



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:52 PM UTC

PDB ID : 3ABL / pdb_00003abl
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (15-s X-ray exposure dataset)
Authors : Aoyama, H.; Muramoto, K.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Ogura, T.; Yoshikawa, S.
Deposited on : 2009-12-16
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

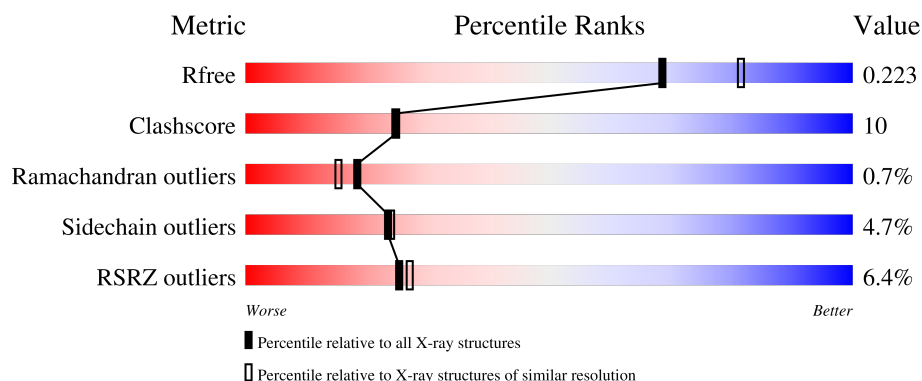
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	514	 64% 31% 5%
1	N	514	 69% 27% 4% 2%
2	B	227	 66% 31% 3% 2%
2	O	227	 69% 26% 4% 1%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	O	229	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-
28	PEK	T	263	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32244 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

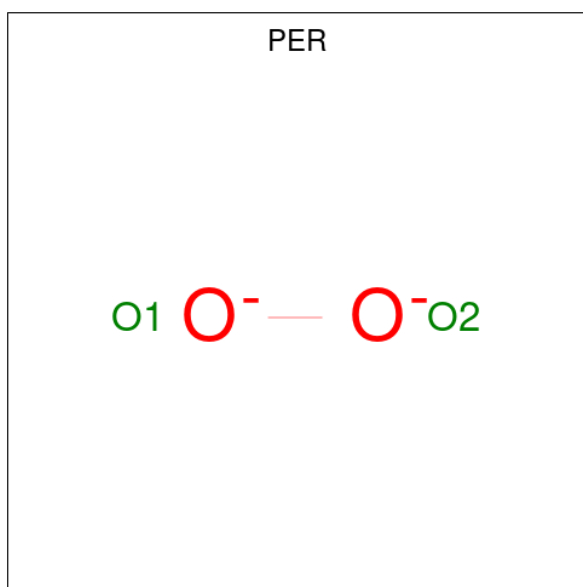
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

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

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

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

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



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

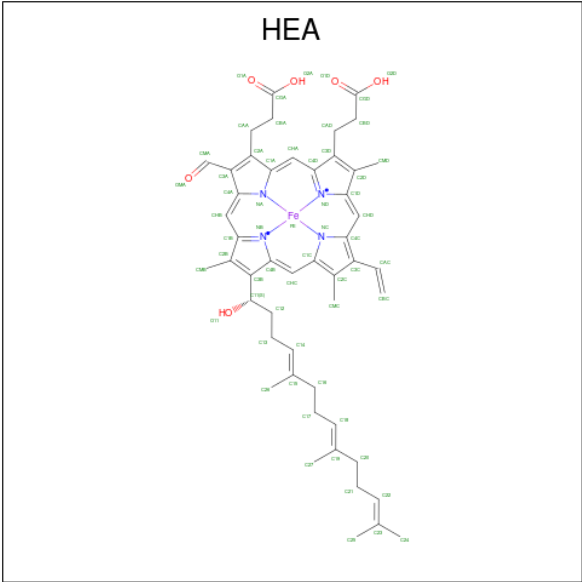
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

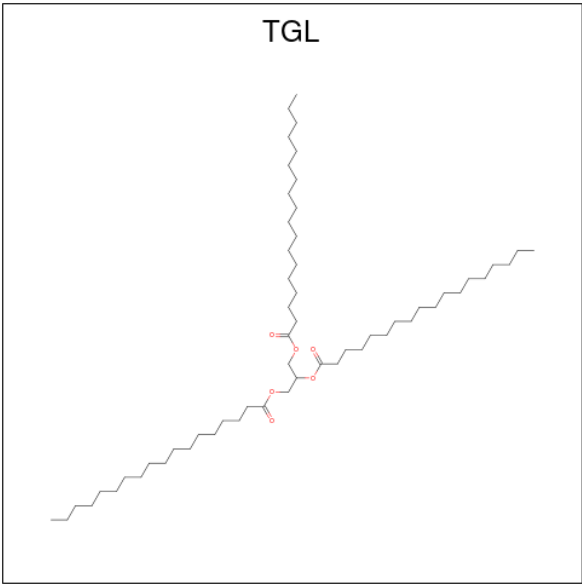
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



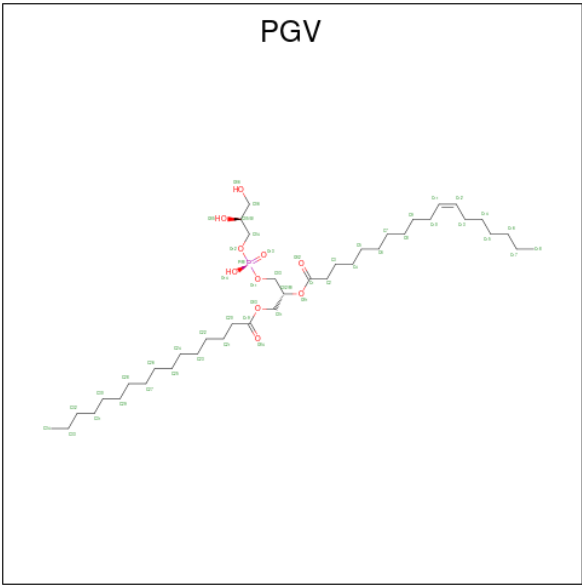
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	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 (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



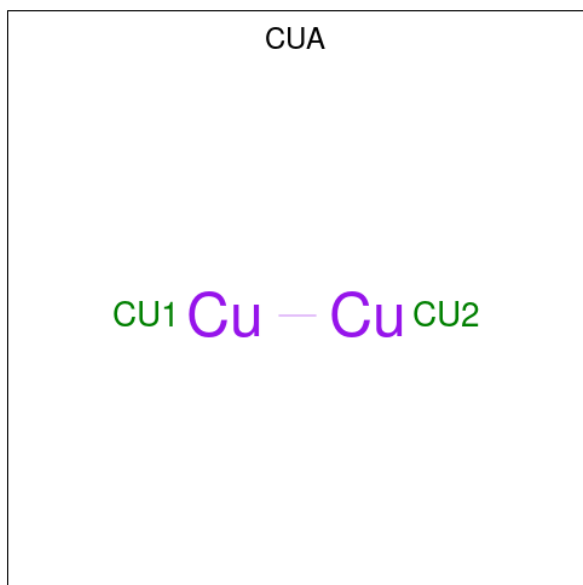
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		

Continued on next page...

Continued from previous page...

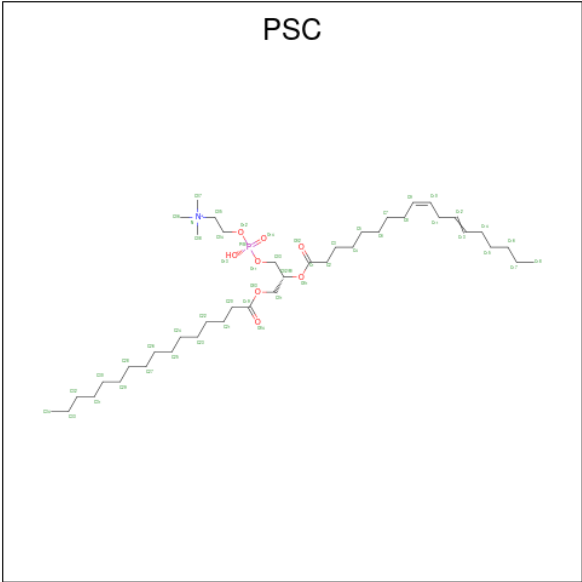
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



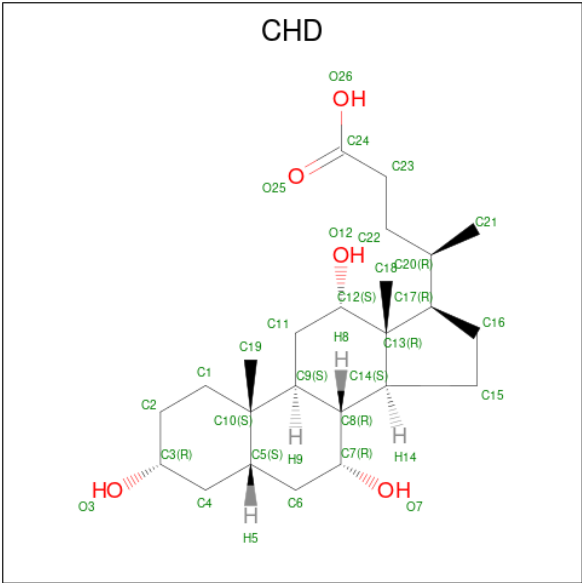
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



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

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



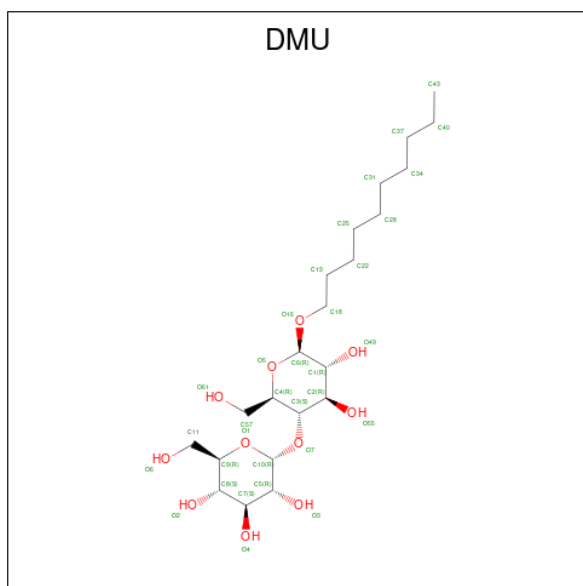
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

Continued on next page...

Continued from previous page...

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

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

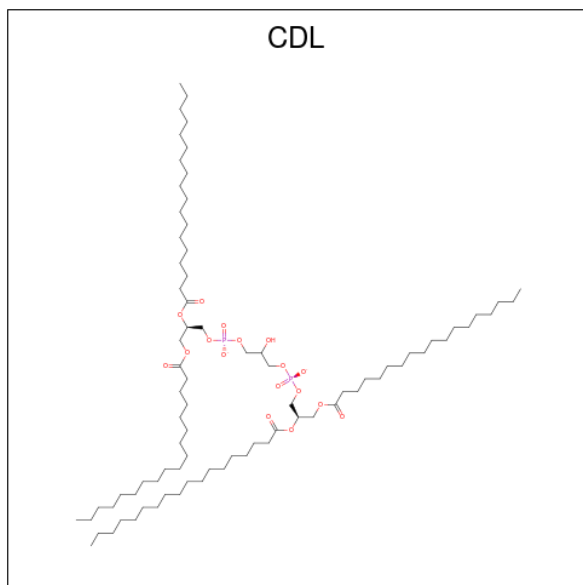


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



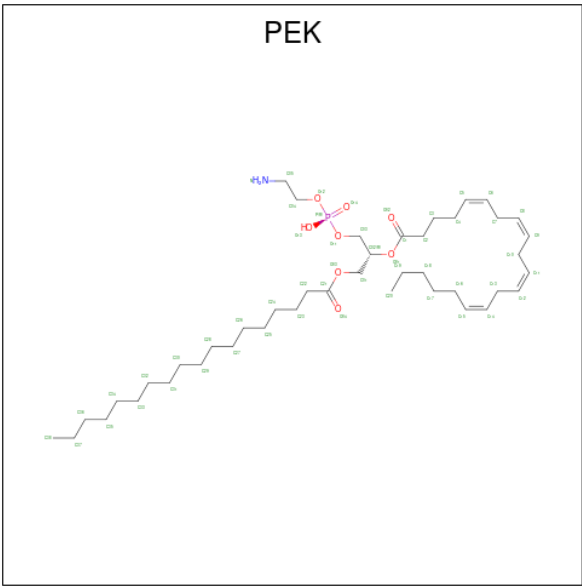
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O P 100 81 17 2	0	0
26	G	1	Total C O P 100 81 17 2	0	0
26	P	1	Total C O P 100 81 17 2	0	0
26	T	1	Total C O P 100 81 17 2	0	0

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

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

- Molecule 28 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE

(CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	219	Total	O	0	0
			219	219		
29	B	139	Total	O	0	0
			139	139		
29	C	105	Total	O	0	0
			105	105		
29	D	110	Total	O	0	0
			110	110		
29	E	68	Total	O	0	0
			68	68		

Continued on next page...

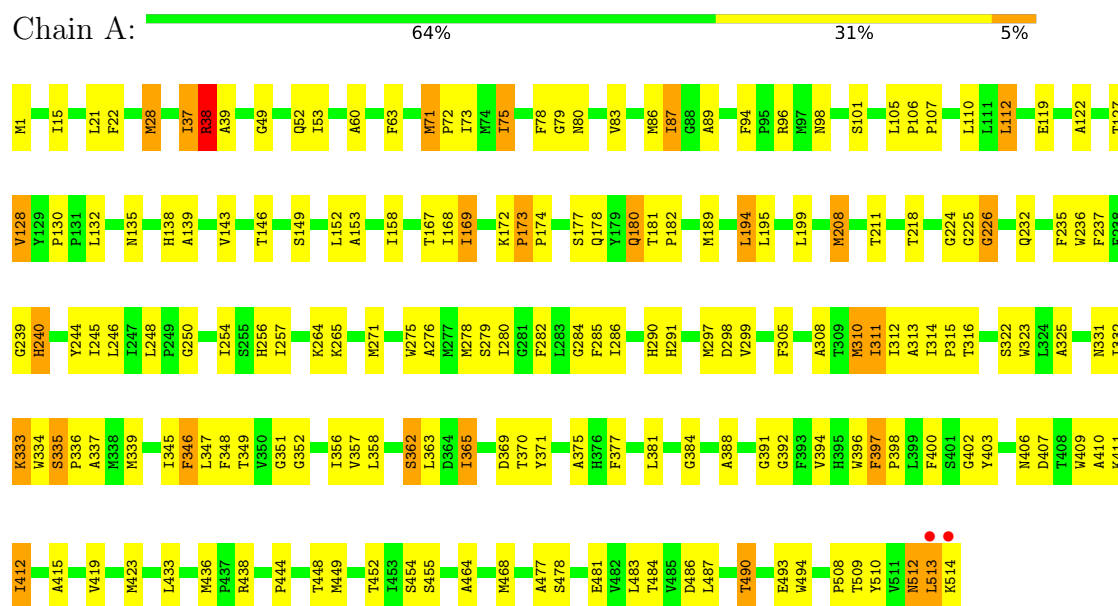
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	F	76	Total 76	O 76	0	0
29	G	45	Total 45	O 45	0	0
29	H	48	Total 48	O 48	0	0
29	I	35	Total 35	O 35	0	0
29	J	21	Total 21	O 21	0	0
29	K	22	Total 22	O 22	0	0
29	L	27	Total 27	O 27	0	0
29	M	18	Total 18	O 18	0	0
29	N	204	Total 204	O 204	0	0
29	O	109	Total 109	O 109	0	0
29	P	106	Total 106	O 106	0	0
29	Q	67	Total 67	O 67	0	0
29	R	52	Total 52	O 52	0	0
29	S	69	Total 69	O 69	0	0
29	T	48	Total 48	O 48	0	0
29	U	38	Total 38	O 38	0	0
29	V	19	Total 19	O 19	0	0
29	W	16	Total 16	O 16	0	0
29	X	16	Total 16	O 16	0	0
29	Y	17	Total 17	O 17	0	0
29	Z	14	Total 14	O 14	0	0

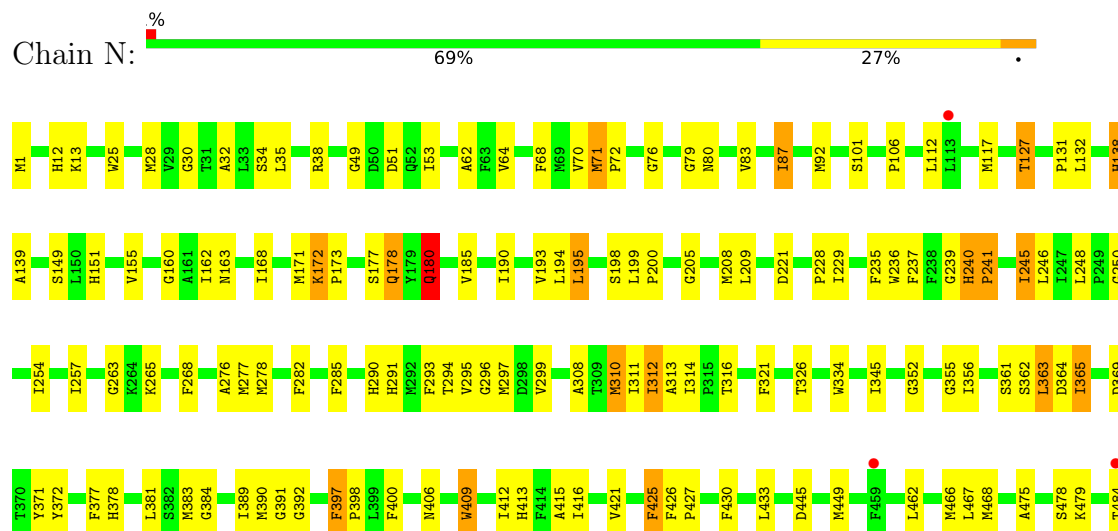
3 Residue-property plots

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

• Molecule 1: Cytochrome c oxidase subunit 1

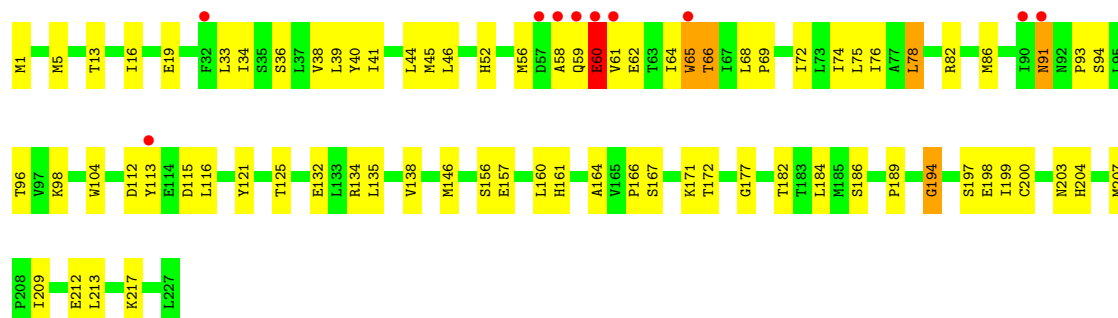


• Molecule 1: Cytochrome c oxidase subunit 1

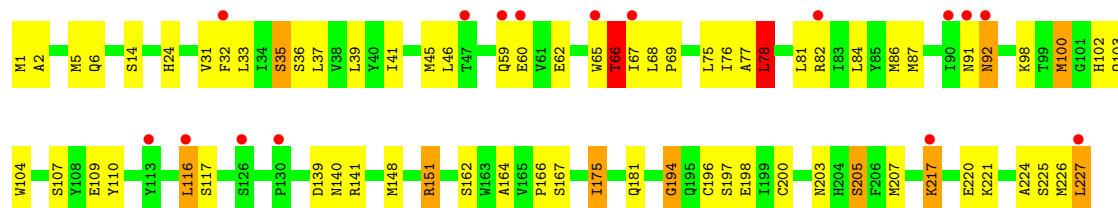




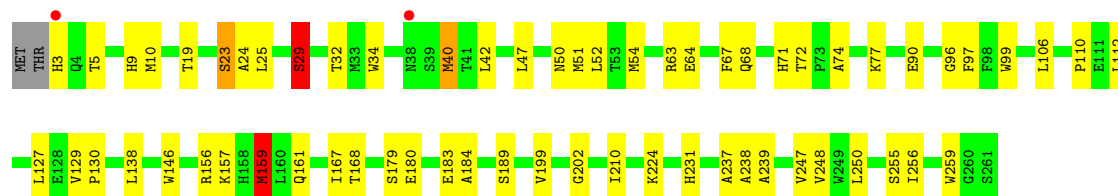
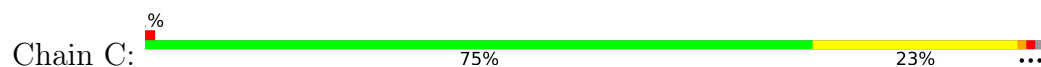
• Molecule 2: Cytochrome c oxidase subunit 2



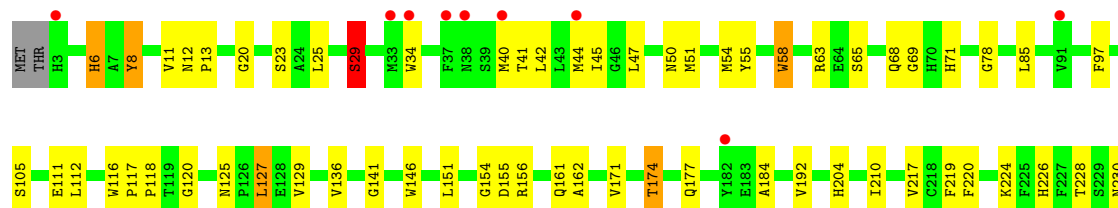
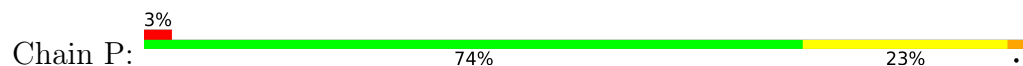
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase subunit 3

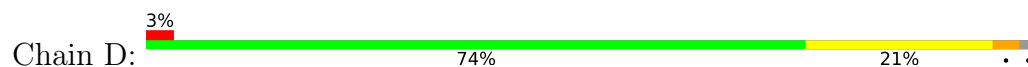


• Molecule 3: Cytochrome c oxidase subunit 3

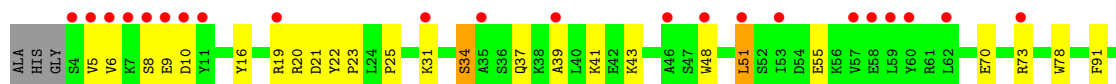
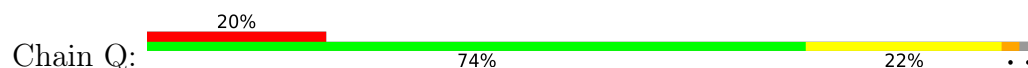




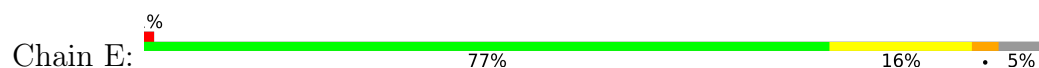
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



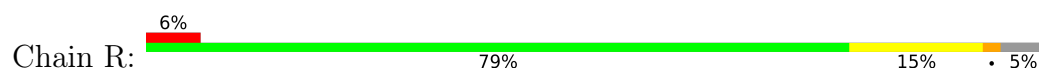
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



- Molecule 5: Cytochrome c oxidase subunit 5A



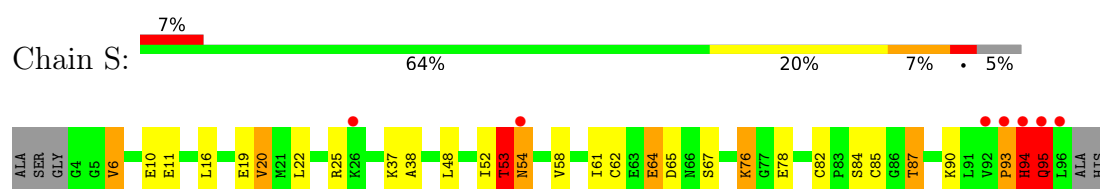
- Molecule 5: Cytochrome c oxidase subunit 5A



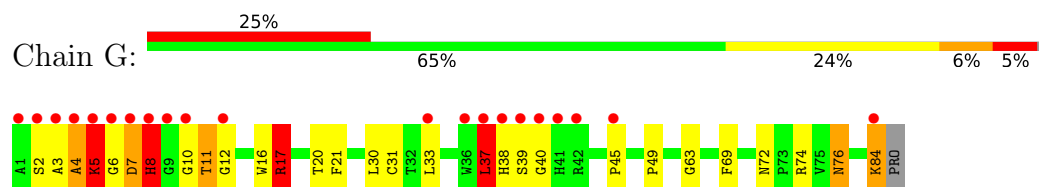
- Molecule 6: Cytochrome c oxidase subunit 5B



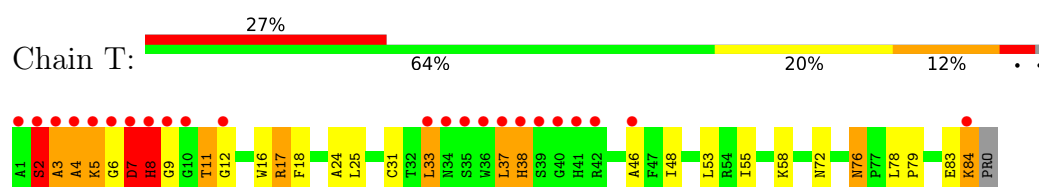
- Molecule 6: Cytochrome c oxidase subunit 5B



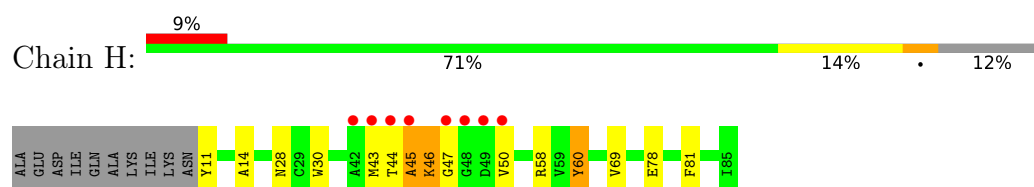
• Molecule 7: Cytochrome c oxidase subunit 6A2



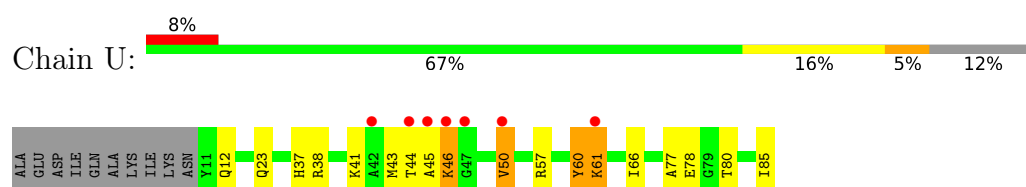
• Molecule 7: Cytochrome c oxidase subunit 6A2



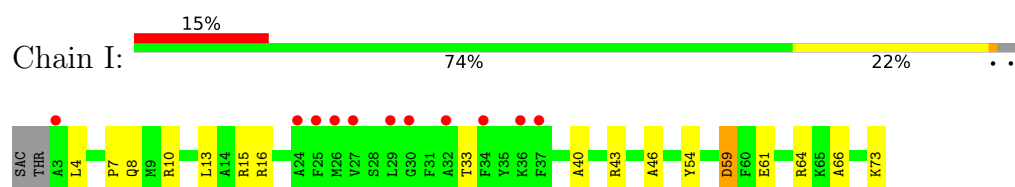
• Molecule 8: Cytochrome c oxidase subunit 6B1



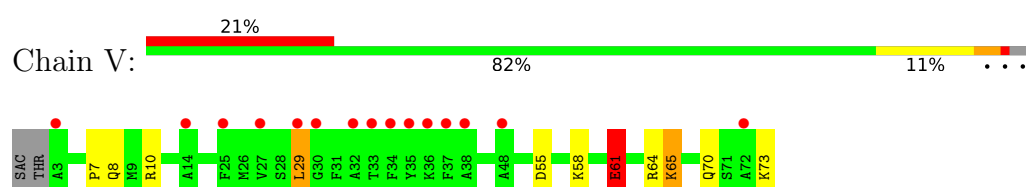
• Molecule 8: Cytochrome c oxidase subunit 6B1



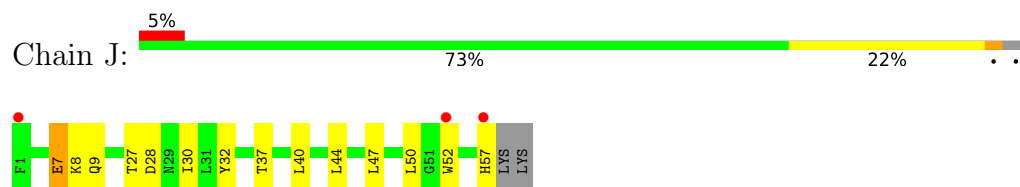
• Molecule 9: Cytochrome c oxidase subunit 6C



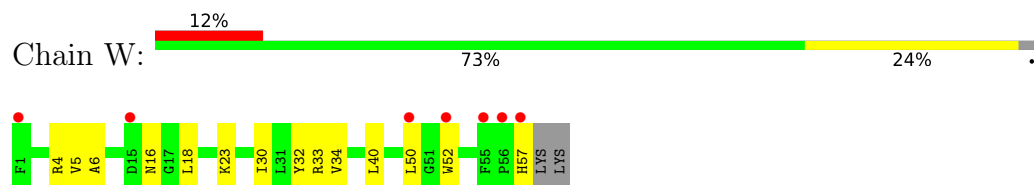
• Molecule 9: Cytochrome c oxidase subunit 6C



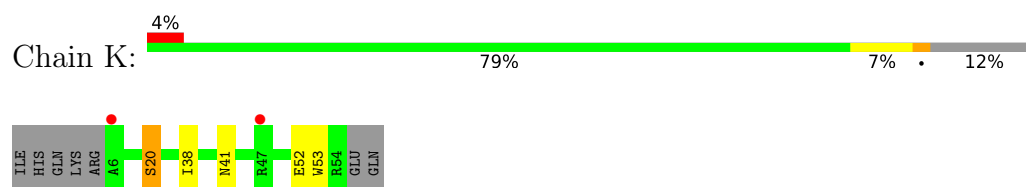
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



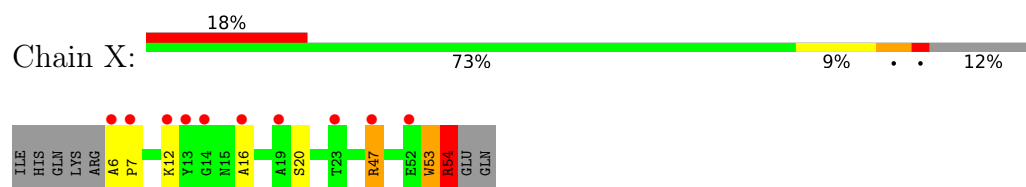
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



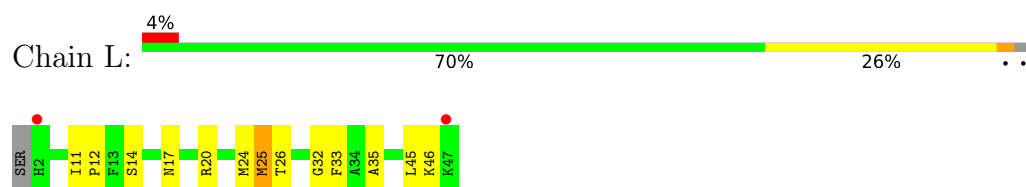
- Molecule 11: Cytochrome c oxidase subunit 7B



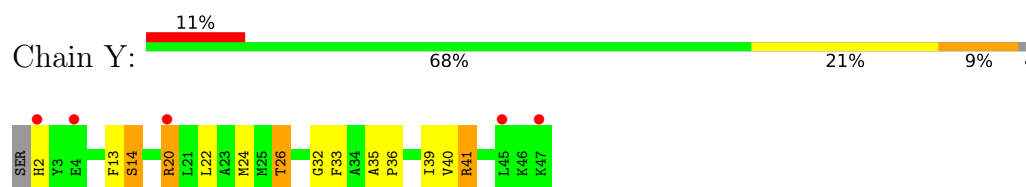
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 12: Cytochrome c oxidase subunit 7C

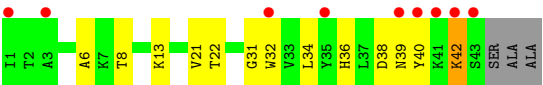


- Molecule 13: Cytochrome c oxidase subunit 8B





● Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.14Å 207.51Å 178.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.10) 98.7 (40.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.176 , 0.210 0.194 , 0.223	Depositor DCC
R_{free} test set	13841 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32244	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	2.10	101/4156 (2.4%)	1.56	55/5678 (1.0%)
1	N	1.85	59/4156 (1.4%)	1.49	49/5678 (0.9%)
2	B	1.93	30/1860 (1.6%)	1.56	15/2534 (0.6%)
2	O	1.61	11/1860 (0.6%)	1.38	7/2534 (0.3%)
3	C	1.75	19/2197 (0.9%)	1.35	11/3005 (0.4%)
3	P	1.76	25/2197 (1.1%)	1.40	18/3005 (0.6%)
4	D	1.86	19/1229 (1.5%)	1.42	8/1658 (0.5%)
4	Q	1.45	5/1229 (0.4%)	1.33	7/1658 (0.4%)
5	E	1.75	13/860 (1.5%)	1.29	4/1167 (0.3%)
5	R	1.46	1/860 (0.1%)	1.27	1/1167 (0.1%)
6	F	1.89	15/733 (2.0%)	1.58	10/996 (1.0%)
6	S	1.70	8/733 (1.1%)	1.56	16/996 (1.6%)
7	G	1.69	6/690 (0.9%)	1.41	6/937 (0.6%)
7	T	1.74	10/690 (1.4%)	1.53	12/937 (1.3%)
8	H	1.70	6/648 (0.9%)	1.42	3/877 (0.3%)
8	U	1.47	1/648 (0.2%)	1.30	1/877 (0.1%)
9	I	1.68	5/598 (0.8%)	1.42	4/792 (0.5%)
9	V	1.38	0/598	1.27	1/792 (0.1%)
10	J	1.53	5/462 (1.1%)	1.29	1/625 (0.2%)
10	W	1.45	4/462 (0.9%)	1.31	2/625 (0.3%)
11	K	1.75	3/398 (0.8%)	1.41	1/546 (0.2%)
11	X	1.29	0/398	1.30	5/546 (0.9%)
12	L	1.85	5/393 (1.3%)	1.39	3/526 (0.6%)
12	Y	1.56	1/393 (0.3%)	1.33	2/526 (0.4%)
13	M	1.88	6/345 (1.7%)	1.46	3/470 (0.6%)
13	Z	1.39	1/345 (0.3%)	1.33	3/470 (0.6%)
All	All	1.78	359/29138 (1.2%)	1.44	248/39622 (0.6%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	S	0	1
All	All	0	2

All (359) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	129	ALA	CA-CB	12.14	1.61	1.52
12	L	35	ALA	CA-CB	11.16	1.67	1.53
1	N	106	PRO	CA-C	11.14	1.62	1.52
4	D	39	ALA	CA-CB	10.99	1.70	1.53
1	N	64	VAL	CA-CB	10.25	1.66	1.54
1	N	139	ALA	CA-CB	10.08	1.70	1.53
13	M	16	ALA	CA-CB	9.77	1.68	1.53
2	O	198	GLU	C-O	9.63	1.34	1.23
2	B	198	GLU	C-O	9.60	1.34	1.23
1	A	235	PHE	N-CA	-9.34	1.35	1.46
7	T	24	ALA	CA-CB	9.32	1.68	1.53
9	I	66	ALA	CA-CB	9.19	1.69	1.53
3	C	250	LEU	N-CA	8.62	1.56	1.46
9	I	46	ALA	CA-CB	8.59	1.66	1.53
1	A	299	VAL	CA-CB	8.58	1.65	1.54
7	G	5	LYS	CA-C	8.45	1.58	1.53
1	N	49	GLY	C-O	8.34	1.29	1.23
2	O	175	ILE	CA-CB	8.32	1.60	1.54
1	A	245	ILE	CA-C	8.17	1.62	1.52
1	A	297	MET	SD-CE	8.15	2.00	1.79
1	A	419	VAL	CA-CB	8.15	1.65	1.54
1	A	352	GLY	N-CA	8.09	1.55	1.45
2	B	194	GLY	C-O	8.00	1.31	1.23
7	T	55	ILE	CA-CB	7.97	1.64	1.54
3	P	184	ALA	CA-CB	7.94	1.65	1.53
1	A	226	GLY	N-CA	7.94	1.53	1.45
12	L	35	ALA	C-O	-7.83	1.17	1.24
2	O	200	CYS	N-CA	7.69	1.53	1.46
1	N	475	ALA	CA-CB	7.65	1.65	1.53
1	N	254	ILE	CA-CB	7.63	1.64	1.54
1	A	331	ASN	N-CA	-7.61	1.37	1.46
6	S	61	ILE	CA-CB	7.61	1.62	1.53
1	N	83	VAL	CA-CB	7.61	1.58	1.54
4	Q	6	VAL	CA-CB	7.61	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	240	HIS	CA-CB	7.49	1.62	1.53
1	A	412	ILE	CA-CB	7.47	1.63	1.54
1	A	119	GLU	CA-C	-7.39	1.45	1.53
1	A	397	PHE	CA-C	7.39	1.60	1.52
1	A	53	ILE	N-CA	-7.34	1.37	1.46
12	Y	32	GLY	N-CA	7.30	1.54	1.45
1	A	494	TRP	N-CA	7.29	1.55	1.46
8	H	81	PHE	C-N	7.28	1.41	1.34
1	A	224	GLY	N-CA	7.26	1.54	1.45
1	A	332	ILE	CA-CB	7.21	1.62	1.54
1	A	388	ALA	CA-CB	7.18	1.64	1.53
3	P	125	ASN	CA-C	7.18	1.60	1.52
1	N	498	CYS	C-O	-7.17	1.19	1.25
1	A	271	MET	N-CA	-7.11	1.37	1.46
2	B	135	LEU	CA-CB	7.11	1.63	1.54
3	P	23	SER	CA-C	7.09	1.62	1.52
13	M	3	ALA	CA-CB	7.06	1.65	1.53
5	E	51	ALA	N-CA	7.04	1.55	1.46
3	P	141	GLY	N-CA	6.99	1.54	1.45
4	D	128	VAL	N-CA	6.96	1.55	1.46
1	N	246	LEU	N-CA	6.92	1.55	1.46
6	F	4	GLY	N-CA	6.90	1.56	1.45
1	N	513	LEU	C-O	6.90	1.32	1.24
1	A	357	VAL	CA-C	6.86	1.61	1.52
6	F	92	VAL	CA-CB	6.84	1.62	1.54
6	F	70	ILE	CA-CB	6.83	1.62	1.54
4	D	12	ALA	CA-CB	6.83	1.65	1.53
2	O	66	THR	CA-C	6.82	1.59	1.52
4	D	29	HIS	CA-C	6.82	1.61	1.52
13	M	22	THR	N-CA	6.79	1.54	1.46
6	S	54	ASN	CB-CG	-6.78	1.35	1.52
3	P	174	THR	CB-CG2	6.78	1.75	1.52
3	P	129	VAL	CA-CB	6.76	1.58	1.53
4	D	92	THR	C-O	-6.75	1.15	1.24
1	A	15	ILE	CA-C	6.73	1.61	1.52
1	A	130	PRO	CA-C	6.71	1.58	1.52
3	P	161	GLN	CB-CG	-6.70	1.32	1.52
1	A	195	LEU	N-CA	6.69	1.54	1.46
1	A	38	ARG	CD-NE	6.66	1.55	1.46
7	T	7	ASP	N-CA	6.66	1.54	1.46
2	B	157	GLU	CA-CB	6.63	1.63	1.53
6	S	76	LYS	CA-C	6.63	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	THR	CA-CB	6.63	1.63	1.53
7	T	53	LEU	C-O	6.61	1.32	1.23
8	H	14	ALA	CA-CB	6.59	1.63	1.53
1	A	323	TRP	N-CA	6.59	1.54	1.46
1	N	268	PHE	C-O	6.57	1.31	1.23
8	H	11	TYR	N-CA	6.57	1.58	1.46
1	A	256	HIS	N-CA	6.57	1.54	1.46
1	A	313	ALA	N-CA	6.47	1.54	1.46
4	D	19	ARG	CZ-NH2	6.46	1.41	1.33
5	E	98	ILE	N-CA	6.44	1.54	1.46
1	A	87	ILE	N-CA	6.42	1.54	1.46
1	N	489	THR	C-O	-6.42	1.15	1.24
2	O	36	SER	CA-C	6.42	1.61	1.52
1	N	38	ARG	C-O	6.42	1.32	1.24
1	A	244	TYR	CA-C	6.41	1.61	1.52
5	R	82	TYR	CA-C	6.36	1.59	1.52
1	A	94	PHE	N-CA	-6.35	1.39	1.46
1	A	189	MET	C-O	-6.31	1.16	1.24
1	N	162	ILE	CA-CB	6.28	1.61	1.54
3	P	204	HIS	N-CA	-6.24	1.38	1.46
1	A	438	ARG	N-CA	6.23	1.54	1.45
3	P	29	SER	CB-OG	-6.23	1.29	1.42
1	A	83	VAL	C-O	-6.22	1.19	1.24
1	N	138	HIS	CA-CB	6.21	1.57	1.53
1	A	78	PHE	C-O	6.20	1.31	1.24
2	B	172	THR	C-O	6.19	1.30	1.24
1	N	297	MET	SD-CE	6.19	1.95	1.79
1	A	248	LEU	CA-C	6.17	1.60	1.52
1	A	122	ALA	CA-CB	6.14	1.60	1.53
7	G	20	THR	N-CA	6.14	1.53	1.46
3	P	238	ALA	CA-CB	6.11	1.62	1.53
1	A	433	LEU	C-O	-6.09	1.17	1.24
3	P	245	VAL	CA-CB	6.09	1.61	1.54
5	E	55	CYS	CA-C	6.09	1.60	1.52
1	A	452	THR	CA-CB	6.08	1.62	1.53
6	F	45	ASP	CA-C	6.08	1.60	1.52
1	A	158	ILE	C-O	-6.08	1.17	1.24
1	A	483	LEU	N-CA	-6.07	1.40	1.46
9	I	40	ALA	CA-CB	6.07	1.62	1.53
1	N	172	LYS	C-N	6.05	1.38	1.33
1	N	295	VAL	CA-CB	6.04	1.61	1.54
1	A	167	THR	CA-CB	6.03	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	40	TYR	CA-C	6.02	1.60	1.52
1	N	163	ASN	C-O	6.01	1.31	1.24
3	C	237	ALA	CA-CB	5.99	1.62	1.53
1	N	326	THR	CA-C	5.98	1.60	1.52
6	S	90	LYS	C-O	-5.97	1.17	1.24
6	F	60	CYS	N-CA	-5.96	1.39	1.46
8	H	78	GLU	C-O	-5.96	1.16	1.24
1	A	110	LEU	C-O	-5.94	1.17	1.24
3	P	219	PHE	N-CA	5.94	1.53	1.46
3	C	247	VAL	C-O	5.94	1.30	1.24
1	A	149	SER	N-CA	-5.93	1.39	1.46
5	E	60	ASP	C-O	5.91	1.30	1.23
1	A	211	THR	N-CA	-5.91	1.39	1.46
1	A	139	ALA	CA-CB	5.90	1.63	1.53
1	A	37	ILE	CA-CB	5.89	1.61	1.54
2	B	160	LEU	N-CA	5.89	1.53	1.45
1	N	509	THR	CA-CB	5.88	1.63	1.53
1	A	508	PRO	C-O	5.88	1.30	1.23
5	E	85	VAL	CA-CB	5.88	1.61	1.54
1	A	339	MET	N-CA	-5.88	1.39	1.46
2	O	100	MET	CA-C	-5.88	1.45	1.52
1	A	75	ILE	CG1-CD1	5.86	1.74	1.51
1	N	276	ALA	CA-CB	5.86	1.62	1.53
10	J	47	LEU	N-CA	5.86	1.53	1.46
2	B	194	GLY	N-CA	5.85	1.51	1.45
1	A	311	ILE	N-CA	-5.85	1.38	1.46
3	C	90	GLU	C-O	-5.84	1.16	1.24
1	A	127	THR	N-CA	5.84	1.53	1.46
1	A	509	THR	CA-CB	5.82	1.62	1.53
3	C	10	MET	N-CA	5.82	1.53	1.46
3	C	184	ALA	CA-CB	5.82	1.62	1.53
13	M	6	ALA	CA-C	-5.82	1.45	1.52
1	N	195	LEU	C-O	5.82	1.30	1.24
1	A	464	ALA	CA-CB	-5.81	1.44	1.53
11	K	20	SER	CA-C	5.81	1.60	1.52
2	B	44	LEU	N-CA	-5.81	1.39	1.46
6	S	6	VAL	CA-CB	5.80	1.60	1.54
3	C	167	ILE	CA-CB	-5.79	1.47	1.54
1	N	364	ASP	C-O	5.79	1.31	1.24
10	W	6	ALA	N-CA	5.78	1.53	1.46
4	D	116	VAL	CA-CB	5.78	1.61	1.54
3	C	72	THR	CA-C	5.77	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	VAL	N-CA	5.76	1.53	1.46
10	J	30	ILE	CA-C	5.75	1.59	1.52
2	B	93	PRO	CA-C	5.75	1.59	1.52
1	A	128	VAL	CA-CB	5.72	1.62	1.54
1	N	389	ILE	C-O	5.71	1.30	1.24
7	T	5	LYS	CB-CG	5.71	1.69	1.52
1	A	226	GLY	C-O	5.70	1.28	1.23
3	C	71	HIS	C-O	5.70	1.30	1.23
1	A	173	PRO	CA-C	-5.69	1.46	1.52
6	F	52	ILE	CA-CB	5.68	1.62	1.54
6	F	60	CYS	CB-SG	5.67	2.00	1.81
5	E	70	VAL	CA-CB	5.65	1.62	1.54
2	B	36	SER	CA-C	5.65	1.60	1.52
1	N	352	GLY	N-CA	5.65	1.53	1.45
1	A	167	THR	N-CA	-5.64	1.39	1.46
1	A	98	ASN	N-CA	5.63	1.53	1.46
2	B	113	TYR	N-CA	5.62	1.53	1.46
2	O	24	HIS	CA-C	5.62	1.60	1.52
6	S	87	THR	CA-CB	5.62	1.62	1.53
1	N	392	GLY	N-CA	5.61	1.52	1.45
3	P	251	PHE	C-O	-5.61	1.17	1.24
3	C	157	LYS	N-CA	-5.60	1.39	1.46
1	N	190	ILE	CA-CB	5.60	1.60	1.54
8	U	77	ALA	N-CA	5.60	1.53	1.46
3	P	65	SER	CA-C	5.59	1.57	1.52
9	I	4	LEU	CA-CB	5.59	1.61	1.53
1	A	146	THR	CB-CG2	5.58	1.71	1.52
3	P	71	HIS	CA-CB	5.58	1.60	1.52
7	T	8	HIS	N-CA	5.58	1.53	1.46
1	N	240	HIS	C-O	-5.57	1.19	1.24
3	P	68	GLN	N-CA	5.57	1.53	1.46
11	K	38	ILE	CA-CB	5.55	1.59	1.54
1	N	185	VAL	C-O	5.55	1.30	1.24
2	B	74	ILE	CA-C	5.55	1.59	1.52
13	M	9	PRO	N-CA	5.55	1.53	1.47
10	W	5	VAL	N-CA	5.55	1.53	1.46
4	D	26	ASP	N-CA	-5.54	1.38	1.46
1	N	149	SER	CA-C	5.54	1.59	1.52
1	A	236	TRP	N-CA	5.52	1.53	1.46
1	N	293	PHE	CA-C	5.51	1.60	1.52
2	B	134	ARG	C-O	5.48	1.30	1.23
1	N	239	GLY	C-O	5.47	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	166	PRO	CA-C	5.47	1.60	1.52
2	B	34	ILE	CA-C	-5.47	1.45	1.52
2	B	112	ASP	CA-C	5.46	1.60	1.52
9	I	7	PRO	N-CA	5.46	1.51	1.46
2	B	207	MET	C-O	-5.45	1.18	1.24
5	E	82	TYR	C-O	-5.45	1.19	1.24
2	B	212	GLU	C-O	-5.45	1.17	1.24
12	L	17	ASN	CA-C	5.45	1.58	1.52
1	A	132	LEU	CA-CB	5.45	1.61	1.53
1	A	232	GLN	N-CA	5.45	1.52	1.46
1	A	246	LEU	N-CA	5.44	1.53	1.46
4	D	27	VAL	C-O	5.44	1.29	1.23
3	C	239	ALA	N-CA	5.43	1.52	1.46
1	N	151	HIS	C-O	-5.43	1.17	1.24
2	B	98	LYS	CE-NZ	5.42	1.65	1.49
7	T	17	ARG	CD-NE	-5.41	1.38	1.46
12	L	32	GLY	N-CA	5.41	1.53	1.45
1	A	423	MET	CA-C	5.40	1.60	1.52
11	K	52	GLU	CA-C	-5.39	1.45	1.52
1	A	298	ASP	C-O	5.38	1.31	1.23
4	D	99	GLU	CA-C	5.38	1.59	1.52
1	A	490	THR	CA-C	-5.38	1.45	1.52
1	A	493	GLU	N-CA	5.38	1.53	1.46
1	N	294	THR	N-CA	5.38	1.53	1.46
1	A	325	ALA	CA-CB	5.37	1.62	1.53
1	A	477	ALA	CA-C	5.37	1.59	1.52
4	D	58	GLU	C-O	-5.36	1.17	1.24
1	N	221	ASP	C-O	-5.36	1.20	1.25
3	P	177	GLN	N-CA	-5.36	1.39	1.46
3	C	238	ALA	CA-CB	5.36	1.61	1.53
10	J	32	TYR	C-O	5.36	1.30	1.24
3	P	156	ARG	C-O	5.35	1.30	1.24
1	A	135	ASN	N-CA	5.35	1.53	1.46
2	B	182	THR	N-CA	5.35	1.52	1.45
1	A	348	PHE	N-CA	5.34	1.52	1.46
3	C	9	HIS	C-O	5.34	1.30	1.24
5	E	64	ALA	CA-CB	5.34	1.61	1.53
1	A	286	ILE	CG1-CD1	5.34	1.72	1.51
2	B	38	VAL	C-O	5.34	1.30	1.24
5	E	51	ALA	CA-CB	5.34	1.61	1.53
7	G	49	PRO	CA-C	5.34	1.58	1.53
10	J	7	GLU	CA-C	-5.34	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	199	ILE	N-CA	5.34	1.52	1.46
1	A	487	LEU	CA-C	-5.33	1.45	1.53
7	G	17	ARG	CD-NE	-5.33	1.38	1.46
1	N	237	PHE	CA-C	5.33	1.59	1.52
1	A	358	LEU	C-O	5.32	1.30	1.24
1	N	415	ALA	CA-C	5.31	1.59	1.52
1	N	79	GLY	N-CA	5.31	1.52	1.45
7	T	2	SER	CA-C	5.31	1.59	1.52
13	Z	22	THR	N-CA	5.30	1.52	1.46
3	P	45	ILE	CA-C	5.30	1.59	1.52
4	D	16	TYR	CA-C	5.30	1.59	1.52
7	G	76	ASN	C-O	5.30	1.30	1.24
1	A	276	ALA	CA-CB	5.29	1.61	1.53
6	F	95	GLN	N-CA	5.29	1.53	1.46
1	N	240	HIS	CA-C	5.29	1.58	1.52
1	N	415	ALA	CA-CB	5.29	1.61	1.53
1	A	335	SER	N-CA	5.29	1.53	1.45
1	A	96	ARG	CA-CB	5.28	1.62	1.53
3	P	245	VAL	CA-C	5.28	1.59	1.52
1	N	314	ILE	C-N	5.27	1.40	1.33
6	F	13	ALA	C-O	5.27	1.30	1.23
8	H	58	ARG	CZ-NH1	5.26	1.40	1.32
4	Q	20	ARG	N-CA	5.26	1.52	1.46
1	A	347	LEU	CA-C	5.26	1.59	1.52
4	Q	5	VAL	CA-CB	5.26	1.61	1.54
4	D	65	LYS	CE-NZ	5.25	1.65	1.49
5	E	42	VAL	CA-C	5.25	1.58	1.52
1	A	349	THR	CA-C	5.24	1.59	1.52
1	A	279	SER	N-CA	5.24	1.52	1.46
13	M	14	GLU	C-O	-5.24	1.17	1.24
3	C	32	THR	CA-CB	5.24	1.61	1.53
6	F	78	GLU	C-O	-5.24	1.17	1.23
2	B	125	THR	CA-CB	5.23	1.61	1.53
1	N	363	LEU	C-O	-5.23	1.17	1.24
2	O	151	ARG	CZ-NH1	5.23	1.40	1.32
1	A	484	THR	CA-C	5.22	1.59	1.52
2	B	72	ILE	CA-CB	-5.22	1.48	1.54
2	B	209	ILE	C-O	-5.22	1.18	1.24
7	T	46	ALA	CA-C	5.22	1.59	1.52
1	N	504	THR	N-CA	-5.22	1.39	1.45
3	P	228	THR	C-O	5.21	1.30	1.23
1	A	333	LYS	CA-C	5.21	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	99	TRP	CA-C	5.20	1.59	1.52
6	S	82	CYS	C-O	-5.20	1.17	1.24
1	A	349	THR	N-CA	-5.20	1.40	1.46
4	D	81	VAL	CA-C	5.20	1.59	1.52
6	F	14	THR	CA-C	5.19	1.59	1.52
3	P	69	GLY	CA-C	5.19	1.58	1.51
1	N	409	TRP	CA-C	5.19	1.59	1.52
2	B	116	LEU	CA-C	5.18	1.59	1.52
2	B	96	THR	C-O	5.16	1.30	1.24
5	E	29	LEU	CA-C	5.16	1.59	1.52
5	E	81	ILE	C-O	5.16	1.30	1.24
3	P	11	VAL	CA-CB	5.16	1.61	1.54
1	A	345	ILE	CA-CB	5.16	1.60	1.54
6	S	16	LEU	C-O	5.16	1.30	1.24
2	B	197	SER	C-O	5.15	1.31	1.23
1	A	392	GLY	N-CA	5.15	1.52	1.45
1	N	180	GLN	N-CA	-5.15	1.40	1.46
1	A	444	PRO	C-O	5.14	1.29	1.23
4	D	21	ASP	CA-CB	5.14	1.61	1.53
1	N	92	MET	CB-CG	5.14	1.67	1.52
1	N	198	SER	N-CA	5.14	1.52	1.46
1	N	371	TYR	CA-CB	5.14	1.62	1.53
1	A	370	THR	N-CA	5.14	1.52	1.45
2	O	103	GLN	CA-C	5.13	1.59	1.52
6	F	70	ILE	C-O	5.13	1.29	1.24
4	D	87	PHE	C-O	-5.12	1.18	1.24
1	A	195	LEU	C-O	5.12	1.29	1.24
1	A	412	ILE	CA-C	5.12	1.59	1.52
6	F	37	LYS	C-O	-5.12	1.17	1.23
12	L	35	ALA	CA-C	5.11	1.58	1.52
1	N	433	LEU	CA-C	5.11	1.59	1.52
10	W	32	TYR	C-O	5.11	1.29	1.24
1	N	257	ILE	N-CA	5.11	1.52	1.46
1	A	73	ILE	CG1-CD1	5.10	1.71	1.51
1	A	63	PHE	C-O	5.09	1.30	1.24
1	A	153	ALA	N-CA	5.09	1.52	1.46
1	A	149	SER	C-O	5.09	1.29	1.24
1	N	425	PHE	N-CA	5.09	1.52	1.46
2	O	194	GLY	C-O	5.09	1.28	1.23
4	Q	8	SER	CA-C	5.09	1.59	1.52
1	A	478	SER	C-O	-5.08	1.17	1.24
1	A	305	PHE	N-CA	5.08	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	160	GLY	C-O	5.08	1.29	1.23
1	A	182	PRO	CA-C	5.08	1.58	1.52
2	B	186	SER	N-CA	5.07	1.52	1.46
3	C	256	ILE	CA-C	5.07	1.59	1.52
4	D	131	ILE	CA-CB	5.07	1.61	1.54
1	A	174	PRO	C-O	-5.07	1.18	1.24
10	J	44	LEU	C-O	-5.07	1.18	1.24
3	P	6	HIS	C-O	5.07	1.30	1.23
4	D	121	LYS	N-CA	5.06	1.52	1.46
3	C	159	MET	N-CA	5.06	1.52	1.46
4	Q	39	ALA	CA-CB	5.06	1.61	1.53
1	A	493	GLU	CA-CB	5.05	1.62	1.53
1	N	365	ILE	CG1-CD1	-5.05	1.32	1.51
6	F	61	ILE	CA-CB	5.05	1.59	1.53
1	A	346	PHE	CD1-CE1	5.04	1.53	1.38
1	N	193	VAL	N-CA	5.04	1.52	1.46
1	N	263	GLY	N-CA	5.04	1.52	1.45
1	N	87	ILE	N-CA	5.04	1.52	1.46
7	G	5	LYS	CB-CG	5.04	1.67	1.52
10	W	40	LEU	N-CA	5.03	1.52	1.46
1	A	39	ALA	CA-C	5.03	1.59	1.52
1	A	308	ALA	CA-CB	-5.03	1.45	1.53
8	H	69	VAL	N-CA	5.02	1.52	1.46
2	B	19	GLU	CB-CG	-5.02	1.37	1.52
3	C	231	HIS	N-CA	-5.02	1.40	1.46
1	N	313	ALA	CA-CB	5.02	1.62	1.53
3	P	85	LEU	CG-CD2	5.02	1.69	1.52
6	F	90	LYS	CA-C	-5.01	1.46	1.52
5	E	70	VAL	N-CA	-5.01	1.39	1.46
7	T	48	ILE	CA-C	-5.00	1.47	1.52
3	C	250	LEU	C-O	-5.00	1.18	1.24

