



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:56 PM EDT

PDB ID : 3X2Q / pdb_00003x2q
Title : X-ray structure of cyanide-bound bovine heart cytochrome c oxidase in the fully oxidized state at 2.0 angstrom resolution
Authors : Yano, N.; Muramoto, K.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2014-12-26
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

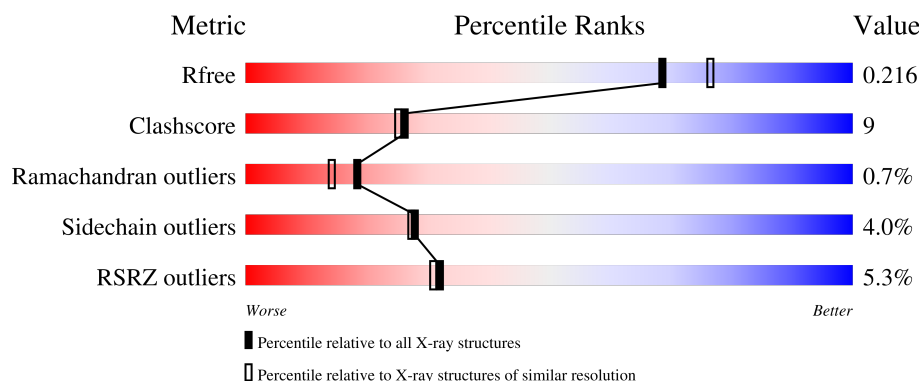
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	514	78% 19% .
1	N	514	5% 81% 18% .
2	B	227	5% 78% 19% .
2	O	227	5% 78% 18% .

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Mol	Chain	Length	Quality of chain
3	C	261	% 82% 15% ..
3	P	261	% 80% 17% ..
4	D	147	% 79% 16% ...
4	Q	147	13% 79% 14% 5% .
5	E	109	2% 83% 11% . .
5	R	109	4% 84% 9% . .
6	F	98	9% 73% 19% 5% .
6	S	98	14% 71% 17% 7% .
7	G	85	21% 72% 16% 11% .
7	T	85	24% 71% 18% 7% . .
8	H	85	13% 80% 9% . . 7%
8	U	85	14% 75% 12% 5% . 7%
9	I	74	4% 84% 12% .
9	V	74	8% 80% 19% .
10	J	59	5% 88% 8% . .
10	W	59	10% 92% 5% . .
11	K	56	2% 77% 9% . 12%
11	X	56	9% 71% 14% . 12%
12	L	47	4% 79% 19% .
12	Y	47	9% 77% 17% . .
13	M	46	11% 72% 20% . 7%
13	Z	46	15% 76% 17% 7%

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
24	CDL	G	103	-	-	X	-
24	CDL	P	306	-	-	X	-
24	CDL	T	102	-	-	X	-
25	PEK	T	101	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32060 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	3	0
			4051	2708	626	681	36			
1	N	514	Total	C	N	O	S	0	3	0
			4051	2708	626	681	36			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			
3	P	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			

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

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, mitochondrial.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	74	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	74	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	0	ACE	-	acetylation	UNP P04038
V	0	ACE	-	acetylation	UNP P04038

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

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

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

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			

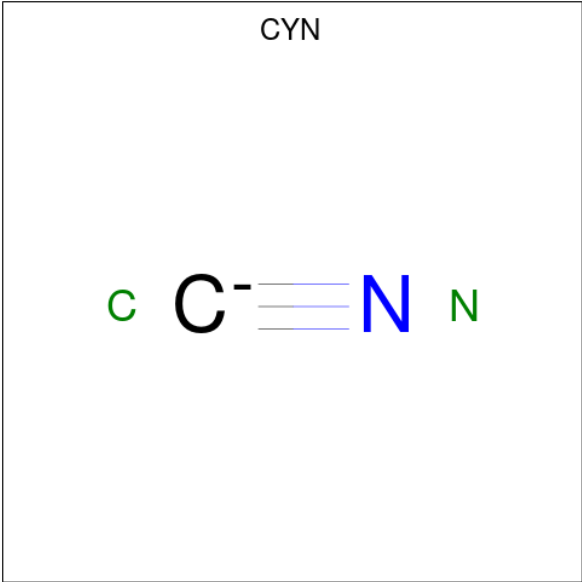
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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, mitochondrial.

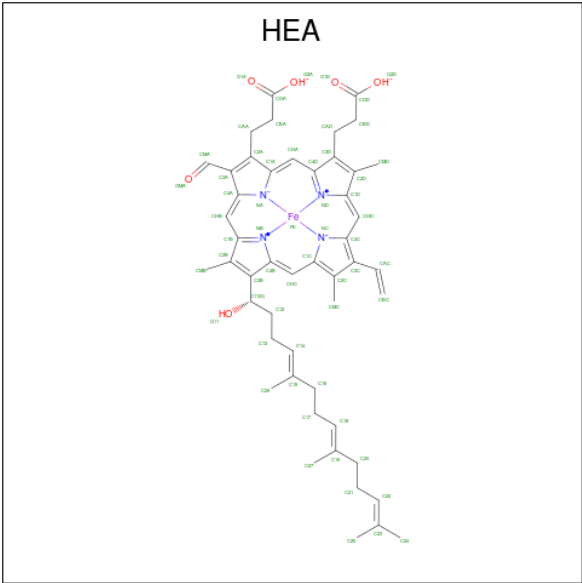
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is CYANIDE ION (CCD ID: CYN) (formula: CN).



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

- Molecule 15 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

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

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

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

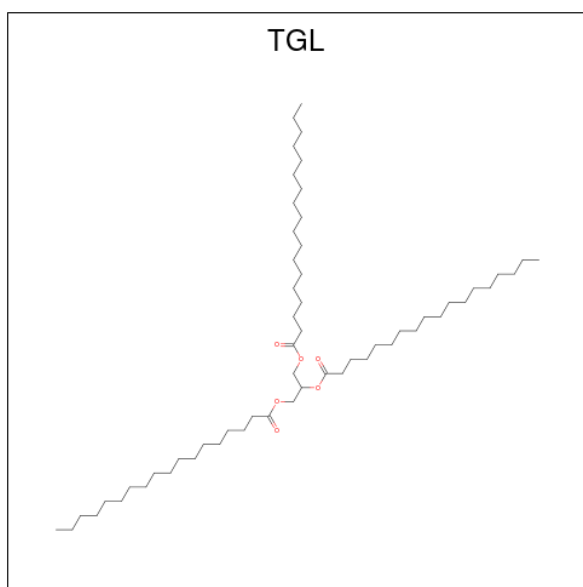
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

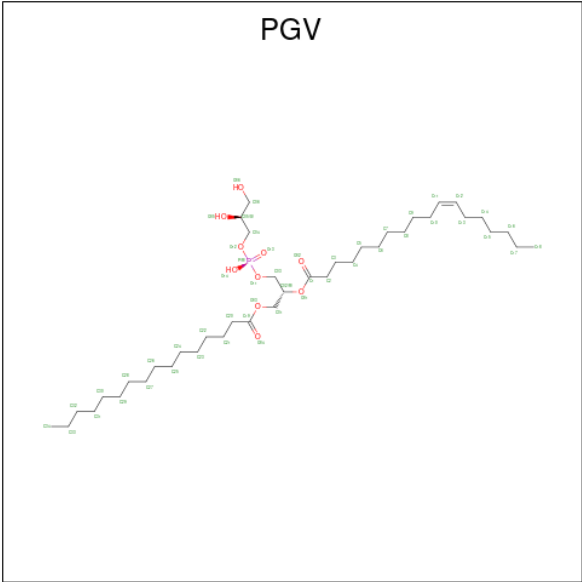
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na		
			1	1	0	0
18	N	1	Total	Na		
			1	1	0	0

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



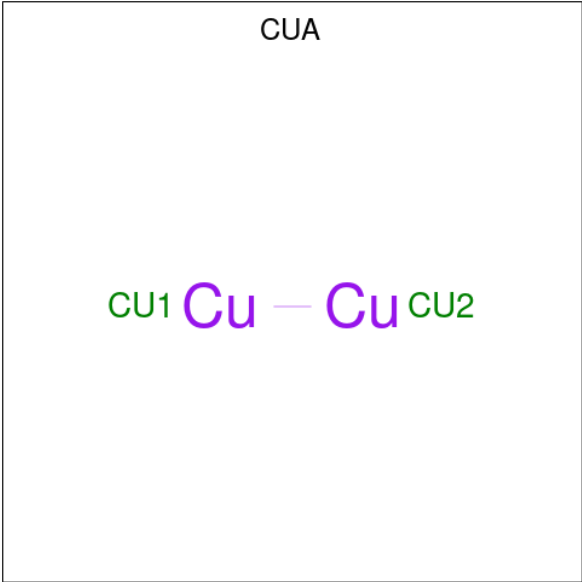
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- 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).



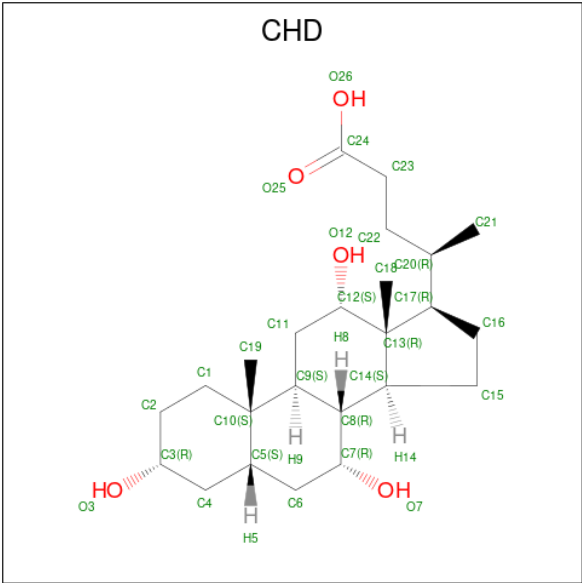
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			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 CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



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

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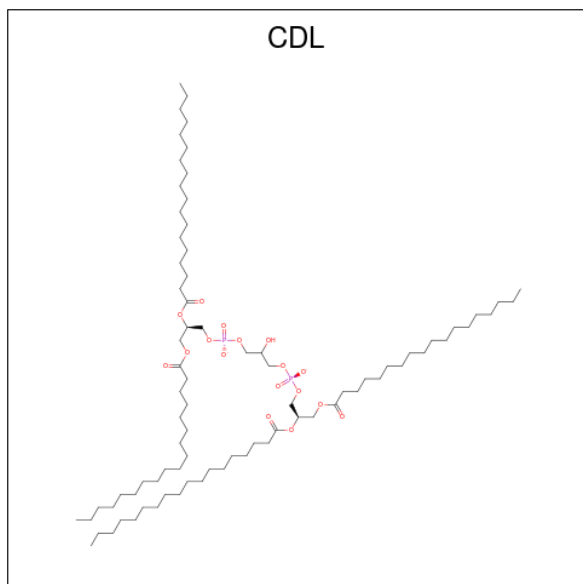
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			29	24	5		
22	O	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

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

- Molecule 24 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



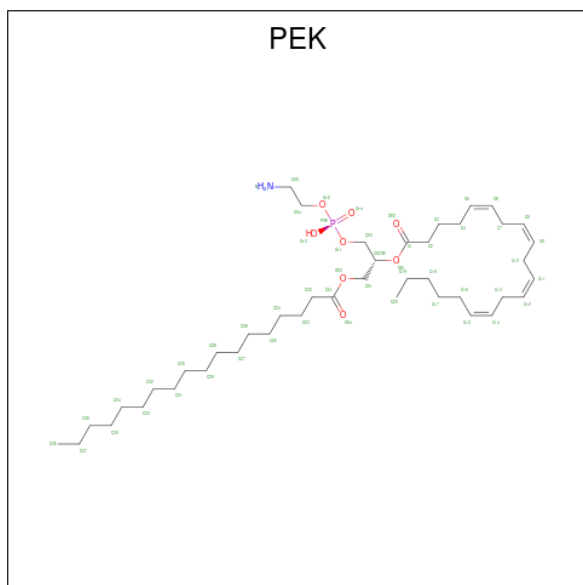
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	C	1	Total	C	O	P	0	0
			100	81	17	2		
24	G	1	Total	C	O	P	0	0
			100	81	17	2		
24	P	1	Total	C	O	P	0	0
			100	81	17	2		

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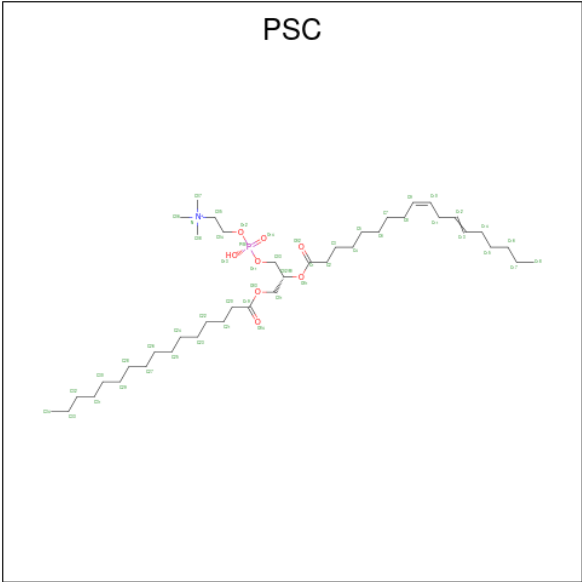
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	T	1	Total	C	O	P	0	0
			100	81	17	2		

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



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).

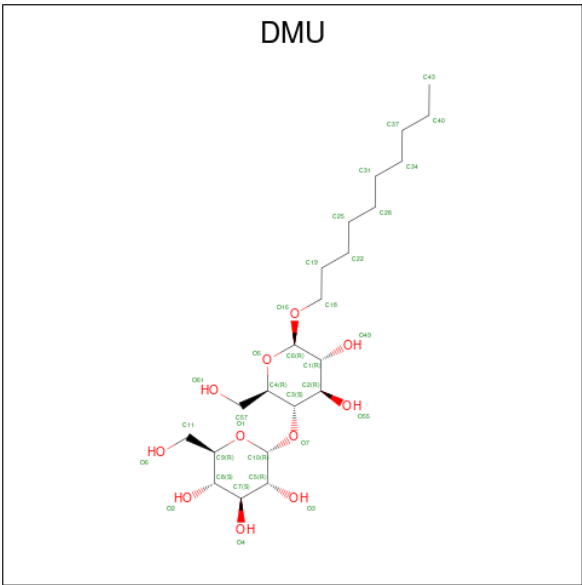


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	188	Total	O	0	0
			188	188		
29	B	121	Total	O	0	0
			121	121		
29	C	77	Total	O	0	0
			77	77		
29	D	78	Total	O	0	0
			78	78		
29	E	58	Total	O	0	0
			58	58		
29	F	58	Total	O	0	0
			58	58		
29	G	27	Total	O	0	0
			27	27		
29	H	34	Total	O	0	0
			34	34		

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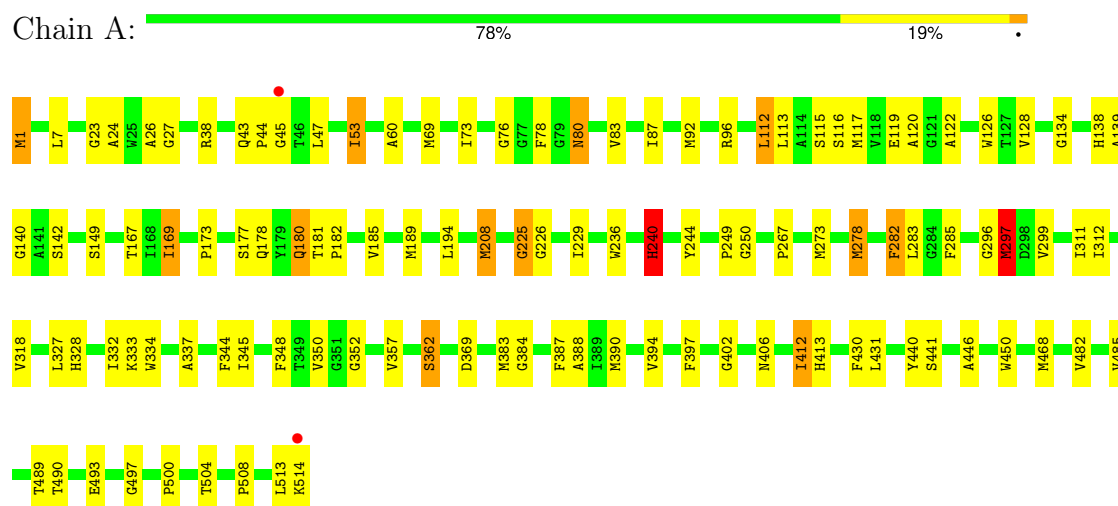
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	I	29	Total 29	O 29	0	0
29	J	15	Total 15	O 15	0	0
29	K	20	Total 20	O 20	0	0
29	L	16	Total 16	O 16	0	0
29	M	14	Total 14	O 14	0	0
29	N	156	Total 156	O 156	0	0
29	O	91	Total 91	O 91	0	0
29	P	76	Total 76	O 76	0	0
29	Q	46	Total 46	O 46	0	0
29	R	42	Total 42	O 42	0	0
29	S	38	Total 38	O 38	0	0
29	T	23	Total 23	O 23	0	0
29	U	28	Total 28	O 28	0	0
29	V	14	Total 14	O 14	0	0
29	W	4	Total 4	O 4	0	0
29	X	15	Total 15	O 15	0	0
29	Y	11	Total 11	O 11	0	0
29	Z	7	Total 7	O 7	0	0

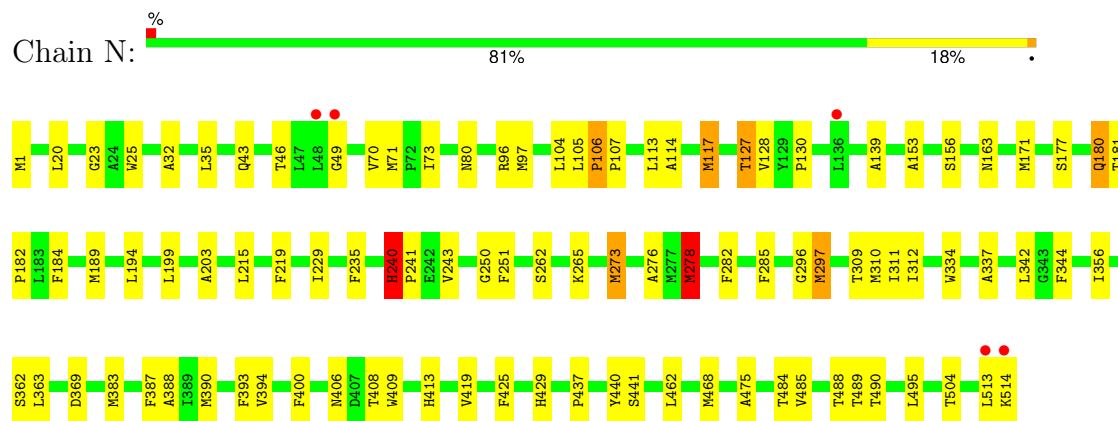
3 Residue-property plots

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.

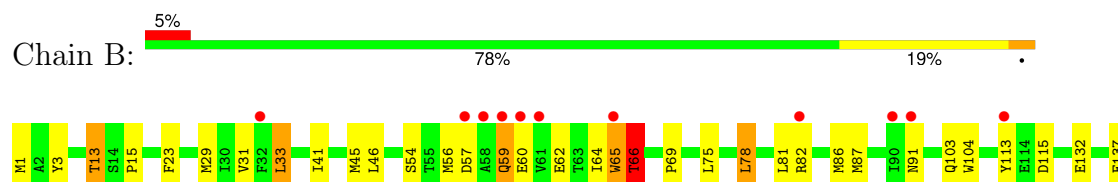
• Molecule 1: Cytochrome c oxidase subunit 1



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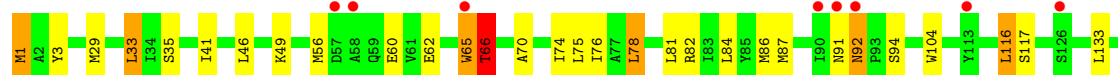
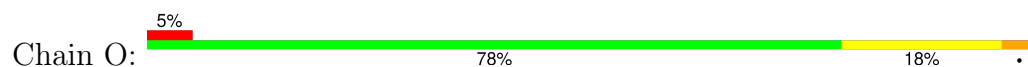


• Molecule 2: Cytochrome c oxidase subunit 2

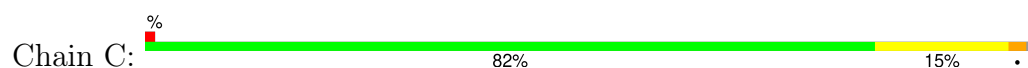




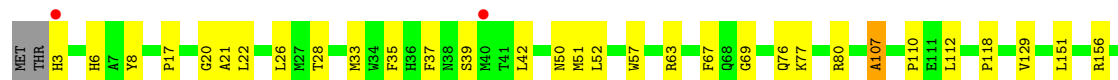
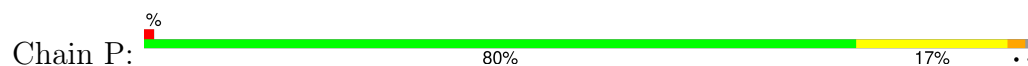
• Molecule 2: Cytochrome c oxidase subunit 2



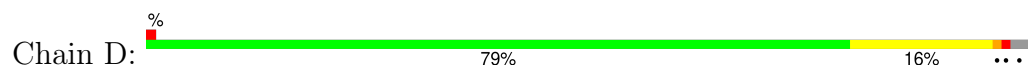
• Molecule 3: Cytochrome c oxidase subunit 3



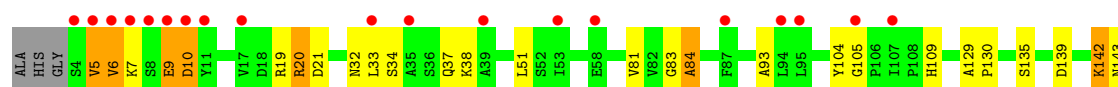
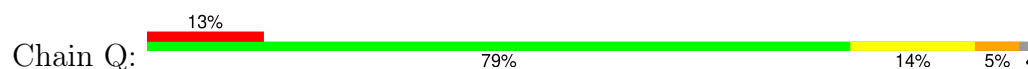
• Molecule 3: Cytochrome c oxidase subunit 3



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

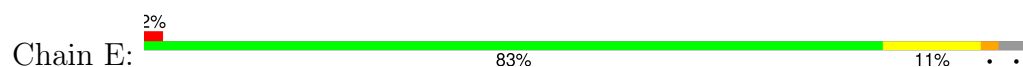


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

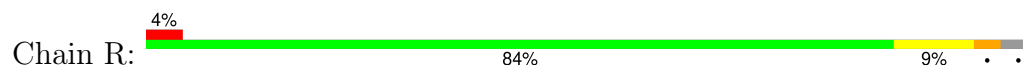




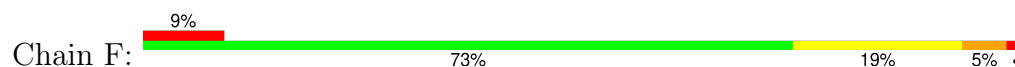
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



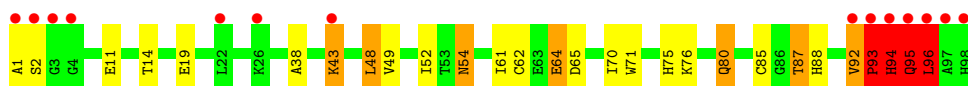
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



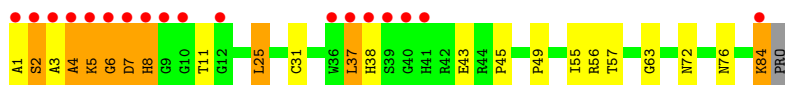
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



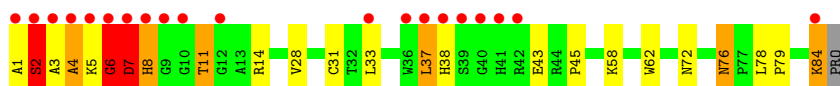
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



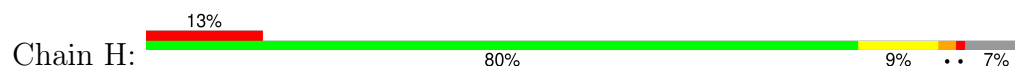
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

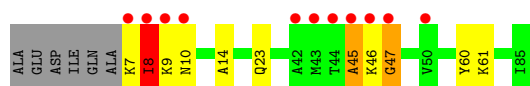


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

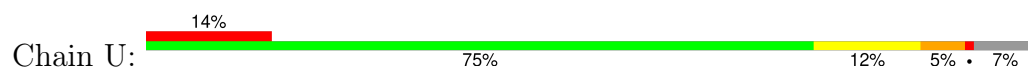


- Molecule 8: Cytochrome c oxidase subunit 6B1

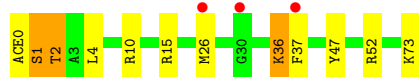
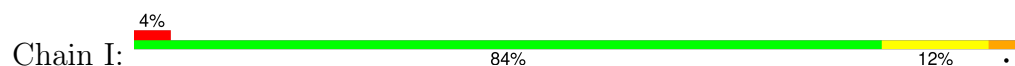




