HG3	2:O:226:MET:O	2.19	0.43
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.54	0.43
13:Z:1:ILE:HG23	13:Z:1:ILE:O	2.19	0.43
6:F:55:LYS:HA	6:F:74:LEU:O	2.19	0.43
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.84	0.43
4:Q:101:HIS:CD2	4:Q:102:TYR:CE2	3.07	0.43
3:C:159:MET:C	3:C:159:MET:SD	2.97	0.42
19:D:523:TGL:HB62	19:D:523:TGL:HA52	2.01	0.42
25:T:1269:CDL:H252	25:T:1269:CDL:H221	1.65	0.42
1:A:352:GLY:N	1:A:380:VAL:HG13	2.33	0.42
1:N:71:MET:CE	1:N:195:LEU:HD21	2.49	0.42
3:C:156:ARG:HE	22:C:271:CHD:C24	2.33	0.42
8:H:45:ALA:C	8:H:47:GLY:H	2.21	0.42
1:N:328:HIS:HB2	2:O:45:MET:SD	2.58	0.42
6:S:25:ARG:HD3	29:S:4617:HOH:O	2.19	0.42
10:W:50:LEU:HD22	10:W:54:SER:OG	2.19	0.42
1:A:129:TYR:HH	1:A:236:TRP:HE1	1.66	0.42
20:C:267:PGV:H12	20:C:267:PGV:H152	1.12	0.42
4:D:20:ARG:HG3	29:D:4124:HOH:O	2.19	0.42
2:O:59:GLN:CG	2:O:59:GLN:O	2.67	0.42
14:A:516:HEA:HHA	14:A:516:HEA:HAD2	1.72	0.42
2:B:33:LEU:HA	2:B:33:LEU:HD12	1.36	0.42
1:N:177:SER:H	1:N:180:GLN:HE21	1.67	0.42
3:P:137:LEU:HD23	3:P:137:LEU:HA	1.83	0.42
19:Q:1523:TGL:H302	19:Q:1523:TGL:H132	1.85	0.42
29:L:4496:HOH:O	13:M:32:TRP:HH2	2.02	0.42
2:O:102:HIS:O	2:O:104:TRP:HA	2.20	0.42
2:O:202:SER:HB2	2:O:203:ASN:ND2	2.15	0.42
24:G:265:PEK:H312	2:O:66:THR:HG23	2.01	0.42
9:V:73:LYS:HB3	9:V:73:LYS:HE3	1.74	0.42
2:B:62:GLU:O	2:B:66:THR:HB	2.20	0.42
14:N:515:HEA:H11	14:N:515:HEA:HHC	1.77	0.42
2:O:22:HIS:CE1	9:V:43:ARG:HG2	2.55	0.42
10:J:31:LEU:HA	10:J:31:LEU:HD12	1.89	0.42
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.91	0.42
29:N:3132:HOH:O	3:P:112:LEU:CD2	2.67	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.55	0.42
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.02	0.42
22:B:1085:CHD:H11	24:S:1265:PEK:H271	2.01	0.42
25:T:1269:CDL:H391	25:T:1269:CDL:H161	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:LEU:HD11	2:B:226:MET:HB3	2.00	0.42
1:N:112:LEU:O	1:N:112:LEU:HD23	2.20	0.42
1:N:409:TRP:HB3	1:N:471:ILE:HG12	2.01	0.42
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.85	0.41
24:G:265:PEK:C38	25:G:269:CDL:H273	2.49	0.41
1:N:431:LEU:HD21	1:N:450:TRP:HB2	2.01	0.41
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.01	0.41
2:O:202:SER:CB	2:O:203:ASN:HD22	2.18	0.41
3:P:58:TRP:CG	20:P:1267:PGV:H41	2.56	0.41
25:T:1269:CDL:OB4	25:T:1269:CDL:H1	2.20	0.41
10:W:32:TYR:OH	22:W:1059:CHD:H213	2.20	0.41
1:A:419:VAL:HG23	19:D:523:TGL:H121	2.01	0.41
4:D:16:TYR:OH	4:D:18:ASP:OD2	2.32	0.41
2:O:40:TYR:O	2:O:43:SER:N	2.54	0.41
3:P:220:PHE:HB2	25:P:1270:CDL:H712	2.00	0.41
3:P:138:LEU:HD12	25:T:1269:CDL:H591	2.02	0.41
24:T:263:PEK:H312	24:T:263:PEK:H282	1.93	0.41
22:B:1085:CHD:H112	22:B:1085:CHD:H12A	1.64	0.41
2:B:146:MET:HA	2:B:213:LEU:HD12	2.01	0.41
3:C:58:TRP:HB2	25:C:270:CDL:H552	2.02	0.41
7:G:3:ALA:CB	24:G:1263:PEK:H382	2.50	0.41
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.20	0.41
10:W:52:TRP:CE2	10:W:57:HIS:CE1	3.08	0.41
1:A:76:GLY:O	1:A:80:ASN:HB2	2.21	0.41
2:B:145:PRO:HA	2:B:214:VAL:O	2.19	0.41
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.75	0.41
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	2.03	0.41
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.01	0.41
2:O:227:LEU:HA	2:O:227:LEU:HD23	1.93	0.41
25:P:1270:CDL:HB21	25:P:1270:CDL:OB6	2.21	0.41
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.55	0.41
24:T:1264:PEK:C11	24:T:1264:PEK:C15	2.98	0.41
1:A:217:THR:HG22	3:C:188:ILE:HG12	2.02	0.41
6:F:92:VAL:HG23	6:F:92:VAL:O	2.20	0.41
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.41
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.03	0.41
3:P:157:LYS:HZ2	24:S:1265:PEK:C05	2.28	0.41
5:R:24:ILE:HG23	5:R:24:ILE:O	2.20	0.41
24:G:1263:PEK:H15	3:P:248:VAL:HG22	2.03	0.41
1:N:321:PHE:CD1	2:O:65:TRP:HB2	2.55	0.41
5:R:8:ASP:HA	26:R:1229:PSC:H071	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1:ALA:HB3	6:S:65:ASP:OD1	2.21	0.41
8:U:11:TYR:HH	8:U:62:SER:CB	2.30	0.41
1:A:378:HIS:HA	1:A:382:SER:CB	2.50	0.41
19:A:521:TGL:H102	19:A:521:TGL:C28	2.48	0.41
1:N:376:HIS:O	1:N:380:VAL:HG22	2.20	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.02	0.41
2:B:42:ILE:HD13	2:B:42:ILE:HG21	1.78	0.41
25:C:270:CDL:H532	25:C:270:CDL:H561	1.41	0.41
1:N:115:SER:O	1:N:121:GLY:HA2	2.21	0.41
6:S:94:HIS:CG	6:S:95:GLN:N	2.86	0.41
1:A:406:ASN:ND2	20:A:524:PGV:H032	2.36	0.41
19:N:1521:TGL:C11	19:N:1521:TGL:H281	2.51	0.41
8:U:46:LYS:HD2	29:U:4404:HOH:O	2.20	0.41
9:V:31:PHE:C	9:V:31:PHE:CD1	2.94	0.41
1:A:377:PHE:O	1:A:381:LEU:HB3	2.21	0.41
25:G:269:CDL:HB32	1:N:304:TYR:CD1	2.56	0.41
19:N:1521:TGL:HC22	29:Q:3606:HOH:O	2.21	0.41
7:T:31:CYS:SG	25:T:1269:CDL:C53	2.95	0.41
3:C:112:LEU:HD13	3:C:118:PRO:HG3	2.02	0.41
3:C:155:ASP:OD2	6:F:2:SER:HA	2.20	0.41
5:R:80:GLU:CD	5:R:80:GLU:H	2.24	0.41
1:A:43:GLN:HB2	1:A:44:PRO:HD2	2.03	0.40
14:A:515:HEA:H11	14:A:515:HEA:HH C	1.86	0.40
19:A:521:TGL:HB91	19:A:521:TGL:HB61	1.46	0.40
25:C:270:CDL:H201	25:C:270:CDL:C64	2.50	0.40
25:C:270:CDL:HB22	25:C:270:CDL:PA1	2.56	0.40
3:C:25:LEU:O	3:C:29:SER:HB2	2.21	0.40
3:C:40:MET:O	3:C:44:MET:HG2	2.21	0.40
8:H:76:ARG:HD2	29:H:4210:HOH:O	2.20	0.40
1:N:444:PRO:HD3	2:O:195:GLN:HE22	1.86	0.40
1:N:68:PHE:HE2	1:N:112:LEU:CD1	2.34	0.40
3:P:249:TRP:HD1	29:P:3165:HOH:O	2.04	0.40
20:A:524:PGV:H152	20:A:524:PGV:C32	2.51	0.40
10:J:16:ASN:OD1	10:J:23:LYS:HE3	2.21	0.40
26:R:1229:PSC:H212	26:R:1229:PSC:C01	2.51	0.40
20:C:268:PGV:H241	20:C:268:PGV:H11	2.03	0.40
3:C:98:PHE:CD2	24:T:263:PEK:H182	2.56	0.40
1:N:398:PRO:HA	1:N:403:TYR:O	2.21	0.40
3:P:8:TYR:CE1	3:P:74:ALA:HB1	2.55	0.40
26:R:1229:PSC:C14	26:R:1229:PSC:H343	2.51	0.40
7:T:35:SER:C	7:T:37:LEU:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:PHE:C	1:A:344:PHE:CD1	2.95	0.40
22:C:271:CHD:H12A	22:C:271:CHD:H112	1.66	0.40
7:G:5:LYS:HD2	24:G:1263:PEK:C38	2.52	0.40
24:T:263:PEK:H271	24:T:263:PEK:H241	1.96	0.40
1:A:160:GLY:HA3	29:A:2648:HOH:O	2.22	0.40
1:A:304:TYR:CD2	1:A:304:TYR:C	2.94	0.40
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.57	0.40
19:N:1521:TGL:H131	19:N:1521:TGL:H302	1.78	0.40
3:P:22:LEU:HD23	3:P:22:LEU:HA	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	495 (97%)	16 (3%)	1 (0%)	47	39
2	B	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	17	8
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	17	8
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	24
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	7	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	0
7	G	81/85 (95%)	66 (82%)	7 (9%)	8 (10%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	1	0
8	H	77/85 (91%)	67 (87%)	4 (5%)	6 (8%)	1	0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	0	1 (2%)	7	1
11	X	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3504/3614 (97%)	3336 (95%)	135 (4%)	33 (1%)	17	8

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	40	GLY
8	H	8	ILE
8	H	46	LYS
3	P	38	ASN
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	U	8	ILE
8	U	10	ASN
7	G	39	SER
8	H	10	ASN
8	H	11	TYR

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Mol	Chain	Res	Type
8	H	45	ALA
7	T	3	ALA
6	F	94	HIS
7	G	6	GLY
2	O	60	GLU
6	S	96	LEU
2	B	33	LEU
7	G	3	ALA
7	G	37	LEU
2	O	92	ASN
1	N	382	SER
11	K	14	GLY
7	T	6	GLY
8	H	47	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	426/426 (100%)	414 (97%)	12 (3%)	43	37
1	N	426/426 (100%)	414 (97%)	12 (3%)	43	37
2	B	210/210 (100%)	200 (95%)	10 (5%)	25	18
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	10
3	C	224/226 (99%)	217 (97%)	7 (3%)	40	33
3	P	224/226 (99%)	218 (97%)	6 (3%)	44	38
4	D	128/129 (99%)	126 (98%)	2 (2%)	62	59
4	Q	128/129 (99%)	125 (98%)	3 (2%)	50	44
5	E	92/95 (97%)	91 (99%)	1 (1%)	73	73
5	R	92/95 (97%)	86 (94%)	6 (6%)	17	9
6	F	81/81 (100%)	76 (94%)	5 (6%)	18	10
6	S	81/81 (100%)	73 (90%)	8 (10%)	8	3
7	G	67/68 (98%)	59 (88%)	8 (12%)	5	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	67/68 (98%)	57 (85%)	10 (15%)	3	0
8	H	71/75 (95%)	67 (94%)	4 (6%)	21	12
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	7
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	7
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	7
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	50
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	10
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	39
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	15
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	39
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	15
13	M	37/38 (97%)	31 (84%)	6 (16%)	2	0
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	2
All	All	3040/3082 (99%)	2900 (95%)	140 (5%)	27	19

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	290	HIS
1	A	312	ILE
1	A	333	LYS
1	A	338	MET
1	A	369	ASP
1	A	380	VAL
1	A	504	THR
1	A	513	LEU
2	B	33	LEU
2	B	42	ILE
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU

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Mol	Chain	Res	Type
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	33	MET
3	C	73	PRO
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	179	SER
3	C	214	PHE
4	D	31	LYS
4	D	51	LEU
5	E	90	ARG
6	F	37	LYS
6	F	48	LEU
6	F	78	GLU
6	F	87	THR
6	F	95	GLN
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
9	I	43	ARG
10	J	50	LEU
11	K	54	ARG
12	L	26	THR
13	M	4	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS

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Mol	Chain	Res	Type
13	M	43	SER
1	N	38	ARG
1	N	109	PHE
1	N	180	GLN
1	N	238	PHE
1	N	264	LYS
1	N	278	MET
1	N	290	HIS
1	N	297	MET
1	N	338	MET
1	N	369	ASP
1	N	380	VAL
1	N	504	THR
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	78	LEU
2	O	86	MET
2	O	94	SER
2	O	113	TYR
2	O	148	MET
2	O	167	SER
2	O	202	SER
2	O	205	SER
2	O	217	LYS
3	P	29	SER
3	P	33	MET
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	31	LYS
4	Q	51	LEU
5	R	5	HIS
5	R	46	LYS
5	R	80	GLU
5	R	90	ARG
5	R	101	PRO
5	R	108	LYS
6	S	37	LYS

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Mol	Chain	Res	Type
6	S	43	LYS
6	S	48	LEU
6	S	53	THR
6	S	64	GLU
6	S	94	HIS
6	S	96	LEU
6	S	98	HIS
7	T	17	ARG
7	T	18	PHE
7	T	35	SER
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	61	SER
7	T	74	ARG
7	T	84	LYS
8	U	9	LYS
8	U	12	GLN
8	U	29	CYS
8	U	41	LYS
8	U	60	TYR
9	V	2	THR
9	V	8	GLN
9	V	26	MET
9	V	37	PHE
10	W	4	ARG
10	W	36	MET
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG
12	Y	26	THR
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 (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN

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Mol	Chain	Res	Type
1	A	180	GLN
1	A	512	ASN
2	B	22	HIS
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
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
11	K	35	GLN
1	N	99	ASN
1	N	178	GLN
1	N	180	GLN
1	N	406	ASN
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	68	GLN
3	P	149	HIS
3	P	207	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
5	R	5	HIS
5	R	78	HIS

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Mol	Chain	Res	Type
5	R	94	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
9	V	8	GLN
9	V	70	GLN
10	W	57	HIS
13	Z	39	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	TPO	G	11	7	8,10,11	2.39	3 (37%)	10,14,16	1.75	3 (30%)
1	FME	A	1	1	8,9,10	1.04	1 (12%)	7,9,11	5.90	4 (57%)
2	FME	O	1	2	8,9,10	1.17	1 (12%)	7,9,11	6.11	2 (28%)
7	TPO	T	11	7	8,10,11	2.23	3 (37%)	10,14,16	2.14	2 (20%)
9	SAC	V	1	9	7,8,9	3.15	2 (28%)	8,9,11	2.22	3 (37%)
9	SAC	I	1	9	7,8,9	2.37	2 (28%)	8,9,11	1.48	2 (25%)
1	FME	N	1	1	8,9,10	1.37	1 (12%)	7,9,11	5.36	4 (57%)
2	FME	B	1	2	8,9,10	2.06	1 (12%)	7,9,11	6.70	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	5.80	1.54	1.46
9	V	1	SAC	OAC-C1A	5.52	1.35	1.23
2	B	1	FME	O1-CN	-4.38	1.09	1.22
9	I	1	SAC	CA-N	4.31	1.52	1.46
9	I	1	SAC	OAC-C1A	4.27	1.32	1.23
7	G	11	TPO	P-OG1	4.09	1.67	1.59
7	G	11	TPO	P-O1P	3.87	1.63	1.50
7	T	11	TPO	P-O1P	3.46	1.61	1.50
1	N	1	FME	CA-N	3.02	1.50	1.46
7	T	11	TPO	P-OG1	2.96	1.64	1.59
2	O	1	FME	O1-CN	-2.59	1.15	1.22
1	A	1	FME	O1-CN	-2.50	1.15	1.22
7	T	11	TPO	P-O3P	2.44	1.64	1.54
7	G	11	TPO	P-O2P	2.30	1.63	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.27	97.80	122.82
2	O	1	FME	CA-N-CN	-15.72	98.64	122.82
1	A	1	FME	CA-N-CN	-14.12	101.11	122.82
1	N	1	FME	CA-N-CN	-13.38	102.24	122.82
7	T	11	TPO	CG2-CB-CA	5.79	124.59	113.16
2	B	1	FME	CG-CB-CA	-4.69	99.92	112.95
1	A	1	FME	CE-SD-CG	4.67	116.44	100.40
2	B	1	FME	C-CA-N	4.38	117.64	109.73
1	A	1	FME	CG-CB-CA	-4.04	101.71	112.95
9	V	1	SAC	C-CA-N	3.69	116.39	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	CA-N-C1A	3.54	129.69	123.15
7	G	11	TPO	O2P-P-OG1	3.40	121.22	105.99
9	I	1	SAC	C-CA-N	3.07	115.26	109.73
1	N	1	FME	O1-CN-N	2.91	132.93	125.27
2	O	1	FME	C-CA-N	2.77	114.72	109.73
1	N	1	FME	CE-SD-CG	2.62	109.39	100.40
7	G	11	TPO	CG2-CB-CA	2.54	118.17	113.16
1	A	1	FME	O-C-CA	-2.27	118.82	124.78
9	I	1	SAC	CB-CA-N	-2.20	105.61	110.55
7	T	11	TPO	O-C-CA	-2.19	119.05	124.78
2	B	1	FME	O-C-CA	-2.18	119.07	124.78
9	V	1	SAC	OAC-C1A-C2A	-2.09	118.18	122.06
7	G	11	TPO	O-C-CA	-2.05	119.42	124.78
1	N	1	FME	O-C-CA	-2.01	119.51	124.78

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0
2	O	1	FME	1	0
7	T	11	TPO	1	0
9	V	1	SAC	1	0
1	N	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
19	TGL	N	1521	-	62,62,62	1.34	6 (9%)	65,65,65	1.47	12 (18%)
20	PGV	P	1268	-	50,50,50	1.28	3 (6%)	53,56,56	1.51	7 (13%)
25	CDL	P	1270	-	99,99,99	1.38	12 (12%)	105,111,111	1.38	14 (13%)
19	TGL	D	523	-	62,62,62	1.61	7 (11%)	65,65,65	1.51	12 (18%)
22	CHD	W	1059	-	29,32,32	1.08	2 (6%)	48,51,51	5.29	34 (70%)
26	PSC	R	1229	-	51,51,51	1.22	3 (5%)	57,59,59	1.01	5 (8%)
24	PEK	G	1263	-	52,52,52	1.18	2 (3%)	55,57,57	1.17	5 (9%)
28	DMU	P	1272	-	34,34,34	1.23	1 (2%)	45,45,45	3.19	23 (51%)
28	DMU	M	526	-	34,34,34	0.85	1 (2%)	45,45,45	3.42	27 (60%)
25	CDL	G	269	-	99,99,99	1.50	14 (14%)	105,111,111	1.50	17 (16%)
20	PGV	C	267	-	50,50,50	0.88	3 (6%)	53,56,56	1.37	4 (7%)
22	CHD	C	525	-	29,32,32	1.87	6 (20%)	48,51,51	5.60	35 (72%)
20	PGV	C	268	-	50,50,50	1.30	3 (6%)	53,56,56	1.46	6 (11%)
22	CHD	J	60	-	29,32,32	0.71	0	48,51,51	5.04	40 (83%)
14	HEA	N	515	1	44,67,67	0.97	3 (6%)	37,103,103	2.40	12 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CDL	C	270	-	99,99,99	1.38	12 (12%)	105,111,111	1.42	15 (14%)
22	CHD	O	229	-	29,32,32	1.29	2 (6%)	48,51,51	5.70	33 (68%)
24	PEK	G	265	-	52,52,52	1.21	3 (5%)	55,57,57	1.24	3 (5%)
28	DMU	G	272	-	34,34,34	1.27	4 (11%)	45,45,45	3.27	23 (51%)
22	CHD	P	1271	-	29,32,32	0.74	0	48,51,51	5.08	37 (77%)
20	PGV	N	1266	-	50,50,50	0.93	1 (2%)	53,56,56	1.36	6 (11%)
19	TGL	Q	1523	-	62,62,62	1.36	6 (9%)	65,65,65	1.24	9 (13%)
25	CDL	T	1269	-	99,99,99	1.38	12 (12%)	105,111,111	1.41	16 (15%)
19	TGL	A	521	-	62,62,62	1.45	7 (11%)	65,65,65	2.37	17 (26%)
19	TGL	L	522	-	62,62,62	1.58	8 (12%)	65,65,65	1.83	16 (24%)
24	PEK	C	264	-	52,52,52	0.89	2 (3%)	55,57,57	1.78	12 (21%)
28	DMU	Z	1526	-	34,34,34	0.97	2 (5%)	45,45,45	3.14	21 (46%)
20	PGV	A	522	-	50,50,50	0.98	2 (4%)	53,56,56	1.28	6 (11%)
21	CUA	B	228	2	0,1,1	0.00	-	-	-	-
22	CHD	P	1525	-	29,32,32	1.46	4 (13%)	48,51,51	5.29	42 (87%)
14	HEA	A	515	1	44,67,67	1.42	8 (18%)	37,103,103	2.35	12 (32%)
15	CYN	N	520	14,16	0,1,1	0.00	-	-	-	-
14	HEA	A	516	1,15	44,67,67	2.54	8 (18%)	37,103,103	3.74	17 (45%)
24	PEK	T	1264	-	52,52,52	0.93	2 (3%)	55,57,57	1.94	8 (14%)
20	PGV	P	1267	-	50,50,50	0.85	2 (4%)	53,56,56	1.42	7 (13%)
26	PSC	E	229	-	51,51,51	1.28	3 (5%)	57,59,59	1.36	6 (10%)
20	PGV	N	1524	-	50,50,50	1.22	2 (4%)	53,56,56	1.27	6 (11%)
19	TGL	N	1522	-	62,62,62	1.59	7 (11%)	65,65,65	1.61	15 (23%)
24	PEK	T	263	-	52,52,52	1.23	2 (3%)	55,57,57	1.18	6 (10%)
15	CYN	A	520	14,16	0,1,1	0.00	-	-	-	-
20	PGV	A	524	-	50,50,50	1.19	2 (4%)	53,56,56	1.34	7 (13%)
24	PEK	S	1265	-	52,52,52	1.34	3 (5%)	55,57,57	1.30	5 (9%)
14	HEA	N	516	1,15	44,67,67	1.82	5 (11%)	37,103,103	3.27	15 (40%)
22	CHD	B	1085	-	29,32,32	1.55	6 (20%)	48,51,51	5.81	35 (72%)
21	CUA	O	228	2	0,1,1	0.00	-	-	-	-
22	CHD	C	271	-	29,32,32	0.86	1 (3%)	48,51,51	5.26	35 (72%)

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
19	TGL	N	1521	-	-	41/65/65/65	-
20	PGV	P	1268	-	-	30/55/55/55	-
25	CDL	P	1270	-	-	69/110/110/110	-
19	TGL	D	523	-	-	37/65/65/65	-
22	CHD	W	1059	-	2/2/12/12	5/7/74/74	0/4/4/4
26	PSC	R	1229	-	-	39/55/55/55	-
24	PEK	G	1263	-	-	27/56/56/56	-
28	DMU	P	1272	-	6/6/10/10	11/19/59/59	0/2/2/2
28	DMU	M	526	-	4/4/10/10	10/19/59/59	0/2/2/2
25	CDL	G	269	-	-	65/110/110/110	-
20	PGV	C	267	-	-	14/55/55/55	-
28	DMU	G	272	-	6/6/10/10	12/19/59/59	0/2/2/2
20	PGV	C	268	-	-	34/55/55/55	-
22	CHD	J	60	-	2/2/12/12	4/7/74/74	0/4/4/4
14	HEA	N	515	1	3/3/7/16	2/24/76/76	-
25	CDL	C	270	-	-	74/110/110/110	-
22	CHD	O	229	-	-	0/7/74/74	0/4/4/4
24	PEK	G	265	-	-	29/56/56/56	-
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
22	CHD	P	1271	-	1/1/12/12	5/7/74/74	0/4/4/4
20	PGV	N	1266	-	-	13/55/55/55	-
19	TGL	Q	1523	-	-	38/65/65/65	-
19	TGL	A	521	-	-	35/65/65/65	-
19	TGL	L	522	-	-	35/65/65/65	-
24	PEK	C	264	-	-	21/56/56/56	-
28	DMU	Z	1526	-	5/5/10/10	9/19/59/59	0/2/2/2
20	PGV	A	522	-	-	15/55/55/55	-
26	PSC	E	229	-	-	32/55/55/55	-
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
14	HEA	A	515	1	3/3/7/16	1/24/76/76	-
14	HEA	A	516	1,15	3/3/7/16	4/24/76/76	-
24	PEK	T	1264	-	-	23/56/56/56	-
20	PGV	P	1267	-	-	14/55/55/55	-
20	PGV	N	1524	-	-	36/55/55/55	-
19	TGL	N	1522	-	-	39/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEK	T	263	-	-	33/56/56/56	-
25	CDL	T	1269	-	-	65/110/110/110	-
20	PGV	A	524	-	-	33/55/55/55	-
24	PEK	S	1265	-	-	25/56/56/56	-
14	HEA	N	516	1,15	3/3/7/16	7/24/76/76	-
22	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
22	CHD	C	271	-	1/1/12/12	5/7/74/74	0/4/4/4

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	516	HEA	C3B-C11	10.38	1.61	1.52
14	A	516	HEA	O11-C11	9.35	1.64	1.42
14	N	516	HEA	O11-C11	7.09	1.59	1.42
19	N	1522	TGL	OG2-CB1	6.85	1.53	1.34
19	L	522	TGL	OG2-CB1	6.42	1.52	1.34
20	P	1268	PGV	O01-C1	6.27	1.52	1.34
20	C	268	PGV	O01-C1	6.10	1.51	1.34
14	N	516	HEA	C3B-C11	6.10	1.57	1.52
24	S	1265	PEK	O03-C21	5.80	1.50	1.33
19	D	523	TGL	OG1-CA1	5.72	1.50	1.33
24	T	263	PEK	O03-C21	5.64	1.49	1.33
19	A	521	TGL	OG1-CA1	5.50	1.49	1.33
25	G	269	CDL	OB6-CB5	5.47	1.49	1.34
20	A	524	PGV	O03-C19	5.47	1.49	1.33
19	L	522	TGL	OG1-CA1	5.41	1.49	1.33
20	N	1524	PGV	O03-C19	5.41	1.49	1.33
19	D	523	TGL	OG2-CB1	5.35	1.49	1.34
25	G	269	CDL	OA8-CA7	5.32	1.48	1.33
25	P	1270	CDL	OA8-CA7	5.31	1.48	1.33
25	C	270	CDL	OA8-CA7	5.31	1.48	1.33
19	D	523	TGL	OB1-CB1	5.30	1.38	1.22
19	N	1522	TGL	OG3-CC1	5.24	1.48	1.33
19	N	1522	TGL	OG1-CA1	5.22	1.48	1.33
25	G	269	CDL	OA6-CA5	5.22	1.49	1.34
19	N	1521	TGL	OG2-CB1	5.22	1.49	1.34
24	G	265	PEK	O03-C21	5.17	1.48	1.33
25	T	1269	CDL	OB6-CB5	5.13	1.48	1.34
24	G	1263	PEK	O03-C21	5.06	1.48	1.33
19	Q	1523	TGL	OG1-CA1	5.04	1.48	1.33
14	A	516	HEA	C3C-C2C	-5.02	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	1265	PEK	O01-C1	4.98	1.48	1.34
24	G	265	PEK	O01-C1	4.95	1.48	1.34
24	T	263	PEK	O01-C1	4.95	1.48	1.34
26	E	229	PSC	O01-C1	4.95	1.48	1.34
22	C	525	CHD	C13-C12	-4.92	1.46	1.54
20	C	268	PGV	O03-C19	4.90	1.47	1.33
19	Q	1523	TGL	OG3-CC1	4.84	1.47	1.33
25	T	1269	CDL	OA6-CA5	4.83	1.47	1.34
28	P	1272	DMU	O16-C6	4.81	1.48	1.40
26	E	229	PSC	O03-C19	4.78	1.47	1.33
19	A	521	TGL	OG3-CC1	4.76	1.47	1.33
19	Q	1523	TGL	OG2-CB1	4.75	1.47	1.34
28	G	272	DMU	O16-C6	4.74	1.48	1.40
22	C	525	CHD	C1-C10	-4.74	1.45	1.54
25	P	1270	CDL	OB6-CB5	4.70	1.47	1.34
25	G	269	CDL	OB8-CB7	4.70	1.47	1.33
19	N	1521	TGL	OG1-CA1	4.69	1.47	1.33
20	N	1266	PGV	O03-C19	4.64	1.46	1.33
24	G	1263	PEK	O01-C1	4.63	1.47	1.34
26	R	1229	PSC	O01-C1	4.62	1.47	1.34
25	T	1269	CDL	OB8-CB7	4.57	1.46	1.33
19	L	522	TGL	OG3-CC1	4.56	1.46	1.33
20	P	1268	PGV	O03-C19	4.56	1.46	1.33
19	A	521	TGL	OG2-CB1	4.52	1.47	1.34
20	N	1524	PGV	O01-C1	4.50	1.47	1.34
25	C	270	CDL	OA6-CA5	4.47	1.46	1.34
19	N	1521	TGL	OG3-CC1	4.33	1.46	1.33
25	C	270	CDL	OB8-CB7	4.31	1.45	1.33
20	A	524	PGV	O01-C1	4.29	1.46	1.34
19	D	523	TGL	OG3-CC1	4.28	1.45	1.33
25	P	1270	CDL	OB8-CB7	4.24	1.45	1.33
26	R	1229	PSC	O03-C19	4.20	1.45	1.33
25	P	1270	CDL	OA6-CA5	4.13	1.46	1.34
20	A	522	PGV	O03-C19	3.94	1.44	1.33
26	R	1229	PSC	C13-C12	3.92	1.54	1.31
26	E	229	PSC	C13-C12	3.86	1.54	1.31
25	C	270	CDL	OB6-CB5	3.85	1.45	1.34
25	T	1269	CDL	OA8-CA7	3.74	1.44	1.33
25	T	1269	CDL	C59-C58	-3.65	1.31	1.51
14	A	515	HEA	C3B-C11	-3.62	1.50	1.52
22	O	229	CHD	C11-C9	3.61	1.59	1.53
19	A	521	TGL	OC1-CC1	-3.60	1.11	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	1270	CDL	C59-C58	-3.48	1.32	1.51
14	N	516	HEA	C3C-C2C	-3.48	1.35	1.40
19	L	522	TGL	C20-CA9	-3.44	1.32	1.51
19	L	522	TGL	C10-CB9	-3.43	1.32	1.51
25	G	269	CDL	C59-C58	-3.42	1.32	1.51
22	B	1085	CHD	C13-C14	-3.39	1.49	1.55
22	B	1085	CHD	C10-C5	-3.34	1.50	1.55
24	T	1264	PEK	O01-C1	3.34	1.43	1.34
25	T	1269	CDL	C42-C41	-3.30	1.33	1.51
19	N	1522	TGL	C10-CB9	-3.30	1.33	1.51
25	C	270	CDL	C62-C61	-3.29	1.33	1.51
22	C	525	CHD	O12-C12	3.27	1.49	1.43
22	W	1059	CHD	C11-C9	3.24	1.59	1.53
25	T	1269	CDL	C62-C61	-3.22	1.33	1.51
22	P	1525	CHD	C16-C17	3.22	1.61	1.54
25	C	270	CDL	C59-C58	-3.21	1.33	1.51
14	A	515	HEA	O11-C11	3.20	1.50	1.42
25	P	1270	CDL	C62-C61	-3.20	1.33	1.51
19	N	1522	TGL	C20-CA9	-3.18	1.33	1.51
14	A	516	HEA	C1B-CHB	3.18	1.49	1.41
14	A	515	HEA	C12-C13	3.13	1.63	1.53
25	G	269	CDL	C42-C41	-3.11	1.34	1.51
25	P	1270	CDL	C19-C18	-3.07	1.34	1.51
19	A	521	TGL	C10-CB9	-3.06	1.34	1.51
19	N	1521	TGL	C10-CB9	-3.06	1.34	1.51
20	C	267	PGV	O03-C19	3.05	1.42	1.33
19	D	523	TGL	C15-CC9	-3.04	1.34	1.51
19	A	521	TGL	C20-CA9	-3.04	1.34	1.51
25	C	270	CDL	C19-C18	-3.02	1.34	1.51
19	Q	1523	TGL	C20-CA9	-3.02	1.34	1.51
25	G	269	CDL	C22-C21	-3.02	1.34	1.51
25	G	269	CDL	C62-C61	-3.01	1.34	1.51
28	Z	1526	DMU	C3-C4	-3.00	1.44	1.52
25	C	270	CDL	C79-C78	-2.99	1.34	1.51
25	P	1270	CDL	C79-C78	-2.96	1.35	1.51
22	C	271	CHD	C20-C17	2.95	1.59	1.54
20	P	1267	PGV	O03-C19	2.95	1.42	1.33
25	T	1269	CDL	C22-C21	-2.95	1.35	1.51
25	T	1269	CDL	C79-C78	-2.94	1.35	1.51
25	P	1270	CDL	C22-C21	-2.92	1.35	1.51
25	C	270	CDL	C22-C21	-2.92	1.35	1.51
25	C	270	CDL	C39-C38	-2.91	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	1059	CHD	C20-C17	2.91	1.59	1.54
25	C	270	CDL	C82-C81	-2.90	1.35	1.51
25	T	1269	CDL	C19-C18	-2.89	1.35	1.51
25	G	269	CDL	C39-C38	-2.88	1.35	1.51
25	P	1270	CDL	C82-C81	-2.87	1.35	1.51
19	Q	1523	TGL	C15-CC9	-2.87	1.35	1.51
19	Q	1523	TGL	C10-CB9	-2.87	1.35	1.51
25	T	1269	CDL	C39-C38	-2.85	1.35	1.51
19	N	1521	TGL	C20-CA9	-2.83	1.35	1.51
24	T	1264	PEK	O03-C01	-2.80	1.38	1.45
20	C	267	PGV	O01-C1	2.79	1.42	1.34
22	B	1085	CHD	C4-C3	2.78	1.57	1.51
25	G	269	CDL	C19-C18	-2.75	1.36	1.51
25	P	1270	CDL	C39-C38	-2.74	1.36	1.51
19	L	522	TGL	C15-CC9	-2.74	1.36	1.51
22	O	229	CHD	C10-C5	-2.70	1.51	1.55
19	D	523	TGL	C20-CA9	-2.69	1.36	1.51
25	G	269	CDL	C17-C16	2.68	1.66	1.51
22	B	1085	CHD	C19-C10	2.68	1.59	1.54
24	C	264	PEK	O01-C1	2.68	1.41	1.34
25	C	270	CDL	C42-C41	-2.67	1.36	1.51
25	T	1269	CDL	C82-C81	-2.67	1.36	1.51
19	N	1521	TGL	C15-CC9	-2.67	1.36	1.51
19	N	1522	TGL	C15-CC9	-2.67	1.36	1.51
25	P	1270	CDL	C42-C41	-2.61	1.37	1.51
25	G	269	CDL	C79-C78	-2.59	1.37	1.51
25	G	269	CDL	C82-C81	-2.58	1.37	1.51
14	A	516	HEA	CAA-C2A	2.55	1.56	1.52
19	D	523	TGL	C10-CB9	-2.53	1.37	1.51
28	M	526	DMU	C3-C4	-2.52	1.46	1.52
24	C	264	PEK	O03-C21	2.50	1.40	1.33
24	S	1265	PEK	P-O11	2.50	1.69	1.59
22	P	1525	CHD	O12-C12	2.50	1.47	1.43
22	C	525	CHD	C19-C10	2.49	1.58	1.54
19	A	521	TGL	C15-CC9	-2.48	1.37	1.51
14	A	515	HEA	CMB-C2B	2.44	1.56	1.51
22	P	1525	CHD	C10-C5	-2.34	1.51	1.55
14	A	516	HEA	C18-C19	2.33	1.38	1.33
22	C	525	CHD	C21-C20	2.32	1.58	1.53
22	C	525	CHD	C11-C12	2.32	1.57	1.53
28	Z	1526	DMU	O16-C6	2.30	1.44	1.40
22	B	1085	CHD	C18-C13	2.28	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	515	HEA	C1C-CHC	2.27	1.47	1.41
14	A	515	HEA	C22-C23	2.26	1.38	1.32
20	A	522	PGV	O06-C06	2.24	1.51	1.42
14	N	515	HEA	CMB-C2B	2.23	1.56	1.51
22	P	1525	CHD	C21-C20	2.21	1.58	1.53
14	N	516	HEA	C1D-C2D	-2.21	1.37	1.42
14	A	515	HEA	CAA-C2A	2.21	1.56	1.52
19	N	1522	TGL	CG3-CG2	2.20	1.57	1.50
24	G	265	PEK	P-O12	2.20	1.68	1.59
20	P	1267	PGV	O01-C1	2.19	1.40	1.34
28	G	272	DMU	C3-C4	-2.18	1.47	1.52
20	C	267	PGV	C03-C02	2.18	1.57	1.50
14	A	515	HEA	CMC-C2C	2.15	1.56	1.51
14	N	516	HEA	C18-C19	2.15	1.38	1.33
14	N	515	HEA	C3C-C2C	-2.13	1.37	1.40
14	N	515	HEA	C3B-C11	-2.12	1.51	1.52
20	C	268	PGV	P-O11	2.11	1.67	1.59
25	G	269	CDL	C16-C15	2.10	1.63	1.51
19	L	522	TGL	CG3-CG2	2.10	1.57	1.50
28	G	272	DMU	O5-C6	2.09	1.47	1.41
19	L	522	TGL	CG1-CG2	2.08	1.57	1.50
14	A	516	HEA	C20-C19	2.07	1.55	1.51
28	G	272	DMU	O1-C10	2.03	1.47	1.41
20	P	1268	PGV	P-O11	2.03	1.67	1.59
22	B	1085	CHD	C1-C10	-2.03	1.50	1.54
14	A	516	HEA	CMB-C2B	2.02	1.55	1.51