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	N-CA-CB	11.59	121.40	110.39
1	A	402	GLY	N-CA-C	-9.74	101.53	115.27
3	C	199	VAL	N-CA-C	9.73	119.76	110.42
4	Q	10	ASP	N-CA-C	-9.49	101.38	113.72
1	A	316	THR	N-CA-C	-9.36	101.16	111.36
4	Q	8	SER	N-CA-C	9.01	121.03	111.03
7	T	76	ASN	CA-C-N	-8.82	111.66	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	76	ASN	C-N-CA	-8.82	111.66	120.31
1	A	49	GLY	N-CA-C	-8.41	99.21	110.74
8	H	14	ALA	CA-C-N	-8.35	112.25	120.52
8	H	14	ALA	C-N-CA	-8.35	112.25	120.52
6	S	94	HIS	N-CA-C	7.95	127.73	110.80
2	B	207	MET	CA-C-N	7.92	128.37	120.52
2	B	207	MET	C-N-CA	7.92	128.37	120.52
6	S	53	THR	CA-C-N	7.80	133.74	120.72
6	S	53	THR	C-N-CA	7.80	133.74	120.72
7	T	8	HIS	N-CA-C	7.76	127.33	110.80
4	D	19	ARG	NE-CZ-NH1	-7.62	113.88	121.50
1	A	284	GLY	N-CA-C	-7.59	105.38	115.32
1	A	105	LEU	CA-C-N	-7.58	112.57	120.38
1	A	105	LEU	C-N-CA	-7.58	112.57	120.38
1	N	62	ALA	N-CA-C	7.58	119.18	111.07
5	R	79	LYS	N-CA-C	7.52	121.37	111.75
4	Q	137	LYS	CD-CE-NZ	-7.48	87.96	111.90
1	N	397	PHE	CA-C-N	7.45	127.32	119.05
1	N	397	PHE	C-N-CA	7.45	127.32	119.05
1	N	355	GLY	N-CA-C	-7.33	103.39	112.77
11	K	41	ASN	CB-CA-C	-7.31	104.64	111.00
2	B	65	TRP	CB-CA-C	7.21	123.29	110.81
1	N	500	PRO	CA-C-N	-7.17	112.93	120.03
1	N	500	PRO	C-N-CA	-7.17	112.93	120.03
7	G	17	ARG	NE-CZ-NH2	-7.16	112.76	119.20
6	F	93	PRO	CA-C-N	7.16	135.21	121.54
6	F	93	PRO	C-N-CA	7.16	135.21	121.54
6	S	20	VAL	N-CA-C	-7.14	103.51	110.72
1	A	153	ALA	N-CA-C	-7.08	103.56	111.28
7	T	7	ASP	N-CA-C	7.07	125.86	110.80
1	A	168	ILE	N-CA-C	6.94	117.70	110.62
2	O	14	SER	CA-C-N	6.91	126.42	119.24
2	O	14	SER	C-N-CA	6.91	126.42	119.24
1	A	208	MET	CG-SD-CE	6.90	116.09	100.90
10	W	18	LEU	CA-C-N	6.87	126.86	119.78
10	W	18	LEU	C-N-CA	6.87	126.86	119.78
1	N	83	VAL	N-CA-CB	6.82	115.77	110.45
9	I	13	LEU	N-CA-C	-6.80	103.94	111.36
1	N	384	GLY	N-CA-C	-6.76	97.15	113.18
2	O	92	ASN	N-CA-C	6.73	124.68	109.81
1	N	513	LEU	N-CA-C	6.71	121.78	112.45
1	A	60	ALA	N-CA-C	-6.60	104.16	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	17	ARG	NE-CZ-NH2	-6.60	113.26	119.20
2	O	78	LEU	CA-C-N	-6.57	112.23	119.19
2	O	78	LEU	C-N-CA	-6.57	112.23	119.19
1	N	345	ILE	N-CA-C	-6.54	104.11	110.72
4	Q	22	TYR	N-CA-C	-6.53	97.65	108.75
1	N	92	MET	N-CA-C	-6.51	100.88	110.52
7	G	76	ASN	CA-C-N	-6.50	113.59	120.03
7	G	76	ASN	C-N-CA	-6.50	113.59	120.03
1	N	445	ASP	N-CA-C	6.50	119.19	111.33
11	X	6	ALA	CA-C-N	6.48	127.94	119.84
11	X	6	ALA	C-N-CA	6.48	127.94	119.84
2	B	177	GLY	N-CA-C	-6.48	106.75	115.36
1	N	412	ILE	N-CA-C	-6.48	104.20	110.42
1	N	25	TRP	N-CA-C	-6.47	104.15	111.07
3	P	141	GLY	N-CA-C	-6.46	104.72	113.37
2	B	39	LEU	N-CA-C	-6.45	104.33	111.36
4	D	102	TYR	CA-C-N	-6.43	114.98	122.63
4	D	102	TYR	C-N-CA	-6.43	114.98	122.63
3	P	156	ARG	N-CA-C	6.43	117.95	111.07
1	A	375	ALA	N-CA-C	-6.42	104.20	111.14
6	S	53	THR	CB-CA-C	-6.42	98.44	114.11
6	S	54	ASN	CB-CA-C	-6.38	96.98	110.31
1	A	415	ALA	N-CA-C	-6.36	104.34	111.28
1	A	239	GLY	CA-C-N	-6.32	111.94	119.78
1	A	239	GLY	C-N-CA	-6.32	111.94	119.78
3	C	24	ALA	N-CA-C	-6.29	104.50	111.36
1	N	71	MET	CG-SD-CE	-6.26	87.14	100.90
6	S	64	GLU	CA-C-N	-6.25	114.11	125.66
6	S	64	GLU	C-N-CA	-6.25	114.11	125.66
1	A	448	THR	N-CA-C	6.21	117.71	111.07
7	G	8	HIS	N-CA-C	6.19	123.98	110.80
3	P	20	GLY	N-CA-C	-6.19	105.00	112.49
4	Q	133	GLY	N-CA-C	6.18	120.68	112.77
5	E	80	GLU	N-CA-C	-6.17	105.25	112.89
1	N	299	VAL	N-CA-C	6.16	116.90	110.62
1	N	70	VAL	N-CA-C	6.15	116.26	110.30
6	F	87	THR	N-CA-CB	6.13	119.05	110.04
10	J	28	ASP	N-CA-C	-6.12	104.69	111.36
6	S	67	SER	N-CA-C	-6.11	105.65	113.23
1	A	240	HIS	N-CA-CB	6.08	117.59	110.42
8	U	66	ILE	N-CA-C	-6.07	104.43	110.62
1	A	101	SER	CA-CB-OG	-6.06	98.98	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	209	LEU	N-CA-C	-6.06	104.68	111.28
4	D	58	GLU	N-CA-C	-6.04	104.78	111.36
2	O	67	ILE	N-CA-C	6.03	116.77	110.62
1	A	454	SER	N-CA-C	-6.02	104.72	111.28
1	A	86	MET	CA-C-N	-5.99	113.36	122.76
1	A	86	MET	C-N-CA	-5.99	113.36	122.76
9	I	40	ALA	N-CA-C	5.99	117.50	110.97
2	B	156	SER	CA-C-N	-5.98	113.28	122.60
2	B	156	SER	C-N-CA	-5.98	113.28	122.60
1	A	351	GLY	N-CA-C	-5.97	105.37	113.37
6	S	53	THR	CA-CB-CG2	5.96	120.63	110.50
3	C	255	SER	N-CA-C	5.96	117.64	111.03
7	T	17	ARG	CB-CG-CD	-5.96	97.60	111.30
1	A	28	MET	N-CA-C	-5.95	104.37	111.69
1	A	180	GLN	N-CA-C	-5.94	104.22	112.30
4	Q	20	ARG	NE-CZ-NH2	-5.90	113.89	119.20
13	M	7	LYS	N-CA-C	5.90	117.71	111.28
4	D	20	ARG	N-CA-C	-5.89	104.93	111.71
1	N	79	GLY	N-CA-C	-5.89	105.67	112.50
7	T	18	PHE	N-CA-C	-5.89	104.94	111.36
1	N	312	ILE	CG1-CB-CG2	-5.88	93.05	110.70
9	V	61	GLU	N-CA-C	-5.88	104.95	111.36
6	F	44	GLU	CA-C-N	-5.87	116.32	122.89
6	F	44	GLU	C-N-CA	-5.87	116.32	122.89
3	C	189	SER	N-CA-C	-5.86	105.89	113.16
1	N	245	ILE	N-CA-C	-5.86	104.80	110.72
1	N	246	LEU	CA-C-N	-5.84	115.24	121.84
1	N	246	LEU	C-N-CA	-5.84	115.24	121.84
3	C	96	GLY	N-CA-C	-5.83	105.73	112.73
1	A	112	LEU	CD1-CG-CD2	-5.82	97.99	110.80
3	C	29	SER	CB-CA-C	-5.82	101.50	110.81
1	A	312	ILE	CA-CB-CG1	-5.81	100.52	110.40
3	P	129	VAL	N-CA-CB	5.81	114.16	110.50
6	S	95	GLN	CA-C-N	5.79	132.13	121.70
6	S	95	GLN	C-N-CA	5.79	132.13	121.70
5	E	90	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	N	205	GLY	N-CA-C	-5.78	105.37	112.77
1	N	391	GLY	N-CA-C	-5.78	105.80	112.50
7	T	2	SER	N-CA-C	-5.77	106.02	114.39
6	S	58	VAL	CA-C-N	-5.76	117.37	122.73
6	S	58	VAL	C-N-CA	-5.76	117.37	122.73
1	A	244	TYR	CA-CB-CG	-5.76	103.53	113.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	479	LYS	N-CA-C	5.76	118.22	111.02
3	P	29	SER	CA-CB-OG	-5.75	99.59	111.10
6	F	93	PRO	N-CA-C	5.75	119.26	111.22
1	A	194	LEU	CA-C-O	-5.74	114.47	120.55
2	B	166	PRO	CA-C-N	5.74	128.75	120.38
2	B	166	PRO	C-N-CA	5.74	128.75	120.38
1	A	79	GLY	N-CA-C	-5.71	105.59	112.49
4	D	10	ASP	N-CA-C	5.70	119.94	113.15
1	A	365	ILE	N-CA-C	-5.70	104.38	110.36
3	P	192	VAL	N-CA-C	-5.65	104.64	112.50
6	F	95	GLN	N-CA-C	5.65	122.83	110.80
3	P	8	TYR	N-CA-C	5.64	118.17	110.55
1	N	381	LEU	N-CA-C	5.64	120.18	111.56
3	C	32	THR	N-CA-C	5.62	117.09	111.07
3	P	151	LEU	N-CA-C	-5.61	105.08	111.14
1	N	310	MET	N-CA-C	5.61	118.16	111.71
11	X	53	TRP	N-CA-C	-5.60	106.99	113.88
4	D	56	LYS	N-CA-C	-5.59	105.26	111.36
3	P	68	GLN	N-CA-C	5.54	120.20	113.38
13	Z	21	VAL	N-CA-C	-5.54	104.97	110.62
1	A	237	PHE	N-CA-C	-5.54	105.40	111.82
1	A	106	PRO	CA-C-N	-5.52	112.92	119.05
1	A	106	PRO	C-N-CA	-5.52	112.92	119.05
1	A	512	ASN	CB-CA-C	-5.52	99.30	109.46
1	N	372	TYR	N-CA-C	-5.51	105.27	111.28
12	L	33	PHE	N-CA-C	5.51	117.28	111.28
11	X	54	ARG	NE-CZ-NH2	5.51	124.16	119.20
2	B	161	HIS	N-CA-C	-5.49	101.15	108.34
1	A	169	ILE	CB-CA-C	-5.48	103.38	112.26
3	C	168	THR	N-CA-C	-5.47	105.40	111.36
1	N	168	ILE	N-CA-C	-5.46	104.12	111.44
1	N	278	MET	N-CA-C	5.46	116.91	111.07
1	N	83	VAL	O-C-N	5.45	123.91	120.42
2	B	132	GLU	CA-C-N	5.45	129.67	122.42
2	B	132	GLU	C-N-CA	5.45	129.67	122.42
1	N	308	ALA	N-CA-C	-5.45	105.50	111.82
1	N	248	LEU	CA-C-N	-5.44	114.07	119.56
1	N	248	LEU	C-N-CA	-5.44	114.07	119.56
7	G	7	ASP	N-CA-C	5.43	122.36	110.80
1	A	280	ILE	N-CA-C	-5.40	105.27	110.72
1	N	30	GLY	N-CA-C	-5.40	106.14	113.37
1	A	384	GLY	N-CA-C	-5.39	100.40	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	MET	CG-SD-CE	-5.39	89.05	100.90
2	B	91	ASN	N-CA-C	5.39	122.41	113.89
2	B	217	LYS	N-CA-C	-5.39	105.44	112.23
1	N	365	ILE	CB-CA-C	-5.39	104.98	111.88
3	P	78	GLY	N-CA-C	-5.38	106.25	112.50
13	M	27	LEU	N-CA-C	5.38	116.95	111.14
1	A	195	LEU	CA-C-O	5.38	126.47	120.82
1	A	257	ILE	N-CA-C	5.38	115.59	110.53
3	P	136	VAL	N-CA-C	5.38	115.58	110.42
1	A	455	SER	CA-C-O	5.36	126.10	120.42
12	Y	41	ARG	N-CA-C	-5.36	105.34	111.07
1	N	466	MET	N-CA-C	-5.36	105.44	111.28
3	P	105	SER	N-CA-C	5.34	118.96	112.23
1	A	275	TRP	N-CA-C	-5.34	105.46	111.28
3	P	120	GLY	N-CA-C	-5.33	107.91	115.43
1	N	316	THR	N-CA-C	-5.33	105.55	111.36
6	F	35	ALA	CA-C-N	5.33	125.25	119.76
6	F	35	ALA	C-N-CA	5.33	125.25	119.76
1	A	362	SER	CA-CB-OG	-5.33	100.45	111.10
1	N	356	ILE	N-CA-C	5.32	116.05	110.62
2	O	65	TRP	N-CA-C	5.32	119.48	113.15
5	E	93	LEU	N-CA-C	-5.31	105.49	111.28
1	A	240	HIS	CA-CB-CG	-5.29	108.52	113.80
6	S	53	THR	OG1-CB-CG2	5.26	119.82	109.30
3	P	217	VAL	N-CA-C	-5.26	105.26	110.62
1	A	410	ALA	N-CA-C	-5.26	105.63	111.36
1	N	250	GLY	N-CA-C	-5.25	106.06	112.77
1	A	71	MET	CG-SD-CE	-5.24	89.36	100.90
5	E	47	ILE	CB-CA-C	-5.24	105.22	112.24
8	H	28	ASN	CB-CA-C	5.24	119.25	110.92
7	T	58	LYS	CA-C-N	-5.23	114.39	119.78
7	T	58	LYS	C-N-CA	-5.23	114.39	119.78
13	Z	8	THR	CA-C-N	5.22	125.22	119.89
13	Z	8	THR	C-N-CA	5.22	125.22	119.89
1	A	322	SER	N-CA-C	-5.22	105.77	111.82
1	N	278	MET	CA-CB-CG	-5.21	103.67	114.10
1	A	312	ILE	CB-CG1-CD1	5.21	124.74	113.80
1	N	416	ILE	N-CA-C	-5.21	105.64	110.53
1	N	475	ALA	N-CA-C	-5.20	105.30	111.69
1	N	509	THR	N-CA-C	-5.20	103.53	110.55
7	G	17	ARG	CB-CG-CD	-5.19	99.36	111.30
3	P	41	THR	N-CA-C	5.19	116.79	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	33	LEU	CA-CB-CG	5.19	134.45	116.30
7	T	83	GLU	N-CA-C	5.18	117.54	110.55
9	I	64	ARG	N-CA-C	-5.17	105.53	111.07
1	N	277	MET	CA-CB-CG	-5.17	103.77	114.10
9	I	59	ASP	N-CA-C	-5.16	105.55	111.07
1	A	52	GLN	N-CA-C	-5.15	105.31	111.03
1	N	101	SER	CA-CB-OG	-5.14	100.81	111.10
1	A	391	GLY	N-CA-C	-5.13	106.20	112.77
6	S	11	GLU	N-CA-C	5.13	116.95	111.36
11	X	47	ARG	CA-CB-CG	5.13	124.36	114.10
3	C	161	GLN	CB-CA-C	-5.11	102.85	110.88
1	A	371	TYR	CA-CB-CG	-5.11	104.70	113.90
13	M	5	PRO	N-CA-C	-5.11	103.43	111.34
1	A	80	ASN	N-CA-C	5.09	116.83	111.28
12	Y	33	PHE	N-CA-C	5.09	116.83	111.28
12	L	25	MET	CA-C-N	5.08	127.04	120.44
12	L	25	MET	C-N-CA	5.08	127.04	120.44
6	F	18	ARG	N-CA-C	5.07	116.50	111.07
3	P	246	ASP	N-CA-C	-5.07	105.84	111.36
1	A	436	MET	CA-C-N	-5.06	115.35	120.21
1	A	436	MET	C-N-CA	-5.06	115.35	120.21
1	A	199	LEU	CA-C-N	-5.05	113.84	119.19
1	A	199	LEU	C-N-CA	-5.05	113.84	119.19
2	B	167	SER	CB-CA-C	-5.05	100.67	110.46
4	Q	113	GLU	N-CA-C	5.05	117.17	111.11
1	N	240	HIS	CA-CB-CG	-5.04	108.76	113.80
3	P	58	TRP	N-CA-C	5.04	116.86	111.36
3	C	74	ALA	N-CA-C	-5.04	105.70	111.14
3	P	161	GLN	N-CA-CB	-5.04	102.76	110.07
3	C	248	VAL	N-CA-C	5.03	115.64	110.36
4	D	80	THR	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	S	93	PRO	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	65	0
1	N	4027	0	4001	62	0
2	B	1824	0	1833	31	0
2	O	1824	0	1833	44	0
3	C	2110	0	2027	33	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	18	0
4	Q	1195	0	1183	17	0
5	E	842	0	838	5	0
5	R	842	0	838	10	0
6	F	717	0	700	16	0
6	S	717	0	700	20	0
7	G	675	0	643	34	0
7	T	675	0	644	43	0
8	H	628	0	580	7	0
8	U	628	0	580	7	0
9	I	585	0	597	11	0
9	V	585	0	597	12	0
10	J	451	0	446	6	0
10	W	451	0	446	6	0
11	K	384	0	366	1	0
11	X	384	0	366	6	0
12	L	380	0	380	11	0
12	Y	380	0	380	14	0
13	M	335	0	352	2	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	2	0	0	1	0
15	N	2	0	0	1	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	120	0	108	9	0
18	N	120	0	108	9	0
19	A	63	0	110	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	15	0
19	L	63	0	110	16	0
19	N	126	0	220	21	0
19	Q	63	0	110	5	0
20	A	102	0	152	10	0
20	C	102	0	152	7	0
20	N	102	0	152	7	0
20	P	102	0	152	8	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	18	0
22	O	52	0	80	12	0
23	B	29	0	37	1	0
23	C	58	0	71	5	0
23	J	29	0	36	3	0
23	O	29	0	36	2	0
23	P	58	0	71	5	0
23	W	29	0	36	4	0
24	C	33	0	37	5	0
24	M	33	0	39	1	0
24	P	33	0	40	2	0
24	Z	33	0	39	2	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	100	0	156	13	0
26	G	100	0	156	24	0
26	P	100	0	156	16	0
26	T	100	0	156	23	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	159	0	231	20	0
28	P	106	0	154	14	0
28	T	53	0	77	21	0
29	A	219	0	0	6	0
29	B	139	0	0	3	0
29	C	105	0	0	2	0
29	D	110	0	0	0	0
29	E	68	0	0	1	0
29	F	76	0	0	3	0
29	G	45	0	0	7	0
29	H	48	0	0	1	0
29	I	35	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	J	21	0	0	1	0
29	K	22	0	0	0	0
29	L	27	0	0	1	0
29	M	18	0	0	0	0
29	N	204	0	0	2	0
29	O	109	0	0	0	0
29	P	106	0	0	2	0
29	Q	67	0	0	3	0
29	R	52	0	0	0	0
29	S	69	0	0	4	0
29	T	48	0	0	4	0
29	U	38	0	0	3	0
29	V	19	0	0	0	0
29	W	16	0	0	0	0
29	X	16	0	0	0	0
29	Y	17	0	0	1	0
29	Z	14	0	0	0	0
All	All	32244	0	31065	602	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 10.

All (602) 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:A:75:ILE:CD1	1:A:75:ILE:CG1	1.74	1.62
3:P:174:THR:CG2	3:P:174:THR:CB	1.74	1.60
28:G:265:PEK:H383	26:G:269:CDL:C27	1.62	1.29
28:P:1265:PEK:H383	26:T:1269:CDL:C27	1.64	1.25
7:T:2:SER:OG	28:T:263:PEK:H302	1.33	1.23
28:G:265:PEK:H383	26:G:269:CDL:H272	1.18	1.15
26:G:269:CDL:H112	26:G:269:CDL:HA21	1.26	1.10
15:A:520:PER:O2	15:A:520:PER:O1	1.70	1.10
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.07	1.09
7:T:84:LYS:HD2	7:T:84:LYS:H	1.13	1.07
15:N:520:PER:O1	15:N:520:PER:O2	1.70	1.07
28:P:1265:PEK:H383	26:T:1269:CDL:H271	1.22	1.06
7:G:84:LYS:H	7:G:84:LYS:HD2	1.19	1.06
22:B:230:PSC:C07	9:I:10:ARG:HH21	1.68	1.05
7:G:5:LYS:HG3	28:G:1263:PEK:H382	1.07	1.04
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG11	1.41	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:1230:PSC:O01	22:O:1230:PSC:H212	1.59	1.02
6:S:95:GLN:HB2	29:S:4411:HOH:O	1.60	1.01
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.40	1.00
6:F:85:CYS:SG	6:F:87:THR:HG23	2.00	1.00
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.25	0.99
9:V:65:LYS:O	11:X:54:ARG:NH1	1.94	0.98
19:N:1522:TGL:H231	19:N:1522:TGL:HA92	1.45	0.97
7:T:2:SER:OG	28:T:263:PEK:C30	2.10	0.97
28:P:1265:PEK:C38	26:T:1269:CDL:C27	2.42	0.96
7:T:5:LYS:CG	28:T:263:PEK:H383	1.94	0.96
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.81	0.95
1:A:486:ASP:OD2	4:D:19:ARG:HD3	1.66	0.95
7:T:5:LYS:HD2	28:T:263:PEK:H381	1.48	0.95
7:G:5:LYS:HB2	28:G:1263:PEK:H361	1.49	0.95
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.47	0.93
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.31	0.93
20:C:267:PGV:H182	26:C:270:CDL:H671	1.50	0.93
7:G:5:LYS:CG	28:G:1263:PEK:H382	1.97	0.92
7:T:5:LYS:HG3	28:T:263:PEK:H383	1.51	0.91
28:G:265:PEK:C38	26:G:269:CDL:C27	2.49	0.90
7:T:31:CYS:SG	26:T:1269:CDL:H551	2.12	0.90
1:N:400:PHE:HB3	19:N:1522:TGL:H283	1.54	0.90
20:A:524:PGV:H152	20:A:524:PGV:H321	1.52	0.89
6:S:52:ILE:O	6:S:94:HIS:CE1	2.26	0.89
7:T:2:SER:HG	28:T:263:PEK:H302	1.36	0.89
26:G:269:CDL:H241	26:G:269:CDL:H541	1.54	0.89
7:G:84:LYS:H	7:G:84:LYS:CD	1.82	0.88
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.09	0.88
22:O:1230:PSC:C07	9:V:10:ARG:HH21	1.86	0.87
4:D:34:SER:H	4:D:37:GLN:HE21	1.20	0.87
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.41	0.86
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.40	0.86
7:T:84:LYS:H	7:T:84:LYS:CD	1.89	0.86
7:G:84:LYS:HD2	7:G:84:LYS:N	1.91	0.84
7:T:72:ASN:H	7:T:76:ASN:HD22	1.25	0.83
7:G:76:ASN:HD21	28:G:264:PEK:HN2	1.23	0.81
22:B:230:PSC:H072	9:I:10:ARG:NH2	1.93	0.80
7:G:5:LYS:HG3	28:G:1263:PEK:C38	2.02	0.80
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.17	0.80
4:Q:109:HIS:HD2	29:Q:3152:HOH:O	1.62	0.80
3:P:25:LEU:O	3:P:29:SER:HB2	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:HD11	29:A:4260:HOH:O	1.80	0.80
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.17	0.80
2:O:82:ARG:HH11	2:O:86:MET:HE1	1.47	0.79
7:T:5:LYS:HD2	28:T:263:PEK:C38	2.13	0.79
3:P:111:GLU:HG3	29:U:4543:HOH:O	1.83	0.79
2:B:41:ILE:HD13	22:B:230:PSC:C34	2.12	0.78
12:L:24:MET:HG3	29:L:4843:HOH:O	1.82	0.78
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.47	0.78
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.64	0.78
2:O:226:MET:O	2:O:227:LEU:C	2.25	0.77
6:S:95:GLN:HA	6:S:95:GLN:HE21	1.50	0.77
1:A:310:MET:HE2	1:A:356:ILE:HG23	1.67	0.77
20:P:1267:PGV:H182	26:P:1270:CDL:H671	1.65	0.76
19:N:1521:TGL:H142	2:O:39:LEU:CD2	2.15	0.76
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.76
22:B:230:PSC:C07	9:I:10:ARG:NH2	2.47	0.75
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.65	0.75
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.68	0.75
7:G:72:ASN:H	7:G:76:ASN:HD22	1.32	0.74
19:N:1521:TGL:H142	2:O:39:LEU:HD22	1.68	0.74
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.51	0.74
22:O:1230:PSC:H072	9:V:10:ARG:HH21	1.50	0.74
28:G:265:PEK:H383	26:G:269:CDL:H273	1.66	0.74
9:I:33:THR:HG22	29:I:4648:HOH:O	1.86	0.74
3:P:55:TYR:HE1	26:P:1270:CDL:H521	1.53	0.73
20:A:524:PGV:H152	20:A:524:PGV:C32	2.17	0.73
7:T:84:LYS:HD2	7:T:84:LYS:N	1.97	0.73
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.18	0.73
7:T:5:LYS:CD	28:T:263:PEK:C38	2.67	0.72
3:C:25:LEU:O	3:C:29:SER:HB2	1.90	0.72
10:W:33:ARG:HG2	23:W:1060:CHD:C15	2.18	0.72
3:P:55:TYR:CE1	26:P:1270:CDL:H521	2.25	0.72
6:F:94:HIS:CE1	29:F:4660:HOH:O	2.42	0.71
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.55	0.71
6:S:94:HIS:CD2	6:S:95:GLN:H	2.07	0.71
2:B:41:ILE:HD13	22:B:230:PSC:H341	1.71	0.71
7:G:45:PRO:HD2	29:G:4665:HOH:O	1.90	0.71
6:S:52:ILE:O	6:S:94:HIS:HE1	1.70	0.71
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.31	0.71
26:T:1269:CDL:H571	26:T:1269:CDL:H782	1.72	0.71
4:Q:78:TRP:HA	19:Q:1523:TGL:HB22	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:1270:CDL:OB9	26:P:1270:CDL:H522	1.92	0.70
19:N:1522:TGL:H231	19:N:1522:TGL:CA9	2.11	0.70
7:T:5:LYS:HB2	28:T:263:PEK:H362	1.74	0.70
28:G:265:PEK:C38	26:G:269:CDL:H272	2.11	0.70
2:O:82:ARG:NH1	2:O:86:MET:HE1	2.07	0.69
28:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.38	0.69
19:Q:1523:TGL:HG11	19:Q:1523:TGL:CC2	2.22	0.69
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.75	0.69
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.57	0.69
6:S:22:LEU:O	6:S:25:ARG:HB3	1.92	0.68
28:G:264:PEK:H101	28:G:264:PEK:H161	1.76	0.68
28:G:265:PEK:C38	26:G:269:CDL:H273	2.22	0.68
12:L:12:PRO:HB2	19:L:522:TGL:HG2	1.75	0.68
2:B:164:ALA:O	2:B:194:GLY:HA3	1.94	0.68
28:P:1265:PEK:C38	26:T:1269:CDL:H273	2.24	0.68
1:N:365:ILE:HD11	29:N:4837:HOH:O	1.94	0.68
2:B:82:ARG:HG2	2:B:86:MET:HE3	1.74	0.68
4:D:34:SER:H	4:D:37:GLN:NE2	1.92	0.67
2:B:58:ALA:O	2:B:62:GLU:HG3	1.94	0.67
6:S:85:CYS:SG	6:S:87:THR:HG23	2.35	0.67
3:C:224:LYS:HE3	26:C:270:CDL:HB31	1.76	0.67
13:Z:42:LYS:HE3	13:Z:42:LYS:HA	1.76	0.67
9:V:61:GLU:HG3	9:V:64:ARG:HH21	1.60	0.66
1:N:468:MET:HE1	18:N:515:HEA:H212	1.77	0.66
7:T:5:LYS:CD	28:T:263:PEK:H381	2.25	0.66
6:F:94:HIS:HE1	29:F:4660:HOH:O	1.76	0.65
1:N:172:LYS:NZ	1:N:178:GLN:HE22	1.95	0.65
3:P:246:ASP:HB2	29:P:4199:HOH:O	1.96	0.65
4:D:78:TRP:HB3	19:D:523:TGL:CB2	2.23	0.65
18:N:515:HEA:HBC1	18:N:515:HEA:HMC3	1.79	0.65
7:T:72:ASN:H	7:T:76:ASN:ND2	1.94	0.65
26:G:269:CDL:H241	26:G:269:CDL:C54	2.27	0.64
7:T:5:LYS:CG	28:T:263:PEK:C38	2.75	0.64
7:G:3:ALA:O	7:G:4:ALA:HB2	1.97	0.64
26:T:1269:CDL:HA21	26:T:1269:CDL:C11	2.27	0.64
26:T:1269:CDL:HA21	26:T:1269:CDL:H111	1.78	0.64
29:B:2351:HOH:O	19:D:523:TGL:HC61	1.98	0.64
19:L:522:TGL:CA9	19:L:522:TGL:H231	2.27	0.64
2:O:141:ARG:H	9:V:70:GLN:HE22	1.46	0.64
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.30	0.64
7:T:17:ARG:HD3	29:T:3300:HOH:O	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:269:CDL:HA21	26:G:269:CDL:C11	2.15	0.64
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.79	0.63
18:N:515:HEA:HBC1	18:N:515:HEA:CMC	2.29	0.63
3:P:174:THR:CG2	3:P:174:THR:CA	2.70	0.63
4:Q:70:GLU:O	4:Q:73:ARG:HG2	1.98	0.63
6:S:64:GLU:O	6:S:65:ASP:HB2	1.97	0.63
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.62	0.63
7:G:37:LEU:HD21	26:G:269:CDL:H352	1.81	0.63
26:G:269:CDL:H541	26:G:269:CDL:C24	2.29	0.62
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.64	0.62
2:O:116:LEU:HD12	2:O:117:SER:N	2.15	0.62
1:A:310:MET:HE1	2:B:76:ILE:HG21	1.80	0.62
20:C:267:PGV:H172	26:C:270:CDL:H652	1.81	0.62
7:G:17:ARG:HD2	29:G:2300:HOH:O	1.98	0.62
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.88	0.62
1:A:468:MET:HE1	18:A:515:HEA:H212	1.81	0.62
2:B:68:LEU:HG	29:B:4723:HOH:O	1.99	0.61
7:T:17:ARG:CD	29:T:3300:HOH:O	2.47	0.61
7:G:3:ALA:O	7:G:4:ALA:CB	2.48	0.61
3:C:5:THR:HG22	6:F:96:LEU:HD13	1.81	0.61
24:C:272:DMU:H29	24:C:272:DMU:O1	2.01	0.61
1:N:177:SER:H	1:N:180:GLN:NE2	1.98	0.61
3:C:3:HIS:HE1	6:F:96:LEU:CD2	2.14	0.61
2:B:59:GLN:C	2:B:60:GLU:HG3	2.26	0.61
20:N:1524:PGV:H22	20:N:1524:PGV:H011	1.83	0.60
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.49	0.60
2:B:62:GLU:O	2:B:66:THR:HB	2.01	0.60
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.83	0.60
19:Q:1523:TGL:H242	19:Q:1523:TGL:HA91	1.84	0.60
1:A:21:LEU:HD23	19:L:522:TGL:H211	1.83	0.60
1:A:278:MET:SD	7:T:5:LYS:HB3	2.42	0.60
18:N:515:HEA:C16	18:N:515:HEA:H272	2.32	0.60
6:S:94:HIS:CD2	6:S:95:GLN:N	2.70	0.60
20:N:1524:PGV:H011	20:N:1524:PGV:C2	2.32	0.59
7:T:5:LYS:HB2	28:T:263:PEK:C36	2.32	0.59
1:N:177:SER:H	1:N:180:GLN:HE21	1.50	0.59
7:G:31:CYS:SG	26:G:269:CDL:H532	2.42	0.59
2:B:59:GLN:O	2:B:60:GLU:HG3	2.03	0.59
7:G:37:LEU:HD23	7:G:38:HIS:ND1	2.17	0.59
20:A:524:PGV:H232	20:A:524:PGV:H31	1.83	0.59
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:269:CDL:H201	1:N:311:ILE:CD1	2.32	0.59
1:A:75:ILE:CD1	1:A:75:ILE:CB	2.76	0.59
19:L:522:TGL:H231	19:L:522:TGL:HA92	1.83	0.59
9:V:55:ASP:OD2	9:V:58:LYS:HB2	2.03	0.59
2:B:41:ILE:HD13	22:B:230:PSC:H342	1.85	0.58
23:C:525:CHD:H42	3:P:127:LEU:HD21	1.84	0.58
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.01	0.58
18:N:516:HEA:HBC1	18:N:516:HEA:HMC3	1.86	0.58
7:G:72:ASN:H	7:G:76:ASN:ND2	2.00	0.58
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.04	0.58
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.39	0.58
26:G:269:CDL:H473	29:G:4638:HOH:O	2.03	0.57
22:O:1230:PSC:H212	22:O:1230:PSC:C02	2.34	0.57
7:T:31:CYS:SG	26:T:1269:CDL:C55	2.90	0.57
4:D:107:ILE:HB	4:D:108:PRO:CD	2.35	0.57
7:T:38:HIS:HE2	26:T:1269:CDL:H111	1.69	0.57
3:P:226:HIS:HE1	26:P:1270:CDL:HB32	1.70	0.56
22:O:1230:PSC:H071	9:V:10:ARG:HH21	1.69	0.56
28:P:1265:PEK:C38	26:T:1269:CDL:H271	2.15	0.56
10:W:52:TRP:O	10:W:57:HIS:HE1	1.88	0.56
1:A:28:MET:CE	18:A:515:HEA:H271	2.36	0.56
1:A:310:MET:HE2	1:A:356:ILE:CG2	2.36	0.56
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.71	0.56
6:S:19:GLU:HG2	29:S:4904:HOH:O	2.06	0.56
7:T:84:LYS:CD	7:T:84:LYS:N	2.64	0.56
19:D:523:TGL:H242	19:D:523:TGL:HA91	1.87	0.55
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.71	0.55
2:B:56:MET:HA	22:B:230:PSC:H202	1.87	0.55
18:N:515:HEA:HHC	18:N:515:HEA:H122	1.87	0.55
3:C:67:PHE:CE1	26:C:270:CDL:H1	2.31	0.55
24:C:272:DMU:H40	7:G:63:GLY:H	1.70	0.55
4:D:78:TRP:N	19:D:523:TGL:HB21	2.21	0.55
22:B:230:PSC:H212	22:B:230:PSC:O01	2.06	0.55
12:Y:35:ALA:O	12:Y:39:ILE:HG13	2.07	0.55
1:A:172:LYS:HZ2	1:A:178:GLN:HE22	1.54	0.55
1:A:514:LYS:HE3	29:A:2385:HOH:O	2.06	0.55
8:H:45:ALA:O	8:H:47:GLY:N	2.34	0.55
3:P:58:TRP:CG	20:P:1267:PGV:H41	2.42	0.54
7:G:21:PHE:CD2	28:G:265:PEK:H222	2.42	0.54
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.20	0.54
4:D:118:LYS:HB3	11:K:53:TRP:HB3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:1522:TGL:HC62	19:N:1522:TGL:HC22	1.89	0.54
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.73	0.54
1:N:488:THR:HB	1:N:495:LEU:HD13	1.90	0.54
19:A:521:TGL:C36	29:A:4497:HOH:O	2.56	0.54
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.90	0.53
26:G:269:CDL:OA7	26:G:269:CDL:H342	2.08	0.53
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.06	0.53
4:D:78:TRP:CA	19:D:523:TGL:HB21	2.38	0.53
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.73	0.53
4:Q:78:TRP:CA	19:Q:1523:TGL:HB22	2.39	0.53
3:C:54:MET:HE1	20:C:267:PGV:H131	1.91	0.53
3:P:210:ILE:HG23	20:P:1267:PGV:H102	1.90	0.53
6:F:64:GLU:O	6:F:65:ASP:HB2	2.07	0.53
3:C:3:HIS:HB2	29:C:4631:HOH:O	2.09	0.53
4:D:68:PHE:HA	4:D:71:MET:HE3	1.91	0.53
20:A:522:PGV:H171	28:G:264:PEK:H352	1.89	0.53
3:P:34:TRP:HE1	24:P:1272:DMU:H29	1.74	0.53
7:T:2:SER:O	28:T:263:PEK:H332	2.09	0.53
1:A:407:ASP:O	1:A:411:LYS:HG3	2.10	0.52
20:P:1267:PGV:H172	26:P:1270:CDL:H662	1.91	0.52
5:R:7:THR:OG1	5:R:10:GLU:HG3	2.08	0.52
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.43	0.52
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.92	0.52
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.73	0.52
3:P:226:HIS:CE1	26:P:1270:CDL:HB32	2.45	0.52
7:T:5:LYS:HB2	28:T:263:PEK:C37	2.39	0.52
5:E:46:LYS:NZ	29:E:4705:HOH:O	2.42	0.52
19:N:1522:TGL:HC62	19:N:1522:TGL:CC2	2.40	0.52
18:N:515:HEA:C16	18:N:515:HEA:C27	2.88	0.51
26:P:1270:CDL:H672	26:P:1270:CDL:H262	1.91	0.51
26:G:269:CDL:H201	1:N:311:ILE:HD12	1.92	0.51
12:L:14:SER:H	19:L:522:TGL:HC31	1.74	0.51
19:A:521:TGL:H361	29:A:4497:HOH:O	2.10	0.51
26:C:270:CDL:H121	26:C:270:CDL:H711	1.91	0.51
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.91	0.51
1:N:76:GLY:O	1:N:80:ASN:HB2	2.09	0.51
2:B:68:LEU:HB2	2:B:69:PRO:HD3	1.92	0.51
5:R:80:GLU:H	5:R:80:GLU:CD	2.18	0.51
7:T:3:ALA:O	7:T:4:ALA:HB2	2.10	0.51
1:A:290:HIS:HD2	1:A:291:HIS:CD2	2.28	0.51
1:A:449:MET:SD	2:B:5:MET:HG2	2.50	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:7:GLU:HG3	29:J:4578:HOH:O	2.11	0.51
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.75	0.51
29:B:2351:HOH:O	19:D:523:TGL:CC6	2.55	0.51
1:N:449:MET:SD	2:O:5:MET:HG2	2.50	0.51
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.93	0.50
19:N:1522:TGL:HA22	12:Y:13:PHE:HB3	1.93	0.50
11:X:7:PRO:O	11:X:12:LYS:HE3	2.10	0.50
1:N:362:SER:HA	2:O:87:MET:HE1	1.94	0.50
19:N:1522:TGL:H162	12:Y:24:MET:HE1	1.93	0.50
10:W:30:ILE:O	10:W:34:VAL:HG23	2.11	0.50
22:B:230:PSC:H343	22:B:230:PSC:C13	2.41	0.50
1:A:28:MET:HE2	18:A:515:HEA:H271	1.92	0.50
19:N:1521:TGL:H142	2:O:39:LEU:HD23	1.94	0.50
3:P:155:ASP:OD1	3:P:155:ASP:C	2.54	0.50
8:U:78:GLU:HG2	8:U:80:THR:HG23	1.93	0.50
12:Y:2:HIS:N	29:Y:4284:HOH:O	2.45	0.50
19:N:1521:TGL:HA52	2:O:32:PHE:CE2	2.46	0.50
10:W:16:ASN:OD1	10:W:23:LYS:HE3	2.11	0.50
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.47	0.50
1:N:513:LEU:O	1:N:514:LYS:HB2	2.12	0.50
20:N:1524:PGV:H061	20:N:1524:PGV:O11	2.12	0.49
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.59	0.49
12:Y:14:SER:O	12:Y:20:ARG:NH2	2.44	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.13	0.49
2:O:41:ILE:O	2:O:45:MET:HG2	2.12	0.49
20:A:524:PGV:H301	20:A:524:PGV:H141	1.94	0.49
19:N:1521:TGL:HC72	29:Q:4417:HOH:O	2.11	0.49
7:T:7:ASP:O	7:T:9:GLY:N	2.46	0.49
19:L:522:TGL:HA92	19:L:522:TGL:C23	2.43	0.49
22:O:1230:PSC:H21	22:O:1230:PSC:H222	1.94	0.49
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.21	0.49
10:J:37:THR:OG1	23:J:60:CHD:H7	2.12	0.49
19:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.95	0.49
19:D:523:TGL:H351	9:I:16:ARG:HH21	1.77	0.49
7:G:38:HIS:CE1	26:G:269:CDL:H111	2.48	0.49
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.12	0.49
3:P:47:LEU:O	3:P:51:MET:HG2	2.13	0.49
23:O:229:CHD:H12	23:O:229:CHD:H212	1.94	0.49
4:Q:130:PRO:HA	4:Q:135:SER:HB2	1.95	0.49
26:T:1269:CDL:OB4	26:T:1269:CDL:H1	2.13	0.49
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:272:DMU:H1	7:G:69:PHE:HZ	1.78	0.48
7:G:30:LEU:HB3	26:G:269:CDL:H531	1.94	0.48
7:T:17:ARG:HD2	29:T:3300:HOH:O	2.12	0.48
12:L:24:MET:SD	19:L:522:TGL:H161	2.54	0.48
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.14	0.48
2:O:82:ARG:HH11	2:O:86:MET:CE	2.22	0.48
2:O:84:LEU:HA	2:O:87:MET:HE2	1.96	0.48
10:W:33:ARG:HG2	23:W:1060:CHD:H151	1.95	0.48
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.96	0.48
26:G:269:CDL:H401	2:O:77:ALA:CB	2.44	0.48
26:C:270:CDL:H831	26:C:270:CDL:H861	1.50	0.48
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.46	0.48
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.44	0.48
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.45	0.48
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.49	0.48
26:G:269:CDL:H371	2:O:81:LEU:HD12	1.96	0.48
8:H:60:TYR:CD1	8:H:60:TYR:C	2.91	0.48
2:O:82:ARG:CG	2:O:86:MET:HE3	2.31	0.48
1:A:38:ARG:HD2	18:A:515:HEA:OMA	2.13	0.48
1:A:311:ILE:HD12	26:T:1269:CDL:H191	1.95	0.48
22:B:230:PSC:H071	5:E:8:ASP:HA	1.96	0.48
18:N:515:HEA:H122	18:N:515:HEA:H262	1.94	0.48
2:O:59:GLN:O	2:O:59:GLN:HG3	2.13	0.48
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.96	0.47
1:N:514:LYS:HE2	29:S:3330:HOH:O	2.13	0.47
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.49	0.47
7:G:10:GLY:HA3	29:G:4761:HOH:O	2.14	0.47
28:G:264:PEK:H161	28:G:264:PEK:C10	2.43	0.47
6:S:53:THR:HG22	6:S:54:ASN:H	1.78	0.47
23:W:1060:CHD:H112	23:W:1060:CHD:H12A	1.63	0.47
1:A:346:PHE:HZ	19:A:521:TGL:H122	1.79	0.47
6:F:55:LYS:HA	6:F:74:LEU:O	2.14	0.47
1:N:377:PHE:CE2	1:N:378:HIS:CE1	3.02	0.47
22:B:230:PSC:H073	5:E:11:PHE:CG	2.50	0.47
24:P:1272:DMU:H25	28:P:1264:PEK:H341	1.97	0.47
8:H:46:LYS:CE	29:H:4804:HOH:O	2.62	0.47
1:N:240:HIS:O	1:N:241:PRO:C	2.58	0.47
3:C:47:LEU:O	3:C:51:MET:HG2	2.15	0.47
19:N:1522:TGL:H251	19:N:1522:TGL:H282	1.54	0.47
2:O:62:GLU:O	2:O:66:THR:HB	2.15	0.47
2:O:100:MET:HB2	2:O:107:SER:OG	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:1270:CDL:H561	26:P:1270:CDL:H532	1.77	0.47
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.42	0.47
7:T:5:LYS:CD	28:T:263:PEK:H383	2.35	0.47
1:A:37:ILE:HG21	18:A:515:HEA:CMA	2.44	0.47
1:A:335:SER:HB2	1:A:336:PRO:HD2	1.97	0.47
20:A:524:PGV:H262	20:A:524:PGV:H71	1.97	0.47
20:C:268:PGV:H062	29:C:4909:HOH:O	2.15	0.47
4:D:12:ALA:CB	6:F:55:LYS:HE3	2.45	0.47
28:G:1263:PEK:H331	28:G:1263:PEK:H372	1.96	0.47
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.38	0.47
26:T:1269:CDL:H761	26:T:1269:CDL:H242	1.97	0.47
3:C:3:HIS:CE1	6:F:96:LEU:CD2	2.97	0.46
20:N:1266:PGV:H181	28:P:1264:PEK:H321	1.96	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.14	0.46
7:T:5:LYS:CB	28:T:263:PEK:H383	2.44	0.46
26:G:269:CDL:H332	2:O:78:LEU:HD12	1.97	0.46
2:O:37:LEU:O	2:O:41:ILE:HG13	2.15	0.46
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.29	0.46
23:B:1086:CHD:H112	23:B:1086:CHD:H12A	1.59	0.46
3:C:52:LEU:HD23	26:C:270:CDL:H362	1.97	0.46
1:A:87:ILE:O	1:A:173:PRO:HD3	2.16	0.46
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.46
19:D:523:TGL:H122	19:D:523:TGL:HB81	1.97	0.46
26:G:269:CDL:H511	26:G:269:CDL:H181	1.97	0.46
20:P:1268:PGV:H51	20:P:1268:PGV:H21	1.71	0.46
1:A:264:LYS:NZ	29:A:4192:HOH:O	2.48	0.46
8:H:45:ALA:C	8:H:47:GLY:H	2.23	0.46
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.96	0.46
3:C:202:GLY:HA3	28:G:264:PEK:H21	1.98	0.46
26:C:270:CDL:H382	26:C:270:CDL:H412	1.60	0.46
4:D:78:TRP:CA	19:D:523:TGL:CB2	2.93	0.46
1:N:28:MET:CE	18:N:515:HEA:H271	2.45	0.46
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.50	0.46
12:L:45:LEU:HD23	12:L:45:LEU:HA	1.77	0.46
2:B:68:LEU:CB	2:B:69:PRO:HD3	2.46	0.46
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.45	0.46
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.03	0.46
2:O:98:LYS:HB2	2:O:109:GLU:HB2	1.97	0.46
28:P:1264:PEK:H383	28:P:1264:PEK:H352	1.37	0.46
26:P:1270:CDL:H822	26:P:1270:CDL:H852	1.64	0.46
7:T:8:HIS:CD2	28:T:263:PEK:H232	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:264:PEK:H32	28:G:264:PEK:C7	2.46	0.46
1:N:87:ILE:O	1:N:173:PRO:HD3	2.16	0.46
6:S:94:HIS:HD2	6:S:95:GLN:H	1.58	0.46
7:G:8:HIS:ND1	28:G:1263:PEK:H312	2.30	0.46
23:J:60:CHD:H112	23:J:60:CHD:H12A	1.61	0.46
6:S:94:HIS:HA	29:S:4898:HOH:O	2.16	0.46
28:T:263:PEK:H332	28:T:263:PEK:H361	1.68	0.46
1:A:396:TRP:O	1:A:397:PHE:C	2.58	0.45
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.31	0.45
10:J:27:THR:O	10:J:27:THR:HG22	2.16	0.45
12:L:11:ILE:CG2	19:L:522:TGL:H272	2.46	0.45
1:A:218:THR:O	1:A:226:GLY:HA3	2.16	0.45
22:B:230:PSC:H073	5:E:11:PHE:CB	2.46	0.45
20:P:1268:PGV:H062	29:P:4599:HOH:O	2.15	0.45
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.44	0.45
2:B:41:ILE:CD1	22:B:230:PSC:H341	2.43	0.45
3:C:224:LYS:CD	26:C:270:CDL:HB32	2.46	0.45
4:D:98:TRP:CE2	24:M:526:DMU:H9	2.51	0.45
1:N:409:TRP:CE2	20:N:1524:PGV:H61	2.52	0.45
22:O:1230:PSC:O01	22:O:1230:PSC:C21	2.47	0.45
22:O:1230:PSC:C07	9:V:10:ARG:NH2	2.68	0.45
12:Y:22:LEU:O	12:Y:26:THR:HB	2.16	0.45
8:H:44:THR:O	8:H:45:ALA:O	2.35	0.45
1:A:172:LYS:NZ	1:A:178:GLN:NE2	2.64	0.45
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.52	0.45
1:A:177:SER:H	1:A:180:GLN:HE21	1.63	0.45
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.45
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.52	0.45
6:F:94:HIS:HB3	6:F:95:GLN:NE2	2.32	0.45
19:L:522:TGL:H252	19:L:522:TGL:H283	1.62	0.45
1:N:378:HIS:CG	1:N:425:PHE:CE2	3.05	0.45
2:O:162:SER:HB3	2:O:197:SER:C	2.42	0.45
5:R:63:SER:O	5:R:67:ILE:HG13	2.17	0.45
26:P:1270:CDL:H791	26:P:1270:CDL:H231	1.99	0.45
9:V:61:GLU:CG	9:V:64:ARG:HH21	2.26	0.45
19:N:1521:TGL:HA52	2:O:32:PHE:HE2	1.82	0.45
13:Z:32:TRP:N	24:Z:1526:DMU:H1	2.32	0.45
22:B:230:PSC:H212	22:B:230:PSC:C1	2.47	0.45
3:C:34:TRP:CD1	3:C:40:MET:HG3	2.52	0.45
7:G:8:HIS:CE1	28:G:1263:PEK:H342	2.52	0.45
1:N:383:MET:HG2	1:N:421:VAL:HG21	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:31:VAL:O	2:O:35:SER:OG	2.34	0.45
6:S:94:HIS:CG	6:S:95:GLN:H	2.27	0.45
23:C:271:CHD:H212	23:C:271:CHD:H12	1.99	0.44
7:G:17:ARG:CD	29:G:2300:HOH:O	2.63	0.44
2:O:217:LYS:HE2	2:O:220:GLU:OE2	2.16	0.44
2:B:52:HIS:CE1	22:B:230:PSC:H211	2.52	0.44
7:G:12:GLY:HA3	29:G:2267:HOH:O	2.16	0.44
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.41	0.44
1:A:334:TRP:HB2	19:D:523:TGL:HG11	2.00	0.44
9:I:54:TYR:OH	9:I:59:ASP:OD1	2.27	0.44
20:P:1267:PGV:H12	20:P:1267:PGV:H152	1.44	0.44
8:U:37:HIS:HD2	29:U:3142:HOH:O	2.00	0.44
1:A:71:MET:N	1:A:72:PRO:CD	2.81	0.44
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.52	0.44
20:A:522:PGV:H261	20:C:267:PGV:H292	1.98	0.44
22:B:230:PSC:H071	9:I:10:ARG:NH2	2.31	0.44
4:D:78:TRP:HA	19:D:523:TGL:HB21	2.00	0.44
10:J:52:TRP:O	10:J:57:HIS:HE1	2.01	0.44
1:N:312:ILE:HG21	1:N:312:ILE:HD13	1.61	0.44
19:A:521:TGL:HA82	19:A:521:TGL:H222	2.00	0.44
13:M:17:ILE:O	13:M:21:VAL:HG23	2.16	0.44
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.98	0.44
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.18	0.44
8:U:60:TYR:CD1	8:U:60:TYR:C	2.96	0.44
2:B:65:TRP:CZ3	22:B:230:PSC:H322	2.53	0.44
19:N:1522:TGL:HC62	19:N:1522:TGL:HC32	1.79	0.44
2:O:59:GLN:O	2:O:59:GLN:CG	2.65	0.44
7:T:12:GLY:HA3	29:T:3267:HOH:O	2.17	0.44
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.82	0.44
19:D:523:TGL:HA32	19:D:523:TGL:HB42	2.00	0.44
1:A:87:ILE:HG13	1:A:89:ALA:HB2	1.99	0.44
3:C:179:SER:O	3:C:183:GLU:HG2	2.17	0.44
12:L:25:MET:HG2	19:L:522:TGL:HA62	2.00	0.44
19:N:1522:TGL:HC31	12:Y:14:SER:H	1.82	0.44
4:Q:16:TYR:CE1	4:Q:25:PRO:HG2	2.52	0.44
4:Q:109:HIS:CD2	29:Q:3152:HOH:O	2.49	0.44
20:A:524:PGV:H232	20:A:524:PGV:H202	1.79	0.43
26:C:270:CDL:PA1	26:C:270:CDL:HB22	2.57	0.43
2:O:102:HIS:O	2:O:104:TRP:HA	2.17	0.43
6:S:94:HIS:HD2	6:S:95:GLN:N	2.12	0.43
6:F:55:LYS:HG3	6:F:73:TRP:CZ3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:73:LYS:HA	9:I:73:LYS:HD2	1.73	0.43
23:P:1525:CHD:H12	23:P:1525:CHD:H212	2.01	0.43
28:P:1264:PEK:H231	28:P:1264:PEK:H262	1.80	0.43
26:T:1269:CDL:H562	26:T:1269:CDL:H762	1.99	0.43
26:T:1269:CDL:H591	26:T:1269:CDL:H561	1.75	0.43
3:C:210:ILE:HD13	20:C:267:PGV:H301	2.00	0.43
3:C:210:ILE:HG12	20:C:267:PGV:H12	2.00	0.43
1:N:508:PRO:HG3	3:P:6:HIS:HB3	2.00	0.43
7:T:8:HIS:ND1	28:T:263:PEK:H321	2.33	0.43
12:Y:41:ARG:HH11	12:Y:41:ARG:HG2	1.82	0.43
13:Z:36:HIS:O	13:Z:39:ASN:HB2	2.18	0.43
19:A:521:TGL:H241	19:A:521:TGL:HA91	1.99	0.43
3:C:159:MET:SD	3:C:159:MET:C	3.01	0.43
23:P:1525:CHD:H152	20:P:1268:PGV:H92	2.01	0.43
9:V:29:LEU:HA	9:V:29:LEU:HD12	1.54	0.43
24:C:272:DMU:H29	24:C:272:DMU:C10	2.49	0.43
1:N:155:VAL:CG2	28:P:1264:PEK:H381	2.48	0.43
4:Q:91:PHE:O	4:Q:94:LEU:HB2	2.18	0.43
8:U:57:ARG:O	8:U:61:LYS:HG3	2.18	0.43
13:Z:31:GLY:C	24:Z:1526:DMU:H1	2.44	0.43
1:N:199:LEU:N	1:N:200:PRO:CD	2.82	0.43
28:P:1265:PEK:H383	26:T:1269:CDL:H272	1.80	0.43
2:B:13:THR:O	2:B:13:THR:HG22	2.19	0.43
3:P:224:LYS:HD3	26:P:1270:CDL:HB31	2.01	0.43
2:B:200:CYS:SG	2:B:204:HIS:HA	2.59	0.43
22:O:1230:PSC:H201	22:O:1230:PSC:H231	1.70	0.43
23:P:1525:CHD:H112	23:P:1525:CHD:H12A	1.74	0.43
28:T:263:PEK:H241	28:T:263:PEK:H271	1.84	0.43
23:C:525:CHD:H112	23:C:525:CHD:H12A	1.72	0.43
19:N:1521:TGL:H101	19:N:1521:TGL:C28	2.49	0.43
26:T:1269:CDL:H221	26:T:1269:CDL:H252	1.48	0.43
26:T:1269:CDL:H342	26:T:1269:CDL:OA7	2.19	0.43
7:G:4:ALA:CB	1:N:282:PHE:HA	2.43	0.43
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.01	0.42
1:N:310:MET:HE1	2:O:76:ILE:CG2	2.49	0.42
3:P:29:SER:HB3	3:P:42:LEU:HD13	2.01	0.42
7:T:8:HIS:HB2	28:T:263:PEK:H282	2.01	0.42
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.18	0.42
1:A:112:LEU:HG	29:A:4496:HOH:O	2.19	0.42
1:A:169:ILE:HG23	7:T:9:GLY:HA3	2.01	0.42
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:224:ALA:C	2:O:226:MET:H	2.27	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.42
26:G:269:CDL:H661	26:G:269:CDL:H631	1.64	0.42
5:R:81:ILE:HG12	9:V:7:PRO:HG2	2.01	0.42
28:P:1265:PEK:H282	28:P:1265:PEK:H311	1.91	0.42
10:J:40:LEU:HD12	23:J:60:CHD:H183	2.01	0.42
1:N:172:LYS:NZ	1:N:178:GLN:NE2	2.63	0.42
19:N:1521:TGL:H211	19:N:1521:TGL:H241	1.78	0.42
2:B:189:PRO:HD2	9:I:54:TYR:OH	2.19	0.42
1:N:430:PHE:HE1	19:N:1521:TGL:HB21	1.83	0.42
3:P:12:ASN:O	3:P:13:PRO:C	2.62	0.42
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.19	0.42
1:A:250:GLY:O	1:A:254:ILE:HG12	2.20	0.42
1:A:486:ASP:OD2	4:D:19:ARG:CD	2.51	0.42
1:A:22:PHE:HA	19:L:522:TGL:HB71	2.02	0.42
3:C:19:THR:O	3:C:23:SER:HB3	2.20	0.42
1:N:426:PHE:HB3	1:N:427:PRO:HD3	2.02	0.42
19:A:521:TGL:H292	19:A:521:TGL:H121	1.26	0.42
4:Q:43:LYS:NZ	4:Q:55:GLU:OE1	2.42	0.42
12:Y:41:ARG:HG2	12:Y:41:ARG:NH1	2.34	0.42
1:A:381:LEU:CD2	18:A:516:HEA:HBC2	2.50	0.41
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.02	0.41
1:A:514:LYS:HG3	6:F:38:ALA:HB2	2.02	0.41
19:N:1522:TGL:H352	29:N:4536:HOH:O	2.19	0.41
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.02	0.41
18:A:515:HEA:H261	18:A:515:HEA:H172	1.78	0.41
2:B:184:LEU:C	2:B:184:LEU:HD23	2.45	0.41
1:N:236:TRP:HA	1:N:236:TRP:CE3	2.55	0.41
3:P:40:MET:O	3:P:44:MET:HG2	2.20	0.41
3:P:171:VAL:HG22	26:P:1270:CDL:H841	2.02	0.41
11:X:16:ALA:O	11:X:20:SER:HB2	2.20	0.41
2:B:64:ILE:HD13	2:B:64:ILE:HA	1.95	0.41
26:C:270:CDL:H231	26:C:270:CDL:H642	2.02	0.41
8:H:43:MET:HE1	8:U:43:MET:HE1	2.02	0.41
7:T:25:LEU:HD23	7:T:25:LEU:HA	1.82	0.41
1:N:514:LYS:HA	6:S:38:ALA:HB3	2.03	0.41
23:O:229:CHD:H112	23:O:229:CHD:H12A	1.68	0.41
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.55	0.41
5:R:26:ALA:O	5:R:30:ARG:HG3	2.21	0.41
1:A:311:ILE:CD1	26:T:1269:CDL:H191	2.51	0.41
6:F:87:THR:HG21	29:F:4882:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:467:LEU:O	1:N:468:MET:C	2.62	0.41
3:P:50:ASN:ND2	3:P:54:MET:HE2	2.36	0.41
3:P:220:PHE:CB	26:P:1270:CDL:H712	2.51	0.41
1:A:314:ILE:HB	1:A:315:PRO:CD	2.51	0.41
1:A:513:LEU:HD13	1:A:513:LEU:O	2.21	0.41
2:B:121:TYR:O	2:B:138:VAL:HA	2.20	0.41
3:C:156:ARG:HE	23:C:271:CHD:C24	2.34	0.41
5:E:72:LYS:HB2	5:E:82:TYR:CD2	2.56	0.41
1:N:51:ASP:OD2	2:O:205:SER:OG	2.37	0.41
22:O:1230:PSC:H071	9:V:10:ARG:NH2	2.33	0.41
1:A:381:LEU:HD13	18:A:515:HEA:HAC	2.03	0.41
10:J:8:LYS:O	10:J:9:GLN:C	2.61	0.41
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.86	0.41
1:A:400:PHE:HB3	19:L:522:TGL:H283	2.03	0.41
1:A:409:TRP:HA	1:A:412:ILE:HD12	2.03	0.41
3:C:3:HIS:HE1	6:F:96:LEU:HD21	1.85	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.41
3:C:138:LEU:HD23	3:C:138:LEU:HA	1.84	0.41
19:D:523:TGL:HC21	19:D:523:TGL:HG12	2.03	0.41
7:G:12:GLY:CA	29:G:2267:HOH:O	2.69	0.41
3:P:116:TRP:HA	3:P:117:PRO:C	2.46	0.41
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.19	0.41
2:B:146:MET:HA	2:B:213:LEU:HD12	2.03	0.41
1:N:171:MET:HE3	3:P:8:TYR:CG	2.56	0.41
1:N:365:ILE:HD11	29:U:4796:HOH:O	2.19	0.41
5:R:105:GLY:O	5:R:108:LYS:HG2	2.20	0.41
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.95	0.40
2:O:139:ASP:OD2	2:O:140:ASN:N	2.53	0.40
3:P:127:LEU:HG	26:T:1269:CDL:OB3	2.20	0.40
3:P:224:LYS:CD	26:P:1270:CDL:HB31	2.51	0.40
23:P:1271:CHD:H162	23:P:1271:CHD:H232	2.03	0.40
5:R:74:LYS:HA	5:R:74:LYS:HD2	1.88	0.40
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.03	0.40
24:C:272:DMU:C11	7:G:63:GLY:H	2.34	0.40
4:D:19:ARG:NH1	4:D:21:ASP:OD2	2.54	0.40
28:P:1265:PEK:C37	26:T:1269:CDL:C27	2.99	0.40
4:Q:37:GLN:O	4:Q:41:LYS:HG2	2.22	0.40
8:U:38:ARG:HG2	8:U:85:ILE:HA	2.04	0.40
1:A:398:PRO:HA	1:A:403:TYR:O	2.20	0.40
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.03	0.40
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.03	0.40
3:C:106:LEU:HD21	3:C:259:TRP:CZ2	2.57	0.40
1:N:12:HIS:CE1	1:N:13:LYS:HG3	2.56	0.40
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.03	0.40
1:N:478:SER:O	13:Z:6:ALA:HB1	2.22	0.40
20:N:1524:PGV:H221	20:N:1524:PGV:H41	2.03	0.40
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.51	0.40
1:A:38:ARG:HD2	1:A:38:ARG:HH11	1.74	0.40
20:A:524:PGV:H151	4:D:87:PHE:CZ	2.57	0.40
9:I:43:ARG:HH11	9:I:43:ARG:HD3	1.61	0.40
1:N:127:THR:HG22	1:N:235:PHE:CE2	2.57	0.40
1:N:131:PRO:O	1:N:132:LEU:C	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	484 (94%)	28 (6%)	0	100	100
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	30	28
2	O	225/227 (99%)	211 (94%)	13 (6%)	1 (0%)	30	28
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	30	28
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	133 (94%)	8 (6%)	1 (1%)	18	15
5	E	102/109 (94%)	99 (97%)	3 (3%)	0	100	100
5	R	102/109 (94%)	101 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	91/98 (93%)	88 (97%)	1 (1%)	2 (2%)	5	2
6	S	91/98 (93%)	86 (94%)	3 (3%)	2 (2%)	5	2
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	0	0
7	T	81/85 (95%)	65 (80%)	10 (12%)	6 (7%)	1	0
8	H	73/85 (86%)	69 (94%)	2 (3%)	2 (3%)	4	1
8	U	73/85 (86%)	66 (90%)	4 (6%)	3 (4%)	2	0
9	I	69/73 (94%)	68 (99%)	1 (1%)	0	100	100
9	V	69/73 (94%)	67 (97%)	2 (3%)	0	100	100
10	J	55/59 (93%)	55 (100%)	0	0	100	100
10	W	55/59 (93%)	55 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	43 (92%)	4 (8%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3478/3614 (96%)	3316 (95%)	136 (4%)	26 (1%)	18	15