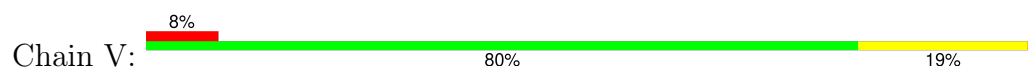
- Molecule 8: Cytochrome c oxidase subunit 6B1



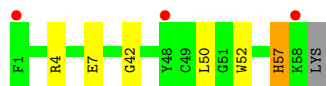
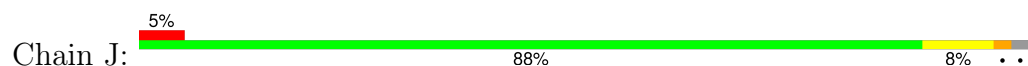
- Molecule 9: Cytochrome c oxidase subunit 6C



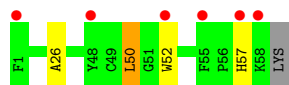
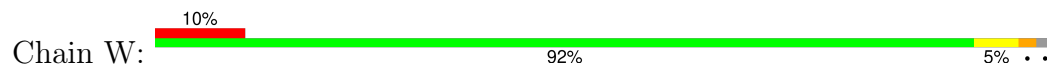
- Molecule 9: Cytochrome c oxidase subunit 6C



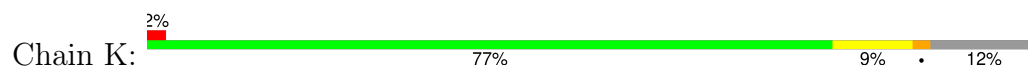
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



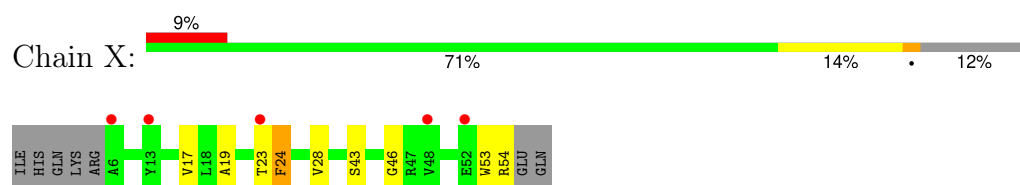
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



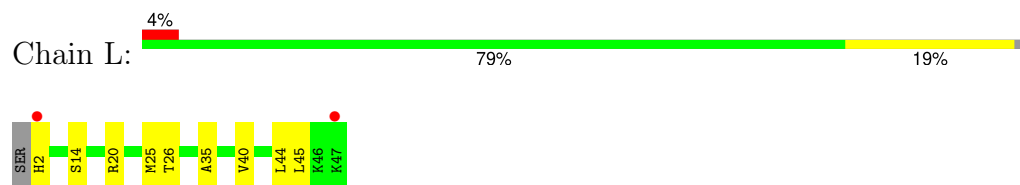
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



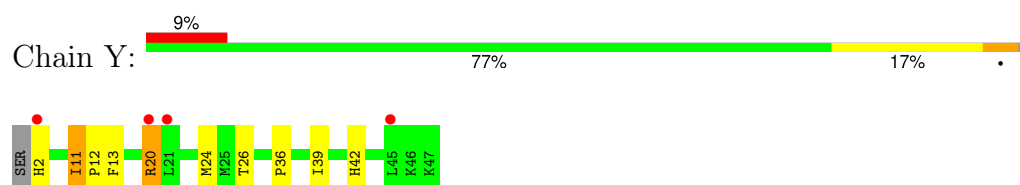
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



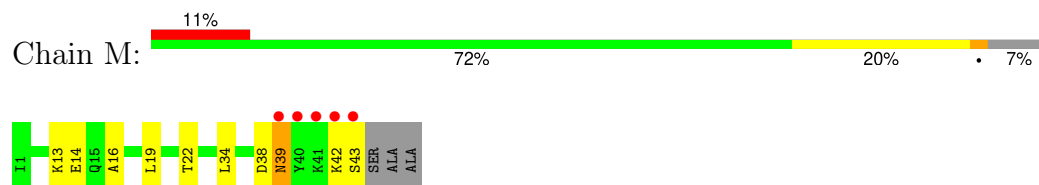
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



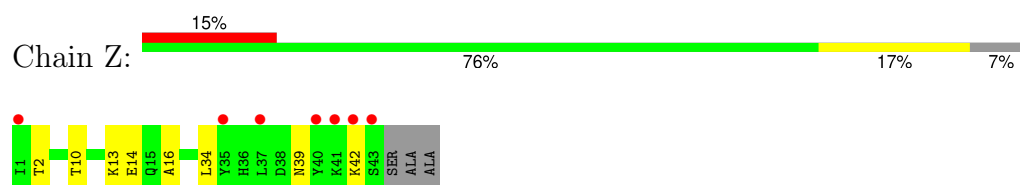
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.68Å 206.68Å 178.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.00) 99.8 (40.00-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.214 0.189 , 0.216	Depositor DCC
R_{free} test set	22864 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32060	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: CDL, DMU, CHD, CU, TPO, PEK, NA, PSC, ACE, PGV, UNX, TGL, CYN, ZN, MG, FME, CUA, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.77	43/4180 (1.0%)	1.41	31/5710 (0.5%)
1	N	1.56	16/4180 (0.4%)	1.28	24/5710 (0.4%)
2	B	1.65	12/1860 (0.6%)	1.37	9/2534 (0.4%)
2	O	1.40	5/1860 (0.3%)	1.27	9/2534 (0.4%)
3	C	1.51	3/2221 (0.1%)	1.21	7/3035 (0.2%)
3	P	1.51	10/2221 (0.5%)	1.20	8/3035 (0.3%)
4	D	1.62	8/1229 (0.7%)	1.31	7/1658 (0.4%)
4	Q	1.21	4/1229 (0.3%)	1.17	6/1658 (0.4%)
5	E	1.49	1/871 (0.1%)	1.18	1/1182 (0.1%)
5	R	1.27	2/871 (0.2%)	1.16	1/1182 (0.1%)
6	F	1.67	10/765 (1.3%)	1.41	6/1038 (0.6%)
6	S	1.56	8/765 (1.0%)	1.40	9/1038 (0.9%)
7	G	1.60	6/690 (0.9%)	1.31	7/937 (0.7%)
7	T	1.52	2/690 (0.3%)	1.31	7/937 (0.7%)
8	H	1.42	1/682 (0.1%)	1.25	2/921 (0.2%)
8	U	1.21	1/682 (0.1%)	1.11	0/921
9	I	1.47	1/612 (0.2%)	1.32	3/812 (0.4%)
9	V	1.19	0/612	1.31	1/812 (0.1%)
10	J	1.43	0/471	1.20	1/636 (0.2%)
10	W	1.24	1/471 (0.2%)	1.18	0/636
11	K	1.55	1/398 (0.3%)	1.35	2/546 (0.4%)
11	X	1.29	2/398 (0.5%)	1.28	3/546 (0.5%)
12	L	1.46	1/393 (0.3%)	1.27	2/526 (0.4%)
12	Y	1.28	0/393	1.21	2/526 (0.4%)
13	M	1.59	3/345 (0.9%)	1.28	0/470
13	Z	1.27	1/345 (0.3%)	1.20	0/470
All	All	1.53	142/29434 (0.5%)	1.29	148/40010 (0.4%)

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
1	N	0	1
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
All	All	0	6

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	198	GLU	C-O	12.35	1.37	1.23
3	P	107	ALA	CA-CB	10.07	1.64	1.53
1	A	297	MET	SD-CE	9.96	2.04	1.79
4	Q	6	VAL	CA-CB	9.10	1.63	1.54
2	O	66	THR	CA-C	8.92	1.61	1.52
11	X	19	ALA	CA-CB	8.80	1.67	1.53
1	A	139	ALA	CA-CB	8.59	1.68	1.53
13	M	16	ALA	CA-CB	8.42	1.66	1.53
2	B	198	GLU	C-O	8.15	1.32	1.23
3	P	129	VAL	CA-CB	8.13	1.59	1.53
1	N	139	ALA	CA-CB	8.04	1.67	1.53
1	N	297	MET	SD-CE	7.85	1.99	1.79
1	A	441	SER	C-O	7.75	1.34	1.24
1	A	120	ALA	CA-CB	7.74	1.63	1.53
11	K	22	ALA	CA-CB	7.71	1.65	1.53
6	S	70	ILE	CA-CB	7.22	1.62	1.54
1	A	388	ALA	CA-CB	7.21	1.64	1.53
2	O	175	ILE	CA-CB	7.09	1.59	1.54
1	A	332	ILE	CA-CB	6.96	1.62	1.54
1	N	106	PRO	CA-C	6.83	1.58	1.52
1	N	182	PRO	C-O	6.78	1.31	1.23
1	N	441	SER	C-O	6.75	1.32	1.24
9	I	4	LEU	CA-CB	6.75	1.63	1.53
1	A	318	VAL	CA-CB	6.74	1.63	1.54
1	N	419	VAL	CA-CB	6.68	1.62	1.54
8	H	8	ILE	CA-CB	6.62	1.63	1.54
1	A	327	LEU	N-CA	6.54	1.54	1.46
6	F	49	VAL	N-CA	-6.51	1.41	1.46
4	D	28	ALA	CA-CB	6.47	1.64	1.53
1	A	181	THR	CA-CB	6.47	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	273	MET	CB-CG	6.33	1.71	1.52
1	A	83	VAL	C-O	-6.31	1.19	1.24
1	A	282	PHE	CA-C	6.31	1.60	1.52
1	N	189	MET	CB-CG	6.28	1.71	1.52
1	A	149	SER	CA-C	6.24	1.61	1.52
4	D	81	VAL	CA-C	6.23	1.60	1.52
4	D	57	VAL	CA-CB	6.19	1.62	1.54
1	A	24	ALA	CA-CB	6.19	1.62	1.53
3	P	6	HIS	C-O	6.18	1.32	1.23
4	D	39	ALA	CA-CB	6.14	1.62	1.53
3	P	21	ALA	CA-CB	6.02	1.62	1.53
1	N	203	ALA	C-O	6.00	1.31	1.24
6	F	68	THR	CA-CB	5.99	1.61	1.53
1	A	485	VAL	C-O	-5.98	1.18	1.24
1	A	240	HIS	CA-C	5.97	1.59	1.52
1	A	412	ILE	CA-C	5.95	1.60	1.52
5	E	26	ALA	CA-CB	5.94	1.62	1.53
12	L	35	ALA	CA-CB	5.91	1.60	1.53
2	B	66	THR	CA-C	5.88	1.58	1.52
7	G	49	PRO	N-CA	5.87	1.51	1.47
6	F	2	SER	CA-C	5.87	1.60	1.52
6	F	2	SER	N-CA	5.86	1.53	1.46
8	U	8	ILE	CA-CB	5.83	1.62	1.54
2	O	200	CYS	N-CA	5.81	1.52	1.46
6	S	94	HIS	N-CA	5.77	1.53	1.46
1	A	446	ALA	CA-C	5.71	1.60	1.52
2	B	57	ASP	CA-C	5.70	1.60	1.52
2	B	167	SER	CB-OG	-5.69	1.30	1.42
6	F	87	THR	CA-CB	5.66	1.62	1.53
5	R	80	GLU	CG-CD	5.66	1.66	1.52
1	N	219	PHE	N-CA	5.65	1.53	1.46
11	X	24	PHE	CA-C	5.62	1.59	1.52
1	A	7	LEU	C-O	5.61	1.30	1.23
10	W	26	ALA	CA-CB	5.61	1.62	1.53
1	A	140	GLY	C-O	5.59	1.30	1.23
7	G	7	ASP	N-CA	5.58	1.53	1.46
1	A	267	PRO	C-O	5.56	1.30	1.23
1	A	441	SER	CA-C	5.54	1.60	1.52
4	D	19	ARG	CZ-NH2	5.54	1.40	1.33
1	A	357	VAL	CA-C	5.54	1.59	1.52
3	P	210	ILE	CA-CB	5.53	1.60	1.54
1	A	482	VAL	CA-CB	5.50	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	276	ALA	CA-CB	5.49	1.62	1.53
2	B	113	TYR	C-O	-5.49	1.17	1.24
2	B	23	PHE	CA-C	5.48	1.59	1.52
1	A	352	GLY	N-CA	5.45	1.52	1.45
6	S	95	GLN	CA-C	5.44	1.60	1.52
6	S	61	ILE	CA-CB	5.44	1.59	1.53
1	A	236	TRP	N-CA	5.42	1.53	1.46
3	C	107	ALA	CA-CB	5.41	1.59	1.53
6	S	93	PRO	CA-CB	5.41	1.60	1.53
6	F	95	GLN	CA-C	5.41	1.60	1.52
7	G	55	ILE	CA-CB	5.40	1.59	1.54
13	M	22	THR	N-CA	5.40	1.52	1.46
3	P	217	VAL	CA-CB	5.40	1.60	1.54
1	A	497	GLY	C-O	5.39	1.31	1.23
7	G	8	HIS	N-CA	5.39	1.53	1.46
2	B	31	VAL	CA-CB	5.39	1.60	1.54
3	P	213	THR	CA-CB	5.37	1.61	1.53
3	P	184	ALA	CA-CB	5.34	1.61	1.53
1	A	508	PRO	C-O	5.33	1.30	1.23
1	A	167	THR	CA-C	5.31	1.59	1.52
6	F	96	LEU	N-CA	5.30	1.53	1.46
7	T	14	ARG	C-O	5.30	1.30	1.24
3	C	8	TYR	N-CA	5.29	1.52	1.45
1	N	163	ASN	CA-C	5.27	1.59	1.52
3	P	238	ALA	CA-CB	5.27	1.61	1.53
1	A	345	ILE	C-O	5.27	1.30	1.24
6	F	67	SER	C-O	-5.27	1.17	1.24
7	G	5	LYS	CA-C	5.24	1.59	1.52
1	A	490	THR	N-CA	5.24	1.51	1.46
3	C	7	ALA	CA-CB	5.24	1.62	1.53
2	B	3	TYR	N-CA	5.23	1.51	1.45
1	A	185	VAL	N-CA	5.23	1.52	1.46
4	D	14	PRO	CA-C	5.23	1.59	1.52
4	D	31	LYS	CD-CE	5.23	1.68	1.52
1	A	182	PRO	CA-C	5.22	1.59	1.52
4	Q	5	VAL	CA-C	5.21	1.59	1.52
4	Q	6	VAL	N-CA	5.20	1.52	1.46
1	A	53	ILE	N-CA	-5.19	1.40	1.46
1	A	250	GLY	N-CA	5.19	1.52	1.45
6	F	37	LYS	C-O	-5.18	1.17	1.23
6	S	96	LEU	N-CA	5.18	1.52	1.46
13	Z	16	ALA	CA-CB	5.17	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	LEU	CA-C	5.17	1.59	1.52
2	B	138	VAL	C-O	5.16	1.30	1.23
3	P	178	ALA	CA-CB	5.16	1.61	1.53
6	F	39	THR	N-CA	5.13	1.51	1.46
4	Q	5	VAL	CA-CB	5.12	1.61	1.54
2	B	33	LEU	CA-C	5.12	1.59	1.52
1	A	134	GLY	N-CA	5.11	1.51	1.45
2	O	174	ALA	CA-CB	5.11	1.60	1.53
1	N	250	GLY	N-CA	5.11	1.52	1.45
2	B	197	SER	CA-CB	5.10	1.60	1.53
1	A	500	PRO	C-O	-5.10	1.18	1.24
1	N	251	PHE	N-CA	5.10	1.52	1.46
1	N	97	MET	CA-C	5.10	1.59	1.52
1	N	130	PRO	CA-C	5.09	1.56	1.52
1	A	169	ILE	CA-CB	5.09	1.61	1.54
4	D	58	GLU	C-O	-5.09	1.18	1.24
1	A	45	GLY	N-CA	5.08	1.50	1.45
1	A	122	ALA	CA-CB	5.08	1.59	1.53
6	S	87	THR	CA-CB	5.08	1.61	1.53
1	A	493	GLU	N-CA	5.06	1.52	1.46
6	S	2	SER	N-CA	5.06	1.52	1.46
7	G	56	ARG	CA-CB	5.06	1.60	1.52
5	R	80	GLU	CB-CG	5.05	1.67	1.52
1	A	92	MET	CB-CG	5.04	1.67	1.52
7	T	28	VAL	CA-C	5.04	1.59	1.52
2	B	59	GLN	CG-CD	5.03	1.64	1.52
1	A	26	ALA	N-CA	5.02	1.52	1.46
13	M	14	GLU	C-O	-5.01	1.18	1.24

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	MET	CG-SD-CE	-14.33	69.37	100.90
2	O	226	MET	N-CA-C	-12.62	98.79	112.93
6	F	2	SER	N-CA-C	8.02	120.70	108.52
4	D	19	ARG	NE-CZ-NH1	-7.88	113.62	121.50
4	Q	105	GLY	CA-C-N	-7.87	112.59	120.31
4	Q	105	GLY	C-N-CA	-7.87	112.59	120.31
1	A	240	HIS	N-CA-CB	7.84	117.84	110.39
1	A	169	ILE	CB-CA-C	-7.77	101.82	112.24
4	D	102	TYR	CA-C-N	-7.49	115.51	123.08
4	D	102	TYR	C-N-CA	-7.49	115.51	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	GLY	N-CA-C	-7.28	105.28	115.32
12	Y	11	ILE	CA-C-N	-7.22	112.62	121.00
12	Y	11	ILE	C-N-CA	-7.22	112.62	121.00
6	F	64	GLU	CA-C-N	-7.21	113.70	126.45
6	F	64	GLU	C-N-CA	-7.21	113.70	126.45
1	A	240	HIS	CA-CB-CG	-7.05	106.75	113.80
6	S	92	VAL	CA-C-N	-7.02	110.14	120.46
6	S	92	VAL	C-N-CA	-7.02	110.14	120.46
1	A	278	MET	CG-SD-CE	-6.95	85.61	100.90
7	G	7	ASP	N-CA-C	6.92	125.55	110.80
7	G	8	HIS	N-CA-C	6.83	125.34	110.80
7	G	57	THR	N-CA-C	-6.77	104.92	113.72
4	D	107	ILE	CB-CG1-CD1	-6.75	99.61	113.80
1	N	199	LEU	CA-C-N	-6.69	112.10	119.19
1	N	199	LEU	C-N-CA	-6.69	112.10	119.19
7	G	2	SER	N-CA-C	-6.65	103.56	112.94
1	N	240	HIS	N-CA-CB	6.63	119.66	110.11
1	A	362	SER	CA-CB-OG	-6.63	97.85	111.10
3	C	80	ARG	CG-CD-NE	-6.60	97.48	112.00
2	B	64	ILE	N-CA-C	-6.55	104.10	110.72
1	A	299	VAL	N-CA-C	6.54	117.29	110.62
2	B	65	TRP	CB-CA-C	6.53	122.11	110.81
2	B	31	VAL	N-CA-C	6.50	116.66	110.42
1	A	45	GLY	N-CA-C	-6.48	103.41	111.70
7	G	25	LEU	CA-C-N	-6.45	112.19	119.28
7	G	25	LEU	C-N-CA	-6.45	112.19	119.28
1	A	249	PRO	N-CA-C	-6.42	104.98	113.65
1	A	112	LEU	CD1-CG-CD2	-6.41	96.71	110.80
1	A	60	ALA	N-CA-C	-6.35	104.43	111.36
1	A	244	TYR	CA-CB-CG	-6.33	102.50	113.90
1	A	80	ASN	N-CA-C	6.29	117.81	111.07
1	A	441	SER	CA-C-O	6.27	127.08	119.31
1	N	475	ALA	N-CA-C	-6.25	104.39	111.14
11	X	43	SER	CA-C-N	-6.23	113.31	120.04
11	X	43	SER	C-N-CA	-6.23	113.31	120.04
1	N	278	MET	CG-SD-CE	-6.22	87.22	100.90
2	O	202	SER	N-CA-C	6.14	118.76	111.33
6	F	93	PRO	CA-C-N	6.13	133.24	121.54
6	F	93	PRO	C-N-CA	6.13	133.24	121.54
6	S	11	GLU	N-CA-C	6.10	118.00	111.36
6	S	49	VAL	CA-C-N	-6.03	113.76	119.85
6	S	49	VAL	C-N-CA	-6.03	113.76	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	59	GLN	N-CA-C	6.01	117.83	111.28
1	N	25	TRP	N-CA-C	-5.97	104.86	111.36
1	N	80	ASN	N-CA-C	5.96	117.77	111.28
2	B	167	SER	CB-CA-C	-5.94	99.63	110.63
3	C	194	GLY	N-CA-C	-5.90	105.46	113.37
2	O	201	GLY	CA-C-N	5.88	128.44	120.38
2	O	201	GLY	C-N-CA	5.88	128.44	120.38
2	O	92	ASN	CA-C-N	5.87	125.78	119.85
2	O	92	ASN	C-N-CA	5.87	125.78	119.85
1	N	153	ALA	N-CA-C	-5.84	104.99	111.36
3	P	193	TYR	N-CA-C	-5.83	104.84	111.14
1	N	181	THR	CA-C-N	-5.82	114.27	120.03
1	N	181	THR	C-N-CA	-5.82	114.27	120.03
2	B	64	ILE	CA-C-N	-5.81	113.01	122.65
2	B	64	ILE	C-N-CA	-5.81	113.01	122.65
9	V	20	HIS	N-CA-C	5.77	118.52	111.82
3	C	107	ALA	CA-C-N	-5.75	114.01	119.76
3	C	107	ALA	C-N-CA	-5.75	114.01	119.76
1	A	189	MET	CA-CB-CG	-5.70	102.70	114.10
1	N	70	VAL	N-CA-C	5.69	115.88	110.42
6	S	64	GLU	CA-C-N	-5.69	115.01	125.02
6	S	64	GLU	C-N-CA	-5.69	115.01	125.02
1	N	388	ALA	N-CA-C	-5.67	105.18	111.36
11	K	39	GLU	CB-CA-C	-5.67	101.45	110.81
1	A	225	GLY	CA-C-N	-5.63	116.69	122.27
1	A	225	GLY	C-N-CA	-5.63	116.69	122.27
1	N	105	LEU	CA-C-N	-5.62	114.59	120.38
1	N	105	LEU	C-N-CA	-5.62	114.59	120.38
3	P	198	PHE	N-CA-C	5.62	117.48	111.36
1	A	226	GLY	N-CA-C	-5.58	104.03	112.41
1	N	429	HIS	N-CA-C	-5.58	105.20	111.28
8	H	14	ALA	CA-C-N	-5.56	114.86	120.31
8	H	14	ALA	C-N-CA	-5.56	114.86	120.31
3	P	57	TRP	N-CA-C	-5.55	105.15	111.14
9	I	52	ARG	CA-C-N	-5.52	114.42	122.86
9	I	52	ARG	C-N-CA	-5.52	114.42	122.86
4	D	74	SER	CA-CB-OG	-5.52	100.07	111.10
2	B	13	THR	N-CA-C	-5.51	106.45	114.12
6	F	87	THR	N-CA-CB	5.49	118.13	109.83
3	P	80	ARG	CG-CD-NE	-5.49	99.91	112.00
4	Q	32	ASN	N-CA-C	5.49	117.47	108.52
1	A	208	MET	CG-SD-CE	5.48	112.96	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	3	TYR	CA-C-N	-5.48	114.13	119.78
2	O	3	TYR	C-N-CA	-5.48	114.13	119.78
7	T	58	LYS	CA-C-N	-5.48	114.14	119.78
7	T	58	LYS	C-N-CA	-5.48	114.14	119.78
9	I	1	SER	CA-CB-OG	-5.47	100.16	111.10
1	A	83	VAL	N-CA-CB	5.45	114.70	110.45
3	P	245	VAL	N-CA-C	5.45	116.18	110.62
1	N	71	MET	CG-SD-CE	-5.42	88.97	100.90
5	R	46	LYS	N-CA-C	-5.42	105.53	111.82
5	E	84	TYR	N-CA-C	-5.42	105.45	111.36
1	N	180	GLN	CA-CB-CG	-5.42	103.27	114.10
1	N	240	HIS	CA-CB-CG	-5.42	108.39	113.80
7	T	7	ASP	N-CA-C	5.42	122.33	110.80
11	X	53	TRP	N-CA-C	-5.40	107.35	114.31
7	T	76	ASN	CA-C-N	-5.38	115.04	120.31
7	T	76	ASN	C-N-CA	-5.38	115.04	120.31
6	S	94	HIS	N-CA-C	5.37	122.24	110.80
7	G	6	GLY	N-CA-C	5.37	125.90	113.18
1	N	189	MET	CA-CB-CG	-5.36	103.39	114.10
1	A	189	MET	CB-CA-C	-5.30	102.56	110.88
1	N	425	PHE	N-CA-C	5.29	119.86	113.41
7	T	2	SER	N-CA-C	-5.27	105.70	113.61
1	A	397	PHE	CA-C-N	-5.26	113.61	119.19
1	A	397	PHE	C-N-CA	-5.26	113.61	119.19
11	K	14	GLY	N-CA-C	5.25	118.99	112.64
4	Q	20	ARG	CG-CD-NE	-5.25	100.46	112.00
3	P	35	PHE	N-CA-C	5.25	117.74	111.71
1	A	119	GLU	CB-CA-C	-5.24	110.51	116.54
3	C	112	LEU	N-CA-C	-5.23	106.58	113.17
2	B	202	SER	N-CA-C	5.23	117.66	111.33
4	Q	9	GLU	N-CA-C	-5.23	107.43	112.97
1	A	96	ARG	NE-CZ-NH2	-5.21	114.51	119.20
2	O	65	TRP	N-CA-C	5.21	119.20	113.21
1	A	78	PHE	N-CA-C	5.21	116.95	111.28
6	S	2	SER	N-CA-C	5.19	115.39	108.38
4	D	19	ARG	NE-CZ-NH2	5.17	123.85	119.20
3	P	20	GLY	N-CA-C	-5.16	106.53	112.73
10	J	42	GLY	N-CA-C	-5.16	106.46	113.37
1	N	184	PHE	N-CA-C	-5.13	105.87	111.82
1	A	362	SER	CB-CA-C	-5.12	102.84	110.88
1	N	127	THR	N-CA-C	-5.11	106.90	113.23
12	L	25	MET	CA-C-N	5.09	127.06	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	25	MET	C-N-CA	5.09	127.06	120.44
7	T	6	GLY	N-CA-C	5.08	125.22	113.18
1	N	362	SER	CA-CB-OG	-5.08	100.94	111.10
3	C	106	LEU	CA-C-N	-5.07	117.01	123.15
3	C	106	LEU	C-N-CA	-5.07	117.01	123.15
1	A	348	PHE	N-CA-C	-5.06	105.84	111.36
4	D	112	GLU	N-CA-C	-5.05	103.38	110.50
3	P	217	VAL	N-CA-C	-5.05	105.58	110.42
1	N	262	SER	N-CA-C	-5.04	106.91	113.16
1	A	126	TRP	N-CA-C	-5.02	106.98	113.01
1	A	181	THR	N-CA-C	-5.01	103.88	110.39
4	Q	84	ALA	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
10	W	57	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4051	0	4029	60	0
1	N	4051	0	4029	58	0
2	B	1824	0	1833	29	0
2	O	1824	0	1833	35	0
3	C	2134	0	2051	33	0
3	P	2134	0	2051	40	0
4	D	1195	0	1183	16	0
4	Q	1195	0	1183	21	0
5	E	852	0	845	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	852	0	845	8	0
6	F	748	0	728	16	0
6	S	748	0	728	29	0
7	G	675	0	643	27	0
7	T	675	0	643	45	0
8	H	662	0	623	9	0
8	U	662	0	623	13	0
9	I	601	0	613	12	0
9	V	601	0	613	10	0
10	J	460	0	459	4	0
10	W	460	0	459	2	0
11	K	384	0	366	3	0
11	X	384	0	366	5	0
12	L	380	0	380	10	0
12	Y	380	0	380	15	0
13	M	335	0	352	2	0
13	Z	335	0	352	2	0
14	A	2	0	0	0	0
14	N	2	0	0	0	0
15	A	120	0	108	7	0
15	N	120	0	108	6	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	1	0
18	N	1	0	0	0	0
19	A	63	0	110	6	0
19	D	63	0	110	12	0
19	L	63	0	110	14	0
19	N	126	0	220	22	0
19	Q	63	0	110	2	0
20	A	102	0	152	8	0
20	C	102	0	152	5	0
20	N	102	0	152	10	0
20	P	102	0	152	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	2	0
22	C	58	0	78	6	0
22	O	29	0	39	1	0
22	P	58	0	78	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	100	0	156	16	0
24	G	100	0	156	26	0
24	P	100	0	156	21	0
24	T	100	0	156	26	0
25	C	53	0	77	6	0
25	G	106	0	154	13	0
25	P	106	0	154	13	0
25	T	53	0	77	22	0
26	E	52	0	80	16	0
26	O	52	0	80	17	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	41	4	0
28	M	33	0	42	0	0
28	P	33	0	42	3	0
28	Z	33	0	42	0	0
29	A	188	0	0	8	0
29	B	121	0	0	4	0
29	C	77	0	0	1	0
29	D	78	0	0	4	0
29	E	58	0	0	2	0
29	F	58	0	0	4	0
29	G	27	0	0	3	0
29	H	34	0	0	0	0
29	I	29	0	0	4	0
29	J	15	0	0	1	0
29	K	20	0	0	1	0
29	L	16	0	0	2	0
29	M	14	0	0	0	0
29	N	156	0	0	3	0
29	O	91	0	0	3	0
29	P	76	0	0	9	0
29	Q	46	0	0	4	0
29	R	42	0	0	1	0
29	S	38	0	0	3	0
29	T	23	0	0	2	0
29	U	28	0	0	3	0
29	V	14	0	0	0	0
29	W	4	0	0	0	0
29	X	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Y	11	0	0	0	0
29	Z	7	0	0	0	0
All	All	32060	0	31341	581	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 9.