All (683) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1085	CHD	C18-C13-C12	-16.45	92.32	109.07
22	P	1271	CHD	C10-C9-C8	14.25	127.12	111.82
22	C	271	CHD	C10-C9-C8	13.69	126.52	111.82
14	A	516	HEA	C4B-C3B-C2B	-12.84	97.89	106.87
22	C	525	CHD	C6-C5-C10	12.69	126.13	112.66
22	B	1085	CHD	C1-C10-C5	12.48	126.22	107.77
22	C	525	CHD	C1-C10-C5	12.36	126.05	107.77
22	B	1085	CHD	C6-C5-C10	12.31	125.73	112.66
22	O	229	CHD	C18-C13-C12	-12.07	96.78	109.07
22	P	1525	CHD	C14-C13-C12	12.06	118.63	107.40
22	O	229	CHD	C1-C10-C5	11.83	125.26	107.77
22	O	229	CHD	C14-C13-C12	11.79	118.38	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	1059	CHD	C10-C9-C8	11.14	123.78	111.82
22	B	1085	CHD	C17-C13-C12	11.00	127.71	117.67
22	J	60	CHD	C10-C9-C8	10.84	123.46	111.82
22	C	525	CHD	C19-C10-C9	-10.69	96.45	111.18
22	O	229	CHD	C6-C5-C10	10.58	123.89	112.66
22	P	1525	CHD	C1-C10-C5	10.53	123.35	107.77
24	T	1264	PEK	C2-C3-C4	10.27	131.53	113.23
22	W	1059	CHD	C13-C17-C20	10.10	131.56	119.50
22	O	229	CHD	C10-C9-C8	10.08	122.64	111.82
22	C	525	CHD	C17-C13-C12	10.03	126.82	117.67
22	B	1085	CHD	C10-C9-C8	10.00	122.56	111.82
22	B	1085	CHD	C14-C13-C12	9.79	116.52	107.40
22	P	1525	CHD	C6-C5-C10	9.70	122.96	112.66
22	O	229	CHD	C5-C4-C3	9.69	126.98	112.76
22	W	1059	CHD	C16-C17-C13	9.45	112.83	103.55
22	C	525	CHD	C4-C3-C2	9.45	121.83	110.55
14	N	516	HEA	CMC-C2C-C1C	-9.42	113.99	128.46
22	O	229	CHD	C19-C10-C9	-9.39	98.24	111.18
14	N	516	HEA	CMC-C2C-C3C	8.93	141.38	124.68
22	P	1525	CHD	C10-C9-C8	8.93	121.40	111.82
22	C	525	CHD	C10-C9-C8	8.86	121.33	111.82
22	W	1059	CHD	C14-C8-C7	8.76	123.42	111.81
19	A	521	TGL	CG2-OG2-CB1	8.66	139.12	117.79
22	C	271	CHD	C15-C14-C8	8.54	130.27	118.33
22	P	1525	CHD	C18-C13-C12	-8.53	100.38	109.07
22	J	60	CHD	C14-C13-C12	8.51	115.33	107.40
22	C	271	CHD	C16-C17-C20	8.45	125.23	112.15
22	C	271	CHD	C6-C5-C10	8.35	121.53	112.66
22	C	271	CHD	C18-C13-C12	-8.31	100.61	109.07
28	M	526	DMU	O1-C9-C8	8.26	124.69	109.69
22	J	60	CHD	C17-C13-C12	8.19	125.14	117.67
22	P	1271	CHD	C6-C5-C10	8.18	121.34	112.66
22	O	229	CHD	O12-C12-C13	-8.14	97.28	111.03
28	M	526	DMU	C18-O16-C6	8.11	127.29	113.84
22	O	229	CHD	C17-C13-C12	8.10	125.06	117.67
22	W	1059	CHD	C5-C6-C7	8.10	123.39	114.46
22	P	1525	CHD	C15-C14-C13	8.05	111.44	103.55
22	P	1525	CHD	C17-C13-C12	8.04	125.00	117.67
22	P	1271	CHD	C15-C14-C8	7.94	129.43	118.33
22	B	1085	CHD	C15-C14-C13	7.84	111.24	103.55
22	J	60	CHD	C1-C2-C3	7.82	120.50	110.47
22	C	271	CHD	C5-C6-C7	7.79	123.06	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1085	CHD	C19-C10-C9	-7.75	100.50	111.18
28	M	526	DMU	O5-C6-C1	7.74	126.73	110.35
22	O	229	CHD	C4-C3-C2	7.65	119.68	110.55
22	B	1085	CHD	C5-C4-C3	7.48	123.74	112.76
22	W	1059	CHD	C1-C2-C3	7.45	120.03	110.47
22	P	1525	CHD	C19-C10-C9	-7.41	100.97	111.18
22	P	1271	CHD	C5-C6-C7	7.37	122.59	114.46
14	A	516	HEA	C26-C15-C16	7.35	127.64	115.27
22	C	525	CHD	C18-C13-C12	-7.33	101.60	109.07
22	C	271	CHD	C14-C13-C12	7.32	114.22	107.40
22	W	1059	CHD	C6-C5-C4	-7.29	102.80	111.19
22	B	1085	CHD	C1-C2-C3	7.28	119.80	110.47
14	N	516	HEA	C26-C15-C16	7.26	127.49	115.27
22	J	60	CHD	C6-C7-C8	7.26	119.22	111.48
22	P	1271	CHD	C1-C10-C5	7.23	118.47	107.77
22	B	1085	CHD	C18-C13-C17	-7.23	99.89	111.21
22	C	271	CHD	C1-C2-C3	7.23	119.75	110.47
22	P	1525	CHD	C6-C7-C8	7.21	119.17	111.48
22	C	271	CHD	C16-C17-C13	7.21	110.62	103.55
22	C	525	CHD	C13-C17-C20	7.20	128.09	119.50
28	G	272	DMU	O1-C9-C8	7.20	122.76	109.69
28	Z	1526	DMU	O1-C9-C8	7.18	122.74	109.69
22	J	60	CHD	C18-C13-C12	-7.18	101.75	109.07
22	P	1525	CHD	C18-C13-C14	-7.18	99.98	111.21
24	C	264	PEK	C2-C3-C4	7.14	125.96	113.23
22	P	1525	CHD	C4-C3-C2	7.10	119.03	110.55
22	W	1059	CHD	C15-C14-C13	7.08	110.49	103.55
28	Z	1526	DMU	O1-C10-C5	7.03	125.23	110.35
22	C	271	CHD	C1-C10-C5	7.02	118.15	107.77
22	P	1525	CHD	C5-C4-C3	7.02	123.07	112.76
28	M	526	DMU	O1-C10-C5	6.99	125.14	110.35
19	A	521	TGL	OG3-CC1-CC2	6.96	133.75	111.91
22	C	525	CHD	C23-C22-C20	-6.96	105.35	114.72
22	C	271	CHD	C15-C14-C13	6.94	110.36	103.55
22	W	1059	CHD	C14-C13-C12	6.94	113.86	107.40
22	J	60	CHD	C4-C5-C10	6.92	120.01	112.66
22	P	1271	CHD	C1-C2-C3	6.91	119.34	110.47
22	C	271	CHD	C11-C12-C13	6.90	118.33	111.24
22	O	229	CHD	C17-C13-C14	6.90	107.05	100.09
28	P	1272	DMU	O1-C10-C5	6.88	124.91	110.35
22	P	1271	CHD	C11-C9-C8	6.87	120.94	110.88
22	W	1059	CHD	C15-C14-C8	6.86	127.92	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	525	CHD	C9-C8-C7	6.83	120.04	111.88
22	J	60	CHD	C5-C6-C7	6.80	121.97	114.46
22	P	1271	CHD	C6-C7-C8	6.78	118.71	111.48
28	P	1272	DMU	O16-C6-C1	6.77	118.87	108.30
14	N	515	HEA	C13-C12-C11	-6.76	104.19	114.35
22	P	1271	CHD	C5-C4-C3	6.76	122.69	112.76
22	J	60	CHD	C6-C5-C10	6.75	119.83	112.66
22	P	1271	CHD	C16-C17-C13	6.72	110.14	103.55
22	P	1271	CHD	C4-C3-C2	6.70	118.55	110.55
22	C	525	CHD	O12-C12-C13	-6.70	99.71	111.03
22	W	1059	CHD	C6-C5-C10	6.69	119.76	112.66
22	C	271	CHD	C5-C4-C3	6.64	122.51	112.76
22	O	229	CHD	C11-C9-C8	6.61	120.55	110.88
22	C	271	CHD	C6-C7-C8	6.60	118.53	111.48
14	A	515	HEA	C13-C12-C11	-6.60	104.44	114.35
22	J	60	CHD	C16-C17-C13	6.59	110.02	103.55
22	W	1059	CHD	C1-C10-C5	6.58	117.50	107.77
22	W	1059	CHD	C5-C4-C3	6.57	122.41	112.76
22	O	229	CHD	C15-C14-C8	6.57	127.51	118.33
22	J	60	CHD	C1-C10-C5	6.56	117.48	107.77
22	W	1059	CHD	C6-C7-C8	6.53	118.45	111.48
28	P	1272	DMU	O1-C9-C8	6.52	121.53	109.69
22	P	1271	CHD	C16-C17-C20	6.51	122.22	112.15
22	C	271	CHD	C4-C5-C10	6.48	119.53	112.66
14	A	516	HEA	CAA-CBA-CGA	-6.47	101.81	112.67
28	Z	1526	DMU	O5-C6-C1	6.47	124.04	110.35
22	C	525	CHD	C17-C13-C14	6.47	106.61	100.09
22	C	525	CHD	C15-C14-C13	6.44	109.87	103.55
22	P	1271	CHD	C18-C13-C12	-6.42	102.53	109.07
22	W	1059	CHD	C4-C3-C2	6.42	118.22	110.55
22	J	60	CHD	C4-C3-C2	6.38	118.18	110.55
28	G	272	DMU	O1-C10-C5	6.38	123.86	110.35
22	O	229	CHD	C18-C13-C17	-6.34	101.29	111.21
26	E	229	PSC	O01-C1-C2	6.34	125.17	111.50
25	G	269	CDL	OB6-CB5-C51	6.32	125.12	111.50
19	A	521	TGL	OG2-CB1-CB2	6.31	125.10	111.50
28	G	272	DMU	O16-C6-C1	6.28	118.10	108.30
22	P	1525	CHD	O7-C7-C6	-6.25	94.43	109.94
22	J	60	CHD	C13-C17-C20	6.22	126.92	119.50
19	A	521	TGL	OG3-CC1-OC1	-6.21	107.92	123.59
22	J	60	CHD	C15-C14-C13	6.20	109.63	103.55
22	P	1525	CHD	C11-C9-C8	6.19	119.93	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	60	CHD	C5-C4-C3	6.13	121.76	112.76
22	P	1271	CHD	C14-C8-C7	6.11	119.91	111.81
20	P	1268	PGV	O01-C1-C2	6.11	124.66	111.50
22	J	60	CHD	C16-C17-C20	6.10	121.58	112.15
22	W	1059	CHD	C4-C5-C10	6.08	119.11	112.66
22	C	271	CHD	C4-C3-C2	6.07	117.80	110.55
22	C	271	CHD	C17-C13-C12	5.99	123.14	117.67
22	O	229	CHD	C1-C10-C9	-5.99	101.94	111.35
22	C	525	CHD	C6-C5-C4	-5.99	104.30	111.19
22	W	1059	CHD	C9-C11-C12	5.97	122.18	114.30
22	O	229	CHD	C11-C12-C13	5.92	117.32	111.24
22	J	60	CHD	C11-C12-C13	5.90	117.30	111.24
22	P	1271	CHD	C15-C14-C13	5.88	109.32	103.55
22	O	229	CHD	C5-C6-C7	5.87	120.94	114.46
22	C	525	CHD	C14-C13-C12	5.87	112.87	107.40
28	G	272	DMU	C18-O16-C6	5.86	123.56	113.84
28	G	272	DMU	O5-C4-C57	5.83	120.94	106.44
22	B	1085	CHD	C14-C8-C9	5.82	117.70	109.71
22	B	1085	CHD	C17-C13-C14	5.81	105.95	100.09
22	W	1059	CHD	C2-C1-C10	5.80	122.73	112.78
19	N	1521	TGL	CG2-OG2-CB1	5.80	132.06	117.79
14	N	515	HEA	C1B-C2B-C3B	-5.72	103.01	107.00
22	B	1085	CHD	C11-C12-C13	5.72	117.12	111.24
14	A	516	HEA	C20-C19-C18	-5.72	109.55	121.12
22	P	1271	CHD	C11-C12-C13	5.71	117.11	111.24
28	M	526	DMU	C2-C3-C4	5.71	124.01	110.93
22	W	1059	CHD	C11-C12-C13	5.70	117.10	111.24
22	W	1059	CHD	C1-C10-C9	-5.70	102.40	111.35
22	C	525	CHD	C11-C12-C13	5.69	117.09	111.24
22	P	1271	CHD	C14-C13-C12	5.67	112.68	107.40
22	C	271	CHD	C11-C9-C8	5.67	119.18	110.88
19	D	523	TGL	OG2-CB1-CB2	-5.66	99.29	111.50
28	P	1272	DMU	O5-C4-C3	5.63	121.62	109.75
28	Z	1526	DMU	O16-C6-C1	5.62	117.08	108.30
22	C	525	CHD	C11-C9-C10	5.60	119.50	113.73
20	C	268	PGV	O01-C1-C2	5.59	123.54	111.50
28	P	1272	DMU	C8-C7-C5	5.58	120.57	110.82
14	A	516	HEA	CMB-C2B-C1B	-5.58	119.89	128.46
22	O	229	CHD	C2-C1-C10	5.56	122.32	112.78
22	B	1085	CHD	C6-C7-C8	5.54	117.39	111.48
22	C	525	CHD	C5-C4-C3	5.53	120.89	112.76
14	A	515	HEA	CAA-CBA-CGA	-5.53	103.39	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	229	CHD	C6-C5-C4	-5.53	104.82	111.19
25	T	1269	CDL	OB6-CB5-C51	5.52	123.40	111.50
22	P	1525	CHD	C18-C13-C17	-5.49	102.62	111.21
22	O	229	CHD	C9-C8-C7	5.48	118.43	111.88
22	J	60	CHD	C15-C14-C8	5.46	125.96	118.33
22	P	1271	CHD	C2-C1-C10	5.46	122.14	112.78
22	C	525	CHD	O3-C3-C4	5.45	120.70	109.85
28	Z	1526	DMU	C8-C7-C5	5.44	120.32	110.82
22	J	60	CHD	C2-C1-C10	5.41	122.06	112.78
22	C	525	CHD	C18-C13-C14	-5.41	102.75	111.21
22	W	1059	CHD	C9-C10-C5	5.40	116.17	108.58
22	W	1059	CHD	C22-C20-C17	5.40	121.43	110.28
22	P	1525	CHD	C17-C13-C14	5.37	105.51	100.09
22	C	525	CHD	C18-C13-C17	-5.33	102.88	111.21
28	G	272	DMU	O5-C4-C3	5.33	120.98	109.75
22	O	229	CHD	C16-C17-C20	5.32	120.39	112.15
22	B	1085	CHD	O12-C12-C13	-5.31	102.05	111.03
22	B	1085	CHD	C4-C3-C2	5.31	116.89	110.55
22	P	1271	CHD	C4-C5-C10	5.31	118.30	112.66
20	P	1268	PGV	O03-C19-C20	5.30	128.55	111.91
22	C	271	CHD	C2-C1-C10	5.27	121.82	112.78
28	G	272	DMU	C8-C7-C5	5.22	119.93	110.82
22	C	525	CHD	C4-C5-C10	-5.20	107.14	112.66
28	Z	1526	DMU	O5-C4-C3	5.15	120.62	109.75
22	P	1525	CHD	O12-C12-C11	-5.15	98.64	109.12
14	A	516	HEA	C17-C18-C19	5.14	140.04	127.66
22	J	60	CHD	C9-C11-C12	5.09	121.02	114.30
28	Z	1526	DMU	O5-C4-C57	5.08	119.08	106.44
24	T	1264	PEK	O03-C01-C02	-5.05	93.73	108.43
14	N	515	HEA	C4B-C3B-C2B	5.04	110.39	106.87
22	B	1085	CHD	C16-C17-C20	5.04	119.94	112.15
25	C	270	CDL	OA6-CA5-C11	5.01	122.30	111.50
20	A	524	PGV	C02-O01-C1	5.00	130.11	117.79
22	O	229	CHD	C18-C13-C14	-4.99	103.40	111.21
22	J	60	CHD	C9-C10-C5	4.98	115.58	108.58
22	W	1059	CHD	C18-C13-C12	-4.96	104.02	109.07
22	C	271	CHD	C14-C8-C7	4.95	118.37	111.81
20	C	268	PGV	O03-C19-C20	4.95	127.44	111.91
22	J	60	CHD	C11-C9-C8	4.94	118.11	110.88
28	Z	1526	DMU	O1-C9-C11	4.93	118.70	106.44
28	P	1272	DMU	O1-C9-C11	4.92	118.67	106.44
22	P	1525	CHD	O12-C12-C13	-4.91	102.72	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	229	CHD	C14-C8-C9	4.91	116.45	109.71
19	L	522	TGL	OG3-CC1-OC1	-4.90	111.22	123.59
28	M	526	DMU	O5-C4-C3	4.90	120.08	109.75
22	C	271	CHD	C18-C13-C17	-4.88	103.58	111.21
24	G	265	PEK	O03-C21-C22	4.85	127.11	111.91
22	J	60	CHD	C14-C8-C7	4.84	118.23	111.81
22	C	271	CHD	C6-C5-C4	-4.83	105.63	111.19
22	W	1059	CHD	C11-C9-C10	4.83	118.70	113.73
24	S	1265	PEK	O03-C21-C22	4.82	127.05	111.91
28	G	272	DMU	O5-C6-C1	4.82	120.56	110.35
22	P	1271	CHD	C22-C23-C24	-4.77	103.34	113.59
14	N	515	HEA	C27-C19-C20	4.76	123.28	115.27
14	A	515	HEA	C26-C15-C16	4.75	123.26	115.27
19	N	1522	TGL	CG2-OG2-CB1	4.73	129.45	117.79
19	L	522	TGL	CG2-OG2-CB1	4.73	129.44	117.79
22	C	271	CHD	C9-C11-C12	4.70	120.50	114.30
28	P	1272	DMU	O5-C4-C57	4.68	118.08	106.44
28	P	1272	DMU	O5-C6-C1	4.66	120.21	110.35
25	G	269	CDL	OA6-CA5-C11	4.65	121.52	111.50
28	G	272	DMU	C2-C3-C4	4.65	121.58	110.93
22	P	1271	CHD	C19-C10-C9	-4.64	104.80	111.18
20	N	1524	PGV	O01-C1-C2	4.63	121.48	111.50
24	G	1263	PEK	O01-C1-C2	4.62	121.46	111.50
14	N	516	HEA	C4B-C3B-C2B	-4.61	103.65	106.87
28	G	272	DMU	O1-C9-C11	4.60	117.86	106.44
22	P	1525	CHD	C2-C1-C10	4.57	120.61	112.78
28	Z	1526	DMU	O7-C10-C5	-4.57	96.27	108.10
19	N	1522	TGL	OG2-CB1-CB2	4.56	121.34	111.50
28	Z	1526	DMU	C2-C3-C4	4.56	121.39	110.93
25	P	1270	CDL	OA6-CA5-C11	4.56	121.33	111.50
22	C	525	CHD	C2-C1-C10	4.55	120.59	112.78
22	C	271	CHD	C22-C23-C24	-4.54	103.82	113.59
19	L	522	TGL	OG3-CC1-CC2	4.52	126.08	111.91
22	W	1059	CHD	C9-C8-C7	4.50	117.25	111.88
22	J	60	CHD	C19-C10-C5	-4.50	102.74	110.36
22	C	271	CHD	C19-C10-C1	-4.49	101.02	108.26
22	C	525	CHD	O7-C7-C6	-4.48	98.82	109.94
22	W	1059	CHD	C18-C13-C14	-4.46	104.22	111.21
22	C	525	CHD	C9-C11-C12	4.45	120.17	114.30
28	P	1272	DMU	C7-C8-C9	4.42	118.13	110.24
22	P	1271	CHD	O12-C12-C11	-4.42	100.11	109.12
25	P	1270	CDL	OB8-CB7-C71	4.41	125.76	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	M	526	DMU	O1-C9-C11	4.40	117.37	106.44
14	N	516	HEA	C20-C21-C22	4.39	126.32	111.88
28	P	1272	DMU	C6-C1-C2	4.38	119.12	110.00
22	P	1525	CHD	O3-C3-C4	4.38	118.57	109.85
28	M	526	DMU	O5-C4-C57	4.37	117.31	106.44
20	C	267	PGV	C27-C26-C25	-4.37	92.25	114.42
19	L	522	TGL	OG1-CG1-CG2	4.37	121.15	108.43
22	P	1271	CHD	O7-C7-C6	-4.34	99.17	109.94
22	P	1271	CHD	C9-C11-C12	4.34	120.04	114.30
22	O	229	CHD	C4-C5-C10	-4.34	108.05	112.66
14	A	516	HEA	C27-C19-C20	4.34	122.57	115.27
22	B	1085	CHD	O12-C12-C11	-4.31	100.34	109.12
22	C	525	CHD	C13-C14-C8	4.30	120.23	114.74
22	P	1525	CHD	C1-C10-C9	-4.30	104.60	111.35
28	M	526	DMU	C8-C7-C5	4.30	118.32	110.82
22	B	1085	CHD	C11-C9-C8	4.29	117.16	110.88
22	P	1271	CHD	C13-C17-C20	4.28	124.61	119.50
22	P	1525	CHD	C22-C20-C17	-4.26	101.48	110.28
22	J	60	CHD	C18-C13-C17	-4.26	104.55	111.21
28	P	1272	DMU	O7-C10-C5	4.24	119.09	108.10
22	C	525	CHD	C22-C20-C17	-4.24	101.52	110.28
22	W	1059	CHD	C19-C10-C5	-4.23	103.18	110.36
14	A	516	HEA	CAD-CBD-CGD	4.23	119.77	112.67
22	P	1271	CHD	C23-C22-C20	-4.22	109.04	114.72
22	B	1085	CHD	C9-C8-C7	4.22	116.92	111.88
28	G	272	DMU	C7-C8-C9	4.19	117.72	110.24
25	T	1269	CDL	OA6-CA5-C11	4.17	120.48	111.50
22	B	1085	CHD	C15-C14-C8	4.16	124.14	118.33
22	P	1525	CHD	C1-C2-C3	4.15	115.79	110.47
28	G	272	DMU	C6-C1-C2	4.14	118.62	110.00
22	J	60	CHD	C22-C20-C17	4.13	118.82	110.28
24	G	265	PEK	O01-C1-C2	4.12	120.38	111.50
14	N	515	HEA	C17-C18-C19	-4.11	117.76	127.66
22	B	1085	CHD	O3-C3-C4	4.09	118.00	109.85
24	T	263	PEK	O01-C1-C2	4.08	120.29	111.50
24	C	264	PEK	C24-C23-C22	-4.08	98.54	113.19
20	N	1266	PGV	O01-C1-O02	-4.06	113.90	123.70
22	W	1059	CHD	C17-C13-C12	4.05	121.37	117.67
14	N	516	HEA	C21-C20-C19	4.05	126.29	112.98
14	A	516	HEA	CBD-CAD-C3D	4.05	119.95	112.49
19	A	521	TGL	OG1-CA1-CA2	4.04	124.60	111.91
14	A	515	HEA	CMC-C2C-C1C	-4.04	122.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	270	CDL	OB8-CB7-C71	4.04	124.58	111.91
22	P	1525	CHD	C19-C10-C5	-4.02	103.55	110.36
22	P	1271	CHD	C17-C13-C14	4.01	104.14	100.09
24	S	1265	PEK	O01-C1-C2	4.00	120.12	111.50
25	G	269	CDL	OA8-CA7-C31	3.96	124.34	111.91
22	B	1085	CHD	C6-C5-C4	-3.95	106.65	111.19
28	P	1272	DMU	C2-C3-C4	3.94	119.96	110.93
25	C	270	CDL	CB4-OB6-CB5	-3.93	108.13	117.79
22	J	60	CHD	C19-C10-C9	-3.91	105.79	111.18
28	M	526	DMU	O3-C5-C7	3.88	119.33	110.35
22	C	525	CHD	C1-C10-C9	-3.87	105.27	111.35
22	B	1085	CHD	O7-C7-C6	-3.85	100.39	109.94
14	A	516	HEA	C1B-C2B-C3B	3.84	109.67	107.00
28	G	272	DMU	O7-C3-C4	3.83	119.95	109.45
22	P	1525	CHD	C11-C12-C13	3.83	115.18	111.24
19	L	522	TGL	OG1-CA1-CA2	3.83	123.92	111.91
20	C	267	PGV	C8-C9-C10	-3.82	97.15	113.79
20	A	522	PGV	O03-C19-C20	3.80	123.82	111.91
26	R	1229	PSC	O01-C1-C2	3.79	119.68	111.50
28	M	526	DMU	O7-C3-C2	3.79	117.36	107.28
20	P	1267	PGV	O03-C19-O04	-3.78	114.05	123.59
28	Z	1526	DMU	C7-C8-C9	3.78	116.98	110.24
20	P	1267	PGV	C8-C9-C10	-3.77	97.36	113.79
22	C	525	CHD	C11-C9-C8	3.76	116.38	110.88
28	P	1272	DMU	C1-C2-C3	3.76	118.27	109.68
19	A	521	TGL	CG3-OG3-CC1	3.75	131.01	117.12
19	N	1521	TGL	CG3-OG3-CC1	3.75	131.01	117.12
28	P	1272	DMU	C18-O16-C6	3.75	120.06	113.84
25	P	1270	CDL	OB8-CB7-OB9	-3.74	114.15	123.59
19	A	521	TGL	CB3-CB2-CB1	-3.74	100.03	113.62
28	G	272	DMU	C6-O5-C4	3.72	121.00	113.69
19	A	521	TGL	OG2-CG2-CG1	3.71	121.83	108.40
22	C	271	CHD	C21-C20-C17	3.71	118.60	112.92
28	Z	1526	DMU	C6-O5-C4	3.71	120.97	113.69
14	N	516	HEA	C1B-C2B-C3B	-3.68	104.44	107.00
22	C	525	CHD	C14-C8-C9	3.66	114.74	109.71
22	P	1525	CHD	C13-C17-C20	3.66	123.86	119.50
25	C	270	CDL	OB8-CB7-OB9	-3.66	114.36	123.59
14	A	516	HEA	C21-C20-C19	3.66	125.01	112.98
22	J	60	CHD	C18-C13-C14	-3.65	105.50	111.21
22	J	60	CHD	C6-C5-C4	-3.64	107.00	111.19
22	J	60	CHD	C11-C9-C10	3.64	117.48	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C18-C13-C17	-3.63	105.52	111.21
22	C	525	CHD	C5-C6-C7	3.63	118.47	114.46
20	N	1266	PGV	O03-C19-C20	3.62	123.27	111.91
28	M	526	DMU	C7-C8-C9	3.62	116.69	110.24
28	P	1272	DMU	O5-C6-O16	3.60	118.51	109.97
19	L	522	TGL	OG2-CB1-CB2	3.60	119.25	111.50
14	N	516	HEA	OMA-CMA-C3A	-3.59	117.08	124.91
22	W	1059	CHD	C11-C9-C8	3.56	116.09	110.88
28	P	1272	DMU	C6-O5-C4	3.56	120.67	113.69
19	A	521	TGL	OG1-CG1-CG2	3.55	118.77	108.43
24	C	264	PEK	O01-C1-O02	-3.55	115.12	123.70
22	B	1085	CHD	C1-C10-C9	-3.54	105.78	111.35
14	A	516	HEA	O11-C11-C12	3.53	123.19	109.55
22	P	1525	CHD	C9-C11-C12	3.52	118.94	114.30
22	O	229	CHD	C15-C14-C13	3.51	107.00	103.55
14	N	516	HEA	C26-C15-C14	-3.50	114.69	123.68
19	A	521	TGL	OG2-CG2-CG3	3.49	121.02	108.40
14	N	516	HEA	C3C-C4C-NC	3.49	113.72	109.21
28	M	526	DMU	O7-C10-C5	-3.49	99.07	108.10
22	C	271	CHD	C23-C22-C20	-3.46	110.06	114.72
22	C	271	CHD	O12-C12-C11	-3.45	102.09	109.12
28	G	272	DMU	O7-C3-C2	3.45	116.46	107.28
22	B	1085	CHD	C11-C9-C10	3.45	117.28	113.73
19	D	523	TGL	OG1-CA1-CA2	3.44	122.70	111.91
19	N	1521	TGL	OG1-CA1-CA2	3.43	122.67	111.91
19	Q	1523	TGL	OG3-CC1-CC2	3.43	122.67	111.91
22	B	1085	CHD	C9-C11-C12	3.42	118.81	114.30
19	D	523	TGL	CG2-OG2-CB1	3.40	126.15	117.79
22	C	525	CHD	C15-C16-C17	3.39	111.86	105.13
22	P	1525	CHD	C14-C8-C9	3.38	114.35	109.71
14	A	516	HEA	C26-C15-C14	-3.36	115.05	123.68
28	G	272	DMU	O7-C10-C5	3.36	116.80	108.10
14	A	515	HEA	C3C-C4C-NC	3.35	113.54	109.21
20	N	1524	PGV	C01-O03-C19	3.34	129.51	117.12
14	N	516	HEA	CAA-CBA-CGA	-3.33	107.08	112.67
28	Z	1526	DMU	C1-C2-C3	3.32	117.27	109.68
28	G	272	DMU	C1-C2-C3	3.32	117.26	109.68
22	J	60	CHD	C9-C8-C7	3.31	115.83	111.88
22	P	1271	CHD	O12-C12-C13	-3.30	105.45	111.03
28	M	526	DMU	C10-C5-C7	3.29	116.85	110.00
24	G	265	PEK	O03-C21-O04	-3.29	115.30	123.59
19	D	523	TGL	CG1-OG1-CA1	3.29	129.29	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1085	CHD	C22-C23-C24	-3.28	106.53	113.59
22	P	1525	CHD	C22-C23-C24	-3.26	106.58	113.59
22	J	60	CHD	O7-C7-C6	-3.26	101.86	109.94
28	P	1272	DMU	O7-C3-C4	3.26	118.38	109.45
19	L	522	TGL	CC3-CC2-CC1	3.25	125.44	113.62
28	P	1272	DMU	C10-O1-C9	3.24	120.05	113.69
24	T	263	PEK	O03-C21-C22	3.20	121.95	111.91
22	P	1271	CHD	C6-C5-C4	-3.20	107.51	111.19
20	N	1266	PGV	O03-C01-C02	3.19	117.73	108.43
14	N	515	HEA	CMD-C2D-C3D	3.19	130.96	124.94
28	M	526	DMU	C57-C4-C3	3.18	122.57	113.33
26	E	229	PSC	O01-C1-O02	-3.17	116.04	123.70
22	P	1525	CHD	C11-C9-C10	3.15	116.98	113.73
22	W	1059	CHD	C23-C22-C20	-3.13	110.50	114.72
28	M	526	DMU	O7-C10-O1	-3.13	101.93	110.67
24	G	1263	PEK	O03-C21-C22	3.13	121.73	111.91
20	C	268	PGV	O04-C19-C20	-3.13	111.53	123.73
14	N	516	HEA	C25-C23-C24	-3.12	107.70	114.60
22	B	1085	CHD	C19-C10-C5	-3.10	105.11	110.36
22	B	1085	CHD	C21-C20-C17	3.10	117.66	112.92
19	N	1522	TGL	OG3-CG3-CG2	3.08	117.41	108.43
14	A	516	HEA	CBA-CAA-C2A	-3.08	106.80	112.48
28	M	526	DMU	O16-C6-C1	3.07	113.09	108.30
26	R	1229	PSC	O03-C19-C20	3.02	121.38	111.91
22	P	1525	CHD	C9-C8-C7	3.01	115.47	111.88
20	A	524	PGV	O01-C02-C03	2.99	119.23	108.40
24	S	1265	PEK	O03-C01-C02	2.98	117.11	108.43
14	A	515	HEA	CMC-C2C-C3C	2.98	130.25	124.68
19	N	1522	TGL	OG1-CA1-CA2	2.97	121.22	111.91
19	N	1522	TGL	OG3-CC1-CC2	2.96	121.19	111.91
28	G	272	DMU	O5-C6-O16	2.96	116.97	109.97
28	G	272	DMU	C10-O1-C9	2.95	119.49	113.69
25	G	269	CDL	C80-C79-C78	2.95	129.40	114.42
22	C	525	CHD	O12-C12-C11	-2.95	103.12	109.12
19	Q	1523	TGL	OG2-CG2-CG3	2.94	119.06	108.40
28	Z	1526	DMU	O3-C5-C7	2.93	117.13	110.35
28	G	272	DMU	C10-C5-C7	2.92	116.08	110.00
20	P	1268	PGV	C03-C02-C01	-2.92	104.88	111.79
22	J	60	CHD	C23-C22-C20	-2.92	110.79	114.72
19	N	1522	TGL	CG3-OG3-CC1	2.92	127.93	117.12
20	A	524	PGV	C3-C2-C1	-2.91	103.02	113.62
19	D	523	TGL	OG2-CB1-OB1	2.91	130.74	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	270	CDL	C52-C51-CB5	-2.91	103.04	113.62
14	N	515	HEA	CBA-CAA-C2A	2.91	117.83	112.48
28	P	1272	DMU	C11-C9-C8	2.90	119.79	113.00
28	M	526	DMU	C31-C28-C25	-2.89	99.75	114.42
20	P	1268	PGV	O04-C19-C20	-2.89	112.47	123.73
20	P	1267	PGV	C27-C26-C25	-2.89	99.77	114.42
22	P	1525	CHD	C16-C17-C13	2.89	106.38	103.55
22	W	1059	CHD	O7-C7-C6	-2.88	102.79	109.94
22	P	1271	CHD	C17-C13-C12	2.87	120.29	117.67
24	C	264	PEK	O04-C21-C22	2.87	134.93	123.73
22	B	1085	CHD	C4-C5-C10	-2.86	109.62	112.66
28	P	1272	DMU	O16-C18-C19	2.85	119.57	109.56
20	A	522	PGV	O03-C19-O04	-2.85	116.39	123.59
24	T	1264	PEK	O01-C1-O02	-2.84	116.83	123.70
25	G	269	CDL	C82-C81-C80	2.84	128.86	114.42
19	N	1521	TGL	OG3-CC1-CC2	2.84	120.82	111.91
25	G	269	CDL	CA6-OA8-CA7	2.84	127.63	117.12
19	N	1522	TGL	OG1-CG1-CG2	2.83	116.69	108.43
14	A	516	HEA	CMB-C2B-C3B	2.82	130.20	124.69
25	P	1270	CDL	OB6-CB4-CB6	2.81	118.59	108.40
20	N	1524	PGV	C02-O01-C1	2.80	124.68	117.79
20	A	522	PGV	C02-O01-C1	2.79	124.67	117.79
26	E	229	PSC	C02-O01-C1	2.78	124.64	117.79
20	C	267	PGV	O14-P-O13	2.78	125.98	112.24
24	T	1264	PEK	C24-C23-C22	-2.77	103.24	113.19
19	Q	1523	TGL	CG2-OG2-CB1	2.77	124.60	117.79
22	O	229	CHD	O12-C12-C11	-2.76	103.51	109.12
22	O	229	CHD	C14-C8-C7	2.75	115.46	111.81
22	C	271	CHD	C17-C13-C14	2.75	102.87	100.09
24	C	264	PEK	O03-C21-C22	-2.75	103.28	111.91
19	L	522	TGL	CB4-CB3-CB2	-2.75	103.32	113.19
22	P	1271	CHD	C19-C10-C1	-2.73	103.86	108.26
22	P	1525	CHD	C4-C5-C10	-2.73	109.76	112.66
19	N	1522	TGL	OG3-CC1-OC1	-2.73	116.71	123.59
20	A	524	PGV	O03-C19-C20	2.72	120.45	111.91
28	G	272	DMU	C11-C9-C8	2.72	119.37	113.00
25	T	1269	CDL	OB8-CB6-CB4	2.71	116.33	108.43
22	J	60	CHD	C14-C8-C9	2.71	113.43	109.71
20	P	1267	PGV	O03-C19-C20	2.71	120.40	111.91
14	A	516	HEA	C17-C16-C15	-2.70	104.09	112.98
25	G	269	CDL	OB8-CB7-C71	2.70	120.37	111.91
24	G	1263	PEK	O03-C21-O04	-2.69	116.81	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	1269	CDL	CA4-OA6-CA5	-2.68	111.19	117.79
25	T	1269	CDL	C83-C82-C81	2.68	128.03	114.42
28	Z	1526	DMU	C10-C5-C7	2.68	115.58	110.00
22	O	229	CHD	C6-C7-C8	2.68	114.34	111.48
22	P	1525	CHD	C21-C20-C22	-2.67	106.19	110.36
24	T	1264	PEK	C3-C2-C1	2.66	123.31	113.62
20	A	524	PGV	O01-C1-C2	2.66	117.22	111.50
22	B	1085	CHD	C2-C1-C10	2.64	117.31	112.78
28	Z	1526	DMU	O5-C6-O16	2.64	116.23	109.97
22	C	271	CHD	C19-C10-C9	-2.64	107.55	111.18
22	P	1525	CHD	C14-C8-C7	2.63	115.30	111.81
24	S	1265	PEK	O03-C21-O04	-2.62	116.97	123.59
25	P	1270	CDL	OA8-CA7-C31	2.61	120.10	111.91
19	A	521	TGL	C15-CC9-CC8	2.60	127.64	114.42
19	N	1522	TGL	OB1-CB1-CB2	-2.60	113.58	123.73
19	A	521	TGL	CG3-CG2-CG1	-2.58	105.68	111.79
26	E	229	PSC	C32-C31-C30	-2.58	101.33	114.42
14	N	516	HEA	C12-C11-C3B	2.58	119.33	112.56
19	D	523	TGL	C10-CB9-CB8	2.57	127.45	114.42
19	Q	1523	TGL	OG2-CB1-CB2	2.56	117.02	111.50
19	N	1522	TGL	C15-CC9-CC8	2.56	127.43	114.42
28	M	526	DMU	O5-C6-O16	2.55	116.02	109.97
20	P	1268	PGV	O02-C1-C2	-2.55	113.78	123.73
25	T	1269	CDL	C39-C38-C37	2.55	127.36	114.42
24	G	1263	PEK	C02-O01-C1	2.54	124.05	117.79
25	G	269	CDL	C19-C18-C17	2.54	127.33	114.42
25	T	1269	CDL	OB8-CB7-C71	2.54	119.87	111.91
28	M	526	DMU	C6-C1-C2	2.54	115.28	110.00
22	J	60	CHD	C17-C13-C14	2.53	102.65	100.09
22	P	1525	CHD	C5-C6-C7	2.53	117.25	114.46
24	C	264	PEK	C30-C29-C28	-2.53	101.60	114.42
22	C	271	CHD	C19-C10-C5	-2.52	106.08	110.36
20	C	268	PGV	C01-O03-C19	2.52	126.45	117.12
14	A	515	HEA	C27-C19-C18	-2.52	117.22	123.68
28	M	526	DMU	O4-C7-C5	2.51	116.16	110.35
25	G	269	CDL	OB8-CB7-OB9	-2.51	117.25	123.59
20	N	1524	PGV	O03-C19-C20	2.50	119.77	111.91
24	C	264	PEK	O01-C02-C01	-2.50	99.34	108.40
28	M	526	DMU	C6-O5-C4	2.50	118.60	113.69
19	L	522	TGL	OB1-CB1-CB2	-2.50	113.98	123.73
22	C	271	CHD	C9-C10-C5	2.50	112.09	108.58
25	T	1269	CDL	OA8-CA7-C31	2.50	119.74	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	1266	PGV	C23-C22-C21	-2.49	101.77	114.42
25	T	1269	CDL	CB6-CB4-CB3	-2.49	105.91	111.79
28	G	272	DMU	O4-C7-C5	2.49	116.10	110.35
19	L	522	TGL	CA5-CA4-CA3	-2.49	101.80	114.42
25	T	1269	CDL	OB8-CB7-OB9	-2.48	117.32	123.59
25	P	1270	CDL	OA6-CA5-OA7	-2.48	117.72	123.70
20	C	268	PGV	O02-C1-C2	-2.48	114.08	123.73
25	C	270	CDL	C53-C52-C51	-2.47	104.30	113.19
14	A	515	HEA	CMB-C2B-C1B	-2.47	124.66	128.46
22	O	229	CHD	C9-C11-C12	2.47	117.56	114.30
20	N	1266	PGV	O03-C19-O04	-2.47	117.37	123.59
20	P	1267	PGV	O14-P-O13	2.47	124.44	112.24
25	G	269	CDL	CB6-CB4-CB3	-2.46	105.98	111.79
22	C	271	CHD	C9-C8-C7	2.45	114.81	111.88
28	Z	1526	DMU	C6-C1-C2	2.45	115.10	110.00
14	A	516	HEA	C13-C14-C15	-2.45	121.77	127.66
25	G	269	CDL	OB7-CB5-C51	-2.45	114.19	123.73
25	C	270	CDL	O1-C1-CB2	2.45	118.14	109.56
22	J	60	CHD	C13-C14-C8	2.44	117.86	114.74
14	A	515	HEA	C26-C15-C14	-2.44	117.42	123.68
14	N	516	HEA	CMB-C2B-C3B	2.44	129.46	124.69
22	P	1271	CHD	C19-C10-C5	-2.43	106.24	110.36
28	Z	1526	DMU	O7-C3-C2	2.42	113.73	107.28
25	G	269	CDL	C17-C16-C15	-2.42	102.16	114.42
25	C	270	CDL	OA8-CA7-C31	2.42	119.49	111.91
19	D	523	TGL	CB3-CB2-CB1	2.41	122.39	113.62
14	A	515	HEA	CAA-C2A-C3A	2.41	132.81	126.86
25	T	1269	CDL	C82-C81-C80	2.41	126.65	114.42
20	A	522	PGV	O03-C01-C02	2.39	115.40	108.43
28	P	1272	DMU	C57-C4-C3	2.39	120.29	113.33
19	N	1522	TGL	CC3-CC2-CC1	2.38	122.29	113.62
14	N	515	HEA	C27-C19-C18	-2.38	117.57	123.68
19	Q	1523	TGL	OG1-CA1-CA2	2.38	119.38	111.91
22	P	1271	CHD	C9-C10-C5	2.38	111.92	108.58
28	Z	1526	DMU	C57-C4-C3	2.38	120.25	113.33
19	A	521	TGL	CB4-CB3-CB2	2.38	121.75	113.19
22	B	1085	CHD	C14-C8-C7	2.37	114.95	111.81
19	N	1521	TGL	OG2-CG2-CG3	2.37	116.98	108.40
22	O	229	CHD	C19-C10-C5	-2.37	106.35	110.36
19	Q	1523	TGL	OG3-CC1-OC1	-2.36	117.63	123.59
20	N	1524	PGV	O01-C1-O02	-2.36	117.99	123.70
28	Z	1526	DMU	C10-O1-C9	2.36	118.31	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	1521	TGL	OG2-CB1-CB2	2.35	116.57	111.50
22	P	1525	CHD	C23-C22-C20	-2.35	111.56	114.72
19	N	1521	TGL	OG2-CG2-CG1	2.35	116.91	108.40
22	P	1271	CHD	C21-C20-C17	2.35	116.52	112.92
24	C	264	PEK	C32-C31-C30	-2.35	102.50	114.42
20	P	1267	PGV	O01-C1-O02	-2.35	118.03	123.70
19	N	1521	TGL	OG1-CA1-OA1	-2.35	117.67	123.59
25	C	270	CDL	C82-C81-C80	2.35	126.34	114.42
25	T	1269	CDL	CB2-C1-CA2	-2.34	105.90	112.79
24	C	264	PEK	O03-C01-C02	-2.34	101.63	108.43
28	Z	1526	DMU	C11-C9-C8	2.33	118.47	113.00
22	J	60	CHD	C1-C10-C9	-2.33	107.69	111.35
25	T	1269	CDL	CB6-OB8-CB7	2.33	125.73	117.12
22	C	271	CHD	C14-C8-C9	2.32	112.90	109.71
24	T	1264	PEK	C03-C02-C01	-2.32	106.30	111.79
19	Q	1523	TGL	CG1-OG1-CA1	2.32	125.70	117.12
25	G	269	CDL	CB6-OB8-CB7	2.32	125.70	117.12
26	R	1229	PSC	O03-C19-O04	-2.32	117.75	123.59
25	G	269	CDL	OA8-CA7-OA9	-2.31	117.76	123.59
22	C	525	CHD	C22-C23-C24	-2.31	108.63	113.59
19	N	1522	TGL	C10-CB9-CB8	2.30	126.10	114.42
28	M	526	DMU	C1-C2-C3	2.30	114.93	109.68
22	O	229	CHD	C16-C17-C13	2.30	105.81	103.55
25	C	270	CDL	C42-C41-C40	2.30	126.09	114.42
28	M	526	DMU	C25-C22-C19	-2.29	102.81	114.42
24	T	263	PEK	O03-C01-C02	2.29	115.09	108.43
22	P	1525	CHD	O7-C7-C8	-2.28	104.32	109.43
22	W	1059	CHD	C19-C10-C1	-2.28	104.58	108.26
14	N	515	HEA	C16-C17-C18	2.28	119.38	111.88
19	N	1522	TGL	CA5-CA4-CA3	-2.28	102.87	114.42
25	P	1270	CDL	C39-C38-C37	2.27	125.95	114.42
14	N	516	HEA	CMD-C2D-C3D	-2.27	120.67	124.94
28	M	526	DMU	O55-C2-C3	2.26	115.94	109.94
19	Q	1523	TGL	CG3-OG3-CC1	2.26	125.48	117.12
24	T	263	PEK	C2-C3-C4	2.26	117.25	113.23
19	L	522	TGL	C15-CC9-CC8	2.26	125.89	114.42
24	C	264	PEK	C11-C10-C9	2.26	123.13	112.02
19	N	1522	TGL	OG2-CG2-CG3	2.25	116.56	108.40
14	N	515	HEA	C26-C15-C16	2.25	119.06	115.27
19	L	522	TGL	C26-C25-C24	-2.25	102.98	114.42
20	P	1267	PGV	O02-C1-C2	2.25	132.51	123.73
25	G	269	CDL	OA6-CA5-OA7	-2.25	118.26	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	522	TGL	CA3-CA2-CA1	-2.25	105.45	113.62
25	T	1269	CDL	C43-C42-C41	2.24	125.81	114.42
22	C	525	CHD	C21-C20-C17	-2.24	109.49	112.92
28	P	1272	DMU	C10-C5-C7	2.24	114.67	110.00
24	T	263	PEK	C01-O03-C21	2.24	125.42	117.12
14	N	515	HEA	CMC-C2C-C3C	2.24	128.87	124.68
28	G	272	DMU	O61-C57-C4	2.24	118.98	111.29
20	A	522	PGV	C7-C6-C5	-2.23	103.11	114.42
22	P	1271	CHD	C11-C9-C10	-2.23	111.43	113.73
22	W	1059	CHD	C21-C20-C17	2.22	116.32	112.92
22	J	60	CHD	O12-C12-C11	-2.22	104.60	109.12
24	C	264	PEK	C26-C25-C24	-2.22	103.16	114.42
14	A	515	HEA	C20-C19-C18	2.22	125.60	121.12
19	D	523	TGL	C13-C12-C11	2.21	125.65	114.42
20	C	268	PGV	O01-C02-C01	2.21	116.41	108.40
19	D	523	TGL	CG3-OG3-CC1	2.21	125.30	117.12
20	N	1266	PGV	O02-C1-C2	2.21	132.34	123.73
25	P	1270	CDL	C40-C39-C38	2.21	125.62	114.42
20	A	524	PGV	C01-O03-C19	2.20	125.28	117.12
22	P	1525	CHD	C15-C14-C8	2.20	121.41	118.33
19	A	521	TGL	OB1-CB1-CB2	-2.20	115.15	123.73
19	N	1521	TGL	CC4-CC3-CC2	-2.20	105.30	113.19
25	T	1269	CDL	OA8-CA7-OA9	-2.19	118.06	123.59
24	T	263	PEK	C02-O01-C1	2.19	123.19	117.79
19	A	521	TGL	C16-C15-CC9	2.19	125.56	114.42
22	B	1085	CHD	C16-C17-C13	2.19	105.70	103.55
25	C	270	CDL	OA8-CA6-CA4	2.18	114.79	108.43
25	P	1270	CDL	C42-C41-C40	2.17	125.45	114.42
20	P	1268	PGV	O01-C02-C03	2.17	116.26	108.40
28	P	1272	DMU	O61-C57-C4	2.17	118.73	111.29
20	C	267	PGV	C14-C13-C12	-2.17	100.01	112.43
25	P	1270	CDL	C52-C51-CB5	-2.17	105.74	113.62
24	T	1264	PEK	C30-C29-C28	-2.17	103.43	114.42
25	P	1270	CDL	CB4-OB6-CB5	-2.17	112.46	117.79
14	A	515	HEA	OMA-CMA-C3A	-2.17	120.19	124.91
22	O	229	CHD	O7-C7-C6	-2.16	104.57	109.94
25	G	269	CDL	C43-C42-C41	2.16	125.41	114.42
24	G	1263	PEK	C01-O03-C21	2.16	125.13	117.12
20	P	1268	PGV	O12-P-O13	-2.16	100.63	109.07
26	R	1229	PSC	O01-C1-O02	-2.15	118.51	123.70
22	O	229	CHD	C19-C10-C1	2.15	111.72	108.26
19	D	523	TGL	OG1-CA1-OA1	-2.14	118.19	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	522	TGL	C24-C23-C22	-2.14	103.56	114.42
22	J	60	CHD	O7-C7-C8	-2.14	104.64	109.43
19	Q	1523	TGL	OG1-CA1-OA1	-2.13	118.20	123.59
25	C	270	CDL	C57-C56-C55	-2.13	103.61	114.42
14	N	515	HEA	CMB-C2B-C3B	2.12	128.85	124.69
22	P	1525	CHD	C9-C10-C5	2.12	111.56	108.58
28	M	526	DMU	O49-C1-C2	2.11	115.24	110.35
24	S	1265	PEK	P-O11-C03	2.11	134.06	121.68
26	E	229	PSC	O01-C02-C03	2.10	116.00	108.40
25	C	270	CDL	C61-C60-C59	-2.10	103.77	114.42
25	T	1269	CDL	OA6-CA5-OA7	-2.10	118.63	123.70
25	P	1270	CDL	OA8-CA6-CA4	2.10	114.54	108.43
22	P	1525	CHD	C21-C20-C17	2.09	116.13	112.92
19	N	1521	TGL	C16-C15-CC9	2.09	125.05	114.42
26	R	1229	PSC	O01-C02-C03	2.09	115.98	108.40
19	L	522	TGL	CB9-CB8-CB7	-2.08	103.84	114.42
24	C	264	PEK	C27-C26-C25	-2.08	103.85	114.42
19	D	523	TGL	OG3-CC1-CC2	2.08	118.44	111.91
19	L	522	TGL	OG3-CG3-CG2	2.07	114.47	108.43
19	A	521	TGL	CC3-CC2-CC1	2.07	121.16	113.62
22	W	1059	CHD	C16-C17-C20	2.07	115.35	112.15
20	N	1524	PGV	O03-C19-O04	-2.07	118.37	123.59
25	C	270	CDL	OA6-CA5-OA7	-2.07	118.70	123.70
19	D	523	TGL	OG3-CC1-OC1	-2.07	118.37	123.59
19	N	1522	TGL	C16-C15-CC9	2.07	124.92	114.42
19	N	1521	TGL	OG3-CC1-OC1	-2.06	118.39	123.59
19	A	521	TGL	OA1-CA1-CA2	-2.06	115.69	123.73
20	A	522	PGV	C21-C20-C19	-2.06	106.14	113.62
22	P	1525	CHD	C16-C17-C20	2.05	115.32	112.15
25	P	1270	CDL	C55-C54-C53	-2.05	104.03	114.42
22	P	1271	CHD	C13-C14-C8	2.04	117.35	114.74
19	N	1521	TGL	CG1-OG1-CA1	2.04	124.69	117.12
26	E	229	PSC	C3-C2-C1	2.04	121.04	113.62
20	A	524	PGV	C8-C9-C10	-2.04	104.91	113.79
25	C	270	CDL	C79-C78-C77	2.03	124.75	114.42
25	G	269	CDL	C18-C17-C16	-2.03	104.12	114.42
25	P	1270	CDL	C82-C81-C80	2.03	124.72	114.42
22	C	271	CHD	C13-C17-C20	2.03	121.92	119.50
28	M	526	DMU	C11-C9-C8	2.02	117.74	113.00
22	J	60	CHD	O12-C12-C13	-2.02	107.61	111.03
24	T	1264	PEK	C28-C27-C26	-2.02	104.19	114.42