All (26) 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	39	SER
7	G	40	GLY
8	H	45	ALA
8	H	46	LYS
6	S	94	HIS
7	T	4	ALA
7	T	8	HIS
8	U	50	VAL
7	G	37	LEU
7	T	7	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	6	GLY
8	U	45	ALA
4	Q	34	SER
6	S	95	GLN
7	T	3	ALA
7	T	37	LEU
6	F	94	HIS
2	O	92	ASN
3	P	232	HIS
7	T	6	GLY
8	U	46	LYS

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%)	417 (98%)	9 (2%)	47	54
1	N	426/426 (100%)	410 (96%)	16 (4%)	29	32
2	B	210/210 (100%)	199 (95%)	11 (5%)	21	20
2	O	210/210 (100%)	194 (92%)	16 (8%)	12	9
3	C	224/226 (99%)	217 (97%)	7 (3%)	35	39
3	P	224/226 (99%)	221 (99%)	3 (1%)	61	69
4	D	128/129 (99%)	126 (98%)	2 (2%)	55	64
4	Q	128/129 (99%)	122 (95%)	6 (5%)	23	24
5	E	91/95 (96%)	88 (97%)	3 (3%)	33	37
5	R	91/95 (96%)	89 (98%)	2 (2%)	45	53
6	F	79/81 (98%)	73 (92%)	6 (8%)	12	9
6	S	79/81 (98%)	71 (90%)	8 (10%)	7	5
7	G	67/68 (98%)	60 (90%)	7 (10%)	7	4
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	6
8	H	67/75 (89%)	65 (97%)	2 (3%)	36	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	67/75 (89%)	60 (90%)	7 (10%)	7	4
9	I	56/57 (98%)	53 (95%)	3 (5%)	20	18
9	V	56/57 (98%)	51 (91%)	5 (9%)	9	6
10	J	48/50 (96%)	47 (98%)	1 (2%)	47	54
10	W	48/50 (96%)	46 (96%)	2 (4%)	26	28
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	46
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	21
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	21
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	9
13	M	37/38 (97%)	30 (81%)	7 (19%)	1	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	4
All	All	3022/3082 (98%)	2881 (95%)	141 (5%)	23	24

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	128	VAL
1	A	138	HIS
1	A	152	LEU
1	A	333	LYS
1	A	362	SER
1	A	363	LEU
1	A	369	ASP
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	61	VAL
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	94	SER
2	B	115	ASP
2	B	171	LYS
3	C	23	SER
3	C	29	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	40	MET
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	180	GLU
4	D	51	LEU
4	D	127	LYS
5	E	46	LYS
5	E	90	ARG
5	E	108	LYS
6	F	37	LYS
6	F	48	LEU
6	F	78	GLU
6	F	84	SER
6	F	87	THR
6	F	95	GLN
7	G	2	SER
7	G	5	LYS
7	G	17	ARG
7	G	33	LEU
7	G	37	LEU
7	G	74	ARG
7	G	84	LYS
8	H	50	VAL
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	61	GLU
10	J	50	LEU
11	K	20	SER
12	L	26	THR
12	L	46	LYS
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
13	M	43	SER
1	N	34	SER
1	N	117	MET
1	N	127	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	138	HIS
1	N	178	GLN
1	N	180	GLN
1	N	228	PRO
1	N	241	PRO
1	N	245	ILE
1	N	265	LYS
1	N	361	SER
1	N	363	LEU
1	N	369	ASP
1	N	484	THR
1	N	485	VAL
1	N	504	THR
2	O	33	LEU
2	O	35	SER
2	O	60	GLU
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	110	TYR
2	O	116	LEU
2	O	148	MET
2	O	167	SER
2	O	205	SER
2	O	217	LYS
2	O	221	LYS
2	O	225	SER
2	O	227	LEU
3	P	29	SER
3	P	127	LEU
3	P	230	ASN
4	Q	9	GLU
4	Q	31	LYS
4	Q	51	LEU
4	Q	121	LYS
4	Q	127	LYS
4	Q	143	ASN
5	R	31	LYS
5	R	80	GLU
6	S	20	VAL
6	S	37	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	S	48	LEU
6	S	53	THR
6	S	78	GLU
6	S	84	SER
6	S	94	HIS
6	S	95	GLN
7	T	2	SER
7	T	8	HIS
7	T	33	LEU
7	T	37	LEU
7	T	38	HIS
7	T	84	LYS
8	U	12	GLN
8	U	41	LYS
8	U	44	THR
8	U	46	LYS
8	U	50	VAL
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	61	GLU
9	V	65	LYS
9	V	73	LYS
10	W	4	ARG
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	14	SER
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	178	GLN
1	A	180	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	422	ASN
1	A	503	HIS
1	A	512	ASN
2	B	10	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	149	HIS
3	C	161	GLN
3	C	230	ASN
4	D	29	HIS
4	D	37	GLN
4	D	109	HIS
4	D	119	GLN
5	E	94	ASN
7	G	76	ASN
8	H	31	GLN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	170	ASN
1	N	178	GLN
1	N	180	GLN
1	N	406	ASN
1	N	422	ASN
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
3	P	161	GLN
3	P	243	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
5	R	78	HIS
5	R	94	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	T	8	HIS
7	T	76	ASN
8	U	28	ASN
8	U	32	ASN
9	V	70	GLN
10	W	29	ASN
10	W	57	HIS
11	X	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TPO	T	11	7	8,10,11	2.34	4 (50%)	10,14,16	1.54	3 (30%)
2	FME	O	1	2	8,9,10	1.09	0	8,9,11	6.03	6 (75%)
1	FME	N	1	1	8,9,10	0.76	0	8,9,11	4.64	3 (37%)
2	FME	B	1	2	8,9,10	1.96	3 (37%)	8,9,11	5.96	5 (62%)
1	FME	A	1	1	8,9,10	1.16	0	8,9,11	4.87	2 (25%)
7	TPO	G	11	7	8,10,11	2.24	4 (50%)	10,14,16	2.25	3 (30%)

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	3.86	1.62	1.50
7	T	11	TPO	P-O1P	3.57	1.61	1.50
7	T	11	TPO	P-OG1	3.42	1.65	1.59
2	B	1	FME	CA-N	3.16	1.51	1.46
2	B	1	FME	O1-CN	-2.94	1.10	1.22
7	G	11	TPO	O-C	2.66	1.30	1.20
7	T	11	TPO	P-O3P	2.65	1.64	1.54
7	T	11	TPO	O-C	2.53	1.29	1.20
7	G	11	TPO	P-OG1	2.45	1.63	1.59
2	B	1	FME	O-C	2.32	1.28	1.20
7	G	11	TPO	P-O2P	2.32	1.63	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CA-N-CN	-15.94	98.31	122.82
2	B	1	FME	CA-N-CN	-14.83	100.01	122.82
1	A	1	FME	CA-N-CN	-13.10	102.67	122.82
1	N	1	FME	CA-N-CN	-12.51	103.58	122.82
2	B	1	FME	C-CA-N	5.30	119.73	109.50
7	G	11	TPO	CG2-CB-CA	4.90	122.81	113.26
2	B	1	FME	CG-CB-CA	-4.76	98.30	112.87
7	G	11	TPO	O2P-P-OG1	3.84	120.81	105.85
2	O	1	FME	C-CA-N	3.56	116.37	109.50
7	T	11	TPO	CG2-CB-CA	3.00	119.11	113.26
2	B	1	FME	O1-CN-N	2.67	132.20	125.32
2	O	1	FME	CG-CB-CA	-2.63	104.82	112.87
7	G	11	TPO	OG1-P-O1P	-2.51	100.39	109.33
7	T	11	TPO	O3P-P-OG1	2.44	115.36	105.85
2	O	1	FME	CE-SD-CG	2.38	112.66	100.32
2	O	1	FME	O1-CN-N	-2.31	119.34	125.32
1	A	1	FME	CG-CB-CA	-2.22	106.09	112.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CB-CA-N	2.18	114.48	110.52
7	T	11	TPO	O-C-CA	-2.15	119.24	124.77
2	B	1	FME	O-C-CA	-2.12	119.32	124.77
1	N	1	FME	O1-CN-N	2.07	130.66	125.32
2	O	1	FME	CB-CA-N	-2.00	106.87	110.52

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-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
1	A	1	FME	CB-CG-SD-CE
1	N	1	FME	CA-CB-CG-SD
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
7	G	11	TPO	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHD	P	1525	-	32,32,32	1.37	5 (15%)	51,51,51	5.48	38 (74%)
19	TGL	A	521	-	62,62,62	1.50	7 (11%)	65,65,65	2.35	14 (21%)
19	TGL	D	523	-	62,62,62	1.65	7 (11%)	65,65,65	1.74	14 (21%)
19	TGL	L	522	-	62,62,62	1.54	7 (11%)	65,65,65	1.87	12 (18%)
20	PGV	C	267	-	50,50,50	0.97	3 (6%)	53,56,56	1.48	11 (20%)
20	PGV	N	1524	-	50,50,50	1.19	2 (4%)	53,56,56	1.27	7 (13%)
23	CHD	O	229	-	32,32,32	1.65	8 (25%)	51,51,51	5.81	31 (60%)
23	CHD	B	1086	-	32,32,32	1.86	9 (28%)	51,51,51	5.23	37 (72%)
28	PEK	G	264	-	52,52,52	0.93	2 (3%)	55,57,57	2.10	12 (21%)
22	PSC	O	1230	-	51,51,51	1.26	3 (5%)	57,59,59	1.29	6 (10%)
19	TGL	N	1522	-	62,62,62	1.55	6 (9%)	65,65,65	1.55	10 (15%)
15	PER	N	520	14,18	1,1,1	1.98	0	-	-	-
24	DMU	Z	1526	-	34,34,34	1.01	2 (5%)	45,45,45	3.27	25 (55%)
18	HEA	A	516	15,1	67,67,67	2.18	23 (34%)	81,103,103	2.46	28 (34%)
20	PGV	A	524	-	50,50,50	1.21	3 (6%)	53,56,56	1.44	8 (15%)
26	CDL	P	1270	-	99,99,99	1.46	13 (13%)	105,111,111	1.45	17 (16%)
28	PEK	P	1264	-	52,52,52	1.06	4 (7%)	55,57,57	1.62	8 (14%)
18	HEA	A	515	1	67,67,67	2.21	23 (34%)	81,103,103	2.82	37 (45%)
23	CHD	J	60	-	32,32,32	0.85	0	51,51,51	4.82	37 (72%)
20	PGV	P	1267	-	50,50,50	0.89	3 (6%)	53,56,56	1.51	11 (20%)
22	PSC	B	230	-	51,51,51	1.40	3 (5%)	57,59,59	1.25	4 (7%)
28	PEK	G	1263	-	52,52,52	1.19	2 (3%)	55,57,57	1.30	5 (9%)
18	HEA	N	515	1	67,67,67	1.99	17 (25%)	81,103,103	2.60	37 (45%)
23	CHD	C	271	-	32,32,32	0.93	2 (6%)	51,51,51	4.95	31 (60%)
18	HEA	N	516	15,1	67,67,67	1.95	24 (35%)	81,103,103	2.18	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	T	1269	-	99,99,99	1.43	12 (12%)	105,111,111	1.51	15 (14%)
24	DMU	M	526	-	34,34,34	0.89	1 (2%)	45,45,45	3.22	25 (55%)
21	CUA	O	228	2	0,1,1	-	-	-	-	-
26	CDL	C	270	-	99,99,99	1.52	13 (13%)	105,111,111	1.63	18 (17%)
23	CHD	P	1271	-	32,32,32	0.94	1 (3%)	51,51,51	5.11	35 (68%)
15	PER	A	520	14,18	1,1,1	1.97	0	-	-	-
24	DMU	C	272	-	34,34,34	1.23	1 (2%)	45,45,45	3.36	23 (51%)
28	PEK	T	263	-	52,52,52	1.32	3 (5%)	55,57,57	1.31	6 (10%)
23	CHD	W	1060	-	32,32,32	0.92	1 (3%)	51,51,51	4.88	36 (70%)
28	PEK	G	265	-	52,52,52	1.19	3 (5%)	55,57,57	1.11	4 (7%)
20	PGV	A	522	-	50,50,50	1.14	2 (4%)	53,56,56	1.41	8 (15%)
26	CDL	G	269	-	99,99,99	1.49	12 (12%)	105,111,111	1.32	13 (12%)
20	PGV	P	1268	-	50,50,50	1.23	2 (4%)	53,56,56	1.44	6 (11%)
21	CUA	B	228	2	0,1,1	-	-	-	-	-
20	PGV	N	1266	-	50,50,50	0.89	1 (2%)	53,56,56	1.66	11 (20%)
20	PGV	C	268	-	50,50,50	1.26	3 (6%)	53,56,56	1.43	5 (9%)
28	PEK	P	1265	-	52,52,52	1.23	2 (3%)	55,57,57	1.33	6 (10%)
24	DMU	P	1272	-	34,34,34	1.26	2 (5%)	45,45,45	3.14	23 (51%)
19	TGL	Q	1523	-	62,62,62	1.46	6 (9%)	65,65,65	1.40	10 (15%)
19	TGL	N	1521	-	62,62,62	1.39	6 (9%)	65,65,65	1.61	12 (18%)
23	CHD	C	525	-	32,32,32	1.71	7 (21%)	51,51,51	5.11	39 (76%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	P	1525	-	-	1/9/74/74	0/4/4/4
19	TGL	A	521	-	-	36/65/65/65	-
19	TGL	D	523	-	-	33/65/65/65	-
19	TGL	L	522	-	-	40/65/65/65	-
20	PGV	C	267	-	-	12/55/55/55	-
23	CHD	O	229	-	1/1/12/12	2/9/74/74	0/4/4/4
20	PGV	N	1524	-	-	30/55/55/55	-
23	CHD	B	1086	-	-	2/9/74/74	0/4/4/4
28	PEK	G	264	-	-	23/56/56/56	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSC	O	1230	-	-	31/55/55/55	-
19	TGL	N	1522	-	-	36/65/65/65	-
24	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
18	HEA	A	516	15,1	-	6/36/76/76	-
20	PGV	A	524	-	-	30/55/55/55	-
26	CDL	P	1270	-	-	65/110/110/110	-
28	PEK	P	1264	-	-	24/56/56/56	-
18	HEA	A	515	1	-	6/36/76/76	-
23	CHD	J	60	-	2/2/12/12	6/9/74/74	0/4/4/4
20	PGV	P	1267	-	-	13/55/55/55	-
22	PSC	B	230	-	-	30/55/55/55	-
28	PEK	G	1263	-	-	32/56/56/56	-
18	HEA	N	515	1	-	10/36/76/76	-
23	CHD	C	271	-	1/1/12/12	7/9/74/74	0/4/4/4
18	HEA	N	516	15,1	-	4/36/76/76	-
26	CDL	T	1269	-	-	60/110/110/110	-
24	DMU	M	526	-	5/5/10/10	9/19/59/59	0/2/2/2
26	CDL	C	270	-	-	64/110/110/110	-
23	CHD	P	1271	-	1/1/12/12	7/9/74/74	0/4/4/4
24	DMU	C	272	-	6/6/10/10	10/19/59/59	0/2/2/2
28	PEK	T	263	-	-	33/56/56/56	-
23	CHD	W	1060	-	2/2/12/12	7/9/74/74	0/4/4/4
28	PEK	G	265	-	-	24/56/56/56	-
20	PGV	A	522	-	-	20/55/55/55	-
26	CDL	G	269	-	-	55/110/110/110	-
20	PGV	P	1268	-	-	31/55/55/55	-
20	PGV	N	1266	-	-	14/55/55/55	-
20	PGV	C	268	-	-	33/55/55/55	-
28	PEK	P	1265	-	-	24/56/56/56	-
24	DMU	P	1272	-	5/5/10/10	11/19/59/59	0/2/2/2
19	TGL	Q	1523	-	-	35/65/65/65	-
19	TGL	N	1521	-	-	31/65/65/65	-
23	CHD	C	525	-	-	2/9/74/74	0/4/4/4

All (256) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	515	HEA	FE-NA	6.21	2.15	1.95
18	N	515	HEA	FE-NA	6.15	2.15	1.95
28	T	263	PEK	O03-C21	6.12	1.51	1.33
18	A	515	HEA	C3A-C4A	-6.01	1.35	1.46
19	N	1522	TGL	OG2-CB1	6.00	1.51	1.34
19	L	522	TGL	OG2-CB1	5.98	1.51	1.34
19	D	523	TGL	OG1-CA1	5.76	1.50	1.33
18	A	515	HEA	CHA-C1A	5.59	1.49	1.38
18	A	515	HEA	C1D-ND	-5.59	1.30	1.40
19	N	1521	TGL	OG2-CB1	5.55	1.50	1.34
20	A	522	PGV	O03-C19	5.54	1.49	1.33
20	C	268	PGV	O01-C1	5.51	1.49	1.34
19	A	521	TGL	OG1-CA1	5.50	1.49	1.33
28	T	263	PEK	O01-C1	5.48	1.49	1.34
22	B	230	PSC	O03-C19	5.46	1.49	1.33
18	A	516	HEA	FE-NC	5.46	2.13	1.95
20	N	1524	PGV	O03-C19	5.42	1.49	1.33
19	A	521	TGL	OG2-CB1	5.38	1.49	1.34
20	P	1268	PGV	O01-C1	5.37	1.49	1.34
19	D	523	TGL	OG2-CB1	5.37	1.49	1.34
19	Q	1523	TGL	OG3-CC1	5.32	1.48	1.33
19	Q	1523	TGL	OG2-CB1	5.30	1.49	1.34
26	C	270	CDL	OA8-CA7	5.29	1.48	1.33
20	A	524	PGV	O03-C19	5.25	1.48	1.33
22	B	230	PSC	O01-C1	5.21	1.49	1.34
19	L	522	TGL	OG1-CA1	5.20	1.48	1.33
28	G	1263	PEK	O03-C21	5.18	1.48	1.33
28	P	1265	PEK	O03-C21	5.16	1.48	1.33
28	G	265	PEK	O01-C1	5.10	1.48	1.34
28	P	1265	PEK	O01-C1	5.09	1.48	1.34
19	D	523	TGL	OG3-CC1	5.09	1.48	1.33
19	N	1522	TGL	OG1-CA1	5.01	1.47	1.33
26	P	1270	CDL	OA8-CA7	4.98	1.47	1.33
19	N	1522	TGL	OG3-CC1	4.98	1.47	1.33
26	C	270	CDL	OA6-CA5	4.97	1.48	1.34
18	N	515	HEA	CHA-C1A	4.92	1.48	1.38
22	O	1230	PSC	O01-C1	4.92	1.48	1.34
18	A	516	HEA	C4D-C3D	-4.90	1.36	1.45
19	N	1521	TGL	OG1-CA1	4.85	1.47	1.33
24	P	1272	DMU	O16-C6	4.80	1.48	1.40
26	G	269	CDL	OA8-CA7	4.79	1.47	1.33
26	G	269	CDL	OA6-CA5	4.76	1.47	1.34
26	C	270	CDL	OB8-CB7	4.71	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	269	CDL	OB8-CB7	4.70	1.47	1.33
26	G	269	CDL	OB6-CB5	4.69	1.47	1.34
28	G	1263	PEK	O01-C1	4.67	1.47	1.34
26	P	1270	CDL	OA6-CA5	4.67	1.47	1.34
28	G	265	PEK	O03-C21	4.65	1.46	1.33
20	C	268	PGV	O03-C19	4.63	1.46	1.33
19	D	523	TGL	OB1-CB1	4.62	1.36	1.22
24	C	272	DMU	O16-C6	4.61	1.47	1.40
19	Q	1523	TGL	OG1-CA1	4.58	1.46	1.33
26	T	1269	CDL	OA6-CA5	4.58	1.47	1.34
18	N	516	HEA	FE-NA	4.55	2.10	1.95
26	P	1270	CDL	OB8-CB7	4.55	1.46	1.33
26	C	270	CDL	OB6-CB5	4.54	1.47	1.34
26	T	1269	CDL	OB8-CB7	4.52	1.46	1.33
20	N	1524	PGV	O01-C1	4.48	1.46	1.34
23	O	229	CHD	C4-C5	4.48	1.61	1.53
18	A	516	HEA	CHB-C4A	4.48	1.47	1.38
26	T	1269	CDL	OB6-CB5	4.47	1.46	1.34
18	N	515	HEA	CHC-C1C	4.34	1.49	1.39
20	P	1268	PGV	O03-C19	4.25	1.45	1.33
18	A	516	HEA	FE-ND	4.22	2.07	1.94
26	P	1270	CDL	OB6-CB5	4.21	1.46	1.34
19	N	1521	TGL	OG3-CC1	4.20	1.45	1.33
18	A	516	HEA	CHD-C1D	4.19	1.46	1.38
22	B	230	PSC	C13-C12	4.17	1.55	1.31
18	A	516	HEA	FE-NA	4.16	2.08	1.95
26	T	1269	CDL	OA8-CA7	4.13	1.45	1.33
18	N	515	HEA	C1A-NA	-4.13	1.31	1.39
20	A	524	PGV	O01-C1	4.11	1.45	1.34
23	C	525	CHD	O12-C12	4.09	1.50	1.43
23	B	1086	CHD	C4-C3	4.05	1.59	1.52
26	G	269	CDL	C59-C58	-4.01	1.31	1.51
22	O	1230	PSC	C13-C12	4.01	1.54	1.31
22	O	1230	PSC	O03-C19	3.99	1.45	1.33
19	A	521	TGL	C10-CB9	-3.97	1.32	1.51
19	N	1521	TGL	C10-CB9	-3.93	1.32	1.51
19	L	522	TGL	C20-CA9	-3.93	1.32	1.51
19	L	522	TGL	C10-CB9	-3.91	1.32	1.51
23	C	525	CHD	C11-C9	3.91	1.60	1.53
18	N	516	HEA	CHD-C1D	3.90	1.46	1.38
18	N	515	HEA	C3A-C4A	-3.89	1.39	1.46
19	L	522	TGL	OG3-CC1	3.85	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C16-C15	3.84	1.59	1.51
26	C	270	CDL	C79-C78	-3.84	1.32	1.51
18	N	516	HEA	C1C-NC	-3.83	1.32	1.39
26	P	1270	CDL	C59-C58	-3.82	1.32	1.51
18	N	516	HEA	CHA-C1A	3.81	1.45	1.38
26	T	1269	CDL	C59-C58	-3.80	1.32	1.51
18	A	515	HEA	C1C-NC	-3.80	1.32	1.39
19	N	1522	TGL	C20-CA9	-3.78	1.33	1.51
18	N	515	HEA	FE-NC	3.75	2.07	1.95
19	A	521	TGL	OG3-CC1	3.74	1.44	1.33
18	A	516	HEA	CHA-C1A	3.74	1.45	1.38
23	B	1086	CHD	C8-C7	-3.74	1.46	1.53
26	T	1269	CDL	C42-C41	-3.73	1.33	1.51
18	N	516	HEA	FE-NC	3.73	2.07	1.95
23	C	525	CHD	C13-C12	-3.70	1.48	1.54
26	C	270	CDL	C59-C58	-3.67	1.33	1.51
26	G	269	CDL	C39-C38	-3.67	1.33	1.51
19	N	1522	TGL	C10-CB9	-3.62	1.33	1.51
18	A	515	HEA	C1A-NA	-3.60	1.32	1.39
26	G	269	CDL	C62-C61	-3.59	1.33	1.51
28	P	1264	PEK	O03-C01	-3.58	1.37	1.45
26	T	1269	CDL	C62-C61	-3.55	1.34	1.51
23	B	1086	CHD	C13-C12	-3.53	1.49	1.54
18	A	515	HEA	C1A-C2A	-3.52	1.39	1.45
26	G	269	CDL	C42-C41	-3.50	1.34	1.51
18	A	516	HEA	CHC-C4B	3.49	1.45	1.38
23	B	1086	CHD	C18-C13	3.49	1.59	1.54
18	N	515	HEA	CHC-C4B	3.48	1.45	1.38
18	N	516	HEA	C12-C11	3.47	1.58	1.53
26	P	1270	CDL	C22-C21	-3.46	1.34	1.51
26	T	1269	CDL	C19-C18	-3.44	1.34	1.51
26	P	1270	CDL	C79-C78	-3.43	1.34	1.51
28	G	264	PEK	O01-C1	3.43	1.44	1.34
18	A	515	HEA	CHB-C4A	3.42	1.45	1.38
18	N	516	HEA	C1A-C2A	-3.41	1.39	1.45
20	N	1266	PGV	O03-C19	3.41	1.43	1.33
28	P	1264	PEK	O01-C1	3.38	1.43	1.34
26	C	270	CDL	C39-C38	-3.38	1.35	1.51
19	D	523	TGL	C15-CC9	-3.38	1.35	1.51
26	P	1270	CDL	C19-C18	-3.37	1.35	1.51
26	C	270	CDL	C62-C61	-3.36	1.35	1.51
26	C	270	CDL	C22-C21	-3.35	1.35	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	269	CDL	C19-C18	-3.34	1.35	1.51
26	P	1270	CDL	C39-C38	-3.31	1.35	1.51
26	C	270	CDL	C82-C81	-3.29	1.35	1.51
19	N	1522	TGL	C15-CC9	-3.29	1.35	1.51
19	Q	1523	TGL	C10-CB9	-3.27	1.35	1.51
26	G	269	CDL	C22-C21	-3.27	1.35	1.51
26	C	270	CDL	C19-C18	-3.27	1.35	1.51
26	P	1270	CDL	C62-C61	-3.26	1.35	1.51
18	A	515	HEA	FE-NC	3.24	2.05	1.95
19	Q	1523	TGL	C15-CC9	-3.24	1.35	1.51
18	A	516	HEA	C1B-C2B	-3.19	1.38	1.44
19	A	521	TGL	C20-CA9	-3.18	1.35	1.51
23	B	1086	CHD	C10-C5	-3.18	1.50	1.55
19	N	1521	TGL	C15-CC9	-3.16	1.36	1.51
18	N	515	HEA	CMB-C2B	3.16	1.57	1.50
24	Z	1526	DMU	C3-C4	-3.15	1.44	1.52
26	T	1269	CDL	C39-C38	-3.15	1.36	1.51
26	P	1270	CDL	C82-C81	-3.15	1.36	1.51
26	P	1270	CDL	C42-C41	-3.14	1.36	1.51
18	A	515	HEA	O11-C11	3.14	1.49	1.42
26	T	1269	CDL	C79-C78	-3.13	1.36	1.51
18	A	516	HEA	CHC-C1C	3.12	1.46	1.39
26	C	270	CDL	C42-C41	-3.12	1.36	1.51
18	A	515	HEA	C4D-C3D	-3.11	1.39	1.45
26	T	1269	CDL	C22-C21	-3.10	1.36	1.51
20	C	267	PGV	O03-C19	3.09	1.42	1.33
18	N	516	HEA	C4B-C3B	-3.08	1.39	1.44
26	T	1269	CDL	C82-C81	-3.07	1.36	1.51
18	A	515	HEA	CHD-C1D	3.06	1.44	1.38
18	N	515	HEA	C1A-C2A	-3.05	1.39	1.45
18	A	515	HEA	CHB-C1B	3.05	1.46	1.39
19	L	522	TGL	C15-CC9	-3.04	1.36	1.51
19	Q	1523	TGL	C20-CA9	-3.03	1.36	1.51
24	M	526	DMU	C3-C4	-3.03	1.44	1.52
18	N	515	HEA	CBA-CGA	3.03	1.57	1.50
26	G	269	CDL	C79-C78	-3.01	1.36	1.51
23	O	229	CHD	C11-C9	3.01	1.58	1.53
18	A	516	HEA	C4A-NA	-3.01	1.34	1.39
18	N	515	HEA	CHD-C1D	3.00	1.44	1.38
26	G	269	CDL	C82-C81	-2.99	1.36	1.51
18	A	516	HEA	C13-C14	2.95	1.59	1.50
19	D	523	TGL	C10-CB9	-2.94	1.37	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C18-C19	2.93	1.39	1.33
20	P	1267	PGV	C03-C02	2.90	1.59	1.50
19	A	521	TGL	C15-CC9	-2.89	1.37	1.51
19	D	523	TGL	C20-CA9	-2.89	1.37	1.51
18	N	516	HEA	CHB-C4A	2.89	1.44	1.38
18	A	516	HEA	C1D-C2D	-2.88	1.38	1.44
18	N	515	HEA	CHA-C4D	2.87	1.45	1.39
18	N	515	HEA	CHB-C1B	2.87	1.45	1.39
23	B	1086	CHD	C13-C14	-2.85	1.50	1.55
28	G	264	PEK	C2-C1	2.83	1.58	1.50
20	P	1267	PGV	O03-C19	2.75	1.41	1.33
23	B	1086	CHD	C15-C14	-2.75	1.48	1.54
23	C	271	CHD	O26-C24	-2.75	1.21	1.30
18	N	516	HEA	CHC-C1C	2.75	1.45	1.39
23	C	271	CHD	C20-C17	2.74	1.59	1.54
19	A	521	TGL	OC1-CC1	-2.74	1.14	1.22
28	P	1264	PEK	C2-C1	2.73	1.58	1.50
23	O	229	CHD	C15-C14	-2.72	1.48	1.54
18	A	515	HEA	CMB-C2B	2.72	1.56	1.50
23	P	1525	CHD	C13-C12	-2.70	1.50	1.54
18	N	516	HEA	CHD-C4C	2.70	1.45	1.39
18	N	515	HEA	C3B-C2B	2.69	1.40	1.34
19	N	1521	TGL	C20-CA9	-2.67	1.38	1.51
18	A	515	HEA	C4A-NA	-2.63	1.34	1.39
23	C	525	CHD	C18-C13	2.61	1.58	1.54
23	P	1271	CHD	C20-C17	2.55	1.58	1.54
23	C	525	CHD	O26-C24	-2.54	1.22	1.30
18	N	516	HEA	CHC-C4B	2.54	1.43	1.38
18	N	516	HEA	FE-NB	2.54	2.02	1.94
18	N	516	HEA	C4B-NB	-2.52	1.35	1.40
23	C	525	CHD	C11-C12	2.52	1.57	1.53
18	A	515	HEA	CAC-C3C	2.52	1.54	1.47
18	A	516	HEA	C1C-NC	-2.51	1.34	1.39
18	A	515	HEA	C16-C15	2.51	1.56	1.51
23	O	229	CHD	C18-C13	2.49	1.58	1.54
23	W	1060	CHD	C11-C9	2.49	1.57	1.53
18	N	516	HEA	C27-C19	-2.48	1.44	1.50
20	P	1267	PGV	O02-C1	2.44	1.29	1.22
23	P	1525	CHD	C16-C17	2.44	1.59	1.54
18	N	516	HEA	C3A-C4A	-2.43	1.41	1.46
23	O	229	CHD	C10-C5	-2.43	1.51	1.55
18	N	516	HEA	CHB-C1B	2.39	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	267	PGV	C03-C02	2.38	1.58	1.50
26	P	1270	CDL	PB2-OB2	2.38	1.68	1.59
18	N	516	HEA	C1A-NA	-2.37	1.35	1.39
24	P	1272	DMU	O1-C10	2.35	1.47	1.41
23	O	229	CHD	C4-C3	2.34	1.56	1.52
24	Z	1526	DMU	O1-C10	2.33	1.47	1.41
18	A	516	HEA	C3A-C4A	-2.33	1.42	1.46
23	P	1525	CHD	C1-C10	-2.33	1.50	1.54
20	C	267	PGV	O01-C1	2.33	1.40	1.34
18	N	516	HEA	CMD-C2D	2.26	1.55	1.50
18	A	516	HEA	CHB-C1B	2.26	1.44	1.39
28	P	1264	PEK	C3-C2	2.24	1.60	1.52
23	P	1525	CHD	C13-C14	-2.21	1.51	1.55
19	L	522	TGL	CG1-CG2	2.21	1.57	1.50
23	B	1086	CHD	C23-C24	2.20	1.55	1.50
26	C	270	CDL	CB2-C1	2.20	1.58	1.51
18	A	516	HEA	C21-C22	2.20	1.57	1.50
18	A	516	HEA	C3A-C2A	2.19	1.42	1.37
28	G	265	PEK	P-O12	2.18	1.67	1.59
18	N	516	HEA	CMA-C3A	2.17	1.50	1.45
18	A	516	HEA	O2D-CGD	-2.17	1.23	1.30
18	A	516	HEA	C26-C15	2.16	1.56	1.50
23	P	1525	CHD	C16-C15	2.15	1.59	1.54
23	C	525	CHD	C4-C3	2.15	1.55	1.52
18	N	516	HEA	C4A-NA	-2.13	1.35	1.39
18	N	516	HEA	C16-C15	2.13	1.55	1.51
28	T	263	PEK	C01-C02	2.12	1.57	1.50
18	A	515	HEA	C4B-C3B	-2.12	1.41	1.44
18	A	515	HEA	FE-ND	2.12	2.01	1.94
18	N	515	HEA	C17-C18	2.10	1.56	1.50
18	N	516	HEA	O11-C11	2.09	1.47	1.42
18	N	515	HEA	FE-ND	2.08	2.01	1.94
18	N	516	HEA	C3D-C2D	2.07	1.41	1.36
18	A	515	HEA	C4C-NC	-2.06	1.35	1.39
23	O	229	CHD	C13-C12	-2.05	1.51	1.54
18	A	515	HEA	CMC-C2C	2.05	1.55	1.50
18	A	515	HEA	CBA-CGA	2.05	1.55	1.50
18	A	516	HEA	O11-C11	2.05	1.47	1.42
23	O	229	CHD	C19-C10	2.04	1.57	1.54
23	B	1086	CHD	C1-C2	-2.03	1.49	1.53
20	A	522	PGV	C3-C2	2.03	1.59	1.52
20	C	268	PGV	P-O11	2.03	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	515	HEA	C3A-C2A	2.03	1.41	1.37
20	A	524	PGV	O02-C1	2.02	1.28	1.22
18	A	515	HEA	CHC-C1C	2.02	1.43	1.39