All (581) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:309:PEK:H383	24:T:102:CDL:C27	1.43	1.46
1:A:297:MET:SD	1:A:297:MET:CE	2.04	1.45
25:C:306:PEK:H383	24:G:103:CDL:C27	1.49	1.38
6:S:43:LYS:H	6:S:43:LYS:CD	1.43	1.26
6:F:95:GLN:HA	29:F:256:HOH:O	1.34	1.25
19:N:610:TGL:HC32	12:Y:20:ARG:NH2	1.53	1.22
24:G:103:CDL:H541	24:G:103:CDL:H241	1.25	1.17
12:L:20:ARG:HH22	19:L:101:TGL:HC32	1.08	1.16
12:L:20:ARG:NH2	19:L:101:TGL:HC32	1.60	1.15
1:A:27:GLY:HA3	15:A:602:HEA:C27	1.78	1.13
25:C:306:PEK:H383	24:G:103:CDL:H273	1.18	1.12
26:E:201:PSC:H072	9:I:10:ARG:HH21	1.10	1.12
19:L:101:TGL:HC62	19:L:101:TGL:HC22	1.32	1.08
25:P:309:PEK:C38	24:T:102:CDL:C27	2.31	1.08
7:G:45:PRO:HD2	29:G:221:HOH:O	1.53	1.08
8:U:9:LYS:HG3	8:U:10:ASN:H	1.14	1.08
25:P:309:PEK:H383	24:T:102:CDL:H272	1.33	1.07
3:P:67:PHE:HE1	24:P:306:CDL:H1	1.15	1.06
25:P:309:PEK:H383	24:T:102:CDL:H273	1.10	1.06
6:S:43:LYS:H	6:S:43:LYS:HD3	1.21	1.05
7:T:5:LYS:HB2	25:T:101:PEK:H362	1.05	1.04
24:G:103:CDL:H241	24:G:103:CDL:C54	1.86	1.04
2:B:41:ILE:HD13	26:E:201:PSC:H342	1.36	1.04
19:L:101:TGL:OC1	19:L:101:TGL:HC41	1.53	1.02
6:S:43:LYS:H	6:S:43:LYS:HD2	1.23	1.01
1:A:27:GLY:HA3	15:A:602:HEA:H273	1.38	1.01
7:G:5:LYS:HG3	25:G:104:PEK:H383	1.38	1.01
6:S:85:CYS:SG	6:S:87:THR:HG23	2.01	1.00
20:P:305:PGV:H182	24:P:306:CDL:H671	1.43	0.98
25:C:306:PEK:C38	24:G:103:CDL:H273	1.94	0.97
6:S:43:LYS:CD	6:S:43:LYS:N	2.26	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:306:PEK:H383	24:G:103:CDL:H271	1.47	0.95
6:S:43:LYS:HE2	29:S:220:HOH:O	1.65	0.95
25:C:306:PEK:C38	24:G:103:CDL:C27	2.44	0.94
24:G:103:CDL:H541	24:G:103:CDL:C24	1.97	0.94
24:P:306:CDL:OB9	24:P:306:CDL:H522	1.68	0.94
1:N:400:PHE:HB3	19:N:610:TGL:H283	1.48	0.93
18:A:606:NA:NA	29:A:709:HOH:O	1.41	0.93
28:G:101:DMU:H36	28:G:101:DMU:H30	1.47	0.93
7:T:5:LYS:CD	25:T:101:PEK:H371	1.98	0.93
26:E:201:PSC:C07	9:I:10:ARG:HH21	1.83	0.92
25:P:304:PEK:H71	25:P:304:PEK:H32	1.51	0.92
3:C:67:PHE:HE1	24:C:303:CDL:H1	1.32	0.92
3:P:3:HIS:HB3	29:P:456:HOH:O	1.71	0.91
7:T:31:CYS:SG	24:T:102:CDL:H532	2.12	0.90
7:T:5:LYS:HB2	25:T:101:PEK:C36	1.99	0.90
7:T:5:LYS:HD2	25:T:101:PEK:H371	1.52	0.89
3:C:63:ARG:HE	24:C:303:CDL:HA22	1.37	0.89
6:S:75:HIS:H	6:S:80:GLN:HE22	1.15	0.89
15:N:602:HEA:C16	15:N:602:HEA:H273	2.00	0.89
19:N:610:TGL:HC32	12:Y:20:ARG:HH22	1.39	0.88
1:A:27:GLY:CA	15:A:602:HEA:H273	2.03	0.88
6:F:85:CYS:SG	6:F:87:THR:HG23	2.14	0.88
20:N:607:PGV:H02	20:N:607:PGV:O14	1.71	0.88
19:L:101:TGL:HC62	19:L:101:TGL:CC2	2.03	0.86
6:S:19:GLU:HG2	29:S:232:HOH:O	1.75	0.86
3:P:67:PHE:CE1	24:P:306:CDL:H1	2.08	0.86
7:T:5:LYS:HD2	25:T:101:PEK:C38	2.06	0.86
19:N:610:TGL:HC32	12:Y:20:ARG:HH21	1.33	0.86
25:P:309:PEK:C38	24:T:102:CDL:H273	2.02	0.85
29:P:463:HOH:O	6:S:96:LEU:HD13	1.77	0.85
25:P:309:PEK:C38	24:T:102:CDL:H272	2.00	0.84
7:T:72:ASN:H	7:T:76:ASN:HD22	1.25	0.84
26:E:201:PSC:H072	9:I:10:ARG:NH2	1.92	0.83
6:F:75:HIS:H	6:F:80:GLN:HE22	1.26	0.83
3:P:160:LEU:HD13	22:P:307:CHD:H181	1.59	0.83
20:P:305:PGV:H182	24:P:306:CDL:C67	2.08	0.83
1:N:117[A]:MET:HE2	12:Y:42:HIS:CD2	2.12	0.82
7:T:2:SER:OG	25:T:101:PEK:H301	1.78	0.82
19:L:101:TGL:OA1	19:L:101:TGL:OG3	1.97	0.82
1:N:484:THR:HG22	13:Z:2:THR:OG1	1.80	0.82
29:P:475:HOH:O	6:S:1:ALA:HB2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:HD21	20:A:609:PGV:H22	1.44	0.82
1:A:27:GLY:HA3	15:A:602:HEA:H271	1.59	0.82
7:T:5:LYS:HD2	25:T:101:PEK:C37	2.09	0.81
8:U:9:LYS:HG3	8:U:10:ASN:N	1.93	0.81
1:A:297:MET:HB2	29:A:884:HOH:O	1.80	0.81
24:T:102:CDL:H111	24:T:102:CDL:HA21	1.63	0.80
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.46	0.80
7:G:72:ASN:H	7:G:76:ASN:HD22	1.27	0.79
24:P:306:CDL:H652	29:P:468:HOH:O	1.81	0.79
25:P:304:PEK:HN2	7:T:76:ASN:HD21	1.31	0.78
6:F:54:ASN:H	6:F:54:ASN:HD22	1.31	0.78
6:F:1:ALA:HB2	29:F:251:HOH:O	1.82	0.78
28:G:101:DMU:H30	28:G:101:DMU:C10	2.13	0.78
3:C:161:GLN:HE22	25:C:306:PEK:H22	1.48	0.78
8:U:7:LYS:O	8:U:8:ILE:HB	1.83	0.78
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.20	0.77
20:P:305:PGV:H172	29:P:468:HOH:O	1.84	0.77
4:D:34:SER:H	4:D:37:GLN:HE21	1.34	0.76
19:D:201:TGL:CG3	29:D:323:HOH:O	2.33	0.75
7:T:45:PRO:HD2	29:T:223:HOH:O	1.85	0.75
6:S:43:LYS:HD2	6:S:43:LYS:N	1.91	0.75
1:A:278:MET:HB3	7:T:5:LYS:HG2	1.69	0.75
7:T:37:LEU:CD2	24:T:102:CDL:H361	2.16	0.75
3:C:160:LEU:HD13	22:C:304:CHD:H181	1.69	0.75
5:E:8:ASP:HA	26:E:201:PSC:H071	1.69	0.75
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.16	0.75
6:F:64:GLU:O	6:F:65:ASP:HB2	1.86	0.74
19:N:610:TGL:H231	19:N:610:TGL:HA92	1.68	0.74
8:H:9:LYS:O	8:H:10:ASN:HB2	1.87	0.74
2:O:56:MET:HA	26:O:303:PSC:H202	1.69	0.74
1:N:513:LEU:O	1:N:514:LYS:HB2	1.88	0.74
15:N:602:HEA:H273	15:N:602:HEA:H161	1.69	0.74
12:L:2:HIS:CD2	29:L:209:HOH:O	2.40	0.74
20:A:609:PGV:C01	20:A:609:PGV:H221	2.17	0.74
19:N:610:TGL:H161	12:Y:24:MET:SD	2.28	0.74
8:U:20:PHE:HE2	8:U:27:ARG:HG2	1.53	0.73
8:H:45:ALA:O	8:H:47:GLY:N	2.18	0.73
7:T:5:LYS:CB	25:T:101:PEK:H362	2.01	0.73
4:Q:34:SER:O	4:Q:38:LYS:HG3	1.88	0.73
4:D:81:VAL:HG11	19:D:201:TGL:HB52	1.70	0.72
9:I:26:MET:HE3	29:I:128:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:31:CYS:SG	24:T:102:CDL:H551	2.29	0.72
9:I:0:ACE:O	9:I:2:THR:HG22	1.89	0.72
2:O:217:LYS:HG3	29:O:485:HOH:O	1.88	0.72
3:P:33[A]:MET:HE3	3:P:39:SER:OG	1.90	0.72
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.72	0.71
1:N:310:MET:HE2	1:N:356:ILE:HG23	1.72	0.71
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.72	0.71
8:U:9:LYS:CG	8:U:10:ASN:H	1.98	0.71
1:N:117[A]:MET:HE3	12:Y:39:ILE:HG23	1.72	0.71
8:U:20:PHE:CE2	8:U:27:ARG:HG2	2.26	0.71
3:P:165:ILE:HG12	25:P:309:PEK:H102	1.72	0.71
4:Q:109:HIS:HD2	29:Q:338:HOH:O	1.72	0.71
24:T:102:CDL:HA21	24:T:102:CDL:C11	2.20	0.71
1:N:273:MET:HE2	29:N:735:HOH:O	1.91	0.70
6:S:43:LYS:HD3	6:S:43:LYS:N	1.99	0.70
7:G:5:LYS:HB2	25:G:104:PEK:H362	1.74	0.70
7:G:38:HIS:CE1	24:G:103:CDL:H111	2.27	0.70
24:C:303:CDL:H242	24:C:303:CDL:H661	1.73	0.70
8:H:7:LYS:O	8:H:8:ILE:HB	1.91	0.70
26:O:303:PSC:H212	26:O:303:PSC:O01	1.92	0.70
7:G:76:ASN:HD21	25:G:102:PEK:HN2	1.38	0.69
19:N:609:TGL:H122	19:N:609:TGL:H302	1.74	0.69
24:C:303:CDL:OB9	24:C:303:CDL:H521	1.92	0.69
2:O:41:ILE:HD13	26:O:303:PSC:H342	1.75	0.69
3:C:63:ARG:HE	24:C:303:CDL:CA2	2.05	0.69
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.75	0.68
1:A:468:MET:HG3	29:A:735:HOH:O	1.93	0.68
20:A:609:PGV:H221	20:A:609:PGV:H012	1.73	0.68
26:O:303:PSC:C07	9:V:10:ARG:HH21	2.07	0.67
1:A:27:GLY:CA	15:A:602:HEA:C27	2.66	0.67
3:P:107:ALA:HB2	20:P:302:PGV:H031	1.77	0.67
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.93	0.67
20:A:609:PGV:C06	29:A:822:HOH:O	2.43	0.67
3:P:63:ARG:HE	24:P:306:CDL:CA2	2.07	0.67
24:T:102:CDL:H541	24:T:102:CDL:H231	1.76	0.67
2:B:87:MET:HE2	29:B:423:HOH:O	1.95	0.67
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.77	0.66
3:P:246:ASP:HB2	29:P:428:HOH:O	1.94	0.66
2:B:183:THR:HG22	29:B:424:HOH:O	1.96	0.66
1:N:406:ASN:HD21	20:N:607:PGV:H21	1.58	0.66
7:T:37:LEU:HD21	24:T:102:CDL:H361	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:303:CDL:HB22	24:C:303:CDL:PA1	2.35	0.66
7:G:45:PRO:CD	29:G:221:HOH:O	2.26	0.66
7:G:3:ALA:HB1	25:G:104:PEK:H382	1.78	0.66
3:P:63:ARG:HE	24:P:306:CDL:HA22	1.58	0.66
26:E:201:PSC:C07	9:I:10:ARG:NH2	2.55	0.66
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.76	0.66
7:T:5:LYS:HD3	25:T:101:PEK:H371	1.78	0.66
24:G:103:CDL:H541	24:G:103:CDL:C23	2.25	0.65
24:G:103:CDL:H571	24:G:103:CDL:H792	1.77	0.65
26:O:303:PSC:H212	26:O:303:PSC:C02	2.26	0.65
1:N:117[A]:MET:CE	12:Y:42:HIS:CD2	2.79	0.65
24:G:103:CDL:H241	24:G:103:CDL:H542	1.77	0.65
3:P:160:LEU:HD13	22:P:307:CHD:C18	2.27	0.65
1:N:177:SER:H	1:N:180:GLN:NE2	1.94	0.64
19:L:101:TGL:OC1	19:L:101:TGL:CC4	2.36	0.64
26:O:303:PSC:H072	9:V:10:ARG:HH21	1.63	0.64
24:G:103:CDL:H201	1:N:311:ILE:CD1	2.27	0.64
19:N:609:TGL:H111	2:O:35:SER:HB3	1.80	0.64
24:P:306:CDL:H672	24:P:306:CDL:H262	1.79	0.64
29:O:452:HOH:O	8:U:61:LYS:HD3	1.98	0.64
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.63	0.64
7:G:5:LYS:CG	25:G:104:PEK:H383	2.19	0.64
1:N:177:SER:H	1:N:180:GLN:HE21	1.46	0.64
1:A:406:ASN:HD21	20:A:609:PGV:C2	2.11	0.63
2:B:78:LEU:HD12	24:T:102:CDL:H352	1.80	0.63
1:A:273:MET:HE2	29:A:738:HOH:O	1.96	0.63
4:D:34:SER:H	4:D:37:GLN:NE2	1.95	0.63
3:P:3:HIS:HD2	29:P:465:HOH:O	1.82	0.63
2:O:225:SER:C	2:O:227:LEU:H	2.06	0.63
1:A:1:FME:HE2	1:A:1:FME:HA	1.80	0.63
19:D:201:TGL:HA91	19:D:201:TGL:C24	2.29	0.63
5:E:11:PHE:CB	26:E:201:PSC:H073	2.28	0.62
19:D:201:TGL:HG32	29:D:323:HOH:O	1.98	0.62
6:S:94:HIS:CD2	6:S:95:GLN:H	2.16	0.62
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.80	0.62
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.81	0.62
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.80	0.62
19:D:201:TGL:HA91	19:D:201:TGL:H242	1.81	0.62
26:O:303:PSC:C22	26:O:303:PSC:H21	2.30	0.61
8:U:9:LYS:O	8:U:10:ASN:HB2	2.01	0.61
7:T:8:HIS:CD2	25:T:101:PEK:H252	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:PHE:HB3	26:E:201:PSC:H073	1.83	0.61
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.01	0.61
7:G:72:ASN:H	7:G:76:ASN:ND2	1.96	0.61
19:A:607:TGL:H252	19:A:607:TGL:HA91	1.82	0.60
29:N:790:HOH:O	4:Q:20:ARG:HG2	2.01	0.60
7:T:3:ALA:HB3	25:T:101:PEK:H361	1.83	0.60
19:L:101:TGL:CA9	19:L:101:TGL:H231	2.31	0.60
1:A:311:ILE:CD1	24:T:102:CDL:H201	2.32	0.60
19:N:610:TGL:CC3	12:Y:20:ARG:HH22	2.14	0.59
26:O:303:PSC:H071	5:R:8:ASP:HA	1.84	0.59
6:S:64:GLU:O	6:S:65:ASP:HB2	2.02	0.59
7:T:3:ALA:O	7:T:4:ALA:CB	2.50	0.59
1:N:117[B]:MET:HE3	10:W:50:LEU:HD21	1.82	0.59
1:N:309:THR:O	1:N:312[B]:ILE:HG22	2.02	0.59
2:B:41:ILE:HD13	26:E:201:PSC:C34	2.23	0.59
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.67	0.59
3:P:224:LYS:CD	24:P:306:CDL:HB31	2.32	0.59
5:E:91:PRO:HD2	29:E:335:HOH:O	2.03	0.59
5:R:79:LYS:HE2	29:R:219:HOH:O	2.03	0.59
19:A:607:TGL:H101	19:A:607:TGL:C28	2.33	0.58
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.84	0.58
20:A:609:PGV:H311	13:M:19:LEU:HD23	1.85	0.58
20:C:302:PGV:H182	24:C:303:CDL:H671	1.85	0.58
4:D:40:LEU:HD22	4:D:58:GLU:HG2	1.85	0.58
11:K:8:ASP:HB2	29:K:108:HOH:O	2.03	0.58
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.33	0.58
11:X:54:ARG:HD3	29:X:114:HOH:O	2.03	0.58
24:G:103:CDL:H541	24:G:103:CDL:H231	1.85	0.58
1:A:1:FME:HA	1:A:1:FME:CE	2.33	0.58
20:C:302:PGV:H172	24:C:303:CDL:H651	1.85	0.58
6:F:1:ALA:HB3	6:S:65:ASP:OD1	2.03	0.58
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.69	0.58
2:B:62:GLU:O	2:B:66:THR:HB	2.04	0.58
9:I:15:ARG:HD3	29:I:122:HOH:O	2.04	0.57
24:P:306:CDL:PA1	24:P:306:CDL:HB22	2.44	0.57
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.03	0.57
1:A:430:PHE:HE1	19:A:607:TGL:HB21	1.69	0.57
20:N:608:PGV:H182	3:P:28:THR:HG22	1.86	0.57
19:D:201:TGL:HG32	19:D:201:TGL:OB1	2.04	0.57
6:S:54:ASN:HD22	6:S:54:ASN:C	2.11	0.57
5:E:90:ARG:HD2	29:E:347:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:26:MET:HG3	29:I:128:HOH:O	2.03	0.57
26:O:303:PSC:H061	5:R:8:ASP:OD1	2.05	0.57
1:N:468:MET:HG3	29:N:732:HOH:O	2.04	0.57
24:G:103:CDL:H112	24:G:103:CDL:HA21	1.87	0.56
1:N:117[A]:MET:HE2	12:Y:42:HIS:HD2	1.69	0.56
1:N:310:MET:HE1	2:O:76:ILE:HG21	1.87	0.56
3:C:67:PHE:CE1	24:C:303:CDL:H1	2.25	0.56
26:O:303:PSC:H343	26:O:303:PSC:H142	1.88	0.56
24:T:102:CDL:H342	24:T:102:CDL:OA7	2.06	0.56
7:G:38:HIS:HE1	24:G:103:CDL:H111	1.69	0.56
10:J:7:GLU:HG3	29:J:110:HOH:O	2.04	0.56
3:P:164:PHE:CD1	22:P:307:CHD:H192	2.40	0.56
1:A:334:TRP:HB2	19:D:201:TGL:HG11	1.88	0.56
7:T:2:SER:OG	25:T:101:PEK:C30	2.53	0.56
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.05	0.56
7:T:37:LEU:HD23	24:T:102:CDL:H361	1.88	0.56
3:C:59:ARG:HG3	24:C:303:CDL:H511	1.88	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.06	0.56
7:T:5:LYS:HD2	25:T:101:PEK:H383	1.88	0.55
7:T:72:ASN:H	7:T:76:ASN:ND2	2.01	0.55
5:E:8:ASP:HA	26:E:201:PSC:C07	2.36	0.55
4:D:31:LYS:NZ	29:D:359:HOH:O	2.26	0.55
6:F:54:ASN:HB3	29:F:226:HOH:O	2.06	0.55
1:A:513:LEU:O	1:A:514:LYS:HB2	2.05	0.55
20:N:607:PGV:H011	20:N:607:PGV:C21	2.37	0.55
2:O:29:MET:HG3	9:V:35:TYR:CD2	2.42	0.55
20:A:609:PGV:H221	20:A:609:PGV:H011	1.89	0.55
20:A:609:PGV:H152	20:A:609:PGV:H321	1.87	0.54
26:O:303:PSC:H21	26:O:303:PSC:H221	1.89	0.54
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.71	0.54
3:C:106:LEU:HD13	20:C:307:PGV:H22	1.88	0.54
1:N:310:MET:CE	1:N:356:ILE:HG23	2.37	0.54
12:L:2:HIS:CG	29:L:209:HOH:O	2.57	0.54
7:G:63:GLY:H	28:G:101:DMU:H34	1.73	0.54
3:P:161:GLN:HE22	25:P:309:PEK:H22	1.73	0.54
24:P:306:CDL:H642	24:P:306:CDL:H242	1.89	0.54
5:E:72:LYS:HB2	5:E:82:TYR:CD2	2.43	0.54
7:T:38:HIS:HE2	24:T:102:CDL:H111	1.73	0.54
4:Q:7:LYS:HB2	4:Q:10:ASP:OD1	2.06	0.54
24:G:103:CDL:H511	24:G:103:CDL:H181	1.89	0.53
3:C:164:PHE:CD1	22:C:304:CHD:H192	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:CYS:SG	24:G:103:CDL:H532	2.48	0.53
8:U:9:LYS:HG3	29:U:123:HOH:O	2.07	0.53
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.89	0.53
2:B:13:THR:OG1	2:B:167:SER:HB3	2.08	0.53
26:E:201:PSC:O13	26:E:201:PSC:H083	2.09	0.53
19:N:609:TGL:C12	19:N:609:TGL:C30	2.86	0.53
3:P:33[A]:MET:HE2	3:P:42:LEU:H	1.73	0.53
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.43	0.53
7:G:3:ALA:O	7:G:4:ALA:HB2	2.08	0.53
1:N:383:MET:O	1:N:387:PHE:HB2	2.07	0.53
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.08	0.53
15:A:602:HEA:HHC	15:A:602:HEA:H122	1.91	0.53
2:B:82:ARG:HG2	2:B:86:MET:HE3	1.91	0.52
15:N:602:HEA:HHC	15:N:602:HEA:H122	1.91	0.52
3:C:107:ALA:HB2	20:C:307:PGV:H031	1.90	0.52
20:N:607:PGV:H011	20:N:607:PGV:H211	1.91	0.52
2:O:56:MET:CA	26:O:303:PSC:H202	2.39	0.52
3:P:156:ARG:HE	22:P:307:CHD:C24	2.22	0.52
7:T:2:SER:O	25:T:101:PEK:H322	2.10	0.52
6:F:64:GLU:O	6:F:65:ASP:CB	2.53	0.52
28:P:301:DMU:H30	7:T:62:TRP:HB3	1.91	0.52
3:P:33[A]:MET:CE	3:P:42:LEU:H	2.23	0.52
19:N:610:TGL:CC3	12:Y:20:ARG:NH2	2.47	0.52
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.75	0.52
3:C:156:ARG:HE	22:C:304:CHD:C24	2.22	0.52