All (39) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	P	1272	DMU	C5
28	P	1272	DMU	C6
28	P	1272	DMU	C9
28	P	1272	DMU	C4
28	P	1272	DMU	C2
28	P	1272	DMU	C10
22	W	1059	CHD	C17
22	W	1059	CHD	C9
28	M	526	DMU	C2
28	M	526	DMU	C4
28	M	526	DMU	C9
28	M	526	DMU	C5
22	J	60	CHD	C17
22	J	60	CHD	C9
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
28	G	272	DMU	C5
28	G	272	DMU	C6
28	G	272	DMU	C9
28	G	272	DMU	C4
28	G	272	DMU	C2
28	G	272	DMU	C3
22	P	1271	CHD	C9
28	Z	1526	DMU	C2
28	Z	1526	DMU	C4
28	Z	1526	DMU	C9
28	Z	1526	DMU	C6
28	Z	1526	DMU	C5
14	A	515	HEA	ND
14	A	515	HEA	NA
14	A	515	HEA	NB
14	A	516	HEA	ND
14	A	516	HEA	NA
14	A	516	HEA	NB
14	N	516	HEA	ND
14	N	516	HEA	NA
14	N	516	HEA	NB
22	C	271	CHD	C9

All (991) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	P	1268	PGV	O12-C04-C05-C06
20	P	1268	PGV	C2-C1-O01-C02
25	P	1270	CDL	CA2-OA2-PA1-OA3
25	P	1270	CDL	CA2-OA2-PA1-OA4
25	P	1270	CDL	CA2-OA2-PA1-OA5
25	P	1270	CDL	C11-CA5-OA6-CA4
25	P	1270	CDL	CB2-OB2-PB2-OB3
22	W	1059	CHD	C13-C17-C20-C22
22	W	1059	CHD	C16-C17-C20-C21
22	W	1059	CHD	C16-C17-C20-C22
26	R	1229	PSC	C03-O11-P-O14
26	R	1229	PSC	C04-O12-P-O11
26	R	1229	PSC	C04-O12-P-O13
26	R	1229	PSC	C04-O12-P-O14
26	R	1229	PSC	O02-C1-O01-C02
24	G	1263	PEK	C03-O11-P-O13
24	G	1263	PEK	O12-C04-C05-N
24	G	1263	PEK	C7-C8-C9-C10
28	M	526	DMU	O5-C6-O16-C18
25	G	269	CDL	O1-C1-CA2-OA2
25	G	269	CDL	CA2-C1-CB2-OB2
25	G	269	CDL	OA9-CA7-OA8-CA6
25	G	269	CDL	C31-CA7-OA8-CA6
25	G	269	CDL	C1-CB2-OB2-PB2
25	G	269	CDL	CB3-OB5-PB2-OB3
25	G	269	CDL	CB3-OB5-PB2-OB4
20	C	268	PGV	C04-C05-C06-O06
20	C	268	PGV	C2-C1-O01-C02
14	N	515	HEA	C14-C15-C16-C17
14	N	515	HEA	C26-C15-C16-C17
25	C	270	CDL	CB2-C1-CA2-OA2
25	C	270	CDL	O1-C1-CB2-OB2
25	C	270	CDL	CA2-OA2-PA1-OA3
25	C	270	CDL	CA2-OA2-PA1-OA4
25	C	270	CDL	CA2-OA2-PA1-OA5
25	C	270	CDL	C11-CA5-OA6-CA4
24	G	265	PEK	O12-C04-C05-N
28	G	272	DMU	C1-C6-O16-C18
28	Z	1526	DMU	C19-C18-O16-C6
19	Q	1523	TGL	CC2-CC1-OG3-CG3
25	T	1269	CDL	C1-CB2-OB2-PB2
25	T	1269	CDL	CB3-OB5-PB2-OB2
25	T	1269	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	CB3-OB5-PB2-OB4
19	A	521	TGL	OB1-CB1-OG2-CG2
19	A	521	TGL	CC2-CC1-OG3-CG3
19	A	521	TGL	OC1-CC1-OG3-CG3
24	C	264	PEK	O12-C04-C05-N
24	C	264	PEK	C11-C12-C13-C14
14	A	516	HEA	C2D-C3D-CAD-CBD
14	A	516	HEA	C4D-C3D-CAD-CBD
14	A	516	HEA	C3B-C11-C12-C13
24	T	1264	PEK	C7-C8-C9-C10
24	T	1264	PEK	C11-C12-C13-C14
24	T	1264	PEK	C12-C13-C14-C15
26	E	229	PSC	C04-O12-P-O11
26	E	229	PSC	C04-O12-P-O13
26	E	229	PSC	C04-O12-P-O14
26	E	229	PSC	C2-C1-O01-C02
20	N	1524	PGV	C03-O11-P-O13
20	N	1524	PGV	C02-C03-O11-P
20	N	1524	PGV	O02-C1-O01-C02
20	N	1524	PGV	C2-C1-O01-C02
24	T	263	PEK	C03-O11-P-O13
24	T	263	PEK	C04-O12-P-O13
20	A	524	PGV	C04-O12-P-O11
20	A	524	PGV	C04-O12-P-O13
20	A	524	PGV	C04-O12-P-O14
20	A	524	PGV	C02-C03-O11-P
20	A	524	PGV	C04-C05-C06-O06
20	A	524	PGV	O02-C1-O01-C02
24	S	1265	PEK	C04-O12-P-O11
24	S	1265	PEK	C04-O12-P-O13
24	S	1265	PEK	C04-O12-P-O14
24	S	1265	PEK	O12-C04-C05-N
14	N	516	HEA	C2D-C3D-CAD-CBD
14	N	516	HEA	C4D-C3D-CAD-CBD
14	N	516	HEA	C3B-C11-C12-C13
14	N	516	HEA	O11-C11-C12-C13
19	Q	1523	TGL	OC1-CC1-OG3-CG3
20	A	524	PGV	O04-C19-O03-C01
19	D	523	TGL	CC2-CC1-OG3-CG3
20	A	524	PGV	C20-C19-O03-C01
19	D	523	TGL	OC1-CC1-OG3-CG3
22	P	1271	CHD	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
22	C	271	CHD	C16-C17-C20-C21
22	P	1271	CHD	C16-C17-C20-C22
25	P	1270	CDL	OA7-CA5-OA6-CA4
25	P	1270	CDL	OB7-CB5-OB6-CB4
25	C	270	CDL	OA7-CA5-OA6-CA4
19	L	522	TGL	OB1-CB1-OG2-CG2
26	E	229	PSC	O02-C1-O01-C02
26	R	1229	PSC	O04-C19-O03-C01
20	N	1524	PGV	C20-C19-O03-C01
25	P	1270	CDL	C51-CB5-OB6-CB4
26	R	1229	PSC	C2-C1-O01-C02
19	L	522	TGL	CB2-CB1-OG2-CG2
20	A	524	PGV	C2-C1-O01-C02
22	J	60	CHD	C16-C17-C20-C22
26	R	1229	PSC	C20-C19-O03-C01
19	L	522	TGL	CA2-CA1-OG1-CG1
26	E	229	PSC	C20-C19-O03-C01
19	N	1522	TGL	CA2-CA1-OG1-CG1
20	P	1268	PGV	C10-C11-C12-C13
24	G	1263	PEK	C4-C5-C6-C7
20	C	267	PGV	C10-C11-C12-C13
24	C	264	PEK	C10-C11-C12-C13
24	C	264	PEK	C13-C14-C15-C16
20	P	1267	PGV	C10-C11-C12-C13
24	T	263	PEK	C4-C5-C6-C7
24	T	263	PEK	C13-C14-C15-C16
24	S	1265	PEK	C4-C5-C6-C7
20	P	1268	PGV	O02-C1-O01-C02
20	C	268	PGV	O02-C1-O01-C02
20	N	1524	PGV	O04-C19-O03-C01
19	N	1522	TGL	OA1-CA1-OG1-CG1
26	R	1229	PSC	C22-C23-C24-C25
22	C	271	CHD	C16-C17-C20-C22
28	M	526	DMU	O5-C4-C57-O61
28	G	272	DMU	O6-C11-C9-O1
28	Z	1526	DMU	O5-C4-C57-O61
25	T	1269	CDL	O1-C1-CA2-OA2
20	N	1524	PGV	O12-C04-C05-O05
25	T	1269	CDL	C31-CA7-OA8-CA6
25	T	1269	CDL	C71-CB7-OB8-CB6
19	A	521	TGL	C13-C14-C29-C30
19	N	1522	TGL	CC3-CC4-CC5-CC6

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Mol	Chain	Res	Type	Atoms
28	P	1272	DMU	C3-C4-C57-O61
25	T	1269	CDL	C11-CA5-OA6-CA4
19	A	521	TGL	CB2-CB1-OG2-CG2
25	C	270	CDL	C62-C63-C64-C65
19	L	522	TGL	CB3-CB4-CB5-CB6
26	E	229	PSC	C20-C21-C22-C23
24	S	1265	PEK	C34-C35-C36-C37
22	P	1271	CHD	C21-C20-C22-C23
26	E	229	PSC	O04-C19-O03-C01
26	R	1229	PSC	C20-C21-C22-C23
20	C	268	PGV	C20-C21-C22-C23
25	C	270	CDL	C38-C39-C40-C41
25	T	1269	CDL	C79-C80-C81-C82
19	L	522	TGL	CC3-CC4-CC5-CC6
28	Z	1526	DMU	O6-C11-C9-O1
24	T	1264	PEK	C1-C2-C3-C4
19	N	1521	TGL	C13-C14-C29-C30
19	D	523	TGL	C17-C18-C19-C33
19	A	521	TGL	C21-C20-CA9-CA8
19	A	521	TGL	CB6-CB7-CB8-CB9
25	T	1269	CDL	OA9-CA7-OA8-CA6
25	T	1269	CDL	OB9-CB7-OB8-CB6
19	N	1522	TGL	CC1-CC2-CC3-CC4
19	L	522	TGL	OA1-CA1-OG1-CG1
28	P	1272	DMU	O5-C6-O16-C18
28	Z	1526	DMU	O5-C6-O16-C18
19	L	522	TGL	CC1-CC2-CC3-CC4
22	C	271	CHD	C17-C20-C22-C23
24	T	1264	PEK	C13-C14-C15-C16
24	T	263	PEK	C7-C8-C9-C10
25	P	1270	CDL	C23-C24-C25-C26
19	N	1522	TGL	CB2-CB1-OG2-CG2
19	D	523	TGL	CB9-C10-C11-C12
25	P	1270	CDL	CB2-C1-CA2-OA2
25	C	270	CDL	CA2-C1-CB2-OB2
20	N	1524	PGV	O12-C04-C05-C06
20	A	524	PGV	O12-C04-C05-C06
25	T	1269	CDL	OA7-CA5-OA6-CA4
19	N	1522	TGL	OB1-CB1-OG2-CG2
20	C	268	PGV	C20-C19-O03-C01
19	D	523	TGL	C13-C14-C29-C30
25	G	269	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
19	Q	1523	TGL	C13-C14-C29-C30
22	J	60	CHD	C13-C17-C20-C22
19	N	1521	TGL	CB1-CB2-CB3-CB4
25	P	1270	CDL	C40-C41-C42-C43
22	P	1271	CHD	C17-C20-C22-C23
24	G	1263	PEK	C33-C34-C35-C36
25	C	270	CDL	C14-C15-C16-C17
20	N	1524	PGV	C20-C21-C22-C23
20	C	268	PGV	O01-C02-C03-O11
20	P	1268	PGV	O12-C04-C05-O05
25	P	1270	CDL	O1-C1-CA2-OA2
25	G	269	CDL	O1-C1-CB2-OB2
22	C	271	CHD	C21-C20-C22-C23
28	P	1272	DMU	C1-C6-O16-C18
19	D	523	TGL	OG1-CG1-CG2-OG2
28	P	1272	DMU	O6-C11-C9-C8
28	M	526	DMU	O6-C11-C9-C8
26	R	1229	PSC	C1-C2-C3-C4
25	T	1269	CDL	CA5-C11-C12-C13
19	Q	1523	TGL	CB9-C10-C11-C12
24	T	263	PEK	C33-C34-C35-C36
25	G	269	CDL	C71-CB7-OB8-CB6
25	P	1270	CDL	CA5-C11-C12-C13
25	P	1270	CDL	CB7-C71-C72-C73
26	R	1229	PSC	C19-C20-C21-C22
24	C	264	PEK	C7-C8-C9-C10
24	S	1265	PEK	C10-C11-C12-C13
28	M	526	DMU	O6-C11-C9-O1
20	N	1524	PGV	O05-C05-C06-O06
20	P	1267	PGV	C12-C13-C14-C15
20	C	268	PGV	O04-C19-O03-C01
25	G	269	CDL	CB5-C51-C52-C53
25	T	1269	CDL	CA7-C31-C32-C33
25	T	1269	CDL	CB5-C51-C52-C53
19	A	521	TGL	CA2-CA1-OG1-CG1
25	T	1269	CDL	CB4-CB3-OB5-PB2
25	G	269	CDL	CA5-C11-C12-C13
20	C	268	PGV	C1-C2-C3-C4
26	E	229	PSC	C1-C2-C3-C4
22	P	1271	CHD	C20-C22-C23-C24
22	J	60	CHD	C16-C17-C20-C21
20	A	524	PGV	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
25	C	270	CDL	C53-C54-C55-C56
28	P	1272	DMU	O16-C18-C19-C22
25	C	270	CDL	C60-C61-C62-C63
25	P	1270	CDL	O1-C1-CB2-OB2
20	C	268	PGV	O12-C04-C05-O05
25	C	270	CDL	O1-C1-CA2-OA2
25	T	1269	CDL	O1-C1-CB2-OB2
20	A	524	PGV	O12-C04-C05-O05
28	G	272	DMU	C3-C4-C57-O61
22	W	1059	CHD	C13-C17-C20-C21
22	J	60	CHD	C13-C17-C20-C21
19	N	1521	TGL	OC1-CC1-OG3-CG3
19	A	521	TGL	OA1-CA1-OG1-CG1
20	C	267	PGV	C12-C13-C14-C15
19	D	523	TGL	CB1-CB2-CB3-CB4
26	R	1229	PSC	C11-C10-C9-C8
24	T	1264	PEK	C4-C5-C6-C7
25	G	269	CDL	C15-C16-C17-C18
25	P	1270	CDL	CA3-OA5-PA1-OA2
25	P	1270	CDL	CB2-OB2-PB2-OB5
24	G	1263	PEK	C03-O11-P-O12
25	G	269	CDL	CB3-OB5-PB2-OB2
25	C	270	CDL	CA3-OA5-PA1-OA2
25	C	270	CDL	CB2-OB2-PB2-OB5
20	N	1524	PGV	C03-O11-P-O12
20	N	1524	PGV	C04-O12-P-O11
24	T	263	PEK	C03-O11-P-O12
19	N	1521	TGL	CC2-CC1-OG3-CG3
25	P	1270	CDL	CA2-C1-CB2-OB2
20	C	268	PGV	O12-C04-C05-C06
25	T	1269	CDL	CA2-C1-CB2-OB2
26	R	1229	PSC	C04-C05-N-C06
20	A	524	PGV	C19-C20-C21-C22
19	Q	1523	TGL	C21-C22-C23-C24
19	N	1521	TGL	CA7-CA8-CA9-C20
25	P	1270	CDL	C11-C12-C13-C14
28	G	272	DMU	O5-C4-C57-O61
22	W	1059	CHD	C17-C20-C22-C23
20	P	1268	PGV	C22-C23-C24-C25
25	P	1270	CDL	C79-C80-C81-C82
26	R	1229	PSC	C2-C3-C4-C5
26	R	1229	PSC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	C23-C24-C25-C26
25	C	270	CDL	C23-C24-C25-C26
25	C	270	CDL	C35-C36-C37-C38
25	C	270	CDL	C39-C40-C41-C42
25	C	270	CDL	C51-C52-C53-C54
19	Q	1523	TGL	C11-C10-CB9-CB8
19	Q	1523	TGL	CC6-CC7-CC8-CC9
25	T	1269	CDL	C36-C37-C38-C39
19	A	521	TGL	CA3-CA4-CA5-CA6
24	C	264	PEK	C16-C17-C18-C19
19	N	1522	TGL	CA2-CA3-CA4-CA5
19	N	1521	TGL	CB3-CB4-CB5-CB6
19	N	1521	TGL	C12-C13-C14-C29
25	P	1270	CDL	C13-C14-C15-C16
25	P	1270	CDL	C83-C84-C85-C86
19	D	523	TGL	C10-C11-C12-C13
26	R	1229	PSC	C4-C5-C6-C7
25	G	269	CDL	C72-C73-C74-C75
24	G	265	PEK	C26-C27-C28-C29
24	G	265	PEK	C28-C29-C30-C31
19	Q	1523	TGL	C23-C24-C25-C26
19	L	522	TGL	CC6-CC7-CC8-CC9
20	A	522	PGV	C23-C24-C25-C26
26	E	229	PSC	C29-C30-C31-C32
19	N	1522	TGL	C12-C13-C14-C29
20	A	524	PGV	C22-C23-C24-C25
19	Q	1523	TGL	CG3-CG2-OG2-CB1
28	P	1272	DMU	C5-C10-O7-C3
19	Q	1523	TGL	CB1-CB2-CB3-CB4
25	P	1270	CDL	C73-C74-C75-C76
25	P	1270	CDL	C77-C78-C79-C80
25	P	1270	CDL	C82-C83-C84-C85
19	D	523	TGL	CA6-CA7-CA8-CA9
25	G	269	CDL	C77-C78-C79-C80
28	G	272	DMU	C28-C31-C34-C37
25	T	1269	CDL	C56-C57-C58-C59
19	N	1522	TGL	CC4-CC5-CC6-CC7
19	N	1522	TGL	C23-C24-C25-C26
24	G	265	PEK	C13-C14-C15-C16
19	N	1521	TGL	CA4-CA5-CA6-CA7
25	P	1270	CDL	C16-C17-C18-C19
25	P	1270	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
20	A	522	PGV	C29-C30-C31-C32
25	C	270	CDL	C81-C82-C83-C84
24	T	263	PEK	C16-C17-C18-C19
19	N	1521	TGL	CA3-CA4-CA5-CA6
20	C	268	PGV	C5-C6-C7-C8
25	C	270	CDL	C41-C42-C43-C44
20	N	1524	PGV	C4-C5-C6-C7
19	N	1522	TGL	CB4-CB5-CB6-CB7
19	N	1522	TGL	C21-C22-C23-C24
25	G	269	CDL	OB9-CB7-OB8-CB6
20	P	1268	PGV	C6-C7-C8-C9
25	C	270	CDL	C18-C19-C20-C21
25	C	270	CDL	C43-C44-C45-C46
25	T	1269	CDL	C54-C55-C56-C57
25	T	1269	CDL	C55-C56-C57-C58
19	L	522	TGL	C12-C13-C14-C29
19	N	1522	TGL	CC9-C15-C16-C17
24	S	1265	PEK	C29-C30-C31-C32
28	P	1272	DMU	C25-C28-C31-C34
25	P	1270	CDL	C72-C73-C74-C75
25	P	1270	CDL	C81-C82-C83-C84
24	G	1263	PEK	C23-C24-C25-C26
20	C	268	PGV	C14-C15-C16-C17
25	C	270	CDL	C21-C22-C23-C24
24	G	265	PEK	C31-C32-C33-C34
19	Q	1523	TGL	CB2-CB3-CB4-CB5
19	Q	1523	TGL	C10-C11-C12-C13
25	T	1269	CDL	C17-C18-C19-C20
19	A	521	TGL	C16-C17-C18-C19
20	N	1524	PGV	C14-C15-C16-C17
19	D	523	TGL	C14-C29-C30-C31
20	C	267	PGV	C13-C14-C15-C16
20	N	1266	PGV	C7-C8-C9-C10
25	T	1269	CDL	C19-C20-C21-C22
20	P	1267	PGV	C7-C8-C9-C10
20	N	1524	PGV	C04-C05-C06-O06
25	G	269	CDL	C11-CA5-OA6-CA4
19	N	1521	TGL	CB6-CB7-CB8-CB9
25	P	1270	CDL	C42-C43-C44-C45
25	P	1270	CDL	C58-C59-C60-C61
25	C	270	CDL	C61-C62-C63-C64
25	T	1269	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	C12-C13-C14-C15
20	A	524	PGV	C11-C10-C9-C8
25	P	1270	CDL	C59-C60-C61-C62
19	D	523	TGL	C11-C10-CB9-CB8
24	G	1263	PEK	C24-C25-C26-C27
20	C	268	PGV	C30-C31-C32-C33
25	C	270	CDL	C63-C64-C65-C66
19	Q	1523	TGL	CC9-C15-C16-C17
19	L	522	TGL	C22-C23-C24-C25
20	P	1267	PGV	C13-C14-C15-C16
24	T	263	PEK	C30-C31-C32-C33
26	R	1229	PSC	C04-C05-N-C07
14	N	516	HEA	C19-C20-C21-C22
19	N	1521	TGL	C11-C12-C13-C14
24	G	1263	PEK	C25-C26-C27-C28
25	G	269	CDL	C61-C62-C63-C64
25	G	269	CDL	C76-C77-C78-C79
25	G	269	CDL	C79-C80-C81-C82
20	C	268	PGV	C22-C23-C24-C25
25	T	1269	CDL	C22-C23-C24-C25
19	N	1521	TGL	C20-C21-C22-C23
25	G	269	CDL	C55-C56-C57-C58
24	G	265	PEK	C25-C26-C27-C28
24	G	265	PEK	C29-C30-C31-C32
28	Z	1526	DMU	C28-C31-C34-C37
19	Q	1523	TGL	C18-C19-C33-C34
19	L	522	TGL	CA5-CA6-CA7-CA8
19	N	1522	TGL	C10-C11-C12-C13
25	G	269	CDL	C18-C19-C20-C21
25	G	269	CDL	C57-C58-C59-C60
20	C	267	PGV	C7-C8-C9-C10
25	C	270	CDL	C16-C17-C18-C19
28	G	272	DMU	C31-C34-C37-C40
28	Z	1526	DMU	C25-C28-C31-C34
19	Q	1523	TGL	C21-C20-CA9-CA8
25	T	1269	CDL	C12-C13-C14-C15
19	A	521	TGL	C15-C16-C17-C18
19	L	522	TGL	C16-C15-CC9-CC8
24	S	1265	PEK	C33-C34-C35-C36
19	D	523	TGL	CB2-CB3-CB4-CB5
25	G	269	CDL	C33-C34-C35-C36
25	G	269	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C59-C60-C61-C62
20	A	524	PGV	C24-C25-C26-C27
19	N	1521	TGL	C21-C20-CA9-CA8
19	N	1521	TGL	C16-C17-C18-C19
19	N	1521	TGL	C14-C29-C30-C31
24	G	1263	PEK	C16-C17-C18-C19
25	C	270	CDL	C11-C12-C13-C14
19	D	523	TGL	C23-C24-C25-C26
20	N	1266	PGV	C29-C30-C31-C32
25	T	1269	CDL	C71-C72-C73-C74
24	T	263	PEK	C31-C32-C33-C34
24	T	263	PEK	C34-C35-C36-C37
25	P	1270	CDL	CA3-CA4-CA6-OA8
25	G	269	CDL	OA7-CA5-OA6-CA4
24	G	265	PEK	C7-C8-C9-C10
26	E	229	PSC	C11-C10-C9-C8
19	Q	1523	TGL	CA4-CA5-CA6-CA7
20	N	1524	PGV	C7-C8-C9-C10
24	T	263	PEK	C22-C23-C24-C25
25	C	270	CDL	C71-C72-C73-C74
19	L	522	TGL	C21-C22-C23-C24
24	G	1263	PEK	C22-C21-O03-C01
25	C	270	CDL	C51-CB5-OB6-CB4
19	N	1521	TGL	CC7-CC8-CC9-C15
19	D	523	TGL	C16-C17-C18-C19
25	T	1269	CDL	C35-C36-C37-C38
24	T	1264	PEK	C26-C27-C28-C29
19	N	1522	TGL	C22-C23-C24-C25
20	C	268	PGV	O05-C05-C06-O06
20	A	524	PGV	O05-C05-C06-O06
25	P	1270	CDL	C35-C36-C37-C38
25	P	1270	CDL	C36-C37-C38-C39
19	Q	1523	TGL	CC7-CC8-CC9-C15
24	C	264	PEK	C34-C35-C36-C37
20	A	522	PGV	C4-C5-C6-C7
26	E	229	PSC	C5-C6-C7-C8
24	T	263	PEK	C25-C26-C27-C28
20	P	1268	PGV	C11-C10-C9-C8
24	G	1263	PEK	C2-C3-C4-C5
24	G	265	PEK	C2-C3-C4-C5
20	N	1266	PGV	C6-C7-C8-C9
25	C	270	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	C	270	CDL	C72-C73-C74-C75
19	A	521	TGL	CC4-CC5-CC6-CC7
19	A	521	TGL	C17-C18-C19-C33
25	P	1270	CDL	C38-C39-C40-C41
25	G	269	CDL	C14-C15-C16-C17
25	C	270	CDL	C19-C20-C21-C22
20	N	1266	PGV	C5-C6-C7-C8
19	Q	1523	TGL	C12-C13-C14-C29
19	N	1521	TGL	C17-C18-C19-C33
20	P	1268	PGV	C30-C31-C32-C33
19	N	1521	TGL	OB1-CB1-OG2-CG2
25	C	270	CDL	OB7-CB5-OB6-CB4
25	G	269	CDL	C38-C39-C40-C41
19	N	1522	TGL	C21-C20-CA9-CA8
25	G	269	CDL	C56-C57-C58-C59
25	T	1269	CDL	C63-C64-C65-C66
19	N	1522	TGL	CA9-C20-C21-C22
26	R	1229	PSC	C04-C05-N-C08
20	A	522	PGV	C19-C20-C21-C22
20	P	1267	PGV	C1-C2-C3-C4
19	N	1522	TGL	C25-C26-C27-C28
24	T	263	PEK	C22-C21-O03-C01
25	T	1269	CDL	C74-C75-C76-C77
19	L	522	TGL	C17-C18-C19-C33
19	L	522	TGL	C25-C26-C27-C28
25	C	270	CDL	C40-C41-C42-C43
19	A	521	TGL	CB5-CB6-CB7-CB8
24	T	1264	PEK	C25-C26-C27-C28
19	D	523	TGL	CA4-CA5-CA6-CA7
25	G	269	CDL	C54-C55-C56-C57
26	E	229	PSC	C24-C25-C26-C27
26	R	1229	PSC	C11-C12-C13-C14
24	G	1263	PEK	C10-C11-C12-C13
24	S	1265	PEK	C7-C8-C9-C10
24	G	1263	PEK	O04-C21-O03-C01
25	C	270	CDL	C59-C60-C61-C62
19	L	522	TGL	C11-C10-CB9-CB8
20	N	1524	PGV	C2-C3-C4-C5
19	A	521	TGL	CG2-CG3-OG3-CC1
20	C	268	PGV	C11-C10-C9-C8
24	G	265	PEK	C15-C16-C17-C18
24	C	264	PEK	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	N	1521	TGL	C25-C26-C27-C28
19	D	523	TGL	C21-C20-CA9-CA8
20	A	524	PGV	C26-C27-C28-C29
28	P	1272	DMU	O6-C11-C9-O1
19	L	522	TGL	CB5-CB6-CB7-CB8
25	G	269	CDL	C36-C37-C38-C39
19	A	521	TGL	CA4-CA5-CA6-CA7
19	N	1521	TGL	CB9-C10-C11-C12
25	G	269	CDL	C83-C84-C85-C86
24	G	1263	PEK	C31-C32-C33-C34
19	L	522	TGL	C10-C11-C12-C13
28	G	272	DMU	O5-C6-O16-C18
26	R	1229	PSC	C27-C28-C29-C30
25	G	269	CDL	C37-C38-C39-C40
24	C	264	PEK	C25-C26-C27-C28
20	N	1524	PGV	C5-C6-C7-C8
24	G	265	PEK	C1-C2-C3-C4
25	T	1269	CDL	CB7-C71-C72-C73
19	N	1521	TGL	CB2-CB1-OG2-CG2
20	P	1268	PGV	O01-C02-C03-O11
25	G	269	CDL	C40-C41-C42-C43
19	Q	1523	TGL	C17-C18-C19-C33
20	A	522	PGV	C7-C8-C9-C10
20	P	1267	PGV	C25-C26-C27-C28
24	G	1263	PEK	O03-C01-C02-O01
19	Q	1523	TGL	OG1-CG1-CG2-OG2
25	C	270	CDL	C42-C43-C44-C45
25	T	1269	CDL	C16-C17-C18-C19
24	T	263	PEK	O04-C21-O03-C01
25	G	269	CDL	C59-C60-C61-C62
19	A	521	TGL	CA5-CA6-CA7-CA8
19	A	521	TGL	CC7-CC8-CC9-C15
20	C	268	PGV	C4-C5-C6-C7
20	P	1267	PGV	C20-C21-C22-C23
20	P	1267	PGV	C28-C29-C30-C31
19	N	1521	TGL	C15-C16-C17-C18
25	P	1270	CDL	C18-C19-C20-C21
25	C	270	CDL	C76-C77-C78-C79
20	A	522	PGV	C5-C6-C7-C8
24	T	1264	PEK	C22-C23-C24-C25
20	P	1268	PGV	C23-C24-C25-C26
24	G	265	PEK	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	R	1229	PSC	C03-O11-P-O12
20	P	1268	PGV	C1-C2-C3-C4
24	G	265	PEK	C22-C21-O03-C01
20	C	268	PGV	C01-C02-C03-O11
25	T	1269	CDL	OB5-CB3-CB4-CB6
24	T	263	PEK	C01-C02-C03-O11
20	P	1268	PGV	C3-C4-C5-C6
25	C	270	CDL	C79-C80-C81-C82
26	E	229	PSC	C23-C24-C25-C26
20	N	1524	PGV	C12-C13-C14-C15
26	R	1229	PSC	C24-C25-C26-C27
25	P	1270	CDL	C12-C13-C14-C15
25	P	1270	CDL	C60-C61-C62-C63
28	G	272	DMU	C5-C10-O7-C3
19	N	1521	TGL	CA6-CA7-CA8-CA9
24	G	265	PEK	C34-C35-C36-C37
19	L	522	TGL	C21-C20-CA9-CA8
24	T	1264	PEK	C33-C34-C35-C36
20	N	1266	PGV	C26-C27-C28-C29
19	D	523	TGL	OG1-CG1-CG2-CG3
26	R	1229	PSC	O03-C01-C02-C03
25	C	270	CDL	CB3-CB4-CB6-OB8
19	Q	1523	TGL	OG1-CG1-CG2-CG3
25	T	1269	CDL	CB3-CB4-CB6-OB8
19	A	521	TGL	OG1-CG1-CG2-CG3
26	E	229	PSC	O03-C01-C02-C03
20	N	1524	PGV	O03-C01-C02-C03
24	T	1264	PEK	C10-C11-C12-C13
25	P	1270	CDL	C19-C20-C21-C22
25	G	269	CDL	C13-C14-C15-C16
25	T	1269	CDL	C62-C63-C64-C65
26	R	1229	PSC	C31-C32-C33-C34
25	C	270	CDL	C58-C59-C60-C61
25	T	1269	CDL	C77-C78-C79-C80
20	N	1524	PGV	O03-C19-C20-C21
24	G	1263	PEK	C1-C2-C3-C4
19	N	1521	TGL	CB7-CB8-CB9-C10
25	C	270	CDL	C17-C18-C19-C20
19	A	521	TGL	C29-C30-C31-C32
19	Q	1523	TGL	CA6-CA7-CA8-CA9
20	C	268	PGV	C31-C32-C33-C34
20	A	524	PGV	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	P	1272	DMU	C22-C25-C28-C31
19	L	522	TGL	C11-C12-C13-C14
26	E	229	PSC	C31-C32-C33-C34
25	P	1270	CDL	C43-C44-C45-C46
19	D	523	TGL	C18-C19-C33-C34
25	P	1270	CDL	C22-C23-C24-C25
25	T	1269	CDL	C20-C21-C22-C23
26	E	229	PSC	C26-C27-C28-C29
19	D	523	TGL	CC2-CC3-CC4-CC5
19	A	521	TGL	C25-C26-C27-C28
19	L	522	TGL	C23-C24-C25-C26
19	D	523	TGL	CG3-CG2-OG2-CB1
26	R	1229	PSC	C03-C02-O01-C1
20	A	524	PGV	C03-C02-O01-C1
19	N	1522	TGL	CA5-CA6-CA7-CA8
19	D	523	TGL	CC4-CC5-CC6-CC7
26	E	229	PSC	C3-C4-C5-C6
25	C	270	CDL	C71-CB7-OB8-CB6
24	G	265	PEK	C10-C11-C12-C13
25	C	270	CDL	C83-C84-C85-C86
25	G	269	CDL	C24-C25-C26-C27
25	G	269	CDL	C31-C32-C33-C34
19	L	522	TGL	C29-C30-C31-C32
20	A	524	PGV	C31-C32-C33-C34
19	Q	1523	TGL	C33-C34-C35-C36
19	N	1521	TGL	OG1-CG1-CG2-OG2
25	G	269	CDL	OA6-CA4-CA6-OA8
25	T	1269	CDL	OB6-CB4-CB6-OB8
19	L	522	TGL	OG2-CG2-CG3-OG3
24	T	263	PEK	O03-C01-C02-O01
24	G	1263	PEK	C30-C31-C32-C33
20	C	267	PGV	C25-C26-C27-C28
24	T	1264	PEK	C35-C36-C37-C38
24	G	265	PEK	O04-C21-O03-C01
25	G	269	CDL	C20-C21-C22-C23
24	T	263	PEK	C29-C30-C31-C32
20	P	1268	PGV	C14-C15-C16-C17
20	P	1267	PGV	C31-C32-C33-C34
25	T	1269	CDL	C24-C25-C26-C27
25	P	1270	CDL	C44-C45-C46-C47
19	A	521	TGL	C21-C22-C23-C24
19	L	522	TGL	CA4-CA5-CA6-CA7

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Mol	Chain	Res	Type	Atoms
19	L	522	TGL	CC5-CC6-CC7-CC8
20	P	1267	PGV	C15-C16-C17-C18
19	Q	1523	TGL	C19-C33-C34-C35
24	C	264	PEK	C4-C5-C6-C7
20	A	524	PGV	C20-C21-C22-C23
19	N	1521	TGL	CC4-CC5-CC6-CC7
20	P	1268	PGV	C01-C02-C03-O11
25	P	1270	CDL	OB5-CB3-CB4-CB6
25	C	270	CDL	OA5-CA3-CA4-CA6
25	C	270	CDL	OB5-CB3-CB4-CB6
25	T	1269	CDL	OA5-CA3-CA4-CA6
20	A	524	PGV	C01-C02-C03-O11
25	T	1269	CDL	C81-C82-C83-C84
20	C	267	PGV	C1-C2-C3-C4
20	P	1268	PGV	C20-C19-O03-C01
19	N	1522	TGL	OG2-CB1-CB2-CB3
20	P	1268	PGV	C02-C03-O11-P
20	A	524	PGV	C05-C04-O12-P
25	C	270	CDL	C80-C81-C82-C83
28	M	526	DMU	C19-C18-O16-C6
20	P	1268	PGV	C24-C25-C26-C27
28	M	526	DMU	C34-C37-C40-C43
28	G	272	DMU	C25-C28-C31-C34
19	Q	1523	TGL	CB6-CB7-CB8-CB9
19	N	1522	TGL	C14-C29-C30-C31
20	C	268	PGV	C21-C22-C23-C24
19	L	522	TGL	CB2-CB3-CB4-CB5
25	P	1270	CDL	CB3-CB4-CB6-OB8
24	G	1263	PEK	O03-C01-C02-C03
25	C	270	CDL	CA3-CA4-CA6-OA8
25	T	1269	CDL	CA3-CA4-CA6-OA8
19	A	521	TGL	CG1-CG2-CG3-OG3
20	A	524	PGV	O03-C01-C02-C03
19	N	1521	TGL	CA5-CA6-CA7-CA8
19	A	521	TGL	CA6-CA7-CA8-CA9
20	A	522	PGV	C31-C32-C33-C34
20	N	1524	PGV	C10-C11-C12-C13
25	C	270	CDL	OB9-CB7-OB8-CB6
19	D	523	TGL	CA5-CA6-CA7-CA8
20	N	1266	PGV	C25-C26-C27-C28
20	C	267	PGV	C15-C16-C17-C18
20	C	267	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
20	N	1266	PGV	C31-C32-C33-C34
20	P	1268	PGV	C13-C14-C15-C16
25	T	1269	CDL	C64-C65-C66-C67
19	L	522	TGL	CA9-C20-C21-C22
26	R	1229	PSC	C9-C10-C11-C12
26	R	1229	PSC	C10-C11-C12-C13
24	G	1263	PEK	C12-C13-C14-C15
24	G	265	PEK	C5-C6-C7-C8
24	G	265	PEK	C11-C10-C9-C8
24	G	265	PEK	C9-C10-C11-C12
24	C	264	PEK	C9-C10-C11-C12
24	T	1264	PEK	C11-C10-C9-C8
24	T	263	PEK	C6-C7-C8-C9
24	T	263	PEK	C9-C10-C11-C12
24	S	1265	PEK	C5-C6-C7-C8
24	S	1265	PEK	C6-C7-C8-C9
24	C	264	PEK	C23-C24-C25-C26
24	S	1265	PEK	C25-C26-C27-C28
25	C	270	CDL	C73-C74-C75-C76
24	G	1263	PEK	C34-C35-C36-C37
24	C	264	PEK	C27-C28-C29-C30
25	T	1269	CDL	C23-C24-C25-C26
22	C	271	CHD	C20-C22-C23-C24
19	D	523	TGL	OG2-CB1-CB2-CB3
25	C	270	CDL	C12-C13-C14-C15
19	L	522	TGL	CB7-CB8-CB9-C10
25	T	1269	CDL	C11-C12-C13-C14
20	C	268	PGV	O03-C01-C02-O01
19	A	521	TGL	OG1-CG1-CG2-OG2
20	N	1266	PGV	C23-C24-C25-C26
19	A	521	TGL	CA7-CA8-CA9-C20
20	P	1268	PGV	C31-C32-C33-C34
25	T	1269	CDL	C38-C39-C40-C41
25	G	269	CDL	CB2-C1-CA2-OA2
28	G	272	DMU	C4-C3-O7-C10
25	T	1269	CDL	C33-C34-C35-C36
19	D	523	TGL	OB1-CB1-OG2-CG2
25	C	270	CDL	C37-C38-C39-C40
28	G	272	DMU	O16-C18-C19-C22
19	N	1522	TGL	C29-C30-C31-C32
19	Q	1523	TGL	CC4-CC5-CC6-CC7
25	G	269	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	C02-C03-O11-P
25	C	270	CDL	C1-CA2-OA2-PA1
25	C	270	CDL	CA4-CA3-OA5-PA1
20	C	268	PGV	C25-C26-C27-C28
20	N	1524	PGV	C31-C32-C33-C34
20	A	524	PGV	C28-C29-C30-C31
25	P	1270	CDL	C71-C72-C73-C74
25	P	1270	CDL	C63-C64-C65-C66
20	C	268	PGV	C28-C29-C30-C31
24	S	1265	PEK	C31-C32-C33-C34
20	N	1524	PGV	C15-C16-C17-C18
19	Q	1523	TGL	C29-C30-C31-C32
25	G	269	CDL	C34-C35-C36-C37
28	M	526	DMU	C28-C31-C34-C37
25	P	1270	CDL	OA5-CA3-CA4-CA6
24	T	263	PEK	C10-C11-C12-C13
25	T	1269	CDL	C41-C42-C43-C44
26	E	229	PSC	C4-C5-C6-C7
24	C	264	PEK	C1-C2-C3-C4
20	P	1268	PGV	C28-C29-C30-C31
25	P	1270	CDL	C24-C25-C26-C27
20	C	268	PGV	C15-C16-C17-C18
24	T	263	PEK	C27-C28-C29-C30
26	E	229	PSC	C03-C02-O01-C1
25	C	270	CDL	C55-C56-C57-C58
24	S	1265	PEK	C30-C31-C32-C33
20	P	1267	PGV	C02-C03-O11-P
24	T	263	PEK	O03-C01-C02-C03
19	D	523	TGL	CB2-CB1-OG2-CG2
19	N	1522	TGL	CC5-CC6-CC7-CC8
25	P	1270	CDL	OA5-CA3-CA4-OA6
24	G	1263	PEK	O01-C02-C03-O11
25	C	270	CDL	OB5-CB3-CB4-OB6
24	T	263	PEK	O01-C02-C03-O11
20	A	522	PGV	C10-C11-C12-C13
20	P	1267	PGV	C22-C23-C24-C25
25	G	269	CDL	C35-C36-C37-C38
20	P	1268	PGV	O04-C19-O03-C01
24	S	1265	PEK	C23-C24-C25-C26
25	P	1270	CDL	OA6-CA4-CA6-OA8
25	P	1270	CDL	OB6-CB4-CB6-OB8
25	C	270	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	OA6-CA4-CA6-OA8
26	E	229	PSC	O03-C01-C02-O01
19	N	1522	TGL	OG2-CG2-CG3-OG3
19	Q	1523	TGL	CA5-CA6-CA7-CA8
19	L	522	TGL	CC4-CC5-CC6-CC7
19	N	1521	TGL	C10-C11-C12-C13
24	T	1264	PEK	C31-C32-C33-C34
24	S	1265	PEK	C22-C23-C24-C25
28	G	272	DMU	C34-C37-C40-C43
19	N	1522	TGL	CB5-CB6-CB7-CB8
28	P	1272	DMU	C4-C3-O7-C10
24	T	1264	PEK	C23-C24-C25-C26
25	C	270	CDL	C32-C33-C34-C35
20	N	1524	PGV	C24-C25-C26-C27
19	N	1521	TGL	C18-C19-C33-C34
19	L	522	TGL	C14-C29-C30-C31
20	N	1524	PGV	C30-C31-C32-C33
28	M	526	DMU	C19-C22-C25-C28
28	M	526	DMU	C25-C28-C31-C34
25	G	269	CDL	CB2-OB2-PB2-OB5
24	G	265	PEK	C03-O11-P-O12
24	T	263	PEK	C04-O12-P-O11
20	P	1268	PGV	C05-C04-O12-P
25	P	1270	CDL	CA4-CA3-OA5-PA1
20	C	267	PGV	C02-C03-O11-P
20	C	268	PGV	C05-C04-O12-P
14	A	515	HEA	C14-C15-C16-C17
25	P	1270	CDL	CA3-OA5-PA1-OA3
25	P	1270	CDL	CB2-OB2-PB2-OB4
26	R	1229	PSC	C03-O11-P-O13
25	G	269	CDL	CA3-OA5-PA1-OA4
25	C	270	CDL	CA3-OA5-PA1-OA3
25	C	270	CDL	CB2-OB2-PB2-OB3
20	N	1524	PGV	C04-O12-P-O13
24	T	263	PEK	C04-O12-P-O14
25	C	270	CDL	CA7-C31-C32-C33
24	G	1263	PEK	C01-C02-C03-O11
26	E	229	PSC	C01-C02-C03-O11
19	D	523	TGL	CA3-CA4-CA5-CA6
19	L	522	TGL	C33-C34-C35-C36
19	N	1521	TGL	C23-C24-C25-C26
19	N	1522	TGL	CB1-CB2-CB3-CB4