All (763) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	229	CHD	C6-C5-C10	16.16	129.86	112.66
23	P	1271	CHD	C10-C9-C8	14.85	128.40	111.84
23	B	1086	CHD	C1-C10-C5	14.66	128.80	107.75
23	C	271	CHD	C10-C9-C8	14.10	127.55	111.84
23	P	1525	CHD	C6-C5-C10	13.07	126.57	112.66
23	C	525	CHD	C19-C10-C9	-13.05	93.64	111.18
23	P	1525	CHD	C1-C10-C5	12.11	125.13	107.75
23	O	229	CHD	C19-C10-C9	-12.10	94.91	111.18
23	W	1060	CHD	C10-C9-C8	11.89	125.10	111.84
23	B	1086	CHD	C14-C13-C12	11.82	118.22	107.42
23	O	229	CHD	C1-C10-C5	11.78	124.65	107.75
23	J	60	CHD	C10-C9-C8	11.44	124.59	111.84
23	O	229	CHD	C17-C13-C12	11.05	127.61	117.67
23	B	1086	CHD	C18-C13-C12	-10.81	98.23	109.06
23	B	1086	CHD	C6-C5-C10	10.76	124.11	112.66
23	C	525	CHD	C1-C10-C5	10.70	123.11	107.75
23	P	1525	CHD	C19-C10-C9	-10.66	96.85	111.18
23	O	229	CHD	C18-C13-C12	-10.60	98.45	109.06
23	C	525	CHD	C6-C5-C10	10.48	123.81	112.66
23	O	229	CHD	C6-C5-C4	-9.70	100.15	111.23
23	P	1271	CHD	C18-C13-C12	-9.59	99.46	109.06
23	C	525	CHD	C10-C9-C8	9.54	122.47	111.84
23	P	1525	CHD	C17-C13-C12	9.44	126.16	117.67
23	O	229	CHD	C9-C8-C7	9.38	123.66	111.86
23	C	271	CHD	C16-C17-C20	9.20	126.10	112.18
28	G	264	PEK	C2-C3-C4	9.16	133.35	113.35
23	P	1525	CHD	C4-C3-C2	9.13	121.75	110.62
23	P	1525	CHD	C18-C13-C17	-9.00	97.09	111.20
23	O	229	CHD	C14-C13-C12	8.97	115.61	107.42
23	P	1525	CHD	C11-C9-C10	8.93	122.77	113.70
23	B	1086	CHD	C10-C9-C8	8.75	121.59	111.84
23	P	1525	CHD	C17-C13-C14	8.68	108.83	100.11
19	A	521	TGL	CG2-OG2-CB1	8.60	138.39	117.80
23	C	271	CHD	C6-C5-C10	8.55	121.75	112.66
23	C	271	CHD	C18-C13-C12	-8.54	100.51	109.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C4-C3-C2	8.44	120.92	110.62
23	C	525	CHD	C17-C13-C12	8.33	125.17	117.67
23	O	229	CHD	C10-C9-C8	8.23	121.01	111.84
23	P	1271	CHD	C6-C5-C10	8.20	121.39	112.66
23	C	271	CHD	C15-C14-C8	8.17	129.56	118.36
23	W	1060	CHD	C1-C10-C5	8.17	119.47	107.75
18	A	516	HEA	C13-C12-C11	-8.09	101.47	114.39
24	M	526	DMU	O5-C6-C1	8.05	126.91	110.37
18	A	515	HEA	C3C-C4C-NC	8.05	116.58	109.80
23	P	1271	CHD	C15-C14-C8	8.04	129.38	118.36
19	A	521	TGL	OG2-CB1-CB2	8.03	128.85	111.48
23	B	1086	CHD	C4-C3-C2	8.00	120.38	110.62
23	W	1060	CHD	C14-C8-C7	7.74	122.12	111.85
18	N	515	HEA	C12-C11-C3B	7.73	124.21	112.12
23	W	1060	CHD	C16-C17-C13	7.69	111.00	103.54
23	P	1271	CHD	C1-C10-C5	7.67	118.76	107.75
23	C	271	CHD	C6-C7-C8	7.67	119.88	111.50
23	P	1271	CHD	C6-C7-C8	7.62	119.82	111.50
23	W	1060	CHD	C13-C17-C20	7.62	128.71	119.48
23	O	229	CHD	C5-C4-C3	7.60	124.17	112.71
23	C	271	CHD	C1-C2-C3	7.59	120.54	110.48
23	J	60	CHD	C1-C10-C5	7.57	118.61	107.75
23	P	1271	CHD	C5-C4-C3	7.50	124.02	112.71
23	C	525	CHD	C14-C13-C12	7.46	114.23	107.42
24	M	526	DMU	O1-C9-C8	7.46	123.14	109.70
23	P	1271	CHD	C11-C9-C8	7.45	121.92	110.89
23	J	60	CHD	C14-C13-C12	7.43	114.21	107.42
23	B	1086	CHD	C17-C13-C14	7.38	107.52	100.11
23	W	1060	CHD	C4-C3-C2	7.37	119.61	110.62
23	J	60	CHD	C6-C7-C8	7.34	119.52	111.50
23	O	229	CHD	C17-C13-C14	7.33	107.47	100.11
23	P	1525	CHD	C9-C8-C7	7.29	121.03	111.86
23	P	1271	CHD	C14-C13-C12	7.23	114.03	107.42
23	J	60	CHD	C13-C17-C20	7.22	128.23	119.48
23	W	1060	CHD	C5-C6-C7	7.22	122.98	114.40
24	Z	1526	DMU	O1-C9-C8	7.20	122.67	109.70
23	B	1086	CHD	C6-C7-C8	7.18	119.34	111.50
23	W	1060	CHD	C6-C5-C10	7.18	120.30	112.66
23	P	1271	CHD	C16-C17-C20	7.16	123.02	112.18
24	C	272	DMU	O1-C9-C8	7.16	122.59	109.70
23	C	271	CHD	C1-C10-C5	7.12	117.97	107.75
24	Z	1526	DMU	O5-C6-C1	7.11	124.97	110.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C6-C5-C10	7.10	120.21	112.66
18	A	515	HEA	C12-C11-C3B	7.09	123.21	112.12
23	B	1086	CHD	C19-C10-C5	-7.06	98.65	110.44
23	C	271	CHD	C14-C13-C12	7.02	113.83	107.42
24	C	272	DMU	O16-C6-C1	7.01	118.92	108.27
24	P	1272	DMU	O16-C6-C1	6.97	118.86	108.27
23	J	60	CHD	C1-C2-C3	6.93	119.66	110.48
19	L	522	TGL	OG3-CC1-OC1	-6.86	106.47	123.63
23	P	1271	CHD	C19-C10-C9	-6.80	102.04	111.18
23	C	525	CHD	C5-C4-C3	6.79	122.94	112.71
23	B	1086	CHD	C9-C11-C12	6.78	123.17	114.29
23	O	229	CHD	C11-C9-C8	6.76	120.90	110.89
24	P	1272	DMU	O1-C9-C8	6.76	121.88	109.70
23	W	1060	CHD	C6-C7-C8	6.73	118.85	111.50
23	C	525	CHD	O12-C12-C13	-6.73	99.65	111.02
26	T	1269	CDL	OB6-CB5-C51	6.65	125.87	111.48
23	C	271	CHD	C5-C4-C3	6.65	122.74	112.71
24	Z	1526	DMU	O16-C6-C1	6.60	118.30	108.27
24	M	526	DMU	O1-C10-C5	6.57	123.87	110.37
23	W	1060	CHD	C17-C13-C12	6.57	123.58	117.67
23	J	60	CHD	C5-C4-C3	6.56	122.60	112.71
23	W	1060	CHD	C9-C11-C12	6.53	122.84	114.29
23	O	229	CHD	C18-C13-C17	-6.49	101.04	111.20
23	J	60	CHD	C17-C13-C12	6.48	123.50	117.67
23	W	1060	CHD	C5-C4-C3	6.47	122.47	112.71
24	C	272	DMU	O1-C10-C5	6.47	123.66	110.37
23	J	60	CHD	C4-C3-C2	6.43	118.46	110.62
23	P	1525	CHD	C10-C9-C8	6.39	118.97	111.84
23	P	1271	CHD	C4-C3-C2	6.39	118.41	110.62
18	N	515	HEA	C3C-C4C-NC	6.37	115.17	109.80
23	O	229	CHD	C18-C13-C14	-6.36	101.23	111.20
24	Z	1526	DMU	O1-C10-C5	6.36	123.43	110.37
23	W	1060	CHD	C15-C14-C8	6.34	127.05	118.36
23	C	525	CHD	C18-C13-C12	-6.32	102.73	109.06
23	P	1525	CHD	O12-C12-C13	-6.31	100.36	111.02
23	P	1525	CHD	C16-C17-C20	6.27	121.66	112.18
23	O	229	CHD	O12-C12-C13	-6.23	100.50	111.02
23	J	60	CHD	C5-C6-C7	6.22	121.80	114.40
20	P	1268	PGV	O03-C19-C20	6.21	130.77	111.83
24	P	1272	DMU	O1-C10-C5	6.20	123.10	110.37
23	J	60	CHD	C16-C17-C13	6.19	109.55	103.54
23	J	60	CHD	C14-C8-C7	6.16	120.02	111.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	CHA-C4D-C3D	-6.15	115.81	124.77
23	P	1271	CHD	C5-C6-C7	6.15	121.71	114.40
23	W	1060	CHD	C14-C13-C12	6.14	113.03	107.42
23	B	1086	CHD	C1-C2-C3	6.13	118.61	110.48
18	A	516	HEA	CHB-C4A-NA	6.13	131.13	124.45
23	J	60	CHD	C15-C14-C13	6.13	109.48	103.54
28	G	264	PEK	O01-C1-O02	-6.13	109.38	123.70
23	P	1525	CHD	C11-C12-C13	6.12	117.49	111.26
23	O	229	CHD	C11-C12-C13	6.08	117.45	111.26
24	C	272	DMU	C18-O16-C6	6.05	124.02	113.68
23	P	1271	CHD	C1-C2-C3	6.05	118.50	110.48
23	C	271	CHD	C17-C13-C12	6.03	123.09	117.67
23	P	1525	CHD	C18-C13-C14	-6.02	101.77	111.20
18	A	515	HEA	C2A-C1A-NA	-6.00	104.53	110.32
23	J	60	CHD	C18-C13-C12	-6.00	103.05	109.06
23	W	1060	CHD	C1-C2-C3	5.98	118.40	110.48
23	C	271	CHD	C5-C6-C7	5.96	121.49	114.40
26	T	1269	CDL	OA6-CA5-C11	5.92	124.30	111.48
24	P	1272	DMU	O5-C4-C3	5.88	121.89	109.72
23	W	1060	CHD	C2-C1-C10	5.87	122.65	112.74
23	C	271	CHD	C15-C14-C13	5.87	109.23	103.54
23	C	525	CHD	C13-C17-C20	5.86	126.58	119.48
23	P	1271	CHD	C2-C1-C10	5.82	122.56	112.74
19	A	521	TGL	OG3-CC1-OC1	-5.81	109.09	123.63
24	M	526	DMU	C2-C3-C4	5.80	123.78	110.93
23	C	525	CHD	C18-C13-C14	-5.80	102.12	111.20
19	N	1521	TGL	CG2-OG2-CB1	5.80	131.67	117.80
23	P	1271	CHD	C17-C13-C14	5.78	105.91	100.11
26	C	270	CDL	CB4-OB6-CB5	-5.77	103.99	117.80
18	A	515	HEA	CHA-C4D-ND	5.76	130.62	124.42
18	A	515	HEA	C26-C15-C16	5.74	125.20	115.23
23	C	271	CHD	C11-C9-C8	5.74	119.40	110.89
23	B	1086	CHD	C19-C10-C9	-5.74	103.47	111.18
23	C	271	CHD	C2-C1-C10	5.74	122.42	112.74
23	O	229	CHD	C16-C17-C20	5.73	120.84	112.18
24	P	1272	DMU	O1-C9-C11	5.71	120.59	106.44
23	J	60	CHD	C2-C1-C10	5.70	122.36	112.74
26	G	269	CDL	OB6-CB5-C51	5.70	123.82	111.48
23	O	229	CHD	C1-C2-C3	5.70	118.03	110.48
23	J	60	CHD	C15-C14-C8	5.67	126.14	118.36
23	C	525	CHD	C2-C1-C10	5.61	122.21	112.74
28	P	1264	PEK	O01-C1-O02	-5.60	110.60	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C17-C13-C14	5.60	105.73	100.11
24	P	1272	DMU	C8-C7-C5	5.56	120.60	110.83
18	N	515	HEA	C27-C19-C18	-5.55	109.37	123.63
23	J	60	CHD	C16-C17-C20	5.55	120.58	112.18
23	J	60	CHD	C11-C12-C13	5.55	116.91	111.26
23	B	1086	CHD	C11-C9-C10	5.54	119.32	113.70
23	P	1271	CHD	C16-C17-C13	5.51	108.89	103.54
24	C	272	DMU	O5-C4-C57	5.51	120.08	106.44
19	A	521	TGL	OG3-CC1-CC2	5.46	128.48	111.83
18	N	515	HEA	C27-C19-C20	5.45	124.69	115.23
19	N	1522	TGL	OG2-CB1-CB2	5.45	123.27	111.48
24	Z	1526	DMU	C8-C7-C5	5.44	120.37	110.83
24	C	272	DMU	O5-C6-C1	5.43	121.52	110.37
23	P	1525	CHD	C5-C4-C3	5.43	120.89	112.71
23	C	525	CHD	C11-C12-C13	5.42	116.77	111.26
20	C	268	PGV	O03-C19-C20	5.41	128.33	111.83
23	P	1525	CHD	C14-C13-C12	5.40	112.35	107.42
24	C	272	DMU	C8-C7-C5	5.37	120.25	110.83
23	C	271	CHD	C17-C13-C14	5.36	105.50	100.11
18	N	515	HEA	CHC-C4B-NB	5.36	130.99	124.37
18	A	516	HEA	C27-C19-C20	5.35	124.52	115.23
23	C	271	CHD	C16-C17-C13	5.35	108.73	103.54
24	C	272	DMU	O5-C4-C3	5.35	120.79	109.72
23	C	271	CHD	C4-C5-C10	5.34	118.34	112.66
23	P	1525	CHD	O3-C3-C4	5.32	120.44	109.84
24	Z	1526	DMU	O5-C4-C3	5.32	120.71	109.72
23	W	1060	CHD	C11-C12-C13	5.30	116.66	111.26
23	O	229	CHD	C13-C14-C8	5.30	121.44	114.72
18	A	515	HEA	C4C-C3C-C2C	-5.30	100.71	107.30
23	J	60	CHD	C4-C5-C10	5.29	118.29	112.66
18	A	516	HEA	C2B-C1B-NB	5.28	116.00	109.90
23	J	60	CHD	C9-C11-C12	5.28	121.20	114.29
23	P	1271	CHD	C14-C8-C7	5.27	118.85	111.85
24	M	526	DMU	C8-C7-C5	5.27	120.08	110.83
23	C	525	CHD	O12-C12-C11	-5.27	98.40	109.12
24	Z	1526	DMU	O5-C4-C57	5.26	119.47	106.44
20	C	268	PGV	O01-C1-C2	5.23	122.80	111.48
23	W	1060	CHD	C1-C10-C9	-5.18	103.30	111.34
23	B	1086	CHD	C15-C14-C8	5.17	125.44	118.36
18	A	516	HEA	C4B-NB-C1B	-5.16	99.09	105.21
23	P	1525	CHD	C6-C5-C4	-5.16	105.33	111.23
23	J	60	CHD	C11-C9-C8	5.16	118.53	110.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	272	DMU	C2-C3-C4	5.16	122.36	110.93
23	W	1060	CHD	C19-C10-C5	-5.16	101.82	110.44
23	C	271	CHD	C4-C3-C2	5.13	116.88	110.62
23	J	60	CHD	C6-C5-C4	-5.11	105.38	111.23
18	A	516	HEA	CMB-C2B-C1B	5.11	133.01	125.03
23	C	525	CHD	C11-C9-C10	5.10	118.88	113.70
23	P	1271	CHD	O7-C7-C6	-5.10	97.17	109.86
19	A	521	TGL	CG3-OG3-CC1	5.10	135.76	117.12
18	A	515	HEA	C2B-C1B-NB	5.09	115.79	109.90
23	P	1525	CHD	C1-C10-C9	-5.09	103.44	111.34
23	B	1086	CHD	C1-C10-C9	-5.06	103.48	111.34
24	Z	1526	DMU	O1-C9-C11	5.05	118.96	106.44
24	M	526	DMU	O5-C4-C3	5.04	120.14	109.72
28	P	1265	PEK	O03-C21-C22	5.02	127.14	111.83
23	C	525	CHD	C9-C11-C12	5.00	120.84	114.29
23	P	1525	CHD	C15-C14-C13	5.00	108.39	103.54
20	N	1266	PGV	O03-C19-C20	4.99	127.06	111.83
19	D	523	TGL	OG2-CB1-CB2	-4.99	100.69	111.48
23	O	229	CHD	C4-C3-C2	4.98	116.70	110.62
23	W	1060	CHD	C6-C5-C4	-4.98	105.54	111.23
19	L	522	TGL	OG3-CC1-CC2	4.98	127.01	111.83
26	C	270	CDL	OA6-CA5-C11	4.97	122.23	111.48
28	P	1264	PEK	O03-C01-C02	-4.96	94.08	108.40
23	C	525	CHD	C9-C8-C7	4.96	118.10	111.86
23	J	60	CHD	C1-C10-C9	-4.96	103.63	111.34
23	C	271	CHD	C11-C12-C13	4.93	116.28	111.26
20	N	1266	PGV	O03-C19-O04	-4.92	111.31	123.63
23	C	271	CHD	C18-C13-C17	-4.92	103.49	111.20
18	A	516	HEA	CMB-C2B-C3B	-4.91	120.77	130.28
23	B	1086	CHD	C18-C13-C14	-4.91	103.51	111.20
23	P	1525	CHD	C9-C11-C12	4.91	120.71	114.29
28	G	1263	PEK	O01-C1-C2	4.90	122.07	111.48
18	N	516	HEA	CHB-C1B-NB	4.90	129.69	124.42
20	C	267	PGV	C27-C26-C25	-4.86	89.79	114.37
23	P	1271	CHD	C9-C11-C12	4.86	120.65	114.29
23	J	60	CHD	C22-C20-C17	4.86	120.40	110.33
24	Z	1526	DMU	C2-C3-C4	4.83	121.63	110.93
23	P	1525	CHD	C19-C10-C5	-4.82	102.39	110.44
23	P	1271	CHD	C18-C13-C17	-4.81	103.66	111.20
23	P	1525	CHD	O12-C12-C11	-4.81	99.33	109.12
23	C	525	CHD	C5-C6-C7	4.79	120.10	114.40
23	C	271	CHD	C6-C5-C4	-4.78	105.76	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	1060	CHD	C15-C14-C13	4.78	108.18	103.54
23	C	271	CHD	C9-C11-C12	4.77	120.53	114.29
20	A	524	PGV	C02-O01-C1	4.76	129.18	117.80
23	P	1525	CHD	C19-C10-C1	4.72	115.81	108.31
28	T	263	PEK	O01-C1-C2	4.72	121.70	111.48
23	J	60	CHD	C9-C10-C5	4.72	115.06	108.51
18	N	515	HEA	C26-C15-C16	4.71	123.41	115.23
19	D	523	TGL	OG2-CB1-OB1	4.71	134.72	123.70
24	P	1272	DMU	O5-C6-C1	4.70	120.02	110.37
26	P	1270	CDL	OA6-CA5-C11	4.70	121.64	111.48
23	C	525	CHD	C18-C13-C17	-4.69	103.86	111.20
23	B	1086	CHD	C17-C13-C12	4.68	121.88	117.67
18	A	516	HEA	CAA-C2A-C1A	4.68	134.36	124.85
18	N	515	HEA	C1D-C2D-C3D	-4.66	102.08	106.98
23	O	229	CHD	C15-C14-C13	4.65	108.05	103.54
23	P	1525	CHD	C6-C7-C8	4.63	116.56	111.50
23	C	271	CHD	C19-C10-C9	-4.62	104.96	111.18
23	B	1086	CHD	C5-C4-C3	4.62	119.68	112.71
23	P	1525	CHD	C22-C20-C17	-4.62	100.76	110.33
26	G	269	CDL	OA6-CA5-C11	4.54	121.30	111.48
20	P	1268	PGV	O01-C1-C2	4.54	121.29	111.48
23	B	1086	CHD	O12-C12-C11	-4.53	99.90	109.12
19	A	521	TGL	OG3-CG3-CG2	4.53	121.46	108.40
23	C	525	CHD	C15-C14-C13	4.52	107.92	103.54
23	B	1086	CHD	C18-C13-C17	-4.50	104.15	111.20
23	W	1060	CHD	C18-C13-C12	-4.48	104.57	109.06
24	P	1272	DMU	O5-C4-C57	4.47	117.51	106.44
19	Q	1523	TGL	OG3-CC1-CC2	4.47	125.45	111.83
23	W	1060	CHD	C11-C9-C8	4.46	117.50	110.89
23	C	271	CHD	O7-C7-C6	-4.46	98.77	109.86
18	A	516	HEA	CHA-C1A-NA	4.45	129.29	124.45
19	N	1521	TGL	OG2-CB1-CB2	4.44	121.10	111.48
23	C	525	CHD	C6-C5-C4	-4.44	106.15	111.23
26	C	270	CDL	OB8-CB7-C71	4.44	125.37	111.83
23	P	1271	CHD	C15-C14-C13	4.44	107.84	103.54
23	O	229	CHD	O12-C12-C11	-4.42	100.12	109.12
18	N	516	HEA	C3D-C4D-ND	4.42	114.63	110.35
19	A	521	TGL	OG1-CA1-CA2	4.42	125.30	111.83
18	N	516	HEA	C2D-C1D-ND	4.42	114.92	109.84
19	D	523	TGL	CG1-OG1-CA1	4.40	133.20	117.12
23	P	1271	CHD	C11-C12-C13	4.40	115.74	111.26
23	W	1060	CHD	C4-C5-C10	4.39	117.34	112.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	516	HEA	C13-C12-C11	-4.39	107.38	114.39
23	W	1060	CHD	C16-C17-C20	4.38	118.81	112.18
19	L	522	TGL	CC3-CC2-CC1	4.37	129.70	113.69
18	N	515	HEA	C2D-C1D-ND	4.36	114.86	109.84
26	C	270	CDL	OA8-CA7-C31	4.36	125.13	111.83
18	N	516	HEA	C17-C18-C19	4.36	137.60	127.62
24	Z	1526	DMU	O7-C10-C5	-4.36	97.37	108.09
23	P	1525	CHD	C4-C5-C10	-4.35	108.03	112.66
18	A	515	HEA	C13-C12-C11	4.35	121.34	114.39
23	P	1271	CHD	C4-C5-C10	4.32	117.26	112.66
24	M	526	DMU	C18-O16-C6	4.32	121.06	113.68
23	W	1060	CHD	C9-C10-C5	4.32	114.51	108.51
18	A	516	HEA	C20-C19-C18	-4.31	111.49	121.17
26	P	1270	CDL	OB8-CB7-C71	4.30	124.96	111.83
19	N	1521	TGL	CG3-OG3-CC1	4.30	132.83	117.12
24	M	526	DMU	O5-C4-C57	4.30	117.09	106.44
23	B	1086	CHD	C15-C14-C13	4.28	107.69	103.54
23	C	525	CHD	C23-C22-C20	-4.27	106.48	114.46
18	A	515	HEA	C4B-NB-C1B	-4.26	100.16	105.21
19	L	522	TGL	OG1-CG1-CG2	4.26	120.68	108.40
22	B	230	PSC	O01-C1-C2	4.24	120.66	111.48
18	N	515	HEA	C1C-CHC-C4B	-4.24	116.28	126.25
19	L	522	TGL	OG1-CA1-CA2	4.22	124.69	111.83
23	B	1086	CHD	C9-C8-C7	4.21	117.15	111.86
23	B	1086	CHD	C14-C8-C9	4.20	115.62	109.75
24	C	272	DMU	C6-C1-C2	4.20	118.85	110.01
23	P	1271	CHD	C11-C9-C10	-4.19	109.45	113.70
18	N	515	HEA	C4C-C3C-C2C	-4.17	102.11	107.30
23	O	229	CHD	C1-C10-C9	-4.17	104.86	111.34
19	L	522	TGL	CG2-OG2-CB1	4.17	127.77	117.80
18	A	515	HEA	C4A-NA-C1A	4.17	112.61	105.82
19	A	521	TGL	OB1-CB1-CB2	-4.16	107.52	123.78
28	G	265	PEK	O03-C21-C22	4.16	124.51	111.83
18	A	516	HEA	C3B-C4B-NB	4.16	114.62	109.84
23	P	1271	CHD	C17-C13-C12	4.14	121.40	117.67
24	P	1272	DMU	C1-C2-C3	4.11	119.02	109.68
18	N	516	HEA	O2A-CGA-CBA	4.11	127.00	114.00
23	B	1086	CHD	C11-C9-C8	4.10	116.96	110.89
24	P	1272	DMU	C7-C8-C9	4.10	117.66	110.23
23	W	1060	CHD	O7-C7-C6	-4.09	99.67	109.86
18	N	516	HEA	O11-C11-C3B	-4.09	103.75	111.26
23	J	60	CHD	C19-C10-C5	-4.09	103.60	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C2D-C1D-ND	4.07	114.52	109.84
18	A	515	HEA	CHD-C1D-ND	-4.07	119.33	124.37
20	N	1524	PGV	O01-C1-C2	4.05	120.24	111.48
23	B	1086	CHD	O12-C12-C13	-4.05	104.19	111.02
23	P	1525	CHD	C13-C17-C20	4.04	124.38	119.48
23	C	525	CHD	C6-C7-C8	4.03	115.90	111.50
18	A	515	HEA	CHB-C4A-NA	4.02	128.84	124.45
24	C	272	DMU	O7-C3-C2	4.02	117.45	107.23
22	O	1230	PSC	O01-C1-C2	4.01	120.16	111.48
24	C	272	DMU	O7-C3-C4	4.01	119.99	109.48
23	P	1525	CHD	C2-C1-C10	3.96	119.43	112.74
24	P	1272	DMU	C6-C1-C2	3.95	118.31	110.01
23	O	229	CHD	C4-C5-C10	-3.94	108.46	112.66
24	Z	1526	DMU	C7-C8-C9	3.93	117.36	110.23
18	N	516	HEA	CMB-C2B-C3B	-3.93	122.67	130.28
24	P	1272	DMU	C6-O5-C4	3.91	121.36	113.72
23	J	60	CHD	C18-C13-C14	-3.89	105.11	111.20
19	D	523	TGL	CG2-OG2-CB1	3.89	127.09	117.80
20	A	524	PGV	C8-C9-C10	-3.88	95.19	113.86
24	C	272	DMU	O1-C9-C11	3.88	116.06	106.44
20	N	1266	PGV	O01-C1-O02	-3.88	114.63	123.70
18	N	516	HEA	CMD-C2D-C1D	3.88	131.09	125.03
24	C	272	DMU	C7-C8-C9	3.86	117.22	110.23
19	D	523	TGL	OG1-CA1-CA2	3.85	123.58	111.83
20	A	522	PGV	O03-C19-C20	3.85	123.58	111.83
24	Z	1526	DMU	O7-C3-C2	3.81	116.92	107.23
24	P	1272	DMU	C2-C3-C4	3.80	119.35	110.93
28	T	263	PEK	O03-C01-C02	3.79	119.32	108.40
18	A	515	HEA	CAD-C3D-C2D	3.77	134.93	127.87
23	P	1271	CHD	O12-C12-C13	-3.76	104.67	111.02
23	P	1271	CHD	C23-C22-C20	-3.76	107.44	114.46
18	N	516	HEA	O1D-CGD-CBD	-3.74	111.23	123.09
18	N	515	HEA	C16-C15-C14	-3.73	112.78	121.17
28	P	1264	PEK	C2-C3-C4	3.73	121.49	113.35
23	O	229	CHD	C14-C8-C9	3.72	114.94	109.75
23	P	1525	CHD	C13-C14-C8	3.71	119.41	114.72
18	N	515	HEA	C2A-C1A-NA	-3.71	106.75	110.32
23	O	229	CHD	C2-C1-C10	3.70	118.98	112.74
23	P	1271	CHD	O12-C12-C11	-3.69	101.61	109.12
28	G	264	PEK	C25-C24-C23	-3.67	95.83	114.37
18	N	516	HEA	C1D-ND-C4D	-3.65	100.88	105.21
23	W	1060	CHD	C22-C20-C17	3.65	117.90	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	CAD-C3D-C4D	-3.64	118.34	124.70
23	P	1525	CHD	O7-C7-C6	-3.64	100.80	109.86
23	C	271	CHD	O12-C12-C11	-3.64	101.72	109.12
23	C	525	CHD	C22-C23-C24	-3.63	102.81	112.49
23	W	1060	CHD	O12-C12-C11	-3.60	101.79	109.12
28	G	264	PEK	C24-C23-C22	-3.60	99.91	113.13
23	B	1086	CHD	C14-C8-C7	3.60	116.62	111.85
18	A	515	HEA	C20-C21-C22	-3.59	94.24	112.02
20	A	524	PGV	O03-C19-C20	3.59	122.79	111.83
28	P	1265	PEK	O01-C1-C2	3.58	119.23	111.48
28	G	265	PEK	O03-C21-O04	-3.57	114.69	123.63
26	C	270	CDL	OB8-CB7-OB9	-3.57	114.70	123.63
18	N	515	HEA	C1B-C2B-C3B	-3.56	102.68	106.80
23	P	1525	CHD	C11-C9-C8	3.55	116.15	110.89
24	C	272	DMU	O7-C10-C5	3.55	116.82	108.09
24	M	526	DMU	C11-C9-C8	3.54	121.71	113.02
26	T	1269	CDL	OA6-CA5-OA7	-3.53	115.45	123.70
26	C	270	CDL	C52-C51-CB5	-3.53	100.77	113.69
23	P	1271	CHD	C21-C20-C17	3.53	118.18	112.88
24	M	526	DMU	O16-C6-C1	3.52	113.62	108.27
28	P	1265	PEK	O03-C21-O04	-3.52	114.83	123.63
23	O	229	CHD	C15-C14-C8	3.51	123.18	118.36
24	P	1272	DMU	C10-O1-C9	3.51	120.58	113.72
26	C	270	CDL	OA8-CA6-CA4	3.51	118.50	108.40
23	W	1060	CHD	C18-C13-C17	-3.50	105.71	111.20
20	P	1267	PGV	C8-C9-C10	-3.46	97.23	113.86
26	P	1270	CDL	OA8-CA7-C31	3.46	122.38	111.83
23	C	525	CHD	C11-C9-C8	3.46	116.01	110.89
23	W	1060	CHD	C13-C14-C8	3.46	119.09	114.72
18	A	515	HEA	C3B-C4B-NB	3.46	113.81	109.84
20	N	1524	PGV	C02-O01-C1	3.45	126.05	117.80
18	N	516	HEA	O2D-CGD-O1D	3.45	132.20	123.33
23	W	1060	CHD	C18-C13-C14	-3.43	105.82	111.20
24	C	272	DMU	C10-O1-C9	3.43	120.42	113.72
22	O	1230	PSC	O03-C19-C20	3.43	122.29	111.83
18	N	515	HEA	C1A-CHA-C4D	-3.42	118.75	126.02
23	J	60	CHD	O12-C12-C11	-3.40	102.21	109.12
23	P	1525	CHD	C14-C8-C9	3.40	114.49	109.75
24	M	526	DMU	O5-C6-O16	3.39	118.06	110.04
24	C	272	DMU	C11-C9-C8	3.39	121.34	113.02
19	Q	1523	TGL	CG3-OG3-CC1	3.37	129.45	117.12
18	N	516	HEA	OMA-CMA-C3A	-3.37	118.01	125.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	C4A-CHB-C1B	-3.37	118.86	126.02
23	B	1086	CHD	C6-C5-C4	-3.37	107.38	111.23
18	A	515	HEA	C1A-CHA-C4D	-3.35	118.90	126.02
24	M	526	DMU	C57-C4-C3	3.34	122.77	113.38
24	C	272	DMU	C6-O5-C4	3.33	120.23	113.72
23	O	229	CHD	O3-C3-C4	3.32	116.45	109.84
19	N	1522	TGL	OG3-CG3-CG2	3.31	117.94	108.40
26	T	1269	CDL	OB6-CB5-OB7	-3.31	115.97	123.70
18	N	515	HEA	CHA-C4D-C3D	-3.30	119.96	124.77
18	N	515	HEA	CAD-C3D-C2D	3.30	134.04	127.87
24	M	526	DMU	O1-C9-C11	3.30	114.61	106.44
26	P	1270	CDL	O1-C1-CA2	-3.30	98.30	109.70
19	N	1521	TGL	OG1-CA1-CA2	3.29	121.86	111.83
18	A	515	HEA	C1D-C2D-C3D	-3.28	103.53	106.98
23	O	229	CHD	C9-C11-C12	3.28	118.59	114.29
23	C	525	CHD	C15-C14-C8	3.27	122.84	118.36
23	J	60	CHD	C18-C13-C17	-3.27	106.09	111.20
19	N	1522	TGL	OG1-CA1-CA2	3.26	121.77	111.83
18	N	516	HEA	C4C-CHD-C1D	-3.25	118.61	126.25
28	G	1263	PEK	O03-C21-C22	3.24	121.72	111.83
24	M	526	DMU	O7-C10-C5	-3.24	100.12	108.09
24	Z	1526	DMU	C6-O5-C4	3.24	120.05	113.72
18	N	516	HEA	C4C-C3C-C2C	-3.23	103.28	107.30
19	Q	1523	TGL	OG1-CA1-OA1	-3.23	115.54	123.63
23	C	525	CHD	C14-C8-C9	3.22	114.25	109.75
24	M	526	DMU	O7-C10-O1	-3.22	102.23	110.69
23	J	60	CHD	C17-C13-C14	3.22	103.34	100.11
19	N	1521	TGL	OG3-CC1-CC2	3.21	121.63	111.83
28	G	265	PEK	O01-C1-C2	3.21	118.42	111.48
24	M	526	DMU	C1-C2-C3	3.19	116.93	109.68
19	Q	1523	TGL	OG2-CB1-CB2	3.19	118.38	111.48
23	C	525	CHD	C13-C14-C8	3.18	118.75	114.72
23	C	271	CHD	C23-C22-C20	-3.16	108.56	114.46
18	A	515	HEA	C1B-C2B-C3B	-3.15	103.15	106.80
20	P	1267	PGV	C27-C26-C25	-3.14	98.48	114.37
23	B	1086	CHD	O3-C3-C4	3.13	116.08	109.84
19	N	1522	TGL	OG1-CG1-CG2	3.13	117.43	108.40
24	Z	1526	DMU	C1-C2-C3	3.13	116.79	109.68
20	N	1524	PGV	O03-C19-C20	3.13	121.38	111.83
28	P	1264	PEK	C03-C02-C01	-3.13	104.50	111.78
28	G	1263	PEK	O03-C01-C02	3.13	117.41	108.40
19	D	523	TGL	C21-C20-CA9	3.12	130.14	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	521	TGL	OG2-CG2-CG1	3.12	119.53	108.34
18	A	515	HEA	CHC-C4B-C3B	-3.11	117.94	125.80
20	P	1267	PGV	O03-C01-C02	3.11	117.37	108.40
18	A	516	HEA	O1A-CGA-CBA	-3.11	113.23	123.09
20	A	522	PGV	O03-C01-C02	3.11	117.35	108.40
24	Z	1526	DMU	C10-O1-C9	3.11	119.79	113.72
20	P	1268	PGV	O04-C19-C20	-3.10	111.66	123.78
23	C	271	CHD	C19-C10-C1	-3.10	103.38	108.31
24	M	526	DMU	C10-C5-C7	3.09	116.51	110.01
26	G	269	CDL	OB6-CB5-OB7	-3.06	116.54	123.70
18	A	515	HEA	CAD-C3D-C4D	-3.05	119.38	124.70
18	N	515	HEA	C4A-NA-C1A	3.05	110.79	105.82
26	P	1270	CDL	OB8-CB7-OB9	-3.05	116.01	123.63
19	D	523	TGL	OG3-CC1-CC2	3.03	121.07	111.83
19	D	523	TGL	CB3-CB2-CB1	3.02	124.76	113.69
23	B	1086	CHD	O7-C7-C6	-3.01	102.37	109.86
18	N	515	HEA	C4A-C3A-C2A	-3.01	104.21	106.81
18	A	516	HEA	CHC-C1C-NC	-3.01	118.41	123.86
23	P	1271	CHD	O3-C3-C4	-3.00	103.86	109.84
18	A	515	HEA	C16-C17-C18	3.00	126.85	112.02
18	A	516	HEA	C4A-NA-C1A	2.98	110.69	105.82
18	N	516	HEA	C3B-C4B-NB	2.98	113.27	109.84
20	A	524	PGV	O01-C02-C01	2.98	119.04	108.34
18	A	515	HEA	CHC-C4B-NB	2.98	128.05	124.37
24	M	526	DMU	C7-C8-C9	2.97	115.62	110.23
19	N	1522	TGL	CC3-CC2-CC1	2.97	124.59	113.69
23	J	60	CHD	O7-C7-C6	-2.97	102.48	109.86
23	C	525	CHD	O3-C3-C4	2.96	115.74	109.84
26	T	1269	CDL	OA8-CA7-C31	2.95	120.83	111.83
28	T	263	PEK	O03-C21-C22	2.95	120.82	111.83
24	P	1272	DMU	O5-C6-O16	2.95	117.00	110.04
23	B	1086	CHD	C13-C17-C20	2.94	123.05	119.48
18	N	515	HEA	CHB-C1B-C2B	-2.94	120.39	125.03
26	G	269	CDL	OA8-CA7-C31	2.93	120.77	111.83
23	C	525	CHD	C16-C17-C20	2.92	116.60	112.18
24	P	1272	DMU	O7-C10-O1	2.92	118.37	110.69
23	B	1086	CHD	O7-C7-C8	-2.91	102.84	109.52
18	N	516	HEA	O1A-CGA-CBA	-2.91	113.85	123.09
24	P	1272	DMU	C10-C5-C7	2.91	116.12	110.01
20	A	522	PGV	C8-C9-C10	-2.90	99.90	113.86
19	Q	1523	TGL	OG1-CA1-CA2	2.90	120.69	111.83
23	O	229	CHD	C11-C9-C10	2.90	116.65	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	CAD-CBD-CGD	-2.90	105.98	113.67
23	B	1086	CHD	C22-C23-C24	-2.89	104.79	112.49
24	Z	1526	DMU	O49-C1-C6	-2.88	103.20	110.08
26	P	1270	CDL	OA8-CA7-OA9	-2.88	116.42	123.63
26	G	269	CDL	OA6-CA5-OA7	-2.88	116.97	123.70
23	C	525	CHD	C1-C10-C9	-2.88	106.87	111.34
18	N	515	HEA	CAA-CBA-CGA	-2.87	106.04	113.67
24	P	1272	DMU	O7-C10-C5	2.87	115.16	108.09
24	M	526	DMU	C10-O1-C9	2.86	119.31	113.72
18	N	515	HEA	CHA-C4D-ND	2.86	127.50	124.42
24	C	272	DMU	C1-C2-C3	2.86	116.16	109.68
24	C	272	DMU	O4-C7-C5	2.84	117.07	110.38
20	C	267	PGV	C8-C9-C10	-2.84	100.23	113.86
24	Z	1526	DMU	C10-C5-C7	2.83	115.97	110.01
19	D	523	TGL	C10-CB9-CB8	2.83	128.68	114.37
20	P	1267	PGV	C3-C2-C1	-2.83	103.33	113.69
19	D	523	TGL	CG3-OG3-CC1	2.83	127.45	117.12
18	A	515	HEA	O2A-CGA-CBA	2.82	122.90	114.00
18	N	516	HEA	C1D-C2D-C3D	-2.82	104.02	106.98
19	L	522	TGL	OG2-CG2-CG1	2.81	118.43	108.34
20	P	1268	PGV	C03-C02-C01	-2.81	105.24	111.78
20	C	268	PGV	O04-C19-C20	-2.80	112.82	123.78
28	T	263	PEK	C01-O03-C21	2.80	127.36	117.12
19	Q	1523	TGL	OG3-CC1-OC1	-2.79	116.64	123.63
18	N	515	HEA	C16-C17-C18	2.78	125.75	112.02
26	C	270	CDL	O1-C1-CB2	2.77	119.27	109.70
20	N	1266	PGV	C01-O03-C19	-2.77	107.00	117.12
19	N	1522	TGL	CG2-OG2-CB1	2.77	124.42	117.80
20	C	267	PGV	C3-C2-C1	-2.77	103.55	113.69
26	P	1270	CDL	CB4-OB6-CB5	-2.76	111.19	117.80
23	W	1060	CHD	C9-C8-C7	2.76	115.33	111.86
23	P	1525	CHD	C23-C22-C20	-2.75	109.33	114.46
19	D	523	TGL	C11-C10-CB9	2.74	128.24	114.37
23	C	525	CHD	C4-C5-C10	-2.74	109.74	112.66
22	B	230	PSC	C29-C28-C27	-2.74	100.52	114.37
23	P	1525	CHD	C1-C2-C3	2.73	114.10	110.48
24	C	272	DMU	O5-C6-O16	2.72	116.47	110.04
18	N	515	HEA	C17-C18-C19	-2.71	121.41	127.62
19	N	1521	TGL	OG3-CG3-CG2	2.71	116.20	108.40
20	C	267	PGV	C4-C3-C2	-2.70	103.20	113.13
18	A	515	HEA	C4C-CHD-C1D	2.69	132.57	126.25
19	N	1522	TGL	OG3-CC1-OC1	-2.69	116.91	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	1267	PGV	O14-P-O13	2.68	124.89	112.44
23	W	1060	CHD	C17-C13-C14	2.67	102.80	100.11
23	W	1060	CHD	C11-C9-C10	2.67	116.42	113.70
24	M	526	DMU	O4-C7-C8	2.67	116.66	110.38
24	Z	1526	DMU	C6-C1-C2	2.67	115.62	110.01
26	P	1270	CDL	OB6-CB4-CB6	2.66	117.90	108.34
26	C	270	CDL	C42-C41-C40	2.66	127.83	114.37
18	A	515	HEA	C3D-C4D-ND	2.66	112.92	110.35
20	P	1267	PGV	C03-C02-C01	-2.66	105.58	111.78
23	C	525	CHD	O7-C7-C6	-2.66	103.25	109.86
26	C	270	CDL	OB6-CB5-C51	2.66	117.23	111.48
23	C	525	CHD	C19-C10-C1	2.64	112.51	108.31
20	N	1524	PGV	O01-C02-C01	2.64	117.83	108.34
22	O	1230	PSC	C31-C30-C29	-2.64	101.02	114.37
28	P	1264	PEK	C24-C23-C22	-2.64	103.43	113.13
24	C	272	DMU	C10-C5-C7	2.64	115.56	110.01
18	A	516	HEA	C4A-C3A-C2A	2.64	109.10	106.81
18	A	515	HEA	CAA-CBA-CGA	-2.63	106.68	113.67
28	G	264	PEK	C26-C25-C24	-2.63	101.06	114.37
18	A	516	HEA	CAA-CBA-CGA	-2.63	106.70	113.67
18	A	516	HEA	C3A-C2A-C1A	-2.61	104.57	107.05
24	Z	1526	DMU	O5-C6-O16	2.61	116.22	110.04
26	T	1269	CDL	OB8-CB7-OB9	-2.61	117.09	123.63
24	Z	1526	DMU	O3-C5-C7	2.61	116.54	110.38
26	G	269	CDL	CA6-OA8-CA7	2.61	126.66	117.12
23	J	60	CHD	C9-C8-C7	2.61	115.14	111.86
20	A	524	PGV	C4-C3-C2	-2.61	103.55	113.13
23	B	1086	CHD	C4-C5-C10	-2.61	109.89	112.66
26	G	269	CDL	OB8-CB7-OB9	-2.60	117.13	123.63
28	T	263	PEK	C02-O01-C1	2.59	124.00	117.80
20	C	267	PGV	O01-C02-C03	-2.59	99.05	108.34
28	G	264	PEK	C31-C30-C29	-2.59	101.30	114.37
28	G	264	PEK	O01-C1-C2	2.58	117.07	111.48
20	N	1266	PGV	C02-O01-C1	2.58	123.97	117.80
26	T	1269	CDL	C83-C82-C81	2.58	127.40	114.37
18	N	515	HEA	CHD-C1D-C2D	-2.57	119.63	126.95
19	N	1521	TGL	CG1-OG1-CA1	2.57	126.51	117.12
24	P	1272	DMU	C57-C4-C3	2.57	120.60	113.38
22	B	230	PSC	O03-C19-C20	2.56	119.64	111.83
23	C	271	CHD	C14-C8-C7	2.56	115.25	111.85
26	P	1270	CDL	C39-C38-C37	2.56	127.29	114.37
26	G	269	CDL	C82-C81-C80	2.55	127.28	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	1269	CDL	C80-C79-C78	2.55	127.24	114.37
18	N	515	HEA	CHA-C1A-NA	2.54	127.22	124.45
23	P	1525	CHD	O7-C7-C8	-2.54	103.70	109.52
18	N	515	HEA	C3A-C2A-C1A	2.54	109.45	107.05
23	J	60	CHD	C19-C10-C9	-2.54	107.77	111.18
20	P	1267	PGV	O01-C1-O02	-2.54	117.77	123.70
20	A	522	PGV	O03-C19-O04	-2.54	117.28	123.63
20	P	1267	PGV	O06-C06-C05	-2.54	98.95	110.38
26	C	270	CDL	OA8-CA7-OA9	-2.53	117.29	123.63
26	P	1270	CDL	C42-C41-C40	2.53	127.15	114.37
20	C	267	PGV	O01-C1-O02	-2.52	117.81	123.70
18	A	515	HEA	CHA-C1A-NA	2.51	127.19	124.45
18	N	515	HEA	C2B-C1B-NB	2.51	112.81	109.90
24	M	526	DMU	C6-O5-C4	2.51	118.61	113.72
24	M	526	DMU	O3-C5-C7	2.50	116.28	110.38
28	P	1265	PEK	O03-C01-C02	2.50	115.61	108.40
24	P	1272	DMU	O7-C3-C4	2.49	116.02	109.48
26	T	1269	CDL	CB6-OB8-CB7	2.49	126.24	117.12
19	Q	1523	TGL	OG2-CG2-CG3	2.49	117.29	108.34
19	A	521	TGL	C15-CC9-CC8	2.49	126.96	114.37
20	N	1266	PGV	O14-P-O11	2.49	118.85	107.57
20	N	1524	PGV	C01-O03-C19	2.49	126.21	117.12
18	N	516	HEA	CHD-C4C-NC	2.48	128.37	123.86
20	N	1266	PGV	O01-C1-C2	2.46	116.80	111.48
19	N	1521	TGL	OG3-CC1-OC1	-2.46	117.48	123.63
26	T	1269	CDL	OB8-CB7-C71	2.45	119.32	111.83
18	A	516	HEA	CMD-C2D-C1D	2.45	128.86	125.03
23	B	1086	CHD	O26-C24-C23	2.45	121.74	114.00
18	A	515	HEA	O1A-CGA-CBA	-2.45	115.33	123.09
18	N	515	HEA	CMD-C2D-C1D	2.45	128.86	125.03
22	B	230	PSC	C02-O01-C1	2.44	123.64	117.80
26	C	270	CDL	C63-C62-C61	2.44	126.71	114.37
18	A	516	HEA	CHB-C1B-C2B	-2.44	121.17	125.03
18	N	515	HEA	O11-C11-C12	-2.44	102.67	109.14
23	C	271	CHD	O12-C12-C13	-2.44	106.90	111.02
20	P	1268	PGV	O03-C19-O04	-2.44	117.53	123.63
24	P	1272	DMU	O7-C3-C2	2.44	113.42	107.23
22	O	1230	PSC	O03-C19-O04	-2.44	117.53	123.63
28	P	1264	PEK	O04-C21-C22	2.44	133.31	123.78
28	G	264	PEK	O02-C1-C2	2.43	133.30	123.78
23	C	525	CHD	O7-C7-C8	-2.43	103.95	109.52
19	N	1522	TGL	OG3-CC1-CC2	2.43	119.25	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	O2A-CGA-CBA	2.42	121.66	114.00
20	A	522	PGV	C24-C23-C22	2.42	126.61	114.37
26	T	1269	CDL	OB8-CB6-CB4	2.42	115.37	108.40
18	A	516	HEA	CHC-C4B-C3B	-2.42	119.70	125.80
20	C	267	PGV	O12-P-O13	-2.42	99.36	108.94
23	P	1525	CHD	C18-C13-C12	-2.41	106.64	109.06
26	G	269	CDL	C83-C82-C81	2.40	126.51	114.37
20	C	268	PGV	O03-C01-C02	2.40	115.32	108.40
19	A	521	TGL	CB7-CB6-CB5	-2.40	102.26	114.37
18	A	516	HEA	C3D-C4D-ND	2.40	112.67	110.35
18	N	515	HEA	C4C-NC-C1C	-2.39	101.92	105.82
23	J	60	CHD	C13-C14-C8	2.39	117.75	114.72
20	N	1266	PGV	O03-C01-C02	2.38	115.27	108.40
19	L	522	TGL	CA5-CA4-CA3	-2.38	102.33	114.37
23	P	1271	CHD	C19-C10-C5	-2.38	106.46	110.44
24	P	1272	DMU	C18-O16-C6	2.38	117.74	113.68
26	C	270	CDL	OB8-CB6-CB4	-2.37	101.56	108.40
19	L	522	TGL	OG2-CB1-CB2	2.37	116.61	111.48
26	P	1270	CDL	CA6-CA4-CA3	-2.37	106.26	111.78
19	N	1522	TGL	CB3-CB2-CB1	2.37	122.38	113.69
26	G	269	CDL	C80-C79-C78	2.37	126.33	114.37
28	P	1264	PEK	O01-C1-C2	2.37	116.60	111.48
23	C	525	CHD	C15-C16-C17	2.36	109.76	105.14
24	P	1272	DMU	O16-C18-C19	2.36	117.36	109.37
18	N	516	HEA	C4B-C3B-C2B	-2.36	103.48	107.44
20	N	1266	PGV	C8-C7-C6	-2.35	102.47	114.37
23	C	271	CHD	C21-C20-C17	2.35	116.41	112.88
26	C	270	CDL	C39-C38-C37	2.35	126.23	114.37
19	D	523	TGL	OG3-CC1-OC1	-2.35	117.76	123.63
18	N	516	HEA	CHD-C1D-C2D	-2.34	120.31	126.95
28	G	264	PEK	O03-C01-C02	-2.33	101.68	108.40
26	P	1270	CDL	CB6-CB4-CB3	-2.33	106.36	111.78
20	N	1266	PGV	C03-C02-C01	-2.32	106.37	111.78
24	Z	1526	DMU	O2-C8-C7	-2.31	104.92	110.38
19	A	521	TGL	OG1-CA1-OA1	-2.31	117.85	123.63
19	N	1522	TGL	CG3-OG3-CC1	2.30	125.54	117.12
23	B	1086	CHD	C13-C14-C8	2.30	117.64	114.72
28	G	1263	PEK	O01-C1-O02	-2.30	118.33	123.70
19	L	522	TGL	CA9-CA8-CA7	-2.30	102.76	114.37
20	A	524	PGV	C01-O03-C19	2.29	125.50	117.12
23	P	1271	CHD	C6-C5-C4	-2.29	108.61	111.23
18	N	516	HEA	C4A-CHB-C1B	-2.29	121.16	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	522	PGV	C28-C27-C26	2.29	125.92	114.37
23	P	1525	CHD	C21-C20-C22	-2.28	106.81	110.34
22	O	1230	PSC	O01-C1-O02	-2.28	118.37	123.70
23	J	60	CHD	C11-C9-C10	2.28	116.02	113.70
23	B	1086	CHD	C21-C20-C22	-2.27	106.82	110.34
24	M	526	DMU	O49-C1-C2	2.27	115.73	110.38
18	A	515	HEA	CHB-C1B-C2B	-2.27	121.44	125.03
24	Z	1526	DMU	C57-C4-C3	2.27	119.75	113.38
26	T	1269	CDL	C23-C22-C21	2.26	125.80	114.37
19	L	522	TGL	CB9-CB8-CB7	-2.26	102.94	114.37
20	P	1267	PGV	O12-P-O13	-2.26	99.98	108.94
18	N	516	HEA	CHB-C1B-C2B	-2.26	121.46	125.03
28	G	264	PEK	C32-C31-C30	-2.26	102.97	114.37
18	N	516	HEA	C2A-C1A-NA	2.26	112.50	110.32
26	P	1270	CDL	OA6-CA5-OA7	-2.25	118.44	123.70
24	Z	1526	DMU	C31-C28-C25	-2.25	102.99	114.37
26	T	1269	CDL	OA8-CA7-OA9	-2.25	118.00	123.63
18	N	515	HEA	CBC-CAC-C3C	-2.24	116.31	127.53
18	A	516	HEA	O2A-CGA-CBA	2.24	121.07	114.00
26	C	270	CDL	CA6-CA4-CA3	-2.23	106.58	111.78
20	A	524	PGV	C3-C2-C1	2.23	121.86	113.69
23	P	1271	CHD	C13-C14-C8	2.22	117.53	114.72
20	C	267	PGV	O06-C06-C05	-2.22	100.38	110.38
20	C	267	PGV	C22-C21-C20	-2.22	104.97	113.13
18	A	516	HEA	C3C-C4C-NC	2.21	111.66	109.80
20	C	267	PGV	O03-C19-O04	-2.21	118.09	123.63
19	N	1521	TGL	CB3-CB2-CB1	2.21	121.78	113.69
26	P	1270	CDL	OB6-CB4-CB3	-2.21	100.42	108.34
28	T	263	PEK	O04-C21-C22	-2.21	115.15	123.78
20	N	1524	PGV	O01-C1-O02	-2.20	118.56	123.70
18	N	516	HEA	CHA-C4D-C3D	-2.20	121.56	124.77
19	Q	1523	TGL	C21-C20-CA9	2.20	125.48	114.37
24	M	526	DMU	C34-C31-C28	-2.20	103.26	114.37
28	P	1265	PEK	P-O11-C03	2.19	133.90	121.35
23	B	1086	CHD	C16-C17-C20	2.18	115.48	112.18
20	P	1267	PGV	C9-C8-C7	-2.18	103.35	114.37
18	A	516	HEA	C4C-CHD-C1D	2.18	131.37	126.25
26	G	269	CDL	OB8-CB7-C71	2.17	118.46	111.83
24	Z	1526	DMU	C11-C9-C8	2.17	118.36	113.02
18	N	515	HEA	C3D-C4D-ND	2.17	112.45	110.35
19	Q	1523	TGL	C16-C15-CC9	2.16	125.30	114.37
28	P	1264	PEK	O02-C1-C2	2.15	132.20	123.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	CA6-CA4-CA3	2.15	116.80	111.78
18	N	515	HEA	CHC-C4B-C3B	-2.14	120.39	125.80
28	G	264	PEK	O12-P-O14	2.13	117.39	108.94
20	C	267	PGV	O14-P-O13	2.13	122.35	112.44
18	A	516	HEA	C1A-CHA-C4D	-2.13	121.50	126.02
19	N	1521	TGL	C15-CC9-CC8	2.13	125.12	114.37
18	A	515	HEA	C16-C15-C14	-2.12	116.41	121.17
26	T	1269	CDL	OB5-PB2-OB3	-2.11	100.57	108.94
20	P	1268	PGV	C21-C20-C19	-2.11	105.96	113.69
20	P	1267	PGV	C10-C11-C12	-2.11	109.04	124.83
19	N	1521	TGL	OG1-CA1-OA1	-2.10	118.36	123.63
19	N	1521	TGL	OG2-CG2-CG3	2.10	115.89	108.34
23	C	525	CHD	O26-C24-C23	2.10	120.64	114.00
26	C	270	CDL	C57-C56-C55	-2.10	103.74	114.37
18	A	515	HEA	O2D-CGD-O1D	-2.10	117.93	123.33
20	A	522	PGV	C03-C02-C01	-2.10	106.89	111.78
18	N	516	HEA	C1B-C2B-C3B	2.09	109.22	106.80
20	A	522	PGV	C3-C2-C1	-2.09	106.03	113.69
23	P	1271	CHD	C16-C15-C14	2.09	109.23	105.14
19	A	521	TGL	C20-CA9-CA8	2.09	124.92	114.37
20	N	1524	PGV	O03-C19-O04	-2.09	118.41	123.63
18	A	515	HEA	C26-C15-C14	-2.08	118.28	123.63
18	N	516	HEA	C3C-C4C-NC	2.08	111.55	109.80
28	G	1263	PEK	C02-O01-C1	2.08	122.77	117.80
26	T	1269	CDL	CA4-OA6-CA5	-2.08	112.83	117.80
28	P	1265	PEK	C33-C32-C31	-2.08	103.87	114.37
19	L	522	TGL	C24-C23-C22	-2.08	103.87	114.37
20	C	268	PGV	O14-P-O13	2.07	122.09	112.44
18	A	515	HEA	C3A-C2A-C1A	2.07	109.00	107.05
24	Z	1526	DMU	C28-C25-C22	-2.07	103.90	114.37
23	O	229	CHD	C19-C10-C5	2.07	113.89	110.44
18	A	515	HEA	C12-C13-C14	-2.07	106.72	112.16
24	M	526	DMU	O7-C3-C2	2.07	112.49	107.23
28	G	264	PEK	C3-C2-C1	-2.07	106.12	113.69
26	C	270	CDL	OA4-PA1-OA3	2.06	122.03	112.44
20	A	524	PGV	O03-C19-O04	-2.05	118.49	123.63
19	Q	1523	TGL	OG3-CG3-CG2	2.05	114.32	108.40
26	P	1270	CDL	OA4-PA1-OA3	2.05	122.00	112.44
18	N	516	HEA	CBD-CAD-C3D	2.05	118.20	112.53
22	O	1230	PSC	C27-C26-C25	-2.05	104.01	114.37
26	P	1270	CDL	C20-C19-C18	2.05	124.72	114.37
18	N	515	HEA	C20-C19-C18	2.05	125.76	121.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	270	CDL	C53-C52-C51	-2.05	105.61	113.13
28	G	265	PEK	C01-O03-C21	2.04	124.58	117.12
19	A	521	TGL	C21-C20-CA9	2.04	124.67	114.37
24	C	272	DMU	C57-C4-C3	2.04	119.11	113.38
23	W	1060	CHD	C16-C15-C14	2.03	109.12	105.14
18	A	515	HEA	CHA-C1A-C2A	2.03	128.07	124.86
23	J	60	CHD	C21-C20-C17	-2.03	109.83	112.88
18	A	516	HEA	CHB-C4A-C3A	-2.03	121.79	125.21
26	G	269	CDL	C20-C19-C18	2.03	124.61	114.37
20	N	1266	PGV	O14-P-O12	-2.03	98.39	107.57
18	N	515	HEA	CMB-C2B-C1B	2.02	128.19	125.03
19	D	523	TGL	C13-C12-C11	2.01	124.53	114.37
26	P	1270	CDL	O1-C1-CB2	2.00	116.61	109.70
19	D	523	TGL	C16-C15-CC9	2.00	124.48	114.37

All (28) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	C	271	CHD	C9
23	J	60	CHD	C9
23	J	60	CHD	C17
23	O	229	CHD	C9
23	P	1271	CHD	C9
23	W	1060	CHD	C9
23	W	1060	CHD	C17
24	C	272	DMU	C6
24	C	272	DMU	C4
24	C	272	DMU	C9
24	C	272	DMU	C2
24	C	272	DMU	C5
24	C	272	DMU	C3
24	M	526	DMU	C4
24	M	526	DMU	C9
24	M	526	DMU	C2
24	M	526	DMU	C5
24	M	526	DMU	C6
24	P	1272	DMU	C6
24	P	1272	DMU	C4
24	P	1272	DMU	C9
24	P	1272	DMU	C2
24	P	1272	DMU	C5
24	Z	1526	DMU	C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	Z	1526	DMU	C9
24	Z	1526	DMU	C2
24	Z	1526	DMU	C5
24	Z	1526	DMU	C6