3:C:254:VAL:CG2	24:G:103:CDL:H672	2.40	0.52
4:D:109:HIS:HD2	29:D:314:HOH:O	1.93	0.52
25:P:304:PEK:H102	25:P:304:PEK:H161	1.92	0.51
3:P:224:LYS:HD3	24:P:306:CDL:HB31	1.92	0.51
4:D:131:ILE:HD13	9:I:47:TYR:CE2	2.45	0.51
24:C:303:CDL:HB22	24:C:303:CDL:OA5	2.10	0.51
2:O:164:ALA:O	2:O:194:GLY:HA3	2.10	0.51
2:B:56:MET:HG2	26:E:201:PSC:H211	1.92	0.51
1:A:43:GLN:HB2	1:A:44:PRO:HD2	1.92	0.51
1:A:76:GLY:O	1:A:80:ASN:HB2	2.11	0.51
1:A:112:LEU:HG	29:A:742:HOH:O	2.11	0.51
1:A:311:ILE:HD12	24:T:102:CDL:H201	1.91	0.51
19:N:610:TGL:HG11	12:Y:12:PRO:HG2	1.93	0.51
26:O:303:PSC:H212	26:O:303:PSC:C01	2.41	0.51
26:O:303:PSC:H21	26:O:303:PSC:H222	1.91	0.51
8:H:9:LYS:O	8:H:10:ASN:CB	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ILE:CD1	26:E:201:PSC:H342	2.26	0.50
19:D:201:TGL:CG3	19:D:201:TGL:OB1	2.59	0.50
12:L:14:SER:H	19:L:101:TGL:HC31	1.75	0.50
8:U:51:SER:HB2	29:U:122:HOH:O	2.10	0.50
19:N:610:TGL:HC31	12:Y:13:PHE:HA	1.93	0.50
7:G:3:ALA:O	7:G:4:ALA:CB	2.59	0.50
26:E:201:PSC:H212	26:E:201:PSC:O01	2.12	0.50
25:G:102:PEK:H71	25:G:102:PEK:H32	1.94	0.50
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.93	0.50
22:C:305:CHD:H152	20:C:307:PGV:H11	1.93	0.50
7:G:3:ALA:CB	25:G:104:PEK:H382	2.40	0.50
1:N:20:LEU:HB3	19:N:610:TGL:H221	1.92	0.50
2:B:56:MET:HA	26:E:201:PSC:H202	1.94	0.50
12:L:20:ARG:HH22	19:L:101:TGL:CC3	2.01	0.50
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.94	0.50
2:O:41:ILE:CD1	26:O:303:PSC:H342	2.41	0.49
3:C:33[A]:MET:HG2	3:C:39:SER:HB3	1.94	0.49
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.57	0.49
3:C:224:LYS:CD	24:C:303:CDL:HB31	2.42	0.49
3:P:50:ASN:HD22	3:P:51[A]:MET:HE2	1.76	0.49
6:S:48:LEU:HG	6:S:92:VAL:HG11	1.94	0.49
1:A:169:ILE:HD12	7:T:7:ASP:O	2.12	0.49
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.49
7:G:5:LYS:CB	25:G:104:PEK:H362	2.43	0.49
1:A:328:HIS:HB2	2:B:45:MET:SD	2.53	0.49
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.48	0.49
3:C:217:VAL:HG22	24:C:303:CDL:H732	1.95	0.49
3:C:254:VAL:HG23	24:G:103:CDL:H672	1.94	0.49
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.43	0.49
1:A:177:SER:H	1:A:180:GLN:HE21	1.61	0.49
8:H:7:LYS:O	8:H:8:ILE:CB	2.61	0.49
9:I:73:LYS:HB3	29:I:121:HOH:O	2.13	0.48
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.13	0.48
3:C:55:TYR:CE1	24:C:303:CDL:H532	2.48	0.48
5:E:5:HIS:HB3	5:E:6:GLU:HG2	1.95	0.48
6:F:50:PRO:HG2	29:F:244:HOH:O	2.13	0.48
8:H:45:ALA:C	8:H:47:GLY:H	2.19	0.48
9:I:0:ACE:O	9:I:2:THR:CG2	2.59	0.48
6:S:19:GLU:CG	29:S:232:HOH:O	2.49	0.48
28:G:101:DMU:H36	28:G:101:DMU:C57	2.30	0.48
19:N:609:TGL:H302	19:N:609:TGL:C12	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:610:TGL:HA22	12:Y:13:PHE:HB3	1.96	0.48
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.96	0.48
7:G:2:SER:O	25:G:104:PEK:H321	2.13	0.48
3:P:51[B]:MET:HE1	24:P:306:CDL:H273	1.94	0.48
2:B:66:THR:HG21	22:B:302:CHD:H3	1.94	0.48
25:G:104:PEK:H051	3:P:77:LYS:HZ1	1.78	0.48
3:P:224:LYS:HD2	24:P:306:CDL:HB31	1.95	0.48
29:A:855:HOH:O	3:C:77:LYS:HE3	2.12	0.48
20:N:607:PGV:H22	20:N:607:PGV:H221	1.95	0.48
7:T:1:ALA:N	29:T:222:HOH:O	2.47	0.48
3:P:52:LEU:HD21	24:P:306:CDL:H411	1.96	0.47
6:S:94:HIS:CD2	6:S:95:GLN:N	2.82	0.47
12:L:20:ARG:HH21	19:L:101:TGL:HC32	1.69	0.47
6:S:94:HIS:HD2	6:S:95:GLN:H	1.60	0.47
1:A:383:MET:O	1:A:387:PHE:HB2	2.14	0.47
19:A:607:TGL:H101	19:A:607:TGL:H281	1.96	0.47
24:T:102:CDL:H592	24:T:102:CDL:H561	1.63	0.47
1:N:106:PRO:N	1:N:107:PRO:HD2	2.30	0.47
1:N:114:ALA:HA	1:N:117[B]:MET:HE3	1.95	0.47
6:S:52:ILE:O	6:S:94:HIS:CE1	2.67	0.47
4:Q:109:HIS:CD2	29:Q:338:HOH:O	2.56	0.47
26:O:303:PSC:H343	26:O:303:PSC:C14	2.44	0.47
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.96	0.47
19:N:609:TGL:H101	19:N:609:TGL:C28	2.44	0.47
7:T:8:HIS:CE1	25:T:101:PEK:H332	2.49	0.47
3:P:151:LEU:HB2	3:P:159:MET:HG3	1.97	0.46
4:Q:130:PRO:HA	4:Q:135:SER:HB2	1.96	0.46
13:M:39:ASN:O	13:M:43:SER:HB2	2.15	0.46
29:O:456:HOH:O	4:Q:129:ALA:HB2	2.15	0.46
10:J:52:TRP:O	10:J:57:HIS:HE1	1.98	0.46
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.98	0.46
24:T:102:CDL:H631	24:T:102:CDL:H662	1.69	0.46
26:E:201:PSC:H62	26:E:201:PSC:H241	1.98	0.46
3:P:164:PHE:CE1	22:P:307:CHD:H192	2.50	0.46
1:A:177:SER:H	1:A:180:GLN:NE2	2.14	0.46
3:C:248:VAL:HG22	25:T:101:PEK:H15	1.98	0.46
3:P:63:ARG:HE	24:P:306:CDL:HA21	1.80	0.46
6:S:43:LYS:HD2	6:S:88:HIS:CE1	2.51	0.46
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.51	0.45
7:T:84:LYS:HZ3	7:T:84:LYS:H	1.64	0.45
6:S:75:HIS:H	6:S:80:GLN:NE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.99	0.45
1:A:87:ILE:O	1:A:173:PRO:HD3	2.16	0.45
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.52	0.45
3:P:37:PHE:CD1	10:W:52:TRP:HZ3	2.34	0.45
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.98	0.45
3:P:22:LEU:O	3:P:26:LEU:HG	2.16	0.45
1:A:283:LEU:HB2	1:A:312[B]:ILE:HD12	1.99	0.45
1:A:344:PHE:CD1	1:A:344:PHE:C	2.95	0.45
24:G:103:CDL:H332	2:O:78:LEU:HD12	1.99	0.45
1:A:113:LEU:HB3	1:A:117[B]:MET:CE	2.46	0.45
1:A:178:GLN:CB	7:T:7:ASP:OD2	2.65	0.45
6:F:92:VAL:HG23	6:F:92:VAL:O	2.16	0.45
8:H:60:TYR:CD1	8:H:60:TYR:C	2.95	0.45
19:L:101:TGL:HC22	19:L:101:TGL:CC6	2.23	0.45
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.99	0.45
4:Q:93:ALA:HB3	11:X:28:VAL:HG22	1.98	0.45
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.45
15:N:602:HEA:H172	15:N:602:HEA:H272	1.31	0.45
24:G:103:CDL:H561	24:G:103:CDL:H592	1.69	0.44
1:N:344:PHE:CD1	1:N:344:PHE:C	2.95	0.44
24:G:103:CDL:H452	2:O:70:ALA:HB1	1.99	0.44
5:R:106:LEU:HD23	5:R:106:LEU:HA	1.79	0.44
1:N:240:HIS:O	1:N:243:VAL:HG22	2.18	0.44
1:N:488:THR:HB	1:N:495:LEU:HD13	1.98	0.44
3:P:51[B]:MET:HB3	24:P:306:CDL:H381	2.00	0.44
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.98	0.44
15:N:602:HEA:HBC1	15:N:602:HEA:HMC3	2.00	0.44
25:P:304:PEK:H32	25:P:304:PEK:C7	2.31	0.44
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.98	0.44
2:B:41:ILE:O	2:B:45:MET:HG2	2.17	0.44
1:N:127:THR:HG22	1:N:235:PHE:CE2	2.53	0.44
2:O:84:LEU:HA	2:O:87:MET:HE2	2.00	0.44
22:P:307:CHD:H112	22:P:307:CHD:H12A	1.84	0.44
24:T:102:CDL:H122	24:T:102:CDL:H362	2.00	0.44
1:N:409:TRP:CE2	20:N:607:PGV:H61	2.53	0.44
20:N:607:PGV:H011	20:N:607:PGV:H221	1.99	0.44
26:O:303:PSC:O02	26:O:303:PSC:H031	2.17	0.44
7:T:3:ALA:HB1	25:T:101:PEK:H382	2.00	0.44
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.83	0.44
1:N:437:PRO:HG2	1:N:440:TYR:CE1	2.53	0.44
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:29:LEU:HD12	9:V:29:LEU:HA	1.81	0.43
1:A:116:SER:HB3	29:A:746:HOH:O	2.17	0.43
19:D:201:TGL:H132	19:D:201:TGL:H302	1.72	0.43
7:G:5:LYS:HB3	1:N:278:MET:SD	2.58	0.43
24:P:306:CDL:HB21	24:P:306:CDL:OB6	2.18	0.43
4:Q:143:ASN:ND2	29:Q:309:HOH:O	2.50	0.43
24:T:102:CDL:H541	24:T:102:CDL:C23	2.43	0.43
7:G:25:LEU:HD23	7:G:25:LEU:HA	1.91	0.43
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.00	0.43
1:N:35:LEU:HD11	1:N:462:LEU:HB2	2.00	0.43
19:N:609:TGL:H111	2:O:35:SER:CB	2.48	0.43
2:B:82:ARG:HH11	2:B:86:MET:HE1	1.84	0.43
3:C:50:ASN:HD22	3:C:51[A]:MET:HE2	1.83	0.43
7:G:4:ALA:CB	1:N:282:PHE:HA	2.45	0.43
1:N:310:MET:HE1	2:O:76:ILE:CG2	2.47	0.43
24:T:102:CDL:H111	24:T:102:CDL:CA2	2.43	0.43
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.99	0.43
15:A:603:HEA:H243	2:B:69:PRO:HB3	2.00	0.43
22:C:304:CHD:H12A	22:C:304:CHD:H112	1.77	0.43
24:G:103:CDL:H351	2:O:81:LEU:HD12	2.01	0.43
22:B:302:CHD:H212	22:B:302:CHD:H12	2.00	0.43
1:N:393:PHE:CD1	15:N:602:HEA:H241	2.53	0.43
7:T:3:ALA:HB1	25:T:101:PEK:C38	2.49	0.43
1:A:113:LEU:HB3	1:A:117[B]:MET:HE3	2.01	0.43
1:A:240:HIS:CD2	1:A:240:HIS:C	2.97	0.43
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.00	0.43
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.18	0.43
3:C:116:TRP:HA	3:C:117:PRO:C	2.42	0.43
19:N:609:TGL:H122	19:N:609:TGL:C30	2.43	0.43
2:O:33:LEU:HD13	9:V:31:PHE:CD1	2.54	0.43
2:B:81:LEU:HD13	24:T:102:CDL:H121	2.00	0.43
5:E:48:ILE:HG21	5:E:89:LEU:HD11	2.00	0.43
24:G:103:CDL:H662	24:G:103:CDL:H631	1.78	0.43
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.18	0.43
11:X:24:PHE:O	11:X:28:VAL:HG12	2.19	0.43
3:C:122:HIS:HA	3:C:123:PRO:HD3	1.88	0.43
4:D:107:ILE:HB	4:D:108:PRO:CD	2.48	0.43
2:O:225:SER:C	2:O:227:LEU:N	2.73	0.43
3:P:217:VAL:HG22	24:P:306:CDL:H732	2.01	0.43
5:R:108:LYS:HB2	5:R:108:LYS:NZ	2.34	0.43
1:A:430:PHE:CE1	19:A:607:TGL:HB21	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:LEU:HD21	22:C:304:CHD:H183	2.02	0.42
19:L:101:TGL:H231	19:L:101:TGL:HA91	1.99	0.42
4:Q:139:ASP:OD2	4:Q:142:LYS:HG3	2.19	0.42
9:V:63:MET:HB3	9:V:68:ILE:HG12	2.00	0.42
1:N:113:LEU:HD13	19:N:610:TGL:H292	2.01	0.42
3:P:69:GLY:HA3	6:S:14:THR:O	2.19	0.42
24:G:103:CDL:H182	24:G:103:CDL:H152	1.69	0.42
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.42
3:P:230:ASN:HB2	29:P:459:HOH:O	2.19	0.42
7:T:3:ALA:CB	25:T:101:PEK:H382	2.50	0.42
25:T:101:PEK:H282	25:T:101:PEK:H312	1.73	0.42
3:C:37:PHE:CD1	10:J:52:TRP:HZ3	2.36	0.42
3:C:76:GLN:NE2	3:C:80:ARG:HH21	2.17	0.42
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.66	0.42
3:P:226:HIS:CE1	24:P:306:CDL:HB32	2.55	0.42
7:T:2:SER:HG	25:T:101:PEK:H301	1.81	0.42
7:T:38:HIS:ND1	7:T:38:HIS:N	2.68	0.42
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.01	0.42
1:A:390:MET:HE2	1:A:413:HIS:CE1	2.53	0.42
2:B:69:PRO:HG2	29:B:474:HOH:O	2.19	0.42
9:V:6:LYS:HA	9:V:7:PRO:HD3	1.87	0.42
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.55	0.42
2:O:116:LEU:HD12	2:O:117:SER:N	2.34	0.42
1:A:297:MET:CE	1:A:297:MET:CB	2.97	0.42
2:B:78:LEU:CD1	24:T:102:CDL:H352	2.47	0.42
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.42
6:F:54:ASN:H	6:F:54:ASN:ND2	2.07	0.42
7:G:3:ALA:HB3	25:G:104:PEK:H361	2.01	0.42
19:L:101:TGL:CA9	19:L:101:TGL:C23	2.97	0.42
1:N:408:THR:HB	20:N:607:PGV:H51	2.01	0.42
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.85	0.42
12:L:45:LEU:HD23	12:L:45:LEU:HA	1.83	0.42
3:P:76:GLN:NE2	29:P:414:HOH:O	2.47	0.42
28:P:301:DMU:H30	7:T:62:TRP:CB	2.48	0.42
2:B:29:MET:SD	9:I:36:LYS:HE3	2.60	0.42
4:D:93:ALA:HB3	11:K:28:VAL:HG22	2.00	0.42
8:U:60:TYR:CD1	8:U:60:TYR:C	2.98	0.42
1:N:215:LEU:HD11	25:P:304:PEK:H271	2.02	0.41
28:P:301:DMU:C57	7:T:62:TRP:HB3	2.50	0.41
6:S:95:GLN:HG3	6:S:96:LEU:H	1.85	0.41
9:V:18:ARG:HH11	9:V:18:ARG:CG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.01	0.41
3:C:224:LYS:HD2	24:C:303:CDL:HB31	2.01	0.41
25:G:104:PEK:H341	29:G:227:HOH:O	2.18	0.41
8:H:8:ILE:HG23	8:H:8:ILE:O	2.20	0.41
19:N:609:TGL:C28	19:N:609:TGL:C10	2.98	0.41
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.01	0.41
22:O:302:CHD:H12	22:O:302:CHD:H212	2.02	0.41
1:A:412:ILE:HG12	4:D:84:ALA:HB3	2.01	0.41
7:G:1:ALA:N	20:P:302:PGV:H321	2.35	0.41
1:N:43:GLN:OE1	4:Q:104:TYR:HB3	2.20	0.41
10:J:4:ARG:HD3	10:J:7:GLU:OE2	2.20	0.41
5:R:5:HIS:CD2	5:R:6:GLU:HG2	2.55	0.41
1:A:334:TRP:CB	19:D:201:TGL:HG11	2.50	0.41
3:C:3:HIS:N	29:C:475:HOH:O	2.52	0.41
3:C:186:PHE:HA	3:C:190:ASP:OD2	2.19	0.41
7:G:84:LYS:H	7:G:84:LYS:HD2	1.86	0.41
19:N:610:TGL:H272	12:Y:11:ILE:CG2	2.50	0.41
2:O:62:GLU:O	2:O:66:THR:HB	2.21	0.41
2:O:74:ILE:HG22	2:O:78:LEU:HD22	2.02	0.41
4:Q:145:TRP:CG	11:X:46:GLY:H	2.38	0.41
19:Q:201:TGL:OB1	29:Q:308:HOH:O	2.22	0.41
1:N:342:LEU:HD13	2:O:46:LEU:HD11	2.03	0.41
2:O:29:MET:HG3	9:V:35:TYR:CG	2.56	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.41
24:C:303:CDL:H222	24:C:303:CDL:H641	2.02	0.41
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.51	0.41
7:G:5:LYS:HG3	25:G:104:PEK:C38	2.28	0.41
1:N:35:LEU:HD11	1:N:462:LEU:HD13	2.02	0.41
2:O:200:CYS:SG	2:O:204:HIS:HA	2.61	0.41
1:A:169:ILE:CD1	7:T:7:ASP:O	2.69	0.41
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.41
7:T:11:TPO:HA	7:T:11:TPO:O2P	2.21	0.41
8:U:9:LYS:CG	29:U:123:HOH:O	2.66	0.41
1:A:115:SER:HB2	1:A:142:SER:O	2.20	0.41
1:A:489:THR:HA	6:F:71:TRP:O	2.21	0.41
29:B:490:HOH:O	4:D:129:ALA:HB2	2.21	0.41
12:L:44:LEU:HD23	12:L:44:LEU:HA	1.87	0.41
1:N:104:LEU:HB2	1:N:156:SER:HB2	2.03	0.41
3:P:223:LEU:HD21	22:P:307:CHD:H183	2.03	0.41
4:Q:83:GLY:HA3	11:X:17:VAL:HG12	2.03	0.41
7:T:6:GLY:O	25:T:101:PEK:H311	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:GLN:HA	2:B:104:TRP:HA	1.88	0.41
22:P:308:CHD:H12	22:P:308:CHD:H212	2.03	0.41
7:G:37:LEU:HD23	7:G:38:HIS:ND1	2.37	0.40
2:O:82:ARG:CG	2:O:86:MET:HE3	2.47	0.40
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.49	0.40
4:Q:81:VAL:HG11	19:Q:201:TGL:HB51	2.03	0.40
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.51	0.40
1:A:350:VAL:HG13	19:A:607:TGL:HB81	2.04	0.40
5:E:86:ILE:O	5:E:90:ARG:HG2	2.22	0.40
1:N:46:THR:HG23	1:N:49:GLY:O	2.21	0.40
20:N:607:PGV:H92	4:Q:84:ALA:HB2	2.02	0.40
3:P:193:TYR:CD2	3:P:193:TYR:C	2.99	0.40
5:R:79:LYS:N	5:R:79:LYS:HD2	2.35	0.40
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.21	0.40
1:A:468:MET:HE2	1:A:468:MET:HB3	2.03	0.40
1:N:117[A]:MET:HE2	1:N:117[A]:MET:HA	2.02	0.40
4:Q:33:LEU:HB2	4:Q:38:LYS:HE2	2.02	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	515/514 (100%)	502 (98%)	12 (2%)	1 (0%)	43	42
1	N	515/514 (100%)	501 (97%)	14 (3%)	0	100	100
2	B	225/227 (99%)	216 (96%)	9 (4%)	0	100	100
2	O	225/227 (99%)	218 (97%)	6 (3%)	1 (0%)	30	27
3	C	260/261 (100%)	256 (98%)	4 (2%)	0	100	100
3	P	260/261 (100%)	255 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	142/147 (97%)	132 (93%)	10 (7%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	5	2
6	S	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	3	1
7	G	81/85 (95%)	70 (86%)	6 (7%)	5 (6%)	1	0
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	1	0
8	H	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	1	0
8	U	77/85 (91%)	71 (92%)	2 (3%)	4 (5%)	1	0
9	I	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
9	V	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	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%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3518/3616 (97%)	3388 (96%)	105 (3%)	25 (1%)	18	14