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C14-C15-C16-C17
24	T	263	PEK	C26-C27-C28-C29
19	L	522	TGL	OG2-CB1-CB2-CB3
24	C	264	PEK	C32-C33-C34-C35
25	C	270	CDL	OA5-CA3-CA4-OA6
25	T	1269	CDL	OB5-CB3-CB4-OB6
26	E	229	PSC	O01-C02-C03-O11
26	E	229	PSC	C22-C23-C24-C25
20	N	1524	PGV	C21-C22-C23-C24
19	Q	1523	TGL	CB4-CB5-CB6-CB7
19	N	1522	TGL	C13-C14-C29-C30
26	R	1229	PSC	O12-C04-C05-N
24	C	264	PEK	C28-C29-C30-C31
26	R	1229	PSC	O03-C01-C02-O01
25	C	270	CDL	OA6-CA4-CA6-OA8
19	A	521	TGL	OG2-CG2-CG3-OG3
20	N	1524	PGV	O03-C01-C02-O01
19	Q	1523	TGL	C16-C17-C18-C19
24	G	1263	PEK	C13-C14-C15-C16
25	C	270	CDL	C13-C14-C15-C16
24	T	1264	PEK	C17-C18-C19-C20
19	N	1522	TGL	C11-C12-C13-C14
25	T	1269	CDL	C13-C14-C15-C16
20	N	1524	PGV	C05-C04-O12-P
24	G	265	PEK	C35-C36-C37-C38
28	Z	1526	DMU	C31-C34-C37-C40
19	A	521	TGL	C18-C19-C33-C34
24	S	1265	PEK	C35-C36-C37-C38
20	A	524	PGV	C25-C26-C27-C28
20	C	268	PGV	C24-C25-C26-C27
25	G	269	CDL	C41-C42-C43-C44
19	L	522	TGL	OG1-CA1-CA2-CA3
20	C	267	PGV	C29-C30-C31-C32
19	N	1522	TGL	C17-C18-C19-C33
24	G	265	PEK	C27-C28-C29-C30
25	T	1269	CDL	C32-C33-C34-C35
20	N	1524	PGV	C01-C02-O01-C1
20	C	267	PGV	C20-C21-C22-C23
26	R	1229	PSC	C15-C16-C17-C18
26	R	1229	PSC	C26-C27-C28-C29
25	T	1269	CDL	C31-C32-C33-C34
20	N	1266	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	C1-CA2-OA2-PA1
20	C	267	PGV	C05-C04-O12-P
25	G	269	CDL	C23-C24-C25-C26
25	G	269	CDL	C71-C72-C73-C74
25	P	1270	CDL	C41-C42-C43-C44
20	A	522	PGV	C6-C7-C8-C9
26	R	1229	PSC	O03-C19-C20-C21
24	S	1265	PEK	C17-C18-C19-C20
19	D	523	TGL	CA9-C20-C21-C22
25	T	1269	CDL	C34-C35-C36-C37
24	G	265	PEK	C3-C4-C5-C6
24	S	1265	PEK	O03-C01-C02-O01
20	P	1268	PGV	C04-O12-P-O11
20	C	268	PGV	C04-O12-P-O11
24	G	265	PEK	C04-O12-P-O11
25	T	1269	CDL	CB2-OB2-PB2-OB5
20	A	524	PGV	C03-O11-P-O12
19	D	523	TGL	CC5-CC6-CC7-CC8
25	G	269	CDL	CA3-CA4-CA6-OA8
19	L	522	TGL	CG1-CG2-CG3-OG3
19	N	1522	TGL	CG1-CG2-CG3-OG3
25	P	1270	CDL	C75-C76-C77-C78
19	A	521	TGL	C11-C12-C13-C14
19	N	1522	TGL	CA6-CA7-CA8-CA9
20	N	1524	PGV	C11-C12-C13-C14
26	E	229	PSC	C27-C28-C29-C30
25	G	269	CDL	C21-C22-C23-C24
24	G	1263	PEK	C29-C30-C31-C32
19	A	521	TGL	CB7-CB8-CB9-C10
24	T	1264	PEK	C3-C4-C5-C6
25	G	269	CDL	OB5-CB3-CB4-CB6
24	G	265	PEK	C01-C02-C03-O11
19	N	1521	TGL	CC6-CC7-CC8-CC9
19	N	1522	TGL	CA3-CA4-CA5-CA6
20	N	1266	PGV	C12-C13-C14-C15
24	C	264	PEK	C2-C3-C4-C5
24	T	263	PEK	C15-C16-C17-C18
19	N	1521	TGL	CB4-CB5-CB6-CB7
24	G	265	PEK	C4-C5-C6-C7
20	N	1524	PGV	C13-C14-C15-C16
19	A	521	TGL	C14-C29-C30-C31
19	N	1522	TGL	CC6-CC7-CC8-CC9

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C15-C16-C17-C18
26	R	1229	PSC	C21-C22-C23-C24
20	N	1524	PGV	C11-C10-C9-C8
19	A	521	TGL	CB2-CB3-CB4-CB5
26	E	229	PSC	C04-C05-N-C08
28	M	526	DMU	C31-C34-C37-C40
24	G	1263	PEK	C9-C10-C11-C12
26	E	229	PSC	C9-C10-C11-C12
26	E	229	PSC	C10-C11-C12-C13
24	G	1263	PEK	C17-C18-C19-C20
25	T	1269	CDL	C53-C54-C55-C56
20	C	267	PGV	C24-C25-C26-C27
20	C	268	PGV	C10-C11-C12-C13
20	N	1266	PGV	C10-C11-C12-C13
20	A	524	PGV	C10-C11-C12-C13
19	L	522	TGL	C19-C33-C34-C35
26	R	1229	PSC	C12-C13-C14-C15
24	S	1265	PEK	C3-C4-C5-C6
24	S	1265	PEK	C14-C15-C16-C17
19	N	1522	TGL	C20-C21-C22-C23
19	N	1521	TGL	CB2-CB3-CB4-CB5
25	G	269	CDL	C12-C13-C14-C15
19	Q	1523	TGL	CB3-CB4-CB5-CB6
19	N	1522	TGL	CA4-CA5-CA6-CA7
19	D	523	TGL	C12-C13-C14-C29
25	T	1269	CDL	CB2-C1-CA2-OA2
26	R	1229	PSC	C28-C29-C30-C31
20	A	522	PGV	O03-C19-C20-C21
19	D	523	TGL	C11-C12-C13-C14
25	P	1270	CDL	C57-C58-C59-C60
19	Q	1523	TGL	OG2-CB1-CB2-CB3
24	C	264	PEK	C14-C15-C16-C17
20	P	1268	PGV	C04-C05-C06-O06
26	E	229	PSC	C30-C31-C32-C33
25	C	270	CDL	C74-C75-C76-C77
20	A	522	PGV	C30-C31-C32-C33
20	N	1524	PGV	O04-C19-C20-C21
19	N	1521	TGL	CB5-CB6-CB7-CB8
19	Q	1523	TGL	CC2-CC3-CC4-CC5
26	R	1229	PSC	O01-C1-C2-C3
26	R	1229	PSC	C7-C8-C9-C10
20	N	1266	PGV	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	G	269	CDL	C52-C53-C54-C55
19	N	1522	TGL	C16-C17-C18-C19
19	A	521	TGL	C10-C11-C12-C13
19	N	1521	TGL	OA1-CA1-OG1-CG1
25	G	269	CDL	C64-C65-C66-C67
20	C	268	PGV	C9-C10-C11-C12
24	T	1264	PEK	C14-C15-C16-C17
24	T	1264	PEK	O01-C1-C2-C3
20	P	1267	PGV	C05-C04-O12-P
24	T	1264	PEK	C15-C16-C17-C18
20	A	524	PGV	C11-C12-C13-C14
14	A	516	HEA	C26-C15-C16-C17
14	N	516	HEA	C26-C15-C16-C17
25	C	270	CDL	C34-C35-C36-C37
25	G	269	CDL	C53-C54-C55-C56
24	C	264	PEK	O01-C1-C2-C3
20	A	522	PGV	C11-C12-C13-C14
19	N	1521	TGL	CG1-CG2-OG2-CB1
25	P	1270	CDL	C21-C22-C23-C24
19	N	1521	TGL	C11-C10-CB9-CB8
25	C	270	CDL	C52-C53-C54-C55
19	N	1521	TGL	OG3-CC1-CC2-CC3
19	D	523	TGL	OG3-CC1-CC2-CC3
19	D	523	TGL	CC1-CC2-CC3-CC4
25	C	270	CDL	C12-C11-CA5-OA6
24	T	263	PEK	C14-C15-C16-C17
25	T	1269	CDL	C37-C38-C39-C40
24	T	263	PEK	O01-C1-C2-C3
24	C	264	PEK	C24-C25-C26-C27
19	N	1521	TGL	CC5-CC6-CC7-CC8
20	P	1268	PGV	C11-C12-C13-C14
28	Z	1526	DMU	C22-C25-C28-C31
20	C	267	PGV	C28-C29-C30-C31
19	A	521	TGL	CC6-CC7-CC8-CC9
19	N	1522	TGL	C11-C10-CB9-CB8
20	C	268	PGV	C29-C30-C31-C32
20	P	1268	PGV	O01-C1-C2-C3
24	S	1265	PEK	O01-C1-C2-C3
20	P	1268	PGV	O05-C05-C06-O06
28	Z	1526	DMU	O6-C11-C9-C8
25	T	1269	CDL	C84-C85-C86-C87
19	N	1522	TGL	CB7-CB8-CB9-C10

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Mol	Chain	Res	Type	Atoms
26	E	229	PSC	C19-C20-C21-C22
19	D	523	TGL	CC7-CC8-CC9-C15
20	A	522	PGV	C9-C10-C11-C12
25	P	1270	CDL	C32-C31-CA7-OA8
25	C	270	CDL	C77-C78-C79-C80
24	T	263	PEK	C24-C25-C26-C27
19	Q	1523	TGL	C11-C12-C13-C14
25	P	1270	CDL	C17-C18-C19-C20
19	N	1521	TGL	CC9-C15-C16-C17
20	P	1267	PGV	C27-C28-C29-C30
25	T	1269	CDL	C80-C81-C82-C83
25	C	270	CDL	C12-C11-CA5-OA7
19	N	1521	TGL	OC1-CC1-CC2-CC3
19	D	523	TGL	OC1-CC1-CC2-CC3
24	T	263	PEK	O02-C1-C2-C3
25	C	270	CDL	C36-C37-C38-C39
20	N	1524	PGV	C29-C30-C31-C32
19	Q	1523	TGL	C20-C21-C22-C23
20	P	1268	PGV	C2-C3-C4-C5
20	A	524	PGV	C4-C5-C6-C7
19	Q	1523	TGL	CA7-CA8-CA9-C20
25	G	269	CDL	CA3-OA5-PA1-OA3
25	C	270	CDL	CB2-OB2-PB2-OB4
24	G	265	PEK	C03-O11-P-O14
24	G	265	PEK	C04-O12-P-O14
25	T	1269	CDL	CB2-OB2-PB2-OB3
25	P	1270	CDL	C76-C77-C78-C79
24	C	264	PEK	O02-C1-C2-C3
25	G	269	CDL	C32-C31-CA7-OA8
20	P	1268	PGV	O02-C1-C2-C3
25	P	1270	CDL	C32-C31-CA7-OA9
20	A	524	PGV	O02-C1-C2-C3
25	G	269	CDL	C84-C85-C86-C87
25	P	1270	CDL	C52-C51-CB5-OB6
20	N	1266	PGV	O03-C19-C20-C21
20	A	522	PGV	C27-C28-C29-C30
24	S	1265	PEK	O02-C1-C2-C3
25	G	269	CDL	C32-C31-CA7-OA9
24	T	1264	PEK	C05-C04-O12-P
24	S	1265	PEK	C05-C04-O12-P
19	D	523	TGL	OB1-CB1-CB2-CB3
25	G	269	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	G	269	CDL	C51-C52-C53-C54
19	D	523	TGL	CA1-CA2-CA3-CA4
24	T	1264	PEK	O02-C1-C2-C3
19	N	1522	TGL	OB1-CB1-CB2-CB3
26	E	229	PSC	C04-C05-N-C06
25	P	1270	CDL	C12-C11-CA5-OA6
26	E	229	PSC	O03-C19-C20-C21
25	P	1270	CDL	C84-C85-C86-C87
24	T	1264	PEK	C24-C25-C26-C27
14	N	516	HEA	C27-C19-C20-C21
25	P	1270	CDL	OB5-CB3-CB4-OB6
20	C	268	PGV	O01-C1-C2-C3
25	G	269	CDL	C63-C64-C65-C66
25	G	269	CDL	C44-C45-C46-C47
28	P	1272	DMU	C19-C18-O16-C6
19	Q	1523	TGL	OG3-CC1-CC2-CC3
20	A	524	PGV	O01-C1-C2-C3
25	P	1270	CDL	C12-C11-CA5-OA7
19	Q	1523	TGL	OC1-CC1-CC2-CC3
24	G	265	PEK	C33-C34-C35-C36
19	D	523	TGL	OG1-CA1-CA2-CA3
25	C	270	CDL	C52-C51-CB5-OB6
20	A	522	PGV	C24-C25-C26-C27
24	T	263	PEK	C3-C4-C5-C6

There are no ring outliers.

42 monomers are involved in 341 short contacts:

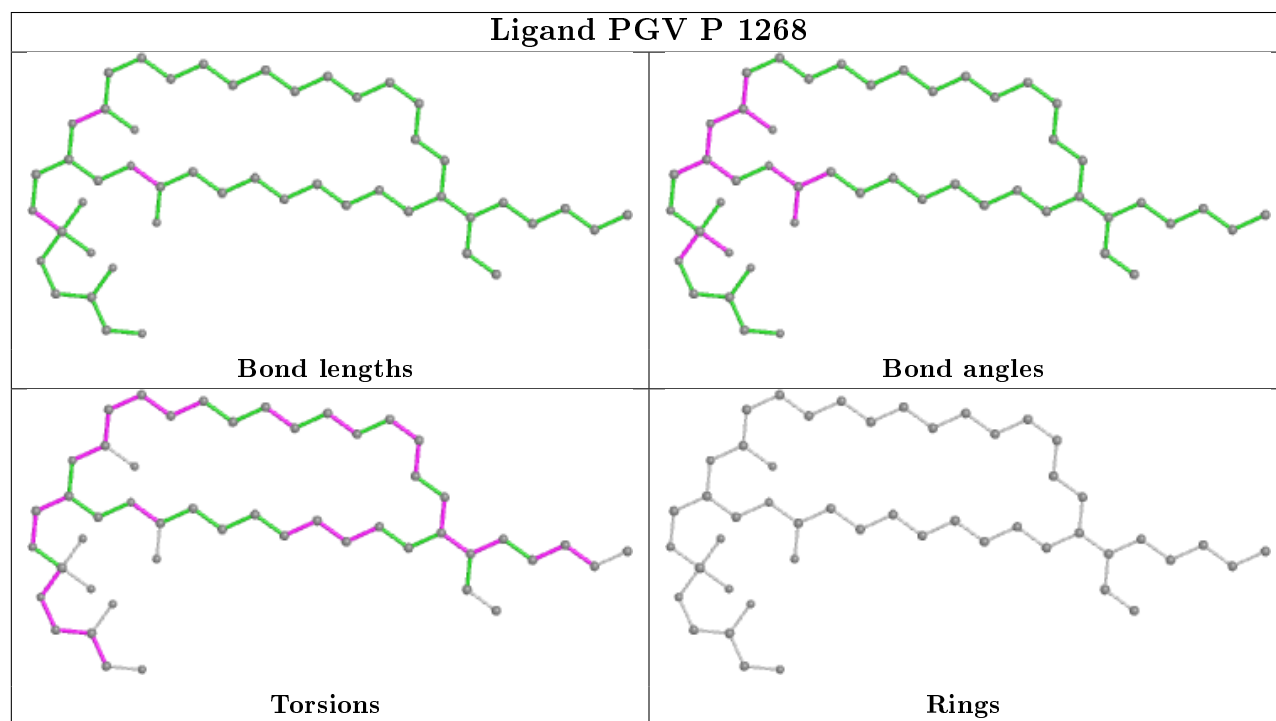
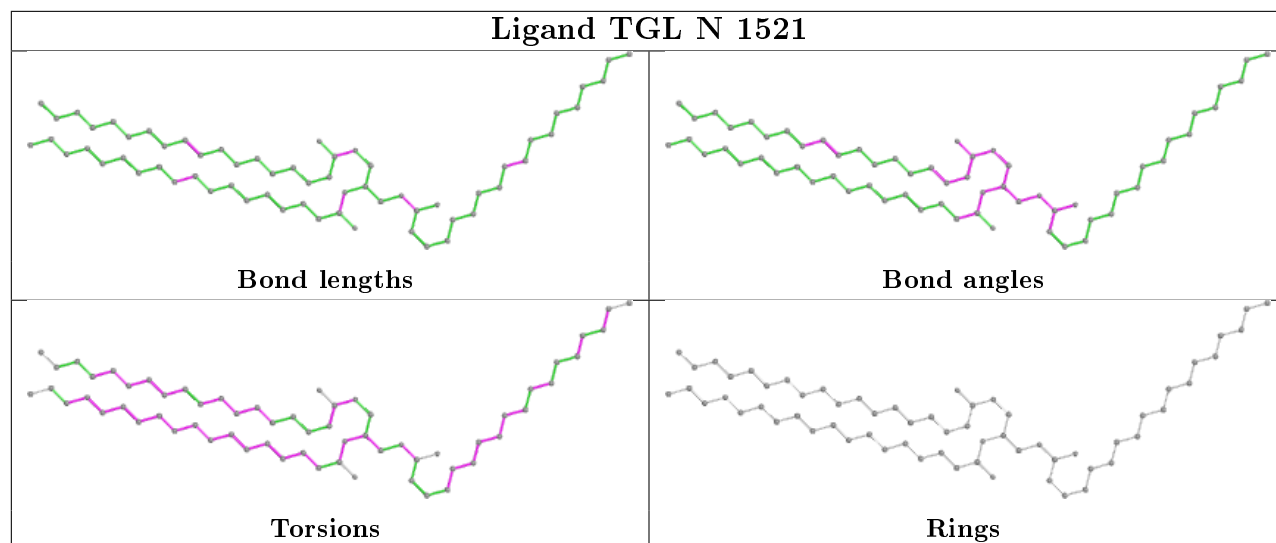
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	1521	TGL	7	0
20	P	1268	PGV	2	0
25	P	1270	CDL	19	0
19	D	523	TGL	13	0
22	W	1059	CHD	6	0
26	R	1229	PSC	14	0
24	G	1263	PEK	11	0
28	P	1272	DMU	5	0
28	M	526	DMU	1	0
25	G	269	CDL	28	0
20	C	267	PGV	3	0
22	C	525	CHD	1	0
20	C	268	PGV	3	0

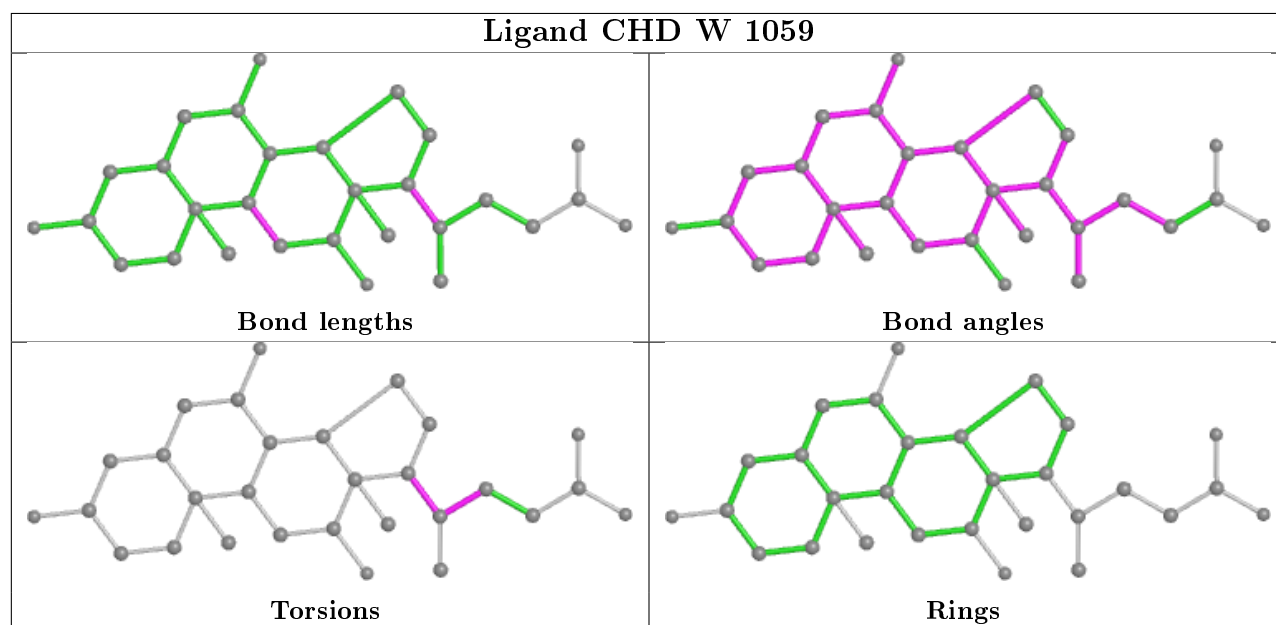
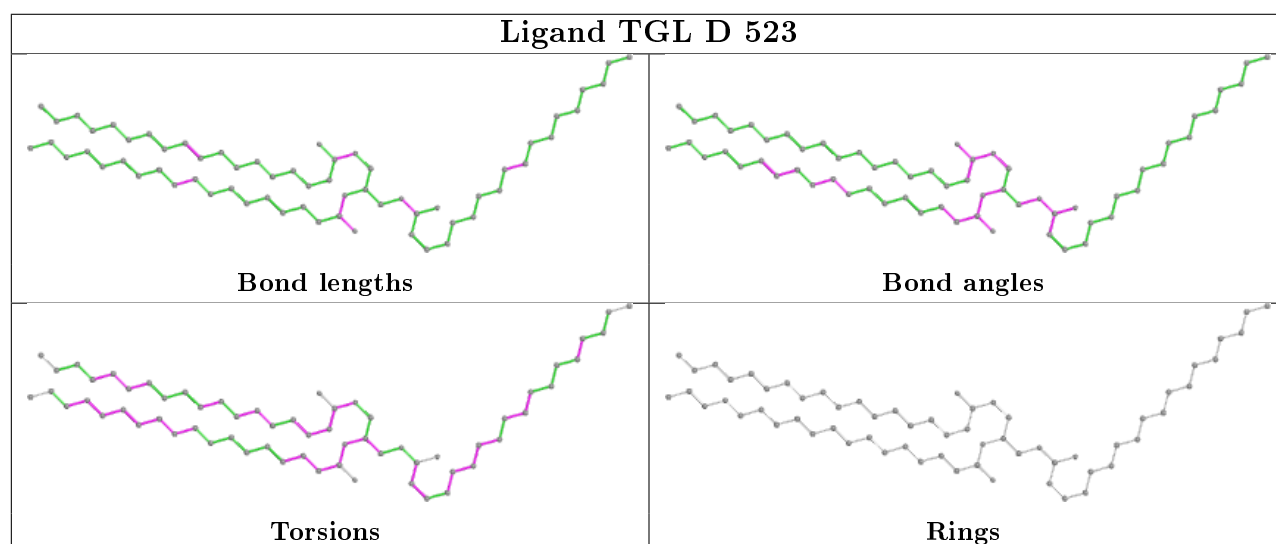
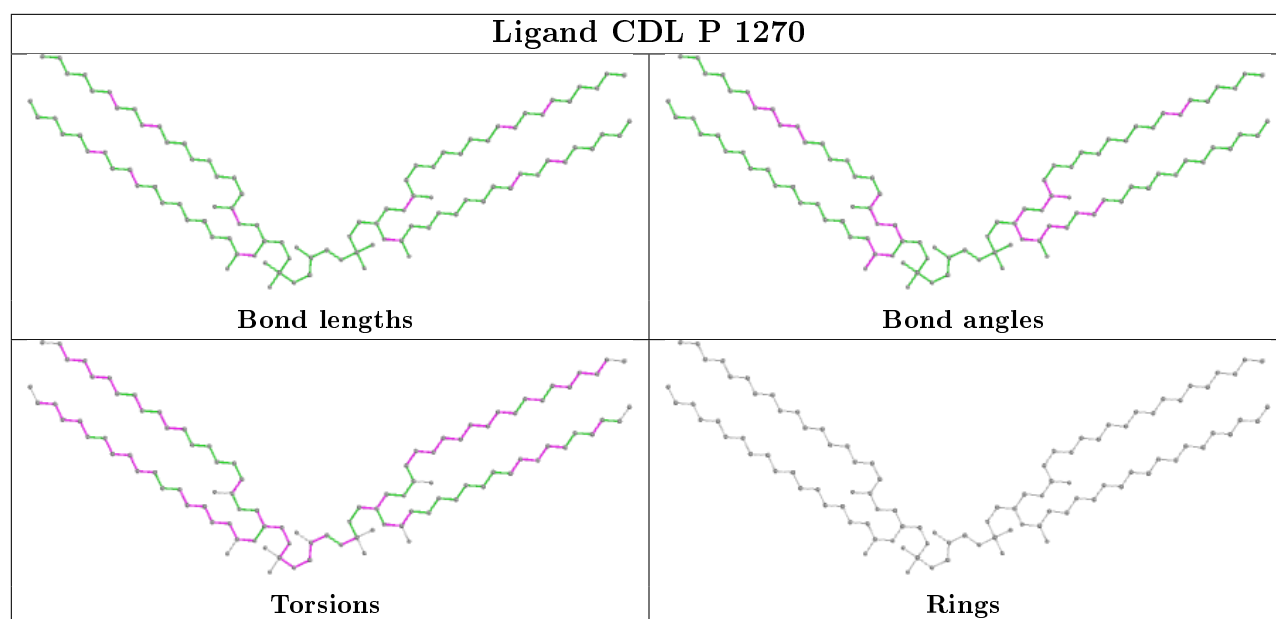
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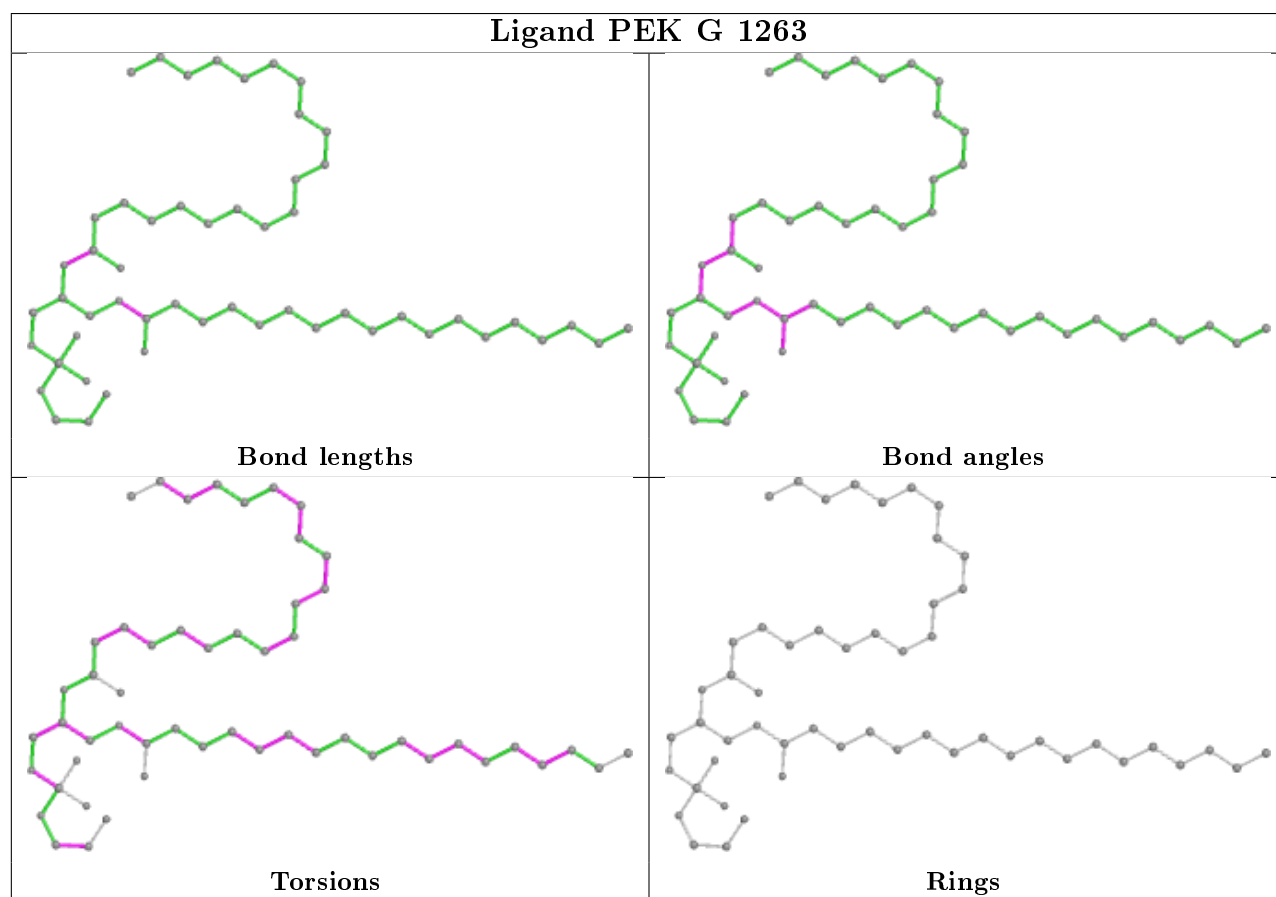
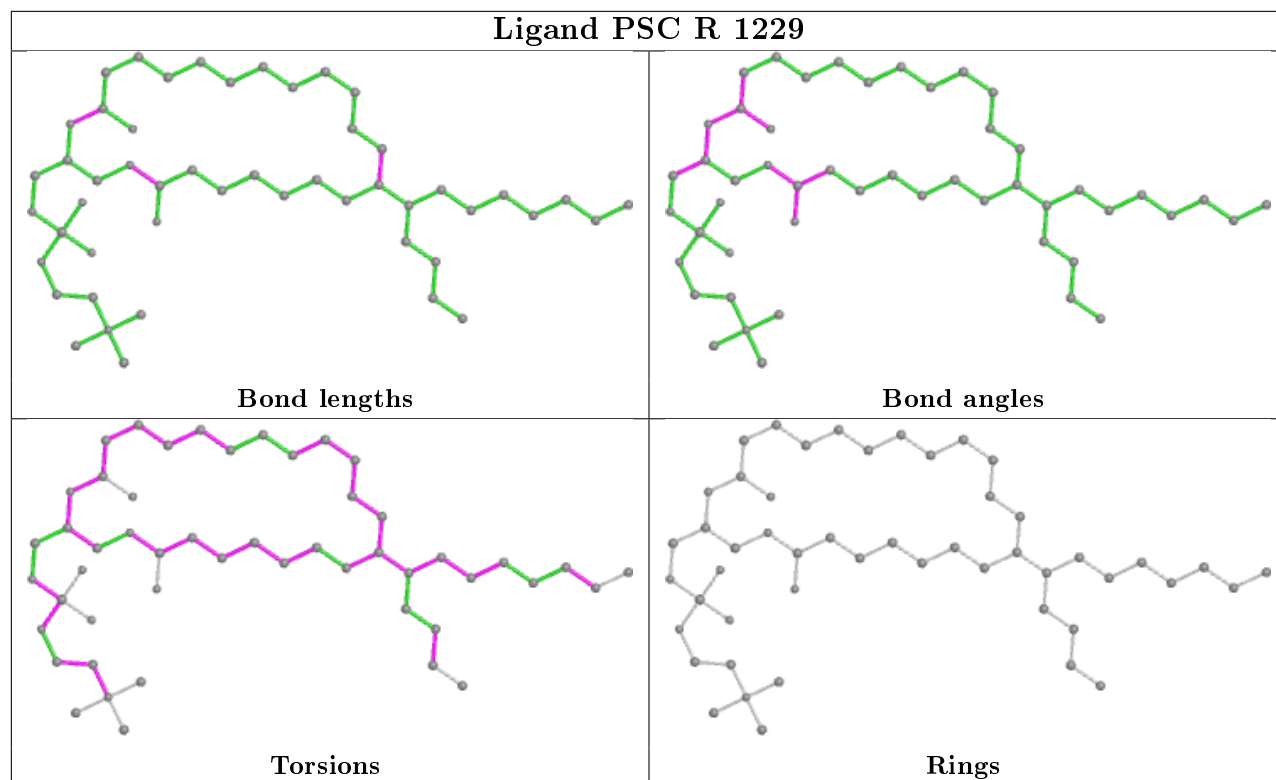
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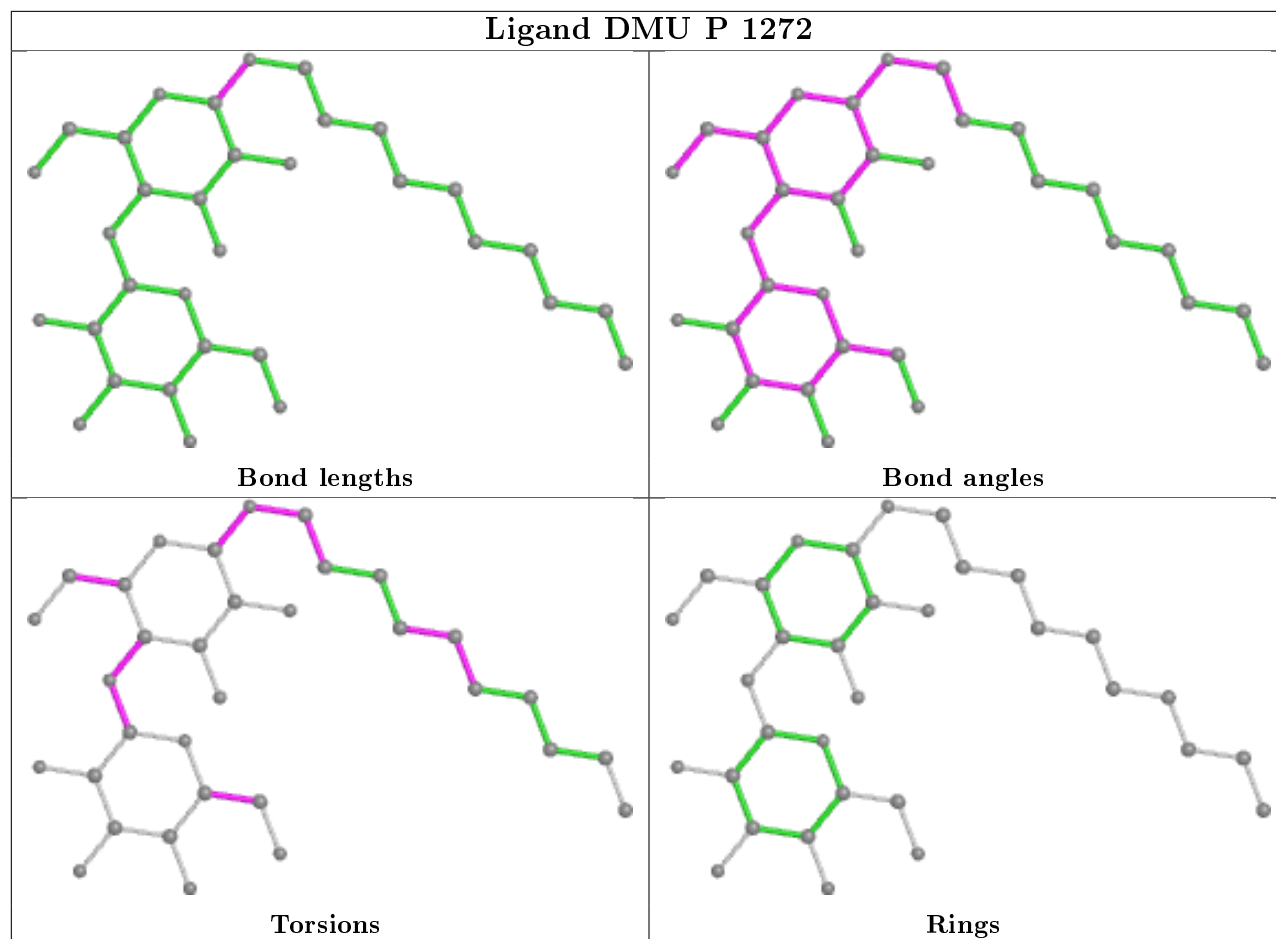
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	J	60	CHD	2	0
14	N	515	HEA	3	0
25	C	270	CDL	21	0
22	O	229	CHD	1	0
24	G	265	PEK	13	0
28	G	272	DMU	3	0
22	P	1271	CHD	4	0
19	Q	1523	TGL	10	0
25	T	1269	CDL	34	0
19	A	521	TGL	7	0
19	L	522	TGL	15	0
24	C	264	PEK	3	0
28	Z	1526	DMU	2	0
20	A	522	PGV	2	0
22	P	1525	CHD	1	0
14	A	515	HEA	5	0
15	N	520	CYN	2	0
14	A	516	HEA	8	0
24	T	1264	PEK	9	0
20	P	1267	PGV	3	0
26	E	229	PSC	16	0
20	N	1524	PGV	7	0
19	N	1522	TGL	15	0
24	T	263	PEK	19	0
20	A	524	PGV	8	0
24	S	1265	PEK	16	0
14	N	516	HEA	10	0
22	B	1085	CHD	3	0
22	C	271	CHD	3	0