All (959) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	515	HEA	C2A-C3A-CMA-OMA
18	A	515	HEA	C4A-C3A-CMA-OMA
18	A	515	HEA	C16-C17-C18-C19
19	A	521	TGL	CB2-CB1-OG2-CG2
19	A	521	TGL	CG2-CG3-OG3-CC1
19	D	523	TGL	CC2-CC1-OG3-CG3
19	D	523	TGL	OC1-CC1-OG3-CG3
19	L	522	TGL	CB2-CB1-OG2-CG2
19	N	1522	TGL	CB2-CB1-OG2-CG2
20	A	524	PGV	C03-O11-P-O12
20	A	524	PGV	C03-O11-P-O14
20	A	524	PGV	C03-C02-O01-C1
20	A	524	PGV	C02-C03-O11-P
20	A	524	PGV	O02-C1-O01-C02
20	A	524	PGV	C2-C1-O01-C02
20	A	524	PGV	O04-C19-O03-C01
20	A	524	PGV	C20-C19-O03-C01
20	C	268	PGV	O01-C02-C03-O11
20	C	268	PGV	C04-C05-C06-O06
20	N	1524	PGV	C03-O11-P-O12
20	N	1524	PGV	C03-O11-P-O14
20	N	1524	PGV	C04-O12-P-O14
20	N	1524	PGV	C02-C03-O11-P
20	N	1524	PGV	O02-C1-O01-C02
20	N	1524	PGV	C2-C1-O01-C02
20	P	1268	PGV	O03-C01-C02-O01
20	P	1268	PGV	C04-C05-C06-O06
22	B	230	PSC	C04-O12-P-O11
22	B	230	PSC	C04-O12-P-O13
22	O	1230	PSC	C03-O11-P-O14
23	J	60	CHD	C16-C17-C20-C22
23	W	1060	CHD	C13-C17-C20-C22
23	W	1060	CHD	C16-C17-C20-C21
23	W	1060	CHD	C16-C17-C20-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	M	526	DMU	O5-C6-O16-C18
24	M	526	DMU	C19-C18-O16-C6
24	Z	1526	DMU	O5-C6-O16-C18
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CA3-OA5-PA1-OA2
26	C	270	CDL	CA3-OA5-PA1-OA3
26	C	270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB3
26	C	270	CDL	CB2-OB2-PB2-OB4
26	C	270	CDL	OB7-CB5-OB6-CB4
26	C	270	CDL	C51-CB5-OB6-CB4
26	G	269	CDL	CA2-OA2-PA1-OA3
26	G	269	CDL	CA2-OA2-PA1-OA5
26	G	269	CDL	CA3-OA5-PA1-OA2
26	G	269	CDL	CA3-OA5-PA1-OA4
26	G	269	CDL	C11-CA5-OA6-CA4
26	G	269	CDL	C1-CB2-OB2-PB2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CA3-OA5-PA1-OA2
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB4
26	P	1270	CDL	CB3-OB5-PB2-OB2
26	P	1270	CDL	CB3-OB5-PB2-OB3
26	P	1270	CDL	C51-CB5-OB6-CB4
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB3-OB5-PB2-OB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
28	G	264	PEK	C6-C7-C8-C9
28	G	265	PEK	O12-C04-C05-N
28	G	265	PEK	C4-C5-C6-C7
28	G	1263	PEK	C03-O11-P-O12
28	G	1263	PEK	C03-O11-P-O13
28	G	1263	PEK	C03-O11-P-O14
28	G	1263	PEK	C04-O12-P-O11
28	G	1263	PEK	C04-O12-P-O13
28	G	1263	PEK	C04-O12-P-O14
28	G	1263	PEK	O03-C01-C02-O01
28	P	1264	PEK	C6-C7-C8-C9
28	P	1265	PEK	C04-O12-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	P	1265	PEK	C04-O12-P-O14
28	P	1265	PEK	C4-C5-C6-C7
28	P	1265	PEK	C6-C7-C8-C9
28	T	263	PEK	C03-O11-P-O12
28	T	263	PEK	C03-O11-P-O13
28	T	263	PEK	O12-C04-C05-N
28	T	263	PEK	C5-C6-C7-C8
28	T	263	PEK	C11-C12-C13-C14
19	Q	1523	TGL	OC1-CC1-OG3-CG3
20	N	1524	PGV	O04-C19-O03-C01
19	N	1521	TGL	CG2-CG3-OG3-CC1
20	N	1524	PGV	C20-C19-O03-C01
19	A	521	TGL	OC1-CC1-OG3-CG3
19	N	1521	TGL	OC1-CC1-OG3-CG3
24	C	272	DMU	O6-C11-C9-O1
24	M	526	DMU	O5-C4-C57-O61
19	A	521	TGL	OB1-CB1-OG2-CG2
19	N	1522	TGL	OB1-CB1-OG2-CG2
26	C	270	CDL	OA7-CA5-OA6-CA4
26	G	269	CDL	OA7-CA5-OA6-CA4
26	P	1270	CDL	OA7-CA5-OA6-CA4
26	P	1270	CDL	OB7-CB5-OB6-CB4
19	A	521	TGL	CC2-CC1-OG3-CG3
19	Q	1523	TGL	CC2-CC1-OG3-CG3
18	A	515	HEA	C26-C15-C16-C17
18	A	515	HEA	C14-C15-C16-C17
19	L	522	TGL	CA2-CA1-OG1-CG1
19	N	1521	TGL	CC2-CC1-OG3-CG3
19	N	1522	TGL	CA2-CA1-OG1-CG1
22	O	1230	PSC	C20-C19-O03-C01
20	N	1524	PGV	C10-C11-C12-C13
28	G	264	PEK	C13-C14-C15-C16
28	T	263	PEK	C13-C14-C15-C16
19	L	522	TGL	CC3-CC4-CC5-CC6
22	O	1230	PSC	O04-C19-O03-C01
19	L	522	TGL	OB1-CB1-OG2-CG2
23	J	60	CHD	C16-C17-C20-C21
26	P	1270	CDL	O1-C1-CB2-OB2
26	T	1269	CDL	O1-C1-CA2-OA2
22	B	230	PSC	C20-C19-O03-C01
24	P	1272	DMU	O6-C11-C9-O1
24	Z	1526	DMU	O5-C4-C57-O61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	L	522	TGL	CC1-CC2-CC3-CC4
19	N	1522	TGL	CC1-CC2-CC3-CC4
19	N	1522	TGL	OA1-CA1-OG1-CG1
19	N	1522	TGL	CC3-CC4-CC5-CC6
24	C	272	DMU	O5-C4-C57-O61
24	Z	1526	DMU	O6-C11-C9-O1
19	L	522	TGL	OA1-CA1-OG1-CG1
19	N	1521	TGL	CB3-CB4-CB5-CB6
18	N	515	HEA	C15-C16-C17-C18
26	C	270	CDL	C83-C84-C85-C86
23	P	1271	CHD	C21-C20-C22-C23
26	P	1270	CDL	C82-C83-C84-C85
19	Q	1523	TGL	CA2-CA1-OG1-CG1
26	T	1269	CDL	C71-CB7-OB8-CB6
19	N	1521	TGL	C21-C20-CA9-CA8
26	C	270	CDL	C38-C39-C40-C41
22	B	230	PSC	C20-C21-C22-C23
26	T	1269	CDL	C79-C80-C81-C82
20	P	1267	PGV	C10-C11-C12-C13
22	O	1230	PSC	C11-C10-C9-C8
28	G	264	PEK	C10-C11-C12-C13
28	G	265	PEK	C7-C8-C9-C10
28	G	265	PEK	C10-C11-C12-C13
28	G	1263	PEK	C4-C5-C6-C7
28	G	1263	PEK	C7-C8-C9-C10
28	G	1263	PEK	C13-C14-C15-C16
28	P	1264	PEK	C7-C8-C9-C10
28	P	1265	PEK	C10-C11-C12-C13
22	B	230	PSC	O04-C19-O03-C01
23	C	271	CHD	C21-C20-C22-C23
26	G	269	CDL	C59-C60-C61-C62
19	Q	1523	TGL	OA1-CA1-OG1-CG1
26	C	270	CDL	CB2-C1-CA2-OA2
26	C	270	CDL	C71-CB7-OB8-CB6
19	Q	1523	TGL	C17-C18-C19-C33
26	T	1269	CDL	C56-C57-C58-C59
26	T	1269	CDL	C73-C74-C75-C76
19	A	521	TGL	C12-C13-C14-C29
22	O	1230	PSC	C20-C21-C22-C23
26	P	1270	CDL	C61-C62-C63-C64
19	D	523	TGL	CB9-C10-C11-C12
28	P	1265	PEK	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	D	523	TGL	C21-C22-C23-C24
24	P	1272	DMU	C1-C6-O16-C18
19	Q	1523	TGL	C21-C22-C23-C24
26	C	270	CDL	O1-C1-CA2-OA2
26	C	270	CDL	C78-C79-C80-C81
20	A	524	PGV	C19-C20-C21-C22
26	G	269	CDL	CA7-C31-C32-C33
23	P	1271	CHD	C17-C20-C22-C23
26	C	270	CDL	OB5-CB3-CB4-OB6
24	M	526	DMU	O6-C11-C9-C8
28	G	265	PEK	C34-C35-C36-C37
20	C	267	PGV	C10-C11-C12-C13
19	A	521	TGL	C21-C20-CA9-CA8
22	B	230	PSC	C19-C20-C21-C22
26	G	269	CDL	CB5-C51-C52-C53
26	P	1270	CDL	CB7-C71-C72-C73
26	G	269	CDL	C79-C80-C81-C82
26	T	1269	CDL	C22-C23-C24-C25
28	T	263	PEK	C33-C34-C35-C36
24	Z	1526	DMU	O16-C18-C19-C22
23	J	60	CHD	C13-C17-C20-C21
22	O	1230	PSC	C04-C05-N-C06
22	O	1230	PSC	C04-C05-N-C08
19	L	522	TGL	CB1-CB2-CB3-CB4
19	N	1522	TGL	CB1-CB2-CB3-CB4
20	A	524	PGV	C1-C2-C3-C4
22	O	1230	PSC	C1-C2-C3-C4
26	G	269	CDL	CA5-C11-C12-C13
28	G	1263	PEK	C21-C22-C23-C24
26	C	270	CDL	OB9-CB7-OB8-CB6
23	W	1060	CHD	C20-C22-C23-C24
19	D	523	TGL	CB1-CB2-CB3-CB4
20	N	1524	PGV	C19-C20-C21-C22
26	T	1269	CDL	CB7-C71-C72-C73
28	G	265	PEK	C1-C2-C3-C4
28	P	1264	PEK	C1-C2-C3-C4
24	C	272	DMU	O5-C6-O16-C18
28	G	265	PEK	C28-C29-C30-C31
19	N	1522	TGL	C20-C21-C22-C23
26	T	1269	CDL	O1-C1-CB2-OB2
28	G	265	PEK	C22-C21-O03-C01
26	T	1269	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	P	1267	PGV	C1-C2-C3-C4
22	O	1230	PSC	C11-C12-C13-C14
28	G	264	PEK	C7-C8-C9-C10
28	P	1264	PEK	C10-C11-C12-C13
28	T	263	PEK	C10-C11-C12-C13
24	P	1272	DMU	O16-C18-C19-C22
26	G	269	CDL	C63-C64-C65-C66
18	N	515	HEA	C16-C17-C18-C19
26	G	269	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CA2-C1-CB2-OB2
28	G	1263	PEK	C33-C34-C35-C36
22	B	230	PSC	C04-C05-N-C08
24	P	1272	DMU	C3-C4-C57-O61
20	C	268	PGV	C2-C1-O01-C02
20	C	268	PGV	O02-C1-O01-C02
24	C	272	DMU	C1-C6-O16-C18
28	G	264	PEK	C4-C5-C6-C7
26	G	269	CDL	O1-C1-CB2-OB2
23	C	271	CHD	C17-C20-C22-C23
20	P	1268	PGV	C02-C03-O11-P
19	D	523	TGL	CG3-CG2-OG2-CB1
26	G	269	CDL	C40-C41-C42-C43
26	T	1269	CDL	C51-CB5-OB6-CB4
28	G	265	PEK	O04-C21-O03-C01
22	B	230	PSC	C02-C01-O03-C19
20	P	1268	PGV	C13-C14-C15-C16
26	C	270	CDL	C58-C59-C60-C61
26	G	269	CDL	C36-C37-C38-C39
26	G	269	CDL	C37-C38-C39-C40
26	G	269	CDL	C75-C76-C77-C78
26	P	1270	CDL	C14-C15-C16-C17
19	N	1521	TGL	CB4-CB5-CB6-CB7
19	N	1521	TGL	C16-C17-C18-C19
20	N	1524	PGV	C2-C3-C4-C5
20	N	1524	PGV	C14-C15-C16-C17
26	C	270	CDL	C57-C58-C59-C60
26	P	1270	CDL	C12-C13-C14-C15
26	P	1270	CDL	C15-C16-C17-C18
26	P	1270	CDL	C17-C18-C19-C20
26	P	1270	CDL	C77-C78-C79-C80
26	T	1269	CDL	C36-C37-C38-C39
28	G	264	PEK	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	524	PGV	C10-C11-C12-C13
19	A	521	TGL	CA5-CA6-CA7-CA8
19	A	521	TGL	CC4-CC5-CC6-CC7
19	L	522	TGL	C18-C19-C33-C34
19	N	1522	TGL	CB5-CB6-CB7-CB8
19	N	1522	TGL	CC6-CC7-CC8-CC9
20	C	267	PGV	C7-C8-C9-C10
20	C	268	PGV	C30-C31-C32-C33
22	O	1230	PSC	C2-C3-C4-C5
26	T	1269	CDL	C61-C62-C63-C64
19	N	1522	TGL	C12-C13-C14-C29
19	N	1522	TGL	C21-C22-C23-C24
19	Q	1523	TGL	CC2-CC3-CC4-CC5
20	A	522	PGV	C27-C28-C29-C30
20	P	1268	PGV	C14-C15-C16-C17
26	C	270	CDL	C16-C17-C18-C19
26	P	1270	CDL	C72-C73-C74-C75
26	T	1269	CDL	C63-C64-C65-C66
28	P	1264	PEK	C25-C26-C27-C28
20	C	268	PGV	O05-C05-C06-O06
20	P	1268	PGV	O05-C05-C06-O06
24	Z	1526	DMU	C28-C31-C34-C37
26	P	1270	CDL	C16-C17-C18-C19
26	P	1270	CDL	C62-C63-C64-C65
26	P	1270	CDL	C73-C74-C75-C76
28	T	263	PEK	C16-C17-C18-C19
19	N	1521	TGL	CA4-CA5-CA6-CA7
26	G	269	CDL	C34-C35-C36-C37
26	T	1269	CDL	C54-C55-C56-C57
19	L	522	TGL	C10-C11-C12-C13
19	N	1521	TGL	CA1-CA2-CA3-CA4
20	C	267	PGV	C1-C2-C3-C4
22	B	230	PSC	C1-C2-C3-C4
19	L	522	TGL	C17-C18-C19-C33
19	N	1522	TGL	C16-C17-C18-C19
20	A	524	PGV	C20-C21-C22-C23
24	C	272	DMU	C28-C31-C34-C37
26	C	270	CDL	C39-C40-C41-C42
26	G	269	CDL	C73-C74-C75-C76
26	P	1270	CDL	C37-C38-C39-C40
19	L	522	TGL	C22-C23-C24-C25
26	G	269	CDL	C77-C78-C79-C80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C63-C64-C65-C66
28	P	1265	PEK	C33-C34-C35-C36
19	Q	1523	TGL	CC6-CC7-CC8-CC9
22	B	230	PSC	C24-C25-C26-C27
24	Z	1526	DMU	C25-C28-C31-C34
26	T	1269	CDL	OB7-CB5-OB6-CB4
19	N	1521	TGL	C11-C12-C13-C14
20	C	268	PGV	C6-C7-C8-C9
20	A	524	PGV	O03-C01-C02-C03
19	A	521	TGL	CB4-CB5-CB6-CB7
19	N	1522	TGL	C23-C24-C25-C26
19	Q	1523	TGL	CC5-CC6-CC7-CC8
26	C	270	CDL	C19-C20-C21-C22
26	P	1270	CDL	C58-C59-C60-C61
26	T	1269	CDL	C19-C20-C21-C22
28	G	264	PEK	C1-C2-C3-C4
19	A	521	TGL	C11-C10-CB9-CB8
19	A	521	TGL	C22-C23-C24-C25
19	N	1522	TGL	CA2-CA3-CA4-CA5
20	C	268	PGV	C26-C27-C28-C29
20	N	1524	PGV	C22-C23-C24-C25
22	O	1230	PSC	C27-C28-C29-C30
26	C	270	CDL	C14-C15-C16-C17
26	G	269	CDL	C35-C36-C37-C38
26	T	1269	CDL	C34-C35-C36-C37
26	T	1269	CDL	C59-C60-C61-C62
28	G	265	PEK	C33-C34-C35-C36
28	P	1264	PEK	C32-C33-C34-C35
28	T	263	PEK	C25-C26-C27-C28
19	L	522	TGL	C21-C20-CA9-CA8
20	P	1267	PGV	C13-C14-C15-C16
28	T	263	PEK	C26-C27-C28-C29
20	P	1268	PGV	C2-C3-C4-C5
26	G	269	CDL	C71-C72-C73-C74
22	O	1230	PSC	C04-C05-N-C07
19	D	523	TGL	CC5-CC6-CC7-CC8
19	Q	1523	TGL	CB6-CB7-CB8-CB9
19	Q	1523	TGL	C16-C15-CC9-CC8
22	B	230	PSC	C30-C31-C32-C33
26	P	1270	CDL	C59-C60-C61-C62
26	T	1269	CDL	C11-C12-C13-C14
20	A	522	PGV	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	P	1264	PEK	C35-C36-C37-C38
20	C	267	PGV	C28-C29-C30-C31
26	T	1269	CDL	C17-C18-C19-C20
20	C	268	PGV	C12-C13-C14-C15
20	P	1267	PGV	C12-C13-C14-C15
28	P	1264	PEK	C15-C16-C17-C18
20	C	268	PGV	C23-C24-C25-C26
26	G	269	CDL	C62-C63-C64-C65
19	L	522	TGL	C25-C26-C27-C28
28	T	263	PEK	C21-C22-C23-C24
20	A	524	PGV	C24-C25-C26-C27
19	A	521	TGL	CC7-CC8-CC9-C15
19	N	1522	TGL	C22-C23-C24-C25
19	Q	1523	TGL	C12-C13-C14-C29
24	Z	1526	DMU	C22-C25-C28-C31
26	P	1270	CDL	C64-C65-C66-C67
19	N	1521	TGL	OB1-CB1-OG2-CG2
18	N	515	HEA	C26-C15-C16-C17
19	A	521	TGL	C11-C12-C13-C14
19	A	521	TGL	C14-C29-C30-C31
19	N	1522	TGL	C11-C12-C13-C14
19	N	1522	TGL	C16-C15-CC9-CC8
19	N	1522	TGL	C17-C18-C19-C33
20	P	1267	PGV	C7-C8-C9-C10
26	G	269	CDL	C58-C59-C60-C61
26	T	1269	CDL	C31-C32-C33-C34
18	N	515	HEA	C14-C15-C16-C17
19	N	1522	TGL	CA3-CA4-CA5-CA6
20	N	1524	PGV	C4-C5-C6-C7
20	N	1266	PGV	C6-C7-C8-C9
22	B	230	PSC	C29-C30-C31-C32
28	P	1264	PEK	C33-C34-C35-C36
19	A	521	TGL	C13-C14-C29-C30
19	N	1521	TGL	C14-C29-C30-C31
19	N	1522	TGL	CB4-CB5-CB6-CB7
26	C	270	CDL	C23-C24-C25-C26
23	J	60	CHD	C13-C17-C20-C22
19	A	521	TGL	CA6-CA7-CA8-CA9
19	A	521	TGL	CC5-CC6-CC7-CC8
19	A	521	TGL	CA9-C20-C21-C22
19	N	1522	TGL	CC4-CC5-CC6-CC7
22	O	1230	PSC	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C81-C82-C83-C84
19	D	523	TGL	CB2-CB3-CB4-CB5
19	D	523	TGL	C19-C33-C34-C35
19	N	1521	TGL	CB9-C10-C11-C12
19	N	1521	TGL	CC7-CC8-CC9-C15
22	O	1230	PSC	C26-C27-C28-C29
19	N	1522	TGL	C25-C26-C27-C28
19	L	522	TGL	CC6-CC7-CC8-CC9
26	G	269	CDL	C54-C55-C56-C57
26	P	1270	CDL	C74-C75-C76-C77
24	P	1272	DMU	O5-C4-C57-O61
20	P	1267	PGV	C24-C25-C26-C27
20	P	1268	PGV	O12-C04-C05-O05
19	N	1521	TGL	C15-C16-C17-C18
26	G	269	CDL	C56-C57-C58-C59
26	P	1270	CDL	C22-C23-C24-C25
28	G	265	PEK	C29-C30-C31-C32
28	T	263	PEK	C29-C30-C31-C32
19	N	1521	TGL	CB2-CB1-OG2-CG2
20	P	1268	PGV	C2-C1-O01-C02
26	T	1269	CDL	C11-CA5-OA6-CA4
20	P	1268	PGV	C3-C4-C5-C6
26	T	1269	CDL	OA7-CA5-OA6-CA4
26	G	269	CDL	C60-C61-C62-C63
20	C	268	PGV	C11-C10-C9-C8
28	G	264	PEK	C2-C3-C4-C5
19	A	521	TGL	CB6-CB7-CB8-CB9
19	N	1521	TGL	CA5-CA6-CA7-CA8
24	M	526	DMU	C28-C31-C34-C37
26	G	269	CDL	C31-C32-C33-C34
23	P	1271	CHD	C20-C22-C23-C24
20	C	268	PGV	C10-C11-C12-C13
28	P	1264	PEK	C13-C14-C15-C16
26	C	270	CDL	C12-C13-C14-C15
26	G	269	CDL	CB7-C71-C72-C73
22	O	1230	PSC	C28-C29-C30-C31
26	T	1269	CDL	C75-C76-C77-C78
19	N	1521	TGL	C10-C11-C12-C13
19	N	1521	TGL	CC5-CC6-CC7-CC8
26	C	270	CDL	C35-C36-C37-C38
20	A	524	PGV	C28-C29-C30-C31
20	N	1266	PGV	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	G	1263	PEK	C22-C23-C24-C25
19	D	523	TGL	C15-C16-C17-C18
19	D	523	TGL	OG1-CG1-CG2-OG2
20	C	268	PGV	O03-C01-C02-O01
20	N	1266	PGV	C11-C10-C9-C8
26	G	269	CDL	OB6-CB4-CB6-OB8
22	B	230	PSC	C28-C29-C30-C31
26	C	270	CDL	C51-C52-C53-C54
28	G	264	PEK	C28-C29-C30-C31
19	D	523	TGL	C17-C18-C19-C33
20	A	522	PGV	C24-C25-C26-C27
28	P	1264	PEK	C30-C31-C32-C33
19	Q	1523	TGL	CA6-CA7-CA8-CA9
24	P	1272	DMU	C19-C22-C25-C28
26	C	270	CDL	C72-C73-C74-C75
19	N	1521	TGL	CC4-CC5-CC6-CC7
19	Q	1523	TGL	CB2-CB3-CB4-CB5
26	T	1269	CDL	C51-C52-C53-C54
20	A	522	PGV	C14-C15-C16-C17
23	W	1060	CHD	C13-C17-C20-C21
28	P	1265	PEK	C25-C26-C27-C28
26	G	269	CDL	C31-CA7-OA8-CA6
19	D	523	TGL	C16-C17-C18-C19
26	P	1270	CDL	C38-C39-C40-C41
26	P	1270	CDL	C71-C72-C73-C74
28	P	1265	PEK	C29-C30-C31-C32
20	N	1266	PGV	C10-C11-C12-C13
28	P	1264	PEK	C4-C5-C6-C7
26	C	270	CDL	C43-C44-C45-C46
28	G	265	PEK	C24-C25-C26-C27
19	L	522	TGL	CA5-CA6-CA7-CA8
20	C	268	PGV	C22-C23-C24-C25
20	P	1268	PGV	C22-C23-C24-C25
26	G	269	CDL	C14-C15-C16-C17
19	Q	1523	TGL	CB5-CB6-CB7-CB8
22	B	230	PSC	C2-C3-C4-C5
26	T	1269	CDL	C55-C56-C57-C58
20	A	524	PGV	C01-C02-C03-O11
20	C	268	PGV	C01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-CA6
26	C	270	CDL	OB5-CB3-CB4-CB6
26	P	1270	CDL	OA5-CA3-CA4-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C35-C36-C37-C38
20	C	268	PGV	C29-C30-C31-C32
22	B	230	PSC	C4-C5-C6-C7
28	G	1263	PEK	C25-C26-C27-C28
28	P	1264	PEK	C26-C27-C28-C29
26	C	270	CDL	C71-C72-C73-C74
26	C	270	CDL	C41-C42-C43-C44
28	P	1265	PEK	C22-C21-O03-C01
20	N	1524	PGV	C11-C12-C13-C14
28	G	264	PEK	C23-C24-C25-C26
28	G	265	PEK	C25-C26-C27-C28
19	L	522	TGL	CC4-CC5-CC6-CC7
20	C	268	PGV	O03-C01-C02-C03
20	N	1524	PGV	O03-C01-C02-C03
20	P	1268	PGV	O03-C01-C02-C03
26	P	1270	CDL	CA3-CA4-CA6-OA8
26	P	1270	CDL	CB3-CB4-CB6-OB8
19	L	522	TGL	C19-C33-C34-C35
20	N	1266	PGV	C12-C13-C14-C15
20	P	1268	PGV	C12-C13-C14-C15
28	G	265	PEK	C15-C16-C17-C18
20	A	522	PGV	C26-C27-C28-C29
20	P	1268	PGV	C26-C27-C28-C29
26	C	270	CDL	C32-C33-C34-C35
19	A	521	TGL	C16-C17-C18-C19
19	D	523	TGL	C13-C14-C29-C30
22	B	230	PSC	C04-C05-N-C07
19	A	521	TGL	CB1-CB2-CB3-CB4
28	P	1265	PEK	O04-C21-O03-C01
20	P	1268	PGV	C6-C7-C8-C9
26	T	1269	CDL	C35-C36-C37-C38
19	D	523	TGL	CC2-CC3-CC4-CC5
19	Q	1523	TGL	CA4-CA5-CA6-CA7
20	C	267	PGV	C29-C30-C31-C32
22	O	1230	PSC	C4-C5-C6-C7
24	C	272	DMU	C4-C3-O7-C10
19	N	1522	TGL	C10-C11-C12-C13
26	G	269	CDL	C18-C19-C20-C21
19	D	523	TGL	CA6-CA7-CA8-CA9
20	C	268	PGV	C4-C5-C6-C7
20	N	1266	PGV	C7-C8-C9-C10
20	P	1267	PGV	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	P	1265	PEK	C15-C16-C17-C18
28	T	263	PEK	C2-C3-C4-C5
19	D	523	TGL	CC6-CC7-CC8-CC9
19	L	522	TGL	C13-C14-C29-C30
26	C	270	CDL	C74-C75-C76-C77
28	P	1265	PEK	C30-C31-C32-C33
18	A	516	HEA	C2A-C3A-CMA-OMA
28	G	1263	PEK	C27-C28-C29-C30
26	G	269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	C71-C72-C73-C74
22	O	1230	PSC	C31-C32-C33-C34
26	C	270	CDL	C79-C80-C81-C82
26	G	269	CDL	C74-C75-C76-C77
20	P	1268	PGV	O02-C1-O01-C02
20	P	1268	PGV	O12-C04-C05-C06
28	T	263	PEK	O01-C02-C03-O11
20	N	1266	PGV	C31-C32-C33-C34
26	C	270	CDL	C82-C83-C84-C85
26	P	1270	CDL	C13-C14-C15-C16
20	P	1268	PGV	C31-C32-C33-C34
19	L	522	TGL	CB4-CB5-CB6-CB7
20	C	268	PGV	C14-C15-C16-C17
26	C	270	CDL	C15-C16-C17-C18
19	D	523	TGL	C16-C15-CC9-CC8
19	L	522	TGL	CA9-C20-C21-C22
19	N	1521	TGL	C13-C14-C29-C30
28	G	265	PEK	C22-C23-C24-C25
28	G	265	PEK	C26-C27-C28-C29
20	C	268	PGV	C31-C32-C33-C34
19	L	522	TGL	CB5-CB6-CB7-CB8
26	T	1269	CDL	C32-C33-C34-C35
28	P	1264	PEK	C16-C17-C18-C19
19	A	521	TGL	OG2-CG2-CG3-OG3
28	T	263	PEK	O03-C01-C02-O01
24	M	526	DMU	C25-C28-C31-C34
26	C	270	CDL	C37-C38-C39-C40
19	L	522	TGL	C33-C34-C35-C36
20	C	267	PGV	C31-C32-C33-C34
26	P	1270	CDL	C44-C45-C46-C47
20	A	522	PGV	C30-C31-C32-C33
26	G	269	CDL	C76-C77-C78-C79
19	A	521	TGL	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	522	PGV	C15-C16-C17-C18
20	N	1266	PGV	C5-C6-C7-C8
22	O	1230	PSC	C2-C1-O01-C02
19	A	521	TGL	C25-C26-C27-C28
19	D	523	TGL	C33-C34-C35-C36
19	D	523	TGL	CA1-CA2-CA3-CA4
28	P	1265	PEK	C13-C14-C15-C16
28	T	263	PEK	C7-C8-C9-C10
22	O	1230	PSC	O03-C19-C20-C21
20	A	522	PGV	C7-C8-C9-C10
26	P	1270	CDL	C42-C43-C44-C45
26	T	1269	CDL	C16-C17-C18-C19
26	T	1269	CDL	C52-C53-C54-C55
20	C	268	PGV	C9-C10-C11-C12
28	G	264	PEK	C27-C28-C29-C30
19	A	521	TGL	CA7-CA8-CA9-C20
20	A	524	PGV	C25-C26-C27-C28
28	G	1263	PEK	C22-C21-O03-C01
19	L	522	TGL	CB2-CB3-CB4-CB5
19	N	1521	TGL	CA7-CA8-CA9-C20
19	Q	1523	TGL	CA5-CA6-CA7-CA8
20	N	1524	PGV	C01-C02-C03-O11
20	A	524	PGV	C31-C32-C33-C34
20	P	1267	PGV	C15-C16-C17-C18
26	T	1269	CDL	CA7-C31-C32-C33
20	C	268	PGV	C15-C16-C17-C18
26	G	269	CDL	C12-C13-C14-C15
28	P	1264	PEK	C3-C4-C5-C6
24	P	1272	DMU	C34-C37-C40-C43
22	O	1230	PSC	C22-C23-C24-C25
20	N	1524	PGV	C24-C25-C26-C27
22	B	230	PSC	C11-C10-C9-C8
26	P	1270	CDL	C19-C20-C21-C22
19	L	522	TGL	CC2-CC3-CC4-CC5
20	A	524	PGV	C12-C13-C14-C15
22	O	1230	PSC	O02-C1-O01-C02
20	N	1524	PGV	C6-C7-C8-C9
19	D	523	TGL	OG1-CG1-CG2-CG3
26	G	269	CDL	CB3-CB4-CB6-OB8
28	G	1263	PEK	O03-C01-C02-C03
28	T	263	PEK	O03-C01-C02-C03
26	T	1269	CDL	C81-C82-C83-C84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	Q	1523	TGL	CB1-CB2-CB3-CB4
28	P	1264	PEK	C31-C32-C33-C34
26	G	269	CDL	C13-C14-C15-C16
26	P	1270	CDL	C41-C42-C43-C44
28	G	264	PEK	C24-C25-C26-C27
26	T	1269	CDL	C20-C21-C22-C23
19	N	1521	TGL	C21-C22-C23-C24
19	N	1522	TGL	C29-C30-C31-C32
19	N	1522	TGL	CA9-C20-C21-C22
19	Q	1523	TGL	CB3-CB4-CB5-CB6
20	C	267	PGV	C02-C03-O11-P
26	P	1270	CDL	CA4-CA3-OA5-PA1
20	C	268	PGV	C21-C22-C23-C24
28	G	1263	PEK	C30-C31-C32-C33
19	L	522	TGL	OG1-CA1-CA2-CA3
19	A	521	TGL	OG1-CG1-CG2-OG2
19	N	1521	TGL	OG1-CG1-CG2-OG2
22	B	230	PSC	C9-C10-C11-C12
22	B	230	PSC	C10-C11-C12-C13
22	O	1230	PSC	C9-C10-C11-C12
28	G	264	PEK	C9-C10-C11-C12
28	G	265	PEK	C5-C6-C7-C8
28	G	265	PEK	C6-C7-C8-C9
28	G	1263	PEK	C11-C10-C9-C8
28	G	1263	PEK	C9-C10-C11-C12
28	G	1263	PEK	C11-C12-C13-C14
28	P	1264	PEK	C9-C10-C11-C12
28	P	1265	PEK	C5-C6-C7-C8
28	P	1265	PEK	C11-C10-C9-C8
28	T	263	PEK	C27-C28-C29-C30
24	P	1272	DMU	C28-C31-C34-C37
19	Q	1523	TGL	CC3-CC4-CC5-CC6
28	G	1263	PEK	C26-C27-C28-C29
19	D	523	TGL	CB4-CB5-CB6-CB7
26	P	1270	CDL	C40-C41-C42-C43
28	P	1265	PEK	C26-C27-C28-C29
26	P	1270	CDL	C36-C37-C38-C39
28	G	265	PEK	C30-C31-C32-C33
26	P	1270	CDL	C84-C85-C86-C87
20	C	268	PGV	C19-C20-C21-C22
20	P	1268	PGV	C23-C24-C25-C26
22	B	230	PSC	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	L	522	TGL	C15-C16-C17-C18
19	D	523	TGL	CA9-C20-C21-C22
19	L	522	TGL	C16-C15-CC9-CC8
22	B	230	PSC	C22-C23-C24-C25
19	L	522	TGL	C11-C10-CB9-CB8
26	T	1269	CDL	C21-C22-C23-C24
26	C	270	CDL	C73-C74-C75-C76
19	A	521	TGL	C16-C15-CC9-CC8
20	P	1268	PGV	C5-C6-C7-C8
19	A	521	TGL	CB9-C10-C11-C12
19	D	523	TGL	OG2-CB1-CB2-CB3
24	P	1272	DMU	C25-C28-C31-C34
26	T	1269	CDL	C37-C38-C39-C40
20	P	1267	PGV	C02-C03-O11-P
19	L	522	TGL	CC5-CC6-CC7-CC8
26	T	1269	CDL	C62-C63-C64-C65
28	G	1263	PEK	O04-C21-O03-C01
28	G	265	PEK	C13-C14-C15-C16
19	D	523	TGL	CA4-CA5-CA6-CA7
19	A	521	TGL	C15-C16-C17-C18
26	P	1270	CDL	C21-C22-C23-C24
20	N	1524	PGV	C01-C02-O01-C1
26	T	1269	CDL	C13-C14-C15-C16
26	C	270	CDL	C84-C85-C86-C87
20	C	268	PGV	C24-C25-C26-C27
26	G	269	CDL	C33-C34-C35-C36
26	P	1270	CDL	C57-C58-C59-C60
19	Q	1523	TGL	OG1-CG1-CG2-CG3
24	M	526	DMU	C34-C37-C40-C43
26	P	1270	CDL	C24-C25-C26-C27
23	C	271	CHD	C20-C22-C23-C24
20	A	522	PGV	C10-C11-C12-C13
22	O	1230	PSC	C23-C24-C25-C26
20	A	524	PGV	C11-C10-C9-C8
20	N	1524	PGV	O03-C01-C02-O01
26	P	1270	CDL	OA6-CA4-CA6-OA8
26	P	1270	CDL	OB6-CB4-CB6-OB8
20	C	268	PGV	C13-C14-C15-C16
28	G	264	PEK	C16-C17-C18-C19
26	C	270	CDL	C36-C37-C38-C39
28	P	1264	PEK	C29-C30-C31-C32
26	C	270	CDL	C1-CA2-OA2-PA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	G	269	CDL	C44-C45-C46-C47
22	B	230	PSC	C5-C6-C7-C8
20	C	267	PGV	C22-C23-C24-C25
22	B	230	PSC	C04-C05-N-C06
26	P	1270	CDL	C51-C52-C53-C54
20	P	1268	PGV	C15-C16-C17-C18
20	A	522	PGV	C12-C13-C14-C15
26	T	1269	CDL	OB5-CB3-CB4-CB6
28	G	1263	PEK	C01-C02-C03-O11
28	T	263	PEK	C01-C02-C03-O11
26	G	269	CDL	C61-C62-C63-C64
28	P	1264	PEK	C2-C1-O01-C02
20	P	1268	PGV	C29-C30-C31-C32
20	A	522	PGV	C5-C6-C7-C8
20	N	1524	PGV	C7-C8-C9-C10
20	P	1268	PGV	C10-C11-C12-C13
26	C	270	CDL	C42-C43-C44-C45
26	P	1270	CDL	C83-C84-C85-C86
20	P	1268	PGV	C05-C04-O12-P
20	A	522	PGV	C23-C24-C25-C26
20	C	267	PGV	C30-C31-C32-C33
26	P	1270	CDL	C78-C79-C80-C81
20	A	524	PGV	O01-C02-C03-O11
20	P	1268	PGV	O01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-OA6
28	G	1263	PEK	O01-C02-C03-O11
28	P	1265	PEK	C24-C25-C26-C27
20	P	1268	PGV	O01-C1-C2-C3
20	C	268	PGV	C7-C8-C9-C10
18	A	516	HEA	C4A-C3A-CMA-OMA
18	N	515	HEA	C4A-C3A-CMA-OMA
18	N	516	HEA	C4A-C3A-CMA-OMA
20	A	524	PGV	C11-C12-C13-C14
19	D	523	TGL	C12-C13-C14-C29
26	T	1269	CDL	C44-C45-C46-C47
19	N	1522	TGL	OG2-CG2-CG3-OG3
19	N	1522	TGL	C21-C20-CA9-CA8
26	C	270	CDL	C59-C60-C61-C62
26	G	269	CDL	C16-C17-C18-C19
19	N	1521	TGL	CB5-CB6-CB7-CB8
19	N	1522	TGL	CG1-CG2-CG3-OG3
23	P	1271	CHD	C16-C17-C20-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	G	269	CDL	C78-C79-C80-C81
19	A	521	TGL	C18-C19-C33-C34
19	D	523	TGL	C11-C10-CB9-CB8
19	Q	1523	TGL	CB4-CB5-CB6-CB7
19	L	522	TGL	CA7-CA8-CA9-C20
20	A	524	PGV	C04-O12-P-O13
20	A	522	PGV	C04-O12-P-O13
20	C	268	PGV	C04-O12-P-O14
20	N	1524	PGV	C04-O12-P-O11
20	N	1524	PGV	C04-O12-P-O13
22	B	230	PSC	C03-O11-P-O14
22	O	1230	PSC	C03-O11-P-O12
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CB2-OB2-PB2-OB5
26	G	269	CDL	CA3-OA5-PA1-OA3
26	G	269	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA3-OA5-PA1-OA3
26	P	1270	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CB2-OB2-PB2-OB5
26	P	1270	CDL	CB3-OB5-PB2-OB4
26	T	1269	CDL	CB3-OB5-PB2-OB4
28	P	1265	PEK	O12-C04-C05-N
28	T	263	PEK	C28-C29-C30-C31
19	Q	1523	TGL	CB7-CB8-CB9-C10
19	Q	1523	TGL	CB9-C10-C11-C12
20	A	522	PGV	C25-C26-C27-C28
26	G	269	CDL	C32-C33-C34-C35
20	N	1524	PGV	C9-C10-C11-C12
20	A	524	PGV	C05-C04-O12-P
20	C	268	PGV	C05-C04-O12-P
20	N	1524	PGV	C05-C04-O12-P
26	T	1269	CDL	CB4-CB3-OB5-PB2
26	C	270	CDL	C77-C78-C79-C80
19	N	1521	TGL	C18-C19-C33-C34
26	G	269	CDL	C20-C21-C22-C23
19	A	521	TGL	CG1-CG2-OG2-CB1
19	Q	1523	TGL	CG3-CG2-OG2-CB1
22	B	230	PSC	C01-C02-O01-C1
28	G	1263	PEK	C32-C33-C34-C35
20	A	524	PGV	C15-C16-C17-C18
19	A	521	TGL	C17-C18-C19-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	OA5-CA3-CA4-OA6
19	A	521	TGL	C20-C21-C22-C23
19	N	1522	TGL	CB7-CB8-CB9-C10
20	N	1524	PGV	C31-C32-C33-C34
28	P	1265	PEK	C22-C23-C24-C25
24	Z	1526	DMU	C19-C22-C25-C28
20	P	1268	PGV	C4-C5-C6-C7
26	G	269	CDL	C52-C51-CB5-OB6
28	T	263	PEK	C1-C2-C3-C4
20	P	1268	PGV	C24-C25-C26-C27
20	P	1268	PGV	C1-C2-C3-C4
28	P	1264	PEK	C34-C35-C36-C37
19	D	523	TGL	OG1-CA1-CA2-CA3
19	D	523	TGL	C18-C19-C33-C34
20	A	524	PGV	C7-C8-C9-C10
23	C	271	CHD	C16-C17-C20-C22
26	P	1270	CDL	CA5-C11-C12-C13
20	N	1266	PGV	C29-C30-C31-C32
19	Q	1523	TGL	C10-C11-C12-C13
19	N	1521	TGL	C23-C24-C25-C26
26	C	270	CDL	CA2-C1-CB2-OB2
18	N	515	HEA	C12-C13-C14-C15
19	A	521	TGL	CB3-CB4-CB5-CB6
28	T	263	PEK	C34-C35-C36-C37
24	C	272	DMU	C31-C34-C37-C40
28	T	263	PEK	C3-C4-C5-C6
28	P	1264	PEK	C17-C18-C19-C20
20	N	1266	PGV	C13-C14-C15-C16
22	O	1230	PSC	O04-C19-C20-C21
19	N	1522	TGL	C11-C10-CB9-CB8
28	T	263	PEK	C35-C36-C37-C38
19	L	522	TGL	C29-C30-C31-C32
24	M	526	DMU	C31-C34-C37-C40
24	Z	1526	DMU	C34-C37-C40-C43
20	A	522	PGV	C02-C01-O03-C19
24	P	1272	DMU	C18-C19-C22-C25
19	Q	1523	TGL	C21-C20-CA9-CA8
28	G	1263	PEK	C02-C03-O11-P
20	N	1266	PGV	C25-C26-C27-C28
26	C	270	CDL	C20-C21-C22-C23
23	J	60	CHD	C22-C23-C24-O25
23	J	60	CHD	C22-C23-C24-O26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C15-C16-C17-C18
28	G	1263	PEK	C10-C11-C12-C13
23	W	1060	CHD	C22-C23-C24-O25
22	B	230	PSC	C03-C02-O01-C1
22	O	1230	PSC	C03-C02-O01-C1
28	G	264	PEK	C32-C33-C34-C35
26	P	1270	CDL	CA7-C31-C32-C33
24	M	526	DMU	O16-C18-C19-C22
18	A	516	HEA	CAD-CBD-CGD-O1D
18	A	516	HEA	CAD-CBD-CGD-O2D
23	B	1086	CHD	C22-C23-C24-O25
26	P	1270	CDL	C20-C21-C22-C23
26	G	269	CDL	OA6-CA4-CA6-OA8
28	P	1265	PEK	O03-C01-C02-O01
22	O	1230	PSC	C10-C11-C12-C13
28	G	265	PEK	C11-C10-C9-C8
28	G	265	PEK	C9-C10-C11-C12
28	G	1263	PEK	C12-C13-C14-C15
28	T	263	PEK	C6-C7-C8-C9
28	T	263	PEK	C9-C10-C11-C12
20	A	524	PGV	C23-C24-C25-C26
20	N	1524	PGV	C5-C6-C7-C8
28	G	264	PEK	C22-C23-C24-C25
18	A	516	HEA	CAA-CBA-CGA-O1A
23	O	229	CHD	C22-C23-C24-O25
28	G	1263	PEK	C34-C35-C36-C37
28	G	265	PEK	O02-C1-O01-C02
20	C	267	PGV	C15-C16-C17-C18
26	G	269	CDL	C17-C18-C19-C20
20	P	1267	PGV	C3-C4-C5-C6
19	D	523	TGL	CC3-CC4-CC5-CC6
22	B	230	PSC	C14-C15-C16-C17
26	T	1269	CDL	C64-C65-C66-C67
19	N	1521	TGL	CA9-C20-C21-C22
20	C	267	PGV	C12-C13-C14-C15
20	C	268	PGV	C02-C03-O11-P
26	C	270	CDL	C1-CB2-OB2-PB2
23	W	1060	CHD	C22-C23-C24-O26
26	T	1269	CDL	CA3-CA4-CA6-OA8
28	G	264	PEK	C35-C36-C37-C38
26	C	270	CDL	C31-C32-C33-C34
19	N	1522	TGL	OG2-CB1-CB2-CB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	O	229	CHD	C22-C23-C24-O26
22	O	1230	PSC	O01-C02-C03-O11
18	A	516	HEA	CAA-CBA-CGA-O2A
19	A	521	TGL	C10-C11-C12-C13
26	T	1269	CDL	C60-C61-C62-C63
26	T	1269	CDL	C72-C73-C74-C75
23	B	1086	CHD	C22-C23-C24-O26
19	Q	1523	TGL	CA3-CA4-CA5-CA6
20	N	1266	PGV	C9-C10-C11-C12
20	A	522	PGV	O03-C19-C20-C21
22	B	230	PSC	O01-C1-C2-C3
26	T	1269	CDL	C52-C51-CB5-OB6
22	B	230	PSC	C26-C27-C28-C29
28	T	263	PEK	C4-C5-C6-C7
26	P	1270	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CB2-C1-CA2-OA2
26	T	1269	CDL	OA9-CA7-OA8-CA6
19	Q	1523	TGL	C19-C33-C34-C35
26	T	1269	CDL	C38-C39-C40-C41
19	Q	1523	TGL	C33-C34-C35-C36
18	N	516	HEA	CAD-CBD-CGD-O1D
23	C	525	CHD	C22-C23-C24-O26
28	G	1263	PEK	C2-C1-O01-C02
19	N	1521	TGL	CB7-CB8-CB9-C10
20	P	1267	PGV	C14-C15-C16-C17
18	N	516	HEA	CAD-CBD-CGD-O2D
24	C	272	DMU	C19-C22-C25-C28
19	N	1522	TGL	C13-C14-C29-C30
28	P	1264	PEK	C2-C3-C4-C5
20	A	522	PGV	C29-C30-C31-C32
22	O	1230	PSC	C12-C13-C14-C15
23	P	1271	CHD	C16-C17-C20-C21
20	N	1524	PGV	C04-C05-C06-O06
19	L	522	TGL	OA1-CA1-CA2-CA3
23	C	271	CHD	C16-C17-C20-C21
19	N	1522	TGL	OG1-CA1-CA2-CA3
20	N	1524	PGV	O03-C19-C20-C21
20	N	1266	PGV	O03-C19-C20-C21
26	T	1269	CDL	C24-C25-C26-C27
20	A	524	PGV	C9-C10-C11-C12
28	T	263	PEK	C24-C25-C26-C27
23	C	525	CHD	C22-C23-C24-O25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	N	1521	TGL	C22-C23-C24-C25
23	P	1271	CHD	C22-C23-C24-O26
20	A	524	PGV	C14-C15-C16-C17
26	C	270	CDL	C64-C65-C66-C67
20	P	1267	PGV	C05-C04-O12-P
26	T	1269	CDL	C31-CA7-OA8-CA6
26	C	270	CDL	C24-C25-C26-C27
19	N	1522	TGL	CA6-CA7-CA8-CA9
19	N	1522	TGL	CA1-CA2-CA3-CA4
20	N	1266	PGV	C20-C21-C22-C23
28	G	264	PEK	C14-C15-C16-C17
28	G	1263	PEK	C16-C17-C18-C19
24	C	272	DMU	C5-C10-O7-C3
19	L	522	TGL	CC7-CC8-CC9-C15
23	P	1271	CHD	C22-C23-C24-O25
26	C	270	CDL	C62-C63-C64-C65
26	C	270	CDL	OB6-CB4-CB6-OB8
20	A	522	PGV	C9-C10-C11-C12
28	P	1265	PEK	C3-C4-C5-C6
26	G	269	CDL	C53-C54-C55-C56
28	G	265	PEK	C2-C1-O01-C02
19	D	523	TGL	OB1-CB1-CB2-CB3
26	T	1269	CDL	C82-C83-C84-C85
19	Q	1523	TGL	C29-C30-C31-C32
28	T	263	PEK	O02-C1-O01-C02
20	P	1268	PGV	C9-C10-C11-C12
28	G	264	PEK	C26-C27-C28-C29
28	T	263	PEK	C2-C1-O01-C02
18	N	515	HEA	CAD-CBD-CGD-O1D
23	C	271	CHD	C22-C23-C24-O26
19	D	523	TGL	CA5-CA6-CA7-CA8
19	L	522	TGL	OG3-CC1-CC2-CC3
28	G	264	PEK	O01-C1-C2-C3
28	P	1264	PEK	O01-C1-C2-C3
22	B	230	PSC	C3-C4-C5-C6
20	P	1268	PGV	C19-C20-C21-C22
20	A	522	PGV	C31-C32-C33-C34
28	P	1265	PEK	O01-C1-C2-C3
19	L	522	TGL	C21-C22-C23-C24
20	C	268	PGV	C25-C26-C27-C28
19	Q	1523	TGL	OG3-CC1-CC2-CC3
28	T	263	PEK	O01-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	C	268	PGV	O12-C04-C05-O05
26	C	270	CDL	CB3-CB4-CB6-OB8
18	N	515	HEA	CAA-CBA-CGA-O2A
19	N	1521	TGL	C17-C18-C19-C33
26	C	270	CDL	C40-C41-C42-C43
18	N	516	HEA	CAA-CBA-CGA-O1A
20	P	1267	PGV	C4-C5-C6-C7
26	C	270	CDL	C52-C51-CB5-OB6
24	C	272	DMU	C18-C19-C22-C25
28	G	264	PEK	C34-C35-C36-C37
26	C	270	CDL	CA7-C31-C32-C33
22	O	1230	PSC	C01-C02-C03-O11
19	Q	1523	TGL	OG2-CB1-CB2-CB3
26	P	1270	CDL	C12-C11-CA5-OA6
26	C	270	CDL	O1-C1-CB2-OB2
19	L	522	TGL	C23-C24-C25-C26
18	N	515	HEA	CAA-CBA-CGA-O1A
19	D	523	TGL	C29-C30-C31-C32
19	L	522	TGL	C11-C12-C13-C14
19	L	522	TGL	CA3-CA4-CA5-CA6
23	C	271	CHD	C22-C23-C24-O25
24	Z	1526	DMU	O6-C11-C9-C8
26	T	1269	CDL	C83-C84-C85-C86
26	T	1269	CDL	C33-C34-C35-C36
26	G	269	CDL	C64-C65-C66-C67
20	C	267	PGV	C13-C14-C15-C16
19	Q	1523	TGL	OG1-CA1-CA2-CA3
24	P	1272	DMU	C5-C10-O7-C3
28	G	264	PEK	O02-C1-C2-C3
18	N	515	HEA	CAD-CBD-CGD-O2D
23	P	1525	CHD	C22-C23-C24-O25
19	Q	1523	TGL	OC1-CC1-CC2-CC3
28	G	264	PEK	O03-C01-C02-O01
19	L	522	TGL	OC1-CC1-CC2-CC3
28	P	1265	PEK	O02-C1-C2-C3
18	A	515	HEA	CAA-CBA-CGA-O2A
28	P	1264	PEK	O02-C1-C2-C3
20	A	522	PGV	C4-C5-C6-C7
20	C	268	PGV	O01-C1-C2-C3
19	L	522	TGL	OG2-CB1-CB2-CB3
20	A	524	PGV	O03-C19-C20-C21
22	O	1230	PSC	O01-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	T	263	PEK	O02-C1-C2-C3

There are no ring outliers.

44 monomers are involved in 284 short contacts:

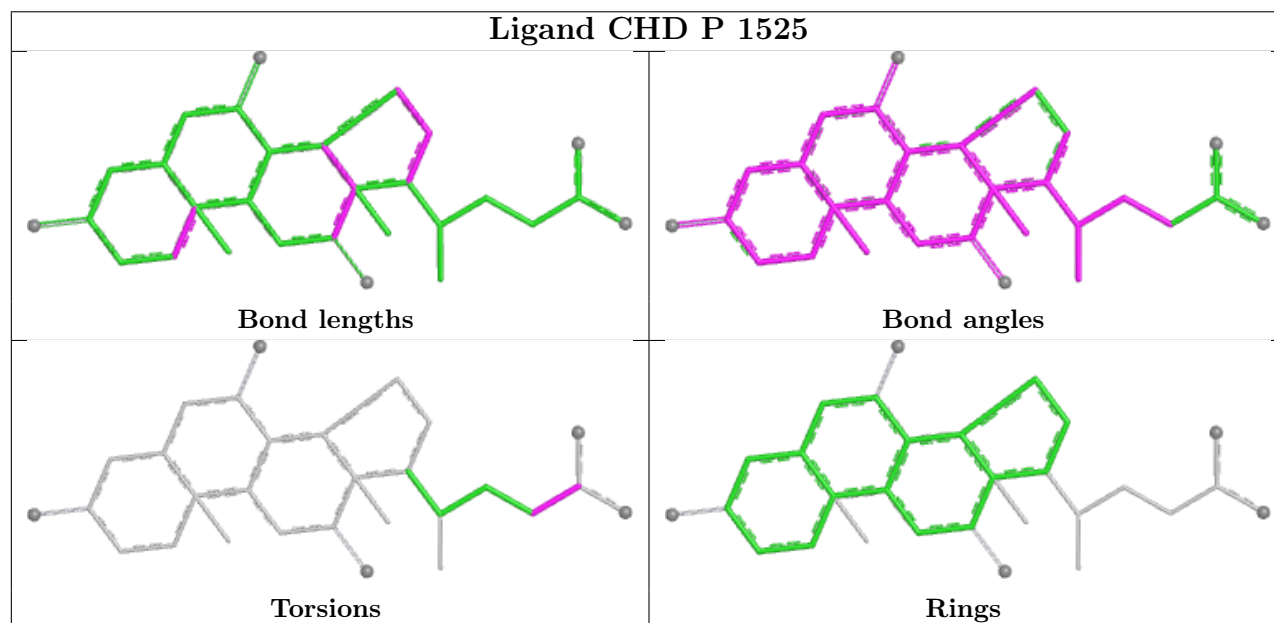
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	P	1525	CHD	3	0
19	A	521	TGL	6	0
19	D	523	TGL	15	0
19	L	522	TGL	16	0
20	C	267	PGV	6	0
20	N	1524	PGV	6	0
23	O	229	CHD	2	0
23	B	1086	CHD	1	0
28	G	264	PEK	6	0
22	O	1230	PSC	12	0
19	N	1522	TGL	12	0
15	N	520	PER	1	0
24	Z	1526	DMU	2	0
18	A	516	HEA	2	0
20	A	524	PGV	8	0
26	P	1270	CDL	16	0
28	P	1264	PEK	6	0
18	A	515	HEA	7	0
23	J	60	CHD	3	0
20	P	1267	PGV	5	0
22	B	230	PSC	18	0
28	G	1263	PEK	7	0
18	N	515	HEA	8	0
23	C	271	CHD	3	0
18	N	516	HEA	1	0
26	T	1269	CDL	23	0
24	M	526	DMU	1	0
26	C	270	CDL	13	0
23	P	1271	CHD	2	0
15	A	520	PER	1	0
24	C	272	DMU	5	0
28	T	263	PEK	21	0
23	W	1060	CHD	4	0
28	G	265	PEK	7	0
20	A	522	PGV	2	0
26	G	269	CDL	24	0

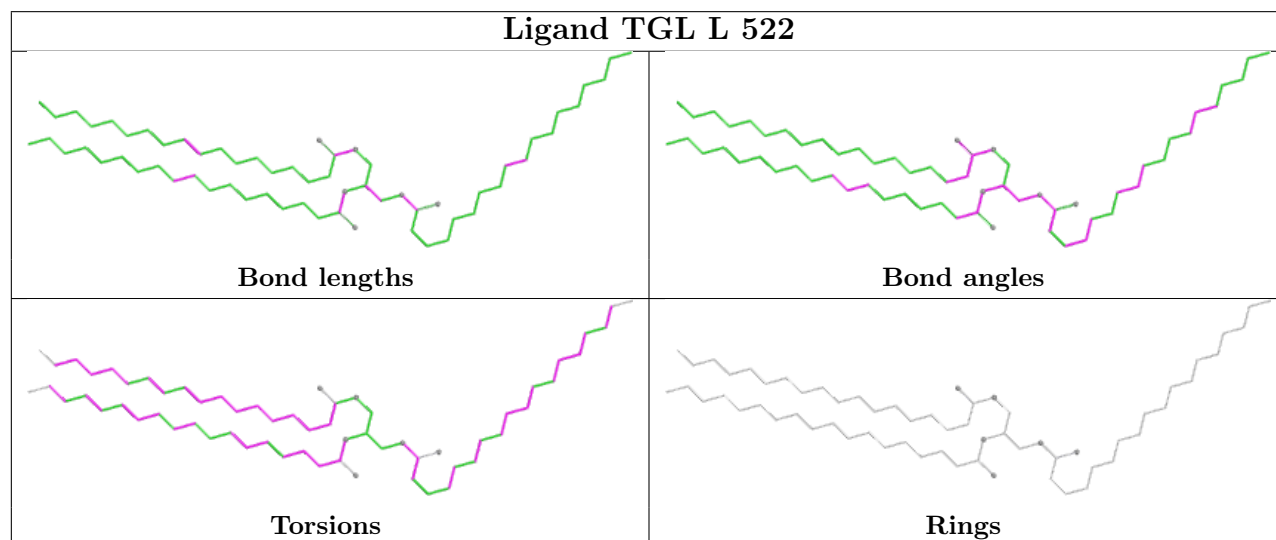
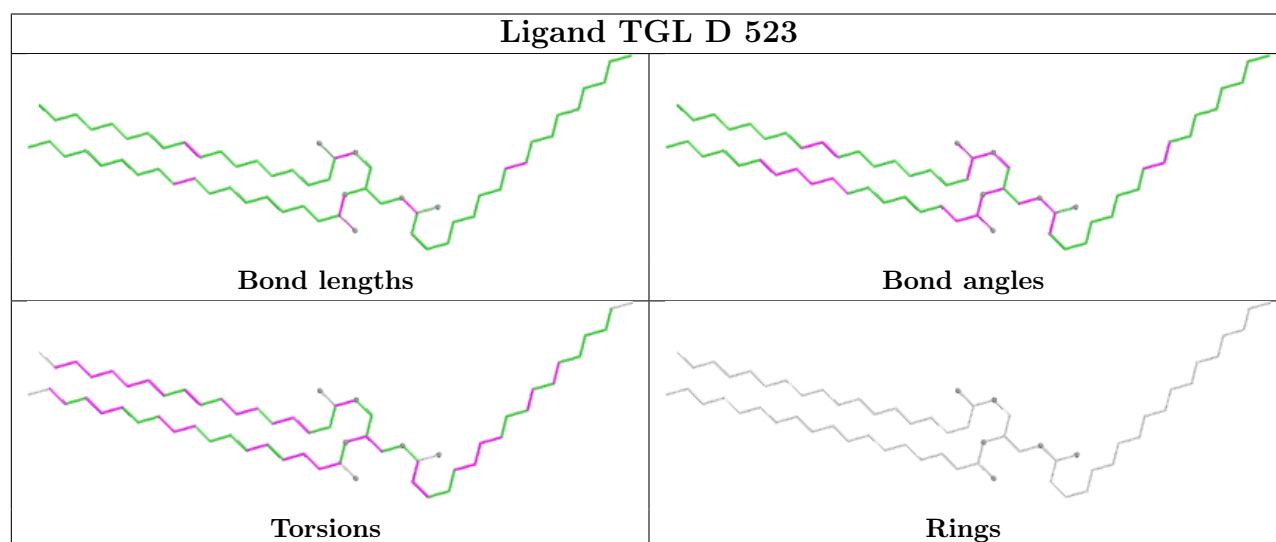
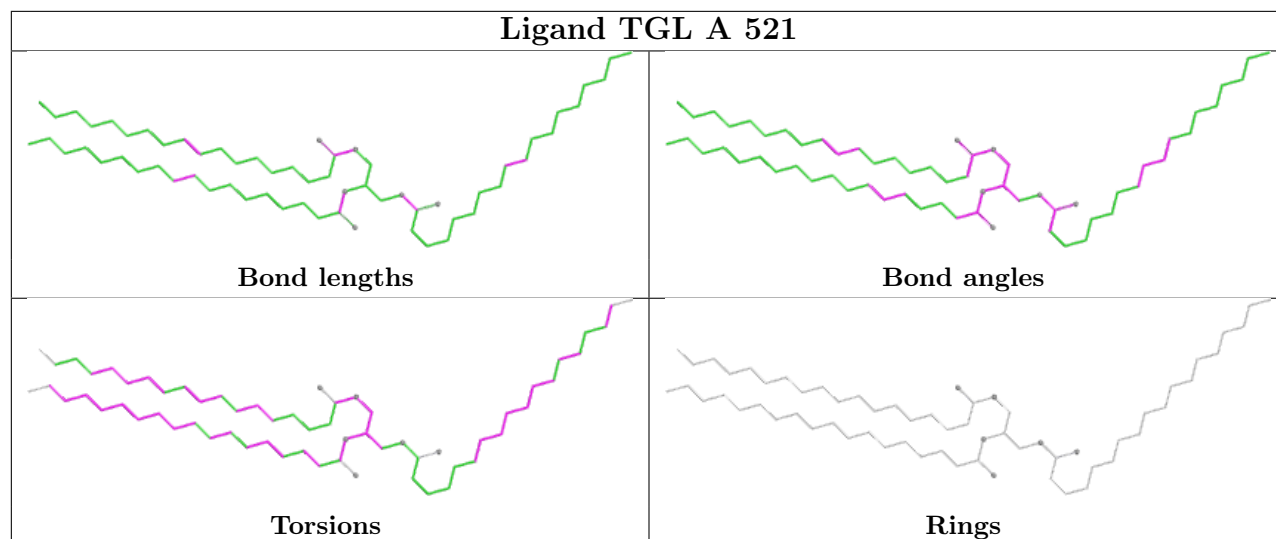
Continued on next page...

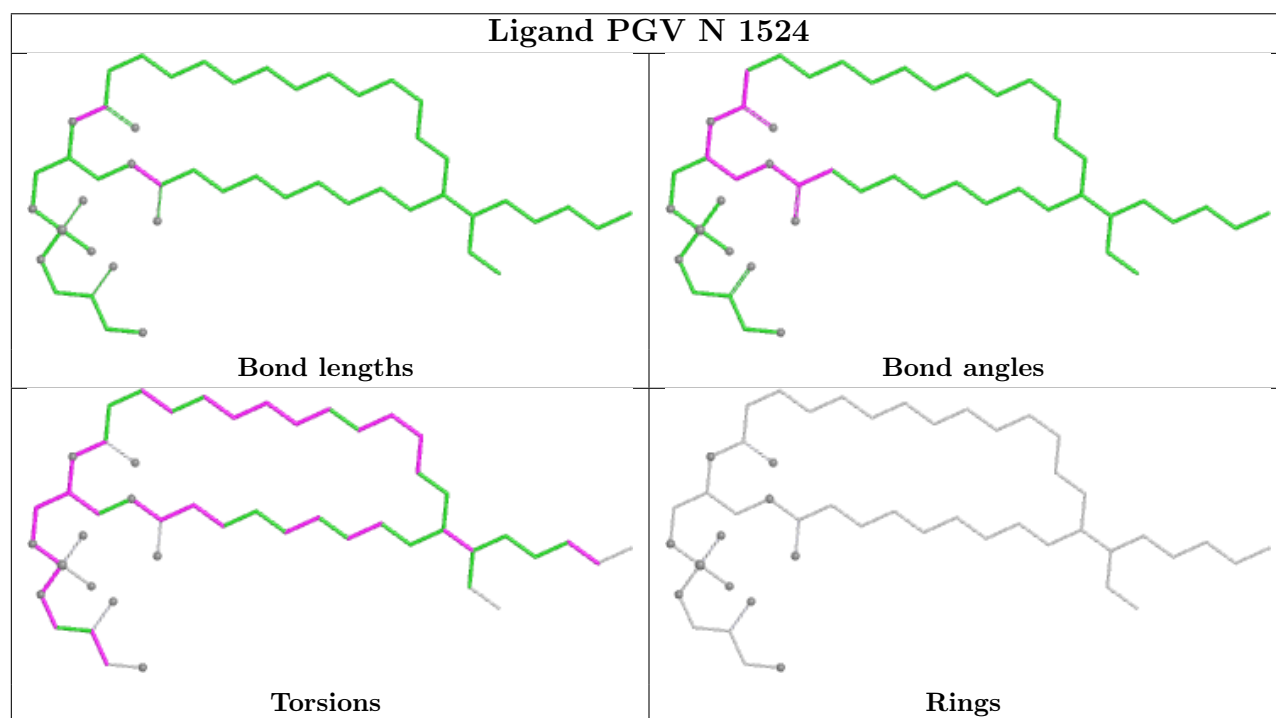
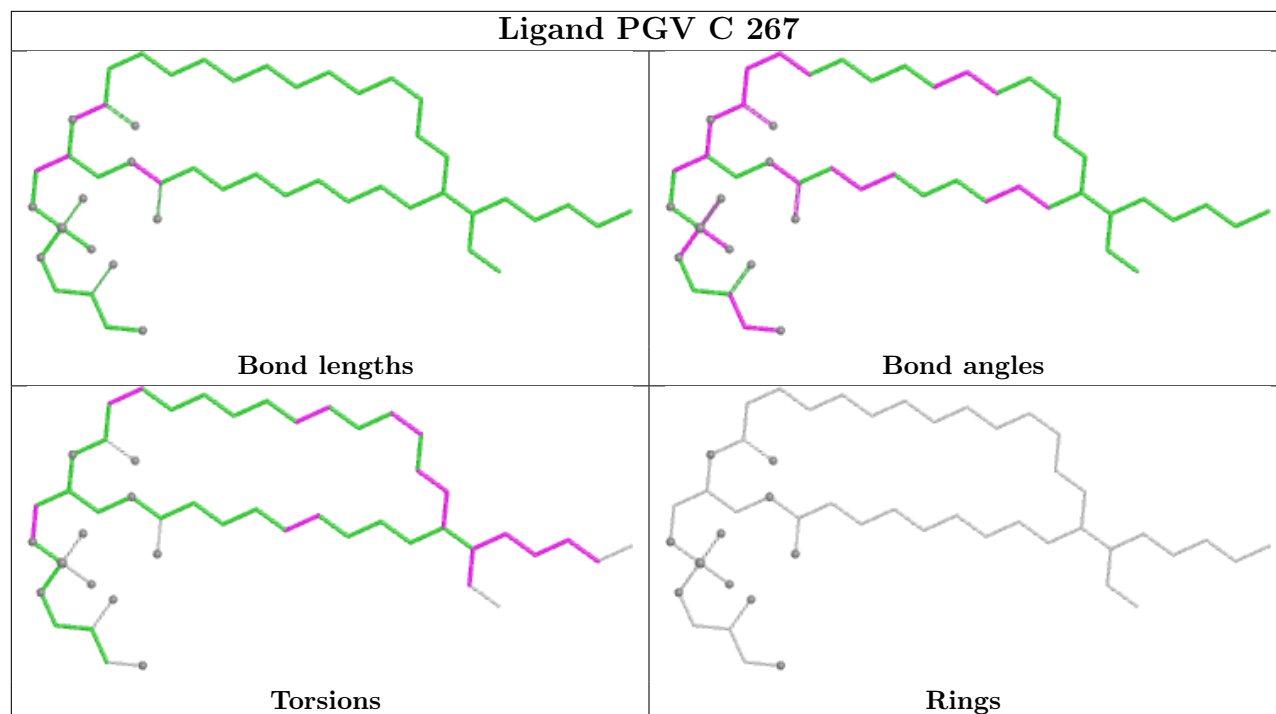
Continued from previous page...