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP
8	H	8	ILE
8	H	45	ALA
8	H	46	LYS
6	S	94	HIS
6	S	96	LEU
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS

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Mol	Chain	Res	Type
8	U	8	ILE
6	F	95	GLN
7	G	37	LEU
7	T	43	GLU
8	U	45	ALA
8	H	47	GLY
6	S	95	GLN
8	U	11	TYR
7	G	8	HIS
7	T	6	GLY
7	G	6	GLY
8	U	10	ASN
1	A	384	GLY
2	O	92	ASN

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	429/426 (101%)	420 (98%)	9 (2%)	47	52
1	N	429/426 (101%)	418 (97%)	11 (3%)	40	44
2	B	210/210 (100%)	198 (94%)	12 (6%)	18	15
2	O	210/210 (100%)	199 (95%)	11 (5%)	21	18
3	C	227/226 (100%)	223 (98%)	4 (2%)	51	58
3	P	227/226 (100%)	221 (97%)	6 (3%)	40	44
4	D	128/129 (99%)	122 (95%)	6 (5%)	23	22
4	Q	128/129 (99%)	122 (95%)	6 (5%)	23	22
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	50
5	R	92/95 (97%)	86 (94%)	6 (6%)	15	12
6	F	81/81 (100%)	77 (95%)	4 (5%)	22	20
6	S	81/81 (100%)	77 (95%)	4 (5%)	22	20
7	G	67/68 (98%)	65 (97%)	2 (3%)	36	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	14
8	H	71/75 (95%)	69 (97%)	2 (3%)	38	41
8	U	71/75 (95%)	64 (90%)	7 (10%)	7	4
9	I	58/58 (100%)	54 (93%)	4 (7%)	14	11
9	V	58/58 (100%)	52 (90%)	6 (10%)	7	4
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	54
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	54
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	44
11	X	39/46 (85%)	38 (97%)	1 (3%)	40	44
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	44
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	8
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	3
All	All	3054/3084 (99%)	2931 (96%)	123 (4%)	28	27

All (123) 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	180	GLN
1	A	297	MET
1	A	333	LYS
1	A	362	SER
1	A	369	ASP
1	A	504	THR
2	B	15	PRO
2	B	33	LEU
2	B	54	SER
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN

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Mol	Chain	Res	Type
2	B	115	ASP
2	B	166	PRO
3	C	40	MET
3	C	104	SER
3	C	127	LEU
3	C	159	MET
4	D	4	SER
4	D	8	SER
4	D	31	LYS
4	D	51	LEU
4	D	58	GLU
4	D	127	LYS
5	E	5	HIS
5	E	90	ARG
6	F	54	ASN
6	F	80	GLN
6	F	87	THR
6	F	96	LEU
7	G	43	GLU
7	G	84	LYS
8	H	8	ILE
8	H	61	LYS
9	I	1	SER
9	I	2	THR
9	I	36	LYS
9	I	37	PHE
10	J	50	LEU
11	K	54	ARG
12	L	26	THR
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
1	N	96	ARG
1	N	117[A]	MET
1	N	117[B]	MET
1	N	128	VAL
1	N	241	PRO
1	N	278	MET
1	N	297	MET
1	N	363	LEU

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Mol	Chain	Res	Type
1	N	369	ASP
1	N	485	VAL
1	N	504	THR
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	116	LEU
2	O	209	ILE
2	O	221	LYS
3	P	17	PRO
3	P	110	PRO
3	P	159	MET
3	P	180	GLU
3	P	230	ASN
3	P	245	VAL
4	Q	5	VAL
4	Q	6	VAL
4	Q	9	GLU
4	Q	10	ASP
4	Q	51	LEU
4	Q	142	LYS
5	R	45	PRO
5	R	79	LYS
5	R	80	GLU
5	R	90	ARG
5	R	108	LYS
5	R	109	VAL
6	S	43	LYS
6	S	48	LEU
6	S	54	ASN
6	S	80	GLN
7	T	2	SER
7	T	33	LEU
7	T	37	LEU
7	T	84	LYS
8	U	8	ILE
8	U	27	ARG

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Mol	Chain	Res	Type
8	U	29	CYS
8	U	40	GLU
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	1	SER
9	V	2	THR
9	V	8	GLN
9	V	29	LEU
9	V	65	LYS
9	V	73	LYS
10	W	50	LEU
11	X	23	THR
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	39	ASN
13	Z	42	LYS

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

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	503	HIS
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
3	C	161	GLN
3	C	222	GLN
4	D	29	HIS
4	D	37	GLN
4	D	76	ASN
4	D	101	HIS
4	D	109	HIS
4	D	119	GLN
4	D	143	ASN
5	E	94	ASN

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Mol	Chain	Res	Type
6	F	54	ASN
6	F	80	GLN
7	G	38	HIS
7	G	76	ASN
8	H	28	ASN
8	H	31	GLN
8	H	32	ASN
10	J	21	HIS
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	413	HIS
1	N	422	ASN
1	N	503	HIS
2	O	24	HIS
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	76	GLN
4	Q	37	GLN
4	Q	143	ASN
5	R	5	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	76	ASN
8	U	28	ASN
8	U	31	GLN
8	U	32	ASN
9	V	20	HIS
10	W	57	HIS
11	X	35	GLN
12	Y	42	HIS

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$
2	FME	O	1	2	8,9,10	0.88	0	8,9,11	4.35	5 (62%)
7	TPO	G	11	7	8,10,11	1.77	2 (25%)	10,14,16	1.52	2 (20%)
1	FME	N	1	1	8,9,10	1.44	1 (12%)	8,9,11	6.15	3 (37%)
2	FME	B	1	2	8,9,10	2.01	1 (12%)	8,9,11	7.80	4 (50%)
1	FME	A	1	1	8,9,10	1.07	0	8,9,11	5.58	3 (37%)
7	TPO	T	11	7	8,10,11	2.14	2 (25%)	10,14,16	1.75	1 (10%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CA-N	4.46	1.53	1.46
7	T	11	TPO	P-O1P	3.45	1.61	1.50
1	N	1	FME	CA-N	3.30	1.51	1.46
7	G	11	TPO	P-O1P	3.21	1.60	1.50
7	T	11	TPO	P-OG1	2.97	1.64	1.59
7	G	11	TPO	O-C	2.11	1.28	1.20

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.20	91.75	122.82
1	N	1	FME	CA-N-CN	-16.07	98.11	122.82
1	A	1	FME	CA-N-CN	-15.24	99.38	122.82
2	O	1	FME	CA-N-CN	-10.62	106.50	122.82
2	B	1	FME	O1-CN-N	6.69	142.60	125.32
2	B	1	FME	CG-CB-CA	-4.81	98.15	112.87
1	N	1	FME	CB-CA-N	4.53	118.78	110.52
7	T	11	TPO	CG2-CB-CA	4.40	121.83	113.26
1	N	1	FME	O1-CN-N	4.03	135.74	125.32
2	O	1	FME	C-CA-N	3.42	116.09	109.50
7	G	11	TPO	CG2-CB-CA	3.31	119.70	113.26
2	O	1	FME	CG-CB-CA	-2.74	104.50	112.87
2	O	1	FME	CB-CA-N	-2.64	105.70	110.52
2	O	1	FME	O1-CN-N	-2.64	118.51	125.32
2	B	1	FME	O-C-CA	-2.57	118.17	124.77
1	A	1	FME	CE-SD-CG	2.54	113.47	100.32
7	G	11	TPO	O2P-P-OG1	2.40	115.21	105.85
1	A	1	FME	CG-CB-CA	-2.04	106.64	112.87

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
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
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
7	T	11	TPO	CA-CB-OG1-P
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
1	N	1	FME	CB-CG-SD-CE
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	1	0
1	A	1	FME	2	0
7	T	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	PGV	P	305	-	50,50,50	0.90	2 (4%)	53,56,56	1.14	5 (9%)
26	PSC	O	303	-	51,51,51	1.21	3 (5%)	57,59,59	1.34	5 (8%)
15	HEA	N	603	1	67,67,67	1.96	21 (31%)	81,103,103	1.81	23 (28%)
14	CYN	A	601	16	1,1,1	0.22	0	-		
22	CHD	C	305	-	32,32,32	1.24	4 (12%)	51,51,51	1.74	12 (23%)
20	PGV	P	302	-	50,50,50	1.15	2 (4%)	53,56,56	1.25	3 (5%)
28	DMU	G	101	-	34,34,34	0.86	2 (5%)	45,45,45	2.45	13 (28%)
22	CHD	C	304	-	32,32,32	0.77	1 (3%)	51,51,51	2.63	23 (45%)
25	PEK	P	309	-	52,52,52	1.21	2 (3%)	55,57,57	1.20	4 (7%)
15	HEA	N	602	1	67,67,67	2.04	23 (34%)	81,103,103	2.72	37 (45%)
25	PEK	C	306	-	52,52,52	1.15	2 (3%)	55,57,57	1.20	5 (9%)
24	CDL	P	306	-	99,99,99	1.49	12 (12%)	105,111,111	1.40	11 (10%)
19	TGL	L	101	-	62,62,62	1.58	7 (11%)	65,65,65	1.68	14 (21%)
14	CYN	N	601	16	1,1,1	0.23	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CDL	G	103	-	99,99,99	1.50	12 (12%)	105,111,111	1.42	17 (16%)
24	CDL	C	303	-	99,99,99	1.49	13 (13%)	105,111,111	1.44	12 (11%)
19	TGL	N	610	-	62,62,62	1.58	6 (9%)	65,65,65	1.68	15 (23%)
25	PEK	P	304	-	52,52,52	0.86	3 (5%)	55,57,57	1.67	9 (16%)
28	DMU	Z	101	-	34,34,34	0.65	0	45,45,45	1.89	10 (22%)
20	PGV	N	608	-	50,50,50	1.05	3 (6%)	53,56,56	1.30	4 (7%)
24	CDL	T	102	-	99,99,99	1.45	12 (12%)	105,111,111	1.38	12 (11%)
28	DMU	M	101	-	34,34,34	0.60	0	45,45,45	1.94	12 (26%)
22	CHD	O	302	-	32,32,32	1.10	3 (9%)	51,51,51	1.69	10 (19%)
25	PEK	G	104	-	52,52,52	1.13	2 (3%)	55,57,57	1.18	6 (10%)
20	PGV	N	607	-	50,50,50	1.03	2 (4%)	53,56,56	1.57	7 (13%)
20	PGV	A	609	-	50,50,50	1.24	2 (4%)	53,56,56	1.47	9 (16%)
22	CHD	P	308	-	32,32,32	1.18	3 (9%)	51,51,51	1.85	17 (33%)
25	PEK	T	101	-	52,52,52	1.22	2 (3%)	55,57,57	1.27	6 (10%)
28	DMU	P	301	-	34,34,34	0.95	1 (2%)	45,45,45	2.39	12 (26%)
26	PSC	E	201	-	51,51,51	1.31	3 (5%)	57,59,59	1.25	4 (7%)
20	PGV	A	608	-	50,50,50	0.97	2 (4%)	53,56,56	1.46	5 (9%)
21	CUA	B	301	2	0,1,1	-	-	-	-	-
19	TGL	A	607	-	62,62,62	1.42	7 (11%)	65,65,65	2.29	16 (24%)
19	TGL	Q	201	-	62,62,62	1.37	6 (9%)	65,65,65	1.48	9 (13%)
22	CHD	B	302	-	32,32,32	1.11	3 (9%)	51,51,51	1.71	11 (21%)
20	PGV	C	302	-	50,50,50	0.93	3 (6%)	53,56,56	1.10	4 (7%)
15	HEA	A	603	1	67,67,67	1.86	19 (28%)	81,103,103	2.24	29 (35%)
25	PEK	G	102	-	52,52,52	0.98	3 (5%)	55,57,57	1.54	8 (14%)
15	HEA	A	602	1	67,67,67	2.14	22 (32%)	81,103,103	2.47	30 (37%)
20	PGV	C	307	-	50,50,50	1.44	4 (8%)	53,56,56	1.45	8 (15%)
19	TGL	D	201	-	62,62,62	1.49	7 (11%)	65,65,65	1.48	14 (21%)
21	CUA	O	301	2	0,1,1	-	-	-	-	-
22	CHD	P	307	-	32,32,32	0.81	1 (3%)	51,51,51	2.97	22 (43%)
19	TGL	N	609	-	62,62,62	1.35	6 (9%)	65,65,65	1.47	10 (15%)

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
20	PGV	P	305	-	-	16/55/55/55	-
26	PSC	O	303	-	-	35/55/55/55	-
15	HEA	N	603	1	-	6/36/76/76	-
22	CHD	C	305	-	-	1/9/74/74	0/4/4/4
20	PGV	P	302	-	-	33/55/55/55	-
28	DMU	G	101	-	-	12/19/59/59	0/2/2/2
22	CHD	C	304	-	-	5/9/74/74	0/4/4/4
15	HEA	N	602	1	-	9/36/76/76	-
25	PEK	C	306	-	-	31/56/56/56	-
24	CDL	P	306	-	-	72/110/110/110	-
19	TGL	L	101	-	-	36/65/65/65	-
24	CDL	G	103	-	-	56/110/110/110	-
24	CDL	C	303	-	-	67/110/110/110	-
19	TGL	N	610	-	-	36/65/65/65	-
25	PEK	P	304	-	-	26/56/56/56	-
28	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
20	PGV	N	608	-	-	13/55/55/55	-
24	CDL	T	102	-	-	54/110/110/110	-
28	DMU	M	101	-	-	7/19/59/59	0/2/2/2
22	CHD	O	302	-	-	2/9/74/74	0/4/4/4
25	PEK	G	104	-	-	32/56/56/56	-
20	PGV	N	607	-	-	29/55/55/55	-
20	PGV	A	609	-	-	32/55/55/55	-
22	CHD	P	308	-	-	1/9/74/74	0/4/4/4
25	PEK	T	101	-	-	36/56/56/56	-
28	DMU	P	301	-	-	7/19/59/59	0/2/2/2
26	PSC	E	201	-	-	36/55/55/55	-
20	PGV	A	608	-	-	10/55/55/55	-
19	TGL	A	607	-	-	36/65/65/65	-
19	TGL	Q	201	-	-	36/65/65/65	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
20	PGV	C	302	-	-	16/55/55/55	-
15	HEA	A	603	1	-	7/36/76/76	-
25	PEK	G	102	-	-	23/56/56/56	-
15	HEA	A	602	1	-	5/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	C	307	-	-	30/55/55/55	-
19	TGL	D	201	-	-	39/65/65/65	-
25	PEK	P	309	-	-	22/56/56/56	-
22	CHD	P	307	-	-	8/9/74/74	0/4/4/4
19	TGL	N	609	-	-	33/65/65/65	-

All (231) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	610	TGL	OG2-CB1	6.08	1.51	1.34
20	C	307	PGV	O01-C1	6.07	1.51	1.34
15	A	602	HEA	C3A-C4A	-6.02	1.35	1.46
19	L	101	TGL	OG2-CB1	5.98	1.51	1.34
15	A	602	HEA	CHA-C1A	5.93	1.50	1.38
20	C	307	PGV	O03-C19	5.86	1.50	1.33
15	N	602	HEA	CHA-C1A	5.52	1.49	1.38
24	P	306	CDL	OA8-CA7	5.44	1.49	1.33
19	N	610	TGL	OG3-CC1	5.43	1.49	1.33
19	A	607	TGL	OG1-CA1	5.33	1.48	1.33
19	L	101	TGL	OG3-CC1	5.27	1.48	1.33
15	N	603	HEA	FE-NB	5.22	2.11	1.94
19	D	201	TGL	OG1-CA1	5.21	1.48	1.33
25	C	306	PEK	O01-C1	5.21	1.49	1.34
24	C	303	CDL	OA8-CA7	5.21	1.48	1.33
25	P	309	PEK	O01-C1	5.20	1.49	1.34
25	T	101	PEK	O03-C21	5.19	1.48	1.33
24	G	103	CDL	OB6-CB5	5.19	1.48	1.34
20	P	302	PGV	O01-C1	5.14	1.48	1.34
24	G	103	CDL	OB8-CB7	5.13	1.48	1.33
19	L	101	TGL	OG1-CA1	5.12	1.48	1.33
19	N	610	TGL	OG1-CA1	5.11	1.48	1.33
19	N	609	TGL	OG2-CB1	5.10	1.48	1.34
19	D	201	TGL	OG3-CC1	5.07	1.48	1.33
24	T	102	CDL	OA6-CA5	5.05	1.48	1.34
25	T	101	PEK	O01-C1	5.04	1.48	1.34
26	E	201	PSC	O03-C19	5.04	1.48	1.33
20	A	609	PGV	O03-C19	5.03	1.48	1.33
25	G	104	PEK	O03-C21	4.98	1.47	1.33
24	G	103	CDL	OA6-CA5	4.98	1.48	1.34
26	E	201	PSC	O01-C1	4.96	1.48	1.34
25	P	309	PEK	O03-C21	4.95	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Q	201	TGL	OG2-CB1	4.94	1.48	1.34
20	A	609	PGV	O01-C1	4.93	1.48	1.34
24	T	102	CDL	OB8-CB7	4.86	1.47	1.33
25	C	306	PEK	O03-C21	4.82	1.47	1.33
19	A	607	TGL	OG2-CB1	4.77	1.47	1.34
24	C	303	CDL	OA6-CA5	4.74	1.47	1.34
24	T	102	CDL	OB6-CB5	4.73	1.47	1.34
15	N	602	HEA	FE-NB	4.72	2.09	1.94
15	N	602	HEA	C3A-C4A	-4.66	1.37	1.46
19	N	609	TGL	OG1-CA1	4.66	1.46	1.33
20	P	302	PGV	O03-C19	4.61	1.46	1.33
24	P	306	CDL	OB6-CB5	4.56	1.47	1.34
24	P	306	CDL	OA6-CA5	4.55	1.47	1.34
26	O	303	PSC	O01-C1	4.54	1.47	1.34
19	Q	201	TGL	OG1-CA1	4.54	1.46	1.33
25	G	104	PEK	O01-C1	4.52	1.47	1.34
15	N	603	HEA	CHD-C1D	4.47	1.47	1.38
15	A	602	HEA	C27-C19	4.45	1.61	1.50
20	N	608	PGV	O03-C19	4.43	1.46	1.33
24	C	303	CDL	OB8-CB7	4.42	1.46	1.33
24	P	306	CDL	OB8-CB7	4.40	1.46	1.33
20	A	608	PGV	O03-C19	4.39	1.46	1.33
19	Q	201	TGL	OG3-CC1	4.37	1.46	1.33
19	L	101	TGL	C20-CA9	-4.37	1.30	1.51
19	D	201	TGL	OG2-CB1	4.34	1.46	1.34
15	A	602	HEA	C1A-C2A	-4.33	1.37	1.45
15	A	603	HEA	FE-NB	4.33	2.08	1.94
24	G	103	CDL	OA8-CA7	4.29	1.45	1.33
15	A	603	HEA	FE-ND	4.26	2.08	1.94
26	O	303	PSC	O03-C19	4.24	1.45	1.33
28	P	301	DMU	O16-C6	4.19	1.47	1.40
15	A	603	HEA	CHD-C1D	4.13	1.46	1.38
20	N	607	PGV	O03-C19	4.02	1.45	1.33
26	E	201	PSC	C13-C12	4.02	1.54	1.31
20	N	607	PGV	O01-C1	4.01	1.45	1.34
24	C	303	CDL	OB6-CB5	4.01	1.45	1.34
26	O	303	PSC	C13-C12	3.98	1.54	1.31
19	N	610	TGL	C20-CA9	-3.96	1.32	1.51
24	C	303	CDL	C59-C58	-3.95	1.32	1.51
15	A	602	HEA	O11-C11	3.95	1.51	1.42
15	A	602	HEA	C1A-NA	-3.93	1.32	1.39
24	G	103	CDL	C59-C58	-3.90	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	609	TGL	C10-CB9	-3.86	1.32	1.51
24	P	306	CDL	C59-C58	-3.80	1.32	1.51
24	C	303	CDL	C79-C78	-3.79	1.32	1.51
15	A	602	HEA	CHC-C1C	3.78	1.47	1.39
19	N	610	TGL	C10-CB9	-3.77	1.33	1.51
15	N	603	HEA	C4B-NB	-3.75	1.33	1.40
15	N	603	HEA	C4C-NC	-3.75	1.32	1.39
20	P	305	PGV	O03-C19	3.75	1.44	1.33
24	T	102	CDL	C59-C58	-3.74	1.33	1.51
24	T	102	CDL	C42-C41	-3.72	1.33	1.51
24	T	102	CDL	C62-C61	-3.67	1.33	1.51
24	C	303	CDL	C62-C61	-3.66	1.33	1.51
24	P	306	CDL	C79-C78	-3.65	1.33	1.51
24	P	306	CDL	C82-C81	-3.64	1.33	1.51
15	A	603	HEA	CHB-C4A	3.62	1.45	1.38
25	G	102	PEK	O01-C1	3.62	1.44	1.34
19	A	607	TGL	C10-CB9	-3.62	1.33	1.51
24	G	103	CDL	C62-C61	-3.60	1.33	1.51
15	N	602	HEA	C1A-C2A	-3.59	1.38	1.45
24	P	306	CDL	C62-C61	-3.58	1.34	1.51
19	A	607	TGL	OG3-CC1	3.56	1.43	1.33
15	N	602	HEA	CHD-C1D	3.54	1.45	1.38
20	C	302	PGV	O03-C19	3.53	1.43	1.33
19	N	609	TGL	OG3-CC1	3.51	1.43	1.33
19	N	609	TGL	C20-CA9	-3.49	1.34	1.51
24	P	306	CDL	C19-C18	-3.47	1.34	1.51
15	A	602	HEA	CMC-C2C	3.46	1.57	1.50
19	A	607	TGL	C20-CA9	-3.46	1.34	1.51
24	C	303	CDL	C82-C81	-3.45	1.34	1.51
15	N	602	HEA	FE-NA	3.44	2.06	1.95
24	P	306	CDL	C22-C21	-3.43	1.34	1.51
19	Q	201	TGL	C20-CA9	-3.43	1.34	1.51
24	T	102	CDL	C19-C18	-3.42	1.34	1.51
24	C	303	CDL	C22-C21	-3.42	1.34	1.51
24	P	306	CDL	C39-C38	-3.40	1.34	1.51
24	C	303	CDL	C19-C18	-3.39	1.34	1.51
24	G	103	CDL	C42-C41	-3.37	1.35	1.51
25	P	304	PEK	O03-C01	-3.37	1.37	1.45
24	G	103	CDL	C19-C18	-3.37	1.35	1.51
19	D	201	TGL	C15-CC9	-3.36	1.35	1.51
15	A	602	HEA	CHD-C1D	3.35	1.45	1.38
24	T	102	CDL	C39-C38	-3.35	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	C10-CB9	-3.34	1.35	1.51
15	A	603	HEA	OMA-CMA	3.33	1.29	1.22
15	N	602	HEA	C4A-NA	-3.33	1.33	1.39
24	T	102	CDL	OA8-CA7	3.31	1.43	1.33
24	T	102	CDL	C79-C78	-3.30	1.35	1.51
24	T	102	CDL	C82-C81	-3.28	1.35	1.51
15	N	603	HEA	CHA-C1A	3.27	1.44	1.38
24	G	103	CDL	C22-C21	-3.27	1.35	1.51
15	N	602	HEA	FE-NC	3.26	2.05	1.95
24	C	303	CDL	C39-C38	-3.26	1.35	1.51
19	Q	201	TGL	C10-CB9	-3.25	1.35	1.51
28	G	101	DMU	O16-C6	3.22	1.45	1.40
24	C	303	CDL	C42-C41	-3.20	1.35	1.51
15	A	602	HEA	FE-NC	3.19	2.05	1.95
19	Q	201	TGL	C15-CC9	-3.18	1.35	1.51
20	A	608	PGV	O01-C1	3.18	1.43	1.34
24	G	103	CDL	C39-C38	-3.17	1.36	1.51
24	T	102	CDL	C22-C21	-3.17	1.36	1.51
19	D	201	TGL	C20-CA9	-3.16	1.36	1.51
15	A	603	HEA	CHC-C4B	3.15	1.44	1.38
15	N	602	HEA	C4C-NC	-3.15	1.33	1.39
19	N	609	TGL	C15-CC9	-3.13	1.36	1.51
24	G	103	CDL	C82-C81	-3.10	1.36	1.51
20	C	302	PGV	O01-C1	3.09	1.43	1.34
15	A	602	HEA	FE-NA	3.07	2.05	1.95
19	L	101	TGL	C15-CC9	-3.03	1.36	1.51
24	G	103	CDL	C79-C78	-3.02	1.36	1.51
15	N	603	HEA	FE-ND	3.02	2.04	1.94
19	D	201	TGL	C10-CB9	-3.01	1.36	1.51
24	P	306	CDL	C42-C41	-2.99	1.36	1.51
19	N	610	TGL	C15-CC9	-2.99	1.36	1.51
15	A	603	HEA	CHA-C1A	2.97	1.44	1.38
15	N	602	HEA	CHA-C4D	2.96	1.45	1.39
15	N	602	HEA	CHD-C4C	2.93	1.46	1.39
15	A	602	HEA	C1D-ND	-2.93	1.35	1.40
22	C	305	CHD	C8-C9	2.92	1.59	1.53
15	A	603	HEA	C4A-NA	-2.88	1.34	1.39
15	N	602	HEA	C1B-NB	-2.88	1.33	1.38
19	A	607	TGL	C15-CC9	-2.87	1.37	1.51
25	G	102	PEK	O03-C21	2.84	1.41	1.33
15	N	603	HEA	C1A-C2A	-2.84	1.40	1.45
15	N	602	HEA	CHC-C4B	2.81	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	602	HEA	C12-C13	2.80	1.62	1.53
15	A	602	HEA	C12-C13	2.79	1.62	1.53
15	N	603	HEA	C12-C13	2.78	1.62	1.53
15	A	603	HEA	C12-C13	2.77	1.62	1.53
15	N	603	HEA	C1B-NB	-2.75	1.33	1.38
15	N	602	HEA	CHC-C1C	2.73	1.45	1.39
15	A	603	HEA	C4D-C3D	-2.72	1.40	1.45
15	N	603	HEA	CHD-C4C	2.71	1.45	1.39
15	N	603	HEA	FE-NC	2.70	2.04	1.95
15	A	603	HEA	O11-C11	2.70	1.48	1.42
15	A	603	HEA	C1C-NC	-2.67	1.34	1.39
15	A	602	HEA	CHB-C4A	2.66	1.43	1.38
15	N	603	HEA	C4B-C3B	-2.65	1.40	1.44
19	D	201	TGL	OB1-CB1	2.65	1.30	1.22
22	O	302	CHD	C11-C9	2.64	1.58	1.53
15	N	603	HEA	C1D-ND	-2.64	1.35	1.40
20	N	608	PGV	O01-C1	2.63	1.41	1.34
15	N	603	HEA	FE-NA	2.62	2.03	1.95
22	P	308	CHD	C8-C7	2.62	1.58	1.53
15	A	602	HEA	CMD-C2D	2.62	1.56	1.50
15	N	603	HEA	C4D-C3D	-2.61	1.40	1.45
22	B	302	CHD	C4-C3	2.58	1.56	1.52
22	P	308	CHD	C6-C5	2.53	1.57	1.53
22	O	302	CHD	C11-C12	2.52	1.57	1.53
15	N	603	HEA	CHA-C4D	2.48	1.44	1.39
15	N	603	HEA	C1A-NA	-2.46	1.35	1.39
25	G	102	PEK	O03-C01	-2.45	1.39	1.45
15	A	602	HEA	CMB-C2B	2.44	1.55	1.50
15	N	602	HEA	C1D-ND	-2.43	1.36	1.40
22	B	302	CHD	C19-C10	2.42	1.58	1.54
25	P	304	PEK	O01-C1	2.42	1.41	1.34
22	B	302	CHD	C6-C7	2.37	1.57	1.52
15	N	603	HEA	C1C-NC	-2.37	1.35	1.39
20	C	307	PGV	P-O11	2.37	1.68	1.59
15	N	603	HEA	C12-C11	2.36	1.57	1.53
15	N	602	HEA	O1A-CGA	2.36	1.29	1.22
15	A	603	HEA	CMD-C2D	2.34	1.55	1.50
19	L	101	TGL	CG3-CG2	2.32	1.58	1.50
15	A	603	HEA	C1D-C2D	-2.30	1.39	1.44
15	A	602	HEA	CHB-C1B	2.30	1.44	1.39
15	N	602	HEA	CHB-C4A	2.29	1.42	1.38
22	C	305	CHD	C8-C14	2.29	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	305	PGV	O01-C1	2.29	1.40	1.34
19	A	607	TGL	OC1-CC1	-2.29	1.15	1.22
15	A	602	HEA	C1C-C2C	-2.28	1.37	1.43
24	C	303	CDL	OB6-CB4	-2.28	1.41	1.46
15	A	602	HEA	C4C-NC	-2.25	1.35	1.39
15	A	603	HEA	CHC-C1C	2.24	1.44	1.39
15	A	603	HEA	C18-C19	2.22	1.38	1.33
15	N	602	HEA	C1A-NA	-2.22	1.35	1.39
22	C	305	CHD	C4-C5	2.21	1.57	1.53
28	G	101	DMU	O1-C10	2.20	1.47	1.41
22	C	305	CHD	O26-C24	-2.17	1.23	1.30
22	O	302	CHD	C6-C7	2.17	1.56	1.52
15	A	602	HEA	FE-ND	2.17	2.01	1.94
22	P	308	CHD	C6-C7	2.15	1.56	1.52
15	N	602	HEA	FE-ND	2.13	2.01	1.94
20	C	307	PGV	C03-C02	2.13	1.57	1.50
15	A	602	HEA	C1C-NC	-2.12	1.35	1.39
20	N	608	PGV	P-O13	2.12	1.58	1.50
22	P	307	CHD	O26-C24	-2.09	1.23	1.30
15	A	603	HEA	C4D-ND	-2.09	1.34	1.38
15	A	603	HEA	C3A-C4A	-2.09	1.42	1.46
15	A	603	HEA	C16-C15	2.09	1.55	1.51
15	N	602	HEA	CBD-CGD	2.08	1.55	1.50
15	N	603	HEA	CHC-C1C	2.07	1.44	1.39
15	A	602	HEA	C1B-NB	-2.05	1.34	1.38
15	N	602	HEA	C4D-ND	-2.04	1.34	1.38
15	N	602	HEA	C1C-NC	-2.03	1.35	1.39
20	C	302	PGV	P-O14	-2.03	1.45	1.55
22	C	304	CHD	O26-C24	-2.02	1.24	1.30
15	N	603	HEA	CBD-CAD	2.01	1.58	1.51
25	P	304	PEK	O01-C02	-2.00	1.41	1.46