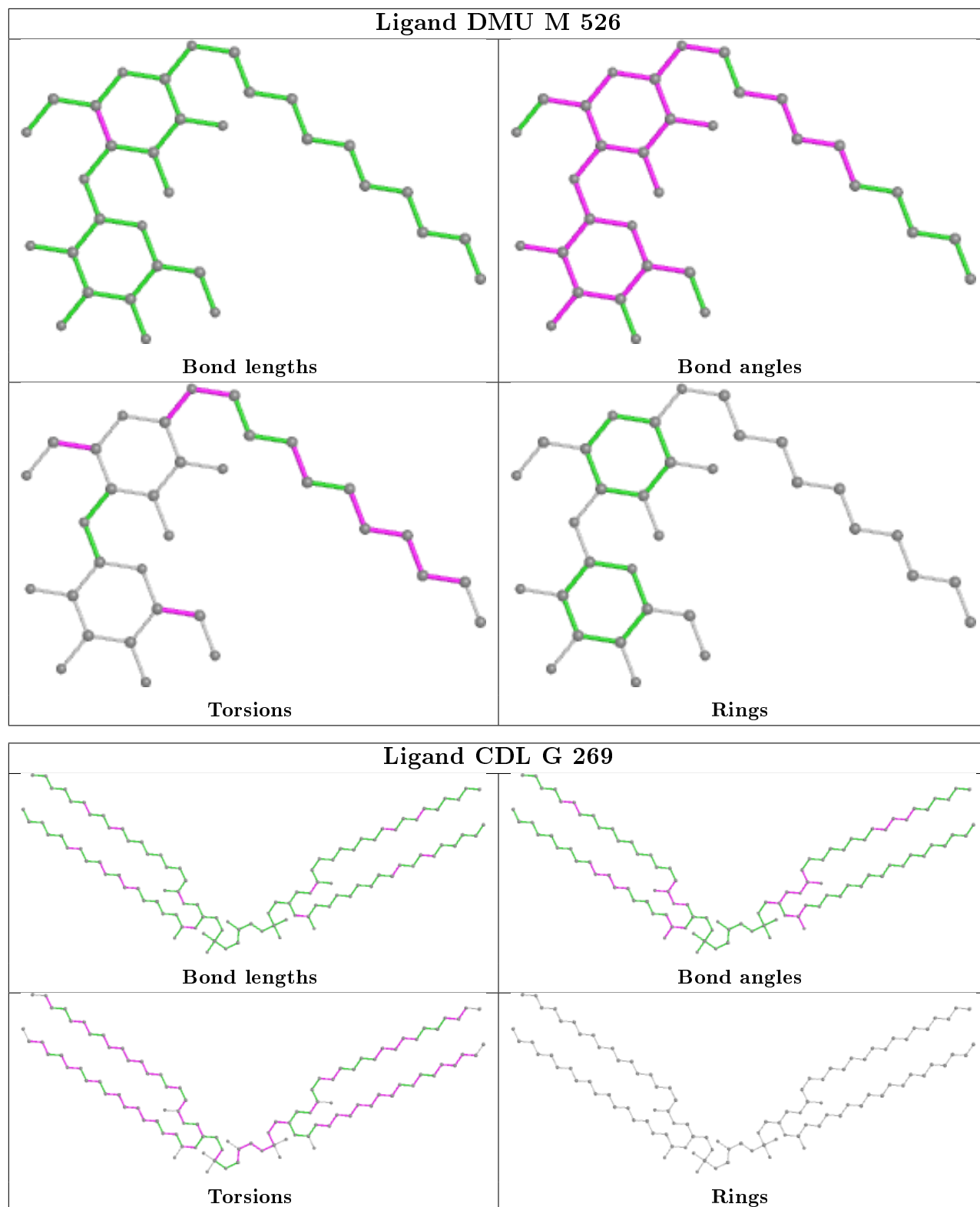
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

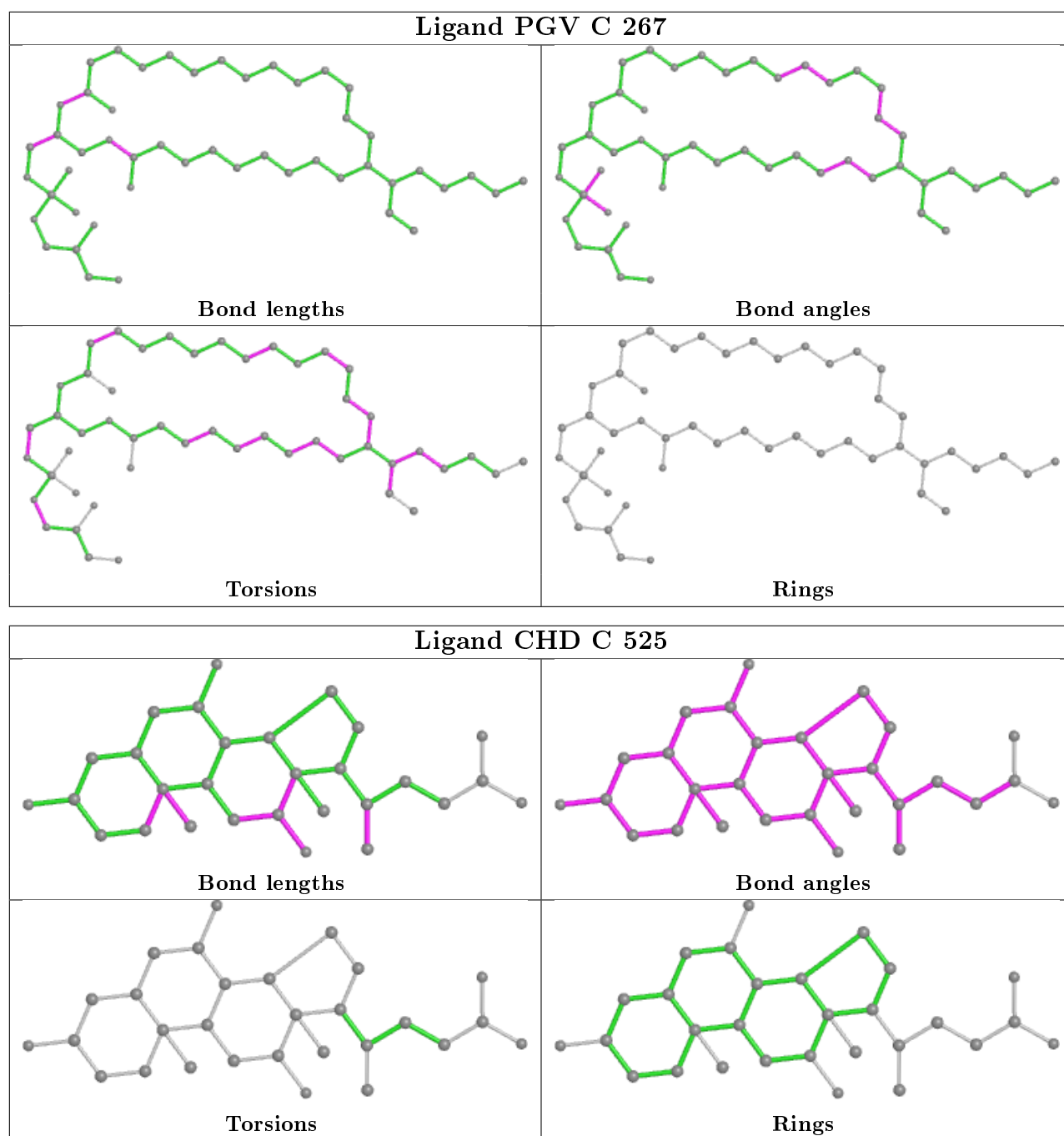


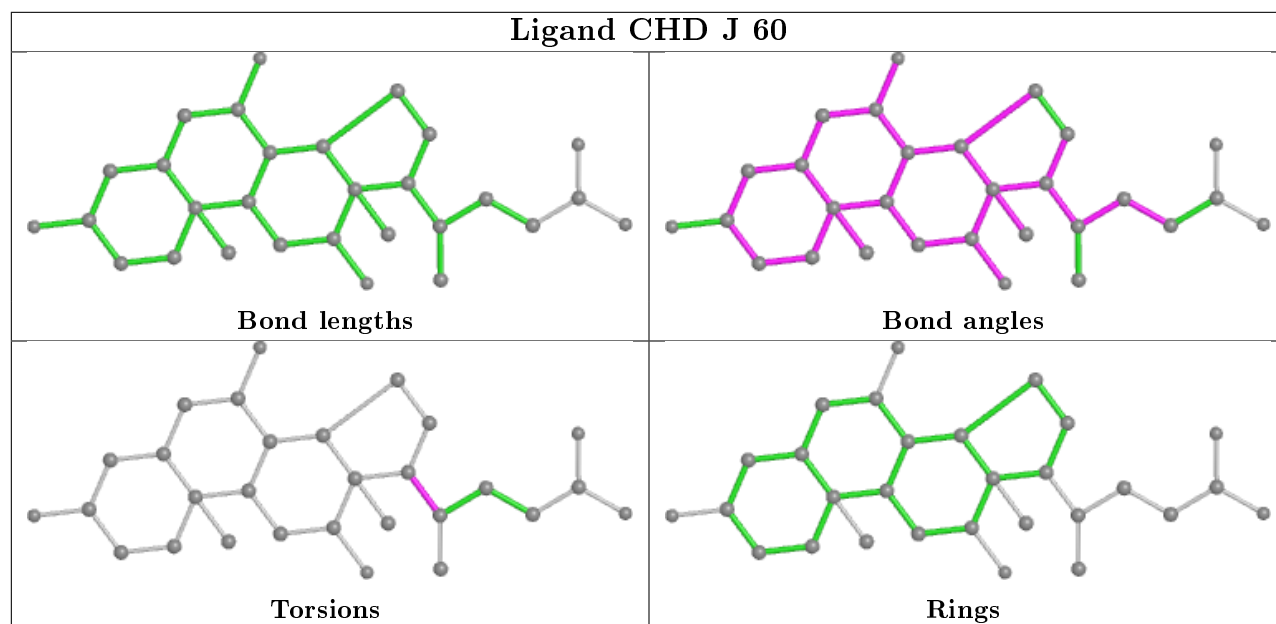
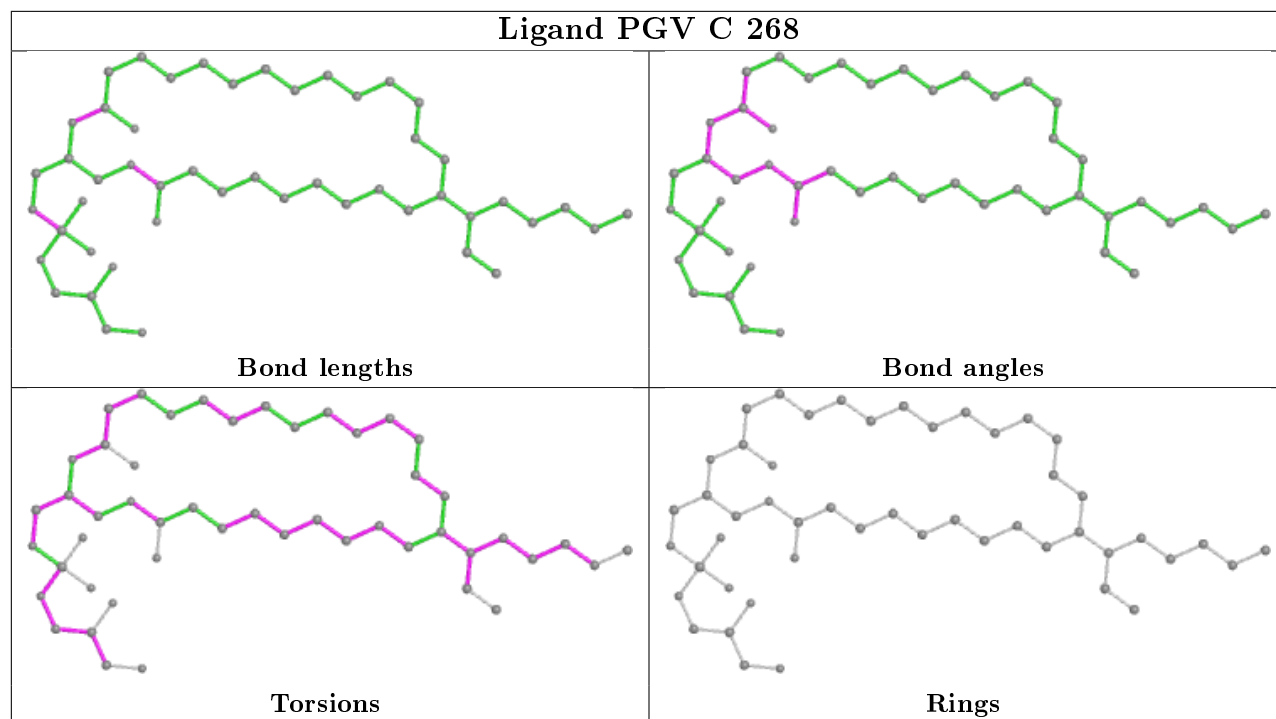


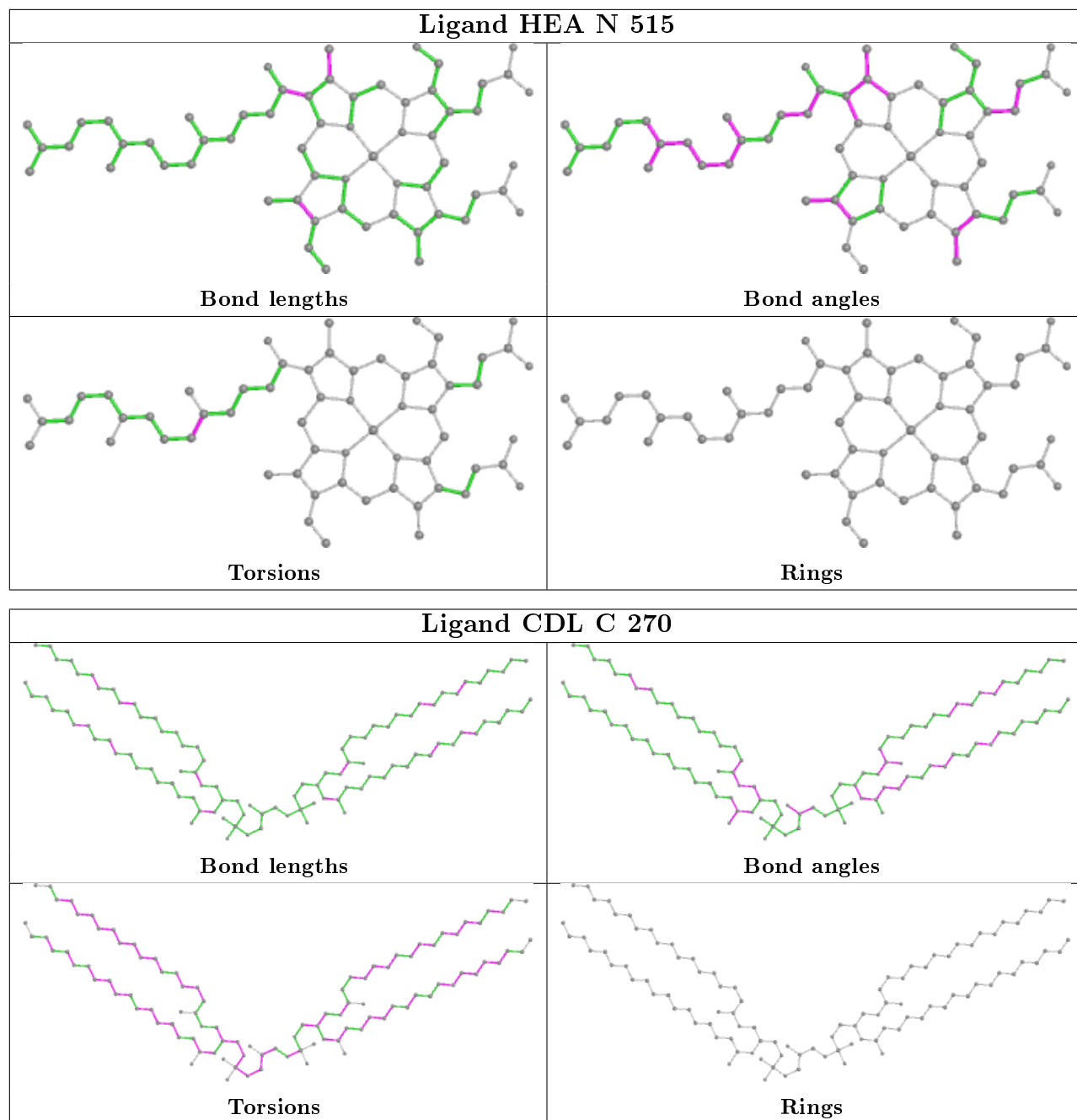


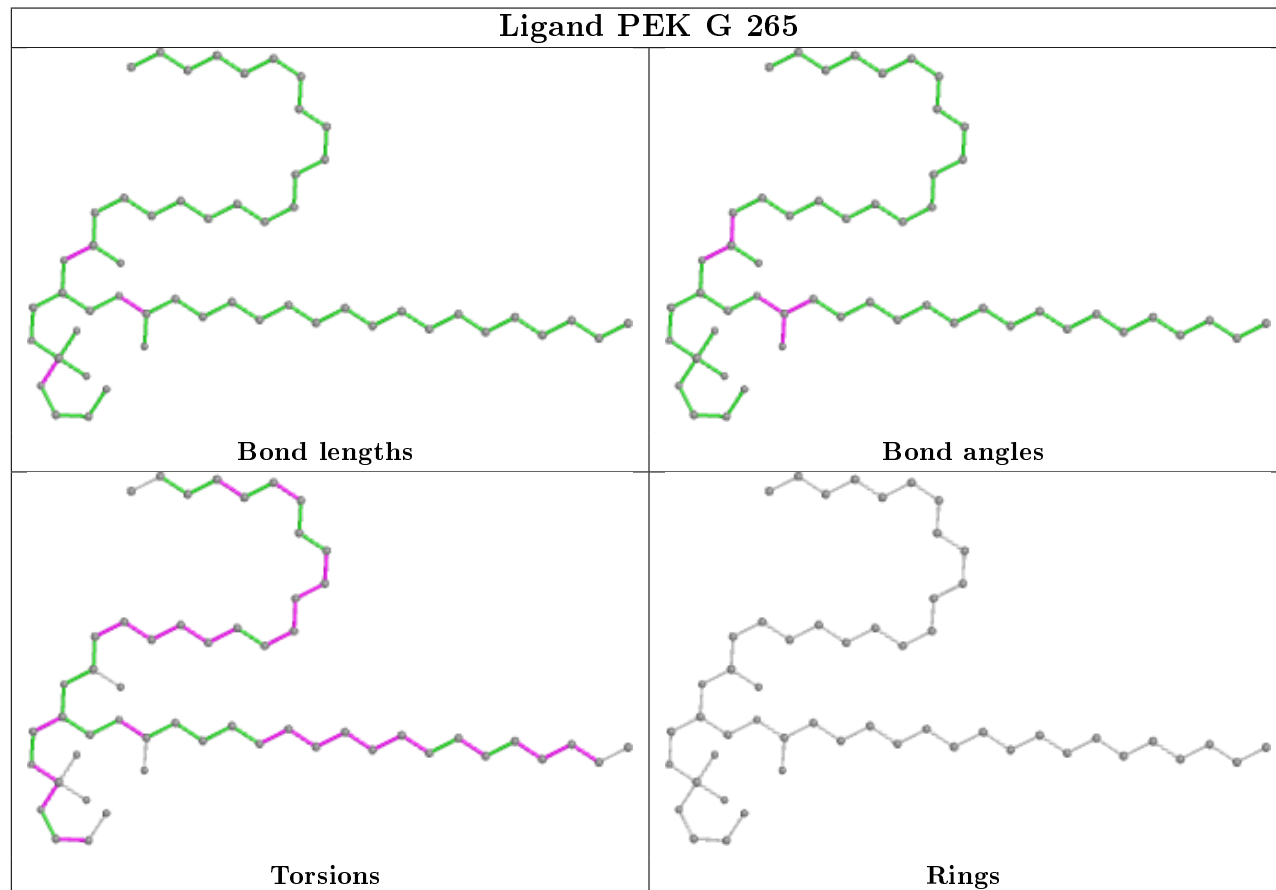
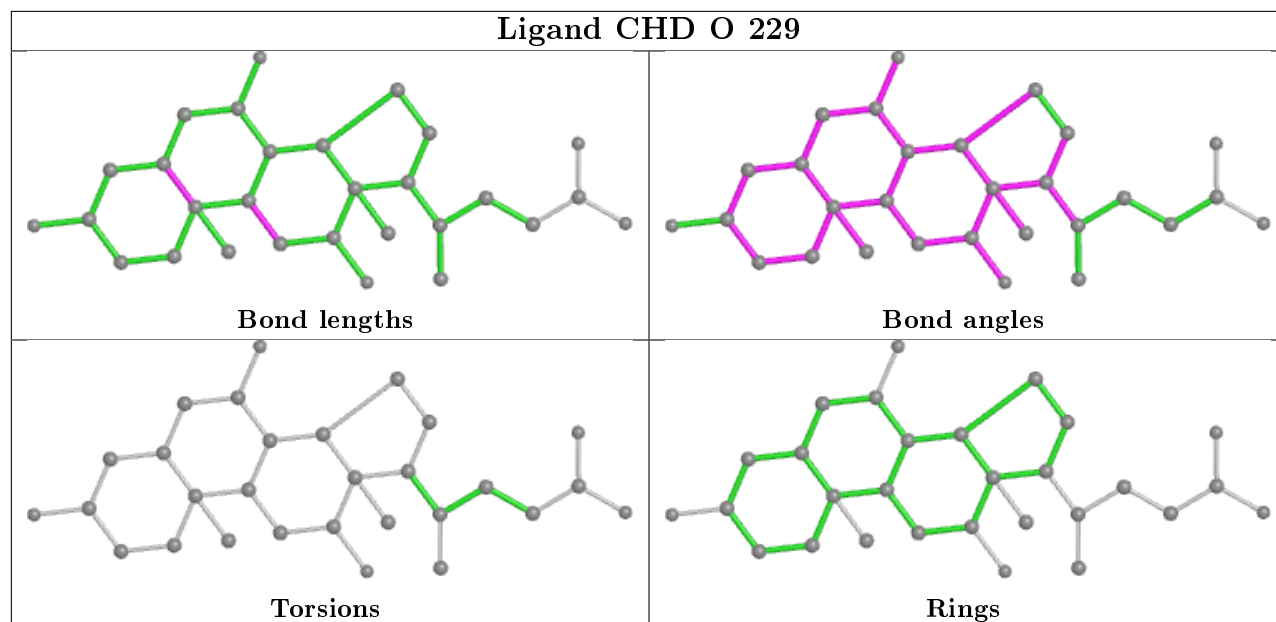




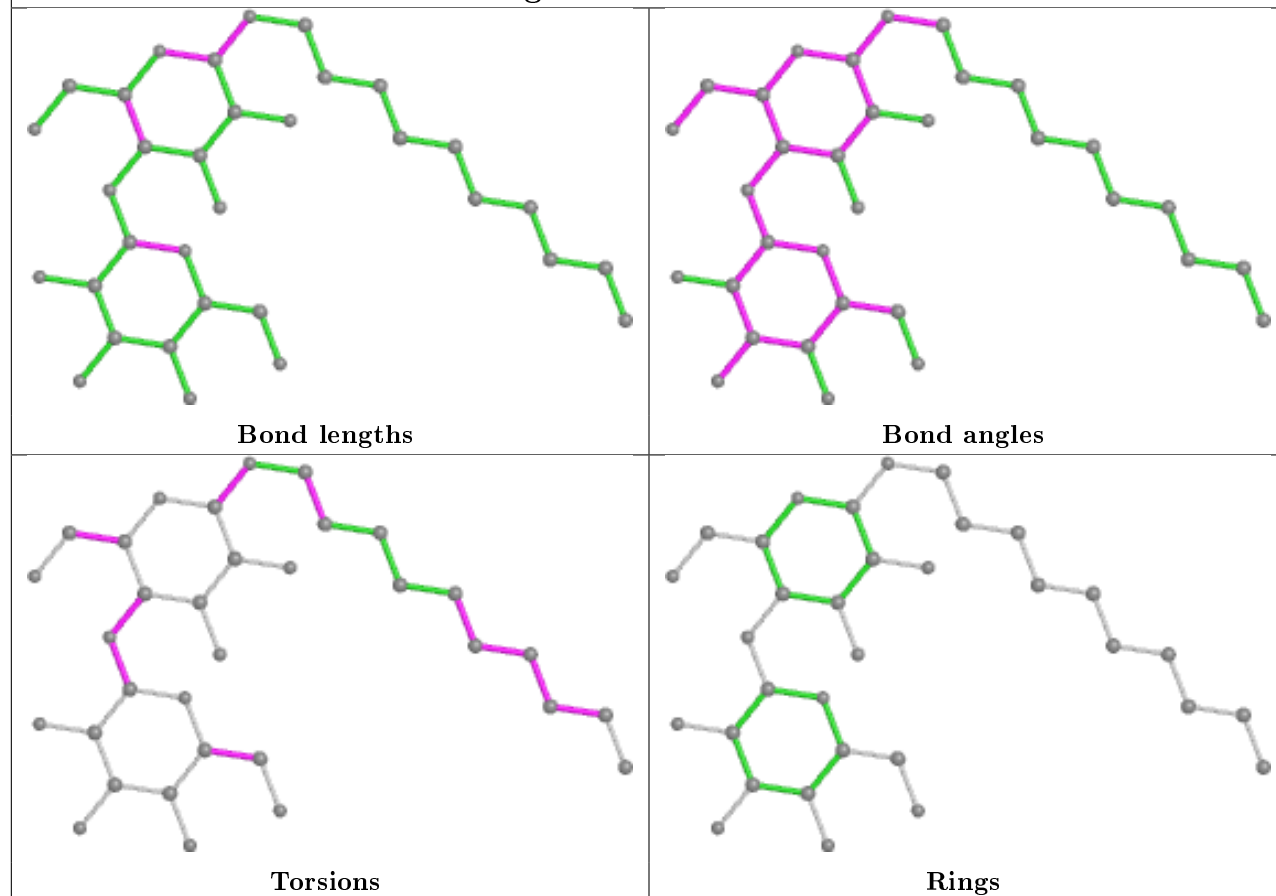




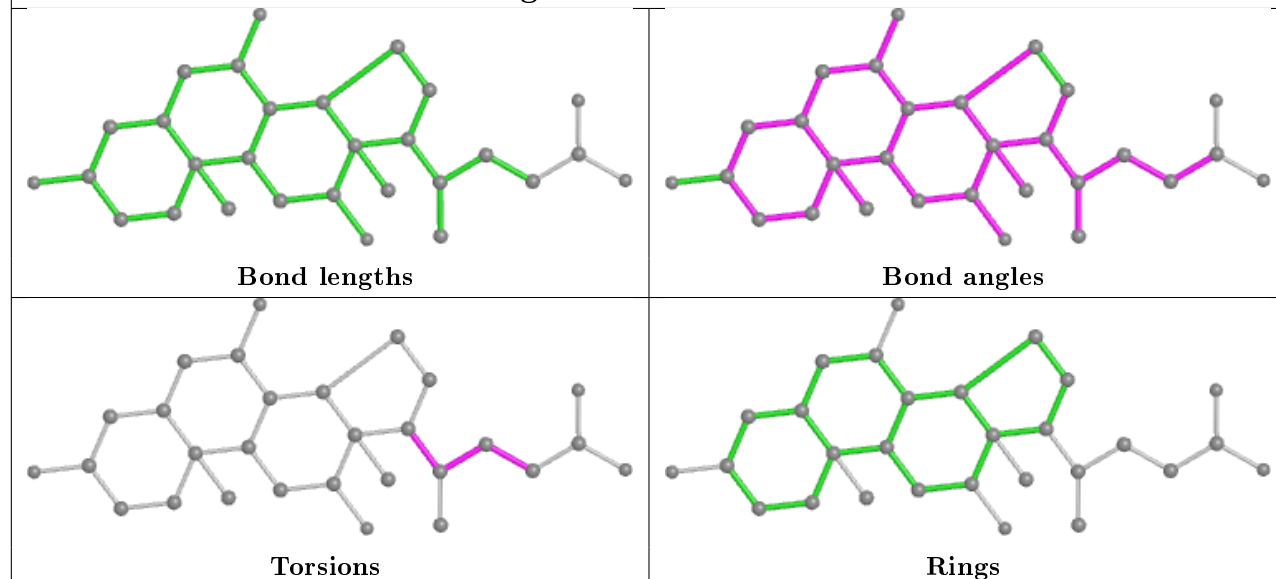


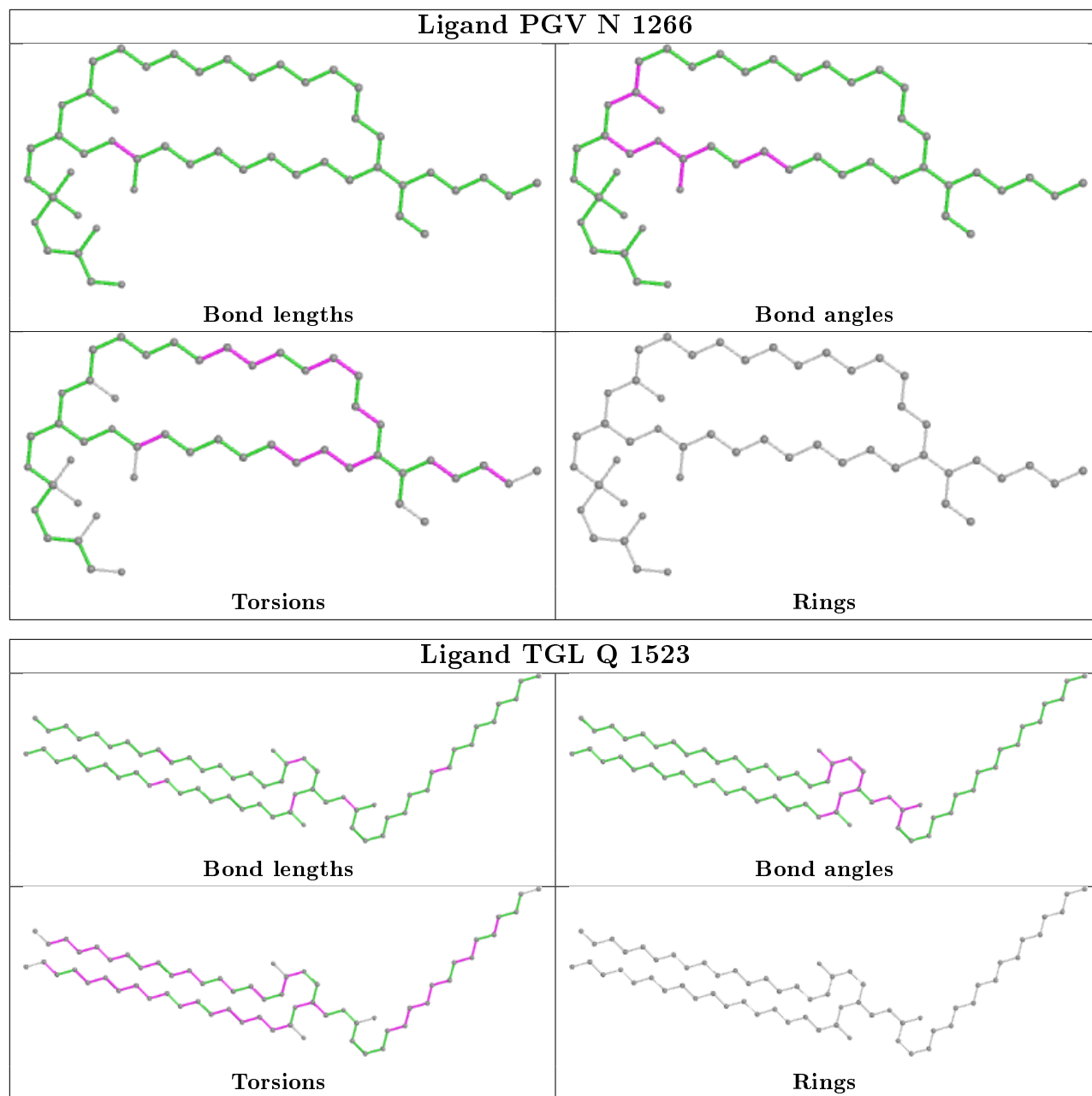


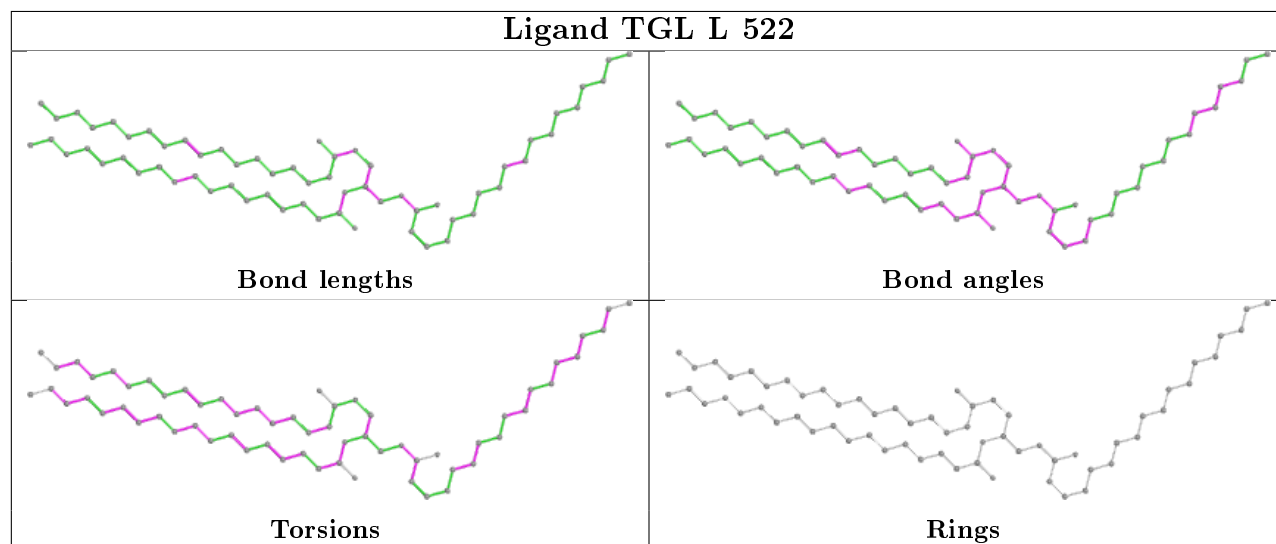
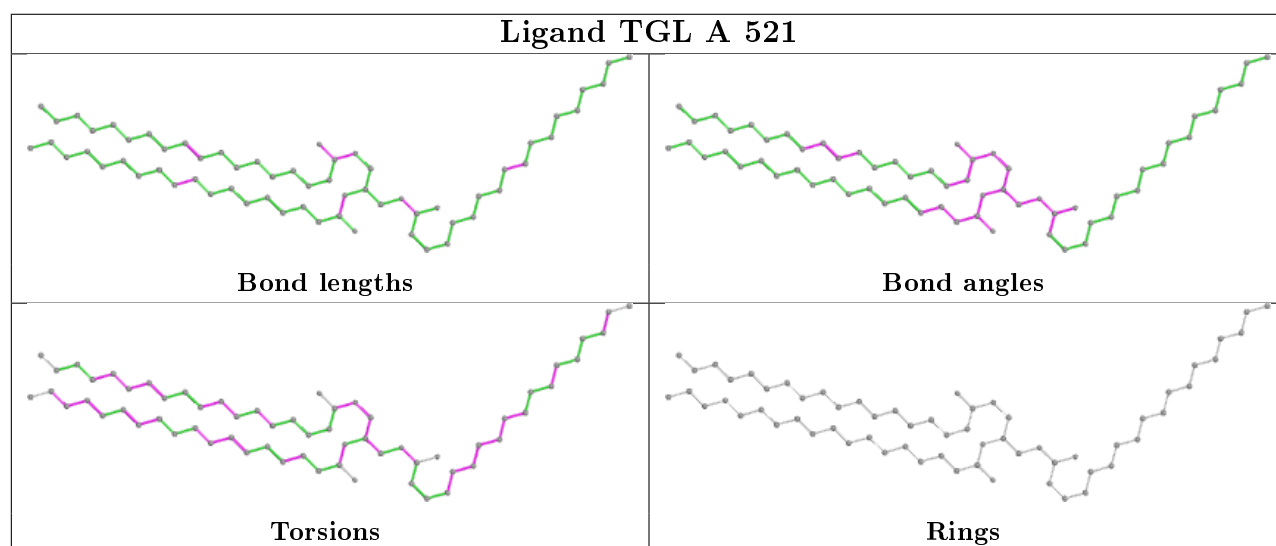
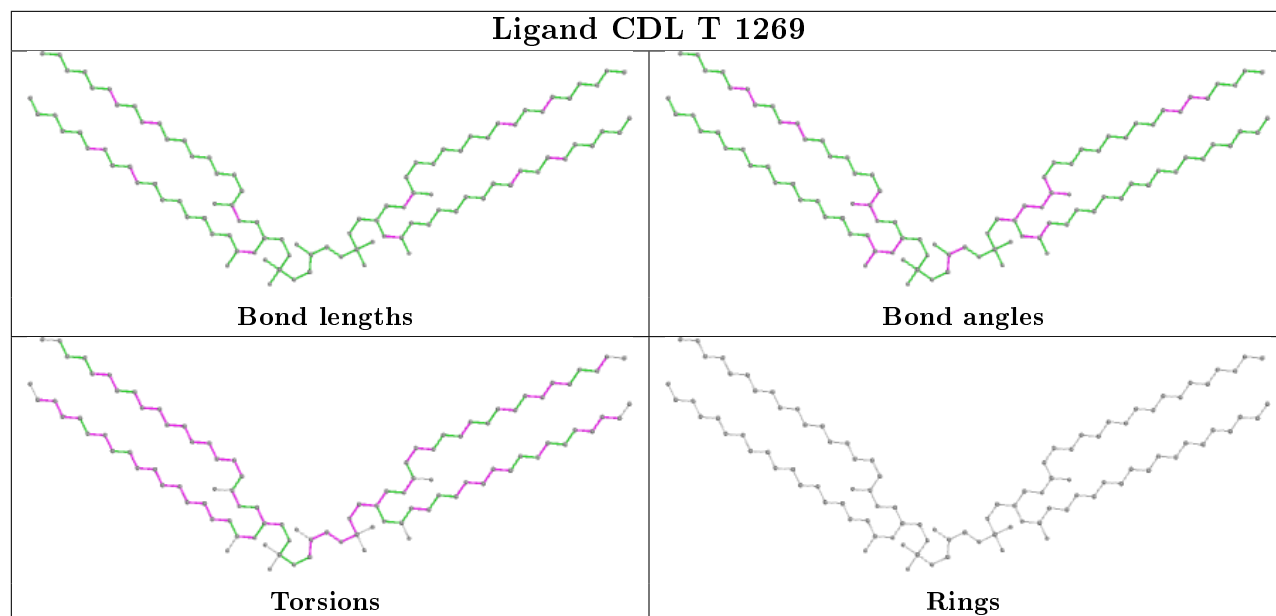
## Ligand DMU G 272