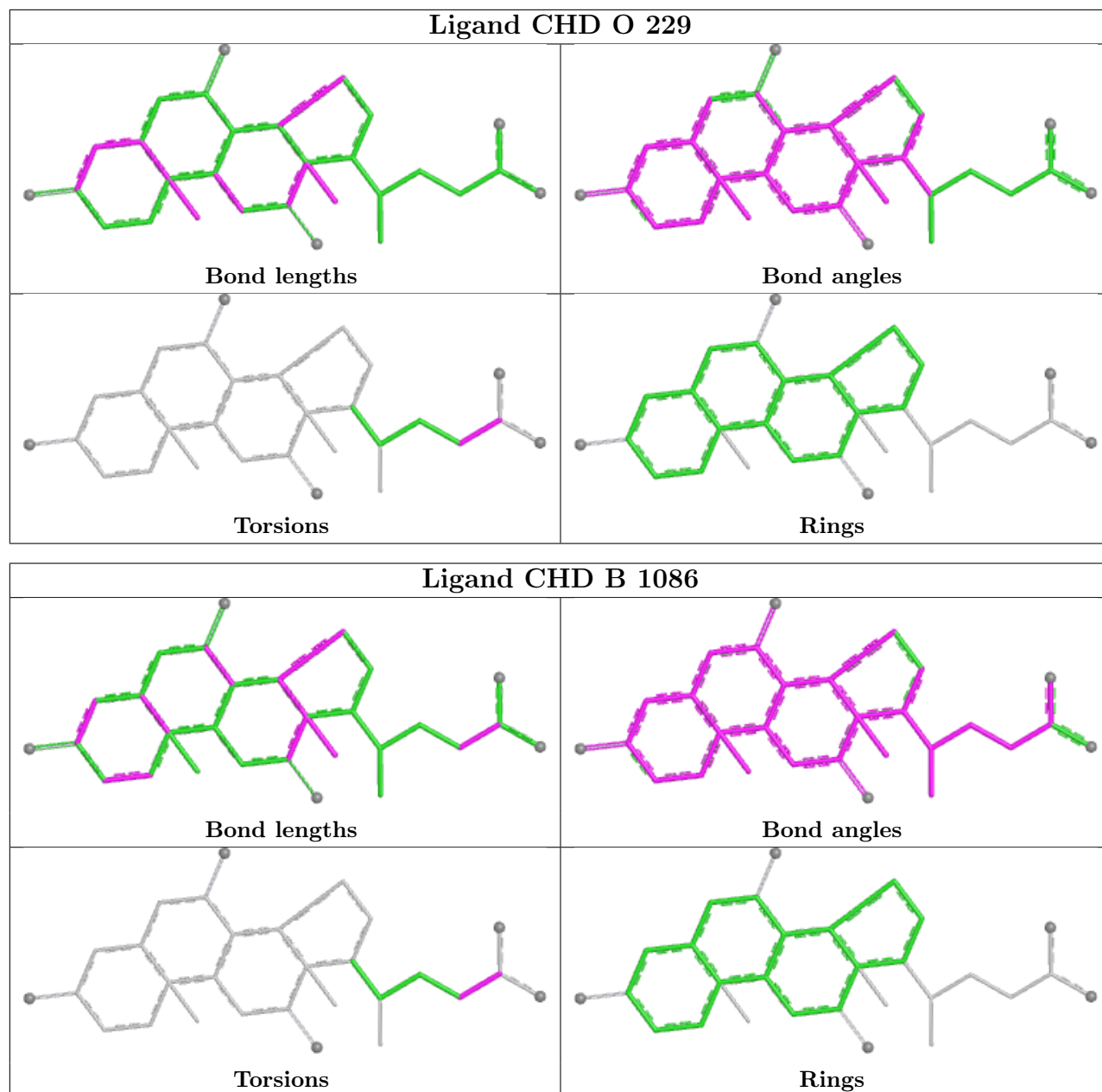
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	P	1268	PGV	3	0
20	N	1266	PGV	1	0
20	C	268	PGV	1	0
28	P	1265	PEK	8	0
24	P	1272	DMU	2	0
19	Q	1523	TGL	5	0
19	N	1521	TGL	9	0
23	C	525	CHD	2	0

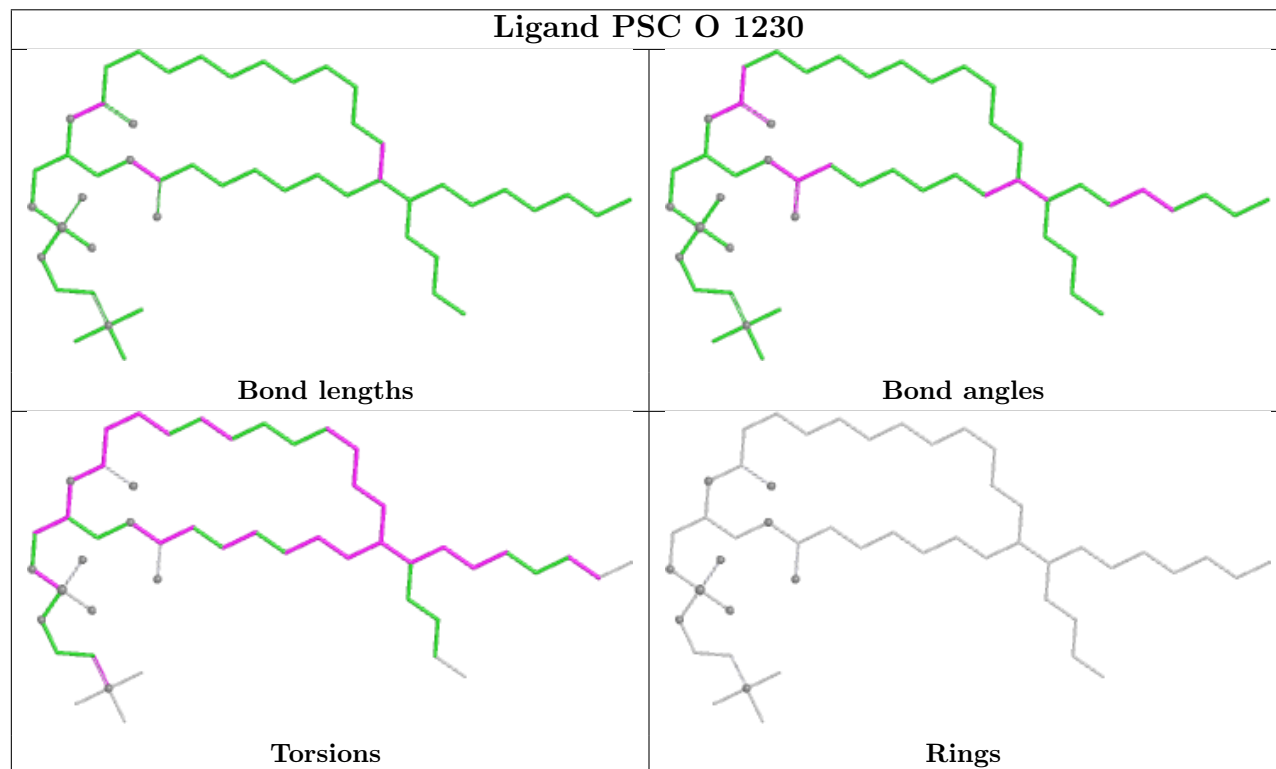
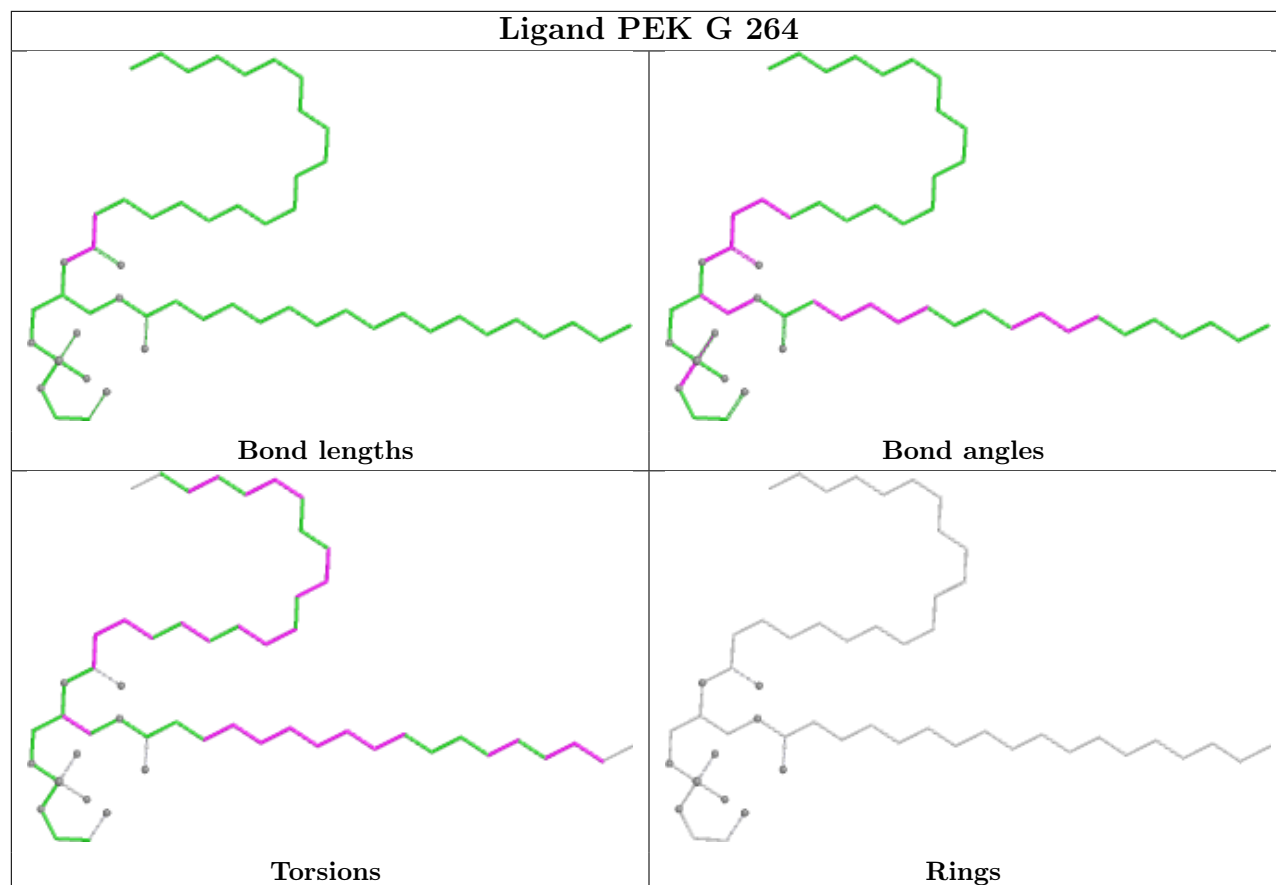
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

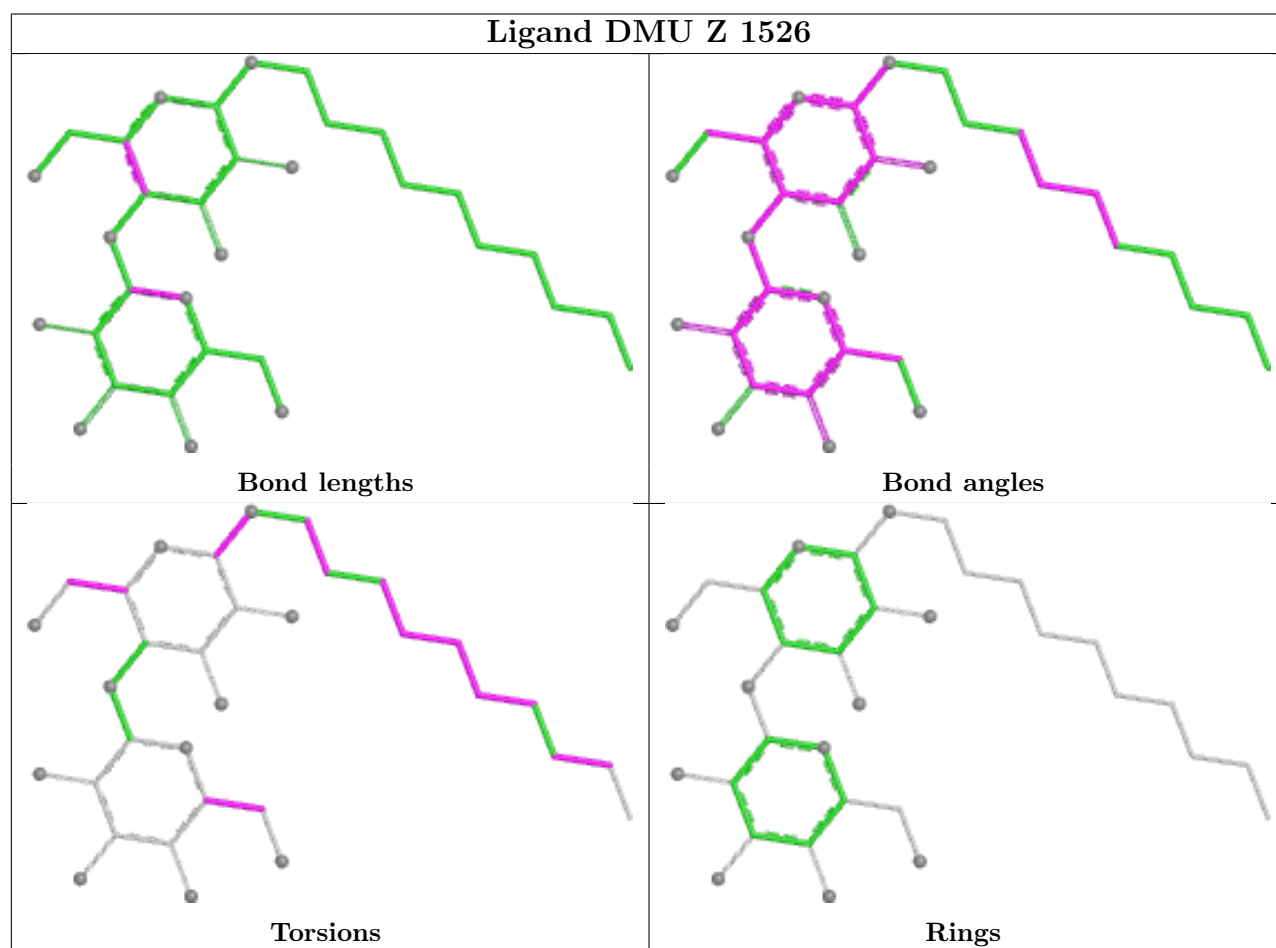
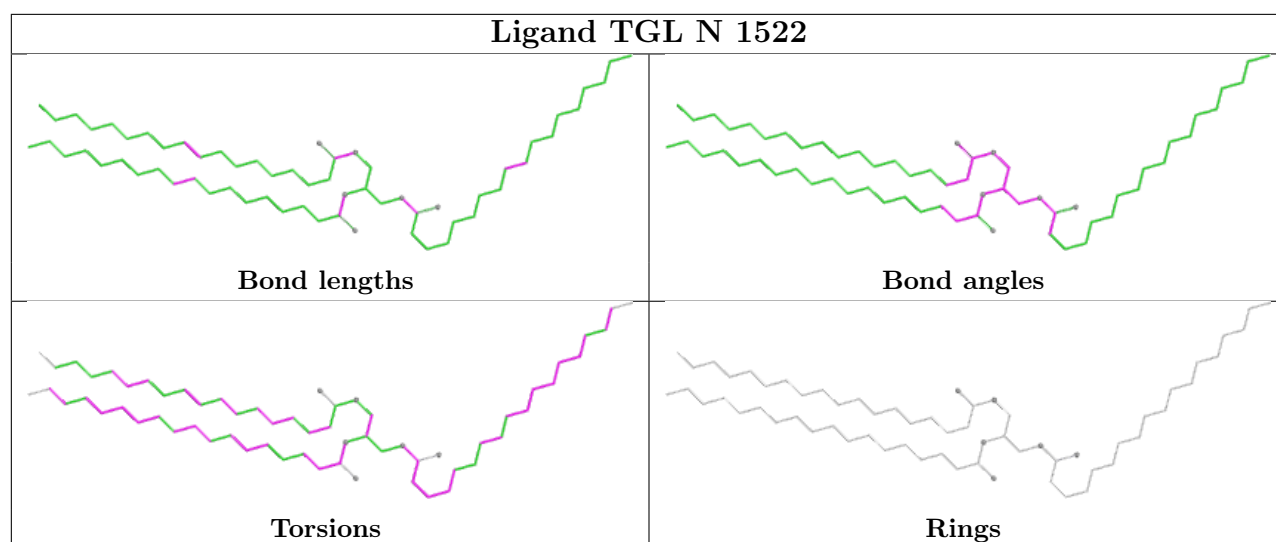


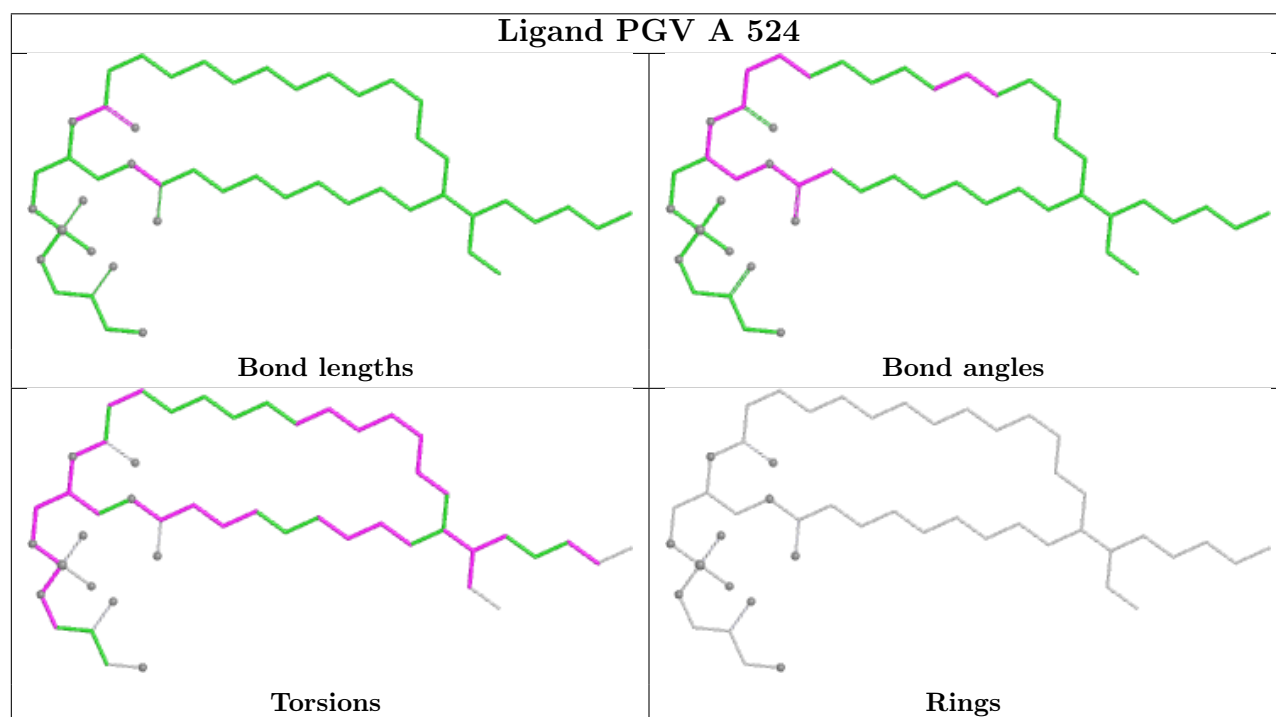
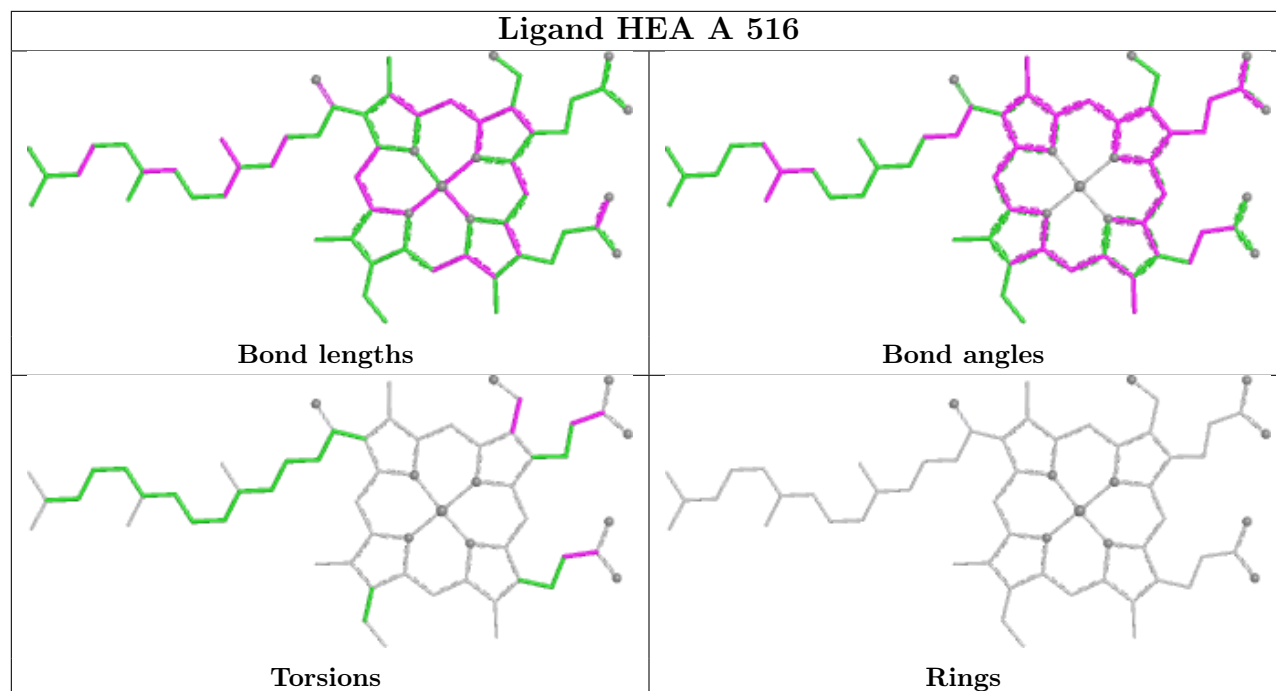


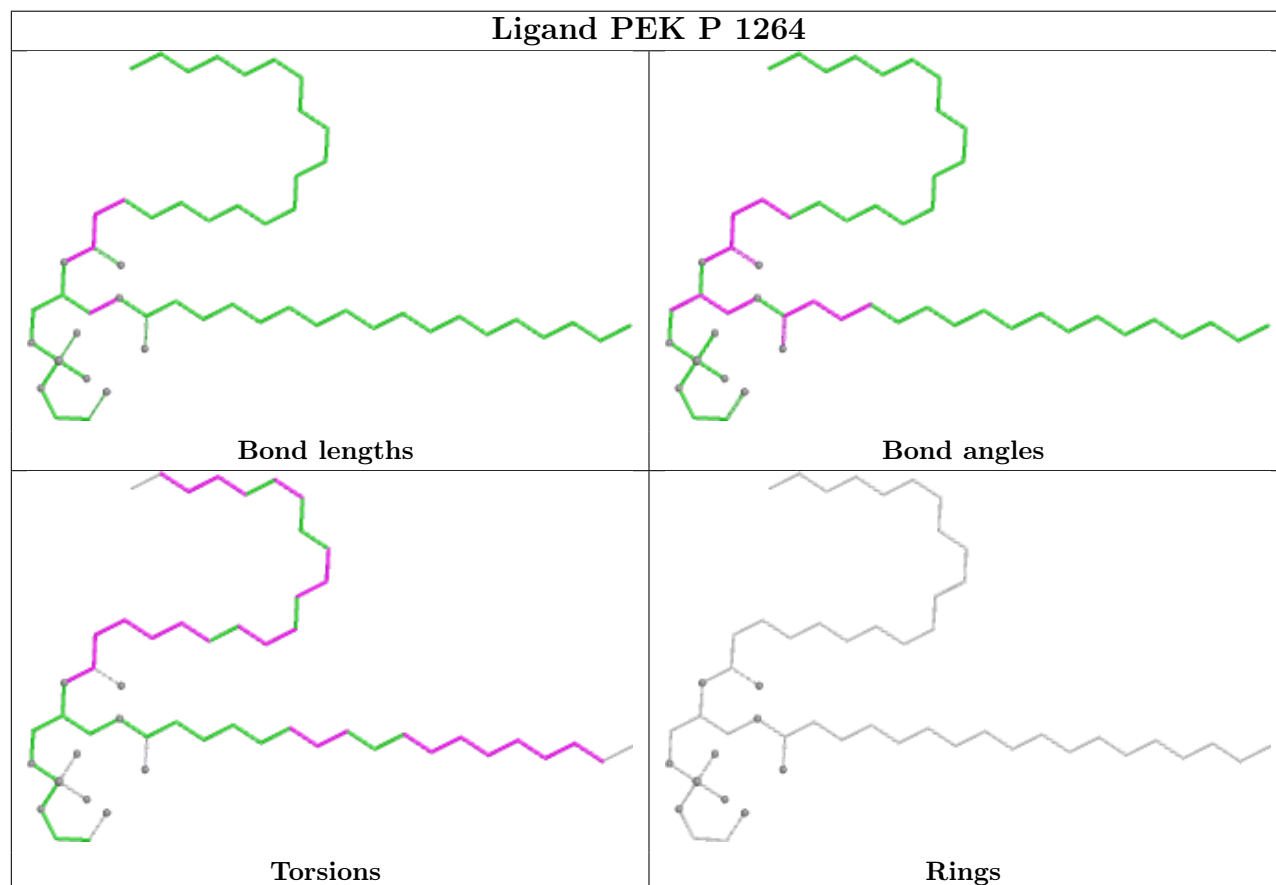
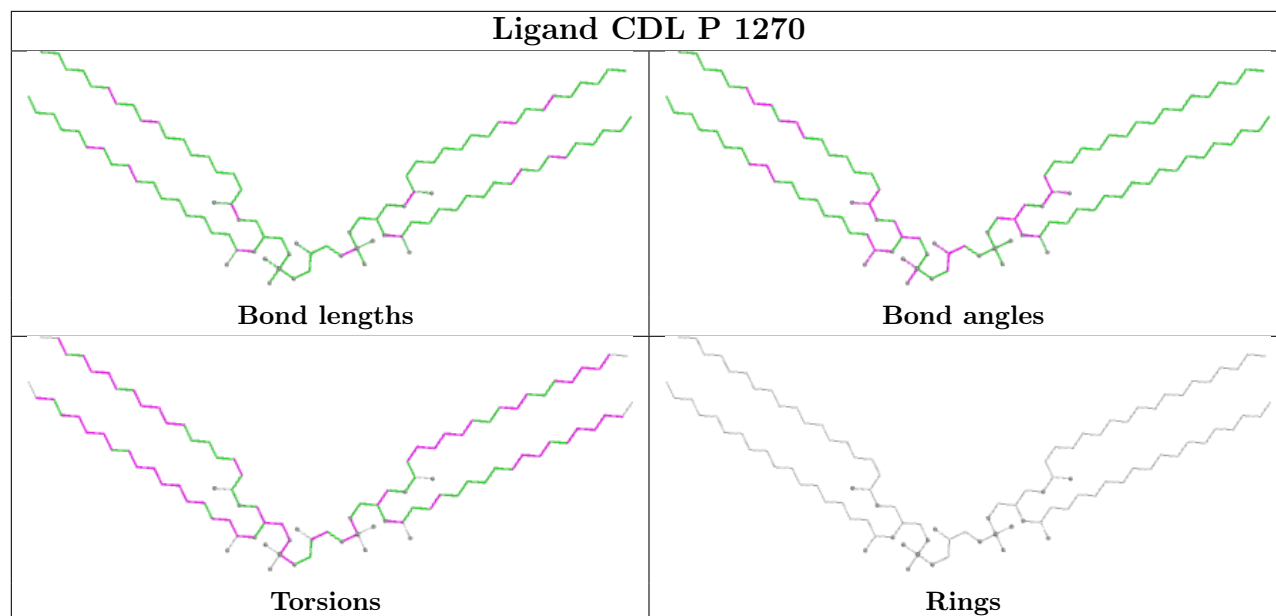


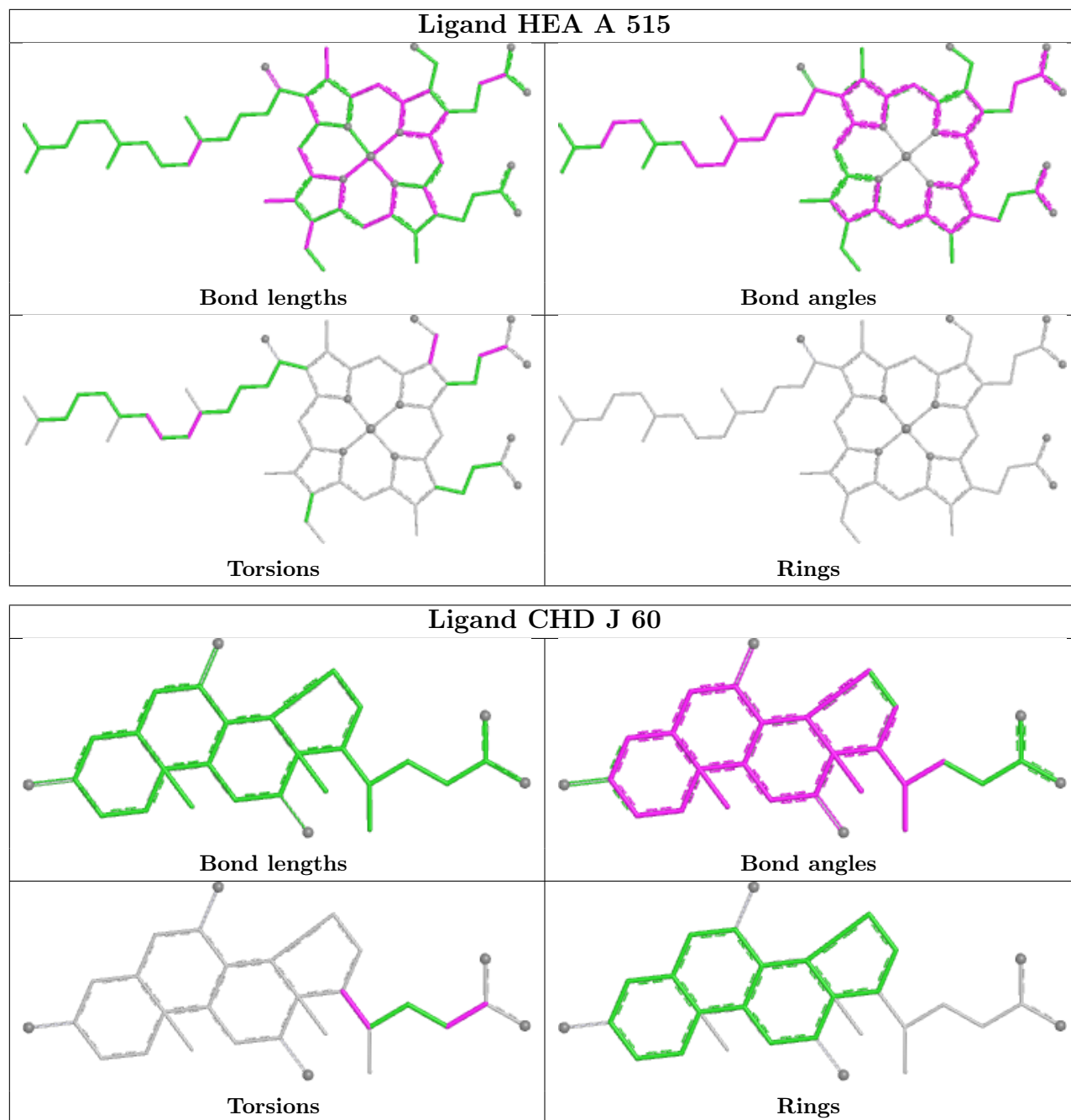


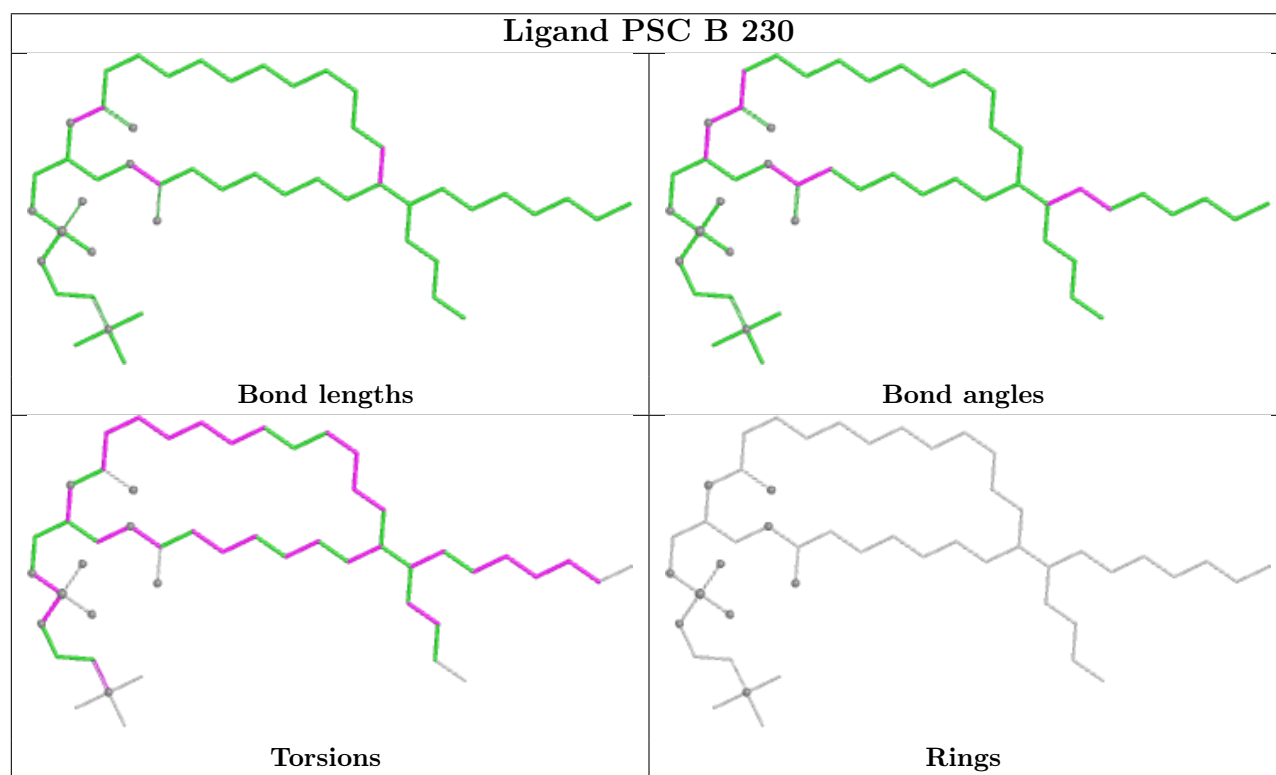
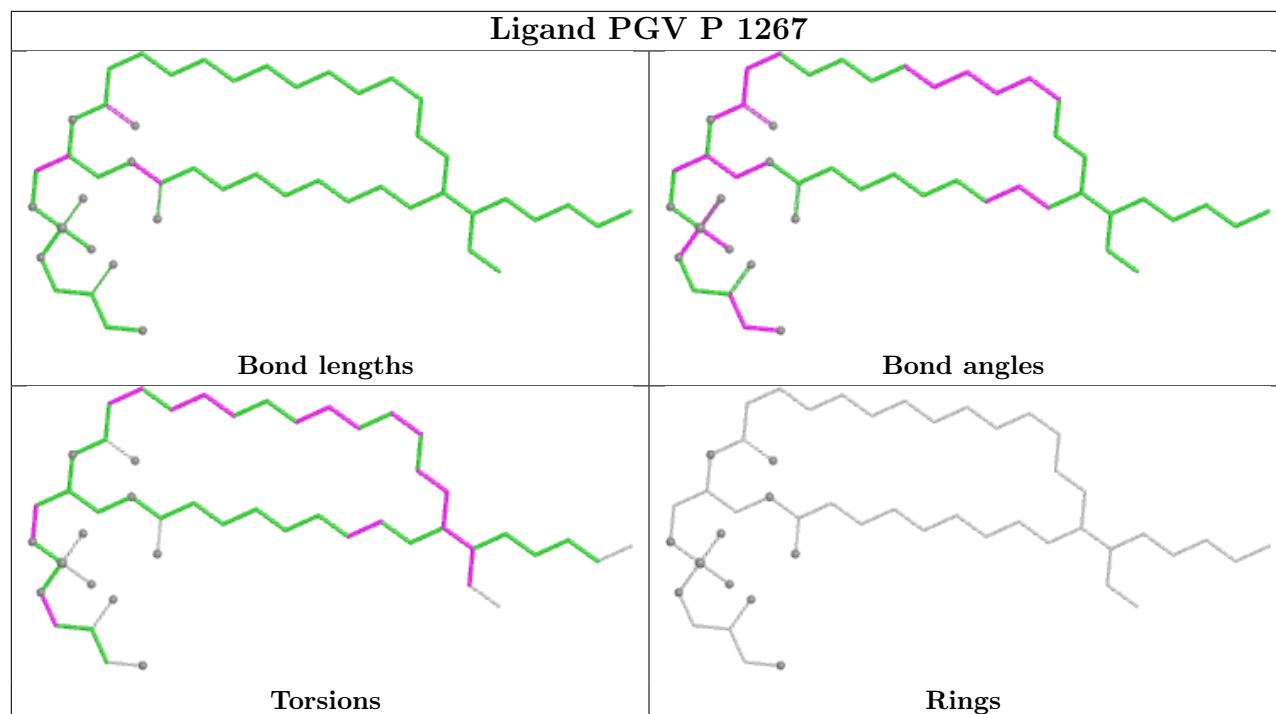


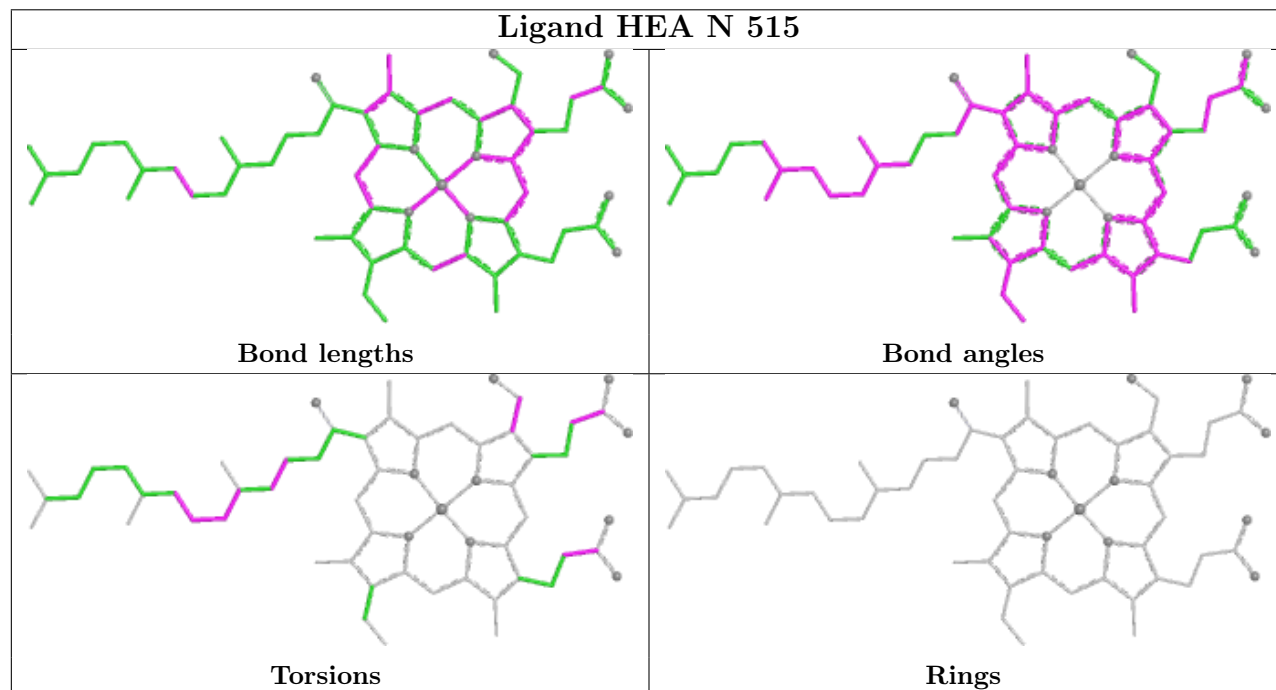
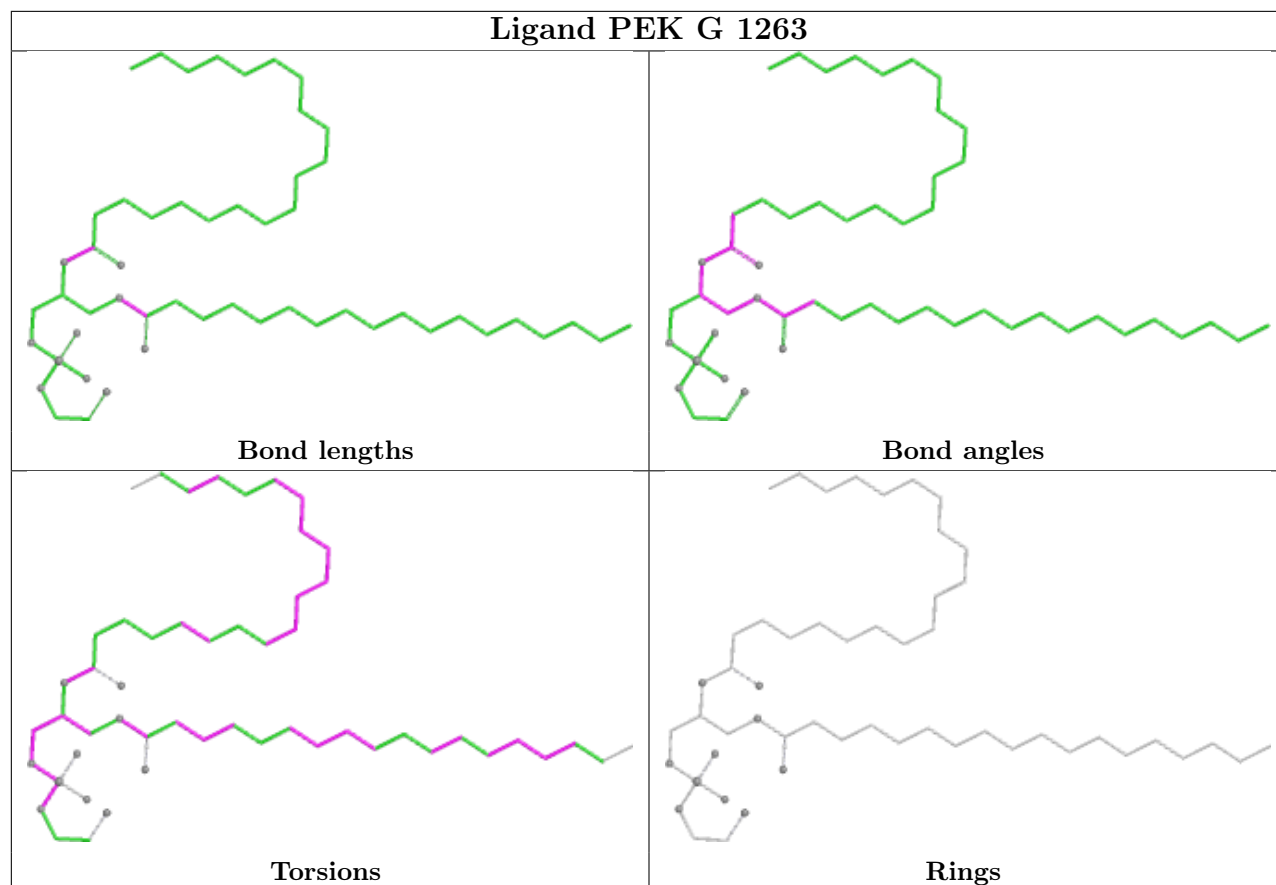


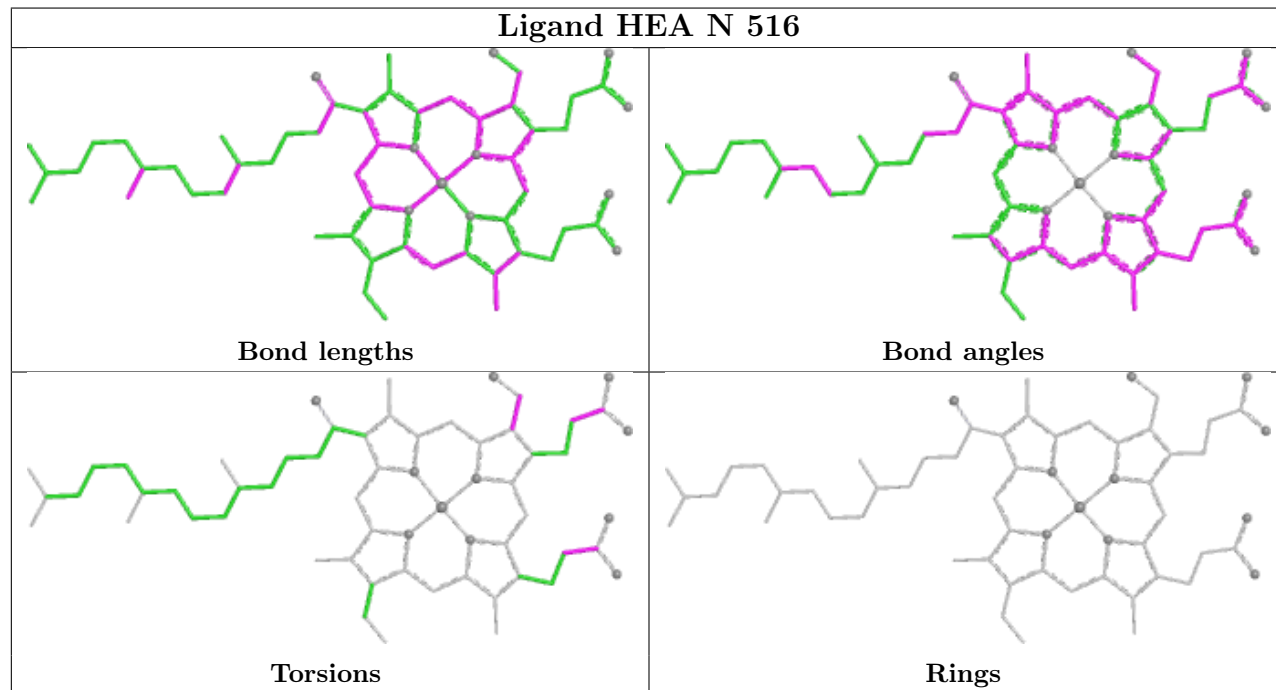
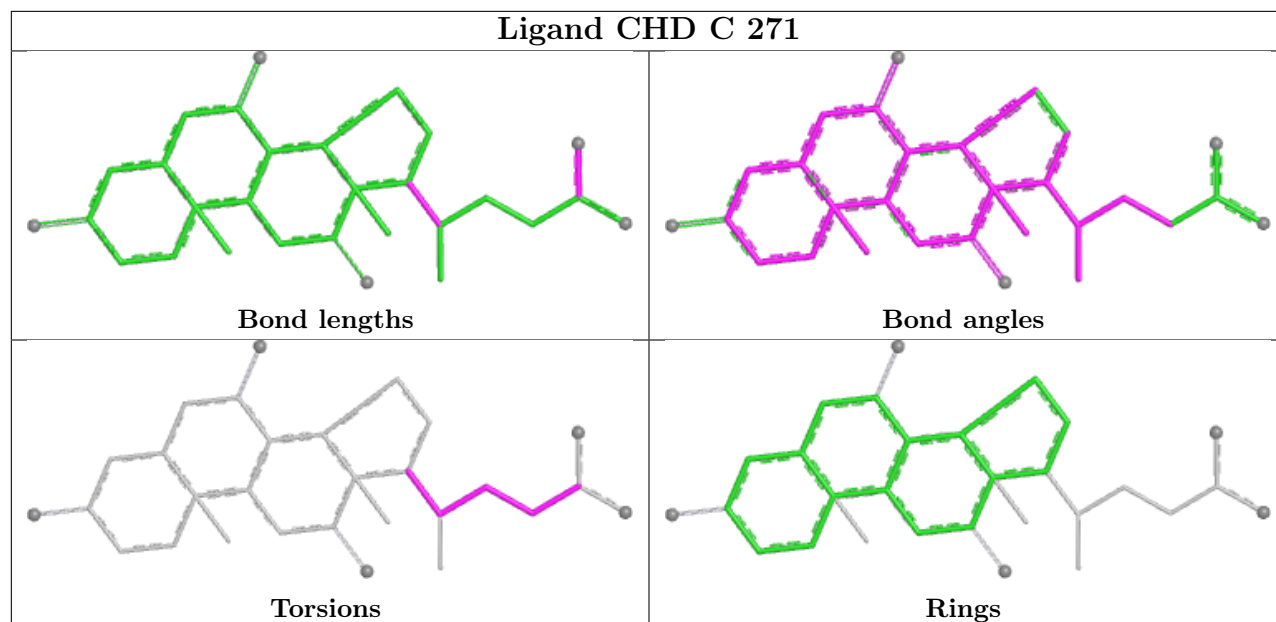


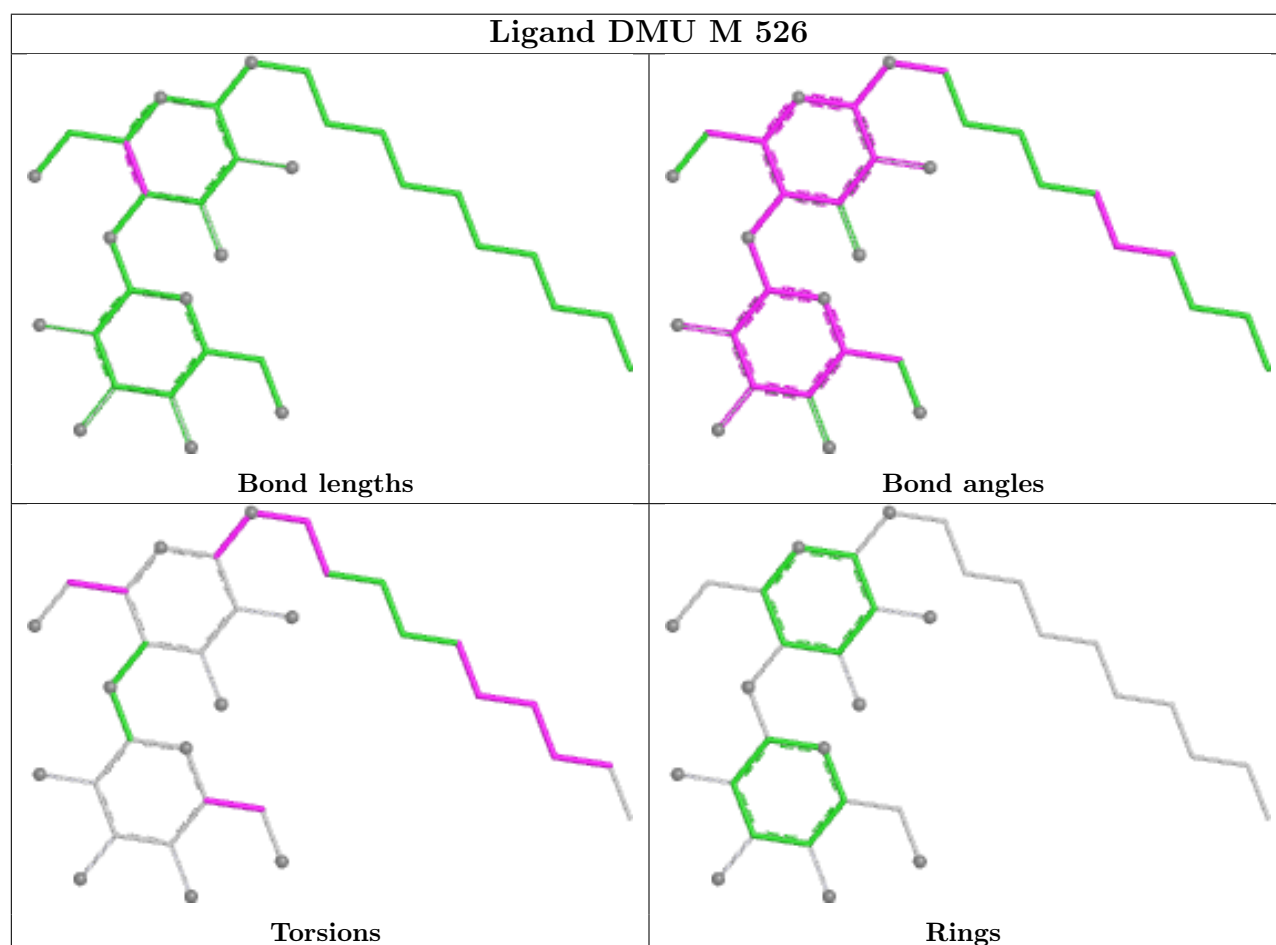
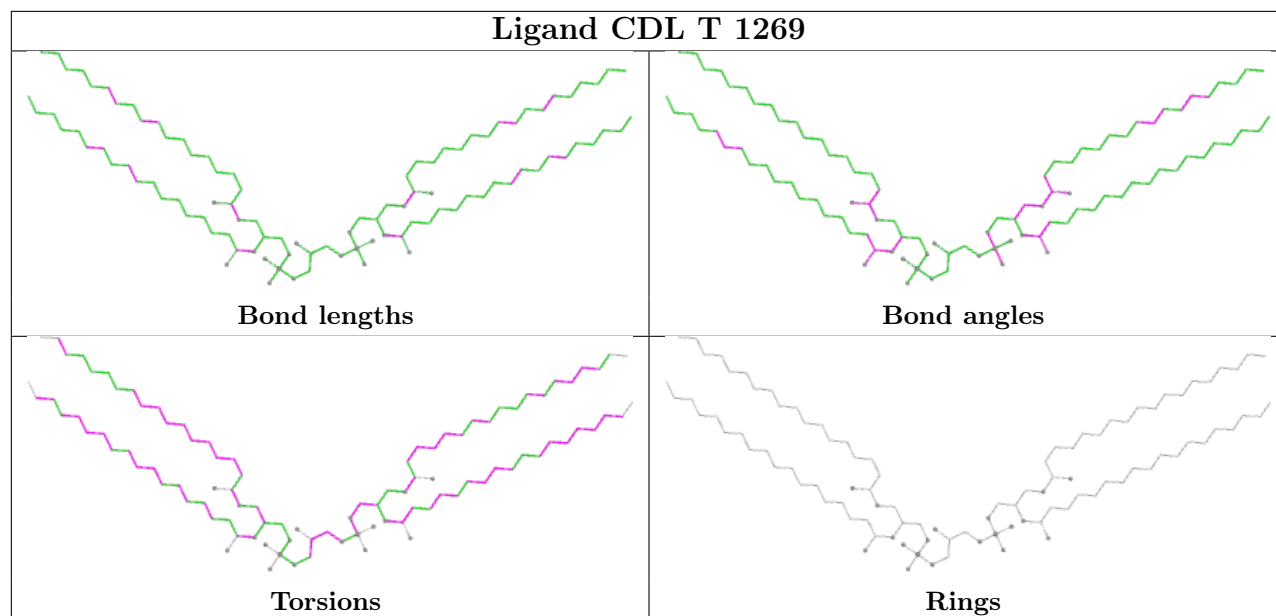


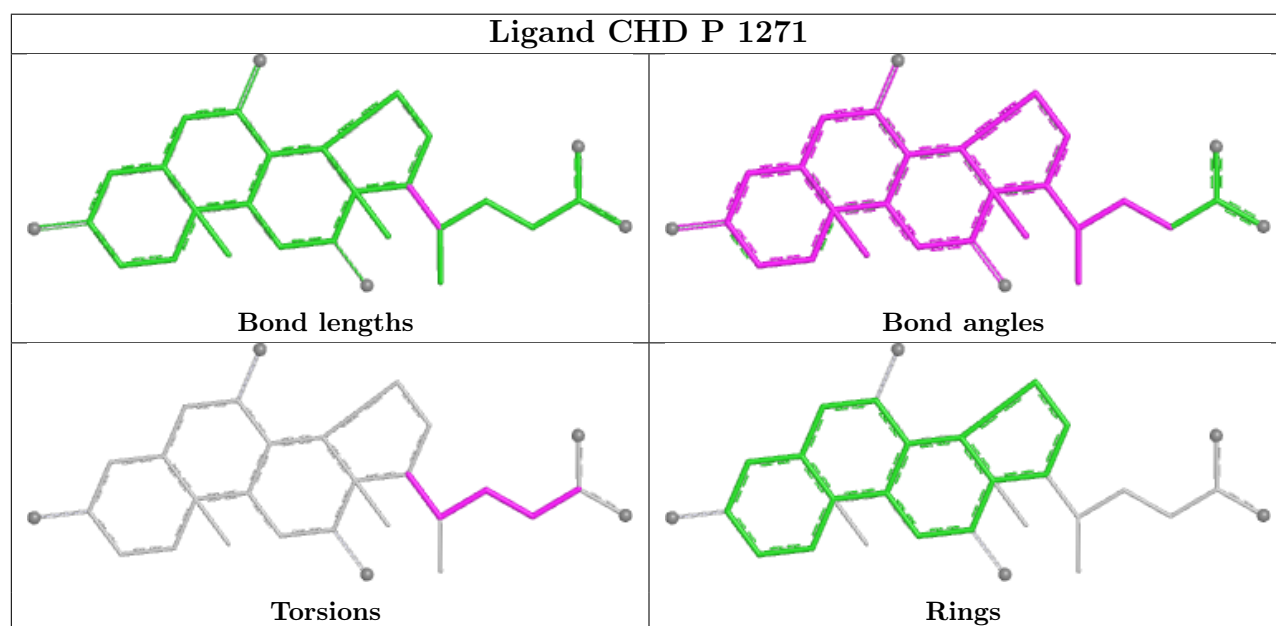
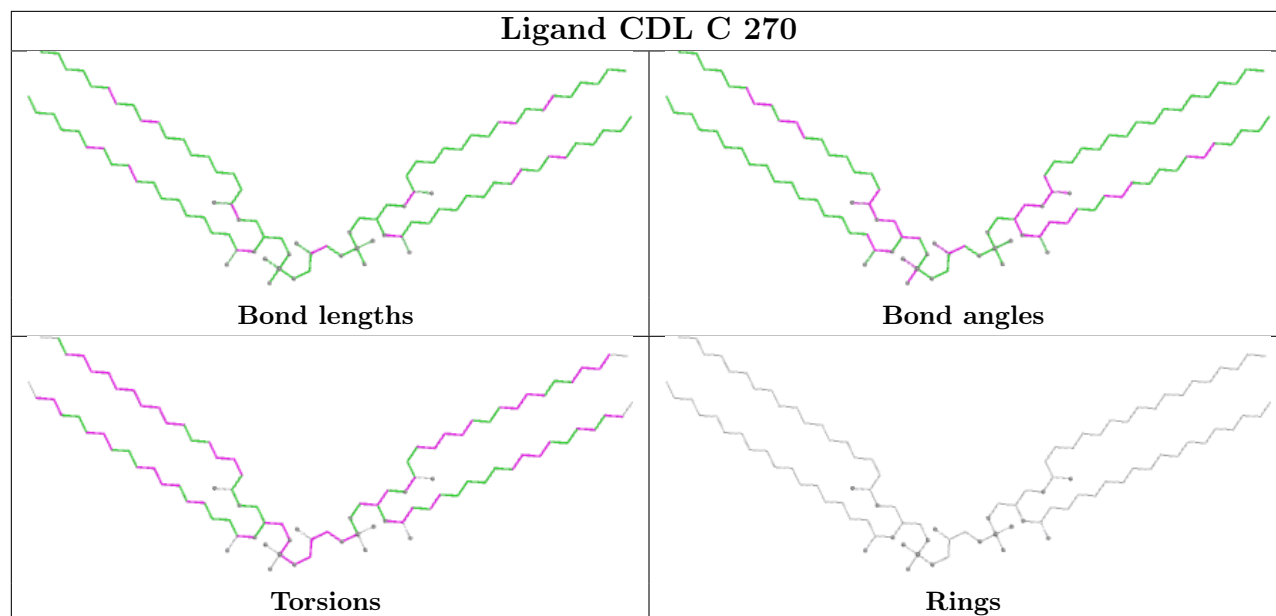