All (483) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602	HEA	C17-C18-C19	-10.69	103.15	127.62
15	A	602	HEA	C20-C19-C18	-9.49	99.87	121.17
28	P	301	DMU	O16-C6-C1	9.42	122.58	108.27
19	A	607	TGL	CG2-OG2-CB1	9.15	139.70	117.80
28	G	101	DMU	O1-C9-C11	8.13	126.60	106.44
15	A	603	HEA	C13-C12-C11	-7.87	101.82	114.39
22	P	307	CHD	C6-C7-C8	7.81	120.03	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	607	TGL	OG2-CB1-CB2	7.41	127.52	111.48
28	P	301	DMU	C18-O16-C6	7.36	126.25	113.68
22	C	304	CHD	C6-C5-C4	-7.28	102.91	111.23
22	P	307	CHD	C14-C13-C12	6.68	113.52	107.42
22	P	307	CHD	C6-C5-C10	6.34	119.40	112.66
15	N	602	HEA	C3C-C4C-NC	6.33	115.13	109.80
15	N	602	HEA	C4B-NB-C1B	6.31	112.67	105.21
28	G	101	DMU	C8-C7-C5	-6.20	99.94	110.83
19	Q	201	TGL	OG2-CB1-CB2	6.18	124.86	111.48
15	A	602	HEA	C27-C19-C18	6.17	139.47	123.63
22	P	307	CHD	C18-C13-C12	-6.05	103.00	109.06
15	A	602	HEA	C2B-C1B-NB	5.89	116.71	109.90
28	M	101	DMU	O2-C8-C9	-5.86	94.89	109.32
24	C	303	CDL	OA6-CA5-C11	5.80	124.03	111.48
24	P	306	CDL	OA6-CA5-C11	5.55	123.50	111.48
19	L	101	TGL	OG3-CC1-CC2	5.54	128.71	111.83
25	G	102	PEK	C2-C3-C4	5.52	125.41	113.35
22	B	302	CHD	C18-C13-C12	-5.38	103.67	109.06
24	G	103	CDL	OA6-CA5-C11	5.33	123.02	111.48
28	G	101	DMU	C7-C8-C9	-5.28	100.65	110.23
25	T	101	PEK	O01-C1-C2	5.28	122.90	111.48
28	Z	101	DMU	C8-C7-C5	-5.25	101.61	110.83
24	T	102	CDL	OB6-CB5-C51	5.25	122.83	111.48
25	P	304	PEK	C2-C3-C4	5.22	124.75	113.35
20	N	607	PGV	O01-C1-C2	5.21	122.76	111.48
20	N	607	PGV	C3-C2-C1	-5.17	94.76	113.69
15	N	602	HEA	C27-C19-C18	-5.12	110.48	123.63
24	T	102	CDL	OA6-CA5-C11	5.11	122.54	111.48
22	P	307	CHD	C6-C5-C4	-5.10	105.40	111.23
19	N	609	TGL	OG2-CB1-CB2	5.09	122.49	111.48
24	G	103	CDL	OB6-CB5-C51	5.09	122.49	111.48
20	P	302	PGV	O01-C1-C2	5.07	122.46	111.48
20	A	608	PGV	O03-C19-O04	-4.95	111.24	123.63
20	C	307	PGV	O01-C1-C2	4.95	122.18	111.48
22	P	307	CHD	C14-C8-C7	4.92	118.38	111.85
25	P	304	PEK	O01-C1-O02	-4.90	112.26	123.70
19	A	607	TGL	OG1-CA1-CA2	4.89	126.74	111.83
15	A	602	HEA	C4B-NB-C1B	-4.88	99.43	105.21
25	G	104	PEK	O01-C1-C2	4.88	122.03	111.48
20	A	608	PGV	O03-C19-C20	4.87	126.69	111.83
26	O	303	PSC	O01-C1-C2	4.87	122.01	111.48
15	A	602	HEA	C25-C23-C24	4.82	125.69	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	603	HEA	C20-C19-C18	-4.81	110.38	121.17
22	C	304	CHD	C19-C10-C1	-4.75	100.76	108.31
22	P	307	CHD	C14-C8-C9	-4.72	103.16	109.75
22	C	304	CHD	C10-C9-C8	4.71	117.09	111.84
22	C	304	CHD	C14-C8-C7	4.70	118.09	111.85
20	C	307	PGV	O03-C19-C20	4.66	126.05	111.83
22	C	304	CHD	C1-C10-C5	4.65	114.43	107.75
22	C	304	CHD	C15-C14-C8	4.63	124.71	118.36
15	N	602	HEA	C2D-C1D-ND	4.63	115.16	109.84
19	A	607	TGL	OG3-CC1-OC1	-4.61	112.10	123.63
20	P	302	PGV	O03-C19-C20	4.57	125.77	111.83
15	A	602	HEA	C2D-C1D-ND	4.54	115.06	109.84
26	E	201	PSC	O01-C1-C2	4.51	121.23	111.48
25	C	306	PEK	O01-C1-C2	4.50	121.21	111.48
28	Z	101	DMU	C7-C8-C9	-4.49	102.09	110.23
19	N	610	TGL	CG2-OG2-CB1	4.49	128.53	117.80
25	P	309	PEK	O01-C1-C2	4.48	121.17	111.48
15	N	603	HEA	C13-C12-C11	-4.47	107.24	114.39
24	C	303	CDL	OB8-CB7-C71	4.44	125.37	111.83
25	P	304	PEK	O03-C01-C02	-4.40	95.71	108.40
25	G	102	PEK	C24-C23-C22	-4.40	96.97	113.13
22	B	302	CHD	C6-C7-C8	4.39	116.29	111.50
22	C	304	CHD	C4-C5-C10	4.38	117.32	112.66
20	A	609	PGV	C02-O01-C1	4.36	128.24	117.80
28	G	101	DMU	O3-C5-C7	4.35	120.63	110.38
22	C	305	CHD	C1-C2-C3	-4.34	104.74	110.48
19	A	607	TGL	OG3-CG3-CG2	4.32	120.84	108.40
19	L	101	TGL	CG2-OG2-CB1	4.30	128.08	117.80
28	M	101	DMU	O1-C9-C8	4.29	117.42	109.70
26	O	303	PSC	O03-C19-C20	4.28	124.89	111.83
19	N	610	TGL	OG2-CB1-CB2	4.27	120.72	111.48
22	P	307	CHD	C15-C14-C8	4.26	124.20	118.36
20	N	608	PGV	O03-C19-C20	4.25	124.79	111.83
24	P	306	CDL	OB8-CB7-C71	4.24	124.76	111.83
19	A	607	TGL	OB1-CB1-CB2	-4.22	107.29	123.78
15	A	603	HEA	C27-C19-C20	4.20	122.53	115.23
22	P	307	CHD	C2-C1-C10	4.18	119.80	112.74
15	N	602	HEA	C27-C19-C20	4.17	122.47	115.23
20	N	608	PGV	O03-C19-O04	-4.17	113.20	123.63
22	C	305	CHD	C5-C4-C3	-4.16	106.43	112.71
25	P	309	PEK	O03-C21-C22	4.16	124.52	111.83
15	N	602	HEA	C2C-C1C-NC	4.16	116.81	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602	HEA	CHA-C4D-C3D	-4.15	118.72	124.77
15	A	602	HEA	CHB-C1B-NB	-4.11	120.00	124.42
19	A	607	TGL	OG3-CC1-CC2	4.10	124.34	111.83
19	L	101	TGL	OG2-CB1-CB2	4.07	120.28	111.48
22	O	302	CHD	O12-C12-C13	-4.06	104.16	111.02
19	D	201	TGL	OG2-CB1-CB2	4.03	120.20	111.48
15	A	603	HEA	CAA-C2A-C1A	4.02	133.03	124.85
15	N	603	HEA	C27-C19-C20	3.99	122.16	115.23
19	A	607	TGL	CG3-OG3-CC1	3.97	131.63	117.12
20	A	609	PGV	O03-C19-C20	3.97	123.93	111.83
15	N	603	HEA	C26-C15-C16	3.95	122.08	115.23
22	P	307	CHD	C1-C10-C5	3.94	113.41	107.75
15	N	602	HEA	C1A-CHA-C4D	-3.93	117.66	126.02
15	A	603	HEA	CMB-C2B-C1B	3.93	131.17	125.03
19	N	609	TGL	CG2-OG2-CB1	3.92	127.17	117.80
22	P	308	CHD	C1-C10-C5	3.91	113.36	107.75
15	A	602	HEA	C17-C18-C19	3.89	136.52	127.62
28	P	301	DMU	O5-C6-C1	-3.88	102.39	110.37
20	A	609	PGV	O01-C1-C2	3.88	119.88	111.48
22	P	308	CHD	C23-C22-C20	-3.88	107.22	114.46
22	P	307	CHD	C9-C8-C7	3.85	116.71	111.86
22	C	304	CHD	C14-C8-C9	-3.83	104.40	109.75
22	P	307	CHD	C19-C10-C9	-3.83	106.03	111.18
15	A	602	HEA	CHA-C4D-C3D	-3.82	119.21	124.77
22	O	302	CHD	C6-C5-C4	-3.81	106.88	111.23
15	A	603	HEA	C12-C11-C3B	-3.80	106.18	112.12
22	C	305	CHD	C11-C12-C13	3.80	115.13	111.26
19	D	201	TGL	OG1-CA1-CA2	3.80	123.41	111.83
28	G	101	DMU	O7-C10-C5	3.78	117.40	108.09
15	N	603	HEA	CAD-CBD-CGD	-3.77	103.66	113.67
28	G	101	DMU	C18-O16-C6	3.77	120.12	113.68
15	N	603	HEA	C2B-C1B-NB	3.77	114.26	109.90
15	A	603	HEA	O2A-CGA-CBA	3.76	125.87	114.00
22	C	304	CHD	C18-C13-C12	-3.75	105.31	109.06
15	N	602	HEA	C2B-C1B-NB	-3.74	105.58	109.90
28	Z	101	DMU	O1-C9-C11	3.73	115.67	106.44
28	G	101	DMU	O16-C6-C1	3.72	113.93	108.27
22	P	307	CHD	C5-C6-C7	3.72	118.83	114.40
22	P	307	CHD	C10-C9-C8	3.71	115.97	111.84
15	A	603	HEA	CHA-C1A-NA	3.70	128.49	124.45
28	P	301	DMU	C8-C7-C5	-3.70	104.33	110.83
15	N	602	HEA	CHC-C4B-NB	3.69	128.94	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	602	HEA	C3B-C4B-NB	3.68	114.07	109.84
19	N	610	TGL	OG1-CA1-CA2	3.68	123.04	111.83
22	C	304	CHD	C6-C5-C10	3.67	116.57	112.66
22	B	302	CHD	C13-C14-C8	-3.67	110.06	114.72
15	N	602	HEA	CMD-C2D-C1D	3.65	130.74	125.03
22	C	304	CHD	C6-C7-C8	3.64	115.48	111.50
22	P	308	CHD	C21-C20-C22	-3.62	104.73	110.34
15	N	602	HEA	CAD-C3D-C2D	3.61	134.63	127.87
15	N	603	HEA	C3D-C4D-ND	3.61	113.84	110.35
15	N	602	HEA	C3D-C4D-ND	3.61	113.84	110.35
20	N	607	PGV	O03-C19-C20	3.59	122.79	111.83
19	A	607	TGL	OG2-CG2-CG1	3.59	121.23	108.34
15	N	602	HEA	CHA-C1A-NA	3.59	128.36	124.45
28	Z	101	DMU	O49-C1-C2	-3.59	101.92	110.38
15	N	602	HEA	C4C-NC-C1C	-3.58	99.98	105.82
22	C	304	CHD	C14-C13-C12	3.58	110.69	107.42
19	N	609	TGL	OG3-CC1-OC1	-3.57	114.70	123.63
28	M	101	DMU	C18-O16-C6	-3.57	107.58	113.68
15	A	603	HEA	CMB-C2B-C3B	-3.57	123.38	130.28
28	P	301	DMU	C10-O1-C9	3.56	120.68	113.72
25	G	102	PEK	O03-C01-C02	-3.56	98.15	108.40
24	G	103	CDL	OA6-CA5-OA7	-3.55	115.41	123.70
20	A	608	PGV	O01-C1-C2	3.52	119.10	111.48
28	M	101	DMU	O3-C5-C7	3.51	118.65	110.38
28	M	101	DMU	O1-C9-C11	3.51	115.13	106.44
19	Q	201	TGL	OG3-CC1-CC2	3.50	122.51	111.83
22	C	304	CHD	C15-C14-C13	3.49	106.93	103.54
15	N	603	HEA	C1B-C2B-C3B	-3.49	102.75	106.80
15	A	603	HEA	C2D-C1D-ND	3.49	113.85	109.84
15	N	602	HEA	C3B-C4B-NB	-3.49	105.83	109.84
22	C	305	CHD	C9-C8-C7	3.46	116.22	111.86
15	A	603	HEA	CAD-CBD-CGD	-3.45	104.51	113.67
24	C	303	CDL	OB8-CB7-OB9	-3.45	115.00	123.63
28	G	101	DMU	C6-O5-C4	3.44	120.44	113.72
22	C	305	CHD	C15-C14-C13	3.44	106.88	103.54
22	O	302	CHD	C9-C8-C7	3.43	116.18	111.86
22	C	304	CHD	C5-C4-C3	3.43	117.88	112.71
22	P	308	CHD	C11-C12-C13	3.42	114.74	111.26
25	P	309	PEK	O03-C21-O04	-3.41	115.09	123.63
15	A	602	HEA	CHA-C4D-ND	3.41	128.09	124.42
15	A	602	HEA	C1D-C2D-C3D	-3.41	103.39	106.98
25	G	104	PEK	O03-C21-C22	3.41	122.22	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	102	PEK	O01-C1-O02	-3.40	115.76	123.70
20	C	307	PGV	O03-C01-C02	3.39	118.17	108.40
20	N	607	PGV	O01-C02-C03	3.39	120.49	108.34
15	A	602	HEA	CMD-C2D-C1D	3.39	130.32	125.03
25	C	306	PEK	O03-C21-C22	3.38	122.14	111.83
15	A	603	HEA	C3D-C4D-ND	3.37	113.61	110.35
20	N	607	PGV	O03-C19-O04	-3.36	115.23	123.63
19	L	101	TGL	CB4-CB3-CB2	-3.35	100.81	113.13
26	E	201	PSC	C02-O01-C1	3.35	125.81	117.80
24	P	306	CDL	OB8-CB7-OB9	-3.35	115.26	123.63
28	Z	101	DMU	O1-C9-C8	3.31	115.66	109.70
22	O	302	CHD	O7-C7-C6	3.30	118.06	109.86
19	N	610	TGL	OG3-CC1-CC2	3.29	121.88	111.83
28	P	301	DMU	C7-C8-C9	-3.28	104.28	110.23
19	Q	201	TGL	OG1-CA1-CA2	3.28	121.82	111.83
24	T	102	CDL	OA6-CA5-OA7	-3.27	116.06	123.70
19	A	607	TGL	CB3-CB2-CB1	-3.26	101.73	113.69
25	P	304	PEK	C01-O03-C21	3.25	129.00	117.12
22	P	307	CHD	C19-C10-C1	-3.25	103.14	108.31
28	Z	101	DMU	O16-C6-C1	3.25	113.21	108.27
15	N	603	HEA	C17-C18-C19	3.24	135.03	127.62
19	L	101	TGL	OG1-CA1-CA2	3.23	121.67	111.83
15	A	602	HEA	O2A-CGA-CBA	3.21	124.16	114.00
24	P	306	CDL	OA6-CA5-OA7	-3.21	116.20	123.70
22	B	302	CHD	O25-C24-C23	-3.19	112.96	123.09
19	Q	201	TGL	OG1-CA1-OA1	-3.17	115.69	123.63
20	N	608	PGV	O01-C1-O02	-3.16	116.33	123.70
15	A	603	HEA	CHB-C1B-NB	-3.15	121.03	124.42
19	L	101	TGL	OG3-CC1-OC1	-3.13	115.80	123.63
15	A	602	HEA	C27-C19-C20	3.12	120.64	115.23
15	N	602	HEA	C13-C14-C15	-3.11	120.50	127.62
20	P	302	PGV	O03-C19-O04	-3.11	115.86	123.63
26	O	303	PSC	O01-C1-O02	-3.10	116.45	123.70
25	T	101	PEK	O01-C1-O02	-3.10	116.47	123.70
26	E	201	PSC	O03-C19-C20	3.10	121.27	111.83
15	N	603	HEA	OMA-CMA-C3A	-3.09	118.64	125.62
20	P	305	PGV	O12-P-O13	-3.09	96.70	108.94
22	P	307	CHD	C9-C10-C5	3.06	112.77	108.51
24	T	102	CDL	OA8-CA7-OA9	-3.06	115.97	123.63
15	N	602	HEA	C3C-C2C-C1C	-3.06	103.56	107.17
22	P	308	CHD	C15-C14-C13	3.05	106.50	103.54
19	N	610	TGL	CG3-OG3-CC1	3.05	128.27	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	301	DMU	C11-C9-C8	3.05	120.51	113.02
15	A	603	HEA	O1A-CGA-CBA	-3.05	113.42	123.09
22	O	302	CHD	C11-C9-C8	3.05	115.41	110.89
15	A	603	HEA	CHB-C4A-NA	3.04	127.76	124.45
24	G	103	CDL	CB6-OB8-CB7	3.04	128.23	117.12
19	D	201	TGL	CG2-OG2-CB1	3.03	125.05	117.80
15	N	602	HEA	C1D-C2D-C3D	-2.99	103.83	106.98
19	Q	201	TGL	OG3-CC1-OC1	-2.99	116.14	123.63
19	D	201	TGL	OG1-CA1-OA1	-2.99	116.15	123.63
28	P	301	DMU	O3-C5-C10	2.99	117.19	110.08
19	N	609	TGL	OG1-CA1-CA2	2.99	120.94	111.83
22	P	308	CHD	C11-C9-C8	2.98	115.30	110.89
15	A	602	HEA	C3C-C4C-NC	2.97	112.30	109.80
25	T	101	PEK	O03-C21-C22	2.97	120.90	111.83
19	D	201	TGL	OG3-CC1-CC2	2.97	120.89	111.83
19	D	201	TGL	C10-CB9-CB8	2.97	129.37	114.37
15	A	603	HEA	C3C-C4C-NC	2.96	112.29	109.80
15	A	603	HEA	O1D-CGD-CBD	-2.96	113.71	123.09
20	A	609	PGV	O03-C19-O04	-2.95	116.24	123.63
24	G	103	CDL	OA8-CA7-C31	2.95	120.83	111.83
15	N	602	HEA	C16-C17-C18	2.95	126.61	112.02
25	P	304	PEK	C24-C23-C22	-2.94	102.33	113.13
22	B	302	CHD	C17-C13-C12	2.93	120.31	117.67
24	P	306	CDL	OB6-CB5-C51	2.90	117.75	111.48
19	D	201	TGL	CG1-OG1-CA1	2.90	127.70	117.12
28	G	101	DMU	C10-C5-C7	2.89	116.09	110.01
28	M	101	DMU	O7-C10-C5	2.88	115.18	108.09
22	C	305	CHD	C22-C23-C24	-2.88	104.81	112.49
22	P	307	CHD	C11-C12-C13	2.88	114.19	111.26
19	Q	201	TGL	CG3-OG3-CC1	2.88	127.63	117.12
25	P	304	PEK	C30-C29-C28	-2.87	99.84	114.37
28	M	101	DMU	O5-C4-C57	2.87	113.56	106.44
24	C	303	CDL	OA8-CA7-C31	2.87	120.59	111.83
22	P	307	CHD	C15-C14-C13	2.86	106.32	103.54
22	P	308	CHD	C22-C20-C17	-2.86	104.40	110.33
24	C	303	CDL	OB6-CB5-C51	2.86	117.67	111.48
19	Q	201	TGL	OG2-CG2-CG3	2.85	118.58	108.34
19	N	610	TGL	OG1-CG1-CG2	2.85	116.62	108.40
15	A	602	HEA	CHD-C1D-ND	-2.84	120.86	124.37
15	N	602	HEA	C4A-C3A-C2A	-2.83	104.36	106.81
15	A	603	HEA	C2B-C1B-NB	2.83	113.17	109.90
28	P	301	DMU	C1-C2-C3	2.83	116.10	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	602	HEA	O1A-CGA-CBA	-2.82	114.14	123.09
24	C	303	CDL	C54-C53-C52	-2.82	100.12	114.37
22	C	304	CHD	C5-C6-C7	2.81	117.75	114.40
24	G	103	CDL	C43-C42-C41	2.81	128.58	114.37
15	A	602	HEA	C1A-CHA-C4D	-2.81	120.05	126.02
19	L	101	TGL	OG1-CG1-CG2	2.80	116.47	108.40
15	A	603	HEA	CMD-C2D-C1D	2.80	129.40	125.03
19	N	610	TGL	C25-C24-C23	-2.79	100.25	114.37
19	N	609	TGL	CG3-OG3-CC1	2.79	127.33	117.12
15	N	602	HEA	CMB-C2B-C3B	-2.79	124.88	130.28
24	C	303	CDL	OA6-CA5-OA7	-2.79	117.19	123.70
19	D	201	TGL	CG3-OG3-CC1	2.77	127.25	117.12
24	P	306	CDL	CB6-CB4-CB3	-2.77	105.32	111.78
28	P	301	DMU	O1-C9-C11	2.77	113.31	106.44
25	T	101	PEK	C01-O03-C21	2.77	127.23	117.12
24	T	102	CDL	OB8-CB6-CB4	2.75	116.33	108.40
19	N	609	TGL	OG3-CC1-CC2	2.75	120.22	111.83
22	P	307	CHD	C16-C17-C13	2.74	106.20	103.54
24	G	103	CDL	OB8-CB7-C71	2.74	120.20	111.83
15	N	602	HEA	CHA-C4D-ND	2.74	127.37	124.42
24	T	102	CDL	CA6-CA4-CA3	-2.74	105.40	111.78
25	G	102	PEK	C26-C25-C24	-2.74	100.52	114.37
19	N	610	TGL	OG3-CC1-OC1	-2.72	116.82	123.63
19	N	610	TGL	C26-C25-C24	-2.72	100.64	114.37
22	C	304	CHD	C19-C10-C9	-2.71	107.53	111.18
24	P	306	CDL	OA8-CA7-C31	2.71	120.10	111.83
22	P	308	CHD	C6-C5-C4	-2.71	108.13	111.23
28	Z	101	DMU	O5-C4-C57	2.71	113.15	106.44
28	Z	101	DMU	C28-C25-C22	-2.71	100.69	114.37
22	C	305	CHD	C9-C11-C12	-2.70	110.76	114.29
24	T	102	CDL	OA8-CA7-C31	2.70	120.07	111.83
20	A	608	PGV	O03-C01-C02	2.69	116.16	108.40
15	A	603	HEA	C1D-C2D-C3D	-2.68	104.16	106.98
24	T	102	CDL	C83-C82-C81	2.68	127.93	114.37
24	G	103	CDL	OB8-CB6-CB4	2.68	116.12	108.40
15	N	602	HEA	C1D-ND-C4D	-2.68	102.04	105.21
22	C	304	CHD	C16-C17-C20	2.67	116.22	112.18
15	N	602	HEA	CAD-C3D-C4D	-2.66	120.05	124.70
19	A	607	TGL	C15-CC9-CC8	2.66	127.81	114.37
22	O	302	CHD	C14-C8-C7	2.65	115.37	111.85
15	N	603	HEA	O11-C11-C3B	-2.65	106.40	111.26
15	A	602	HEA	C3C-C2C-C1C	-2.65	104.05	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	603	HEA	CHC-C1C-C2C	-2.64	119.76	127.43
15	A	603	HEA	CAA-CBA-CGA	-2.63	106.68	113.67
28	Z	101	DMU	O3-C5-C7	2.63	116.58	110.38
20	C	302	PGV	O03-C19-O04	-2.63	117.05	123.63
15	A	602	HEA	CMB-C2B-C1B	2.62	129.13	125.03
15	N	602	HEA	C20-C19-C18	2.62	127.04	121.17
28	M	101	DMU	O7-C3-C4	-2.60	102.66	109.48
15	A	603	HEA	CAD-C3D-C2D	2.60	132.73	127.87
19	N	610	TGL	CC3-CC2-CC1	2.60	123.20	113.69
22	B	302	CHD	C6-C5-C4	-2.60	108.26	111.23
15	N	602	HEA	CHB-C1B-NB	2.58	127.20	124.42
19	D	201	TGL	OG3-CC1-OC1	-2.58	117.18	123.63
19	D	201	TGL	C11-C10-CB9	2.57	127.38	114.37
20	C	302	PGV	C22-C21-C20	-2.57	103.68	113.13
15	N	602	HEA	C12-C11-C3B	2.57	116.13	112.12
19	N	609	TGL	OB1-CB1-CB2	-2.56	113.77	123.78
15	A	603	HEA	CHB-C4A-C3A	-2.56	120.89	125.21
20	N	607	PGV	C5-C4-C3	-2.56	101.44	114.37
15	N	602	HEA	CHD-C1D-C2D	-2.56	119.68	126.95
15	N	603	HEA	C2A-C1A-NA	2.55	112.78	110.32
25	P	304	PEK	C28-C27-C26	-2.55	101.48	114.37
15	N	603	HEA	CHC-C1C-NC	2.54	128.47	123.86
28	P	301	DMU	O7-C10-C5	2.54	114.34	108.09
19	L	101	TGL	OG3-CG3-CG2	2.54	115.72	108.40
24	G	103	CDL	C83-C82-C81	2.54	127.19	114.37
22	P	308	CHD	C4-C5-C10	-2.53	109.97	112.66
15	A	602	HEA	C2C-C1C-NC	2.53	114.19	110.14
22	P	308	CHD	O26-C24-O25	-2.52	116.86	123.33
15	N	603	HEA	C21-C20-C19	2.52	121.52	113.19
22	O	302	CHD	O26-C24-C23	2.51	121.93	114.00
25	G	104	PEK	O01-C1-O02	-2.51	117.84	123.70
22	B	302	CHD	C22-C23-C24	-2.50	105.81	112.49
22	P	308	CHD	C6-C5-C10	2.49	115.31	112.66
22	P	308	CHD	C5-C4-C3	-2.49	108.95	112.71
24	C	303	CDL	C52-C51-CB5	-2.49	104.56	113.69
20	A	609	PGV	O01-C02-C03	2.49	117.28	108.34
24	P	306	CDL	C53-C52-C51	-2.48	104.00	113.13
24	C	303	CDL	CB4-OB6-CB5	-2.48	111.86	117.80
20	P	305	PGV	C03-C02-C01	-2.48	106.01	111.78
24	P	306	CDL	C42-C41-C40	2.48	126.88	114.37
22	P	307	CHD	C21-C20-C17	2.46	116.57	112.88
28	M	101	DMU	C7-C8-C9	-2.46	105.78	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	303	CDL	C39-C38-C37	2.46	126.79	114.37
20	A	609	PGV	C8-C9-C10	-2.46	102.05	113.86
22	O	302	CHD	C15-C16-C17	2.46	109.95	105.14
19	N	609	TGL	CB3-CB2-CB1	-2.45	104.73	113.69
22	C	305	CHD	C5-C6-C7	-2.44	111.49	114.40
19	L	101	TGL	OB1-CB1-CB2	-2.44	114.22	123.78
15	N	603	HEA	O2A-CGA-O1A	-2.44	117.05	123.33
22	C	304	CHD	C21-C20-C17	2.44	116.55	112.88
19	Q	201	TGL	OG2-CB1-OB1	-2.43	118.02	123.70
20	C	302	PGV	O06-C06-C05	-2.43	99.46	110.38
22	P	307	CHD	C5-C4-C3	-2.42	109.05	112.71
25	P	304	PEK	C03-C02-C01	-2.42	106.14	111.78
15	A	603	HEA	CHA-C4D-C3D	-2.40	121.27	124.77
15	N	603	HEA	C4D-C3D-C2D	-2.40	103.39	106.89
25	G	104	PEK	O03-C01-C02	2.40	115.33	108.40
20	A	609	PGV	O03-C01-C02	2.39	115.30	108.40
22	C	305	CHD	C15-C14-C8	2.39	121.64	118.36
15	N	602	HEA	C4C-C3C-C2C	-2.39	104.33	107.30
28	Z	101	DMU	O2-C8-C9	-2.39	103.45	109.32
19	L	101	TGL	C26-C25-C24	-2.38	102.31	114.37
28	G	101	DMU	O1-C10-C5	2.38	115.27	110.37
19	N	610	TGL	OG3-CG3-CG2	2.37	115.24	108.40
19	L	101	TGL	OG1-CA1-OA1	-2.37	117.69	123.63
15	A	602	HEA	C12-C11-C3B	2.37	115.83	112.12
20	A	608	PGV	O01-C1-O02	-2.37	118.16	123.70
20	A	609	PGV	C01-O03-C19	2.37	125.77	117.12
22	P	308	CHD	C16-C15-C14	-2.36	100.52	105.14
19	A	607	TGL	CB7-CB6-CB5	-2.36	102.43	114.37
20	C	307	PGV	O01-C02-C03	2.35	116.78	108.34
15	A	603	HEA	C1A-CHA-C4D	-2.35	121.03	126.02
22	C	304	CHD	C4-C3-C2	2.35	113.48	110.62
22	P	307	CHD	C23-C22-C20	-2.34	110.08	114.46
20	N	608	PGV	O01-C1-C2	2.34	116.55	111.48
24	T	102	CDL	OB8-CB7-C71	2.34	118.98	111.83
25	C	306	PEK	C2-C3-C4	-2.33	108.25	113.35
24	G	103	CDL	OB8-CB7-OB9	-2.33	117.79	123.63
15	A	603	HEA	CHA-C1A-C2A	-2.33	121.19	124.86
22	P	308	CHD	C16-C17-C20	2.32	115.69	112.18
15	A	602	HEA	C20-C21-C22	-2.32	100.54	112.02
15	A	602	HEA	C3D-C4D-ND	2.32	112.59	110.35
25	C	306	PEK	C01-O03-C21	2.32	125.59	117.12
22	C	304	CHD	C22-C23-C24	-2.32	106.31	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	304	PEK	O01-C1-C2	2.31	116.47	111.48
19	L	101	TGL	C15-CC9-CC8	2.31	126.02	114.37
25	T	101	PEK	O03-C01-C02	2.30	115.04	108.40
25	T	101	PEK	O03-C21-O04	-2.30	117.88	123.63
25	G	102	PEK	C25-C24-C23	-2.30	102.75	114.37
22	C	304	CHD	C16-C17-C13	2.30	105.77	103.54
15	N	603	HEA	C20-C19-C18	-2.30	116.01	121.17
22	O	302	CHD	C15-C14-C13	2.29	105.77	103.54
19	N	610	TGL	C15-CC9-CC8	2.29	125.94	114.37
15	N	603	HEA	C12-C13-C14	-2.29	106.16	112.16
24	G	103	CDL	C79-C78-C77	2.28	125.91	114.37
19	A	607	TGL	OG1-CA1-OA1	-2.27	117.94	123.63
25	G	104	PEK	O03-C21-O04	-2.27	117.95	123.63
15	N	603	HEA	CMB-C2B-C1B	2.27	128.58	125.03
24	T	102	CDL	C82-C81-C80	2.26	125.81	114.37
15	N	602	HEA	CMC-C2C-C1C	2.26	128.87	125.42
24	G	103	CDL	C82-C81-C80	2.26	125.81	114.37
22	P	308	CHD	C17-C13-C14	-2.26	97.84	100.11
15	A	602	HEA	C1D-ND-C4D	-2.26	102.53	105.21
20	P	305	PGV	O06-C06-C05	-2.25	100.23	110.38
19	L	101	TGL	CA3-CA2-CA1	-2.25	105.43	113.69
28	P	301	DMU	O1-C10-C5	2.25	115.00	110.37
22	C	305	CHD	O26-C24-O25	-2.24	117.56	123.33
24	T	102	CDL	CB6-OB8-CB7	2.24	125.31	117.12
24	G	103	CDL	C40-C39-C38	2.23	125.64	114.37
28	G	101	DMU	C10-O7-C3	-2.23	112.69	117.98
22	O	302	CHD	O25-C24-C23	-2.22	116.04	123.09
25	G	104	PEK	C01-O03-C21	2.22	125.23	117.12
19	N	610	TGL	OG1-CA1-OA1	-2.22	118.08	123.63
22	P	308	CHD	C11-C9-C10	-2.21	111.46	113.70
25	P	309	PEK	O03-C01-C02	2.21	114.76	108.40
19	N	610	TGL	OB1-CB1-CB2	-2.21	115.15	123.78
22	P	308	CHD	C16-C17-C13	2.19	105.66	103.54
15	N	602	HEA	C1B-C2B-C3B	2.19	109.33	106.80
22	B	302	CHD	C10-C9-C8	2.18	114.27	111.84
15	A	602	HEA	CMB-C2B-C3B	-2.18	126.05	130.28
15	A	602	HEA	O2D-CGD-O1D	-2.18	117.73	123.33
25	G	102	PEK	C11-C10-C9	2.18	122.75	112.02
19	D	201	TGL	C21-C20-CA9	2.17	125.36	114.37
19	A	607	TGL	OA1-CA1-CA2	-2.17	115.31	123.78
28	M	101	DMU	C28-C25-C22	-2.17	103.42	114.37
15	A	602	HEA	CAA-CBA-CGA	-2.16	107.92	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	103	CDL	OA8-CA7-OA9	-2.16	118.22	123.63
26	O	303	PSC	O03-C19-O04	-2.16	118.22	123.63
24	C	303	CDL	OA8-CA6-CA4	2.15	114.61	108.40
24	G	103	CDL	C80-C79-C78	2.15	125.25	114.37
25	C	306	PEK	O03-C21-O04	-2.15	118.25	123.63
28	G	101	DMU	C10-O1-C9	2.15	117.92	113.72
20	P	305	PGV	C8-C9-C10	-2.15	103.54	113.86
20	P	305	PGV	O03-C19-O04	-2.14	118.27	123.63
28	G	101	DMU	O3-C5-C10	2.13	115.16	110.08
15	A	603	HEA	CHC-C1C-C2C	-2.13	121.23	127.43
19	L	101	TGL	OC1-CC1-CC2	-2.12	115.48	123.78
19	N	609	TGL	C15-CC9-CC8	2.12	125.09	114.37
24	T	102	CDL	C80-C79-C78	2.12	125.09	114.37
22	C	304	CHD	C23-C22-C20	-2.12	110.50	114.46
20	C	307	PGV	O04-C19-C20	-2.12	115.50	123.78
24	P	306	CDL	CA6-OA8-CA7	2.11	124.84	117.12
26	E	201	PSC	C08-N-C06	2.11	114.52	108.98
26	O	303	PSC	C29-C28-C27	-2.10	103.73	114.37
22	C	305	CHD	C14-C8-C9	2.10	112.68	109.75
19	A	607	TGL	C16-C15-CC9	2.10	124.97	114.37
22	B	302	CHD	C11-C12-C13	2.09	113.39	111.26
15	N	602	HEA	O2A-CGA-CBA	2.09	120.60	114.00
19	N	609	TGL	C16-C15-CC9	2.09	124.92	114.37
28	M	101	DMU	O1-C10-C5	-2.09	106.08	110.37
24	G	103	CDL	C39-C38-C37	2.09	124.91	114.37
15	A	602	HEA	CMC-C2C-C1C	2.08	128.58	125.42
22	B	302	CHD	C14-C8-C9	2.07	112.64	109.75
20	C	307	PGV	O03-C19-O04	-2.07	118.45	123.63
19	N	610	TGL	OG2-CG2-CG3	2.07	115.76	108.34
15	N	602	HEA	CHB-C4A-C3A	-2.06	121.73	125.21
15	N	603	HEA	C3B-C4B-NB	2.06	112.21	109.84
20	C	307	PGV	C01-O03-C19	2.05	124.62	117.12
20	C	302	PGV	C8-C9-C10	-2.05	104.02	113.86
19	D	201	TGL	C20-CA9-CA8	2.05	124.71	114.37
28	M	101	DMU	C22-C19-C18	-2.04	104.58	113.47
15	N	602	HEA	O2A-CGA-O1A	-2.04	118.08	123.33
19	D	201	TGL	CC3-CC2-CC1	-2.04	106.21	113.69
15	N	603	HEA	O2A-CGA-CBA	2.04	120.45	114.00
20	A	609	PGV	C6-C5-C4	-2.04	104.05	114.37
24	C	303	CDL	C61-C60-C59	-2.04	104.05	114.37
19	Q	201	TGL	C16-C15-CC9	2.04	124.67	114.37
20	N	607	PGV	C02-O01-C1	2.04	122.67	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	603	HEA	O2D-CGD-CBD	2.03	120.42	114.00
24	G	103	CDL	C23-C22-C21	2.03	124.64	114.37
19	D	201	TGL	C16-C15-CC9	2.03	124.63	114.37
19	A	607	TGL	CG1-OG1-CA1	2.03	124.54	117.12
25	G	102	PEK	C28-C27-C26	-2.03	104.11	114.37
24	P	306	CDL	OB6-CB4-CB6	2.03	115.61	108.34
15	A	603	HEA	C1D-ND-C4D	-2.02	102.81	105.21
20	C	307	PGV	P-O11-C03	2.02	132.94	121.35
15	N	602	HEA	C13-C12-C11	-2.02	111.17	114.39
15	N	603	HEA	O1D-CGD-CBD	-2.02	116.70	123.09
22	C	305	CHD	C16-C17-C20	-2.01	109.14	112.18
22	C	304	CHD	C9-C11-C12	-2.01	111.67	114.29
22	B	302	CHD	O26-C24-C23	2.00	120.33	114.00
15	A	603	HEA	O2D-CGD-CBD	2.00	120.32	114.00