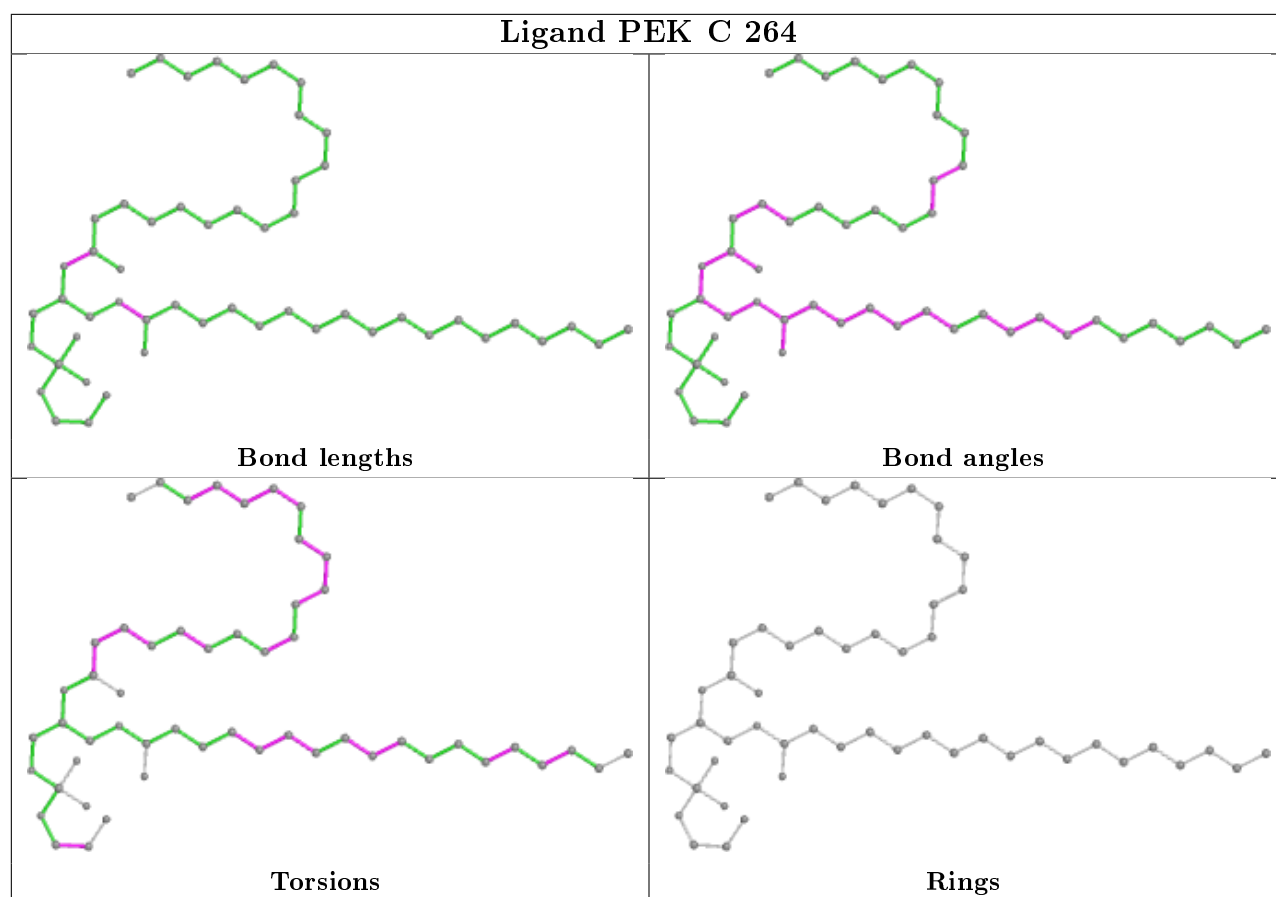


## Ligand CHD P 1271

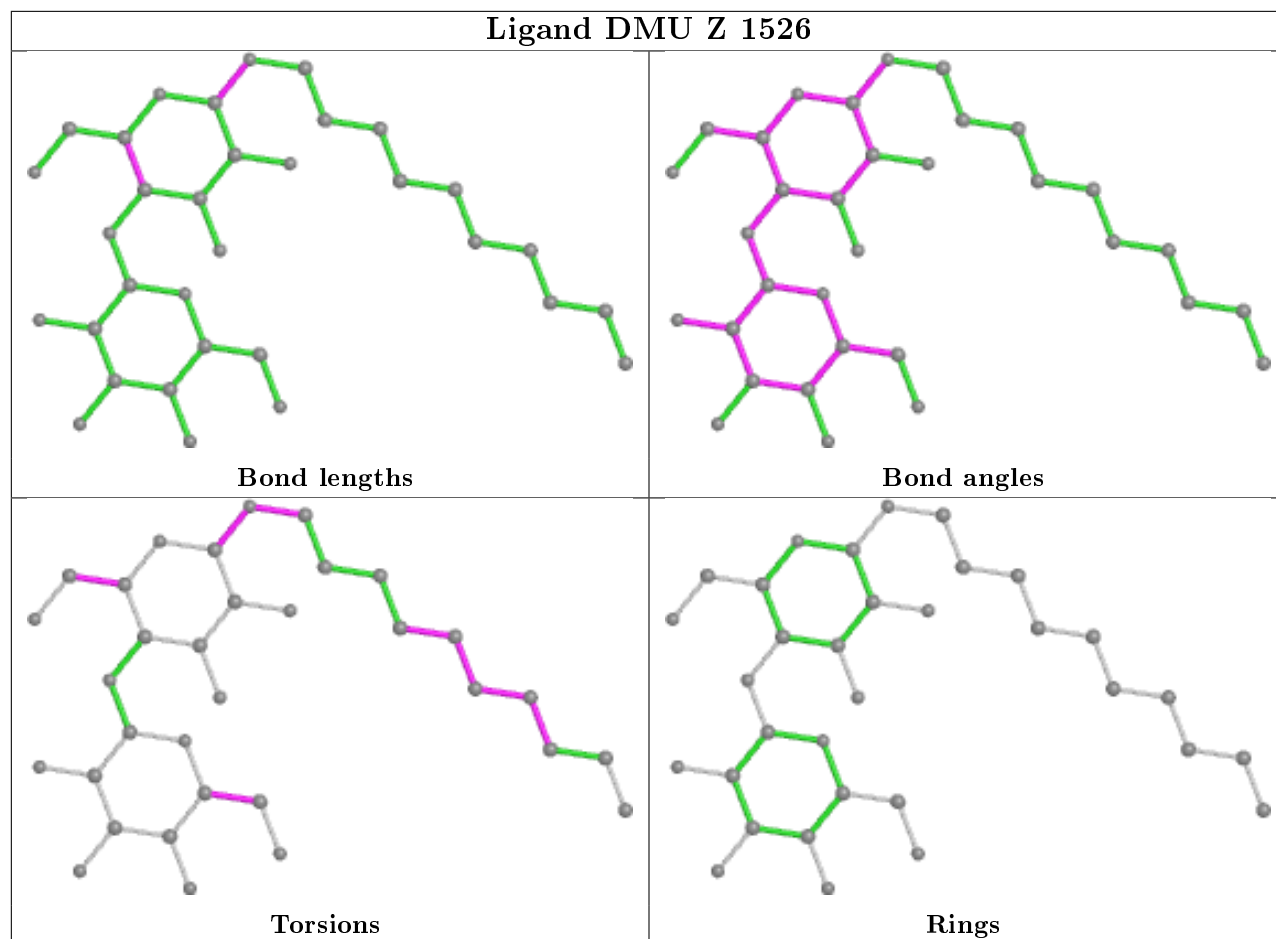




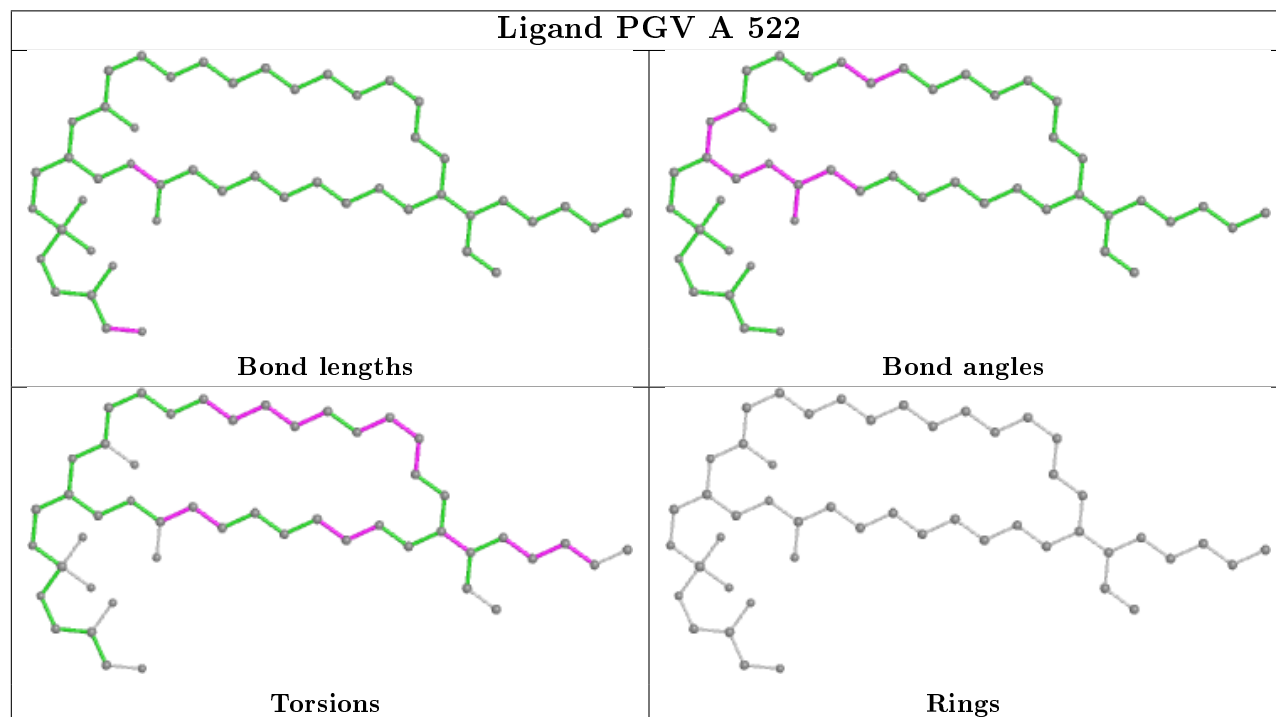


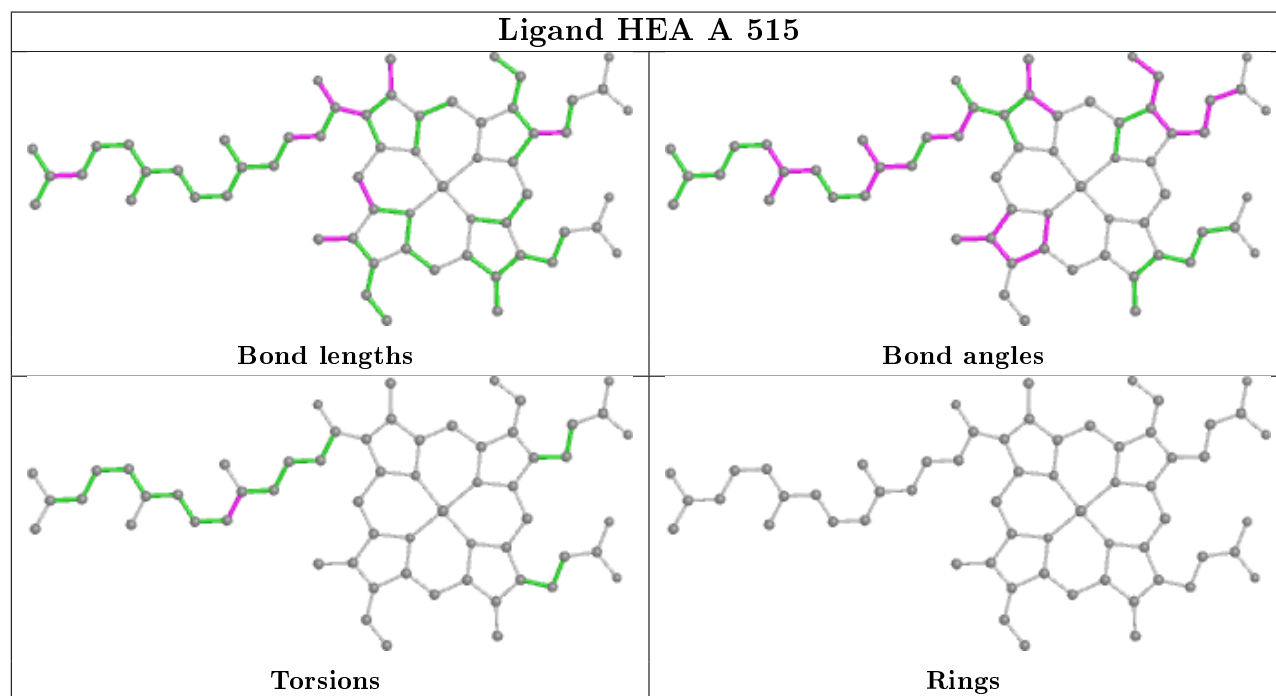
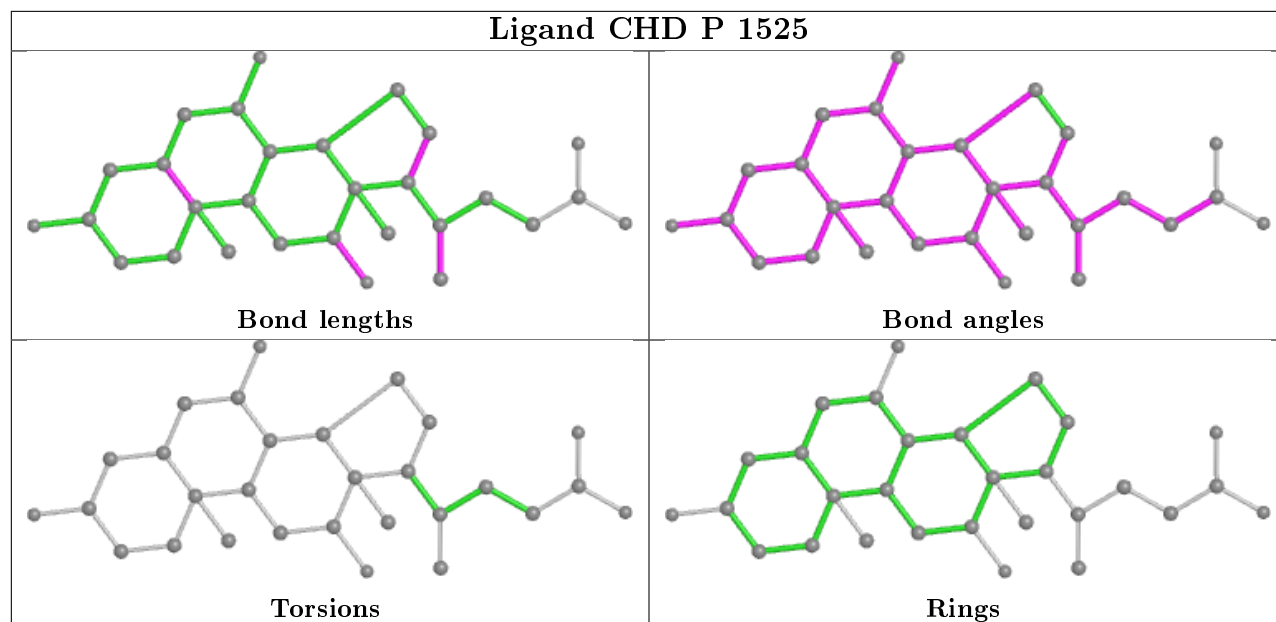


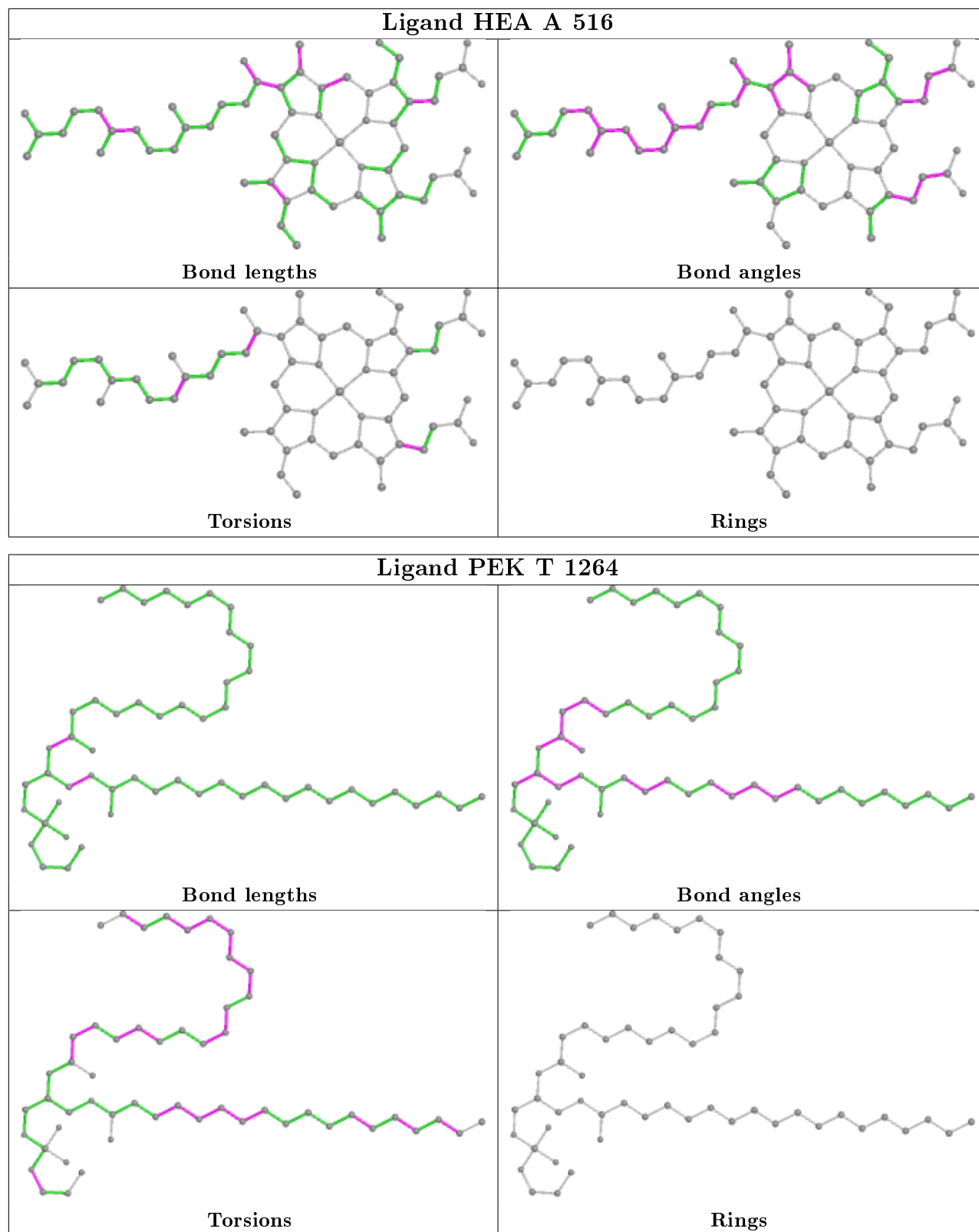
## Ligand DMU Z 1526



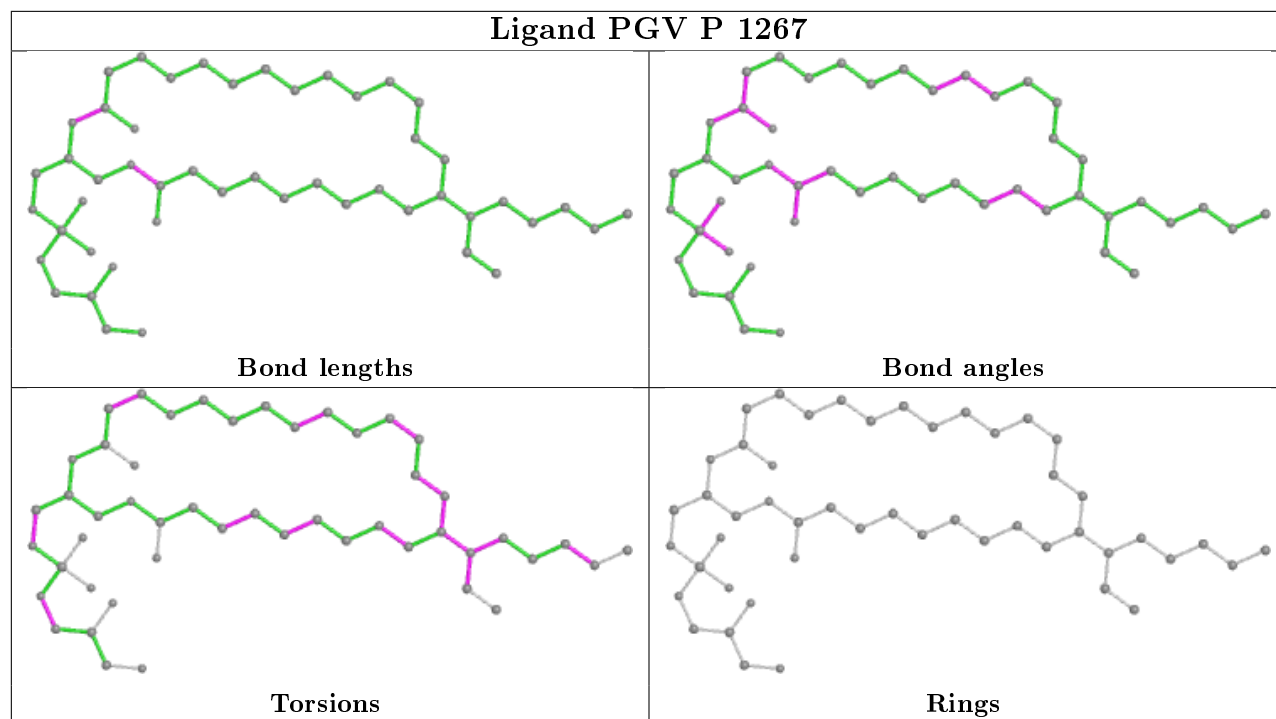
## Ligand PGV A 522



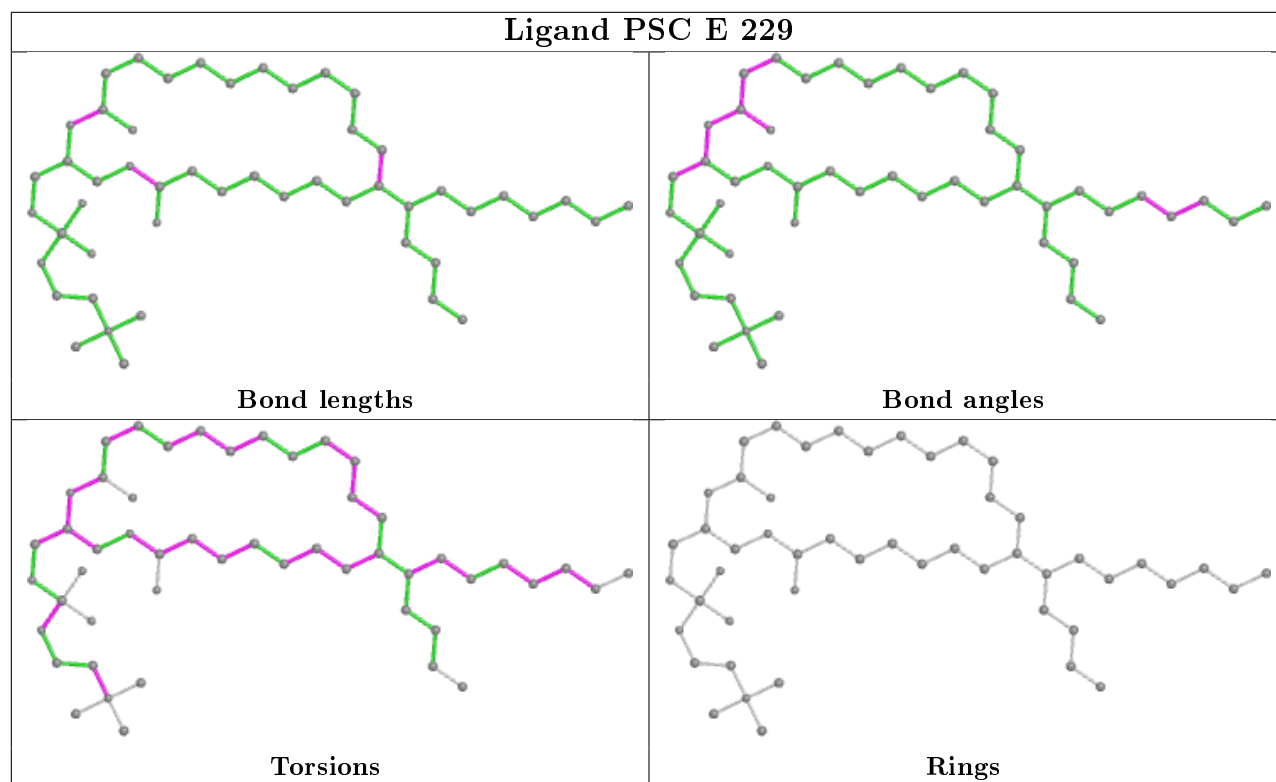




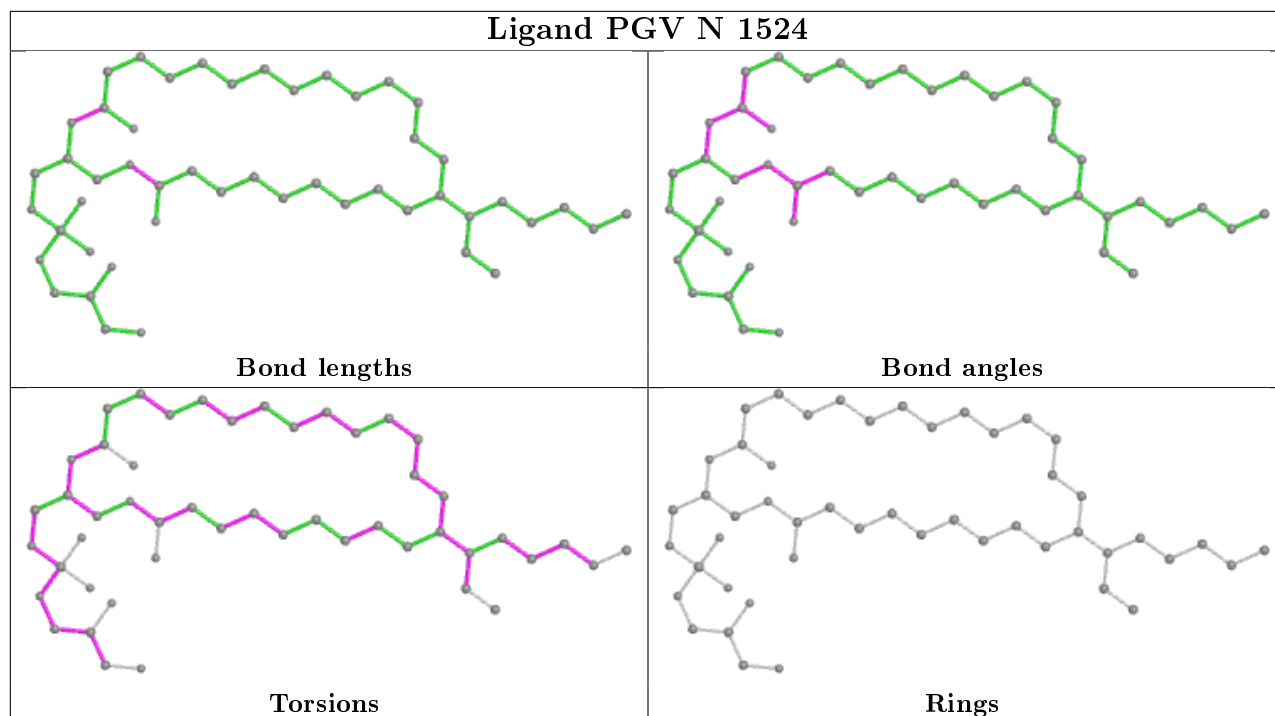
## Ligand PGV P 1267



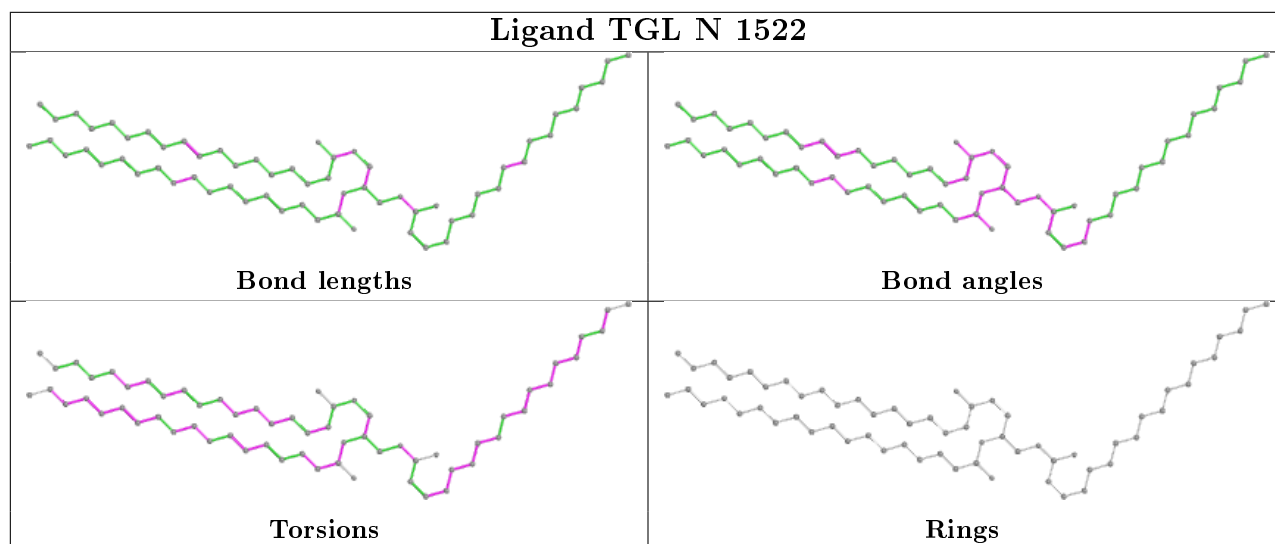
## Ligand PSC E 229

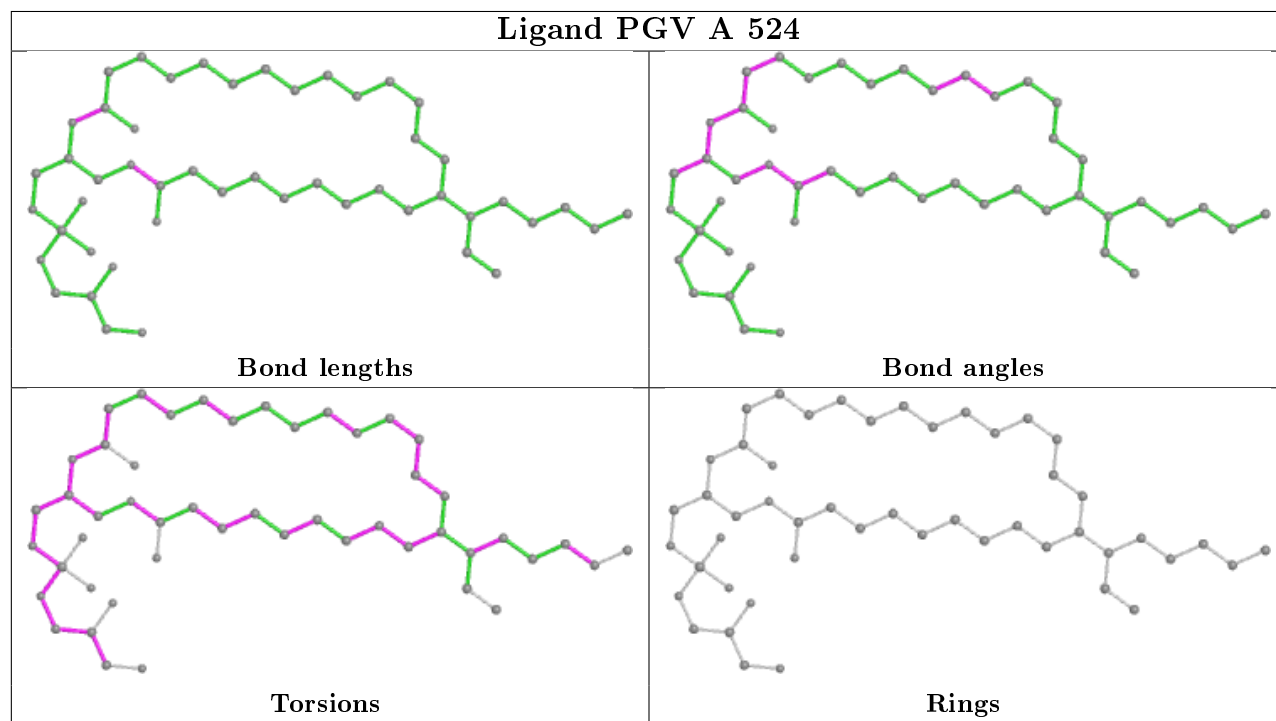
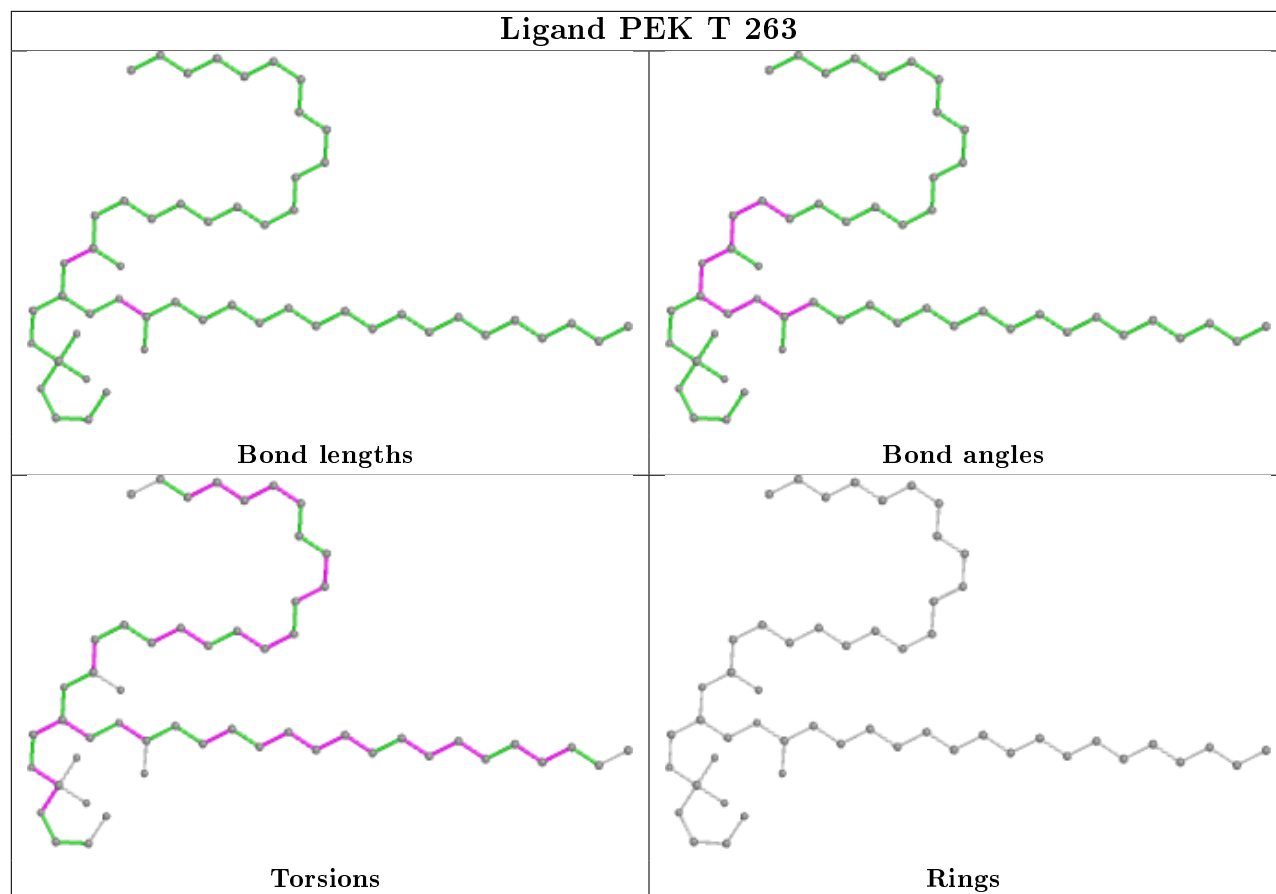


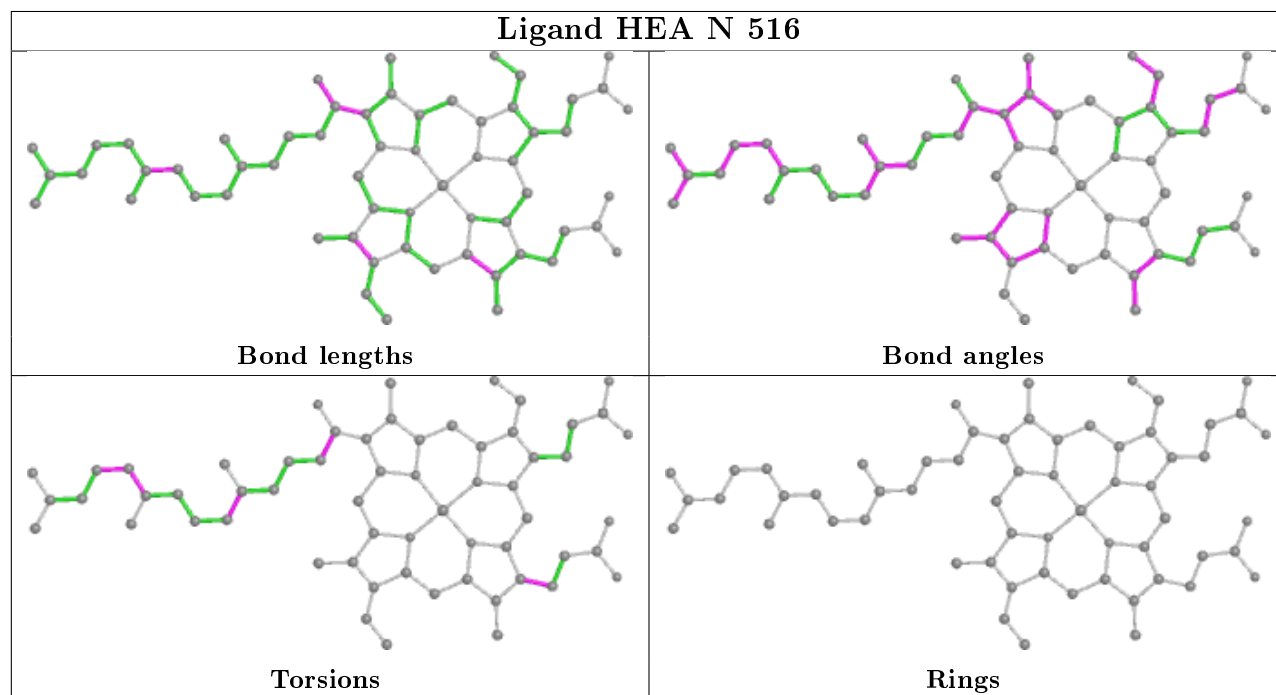
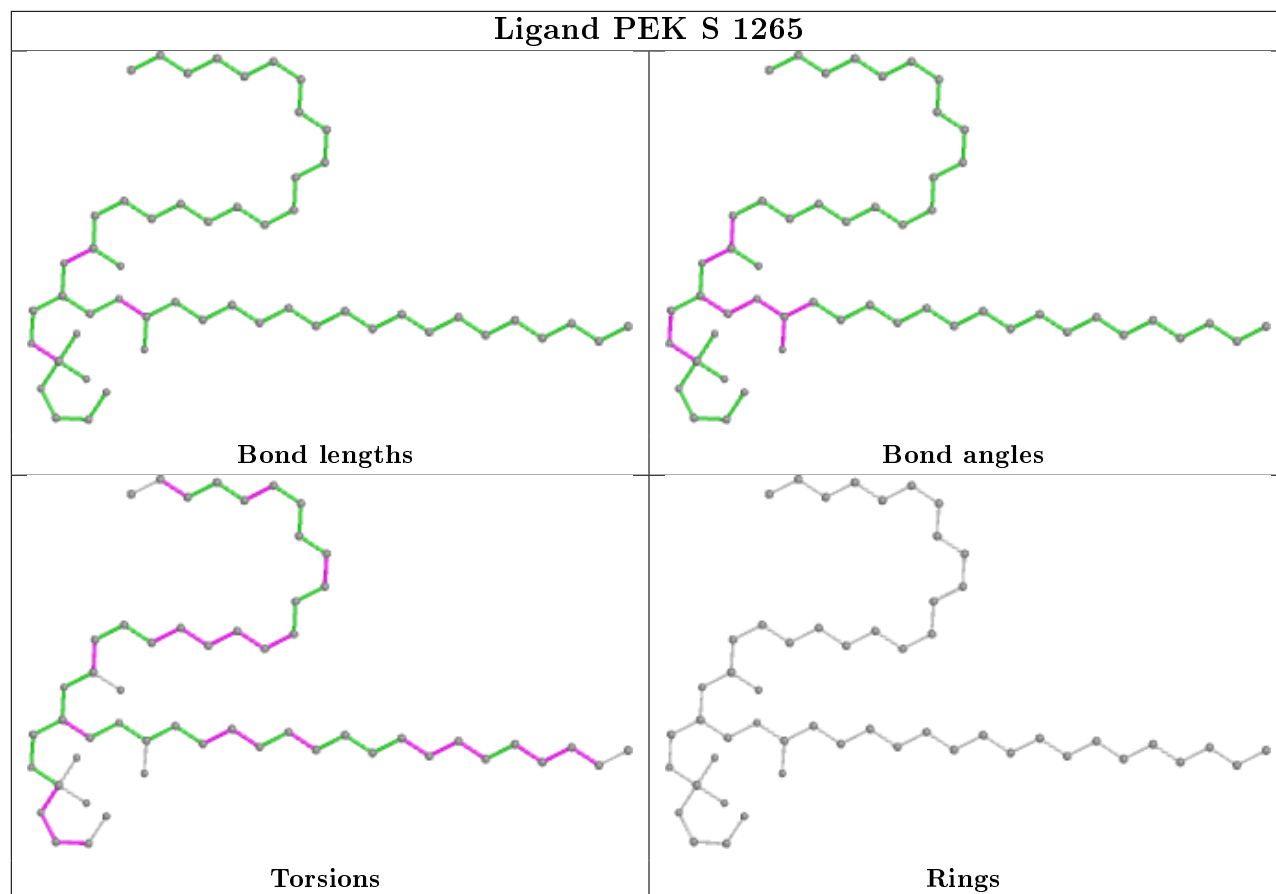
## Ligand PGV N 1524

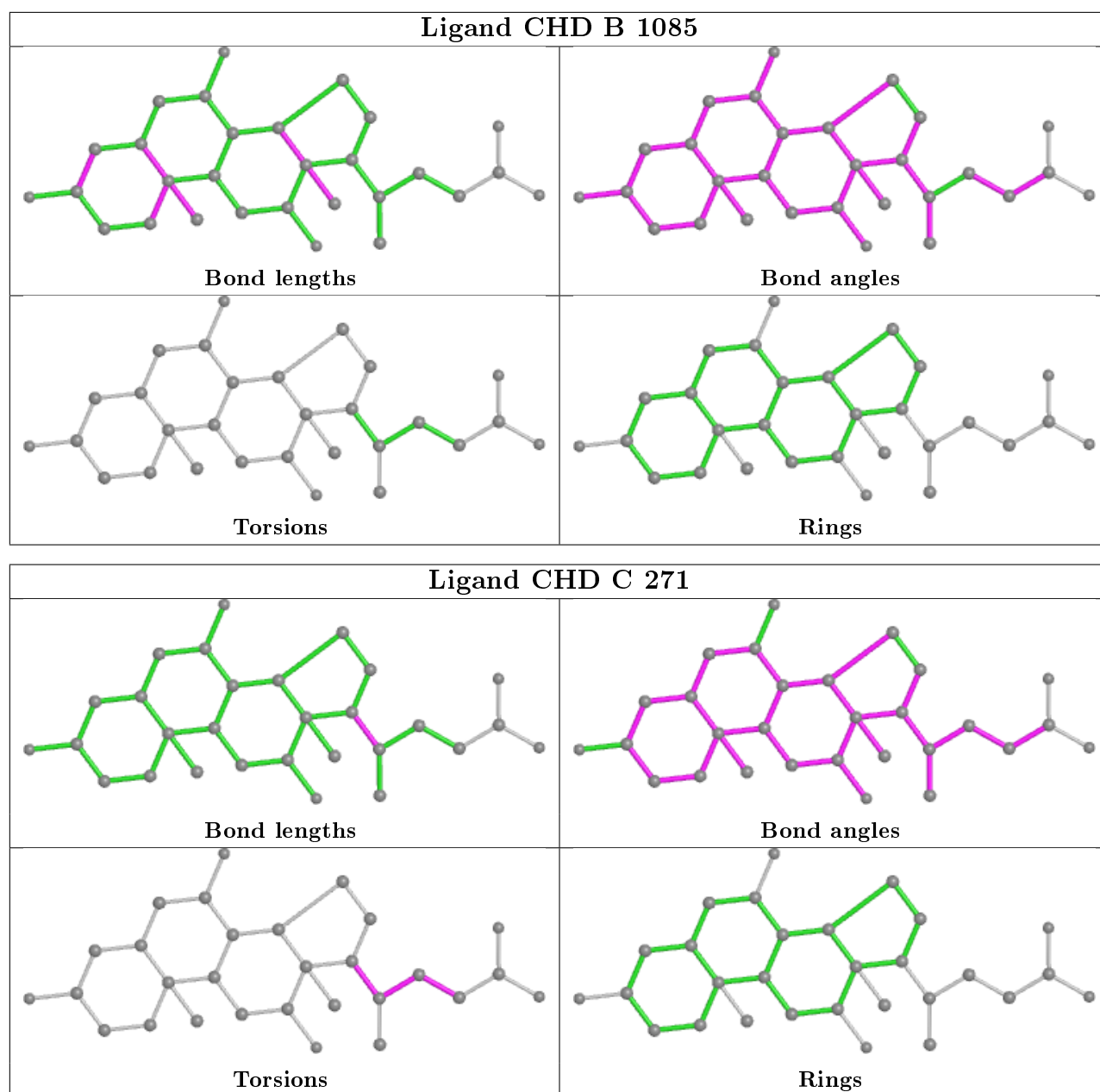


## Ligand TGL N 1522









## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	0.50	48 (9%) 8 9	23, 29, 40, 63	0
1	N	513/514 (99%)	0.29	29 (5%) 23 25	30, 36, 47, 68	0
2	B	226/227 (99%)	-0.33	3 (1%) 77 79	24, 35, 59, 78	0
2	O	226/227 (99%)	-0.07	5 (2%) 62 66	33, 45, 70, 88	0
3	C	259/261 (99%)	-0.43	1 (0%) 92 93	26, 32, 43, 62	0
3	P	259/261 (99%)	-0.44	3 (1%) 79 81	29, 36, 47, 67	0
4	D	144/147 (97%)	-0.44	1 (0%) 87 89	30, 37, 56, 70	0
4	Q	144/147 (97%)	1.22	28 (19%) 1 0	39, 52, 76, 118	0
5	E	105/109 (96%)	-0.03	2 (1%) 66 71	31, 38, 63, 99	0
5	R	105/109 (96%)	0.22	5 (4%) 30 33	36, 43, 68, 103	0
6	F	98/98 (100%)	0.34	8 (8%) 11 12	29, 39, 80, 127	0
6	S	98/98 (100%)	0.50	11 (11%) 5 5	34, 43, 86, 123	0
7	G	83/85 (97%)	0.70	15 (18%) 1 1	29, 39, 110, 113	0
7	T	83/85 (97%)	0.67	18 (21%) 0 0	29, 42, 102, 110	0
8	H	79/85 (92%)	0.32	12 (15%) 2 1	30, 41, 90, 112	0
8	U	79/85 (92%)	0.87	16 (20%) 1 0	37, 48, 94, 113	0
9	I	72/73 (98%)	0.21	6 (8%) 11 11	34, 46, 80, 83	0
9	V	72/73 (98%)	0.77	11 (15%) 2 1	39, 55, 82, 85	0
10	J	58/59 (98%)	0.21	8 (13%) 2 2	31, 41, 65, 96	0
10	W	58/59 (98%)	0.53	11 (18%) 1 0	34, 45, 69, 107	0
11	K	49/56 (87%)	-0.38	0 100 100	33, 41, 52, 62	0
11	X	49/56 (87%)	1.13	12 (24%) 0 0	44, 51, 64, 76	0
12	L	46/47 (97%)	-0.44	1 (2%) 62 66	29, 34, 50, 79	0
12	Y	46/47 (97%)	0.04	3 (6%) 18 20	34, 45, 61, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.22	3 (6%) 16 18	30, 34, 71, 101	0
13	Z	43/46 (93%)	0.45	7 (16%) 1 1	41, 46, 90, 112	0
All	All	3550/3614 (98%)	0.18	267 (7%) 14 15	23, 38, 69, 127	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	30.7
6	S	97	ALA	13.6
4	Q	5	VAL	13.4
4	Q	4	SER	12.7
6	F	96	LEU	10.9
7	G	2	SER	10.6
6	F	97	ALA	10.4
6	F	98	HIS	10.4
4	Q	8	SER	9.9
7	G	3	ALA	9.8
4	Q	7	LYS	9.6
8	U	7	LYS	9.5
6	F	2	SER	8.8
7	T	1	ALA	8.1
6	S	96	LEU	8.1
13	Z	43	SER	8.0
8	H	46	LYS	7.9
10	J	58	LYS	7.8
8	U	8	ILE	7.6
10	W	58	LYS	7.3
8	H	44	THR	7.2
6	F	1	ALA	7.2
6	S	94	HIS	7.0
6	S	2	SER	6.8
8	H	47	GLY	6.6
7	G	5	LYS	6.2
5	R	109	VAL	6.1
11	X	7	PRO	6.1
7	G	42	ARG	6.1
6	F	95	GLN	5.8
5	R	5	HIS	5.8
8	H	7	LYS	5.8
8	H	45	ALA	5.7
7	T	5	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
10	J	1	PHE	5.6
11	X	6	ALA	5.6
6	S	98	HIS	5.5
11	X	13	TYR	5.4
13	M	43	SER	5.4
6	S	1	ALA	5.4
5	E	5	HIS	5.4
8	U	44	THR	5.1
7	T	42	ARG	5.1
9	V	30	GLY	4.9
7	T	36	TRP	4.7
7	T	2	SER	4.7
9	I	25	PHE	4.6
4	Q	147	LYS	4.5
7	G	40	GLY	4.4
1	A	66	ILE	4.4
9	V	29	LEU	4.4
13	Z	32	TRP	4.4
8	U	45	ALA	4.3
7	T	4	ALA	4.3
7	G	8	HIS	4.3
7	G	1	ALA	4.3
5	E	109	VAL	4.2
7	T	39	SER	4.2
10	W	57	HIS	4.2
7	T	40	GLY	4.1
10	W	52	TRP	4.1
9	I	37	PHE	4.1
9	V	37	PHE	4.1
2	O	113	TYR	4.0
12	Y	47	LYS	4.0
1	A	73	ILE	4.0
8	H	43	MET	3.9
9	I	30	GLY	3.9
9	V	2	THR	3.9
5	R	96	LEU	3.8
8	U	9	LYS	3.8
4	Q	58	GLU	3.8
1	N	3	ILE	3.8
9	I	29	LEU	3.8
8	U	10	ASN	3.8
4	Q	53	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
6	S	95	GLN	3.7
9	V	33	THR	3.7
13	Z	35	TYR	3.6
13	Z	40	TYR	3.6
7	G	84	LYS	3.5
1	A	195	LEU	3.5
7	T	8	HIS	3.5
12	L	2	HIS	3.5
6	S	93	PRO	3.5
8	U	47	GLY	3.5
1	A	202	LEU	3.4
1	N	66	ILE	3.4
1	A	199	LEU	3.4
4	Q	62	LEU	3.4
4	Q	46	ALA	3.4
1	A	243	VAL	3.4
8	H	48	GLY	3.3
4	Q	48	TRP	3.3
10	J	52	TRP	3.3
8	U	48	GLY	3.3
10	W	26	ALA	3.3
7	G	37	LEU	3.3
1	N	62	ALA	3.3
4	Q	138	TRP	3.2
8	U	55	TRP	3.2
4	Q	33	LEU	3.2
7	T	84	LYS	3.1
4	Q	30	VAL	3.1
8	U	42	ALA	3.1
1	A	75	ILE	3.1
13	Z	39	ASN	3.1
8	U	49	ASP	3.1
3	P	3	HIS	3.1
7	G	7	ASP	3.0
4	Q	51	LEU	3.0
1	A	64	VAL	3.0
1	A	237	PHE	3.0
7	G	4	ALA	3.0
11	X	23	THR	3.0
6	F	3	GLY	3.0
6	F	94	HIS	3.0
2	O	217	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	67	PHE	3.0
1	N	377	PHE	3.0
4	Q	102	TYR	3.0
11	X	52	GLU	2.9
1	N	75	ILE	2.9
13	Z	13	LYS	2.9
1	A	70	VAL	2.9
8	U	11	TYR	2.9
11	X	16	ALA	2.9
1	N	70	VAL	2.9
1	A	194	LEU	2.9
9	V	26	MET	2.9
7	T	6	GLY	2.8
7	T	43	GLU	2.8
9	V	25	PHE	2.8
9	I	33	THR	2.8
13	Z	42	LYS	2.8
1	A	62	ALA	2.8
10	W	1	PHE	2.8
1	N	373	VAL	2.8
7	T	10	GLY	2.8
8	U	43	MET	2.8
1	N	246	LEU	2.8
4	Q	40	LEU	2.8
1	A	197	LEU	2.7
2	B	59	GLN	2.7
8	H	8	ILE	2.7
4	Q	39	ALA	2.7
7	T	3	ALA	2.7
1	A	71	MET	2.7
1	N	2	PHE	2.7
1	N	201	VAL	2.7
10	J	57	HIS	2.7
1	A	246	LEU	2.7
12	Y	19	TRP	2.6
4	Q	97	ILE	2.6
1	A	235	PHE	2.6
13	M	40	TYR	2.6
10	W	30	ILE	2.6
1	A	236	TRP	2.6
1	A	385	ALA	2.6
4	Q	49	SER	2.6