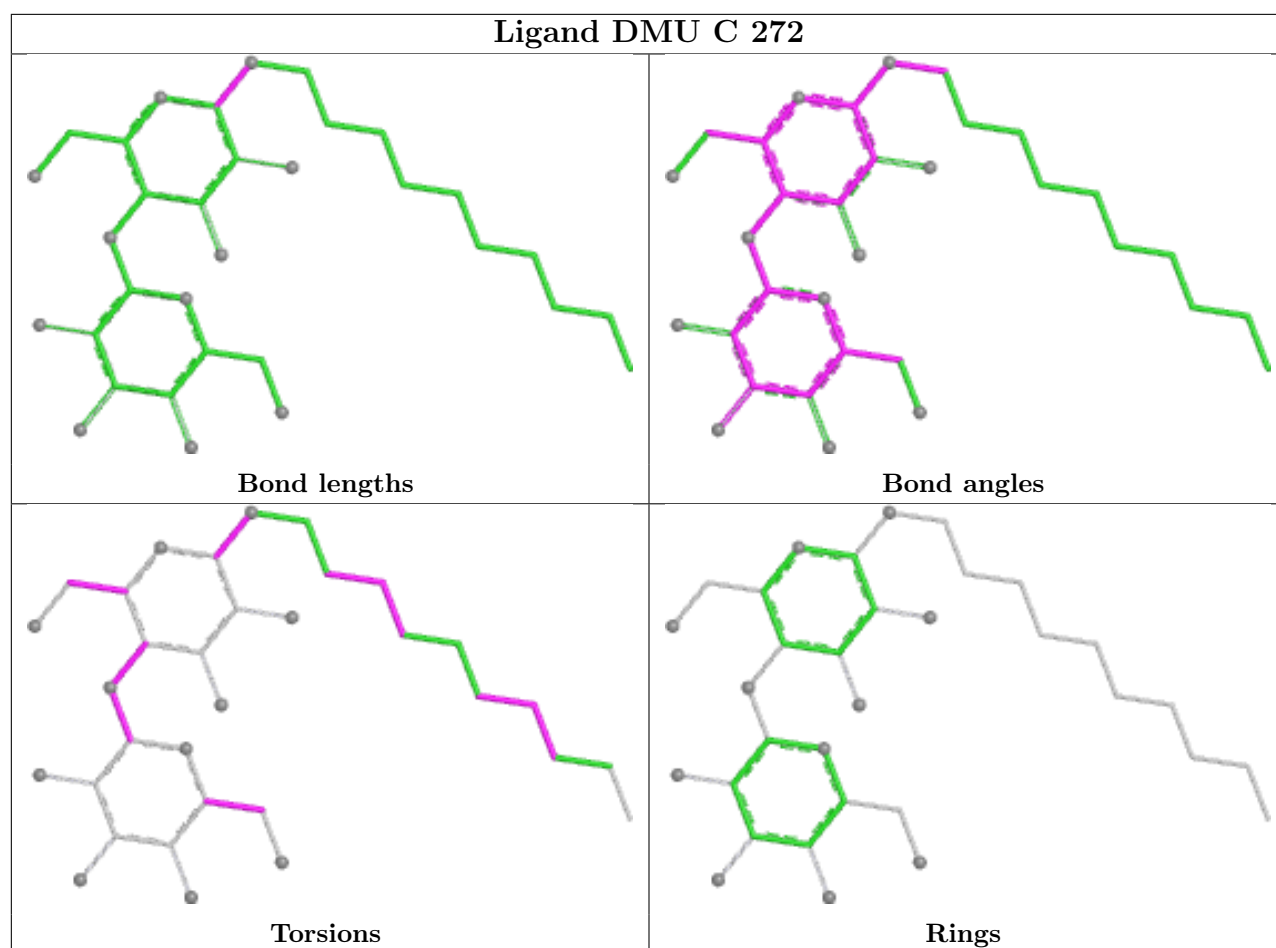




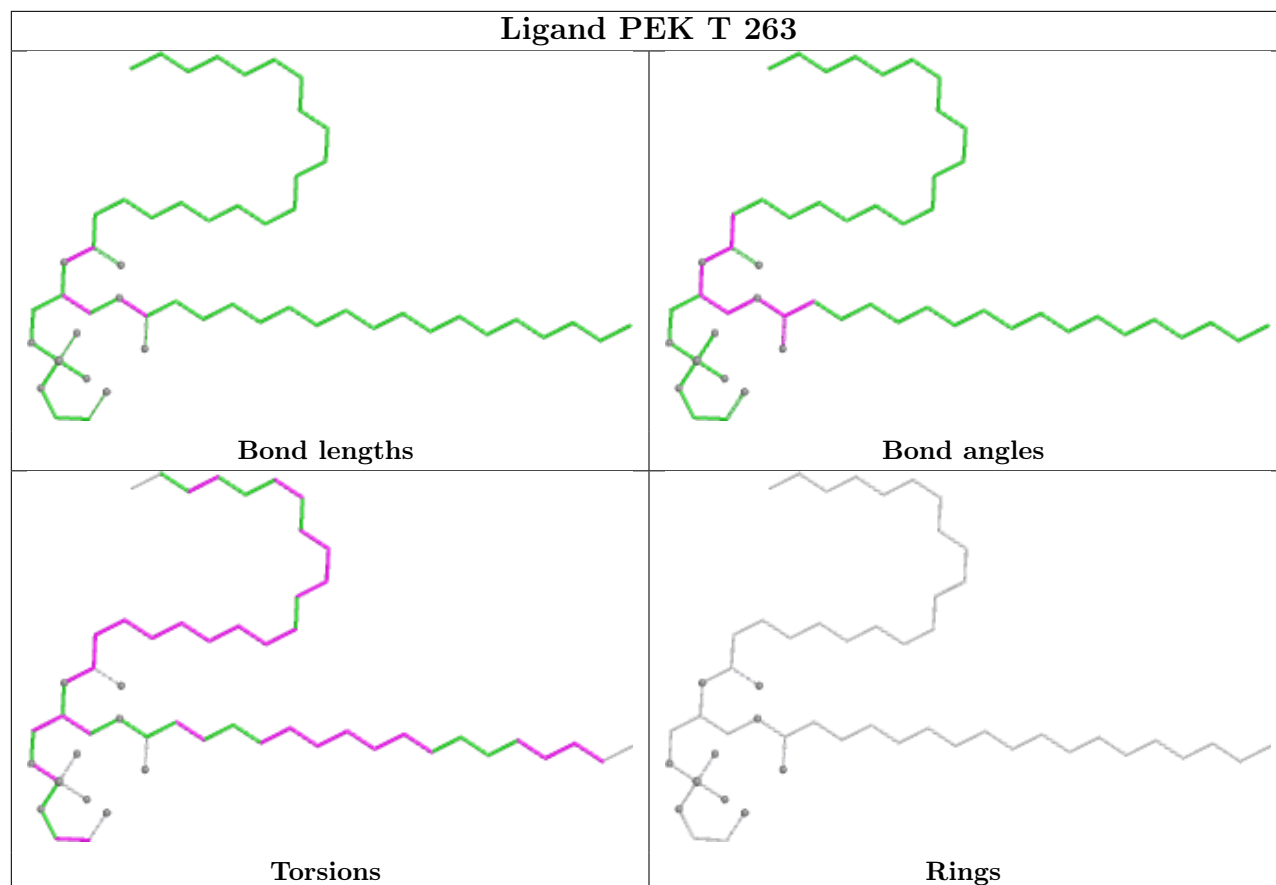




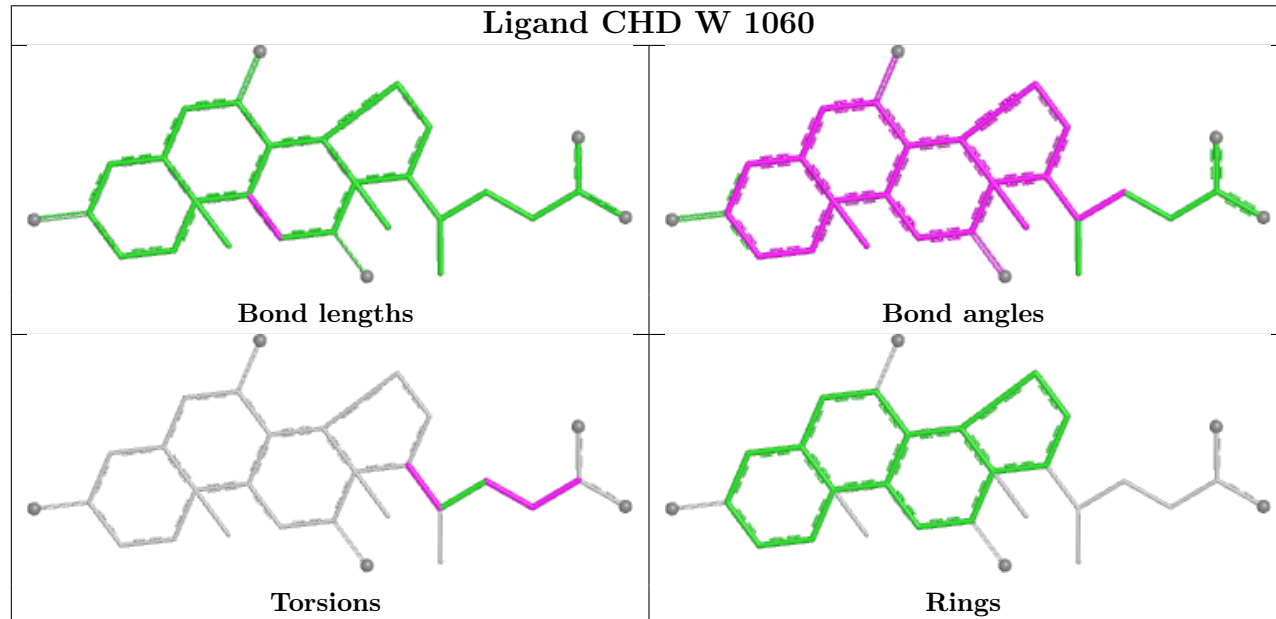


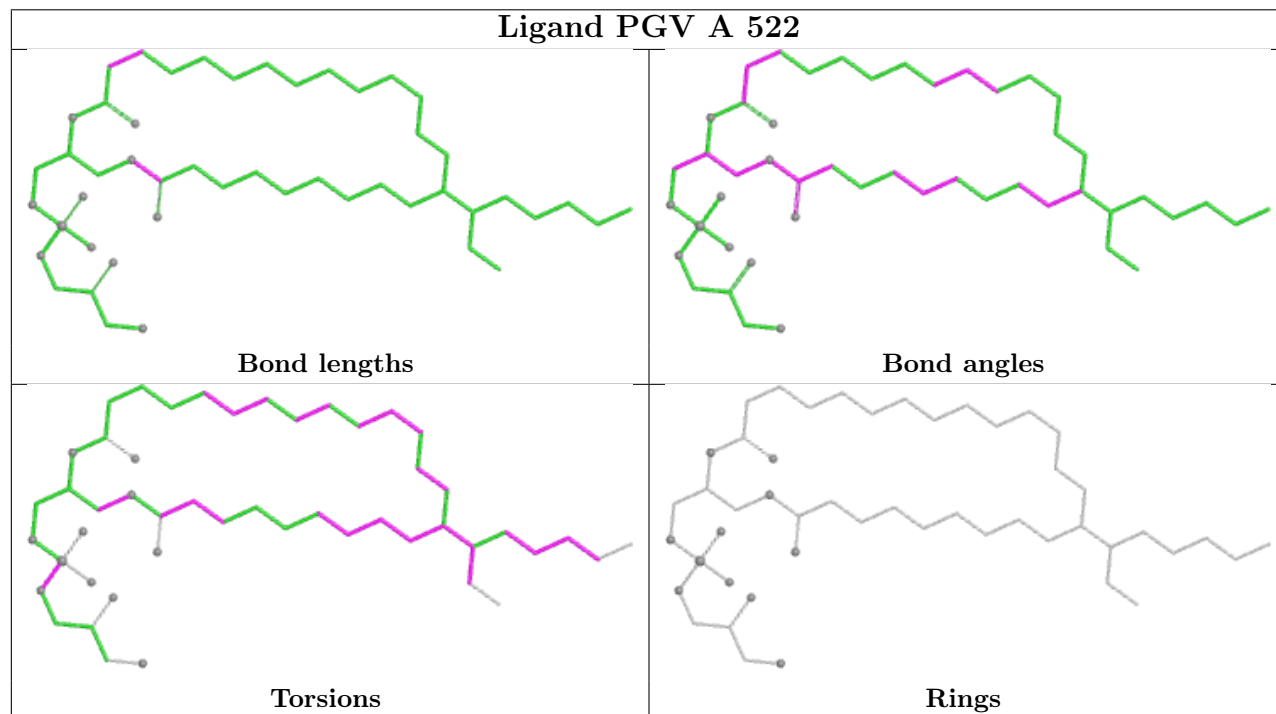
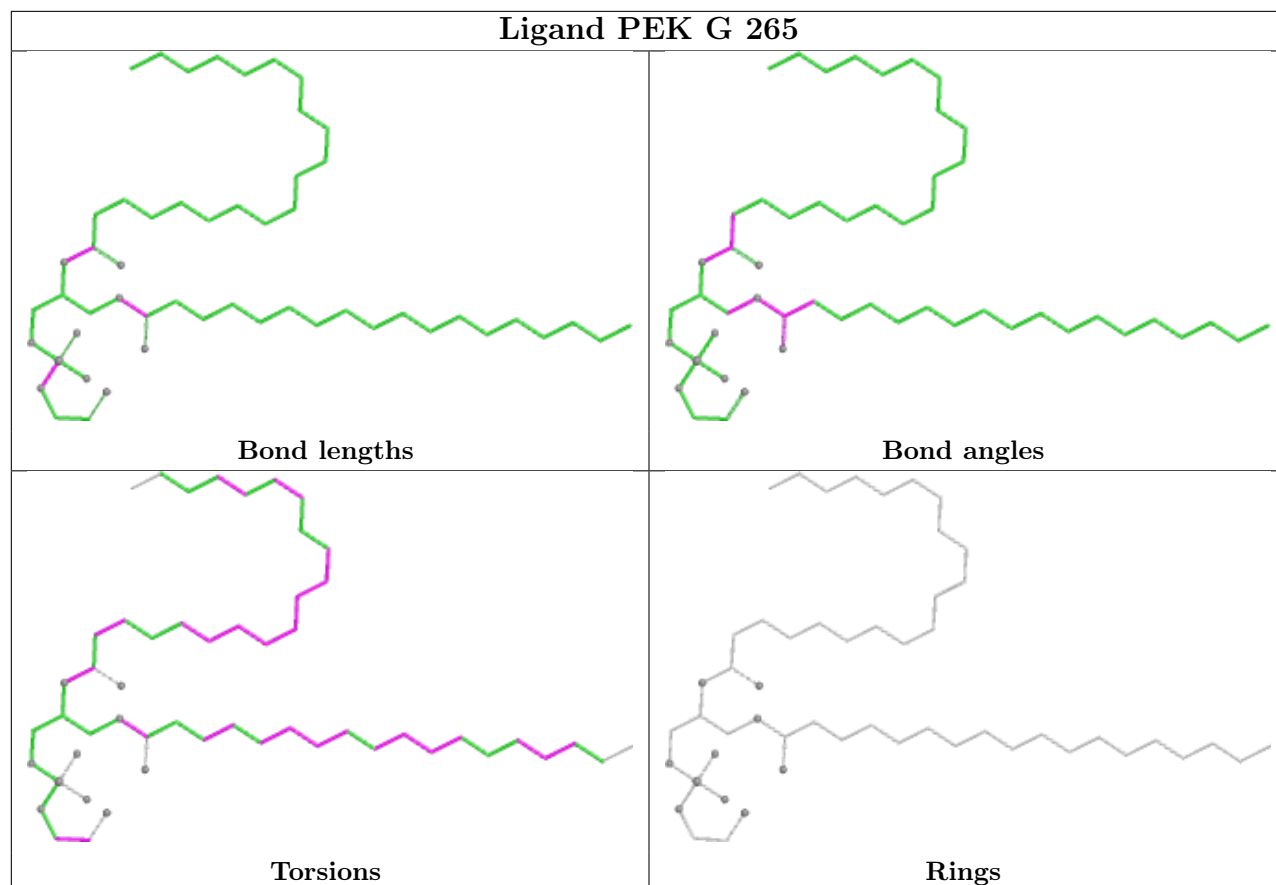


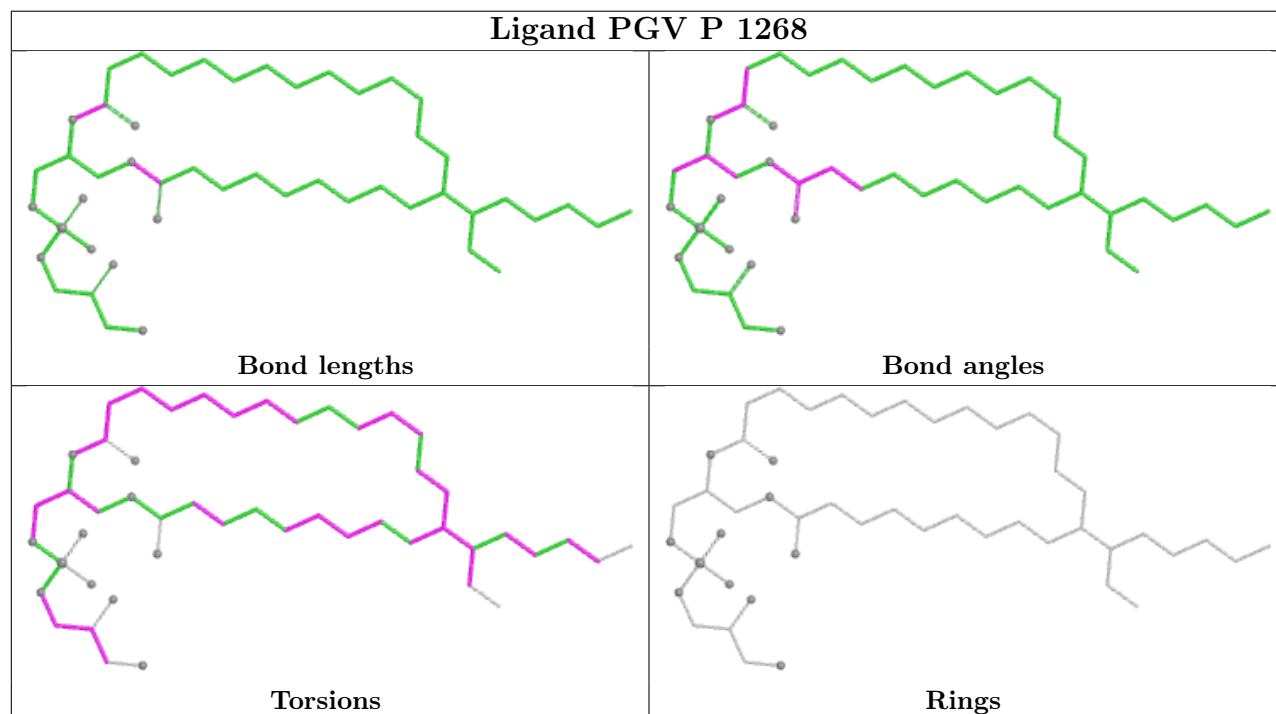
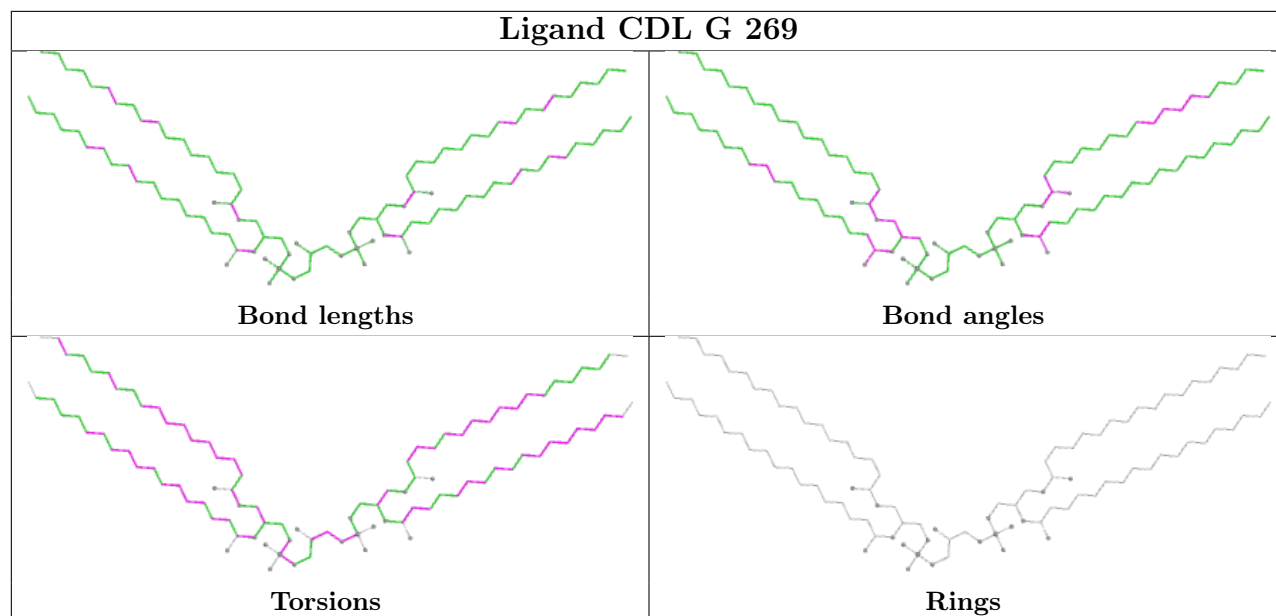
Ligand PEK T 263



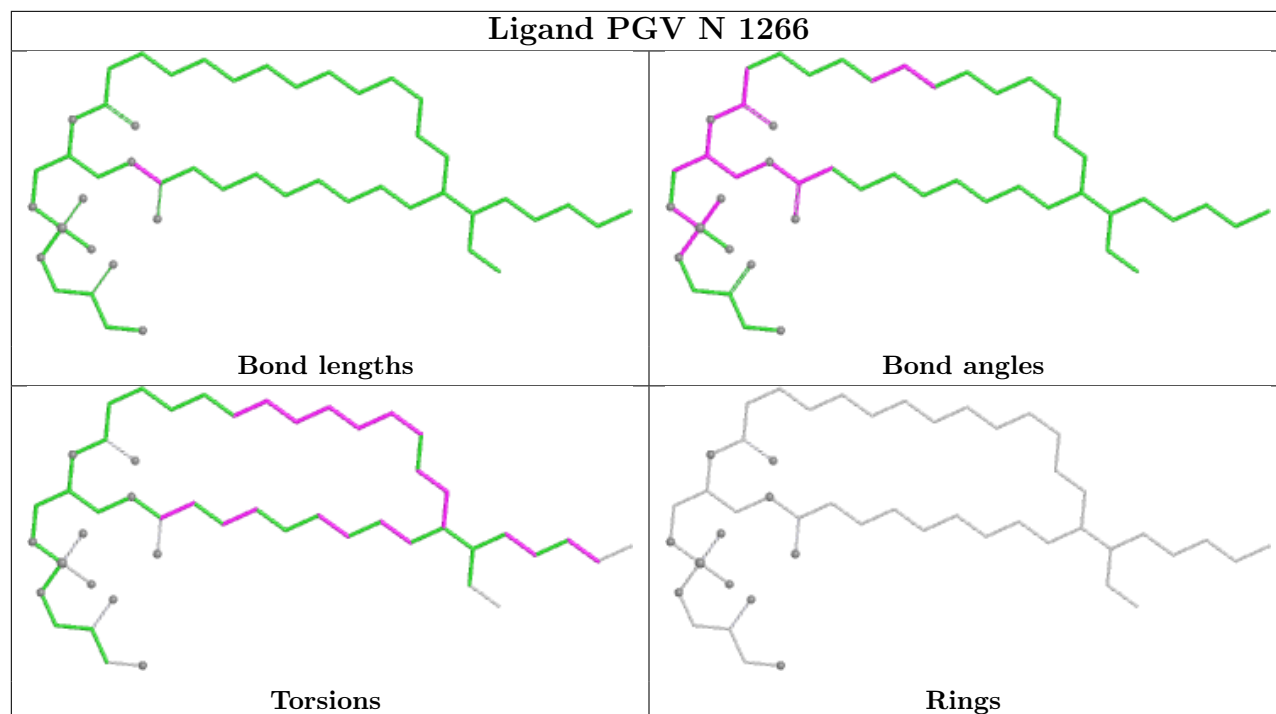
Ligand CHD W 1060



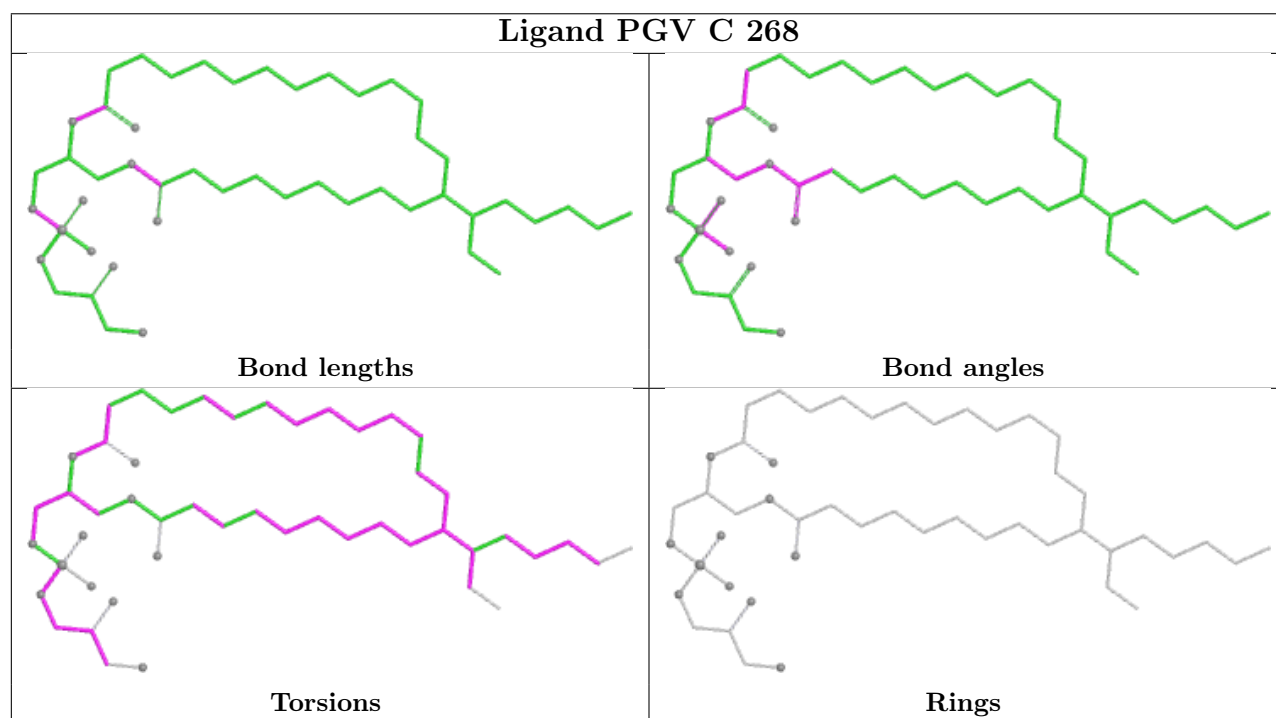


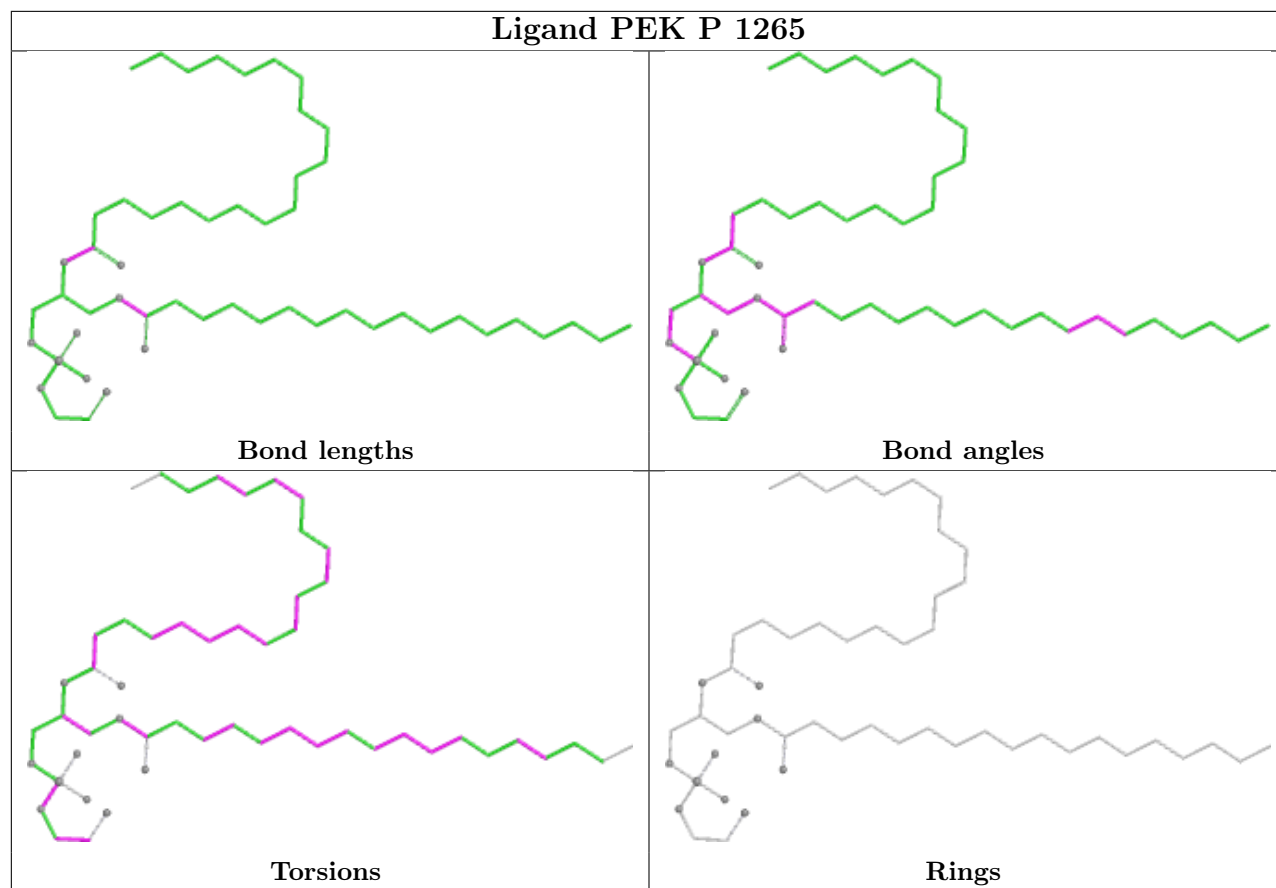


Ligand PGV N 1266

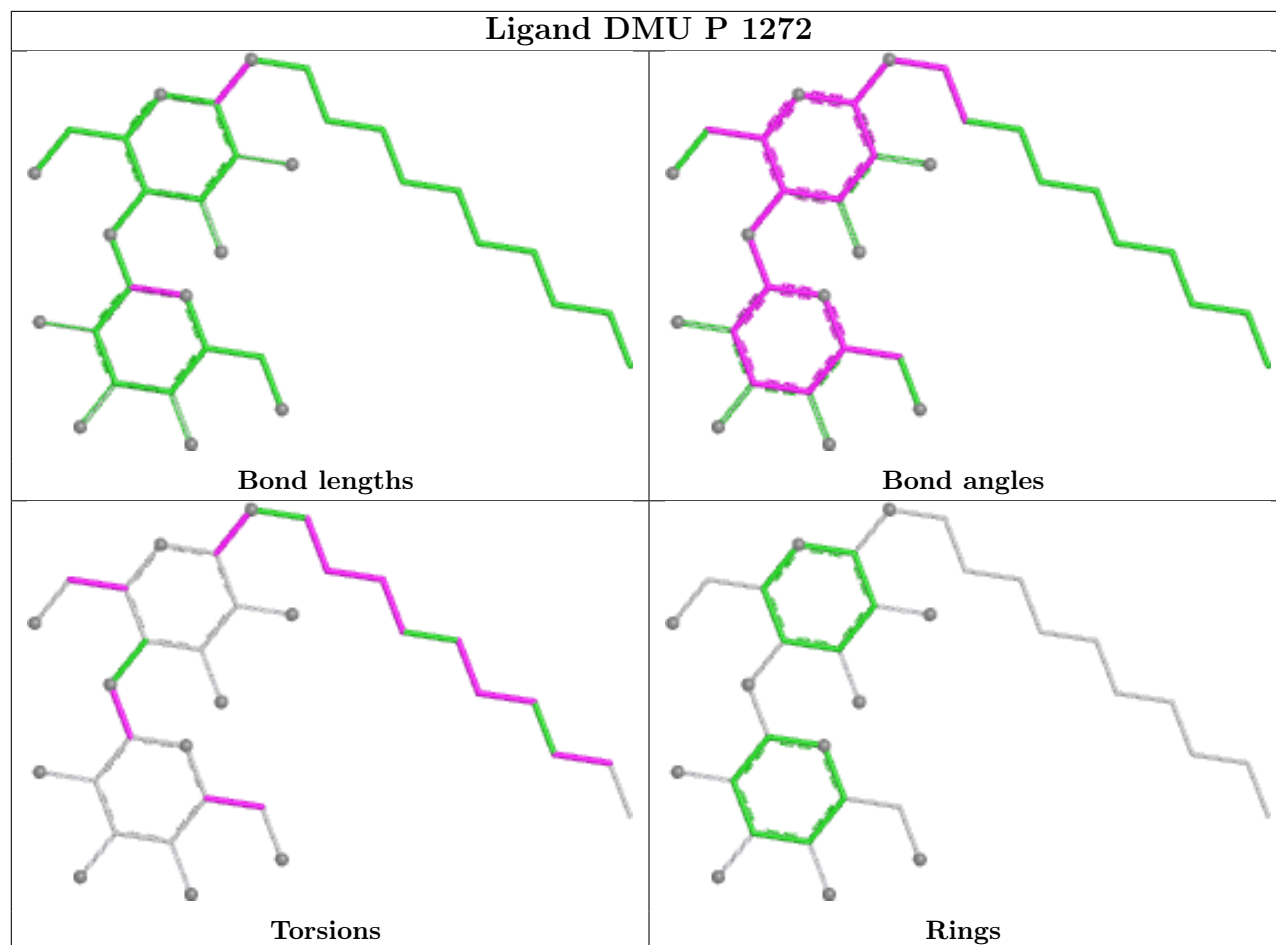


Ligand PGV C 268

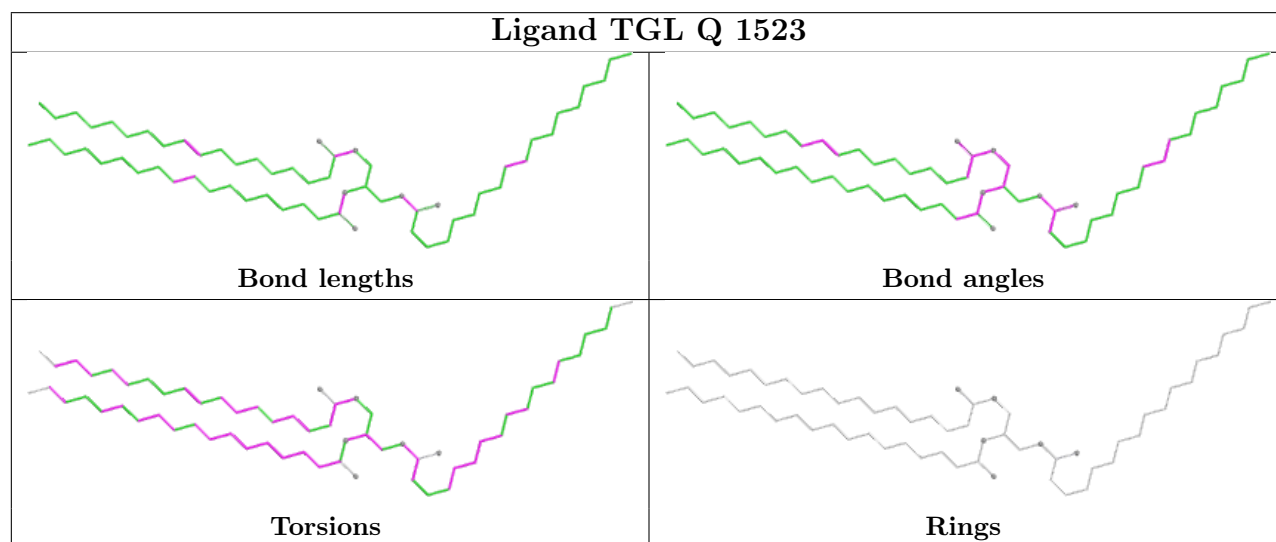


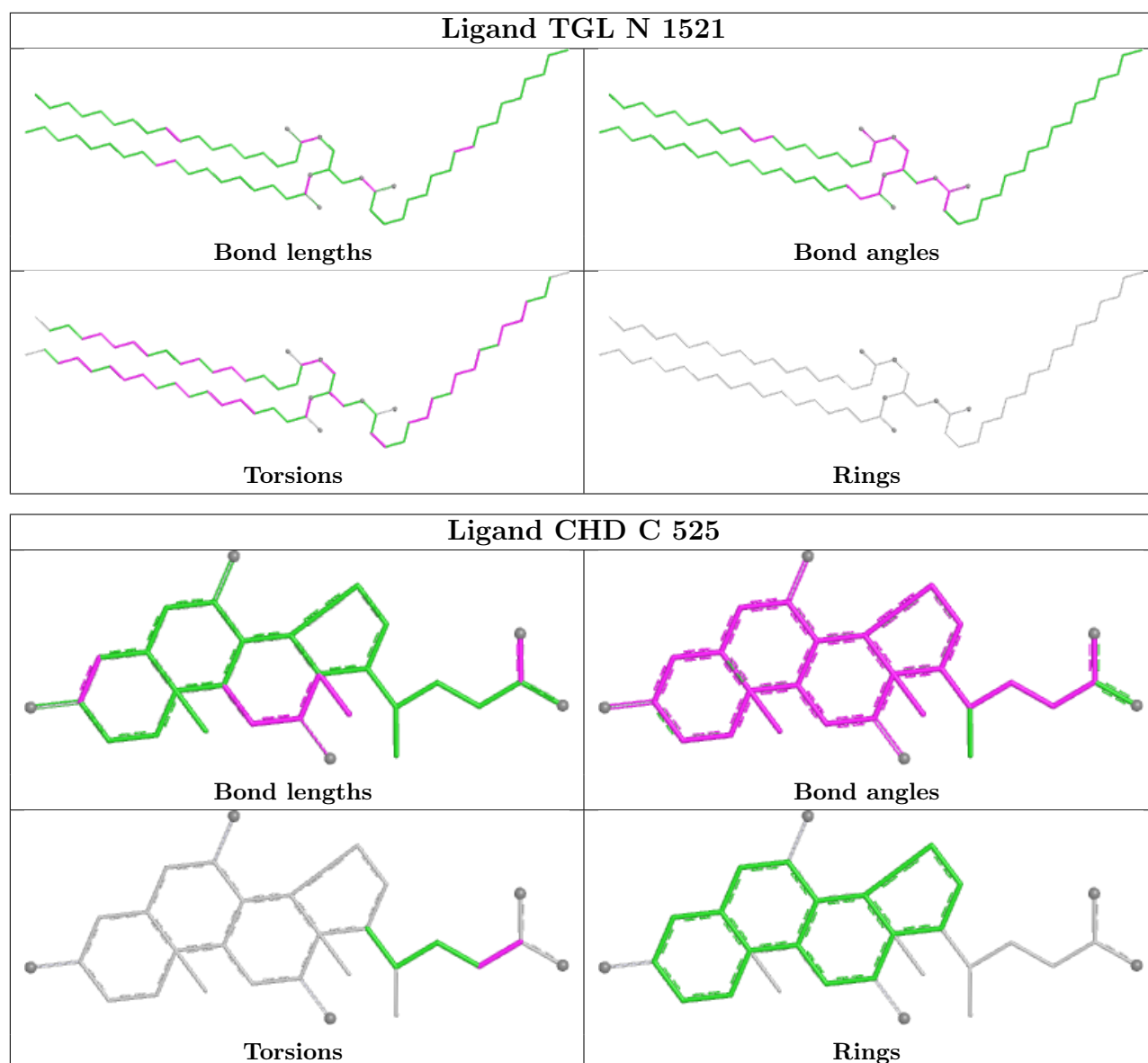


Ligand DMU P 1272



Ligand TGL Q 1523





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.46	2 (0%) 88 90	20, 25, 32, 63	0
1	N	513/514 (99%)	0.12	5 (0%) 79 81	24, 31, 38, 63	0
2	B	226/227 (99%)	0.02	10 (4%) 39 41	21, 29, 49, 77	0
2	O	226/227 (99%)	0.62	16 (7%) 22 23	28, 37, 56, 77	0
3	C	259/261 (99%)	-0.18	2 (0%) 82 84	22, 28, 40, 63	0
3	P	259/261 (99%)	0.26	9 (3%) 47 49	25, 32, 43, 63	0
4	D	144/147 (97%)	0.10	4 (2%) 55 57	25, 31, 48, 64	0
4	Q	144/147 (97%)	1.42	29 (20%) 3 3	33, 44, 67, 108	0
5	E	104/109 (95%)	-0.05	1 (0%) 79 81	26, 31, 51, 65	0
5	R	104/109 (95%)	0.74	6 (5%) 29 30	31, 38, 58, 74	0
6	F	93/98 (94%)	0.34	5 (5%) 31 33	23, 34, 52, 94	0
6	S	93/98 (94%)	0.80	7 (7%) 20 21	29, 38, 59, 91	0
7	G	83/85 (97%)	1.19	21 (25%) 1 2	25, 35, 94, 102	0
7	T	83/85 (97%)	1.46	23 (27%) 1 1	27, 38, 93, 100	0
8	H	75/85 (88%)	0.46	8 (10%) 11 11	28, 36, 69, 75	0
8	U	75/85 (88%)	0.82	7 (9%) 14 15	32, 41, 72, 76	0
9	I	71/73 (97%)	0.78	11 (15%) 5 5	28, 38, 65, 70	0
9	V	71/73 (97%)	1.34	15 (21%) 2 2	30, 48, 65, 75	0
10	J	57/59 (96%)	0.49	3 (5%) 32 34	28, 37, 57, 70	0
10	W	57/59 (96%)	1.29	7 (12%) 8 8	33, 42, 62, 79	0
11	K	49/56 (87%)	0.54	2 (4%) 41 43	28, 35, 47, 55	0
11	X	49/56 (87%)	1.50	10 (20%) 3 3	38, 45, 60, 71	0
12	L	46/47 (97%)	0.13	2 (4%) 40 41	26, 31, 51, 75	0
12	Y	46/47 (97%)	1.14	5 (10%) 10 11	33, 39, 60, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.42	5 (11%) 9 10	27, 30, 65, 89	0
13	Z	43/46 (93%)	1.35	9 (20%) 2 2	35, 39, 77, 95	0
All	All	3526/3614 (97%)	0.34	224 (6%) 25 27	20, 33, 58, 108	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	13.1
6	S	96	LEU	11.6
4	Q	4	SER	7.7
7	T	3	ALA	7.6
2	O	227	LEU	7.2
7	G	5	LYS	6.9
4	Q	5	VAL	6.6
7	T	36	TRP	6.4
6	S	95	GLN	6.4
6	S	94	HIS	6.3
7	G	36	TRP	6.2
7	G	4	ALA	6.2
7	T	4	ALA	6.2
7	G	3	ALA	6.1
7	G	7	ASP	5.8
4	Q	8	SER	5.8
12	L	2	HIS	5.7
7	T	37	LEU	5.3
7	T	38	HIS	5.3
7	T	9	GLY	5.3
2	B	59	GLN	5.2
7	T	5	LYS	5.2
6	F	96	LEU	5.1
6	S	93	PRO	5.1
7	T	8	HIS	5.0
7	T	10	GLY	5.0
2	O	113	TYR	5.0
2	B	60	GLU	4.9
7	G	6	GLY	4.7
7	G	9	GLY	4.7
7	G	1	ALA	4.7
7	T	2	SER	4.6
6	F	94	HIS	4.6
4	Q	7	LYS	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	P	3	HIS	4.5
9	V	3	ALA	4.5
7	G	8	HIS	4.4
7	T	1	ALA	4.3
7	G	10	GLY	4.3
9	V	36	LYS	4.3
10	W	52	TRP	4.2
8	H	47	GLY	4.2
9	I	29	LEU	4.2
13	M	43	SER	4.1
2	B	91	ASN	4.1
13	Z	43	SER	4.1
8	U	45	ALA	4.0
7	T	6	GLY	4.0
9	I	30	GLY	4.0
4	D	4	SER	4.0
7	G	2	SER	4.0
7	G	38	HIS	4.0
7	G	37	LEU	4.0
7	T	42	ARG	4.0
7	T	84	LYS	4.0
9	V	37	PHE	3.9
2	O	65	TRP	3.8
8	U	46	LYS	3.8
7	T	7	ASP	3.8
7	T	39	SER	3.8
2	O	91	ASN	3.7
12	Y	20	ARG	3.6
10	W	1	PHE	3.6
13	Z	40	TYR	3.6
7	G	12	GLY	3.6
10	W	57	HIS	3.6
1	N	513	LEU	3.6
7	T	40	GLY	3.6
2	B	32	PHE	3.5
11	X	6	ALA	3.5
11	X	13	TYR	3.5
2	O	60	GLU	3.5
7	T	12	GLY	3.4
2	O	59	GLN	3.4
11	X	47	ARG	3.4
10	W	56	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	90	ILE	3.4
12	Y	45	LEU	3.3
8	U	47	GLY	3.3
1	A	513	LEU	3.2
6	F	93	PRO	3.2
13	Z	32	TRP	3.2
5	R	96	LEU	3.2
4	Q	9	GLU	3.2
11	X	52	GLU	3.2
13	Z	41	LYS	3.2
3	P	38	ASN	3.2
11	X	7	PRO	3.1
4	Q	53	ILE	3.1
2	B	113	TYR	3.1
1	N	113	LEU	3.1
6	F	95	GLN	3.1
7	G	41	HIS	3.0
5	R	109	VAL	3.0
12	Y	47	LYS	3.0
2	B	61	VAL	3.0
4	Q	51	LEU	3.0
3	P	37	PHE	3.0
4	Q	46	ALA	3.0
8	U	42	ALA	3.0
13	M	42	LYS	3.0
2	B	65	TRP	3.0
8	H	45	ALA	2.9
7	G	84	LYS	2.9
4	Q	58	GLU	2.9
9	I	25	PHE	2.9
9	V	34	PHE	2.9
4	Q	48	TRP	2.9
3	C	3	HIS	2.8
9	I	27	VAL	2.8
11	K	6	ALA	2.8
9	V	33	THR	2.8
4	D	5	VAL	2.8
3	C	38	ASN	2.8
9	I	26	MET	2.8
8	H	50	VAL	2.8
12	Y	2	HIS	2.7
4	Q	10	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	V	25	PHE	2.7
1	N	514	LYS	2.7
13	M	39	ASN	2.7
2	O	217	LYS	2.7
4	Q	35	ALA	2.7
8	H	43	MET	2.7
7	G	40	GLY	2.7
9	I	3	ALA	2.7
7	T	41	HIS	2.7
4	Q	57	VAL	2.7
9	I	37	PHE	2.6
9	V	72	ALA	2.6
7	G	39	SER	2.6
9	V	27	VAL	2.6
4	Q	115	TRP	2.6
5	R	7	THR	2.6
7	T	33	LEU	2.6
8	U	61	LYS	2.6
4	Q	121	LYS	2.6
8	U	44	THR	2.6
7	T	35	SER	2.6
10	W	50	LEU	2.6
13	Z	1	ILE	2.5
13	Z	35	TYR	2.5
3	P	33	MET	2.5
13	M	41	LYS	2.5
13	Z	39	ASN	2.5
4	D	19	ARG	2.5
13	Z	3	ALA	2.5
13	M	40	TYR	2.5
4	Q	19	ARG	2.5
10	J	57	HIS	2.5
8	H	42	ALA	2.5
2	O	32	PHE	2.5
10	W	55	PHE	2.5
8	H	44	THR	2.4
11	X	23	THR	2.4
5	R	91	PRO	2.4
2	O	116	LEU	2.4
4	Q	111	PHE	2.4
12	Y	4	GLU	2.4
6	S	92	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	V	48	ALA	2.4
7	T	34	ASN	2.4
10	W	15	ASP	2.4
8	U	50	VAL	2.4
7	G	42	ARG	2.4
7	G	33	LEU	2.4
8	H	48	GLY	2.4
4	Q	39	ALA	2.3
6	S	54	ASN	2.3
10	J	1	PHE	2.3
11	K	47	ARG	2.3
2	O	126	SER	2.3
9	V	14	ALA	2.3
9	I	36	LYS	2.3
9	I	24	ALA	2.3
11	X	16	ALA	2.3
4	Q	31	LYS	2.3
2	O	67	ILE	2.3
5	E	109	VAL	2.3
2	O	92	ASN	2.3
5	R	90	ARG	2.3
2	B	57	ASP	2.3
2	B	58	ALA	2.3
3	P	182	TYR	2.3
10	J	52	TRP	2.3
6	F	52	ILE	2.2
3	P	91	VAL	2.2
2	B	90	ILE	2.2
4	D	143	ASN	2.2
13	Z	42	LYS	2.2
3	P	40	MET	2.2
9	V	30	GLY	2.2
4	Q	59	LEU	2.2
9	I	34	PHE	2.2
3	P	44	MET	2.2
11	X	14	GLY	2.2
11	X	19	ALA	2.2
5	R	79	LYS	2.2
4	Q	138	TRP	2.2
1	N	484	THR	2.2
8	H	49	ASP	2.2
9	I	32	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	V	29	LEU	2.1
2	O	130	PRO	2.1
7	T	46	ALA	2.1
4	Q	62	LEU	2.1
4	Q	94	LEU	2.1
4	Q	102	TYR	2.1
4	Q	106	PRO	2.1
4	Q	73	ARG	2.1
12	L	47	LYS	2.1
4	Q	60	TYR	2.1
7	G	45	PRO	2.1
6	S	26	LYS	2.1
11	X	12	LYS	2.1
3	P	34	TRP	2.1
9	V	32	ALA	2.1
9	V	38	ALA	2.1
2	O	47	THR	2.0
9	V	35	TYR	2.0
1	N	459	PHE	2.0
2	O	82	ARG	2.0
1	A	514	LYS	2.0
4	Q	11	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	T	11	11/12	0.42	0.29	70,77,97,98	0
7	TPO	G	11	11/12	0.57	0.31	68,74,91,92	0
1	FME	N	1	10/11	0.83	0.18	48,54,69,70	0
1	FME	A	1	10/11	0.86	0.16	42,48,68,76	0
2	FME	O	1	10/11	0.94	0.12	36,37,46,55	0
2	FME	B	1	10/11	0.95	0.10	27,29,39,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	CHD	W	1060	29/29	0.67	0.28	107,109,111,111	0
24	DMU	P	1272	33/33	0.68	0.26	89,103,109,111	0
28	PEK	G	265	53/53	0.69	0.30	45,91,106,111	0
28	PEK	G	1263	53/53	0.72	0.32	50,107,128,129	0
28	PEK	T	263	53/53	0.73	0.28	48,93,126,127	0
23	CHD	J	60	29/29	0.74	0.29	99,100,106,106	0
28	PEK	P	1265	53/53	0.74	0.28	42,86,105,108	0
24	DMU	C	272	33/33	0.74	0.23	70,99,105,105	0
20	PGV	P	1268	51/51	0.75	0.27	64,97,112,113	0
20	PGV	A	524	51/51	0.76	0.26	33,71,98,101	0
26	CDL	G	269	100/100	0.76	0.26	62,86,114,116	0
19	TGL	N	1522	63/63	0.77	0.25	45,73,89,92	0
26	CDL	T	1269	100/100	0.77	0.23	52,85,111,116	0
22	PSC	O	1230	52/52	0.77	0.27	41,93,121,122	0
19	TGL	Q	1523	63/63	0.78	0.27	53,78,92,94	0
26	CDL	P	1270	100/100	0.79	0.25	43,87,117,123	0
20	PGV	C	268	51/51	0.79	0.26	59,88,104,105	0
19	TGL	D	523	63/63	0.80	0.25	41,69,96,98	0
19	TGL	L	522	63/63	0.80	0.23	36,66,84,86	0
26	CDL	C	270	100/100	0.80	0.24	43,84,127,129	0
19	TGL	A	521	63/63	0.80	0.24	47,71,92,98	0
20	PGV	N	1524	51/51	0.80	0.21	43,72,104,106	0
22	PSC	B	230	52/52	0.81	0.25	39,96,121,123	0
19	TGL	N	1521	63/63	0.81	0.23	53,75,92,94	0
23	CHD	P	1271	29/29	0.82	0.18	68,74,77,78	0
25	UNX	C	262	1/1	0.83	0.35	39,39,39,39	0
23	CHD	C	271	29/29	0.84	0.17	59,69,71,72	0
25	UNX	P	1262	1/1	0.84	0.42	40,40,40,40	0
24	DMU	Z	1526	33/33	0.85	0.14	42,51,63,65	0
23	CHD	P	1525	29/29	0.92	0.09	25,33,39,39	0
24	DMU	M	526	33/33	0.92	0.11	35,44,55,60	0
23	CHD	C	525	29/29	0.94	0.08	24,32,36,43	0
28	PEK	P	1264	53/53	0.94	0.14	26,47,80,82	0
28	PEK	G	264	53/53	0.95	0.12	23,43,71,73	0
20	PGV	N	1266	51/51	0.95	0.12	28,41,63,64	0
23	CHD	O	229	29/29	0.95	0.07	21,25,34,39	0
23	CHD	B	1086	29/29	0.95	0.08	23,28,35,44	0

Continued on next page...