There are no chirality outliers.

All (963) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	602	HEA	C16-C17-C18-C19
15	A	603	HEA	C2A-C3A-CMA-OMA
15	N	602	HEA	C2A-C3A-CMA-OMA
19	A	607	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	CC2-CC1-OG3-CG3
20	A	609	PGV	C03-O11-P-O12
20	A	609	PGV	C03-O11-P-O13
20	A	609	PGV	C03-O11-P-O14
20	A	609	PGV	C04-O12-P-O13
20	A	609	PGV	C02-C03-O11-P
20	A	609	PGV	C04-C05-C06-O06
20	A	609	PGV	O02-C1-O01-C02
20	A	609	PGV	C2-C1-O01-C02
20	C	307	PGV	C2-C1-O01-C02
20	N	607	PGV	C04-O12-P-O11
20	N	607	PGV	C02-C03-O11-P
20	N	607	PGV	C04-C05-C06-O06
20	N	607	PGV	O02-C1-O01-C02
20	N	607	PGV	C2-C1-O01-C02
20	P	302	PGV	C03-O11-P-O13
20	P	302	PGV	C2-C1-O01-C02
24	C	303	CDL	CA2-C1-CB2-OB2
24	C	303	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
24	C	303	CDL	CA2-OA2-PA1-OA4
24	C	303	CDL	CA2-OA2-PA1-OA5
24	C	303	CDL	CA3-OA5-PA1-OA2
24	C	303	CDL	OA7-CA5-OA6-CA4
24	C	303	CDL	C11-CA5-OA6-CA4
24	C	303	CDL	CB2-OB2-PB2-OB3
24	C	303	CDL	CB2-OB2-PB2-OB4
24	C	303	CDL	CB2-OB2-PB2-OB5
24	G	103	CDL	C11-CA5-OA6-CA4
24	G	103	CDL	C1-CB2-OB2-PB2
24	G	103	CDL	CB3-OB5-PB2-OB2
24	G	103	CDL	CB3-OB5-PB2-OB3
24	G	103	CDL	CB3-OB5-PB2-OB4
24	P	306	CDL	CA2-OA2-PA1-OA3
24	P	306	CDL	CA2-OA2-PA1-OA4
24	P	306	CDL	CA2-OA2-PA1-OA5
24	P	306	CDL	CA3-OA5-PA1-OA2
24	P	306	CDL	CA3-OA5-PA1-OA3
24	P	306	CDL	CA3-OA5-PA1-OA4
24	P	306	CDL	OA7-CA5-OA6-CA4
24	P	306	CDL	C11-CA5-OA6-CA4
24	P	306	CDL	CB2-OB2-PB2-OB4
24	P	306	CDL	CB2-OB2-PB2-OB5
24	T	102	CDL	CA2-C1-CB2-OB2
24	T	102	CDL	C1-CB2-OB2-PB2
24	T	102	CDL	CB3-OB5-PB2-OB2
24	T	102	CDL	CB3-OB5-PB2-OB3
24	T	102	CDL	CB3-OB5-PB2-OB4
25	C	306	PEK	C03-O11-P-O12
25	C	306	PEK	C03-O11-P-O14
25	C	306	PEK	C04-O12-P-O11
25	C	306	PEK	C04-O12-P-O13
25	C	306	PEK	C04-O12-P-O14
25	G	102	PEK	C11-C12-C13-C14
25	G	104	PEK	O03-C01-C02-O01
25	G	104	PEK	O12-C04-C05-N
25	P	309	PEK	C04-O12-P-O11
25	P	309	PEK	C04-O12-P-O13
25	P	309	PEK	O12-C04-C05-N
25	T	101	PEK	C03-O11-P-O12
25	T	101	PEK	C03-O11-P-O13
25	T	101	PEK	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
25	T	101	PEK	C04-O12-P-O11
25	T	101	PEK	C04-O12-P-O13
25	T	101	PEK	C04-O12-P-O14
25	T	101	PEK	O03-C01-C02-O01
25	T	101	PEK	O12-C04-C05-N
25	T	101	PEK	C6-C7-C8-C9
26	E	201	PSC	C03-O11-P-O14
26	E	201	PSC	C03-C02-O01-C1
26	O	303	PSC	C04-O12-P-O11
26	O	303	PSC	C04-O12-P-O13
26	O	303	PSC	O12-C04-C05-N
28	G	101	DMU	O5-C6-O16-C18
28	P	301	DMU	C1-C6-O16-C18
19	D	201	TGL	OC1-CC1-OG3-CG3
20	A	609	PGV	O04-C19-O03-C01
20	N	607	PGV	O04-C19-O03-C01
20	A	609	PGV	C20-C19-O03-C01
20	N	607	PGV	C20-C19-O03-C01
19	Q	201	TGL	OC1-CC1-OG3-CG3
26	O	303	PSC	O04-C19-O03-C01
19	A	607	TGL	OB1-CB1-OG2-CG2
20	C	307	PGV	O02-C1-O01-C02
24	G	103	CDL	OA7-CA5-OA6-CA4
26	E	201	PSC	C02-C01-O03-C19
19	Q	201	TGL	CA2-CA1-OG1-CG1
19	Q	201	TGL	CC2-CC1-OG3-CG3
26	O	303	PSC	C20-C19-O03-C01
20	C	302	PGV	C10-C11-C12-C13
20	C	307	PGV	C10-C11-C12-C13
20	P	302	PGV	C10-C11-C12-C13
25	G	102	PEK	C13-C14-C15-C16
25	G	104	PEK	C7-C8-C9-C10
25	G	104	PEK	C13-C14-C15-C16
25	P	304	PEK	C13-C14-C15-C16
26	E	201	PSC	C11-C10-C9-C8
20	P	302	PGV	O02-C1-O01-C02
26	E	201	PSC	C04-C05-N-C06
24	C	303	CDL	O1-C1-CB2-OB2
24	G	103	CDL	O1-C1-CB2-OB2
24	P	306	CDL	O1-C1-CA2-OA2
24	P	306	CDL	O1-C1-CB2-OB2
24	T	102	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
19	N	610	TGL	CA2-CA1-OG1-CG1
28	G	101	DMU	O6-C11-C9-O1
19	Q	201	TGL	OA1-CA1-OG1-CG1
24	P	306	CDL	C51-CB5-OB6-CB4
24	T	102	CDL	C11-CA5-OA6-CA4
24	C	303	CDL	C62-C63-C64-C65
24	P	306	CDL	OB7-CB5-OB6-CB4
28	Z	101	DMU	O6-C11-C9-O1
15	N	602	HEA	C15-C16-C17-C18
20	N	607	PGV	C05-C04-O12-P
28	P	301	DMU	O5-C4-C57-O61
28	M	101	DMU	O6-C11-C9-C8
22	P	307	CHD	C21-C20-C22-C23
24	T	102	CDL	C79-C80-C81-C82
19	N	610	TGL	OA1-CA1-OG1-CG1
28	P	301	DMU	O5-C6-O16-C18
19	Q	201	TGL	C16-C15-CC9-CC8
19	L	101	TGL	C20-C21-C22-C23
22	C	304	CHD	C17-C20-C22-C23
22	P	307	CHD	C17-C20-C22-C23
28	Z	101	DMU	O6-C11-C9-C8
20	P	305	PGV	C10-C11-C12-C13
25	C	306	PEK	C4-C5-C6-C7
25	G	102	PEK	C7-C8-C9-C10
25	G	102	PEK	C10-C11-C12-C13
25	G	104	PEK	C4-C5-C6-C7
25	T	101	PEK	C13-C14-C15-C16
26	O	303	PSC	C11-C10-C9-C8
26	O	303	PSC	C11-C12-C13-C14
24	T	102	CDL	C56-C57-C58-C59
19	D	201	TGL	C13-C14-C29-C30
19	L	101	TGL	CC3-CC4-CC5-CC6
19	N	609	TGL	C12-C13-C14-C29
24	T	102	CDL	OA7-CA5-OA6-CA4
26	O	303	PSC	O02-C1-O01-C02
24	C	303	CDL	CB2-C1-CA2-OA2
24	G	103	CDL	CA2-C1-CB2-OB2
24	P	306	CDL	CB2-C1-CA2-OA2
19	A	607	TGL	CC2-CC1-OG3-CG3
19	L	101	TGL	CA2-CA1-OG1-CG1
19	N	609	TGL	CC2-CC1-OG3-CG3
24	G	103	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
24	T	102	CDL	C31-CA7-OA8-CA6
25	T	101	PEK	C22-C21-O03-C01
26	E	201	PSC	C20-C19-O03-C01
24	G	103	CDL	C15-C16-C17-C18
24	T	102	CDL	C15-C16-C17-C18
19	Q	201	TGL	CB9-C10-C11-C12
26	E	201	PSC	C20-C21-C22-C23
20	C	307	PGV	C20-C21-C22-C23
24	G	103	CDL	C56-C57-C58-C59
20	P	302	PGV	O12-C04-C05-O05
28	M	101	DMU	O6-C11-C9-O1
19	N	609	TGL	OC1-CC1-OG3-CG3
24	G	103	CDL	OA9-CA7-OA8-CA6
26	E	201	PSC	O04-C19-O03-C01
28	P	301	DMU	C3-C4-C57-O61
19	Q	201	TGL	C21-C22-C23-C24
26	O	303	PSC	C2-C1-O01-C02
19	D	201	TGL	C21-C22-C23-C24
26	E	201	PSC	C1-C2-C3-C4
24	T	102	CDL	C73-C74-C75-C76
19	A	607	TGL	C12-C13-C14-C29
24	G	103	CDL	C63-C64-C65-C66
24	P	306	CDL	C82-C83-C84-C85
25	G	102	PEK	C4-C5-C6-C7
25	P	309	PEK	C7-C8-C9-C10
25	T	101	PEK	C7-C8-C9-C10
25	T	101	PEK	C10-C11-C12-C13
28	G	101	DMU	C3-C4-C57-O61
24	T	102	CDL	C22-C23-C24-C25
25	T	101	PEK	C28-C29-C30-C31
28	G	101	DMU	O6-C11-C9-C8
20	A	609	PGV	C1-C2-C3-C4
24	G	103	CDL	C41-C42-C43-C44
28	P	301	DMU	O6-C11-C9-C8
24	G	103	CDL	C22-C23-C24-C25
20	A	608	PGV	C26-C27-C28-C29
19	A	607	TGL	CA1-CA2-CA3-CA4
19	A	607	TGL	CB1-CB2-CB3-CB4
19	D	201	TGL	CB1-CB2-CB3-CB4
19	N	609	TGL	CA1-CA2-CA3-CA4
24	G	103	CDL	CA5-C11-C12-C13
24	G	103	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	P	306	CDL	CB7-C71-C72-C73
24	T	102	CDL	CB5-C51-C52-C53
19	A	607	TGL	OC1-CC1-OG3-CG3
24	T	102	CDL	OA9-CA7-OA8-CA6
19	N	609	TGL	CA9-C20-C21-C22
22	C	304	CHD	C21-C20-C22-C23
20	C	307	PGV	C19-C20-C21-C22
20	P	302	PGV	C1-C2-C3-C4
26	O	303	PSC	C19-C20-C21-C22
20	C	307	PGV	O12-C04-C05-O05
24	C	303	CDL	O1-C1-CA2-OA2
25	G	104	PEK	C22-C21-O03-C01
25	T	101	PEK	O04-C21-O03-C01
20	C	307	PGV	C1-C2-C3-C4
19	N	609	TGL	OB1-CB1-OG2-CG2
26	E	201	PSC	C28-C29-C30-C31
26	E	201	PSC	C11-C12-C13-C14
19	N	609	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	OA1-CA1-OG1-CG1
24	T	102	CDL	CA7-C31-C32-C33
20	C	307	PGV	C2-C3-C4-C5
20	N	607	PGV	C19-C20-C21-C22
20	C	307	PGV	O12-C04-C05-C06
24	P	306	CDL	CA2-C1-CB2-OB2
26	E	201	PSC	C04-C05-N-C07
26	O	303	PSC	C04-C05-N-C06
26	O	303	PSC	C04-C05-N-C07
26	O	303	PSC	C04-C05-N-C08
19	L	101	TGL	CC1-CC2-CC3-CC4
25	G	102	PEK	C1-C2-C3-C4
20	N	607	PGV	C10-C11-C12-C13
25	P	304	PEK	C4-C5-C6-C7
28	G	101	DMU	O5-C4-C57-O61
20	N	607	PGV	O12-C04-C05-O05
25	G	104	PEK	O04-C21-O03-C01
20	C	307	PGV	C04-C05-C06-O06
19	A	607	TGL	CG1-CG2-OG2-CB1
19	D	201	TGL	CG3-CG2-OG2-CB1
19	A	607	TGL	C16-C15-CC9-CC8
19	N	609	TGL	C22-C23-C24-C25
24	T	102	CDL	C63-C64-C65-C66
26	E	201	PSC	C04-C05-N-C08