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Mol	Chain	Res	Type	RSRZ
7	G	9	GLY	2.6
3	P	38	ASN	2.6
1	A	193	VAL	2.6
1	A	161	ALA	2.6
7	T	41	HIS	2.6
1	A	65	MET	2.6
10	J	2	GLU	2.5
1	N	202	LEU	2.5
7	G	43	GLU	2.5
2	O	47	THR	2.5
4	Q	43	LYS	2.5
1	N	67	PHE	2.5
1	N	71	MET	2.5
1	N	193	VAL	2.5
1	A	153	ALA	2.5
10	W	55	PHE	2.5
4	D	147	LYS	2.4
1	A	241	PRO	2.4
4	Q	124	LEU	2.4
1	N	243	VAL	2.4
1	N	388	ALA	2.4
9	V	53	ASN	2.4
1	A	238	PHE	2.4
5	R	52	LEU	2.4
8	U	46	LYS	2.4
8	H	42	ALA	2.4
10	J	56	PRO	2.4
1	A	126	TRP	2.4
1	N	383	MET	2.4
7	T	33	LEU	2.4
7	T	37	LEU	2.4
10	W	56	PRO	2.4
1	N	384	GLY	2.4
1	A	74	MET	2.3
1	A	192	ALA	2.3
3	C	92	LEU	2.3
9	V	31	PHE	2.3
1	N	241	PRO	2.3
8	H	50	VAL	2.3
4	Q	140	TYR	2.3
10	W	48	TYR	2.3
1	A	196	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	197	LEU	2.3
1	A	201	VAL	2.3
11	X	35	GLN	2.3
12	Y	20	ARG	2.3
6	S	44	GLU	2.3
11	X	19	ALA	2.3
1	A	440	TYR	2.3
10	W	2	GLU	2.3
1	A	203	ALA	2.2
1	A	191	THR	2.2
4	Q	134	PHE	2.2
3	P	91	VAL	2.2
11	X	15	ASN	2.2
10	J	48	TYR	2.2
11	X	9	PHE	2.2
1	N	245	ILE	2.2
10	J	30	ILE	2.2
6	S	3	GLY	2.2
7	G	41	HIS	2.2
1	A	389	ILE	2.2
1	A	198	SER	2.2
1	A	68	PHE	2.2
1	A	188	VAL	2.2
1	A	386	VAL	2.2
9	I	34	PHE	2.2
1	N	285	PHE	2.2
8	U	52	VAL	2.2
9	V	34	PHE	2.2
9	V	65	LYS	2.2
1	A	381	LEU	2.1
1	A	78	PHE	2.1
7	T	9	GLY	2.1
4	Q	52	SER	2.1
2	B	199	ILE	2.1
1	A	383	MET	2.1
8	H	9	LYS	2.1
1	A	63	PHE	2.1
2	O	226	MET	2.1
4	Q	44	GLU	2.1
8	U	85	ILE	2.1
1	N	196	LEU	2.1
6	S	43	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	O	59	GLN	2.1
7	G	6	GLY	2.1
1	N	158	ILE	2.1
1	N	199	LEU	2.1
2	B	60	GLU	2.1
1	N	126	TRP	2.1
1	N	73	ILE	2.0
1	N	385	ALA	2.0
1	A	377	PHE	2.0
5	R	11	PHE	2.0
1	A	157	SER	2.0
10	W	4	ARG	2.0
13	M	39	ASN	2.0
1	A	200	PRO	2.0
11	X	36	ILE	2.0
4	Q	10	ASP	2.0
8	H	49	ASP	2.0
11	X	47	ARG	2.0
1	A	105	LEU	2.0
1	A	388	ALA	2.0
1	N	381	LEU	2.0
1	A	239	GLY	2.0
4	Q	128	VAL	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.14	0.56	88,90,92,93	0
7	TPO	G	11	11/12	0.45	0.32	74,82,105,105	0
7	TPO	T	11	11/12	0.54	0.26	75,82,101,102	0
9	SAC	I	1	9/10	0.80	0.28	77,82,84,85	0
1	FME	N	1	10/11	0.87	0.23	50,54,74,77	0
1	FME	A	1	10/11	0.92	0.14	46,51,63,76	0
2	FME	O	1	10/11	0.95	0.14	41,42,49,55	0
2	FME	B	1	10/11	0.96	0.13	31,33,40,56	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
28	DMU	G	272	33/33	0.54	0.31	85,116,119,121	0
24	PEK	T	263	53/53	0.54	0.38	54,103,127,128	0
19	TGL	N	1522	63/63	0.55	0.33	54,76,92,95	0
24	PEK	G	265	53/53	0.55	0.27	51,91,109,114	0
28	DMU	P	1272	33/33	0.56	0.35	104,118,124,125	0
24	PEK	S	1265	53/53	0.59	0.30	50,87,111,114	0
23	UNX	C	262	1/1	0.64	0.58	49,49,49,49	0
25	CDL	G	269	100/100	0.64	0.34	72,99,122,124	0
25	CDL	T	1269	100/100	0.65	0.32	66,96,122,126	0
24	PEK	G	1263	53/53	0.66	0.37	59,107,131,132	0
20	PGV	P	1268	51/51	0.67	0.31	64,100,119,121	0
22	CHD	W	1059	29/29	0.67	0.47	107,115,119,120	0
26	PSC	R	1229	52/52	0.67	0.32	53,109,133,136	0
20	PGV	N	1524	51/51	0.68	0.33	54,81,117,119	0
25	CDL	P	1270	100/100	0.68	0.37	46,100,119,122	0
20	PGV	C	268	51/51	0.69	0.29	60,91,117,117	0
19	TGL	L	522	63/63	0.69	0.27	43,68,84,87	0
19	TGL	Q	1523	63/63	0.72	0.22	67,83,98,100	0
26	PSC	E	229	52/52	0.72	0.33	53,106,131,133	0
22	CHD	J	60	29/29	0.72	0.28	105,109,113,114	0
20	PGV	A	524	51/51	0.75	0.28	45,75,117,118	0
25	CDL	C	270	100/100	0.75	0.31	49,96,120,122	0
19	TGL	N	1521	63/63	0.76	0.23	71,92,105,109	0
19	TGL	D	523	63/63	0.77	0.22	48,70,93,94	0
28	DMU	Z	1526	33/33	0.78	0.26	44,59,75,75	0
23	UNX	P	262	1/1	0.80	0.60	49,49,49,49	0
19	TGL	A	521	63/63	0.81	0.21	49,82,106,110	0
22	CHD	C	271	29/29	0.85	0.31	72,84,87,90	0
15	CYN	N	520	2/2	0.88	0.15	42,42,42,43	0
28	DMU	M	526	33/33	0.89	0.16	36,51,69,71	0
22	CHD	P	1271	29/29	0.91	0.22	68,86,90,91	0
18	NA	N	519	1/1	0.92	0.06	40,40,40,40	0

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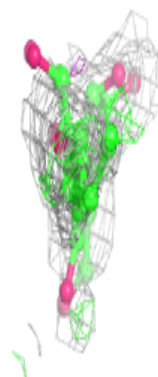
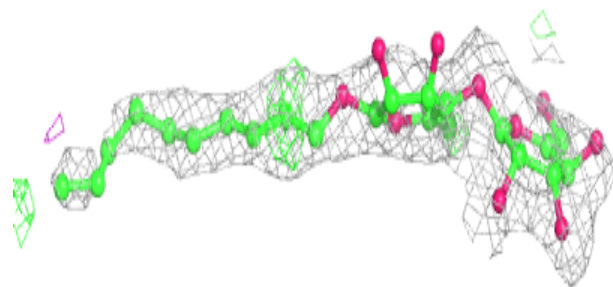
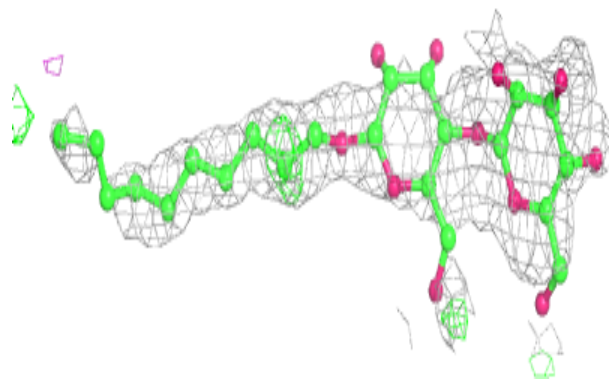
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	MG	N	518	1/1	0.92	0.12	33,33,33,33	0
22	CHD	P	1525	29/29	0.94	0.11	28,38,43,51	0
24	PEK	T	1264	53/53	0.94	0.15	30,54,83,85	0
24	PEK	C	264	53/53	0.95	0.13	27,50,76,79	0
22	CHD	B	1085	29/29	0.95	0.09	29,34,40,50	0
22	CHD	O	229	29/29	0.95	0.08	27,34,42,45	0
14	HEA	N	516	60/60	0.96	0.19	32,40,54,57	0
20	PGV	C	267	51/51	0.96	0.13	23,36,72,75	0
22	CHD	C	525	29/29	0.96	0.11	25,35,39,46	0
20	PGV	N	1266	51/51	0.97	0.15	28,43,70,75	0
20	PGV	P	1267	51/51	0.97	0.13	29,40,77,85	0
20	PGV	A	522	51/51	0.97	0.17	25,36,68,72	0
14	HEA	N	515	60/60	0.97	0.20	30,36,50,52	0
18	NA	A	519	1/1	0.97	0.09	30,30,30,30	0
14	HEA	A	516	60/60	0.97	0.17	23,35,51,52	0
15	CYN	A	520	2/2	0.98	0.13	31,31,31,31	0
17	MG	A	518	1/1	0.98	0.17	25,25,25,25	0
21	CUA	O	228	2/2	0.98	0.09	36,36,36,37	0
14	HEA	A	515	60/60	0.98	0.20	18,27,40,45	0
27	ZN	F	99	1/1	0.99	0.07	35,35,35,35	0
21	CUA	B	228	2/2	0.99	0.14	28,28,28,28	0
16	CU	N	517	1/1	0.99	0.16	37,37,37,37	0
27	ZN	S	99	1/1	0.99	0.07	38,38,38,38	0
16	CU	A	517	1/1	1.00	0.17	31,31,31,31	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.

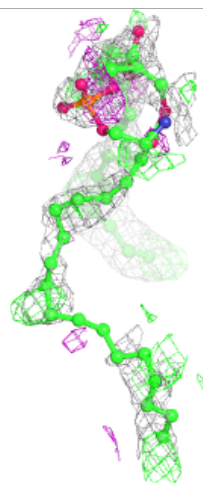
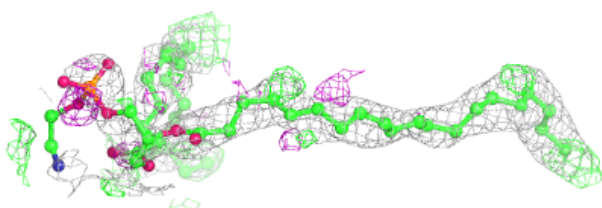
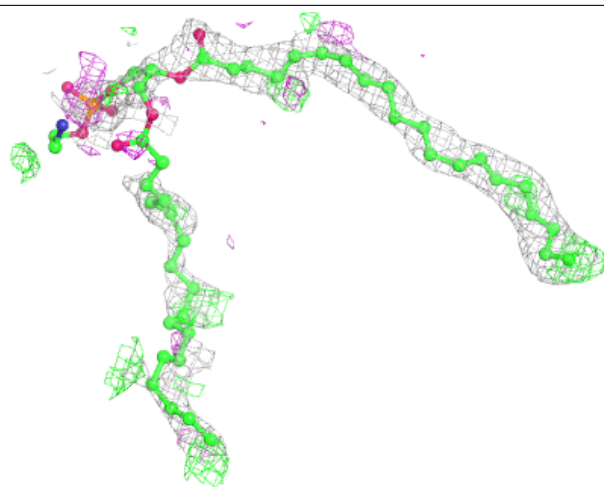
**Electron density around DMU G 272:**

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



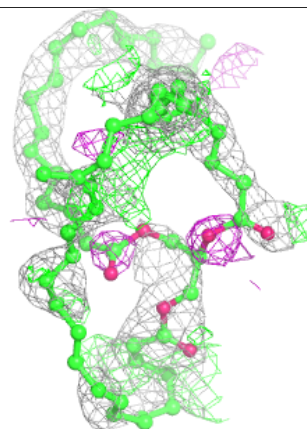
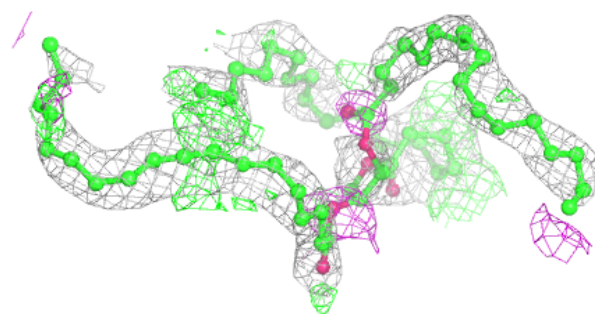
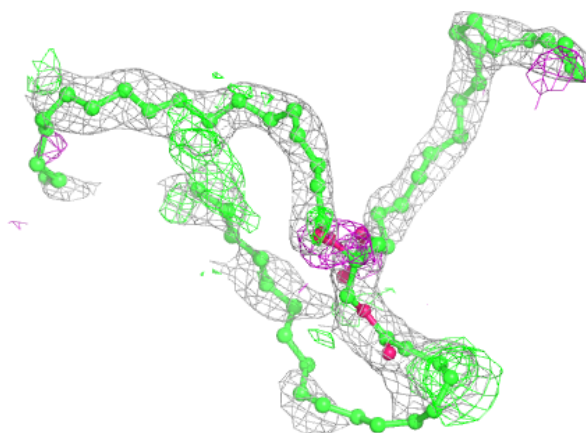
**Electron density around PEK T 263:**

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



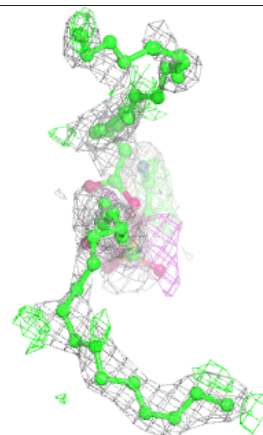
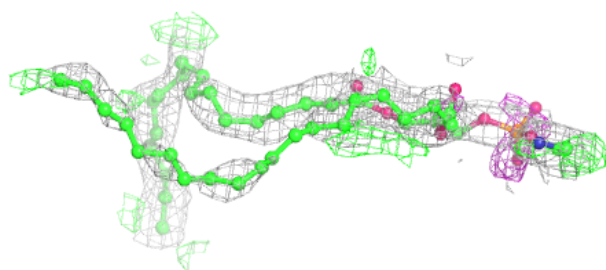
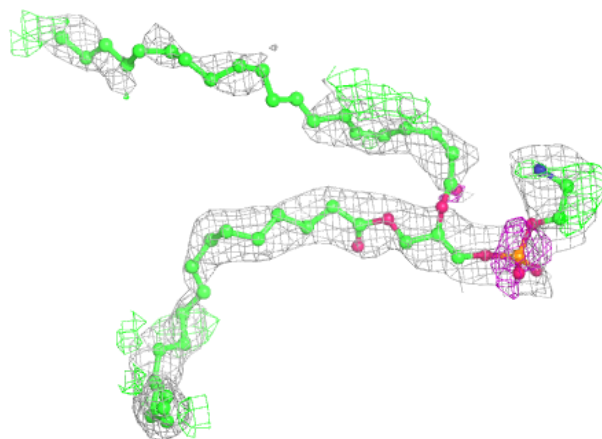
**Electron density around TGL N 1522:**

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

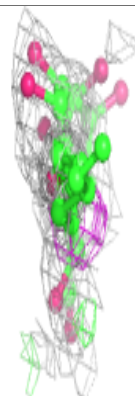
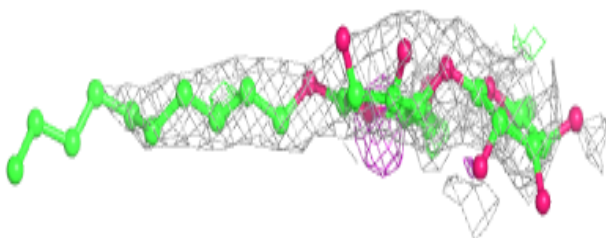
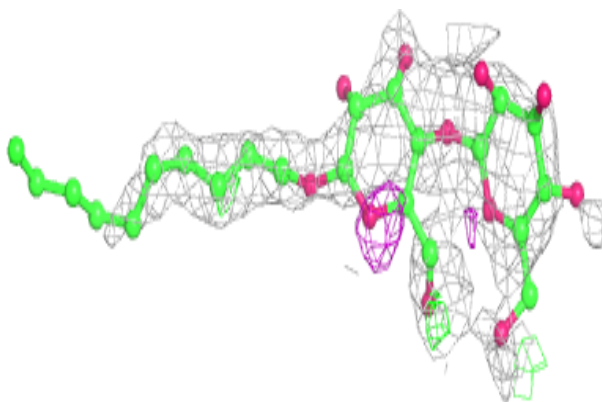


**Electron density around PEK G 265:**

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

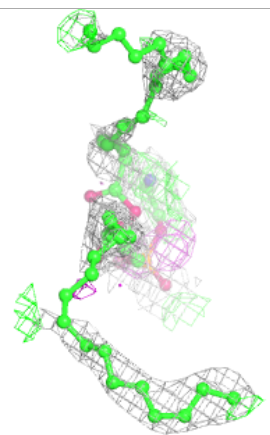
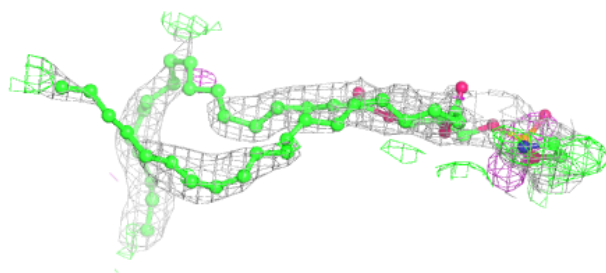
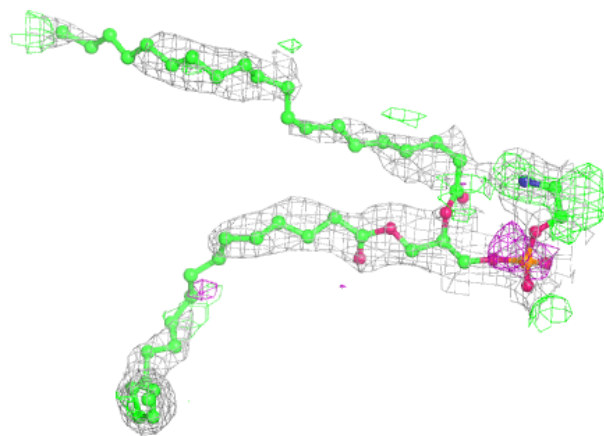
**Electron density around DMU P 1272:**

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



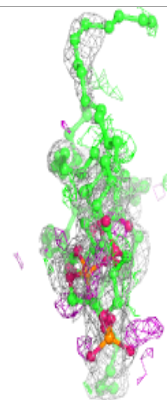
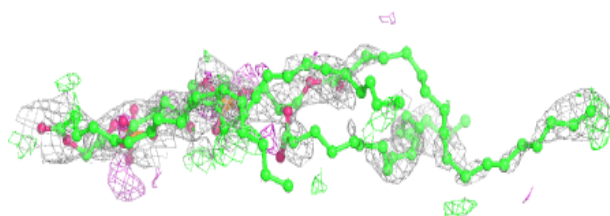
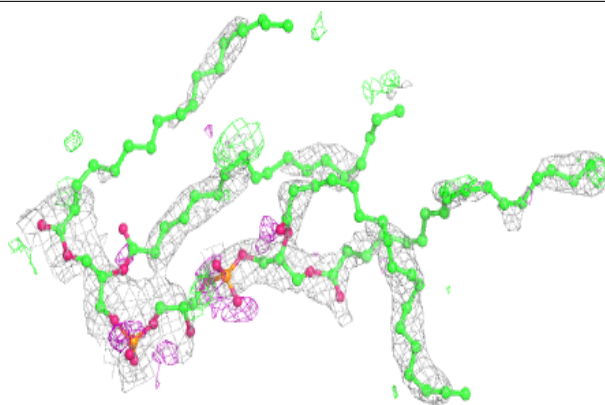
**Electron density around PEK S 1265:**

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

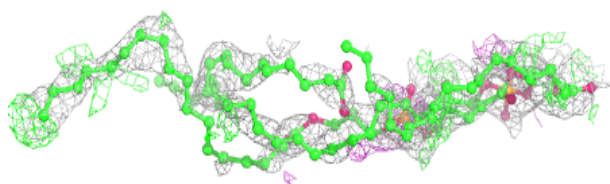
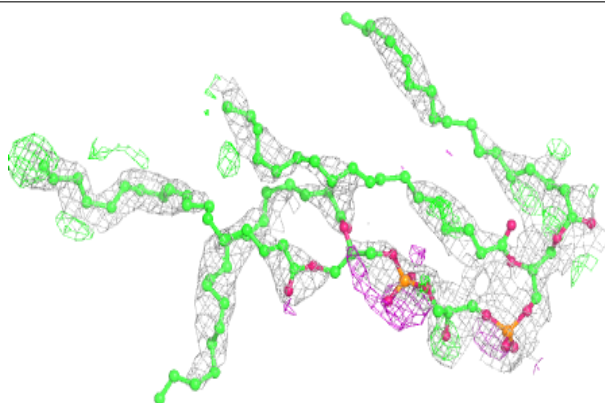


**Electron density around CDL G 269:**

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

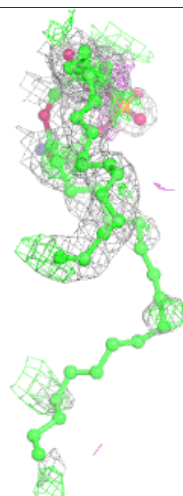
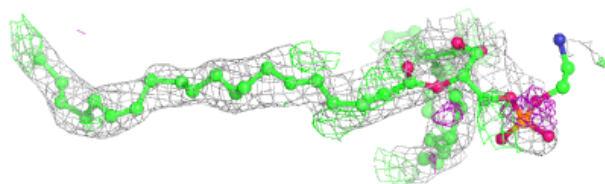
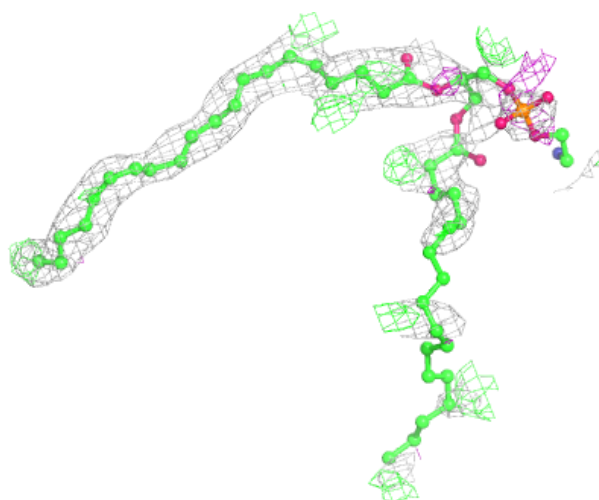
**Electron density around CDL T 1269:**

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



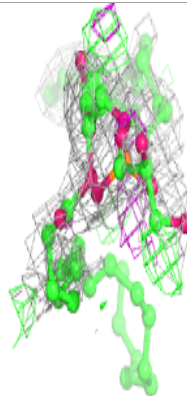
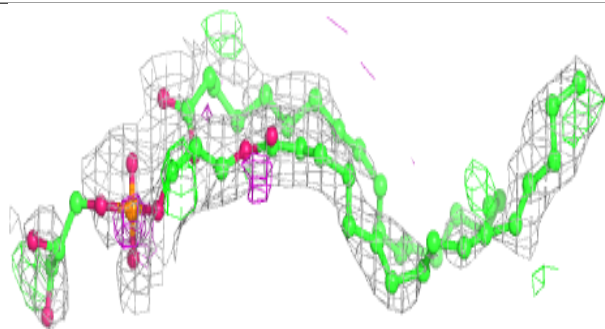
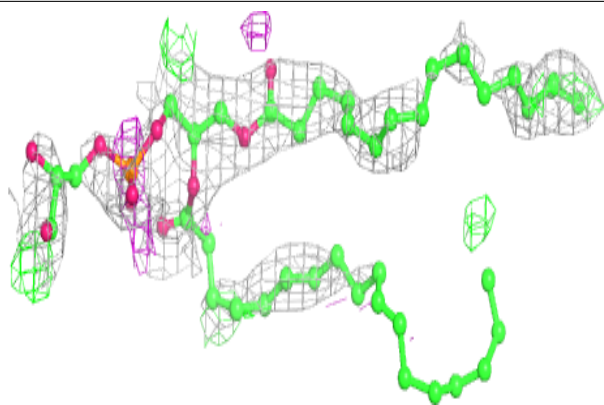
**Electron density around PEK G 1263:**

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

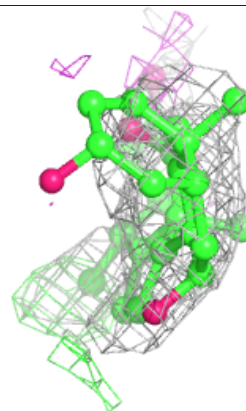
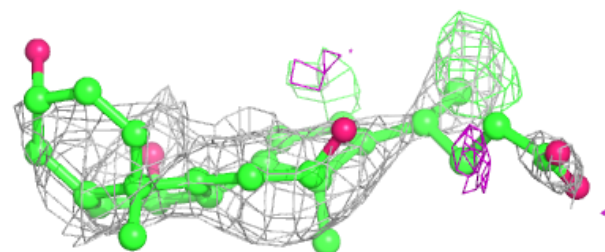
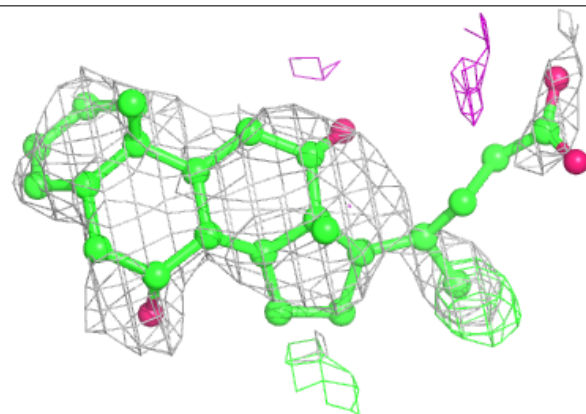


**Electron density around PGV P 1268:**

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

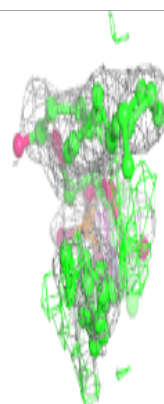
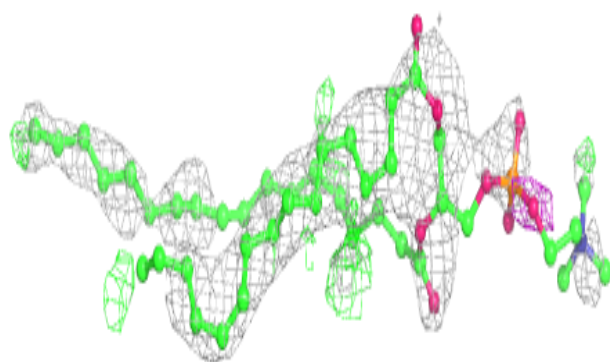
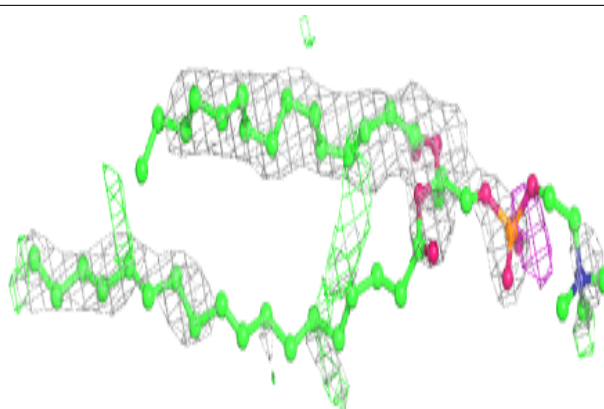
**Electron density around CHD W 1059:**

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

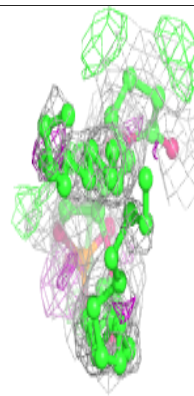
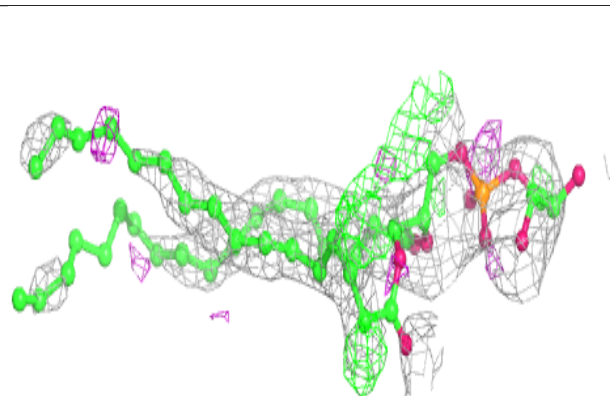
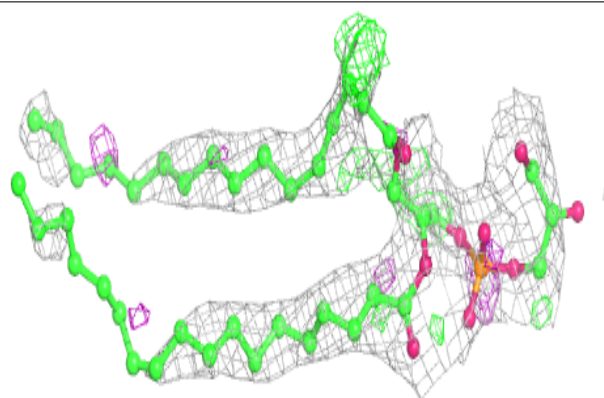


**Electron density around PSC R 1229:**

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

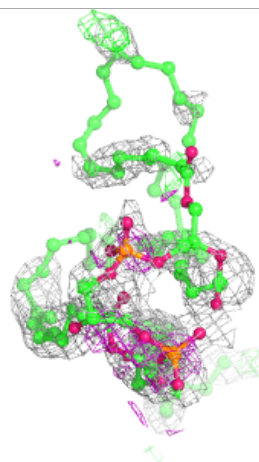
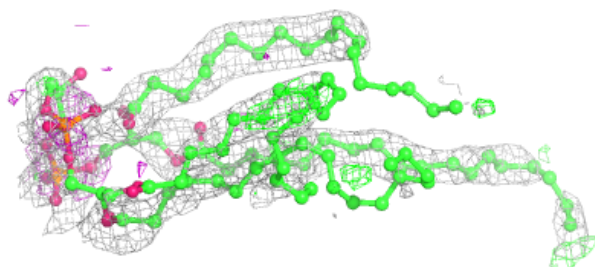
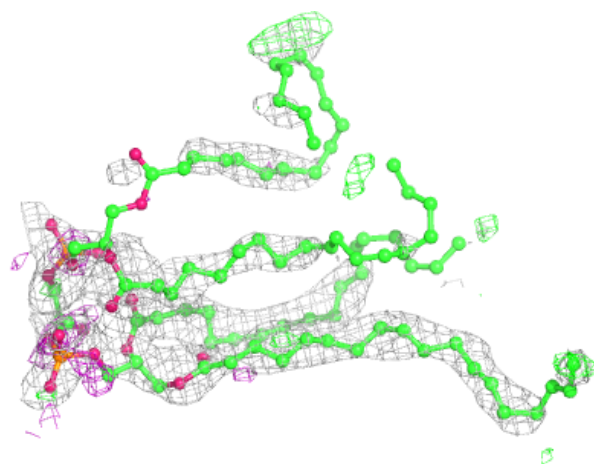
**Electron density around PGV N 1524:**

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



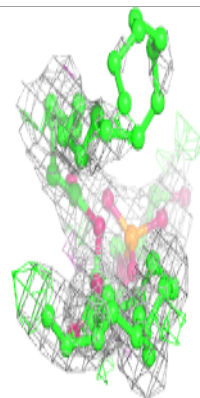
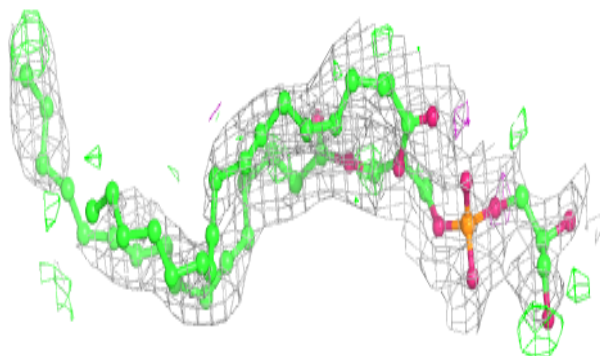
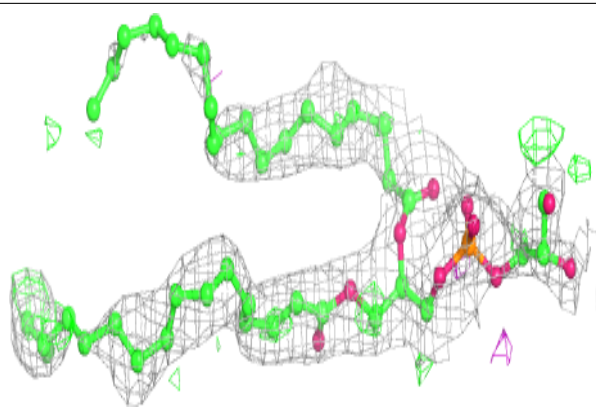
**Electron density around CDL P 1270:**

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

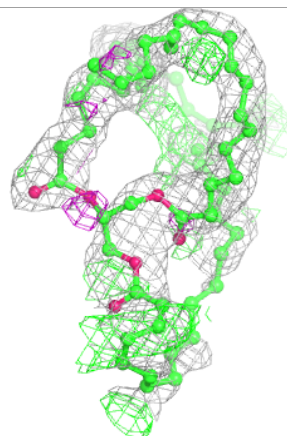
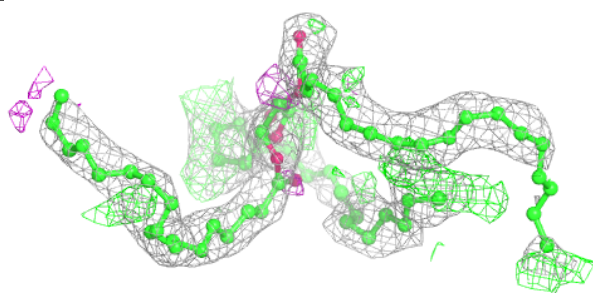
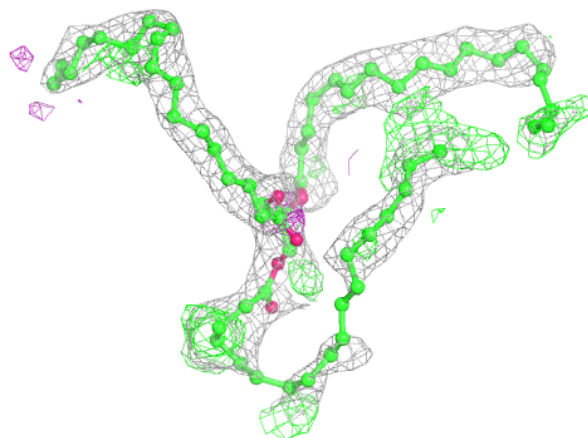


**Electron density around PGV C 268:**

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

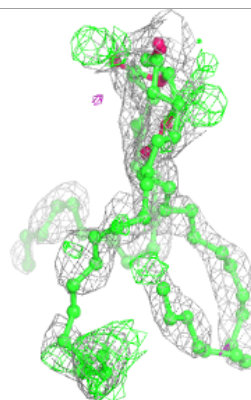
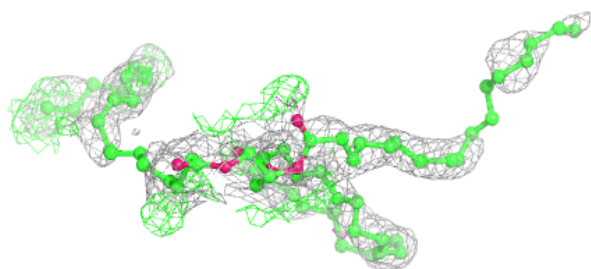
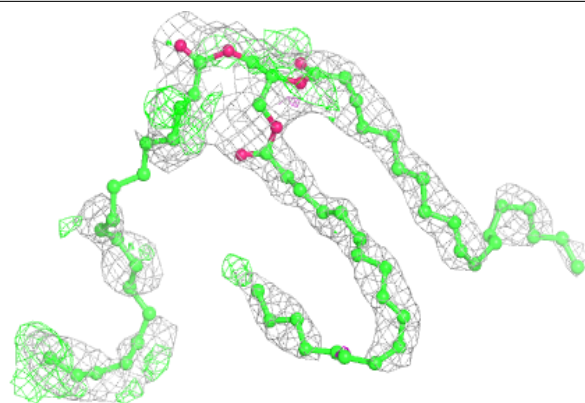
**Electron density around TGL L 522:**