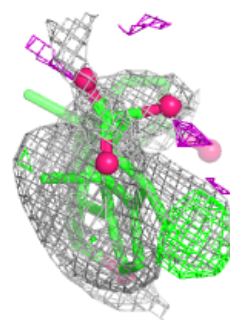
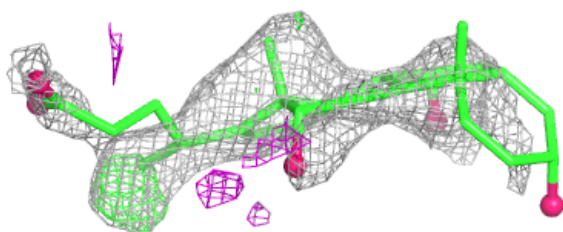
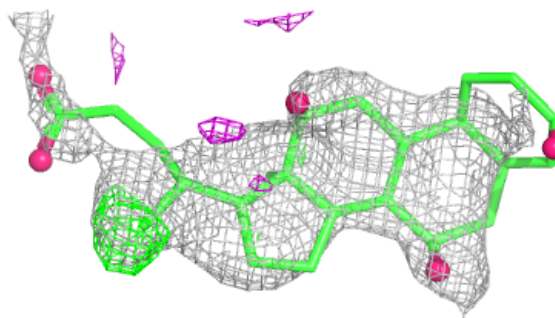
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	NA	N	1519	1/1	0.95	0.08	30,30,30,30	0
16	MG	N	1518	1/1	0.95	0.05	29,29,29,29	0
20	PGV	P	1267	51/51	0.96	0.10	21,37,76,85	0
15	PER	N	520	2/2	0.96	0.10	20,20,20,27	0
20	PGV	A	522	51/51	0.96	0.10	25,37,63,68	0
20	PGV	C	267	51/51	0.96	0.10	20,31,74,77	0
18	HEA	N	515	60/60	0.97	0.08	22,28,54,56	0
18	HEA	N	516	60/60	0.98	0.07	23,28,35,38	0
15	PER	A	520	2/2	0.98	0.12	16,16,16,19	0
18	HEA	A	515	60/60	0.98	0.06	16,23,46,47	0
21	CUA	O	228	2/2	0.98	0.04	31,31,31,32	0
17	NA	A	519	1/1	0.98	0.04	25,25,25,25	0
14	CU	A	517	1/1	0.99	0.03	24,24,24,24	0
21	CUA	B	228	2/2	0.99	0.03	23,23,23,26	0
16	MG	A	518	1/1	0.99	0.03	21,21,21,21	0
27	ZN	S	99	1/1	0.99	0.03	34,34,34,34	0
18	HEA	A	516	60/60	0.99	0.05	13,22,29,32	0
27	ZN	F	99	1/1	1.00	0.01	30,30,30,30	0
14	CU	N	517	1/1	1.00	0.05	30,30,30,30	0

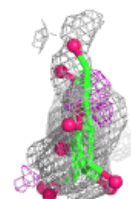
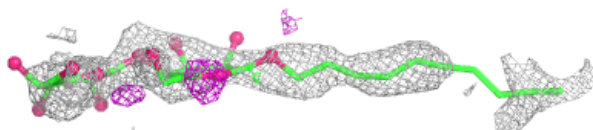
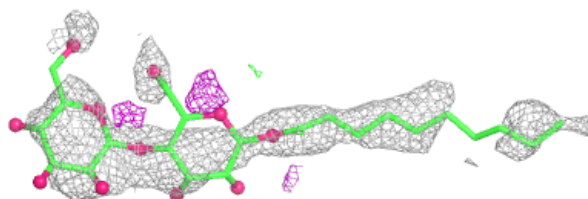
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD W 1060:

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

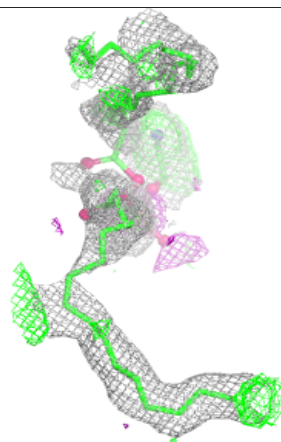
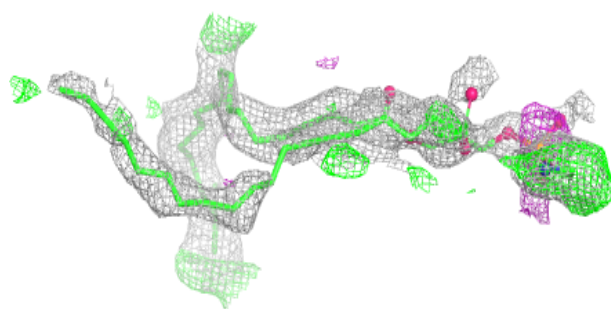
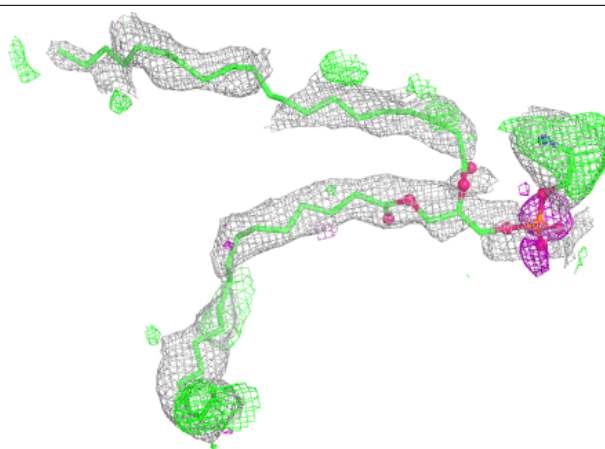
**Electron density around DMU P 1272:**

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



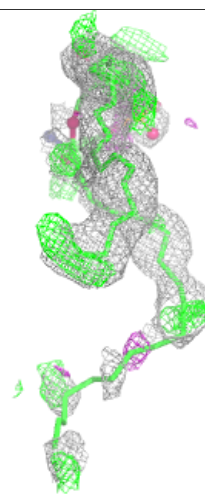
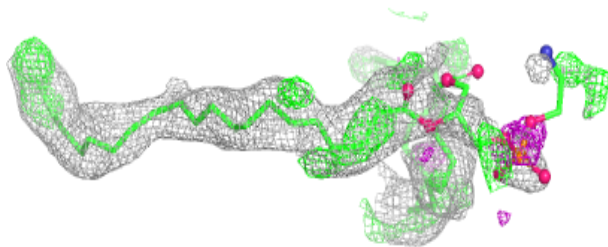
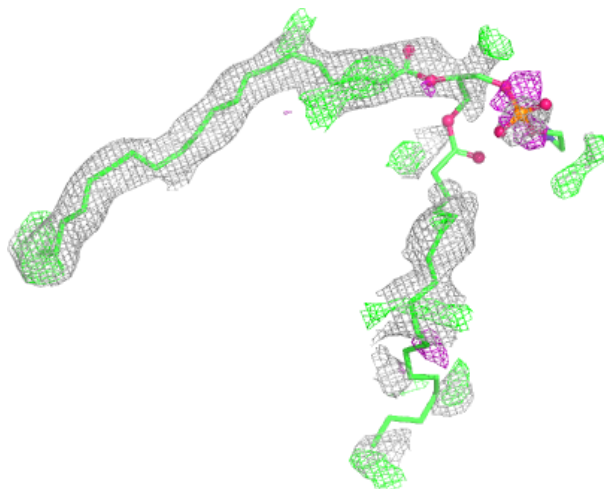
Electron density around PEK G 265:

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



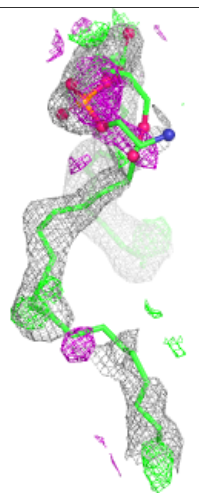
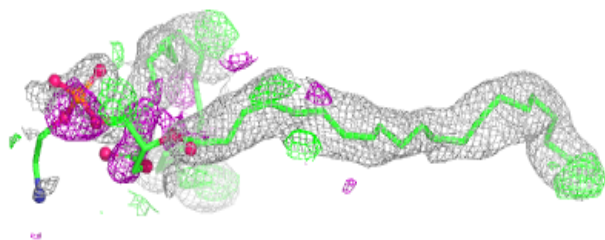
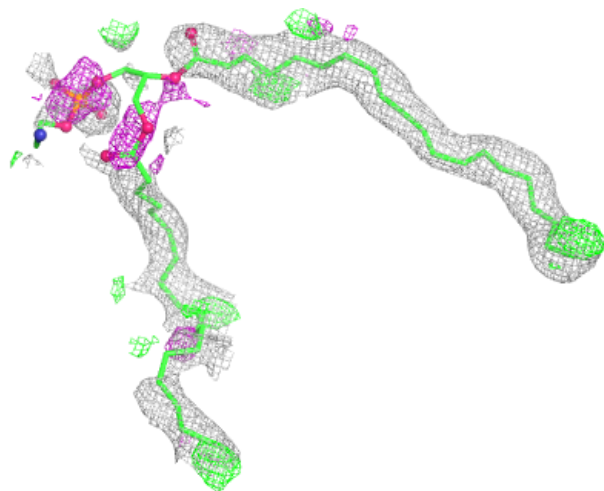
Electron density around PEK G 1263:

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



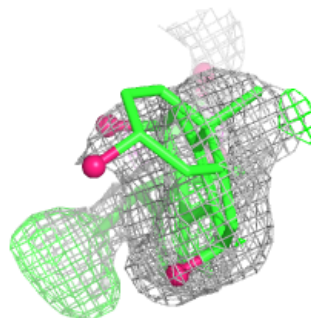
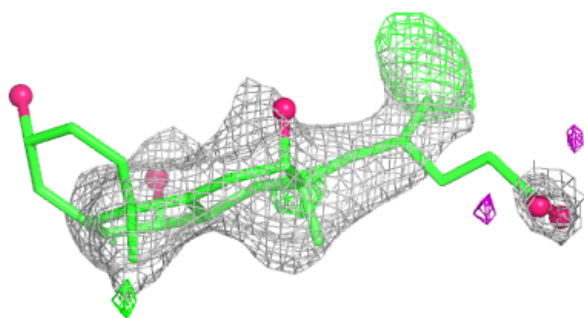
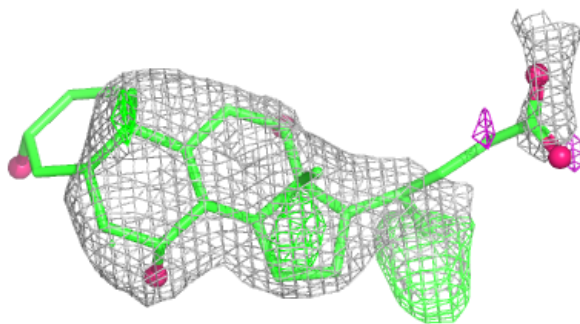
Electron density around PEK T 263:

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



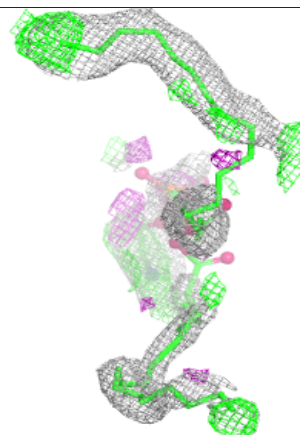
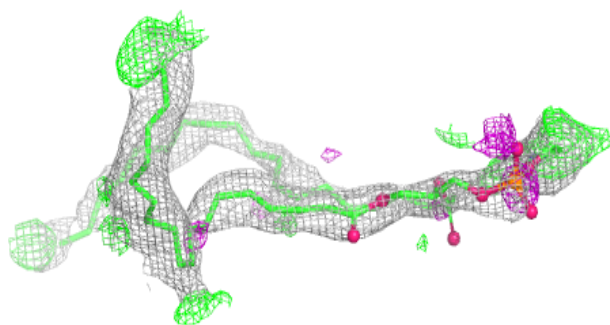
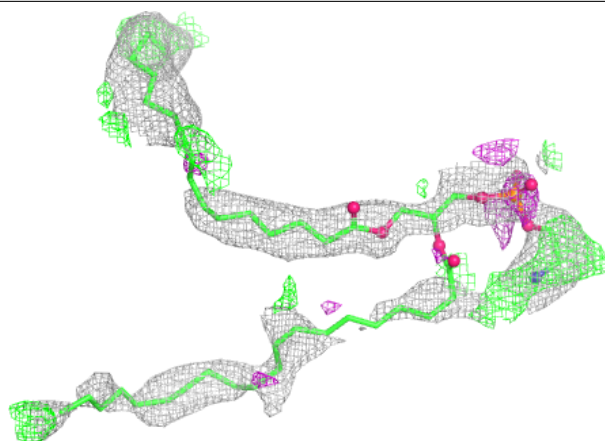
Electron density around CHD J 60:

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

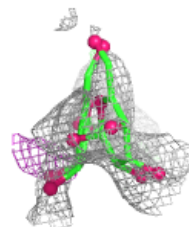
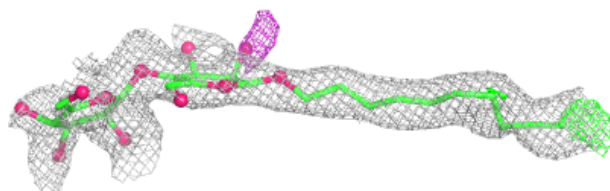
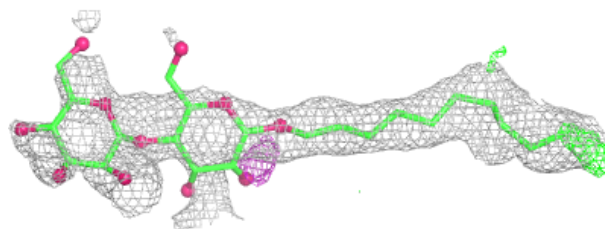


Electron density around PEK P 1265:

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

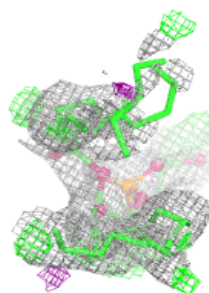
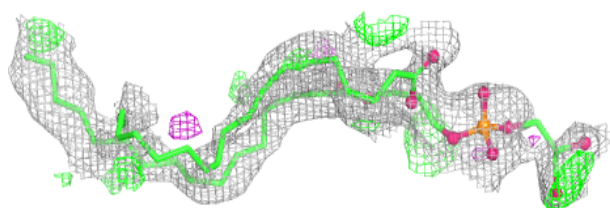
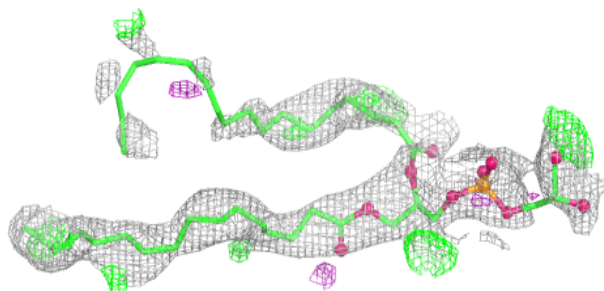
**Electron density around DMU C 272:**

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

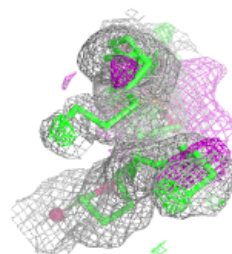
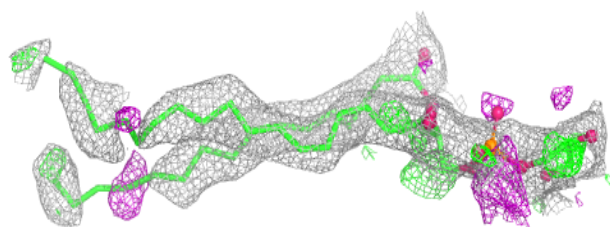
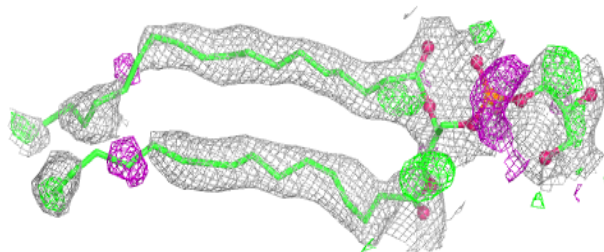


Electron density around PGV P 1268:

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

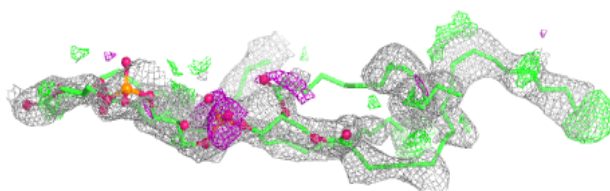
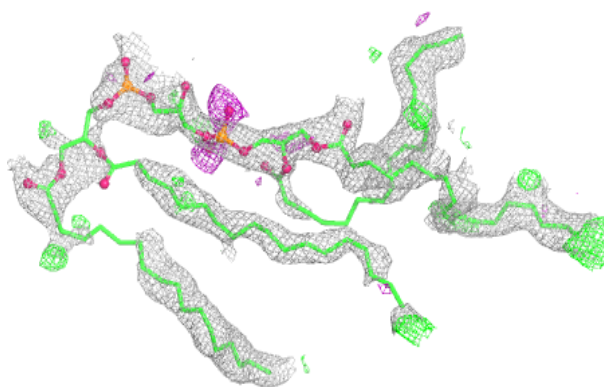
**Electron density around PGV A 524:**

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

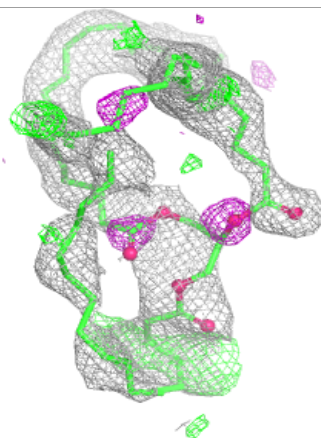
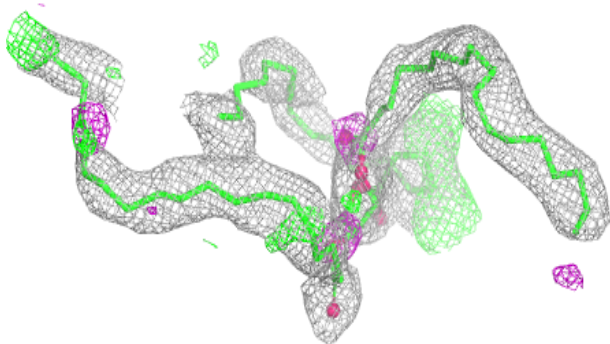
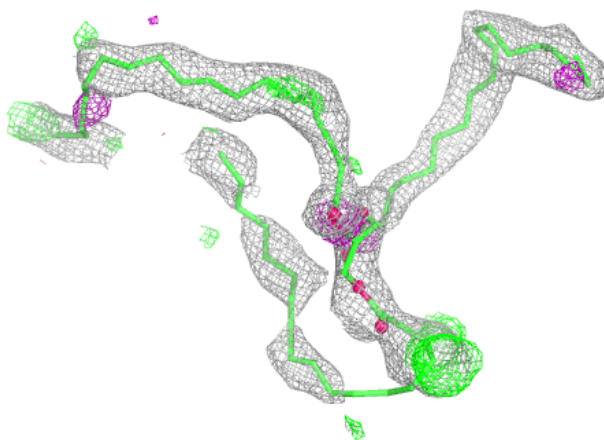


Electron density around CDL G 269:

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

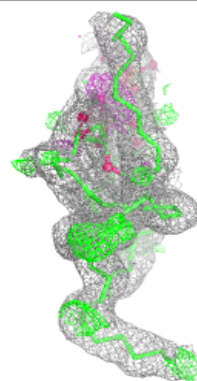
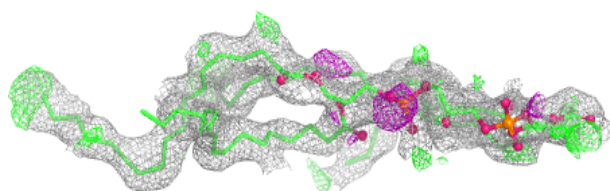
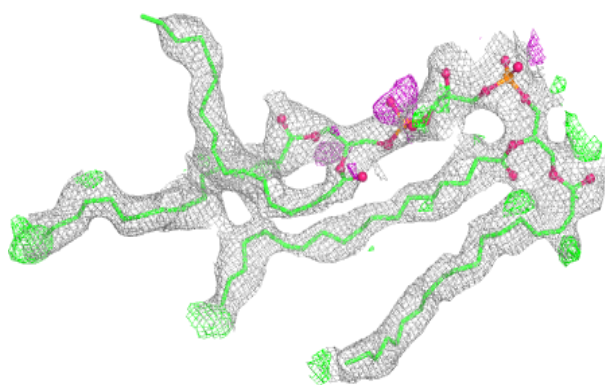
**Electron density around TGL N 1522:**

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

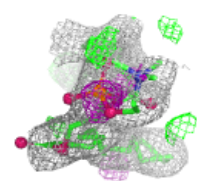
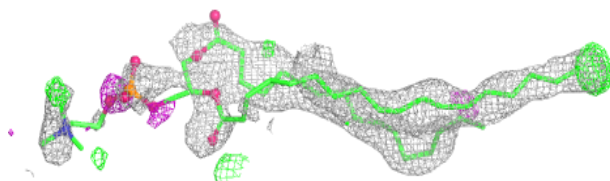
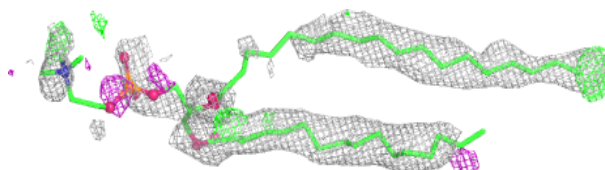


Electron density around CDL T 1269:

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

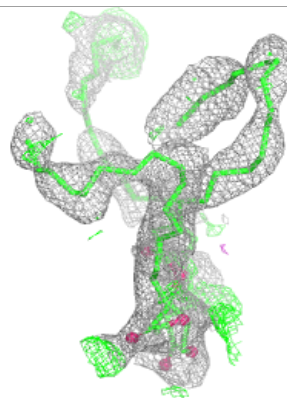
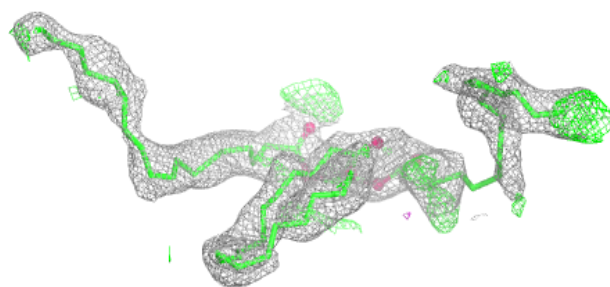
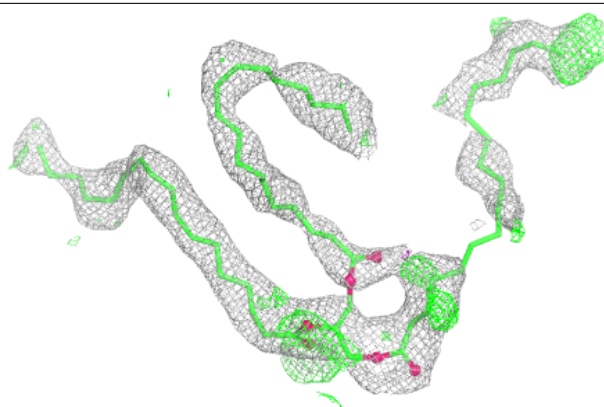
**Electron density around PSC O 1230:**

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

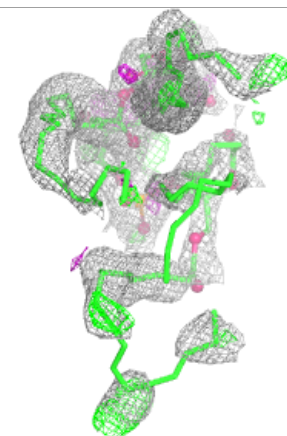
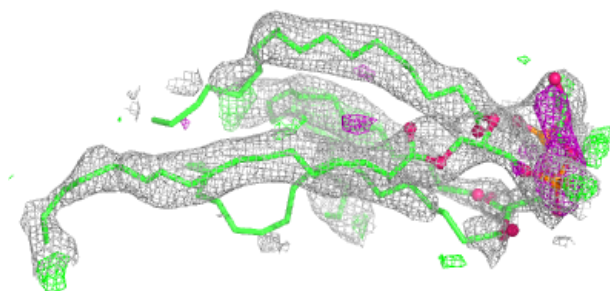
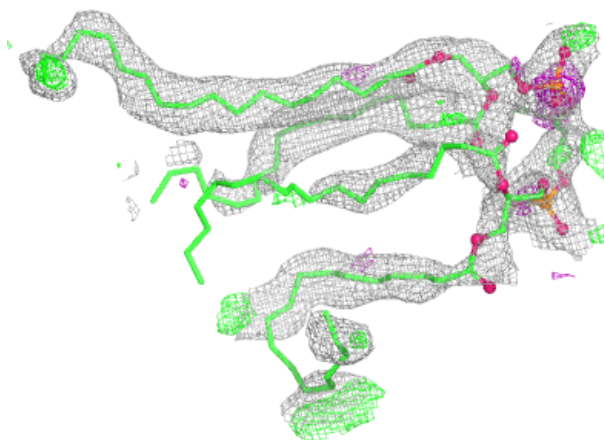


Electron density around TGL Q 1523:

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

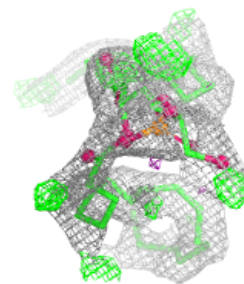
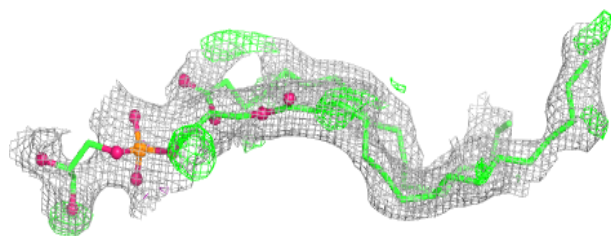
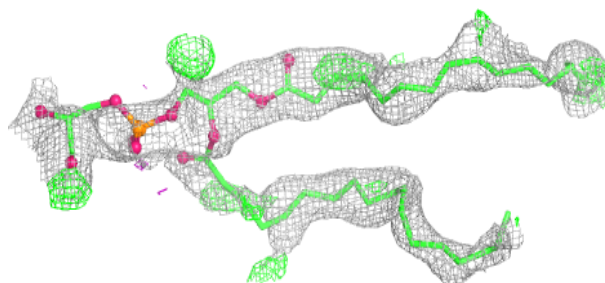
**Electron density around CDL P 1270:**

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

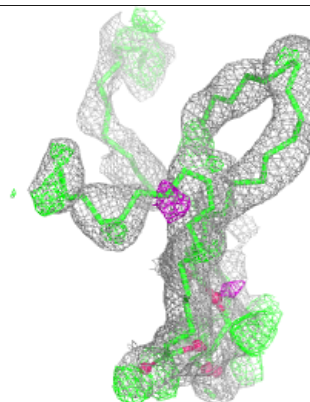
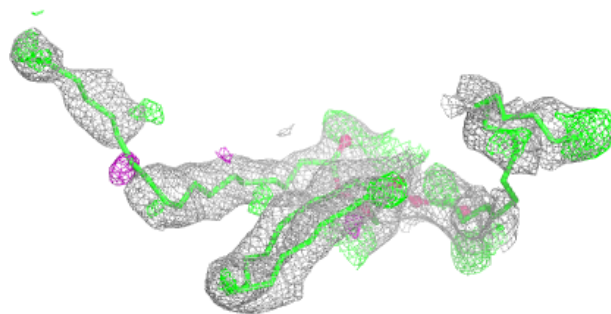
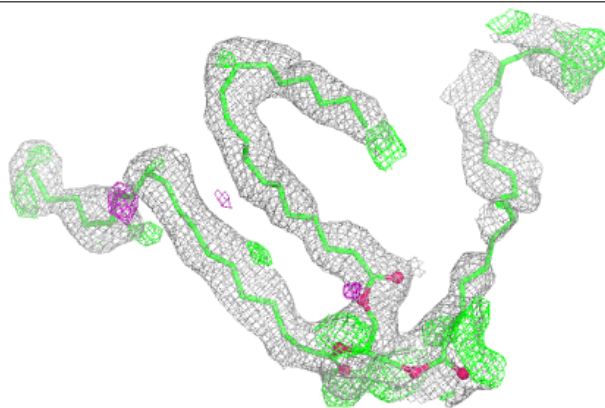


Electron density around PGV C 268:

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

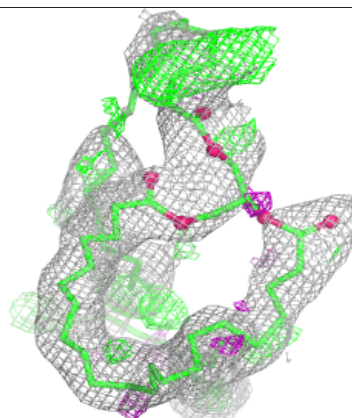
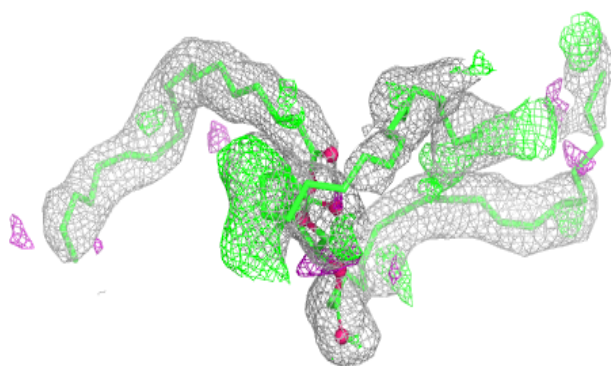
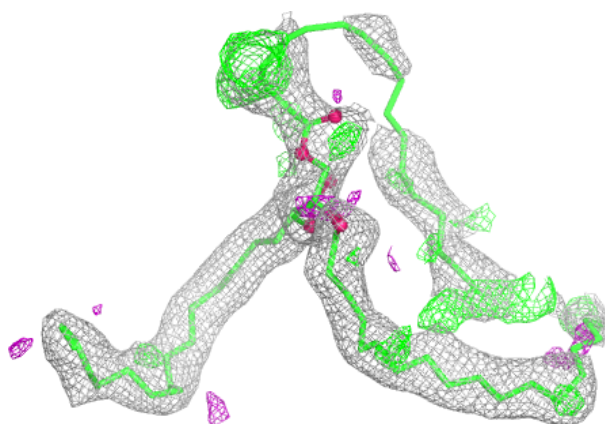
**Electron density around TGL D 523:**

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



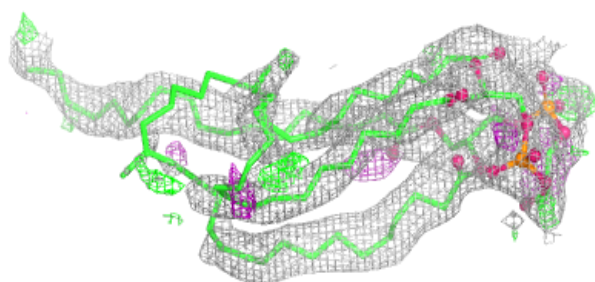
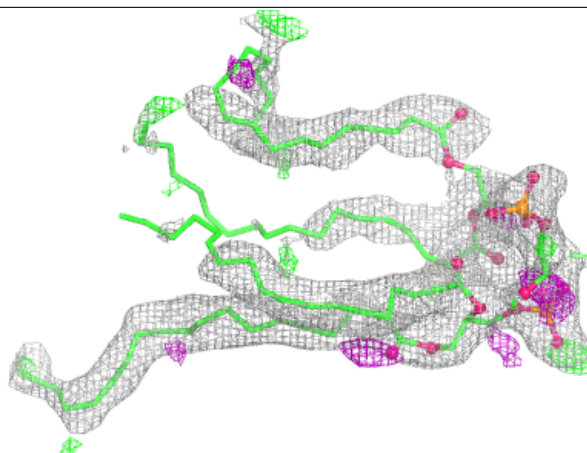
Electron density around TGL L 522:

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



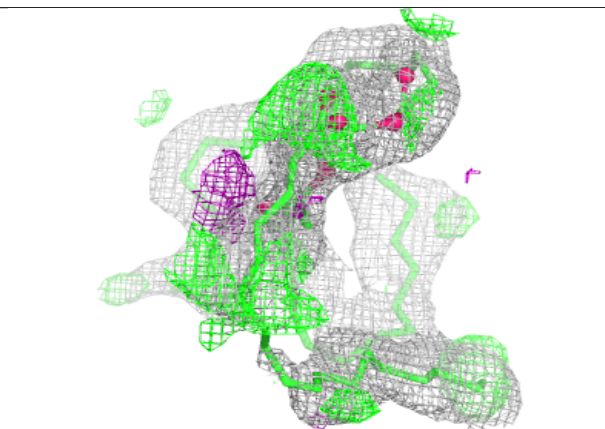
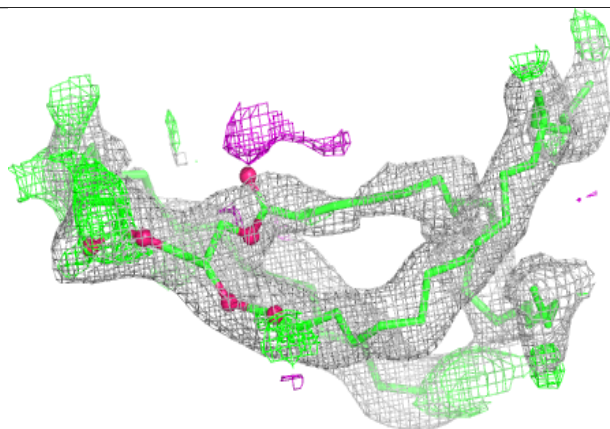
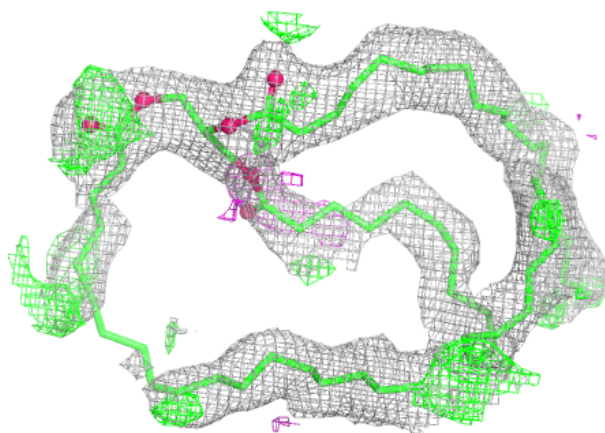
Electron density around CDL C 270:

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

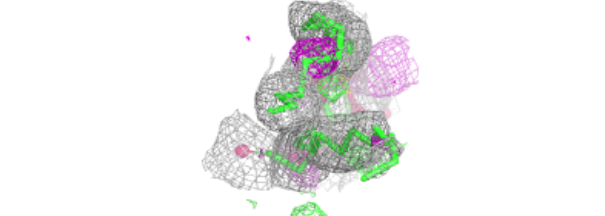
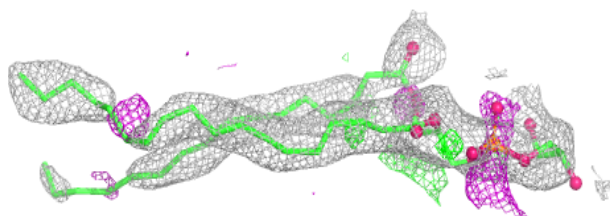
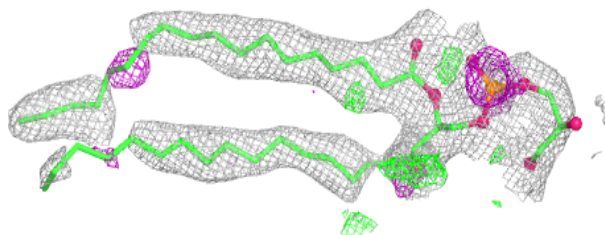


Electron density around TGL A 521:

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

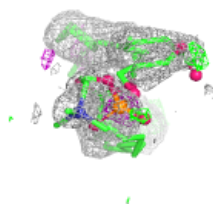
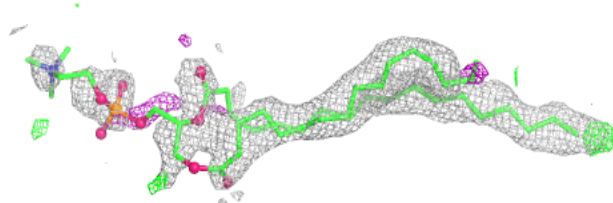
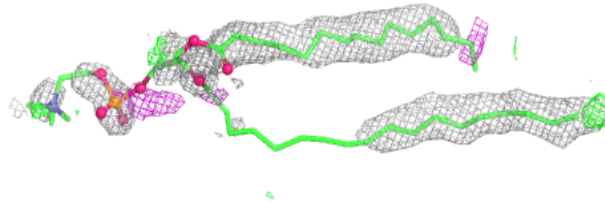
**Electron density around PGV N 1524:**

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

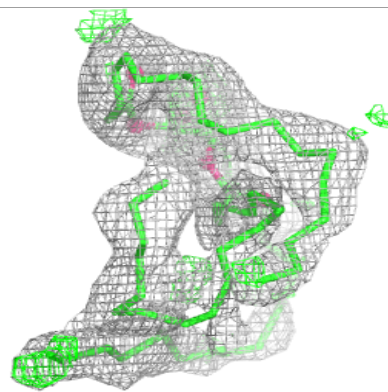
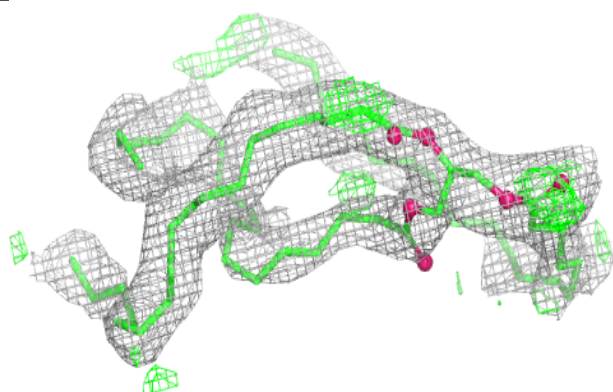
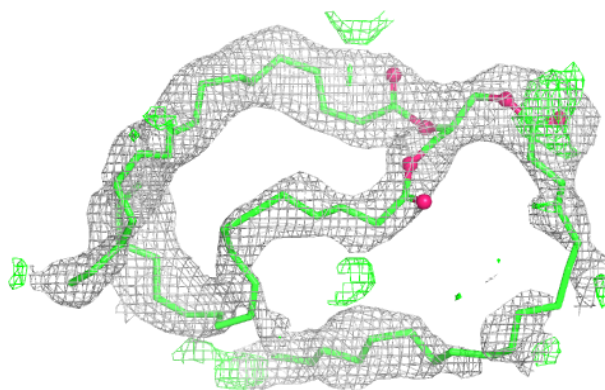


Electron density around PSC B 230:

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

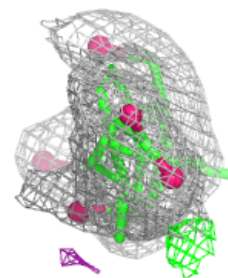
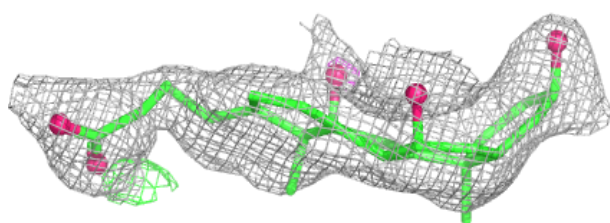
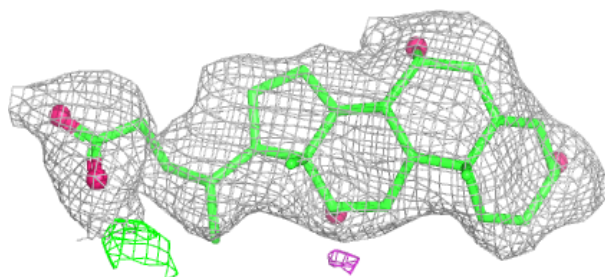
**Electron density around TGL N 1521:**

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

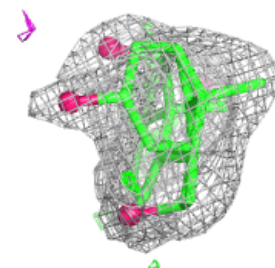
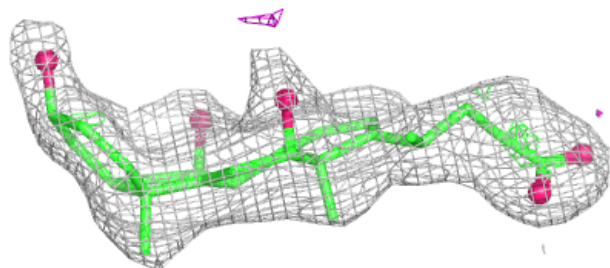
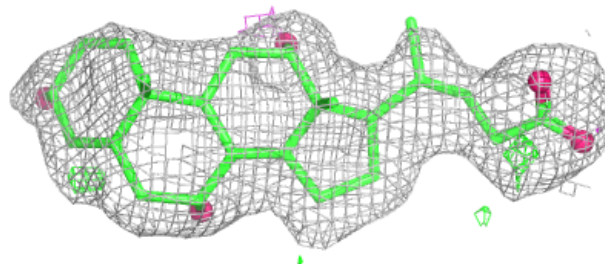


Electron density around CHD P 1271:

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

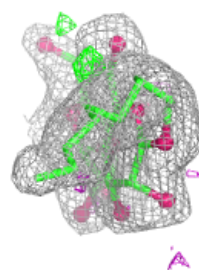
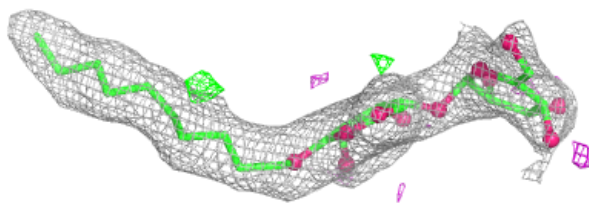
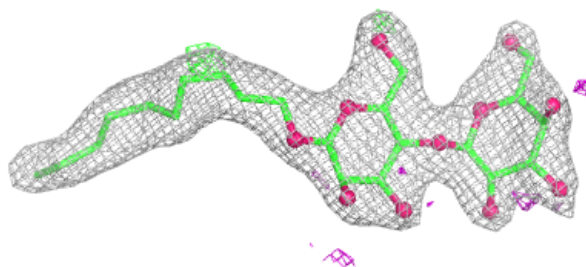
**Electron density around CHD C 271:**

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

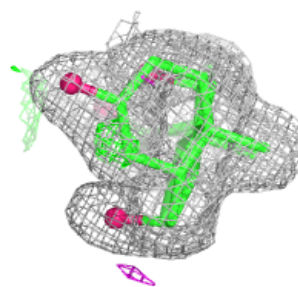
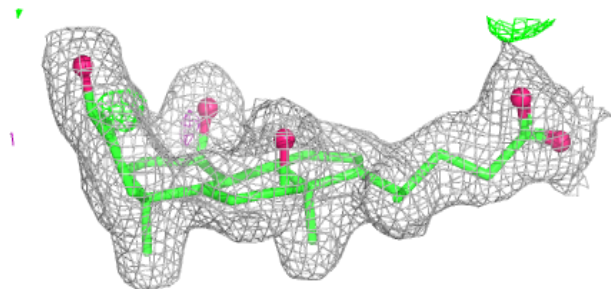
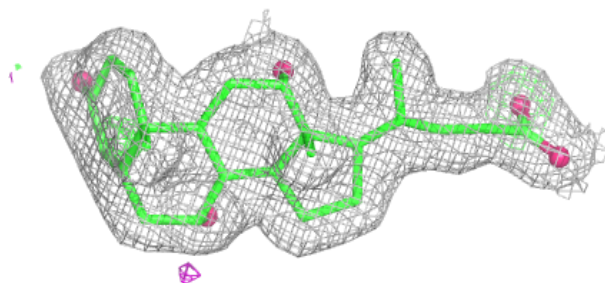


Electron density around DMU Z 1526:

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

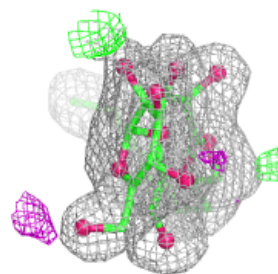
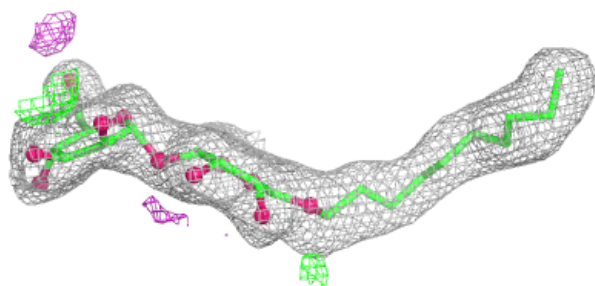
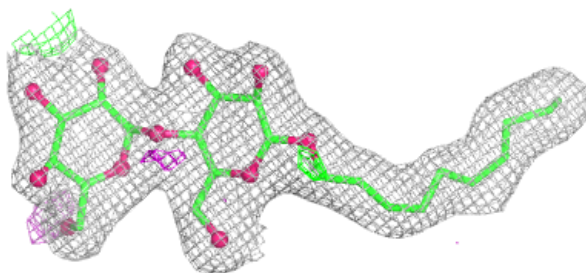
**Electron density around CHD P 1525:**

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

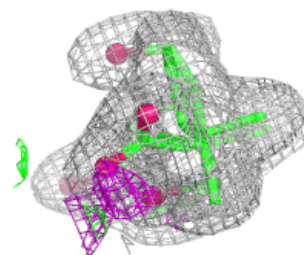
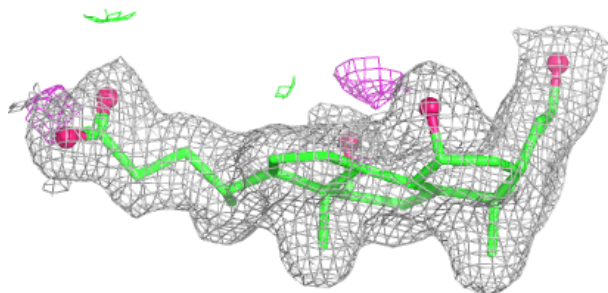
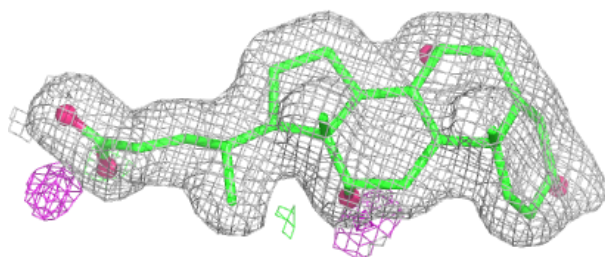


Electron density around DMU M 526:

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

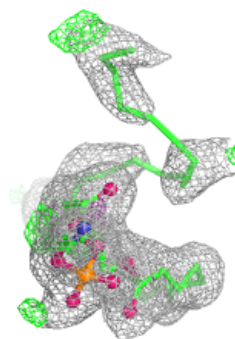
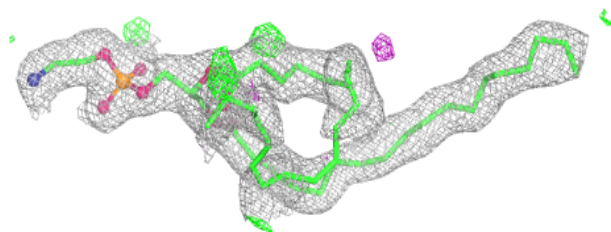
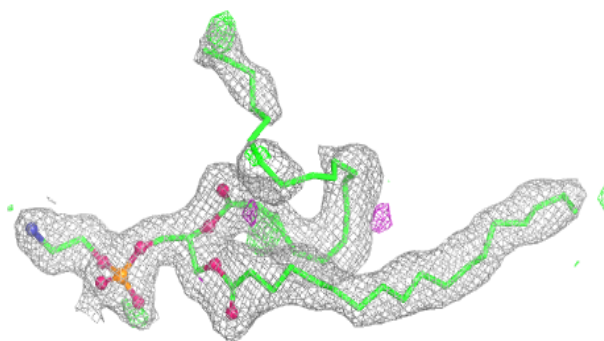
**Electron density around CHD C 525:**

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

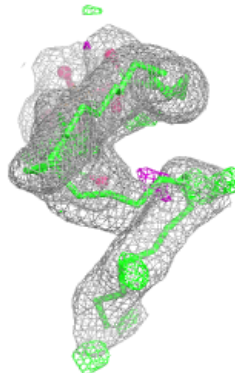
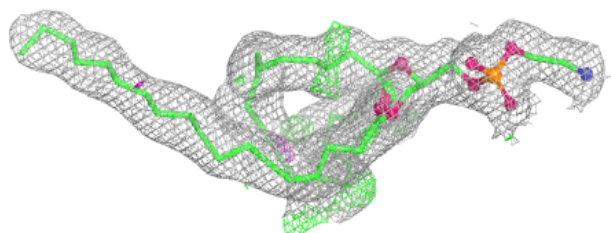
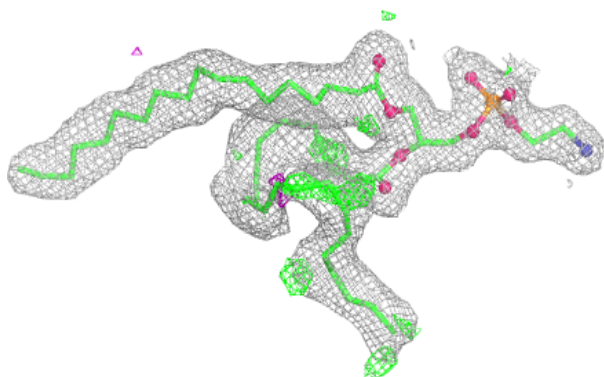


Electron density around PEK P 1264:

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

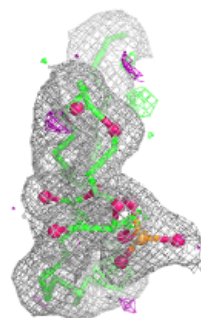
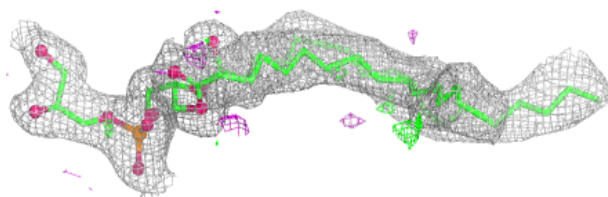
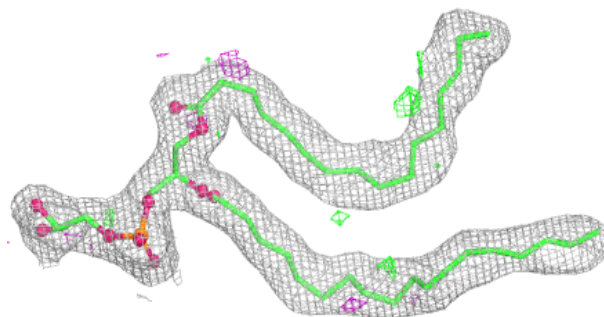
**Electron density around PEK G 264:**

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

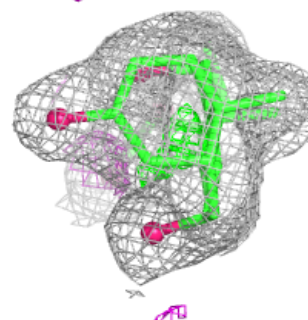
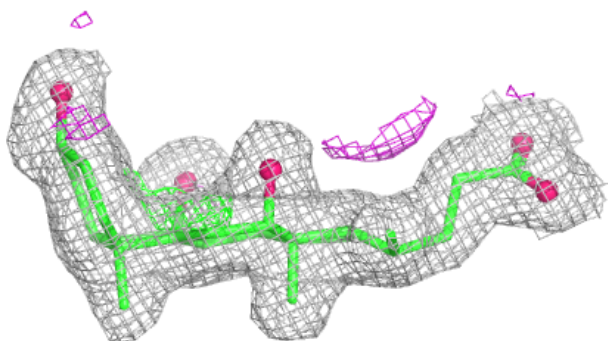
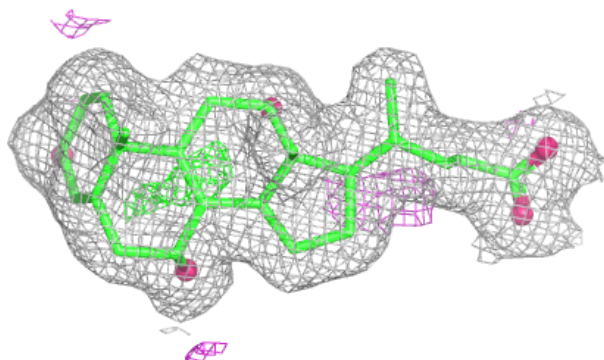


Electron density around PGV N 1266:

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

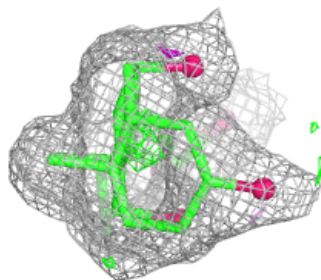
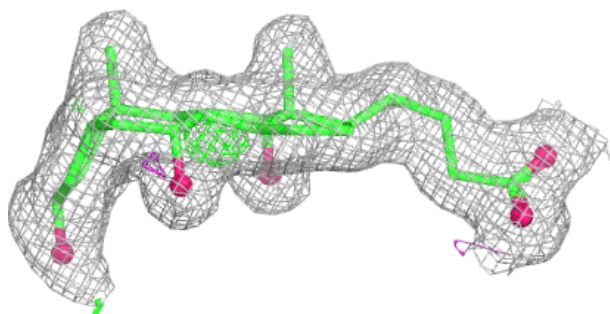
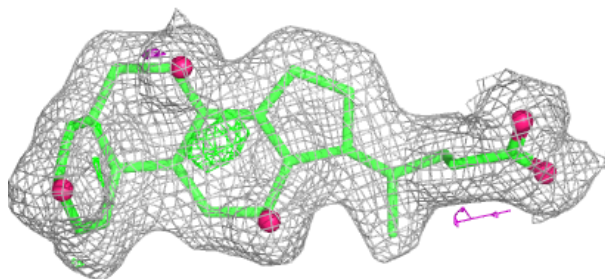
**Electron density around CHD O 229:**

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

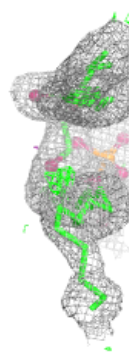
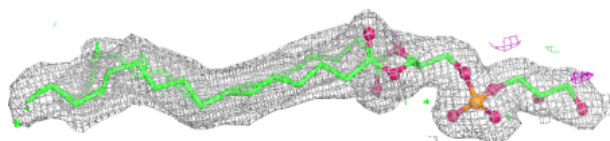
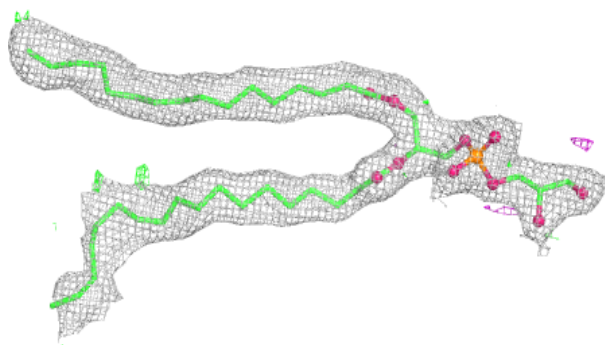


Electron density around CHD B 1086:

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

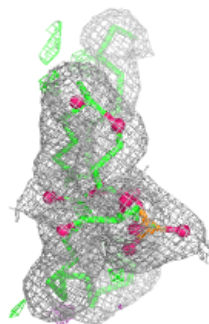
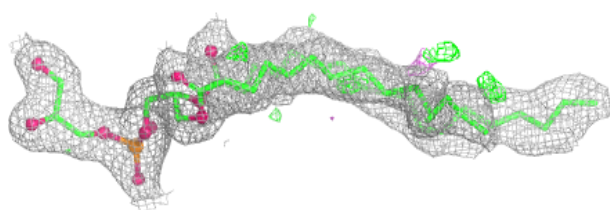
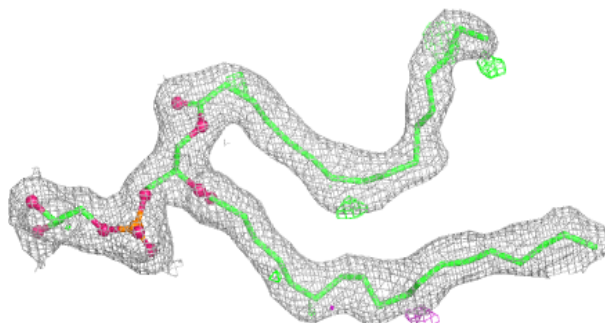
**Electron density around PGV P 1267:**

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

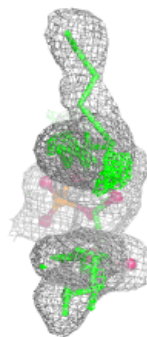
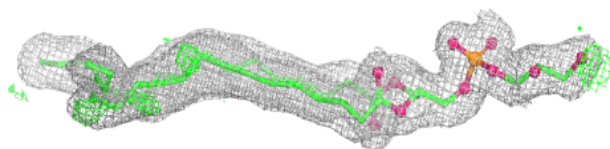
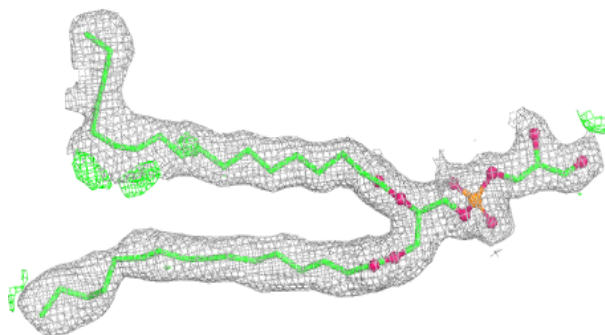


Electron density around PGV A 522:

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

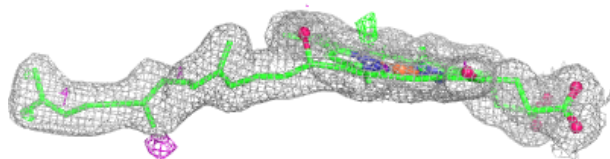
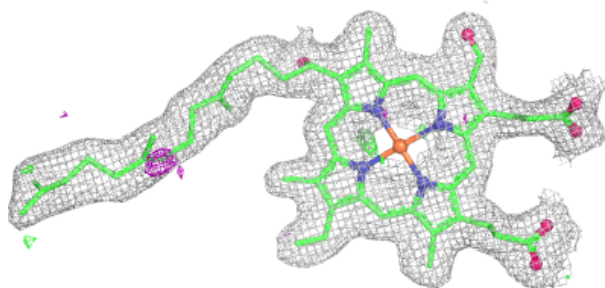
**Electron density around PGV C 267:**

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

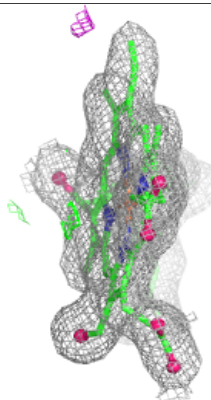
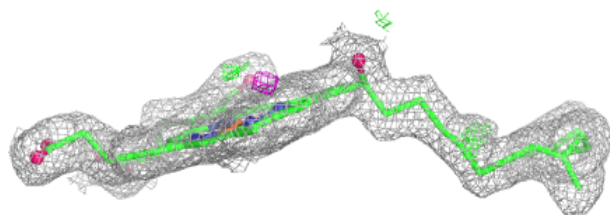
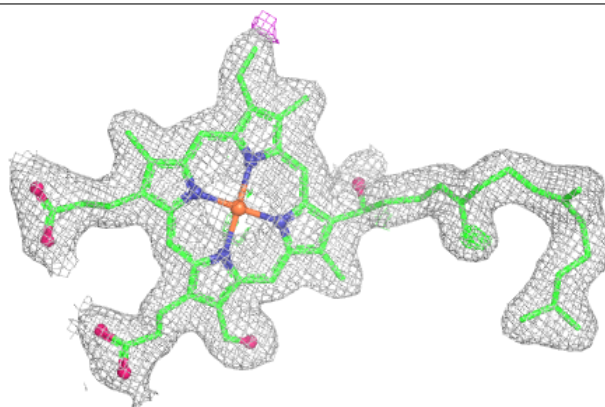


Electron density around HEA N 515:

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

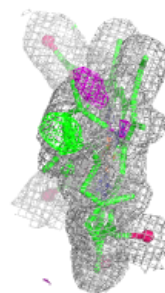
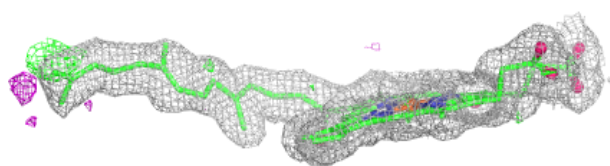
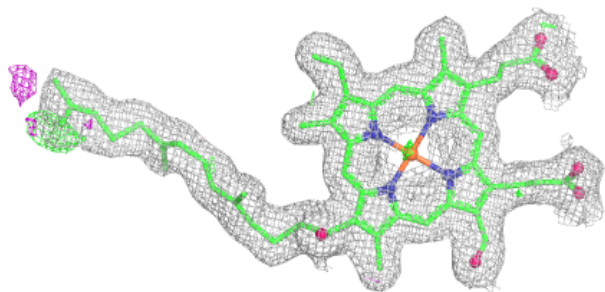
**Electron density around HEA N 516:**

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

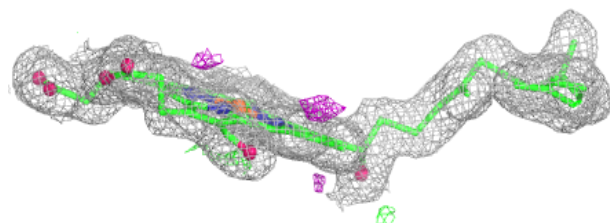
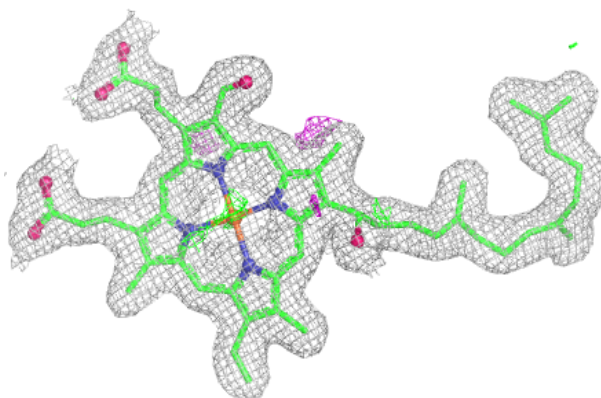


Electron density around HEA A 515:

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

**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.