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

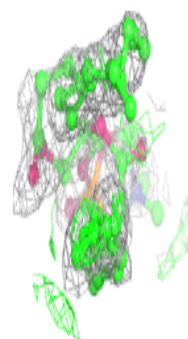
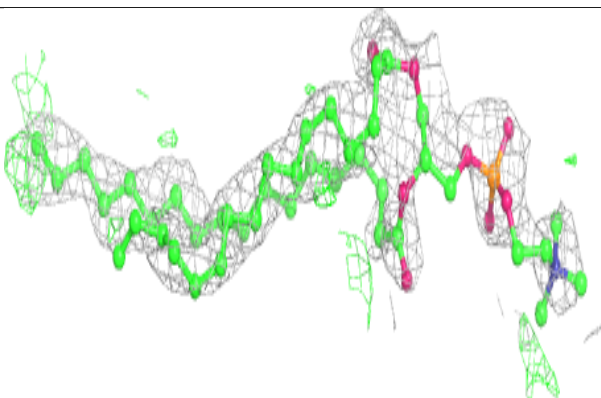
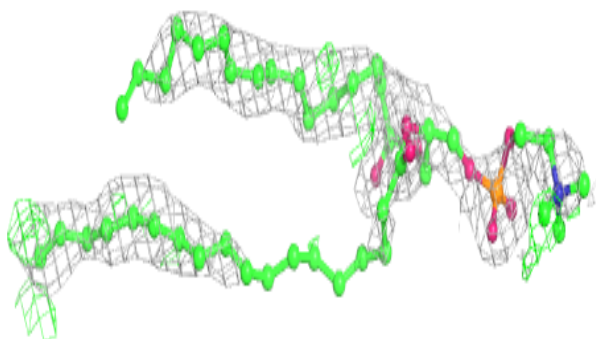


**Electron density around TGL Q 1523:**

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

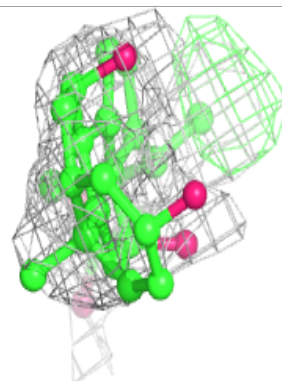
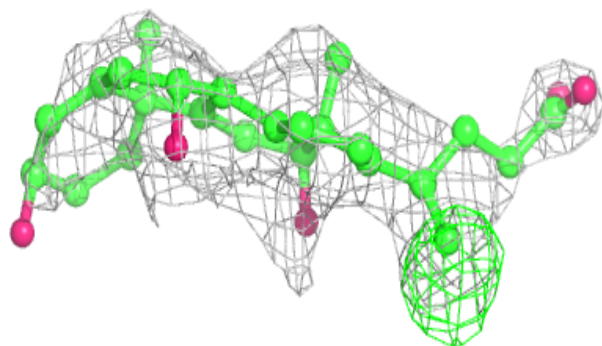
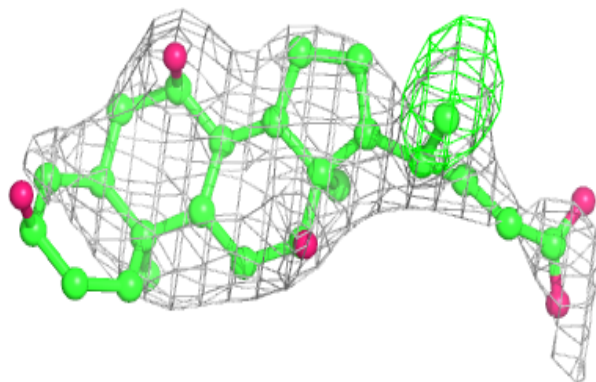
**Electron density around PSC E 229:**

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

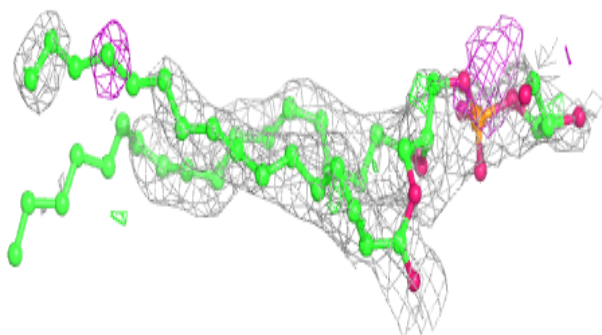
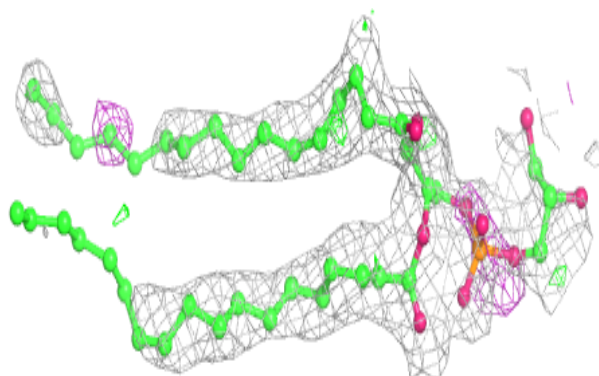


**Electron density around CHD J 60:**

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

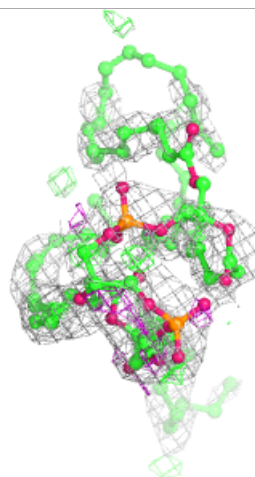
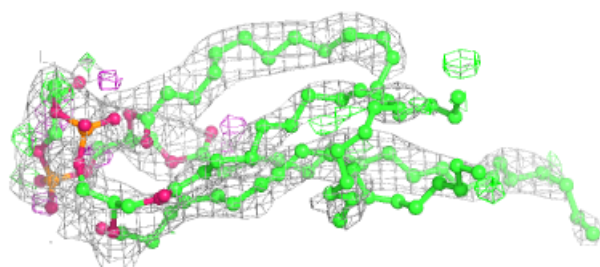
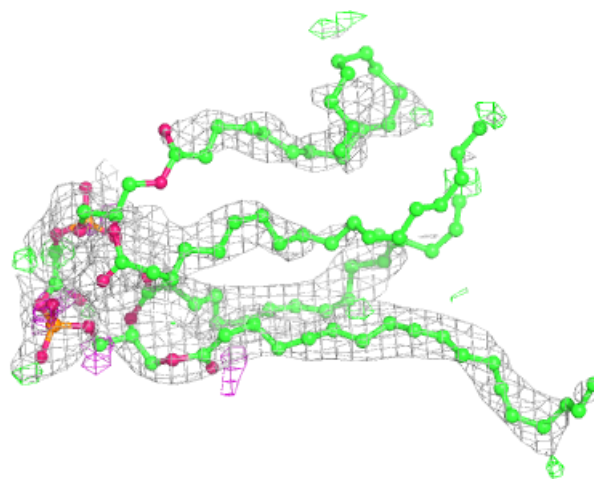
**Electron density around PGV A 524:**

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



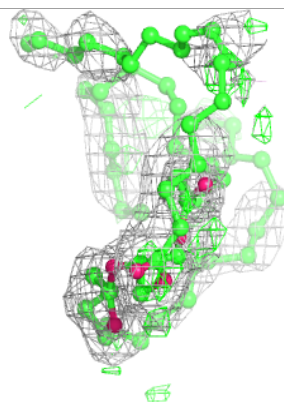
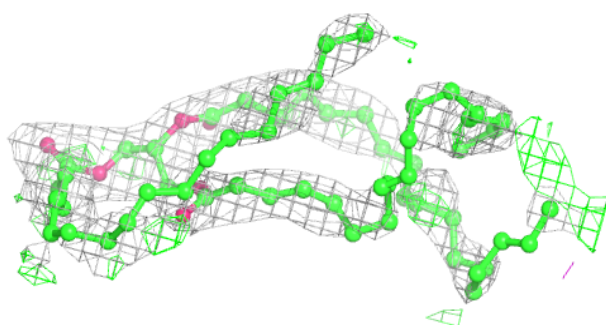
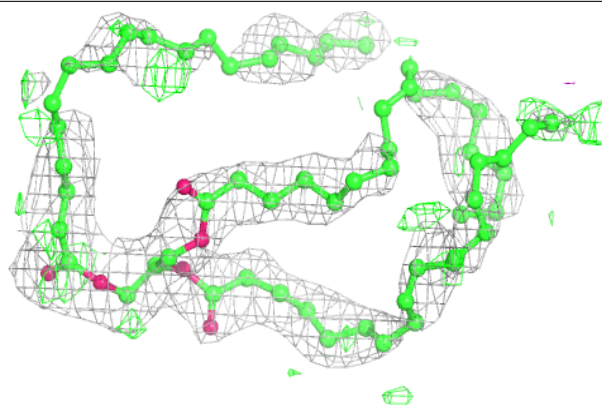
**Electron density around CDL C 270:**

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

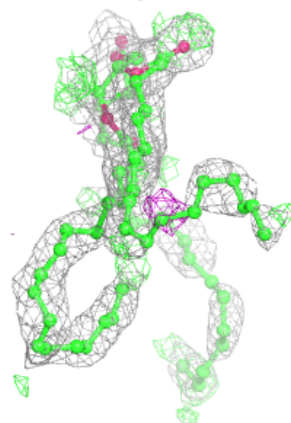
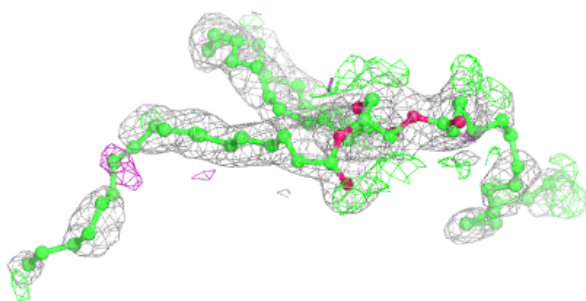
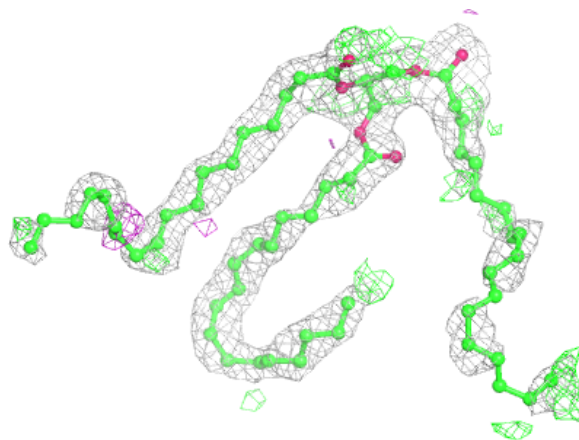


**Electron density around TGL N 1521:**

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

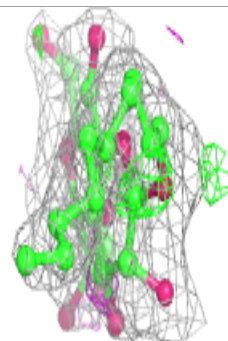
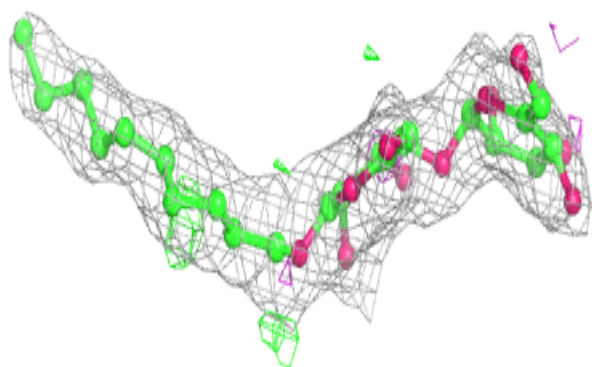
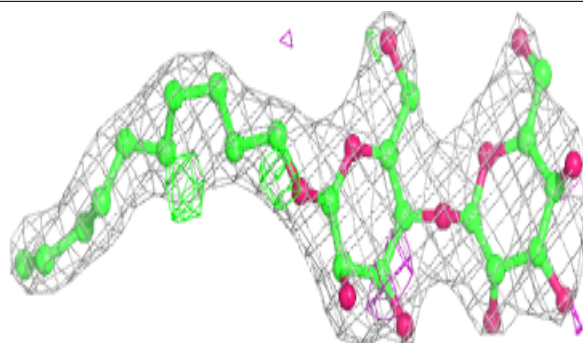
**Electron density around TGL D 523:**

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

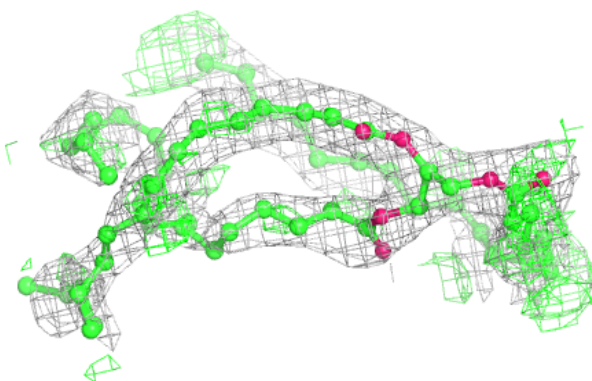
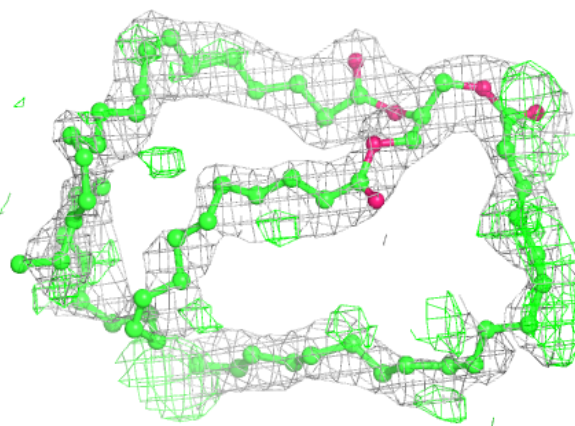


**Electron density around DMU Z 1526:**

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

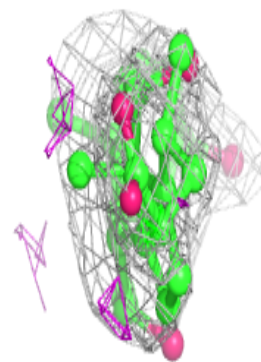
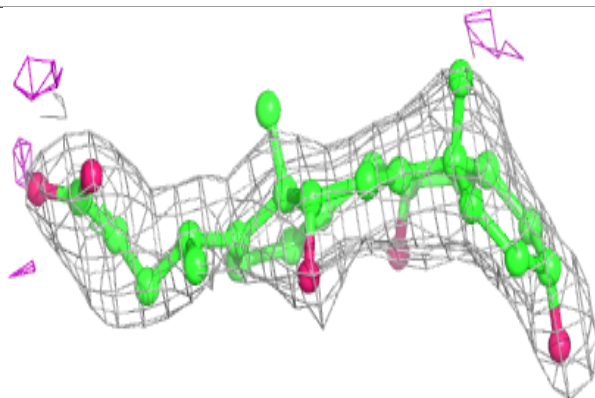
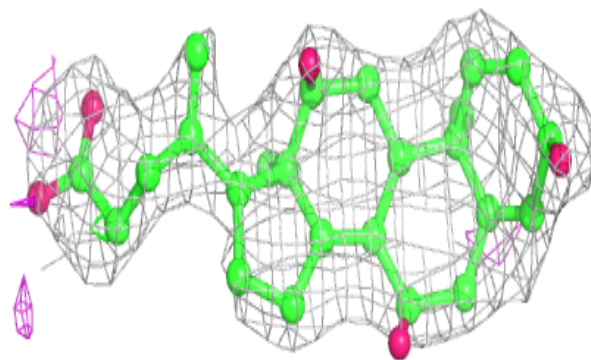
**Electron density around TGL A 521:**

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

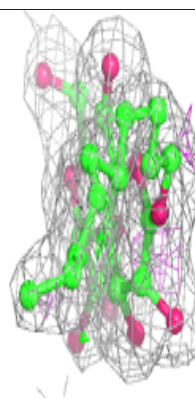
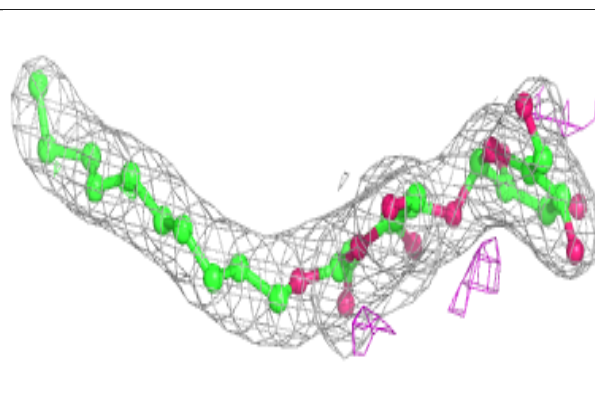
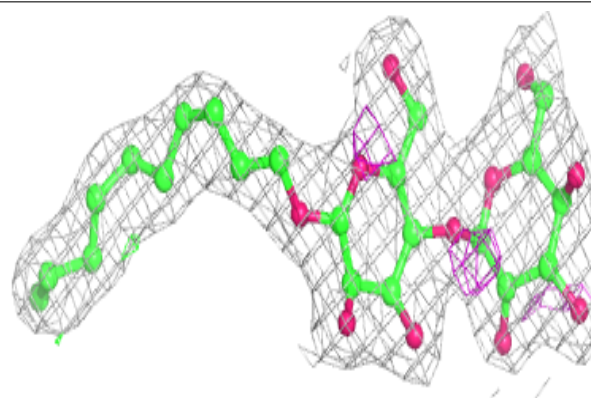


**Electron density around CHD C 271:**

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

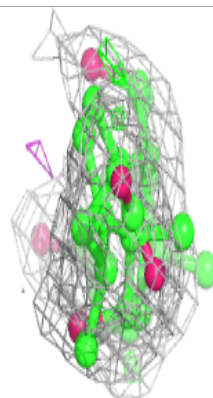
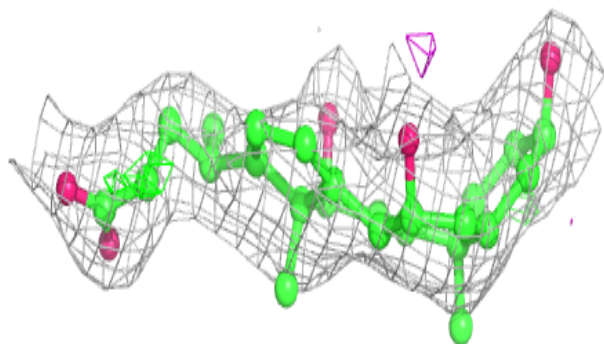
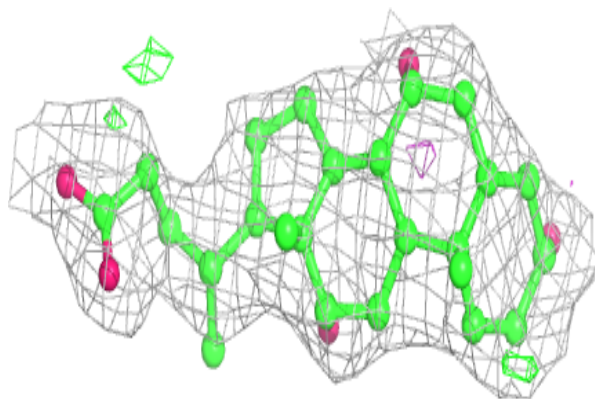
**Electron density around DMU M 526:**

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

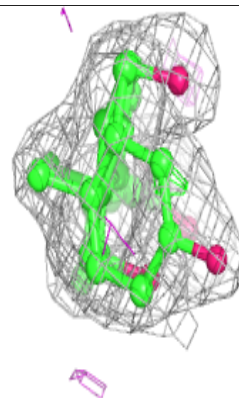
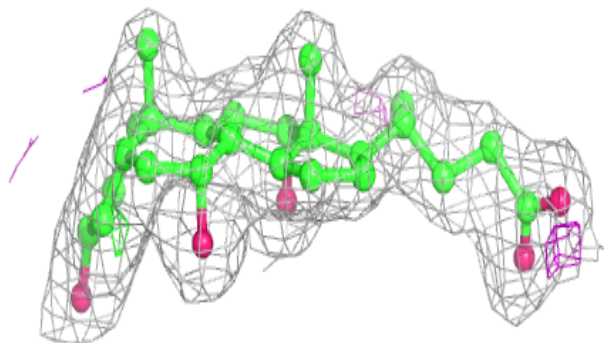
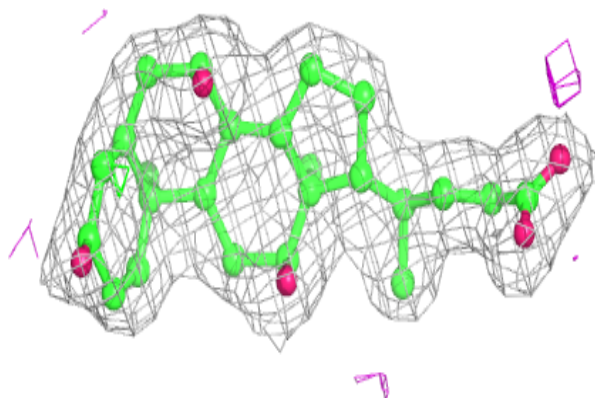


**Electron density around CHD P 1271:**

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

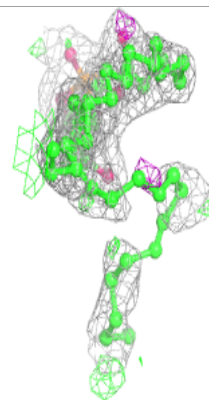
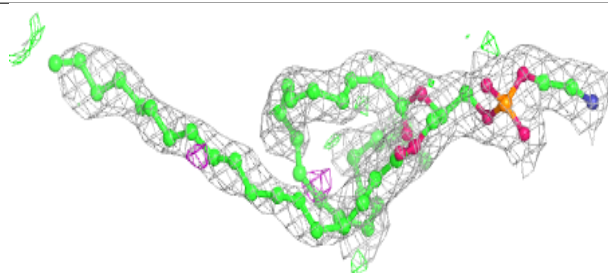
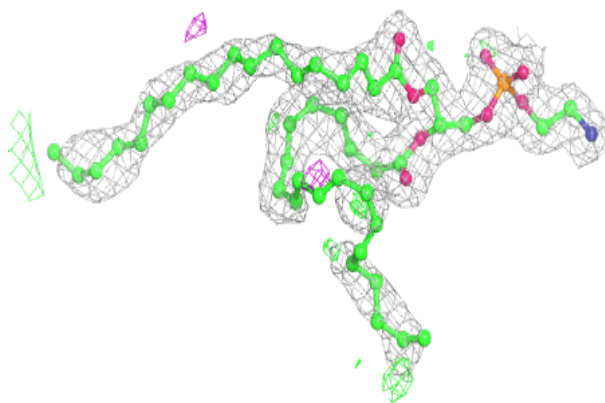
**Electron density around CHD P 1525:**

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

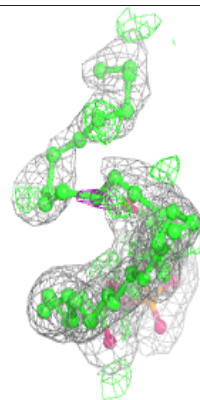
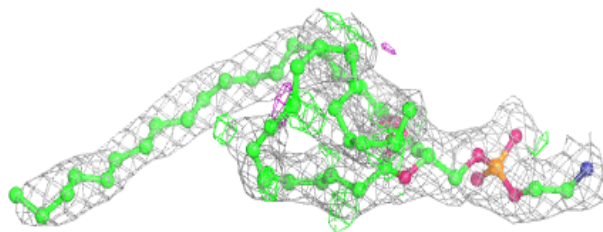
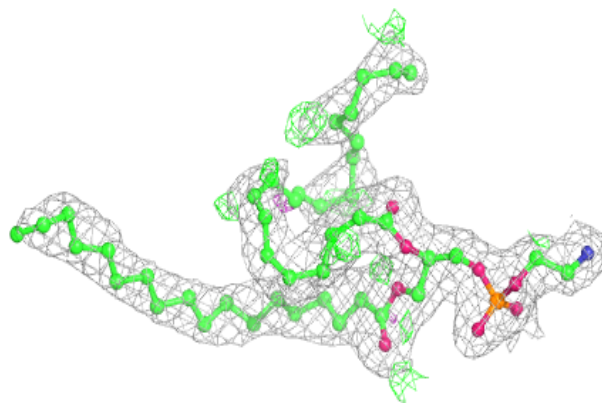


**Electron density around PEK T 1264:**

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

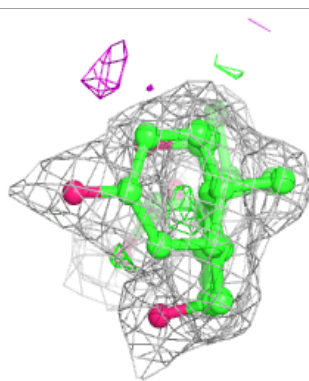
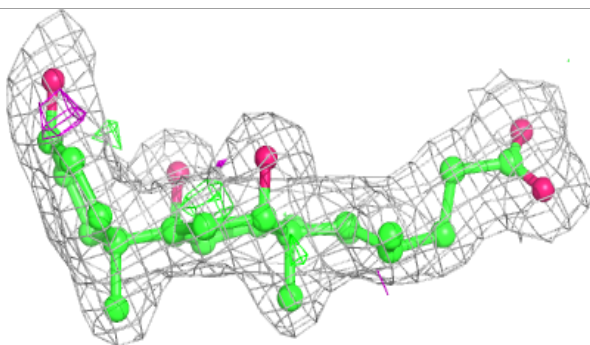
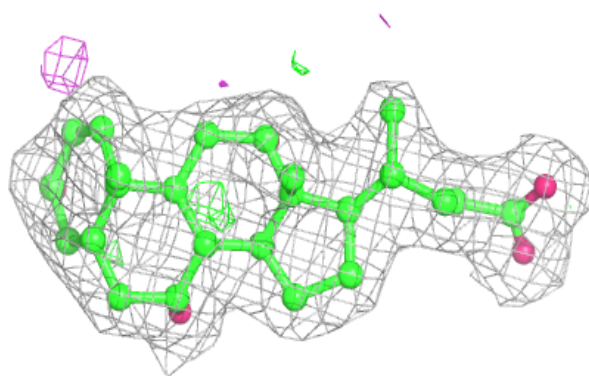
**Electron density around PEK C 264:**

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

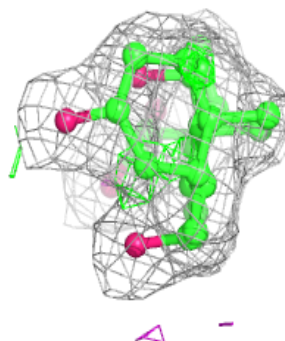
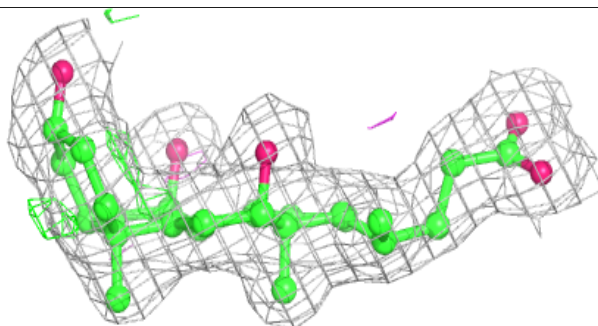
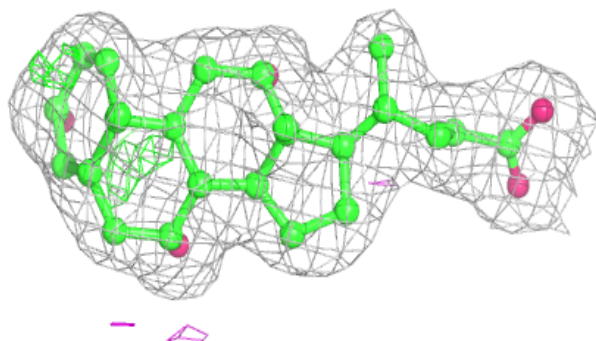


**Electron density around CHD B 1085:**

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

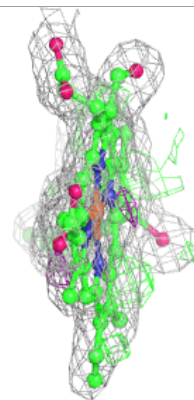
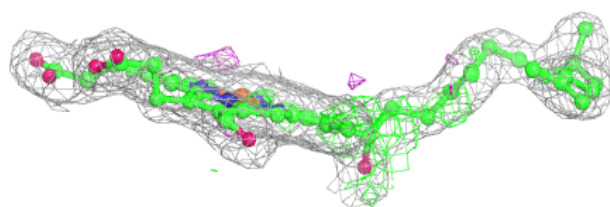
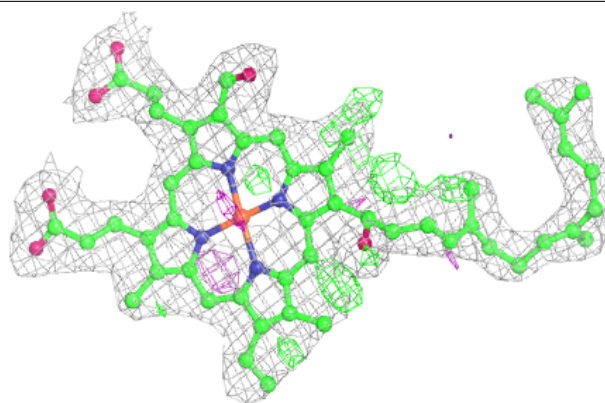
**Electron density around CHD O 229:**

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

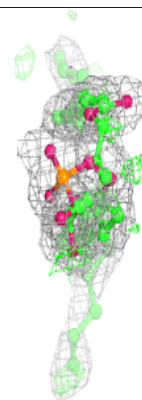
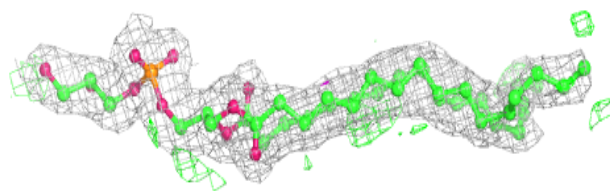
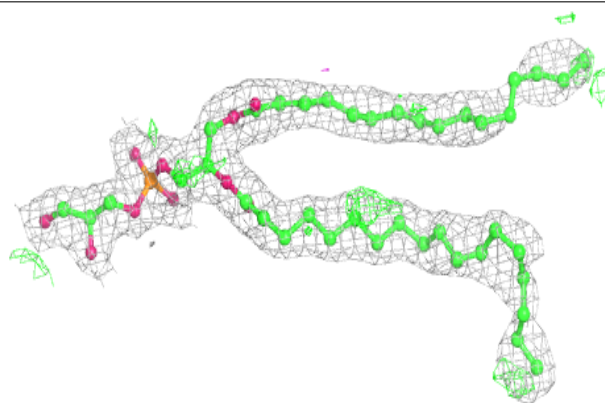


**Electron density around HEA N 516:**

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

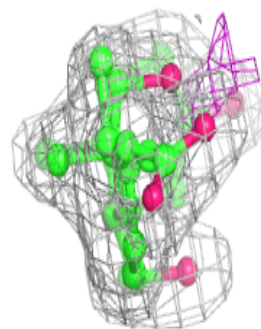
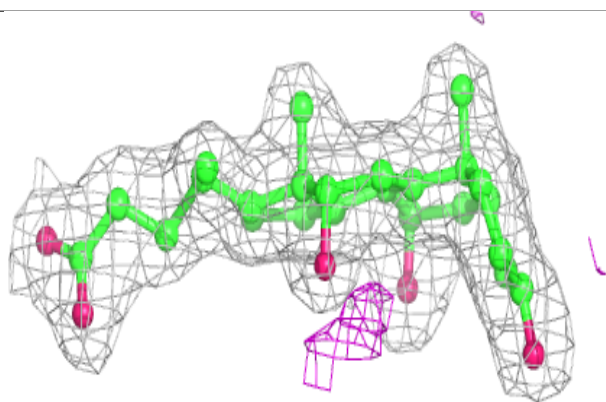
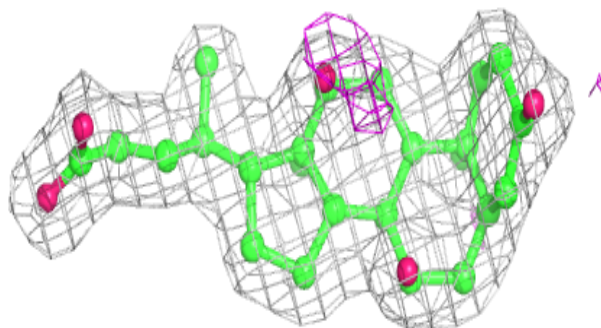
**Electron density around PGV C 267:**

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

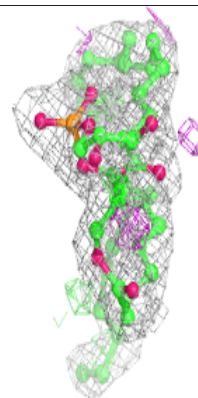
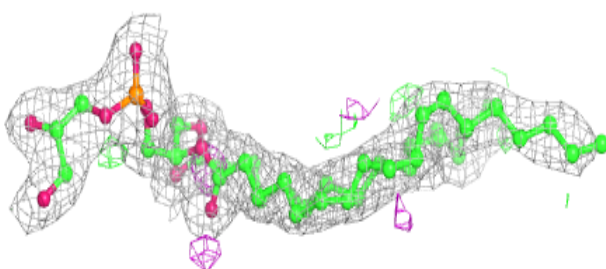
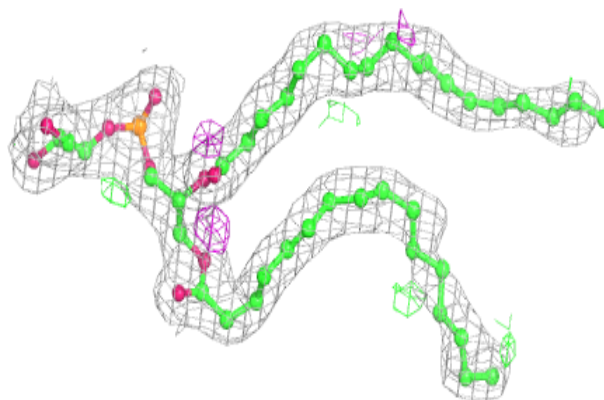


**Electron density around CHD C 525:**

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

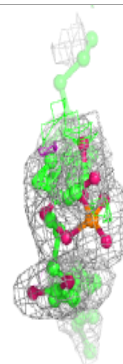
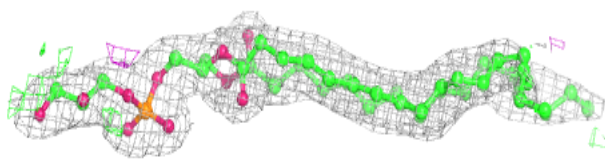
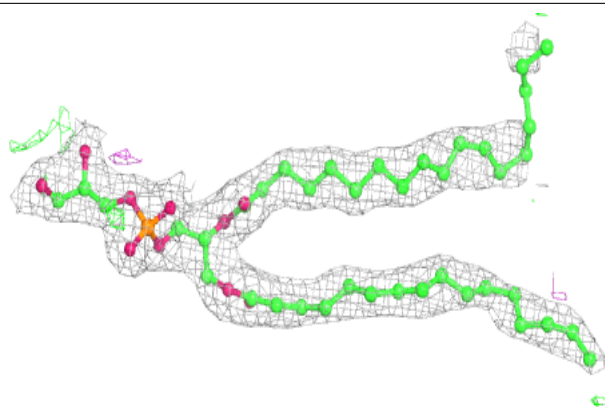
**Electron density around PGV N 1266:**

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

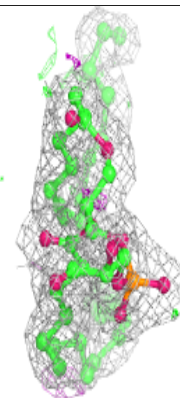
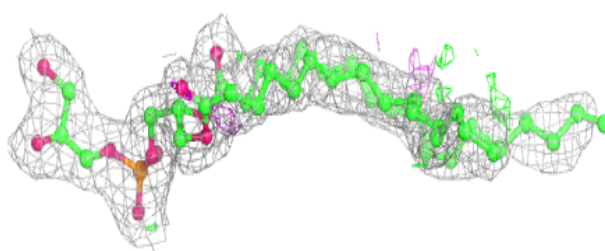
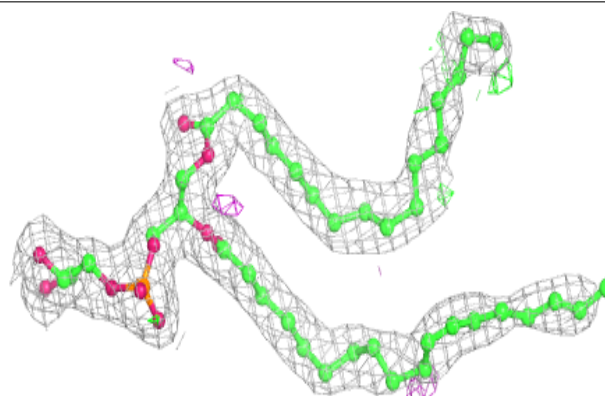


**Electron density around PGV P 1267:**

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

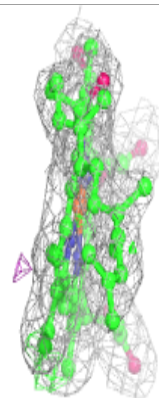
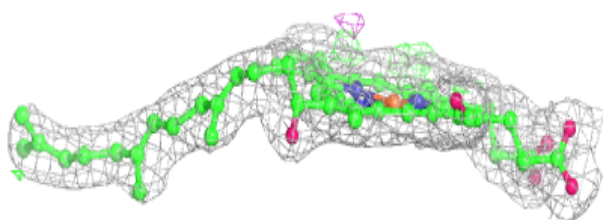
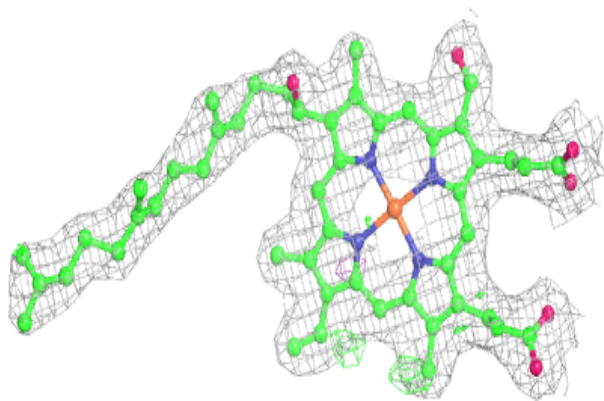
**Electron density around PGV A 522:**

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

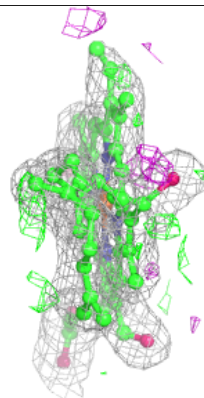
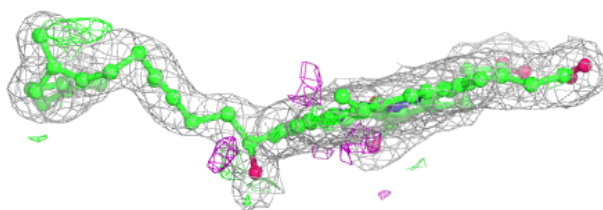
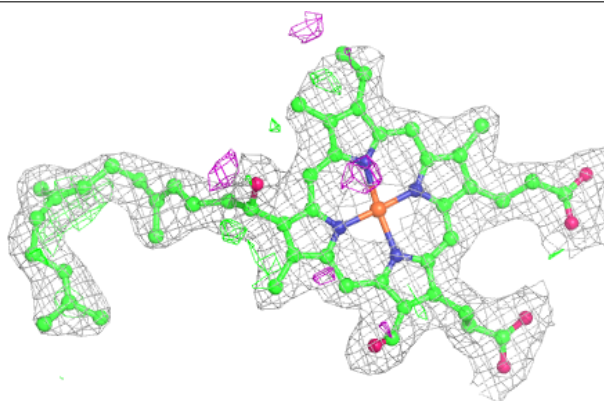


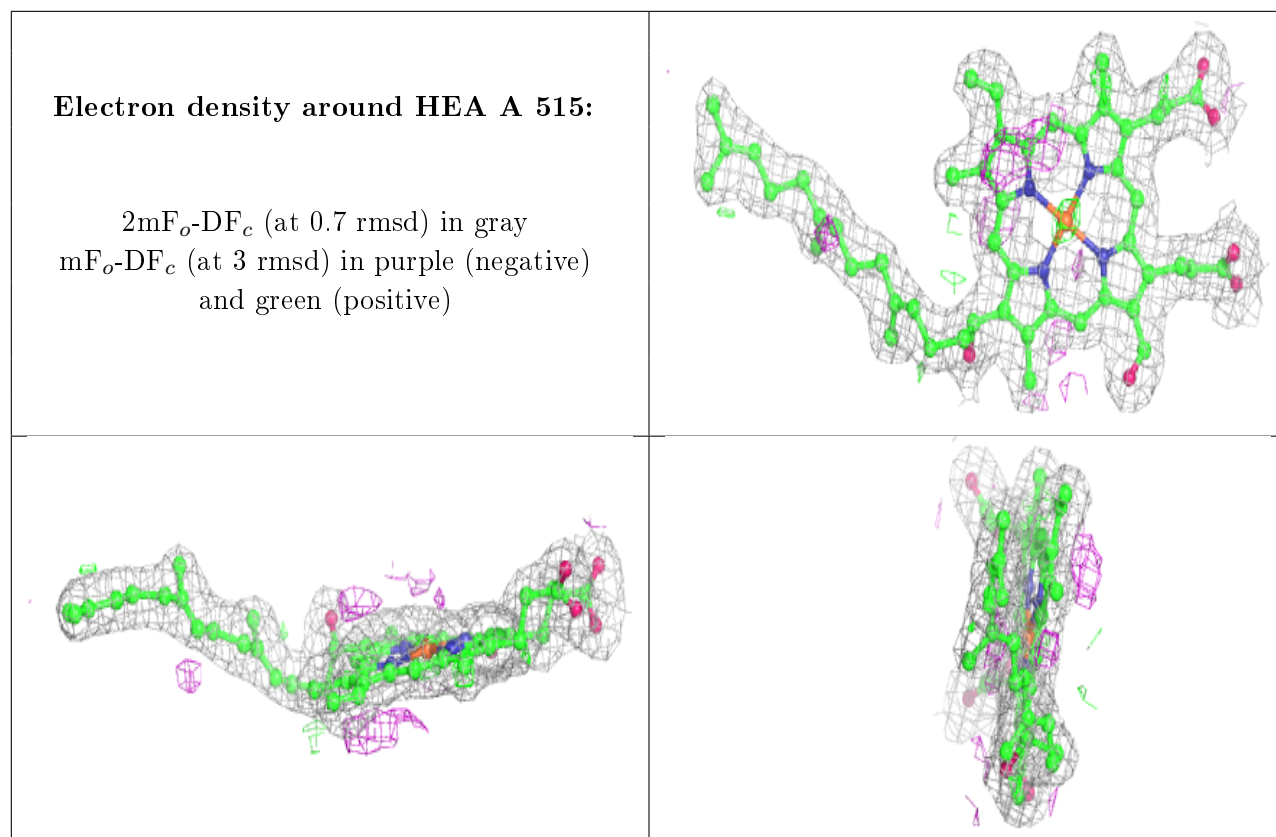
**Electron density around HEA N 515:**

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

**Electron density around HEA A 516:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.