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Mol	Chain	Res	Type	Atoms
19	N	609	TGL	CA5-CA6-CA7-CA8
24	P	306	CDL	C51-C52-C53-C54
24	T	102	CDL	C18-C19-C20-C21
26	O	303	PSC	C22-C23-C24-C25
19	D	201	TGL	C17-C18-C19-C33
19	L	101	TGL	C16-C15-CC9-CC8
20	N	608	PGV	C26-C27-C28-C29
24	G	103	CDL	C72-C73-C74-C75
25	C	306	PEK	C29-C30-C31-C32
25	G	104	PEK	C27-C28-C29-C30
25	G	104	PEK	C10-C11-C12-C13
19	L	101	TGL	CC6-CC7-CC8-CC9
24	P	306	CDL	C58-C59-C60-C61
24	T	102	CDL	C59-C60-C61-C62
19	A	607	TGL	CB3-CB4-CB5-CB6
19	D	201	TGL	CA6-CA7-CA8-CA9
19	N	610	TGL	CA3-CA4-CA5-CA6
24	P	306	CDL	C37-C38-C39-C40
24	T	102	CDL	C82-C83-C84-C85
20	A	609	PGV	O05-C05-C06-O06
20	C	307	PGV	O05-C05-C06-O06
20	N	607	PGV	O05-C05-C06-O06
28	G	101	DMU	C19-C18-O16-C6
19	L	101	TGL	CB6-CB7-CB8-CB9
20	C	302	PGV	C7-C8-C9-C10
20	P	302	PGV	C29-C30-C31-C32
25	T	101	PEK	C32-C33-C34-C35
19	Q	201	TGL	CB1-CB2-CB3-CB4
24	C	303	CDL	CB7-C71-C72-C73
24	P	306	CDL	CA5-C11-C12-C13
19	A	607	TGL	CB4-CB5-CB6-CB7
20	A	609	PGV	C14-C15-C16-C17
25	G	104	PEK	C2-C3-C4-C5
19	N	610	TGL	CC3-CC4-CC5-CC6
20	C	307	PGV	C6-C7-C8-C9
24	G	103	CDL	C61-C62-C63-C64
24	C	303	CDL	C51-CB5-OB6-CB4
19	D	201	TGL	CC2-CC3-CC4-CC5
19	N	610	TGL	CB4-CB5-CB6-CB7
20	A	608	PGV	C29-C30-C31-C32
19	A	607	TGL	C14-C29-C30-C31
20	C	307	PGV	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
24	G	103	CDL	O1-C1-CA2-OA2
19	D	201	TGL	C21-C20-CA9-CA8
19	L	101	TGL	C21-C20-CA9-CA8
19	N	610	TGL	CC6-CC7-CC8-CC9
19	Q	201	TGL	CA2-CA3-CA4-CA5
24	C	303	CDL	C17-C18-C19-C20
19	N	610	TGL	CB9-C10-C11-C12
19	N	610	TGL	C16-C15-CC9-CC8
19	Q	201	TGL	C17-C18-C19-C33
24	C	303	CDL	C19-C20-C21-C22
24	T	102	CDL	CA5-C11-C12-C13
19	N	609	TGL	C17-C18-C19-C33
19	N	610	TGL	C11-C10-CB9-CB8
24	P	306	CDL	C14-C15-C16-C17
25	G	102	PEK	C25-C26-C27-C28
24	P	306	CDL	C83-C84-C85-C86
26	O	303	PSC	C29-C30-C31-C32
20	P	302	PGV	O12-C04-C05-C06
20	N	607	PGV	C22-C23-C24-C25
26	E	201	PSC	C24-C25-C26-C27
19	A	607	TGL	C11-C10-CB9-CB8
19	N	609	TGL	C16-C17-C18-C19
19	N	609	TGL	C14-C29-C30-C31
19	N	610	TGL	CA9-C20-C21-C22
19	N	610	TGL	C23-C24-C25-C26
19	Q	201	TGL	CC6-CC7-CC8-CC9
20	C	302	PGV	C14-C15-C16-C17
24	C	303	CDL	C76-C77-C78-C79
24	T	102	CDL	C54-C55-C56-C57
25	G	104	PEK	C33-C34-C35-C36
19	A	607	TGL	CB6-CB7-CB8-CB9
19	N	610	TGL	CB5-CB6-CB7-CB8
20	C	307	PGV	C26-C27-C28-C29
24	C	303	CDL	C41-C42-C43-C44
24	C	303	CDL	C60-C61-C62-C63
24	T	102	CDL	C55-C56-C57-C58
24	P	306	CDL	C61-C62-C63-C64
25	T	101	PEK	C34-C35-C36-C37
26	E	201	PSC	C29-C30-C31-C32
19	A	607	TGL	CA9-C20-C21-C22
20	N	608	PGV	C23-C24-C25-C26
20	P	302	PGV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
26	E	201	PSC	C13-C14-C15-C16
20	A	609	PGV	C10-C11-C12-C13
25	C	306	PEK	C10-C11-C12-C13
25	T	101	PEK	C4-C5-C6-C7
20	P	302	PGV	C3-C4-C5-C6
24	P	306	CDL	C42-C43-C44-C45
25	P	309	PEK	C33-C34-C35-C36
19	A	607	TGL	C17-C18-C19-C33
19	N	609	TGL	CC7-CC8-CC9-C15
20	C	302	PGV	C27-C28-C29-C30
20	C	307	PGV	C22-C23-C24-C25
19	D	201	TGL	CA2-CA3-CA4-CA5
24	C	303	CDL	C71-C72-C73-C74
24	C	303	CDL	C81-C82-C83-C84
19	L	101	TGL	OB1-CB1-OG2-CG2
24	C	303	CDL	OB7-CB5-OB6-CB4
24	C	303	CDL	C72-C73-C74-C75
19	A	607	TGL	CA5-CA6-CA7-CA8
19	N	609	TGL	C20-C21-C22-C23
25	T	101	PEK	C27-C28-C29-C30
25	T	101	PEK	C33-C34-C35-C36
20	P	302	PGV	C19-C20-C21-C22
19	L	101	TGL	CC4-CC5-CC6-CC7
24	G	103	CDL	C54-C55-C56-C57
25	G	104	PEK	C30-C31-C32-C33
25	P	304	PEK	C31-C32-C33-C34
24	P	306	CDL	C72-C73-C74-C75
25	G	104	PEK	C25-C26-C27-C28
20	P	302	PGV	C23-C24-C25-C26
24	T	102	CDL	C11-C12-C13-C14
28	Z	101	DMU	C25-C28-C31-C34
28	G	101	DMU	C1-C6-O16-C18
24	C	303	CDL	C16-C17-C18-C19
25	G	104	PEK	C34-C35-C36-C37
19	N	610	TGL	CC1-CC2-CC3-CC4
19	N	609	TGL	CC4-CC5-CC6-CC7
24	C	303	CDL	C58-C59-C60-C61
24	G	103	CDL	C38-C39-C40-C41
25	G	102	PEK	C24-C25-C26-C27
19	N	610	TGL	C22-C23-C24-C25
20	C	307	PGV	C30-C31-C32-C33
20	P	302	PGV	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	P	302	PGV	C14-C15-C16-C17
25	G	104	PEK	C31-C32-C33-C34
25	G	104	PEK	C32-C33-C34-C35
28	M	101	DMU	C19-C22-C25-C28
19	D	201	TGL	C12-C13-C14-C29
19	L	101	TGL	CB2-CB1-OG2-CG2
19	N	610	TGL	CB2-CB1-OG2-CG2
25	G	104	PEK	C2-C1-O01-C02
19	N	609	TGL	CB4-CB5-CB6-CB7
26	O	303	PSC	C20-C21-C22-C23
19	N	610	TGL	CA2-CA3-CA4-CA5
19	N	610	TGL	C17-C18-C19-C33
24	C	303	CDL	C53-C54-C55-C56
24	G	103	CDL	C78-C79-C80-C81
24	P	306	CDL	C60-C61-C62-C63
25	P	309	PEK	C28-C29-C30-C31
20	N	608	PGV	C11-C10-C9-C8
25	P	309	PEK	C2-C3-C4-C5
25	G	102	PEK	C23-C24-C25-C26
19	A	607	TGL	CB9-C10-C11-C12
19	L	101	TGL	C22-C23-C24-C25
19	Q	201	TGL	CB5-CB6-CB7-CB8
25	C	306	PEK	C25-C26-C27-C28
19	N	609	TGL	C15-C16-C17-C18
20	N	607	PGV	C2-C3-C4-C5
19	N	609	TGL	CA3-CA4-CA5-CA6
19	N	609	TGL	CA2-CA3-CA4-CA5
28	P	301	DMU	C28-C31-C34-C37
20	C	307	PGV	O01-C02-C03-O11
24	P	306	CDL	C36-C37-C38-C39
25	P	309	PEK	C34-C35-C36-C37
20	A	609	PGV	C21-C22-C23-C24
24	P	306	CDL	C73-C74-C75-C76
26	O	303	PSC	C2-C3-C4-C5
24	G	103	CDL	CB5-C51-C52-C53
19	L	101	TGL	C12-C13-C14-C29
19	N	610	TGL	C14-C29-C30-C31
20	P	305	PGV	C22-C23-C24-C25
24	P	306	CDL	C80-C81-C82-C83
25	G	104	PEK	C15-C16-C17-C18
25	P	304	PEK	C15-C16-C17-C18
19	Q	201	TGL	C12-C13-C14-C29

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Mol	Chain	Res	Type	Atoms
19	Q	201	TGL	CC4-CC5-CC6-CC7
19	D	201	TGL	CA2-CA1-OG1-CG1
20	A	609	PGV	C7-C8-C9-C10
24	T	102	CDL	C36-C37-C38-C39
26	E	201	PSC	C26-C27-C28-C29
19	Q	201	TGL	C19-C33-C34-C35
28	Z	101	DMU	C19-C22-C25-C28
19	D	201	TGL	CC6-CC7-CC8-CC9
19	L	101	TGL	C21-C22-C23-C24
19	Q	201	TGL	CB2-CB3-CB4-CB5
20	P	305	PGV	C14-C15-C16-C17
24	P	306	CDL	C12-C13-C14-C15
24	P	306	CDL	C71-C72-C73-C74
25	P	304	PEK	C26-C27-C28-C29
24	G	103	CDL	C18-C19-C20-C21
24	P	306	CDL	C15-C16-C17-C18
25	G	104	PEK	C16-C17-C18-C19
19	N	610	TGL	OB1-CB1-OG2-CG2
24	C	303	CDL	C12-C13-C14-C15
24	C	303	CDL	C83-C84-C85-C86
24	G	103	CDL	C57-C58-C59-C60
19	D	201	TGL	C11-C10-CB9-CB8
20	P	302	PGV	C26-C27-C28-C29
19	L	101	TGL	C18-C19-C33-C34
24	G	103	CDL	C62-C63-C64-C65
20	N	608	PGV	C10-C11-C12-C13
25	P	304	PEK	C1-C2-C3-C4
19	D	201	TGL	C18-C19-C33-C34
24	C	303	CDL	C36-C37-C38-C39
24	C	303	CDL	C42-C43-C44-C45
20	C	302	PGV	C25-C26-C27-C28
20	P	305	PGV	C27-C28-C29-C30
24	C	303	CDL	C73-C74-C75-C76
24	T	102	CDL	C80-C81-C82-C83
24	P	306	CDL	C16-C17-C18-C19
25	G	102	PEK	C2-C3-C4-C5
20	C	307	PGV	C01-C02-C03-O11
24	C	303	CDL	OA5-CA3-CA4-CA6
24	G	103	CDL	OA5-CA3-CA4-CA6
25	G	104	PEK	O02-C1-O01-C02
20	C	302	PGV	C22-C23-C24-C25
20	P	302	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
28	G	101	DMU	O16-C18-C19-C22
25	P	304	PEK	C25-C26-C27-C28
24	P	306	CDL	C78-C79-C80-C81
25	G	102	PEK	C16-C17-C18-C19
19	N	610	TGL	C25-C26-C27-C28
28	M	101	DMU	C22-C25-C28-C31
24	T	102	CDL	C41-C42-C43-C44
20	P	305	PGV	C1-C2-C3-C4
20	A	609	PGV	O03-C01-C02-C03
24	C	303	CDL	CB3-CB4-CB6-OB8
24	C	303	CDL	C13-C14-C15-C16
24	T	102	CDL	C71-C72-C73-C74
25	C	306	PEK	C24-C25-C26-C27
20	A	609	PGV	C24-C25-C26-C27
24	C	303	CDL	C11-C12-C13-C14
28	G	101	DMU	C2-C3-O7-C10
19	D	201	TGL	C10-C11-C12-C13
20	P	302	PGV	C25-C26-C27-C28
24	G	103	CDL	C36-C37-C38-C39
19	N	609	TGL	C21-C20-CA9-CA8
24	T	102	CDL	C75-C76-C77-C78
19	L	101	TGL	C19-C33-C34-C35
19	N	609	TGL	CB9-C10-C11-C12
19	Q	201	TGL	CA6-CA7-CA8-CA9
25	P	309	PEK	C25-C26-C27-C28
19	D	201	TGL	OA1-CA1-OG1-CG1
20	C	302	PGV	C28-C29-C30-C31
20	A	608	PGV	C19-C20-C21-C22
19	A	607	TGL	C16-C17-C18-C19
20	N	607	PGV	C03-C02-O01-C1
19	N	609	TGL	C21-C22-C23-C24
24	T	102	CDL	C39-C40-C41-C42
20	A	609	PGV	C11-C10-C9-C8
20	P	305	PGV	C12-C13-C14-C15
25	P	304	PEK	C2-C3-C4-C5
24	T	102	CDL	C31-C32-C33-C34
25	P	304	PEK	C32-C33-C34-C35
25	P	309	PEK	C22-C23-C24-C25
19	N	610	TGL	CC9-C15-C16-C17
25	P	304	PEK	C10-C11-C12-C13
20	A	608	PGV	C14-C15-C16-C17
20	C	307	PGV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
20	N	607	PGV	O12-C04-C05-C06
25	C	306	PEK	O01-C02-C03-O11
19	L	101	TGL	CA5-CA6-CA7-CA8
20	N	607	PGV	C24-C25-C26-C27
19	A	607	TGL	C21-C22-C23-C24
19	L	101	TGL	C29-C30-C31-C32
19	N	610	TGL	CC4-CC5-CC6-CC7
24	P	306	CDL	C77-C78-C79-C80
25	C	306	PEK	C33-C34-C35-C36
25	G	104	PEK	C22-C23-C24-C25
19	A	607	TGL	CC4-CC5-CC6-CC7
19	D	201	TGL	C22-C23-C24-C25
19	D	201	TGL	C24-C25-C26-C27
19	N	610	TGL	C21-C22-C23-C24
28	G	101	DMU	C4-C3-O7-C10
24	C	303	CDL	C61-C62-C63-C64
24	P	306	CDL	C74-C75-C76-C77
28	Z	101	DMU	C22-C25-C28-C31
24	T	102	CDL	C71-CB7-OB8-CB6
19	D	201	TGL	C15-C16-C17-C18
19	Q	201	TGL	C33-C34-C35-C36
20	P	302	PGV	C15-C16-C17-C18
20	A	608	PGV	C30-C31-C32-C33
20	N	608	PGV	C24-C25-C26-C27
25	C	306	PEK	C26-C27-C28-C29
20	N	608	PGV	C31-C32-C33-C34
19	L	101	TGL	CC7-CC8-CC9-C15
24	T	102	CDL	C61-C62-C63-C64
20	C	307	PGV	C11-C10-C9-C8
25	G	102	PEK	C15-C16-C17-C18
26	O	303	PSC	C24-C25-C26-C27
19	A	607	TGL	C20-C21-C22-C23
24	T	102	CDL	C81-C82-C83-C84
25	T	101	PEK	C26-C27-C28-C29
24	C	303	CDL	C24-C25-C26-C27
24	P	306	CDL	C24-C25-C26-C27
25	P	304	PEK	C7-C8-C9-C10
19	N	610	TGL	CC2-CC3-CC4-CC5
20	P	302	PGV	C22-C23-C24-C25
19	D	201	TGL	C11-C12-C13-C14
24	P	306	CDL	C21-C22-C23-C24
20	A	609	PGV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
20	N	607	PGV	C23-C24-C25-C26
20	P	302	PGV	C7-C8-C9-C10
20	C	307	PGV	C02-C03-O11-P
20	P	302	PGV	C02-C03-O11-P
20	P	302	PGV	C05-C04-O12-P
25	T	101	PEK	C25-C26-C27-C28
26	O	303	PSC	C28-C29-C30-C31
19	N	610	TGL	C29-C30-C31-C32
19	Q	201	TGL	C21-C20-CA9-CA8
24	G	103	CDL	C20-C21-C22-C23
26	E	201	PSC	C19-C20-C21-C22
26	O	303	PSC	C1-C2-C3-C4
20	N	607	PGV	C01-C02-C03-O11
24	P	306	CDL	OA5-CA3-CA4-CA6
24	T	102	CDL	OA5-CA3-CA4-CA6
19	D	201	TGL	C19-C33-C34-C35
19	L	101	TGL	C10-C11-C12-C13
20	A	608	PGV	C31-C32-C33-C34
20	P	302	PGV	C31-C32-C33-C34
25	G	102	PEK	C17-C18-C19-C20
28	Z	101	DMU	C34-C37-C40-C43
24	T	102	CDL	C44-C45-C46-C47
28	M	101	DMU	O5-C4-C57-O61
24	C	303	CDL	C84-C85-C86-C87
24	T	102	CDL	C24-C25-C26-C27
24	G	103	CDL	C14-C15-C16-C17
24	G	103	CDL	C31-C32-C33-C34
24	G	103	CDL	C74-C75-C76-C77
19	D	201	TGL	CB9-C10-C11-C12
24	P	306	CDL	C13-C14-C15-C16
20	P	302	PGV	C30-C31-C32-C33
24	C	303	CDL	C59-C60-C61-C62
19	N	610	TGL	C11-C12-C13-C14
24	T	102	CDL	C16-C17-C18-C19
24	T	102	CDL	C62-C63-C64-C65
24	P	306	CDL	C79-C80-C81-C82
19	Q	201	TGL	C16-C17-C18-C19
25	P	304	PEK	C16-C17-C18-C19
24	C	303	CDL	CA5-C11-C12-C13
19	A	607	TGL	CC5-CC6-CC7-CC8
25	T	101	PEK	C29-C30-C31-C32
19	Q	201	TGL	OG1-CG1-CG2-CG3

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Mol	Chain	Res	Type	Atoms
19	Q	201	TGL	CG1-CG2-CG3-OG3
25	G	104	PEK	O03-C01-C02-C03
26	O	303	PSC	O03-C01-C02-C03
19	L	101	TGL	C11-C12-C13-C14
26	E	201	PSC	C23-C24-C25-C26
19	Q	201	TGL	CA9-C20-C21-C22
25	G	102	PEK	C27-C28-C29-C30
20	A	609	PGV	O01-C02-C03-O11
20	P	302	PGV	O01-C02-C03-O11
24	P	306	CDL	OA5-CA3-CA4-OA6
24	T	102	CDL	OA5-CA3-CA4-OA6
25	T	101	PEK	O01-C02-C03-O11
20	P	305	PGV	C02-C03-O11-P
24	C	303	CDL	C1-CA2-OA2-PA1
19	A	607	TGL	C22-C23-C24-C25
20	P	305	PGV	C26-C27-C28-C29
19	D	201	TGL	CA5-CA6-CA7-CA8
24	P	306	CDL	C59-C60-C61-C62
19	A	607	TGL	OG1-CG1-CG2-OG2
19	D	201	TGL	OG1-CG1-CG2-OG2
19	Q	201	TGL	OG2-CG2-CG3-OG3
24	G	103	CDL	OB6-CB4-CB6-OB8
24	P	306	CDL	OB6-CB4-CB6-OB8
24	T	102	CDL	OB6-CB4-CB6-OB8
26	O	303	PSC	O03-C01-C02-O01
25	C	306	PEK	C11-C10-C9-C8
25	C	306	PEK	C9-C10-C11-C12
25	G	102	PEK	C9-C10-C11-C12
25	G	104	PEK	C9-C10-C11-C12
25	G	104	PEK	C11-C12-C13-C14
25	G	104	PEK	C12-C13-C14-C15
25	P	304	PEK	C5-C6-C7-C8
25	P	304	PEK	C9-C10-C11-C12
25	P	309	PEK	C9-C10-C11-C12
25	T	101	PEK	C5-C6-C7-C8
25	T	101	PEK	C9-C10-C11-C12
25	T	101	PEK	C12-C13-C14-C15
26	E	201	PSC	C9-C10-C11-C12
26	E	201	PSC	C10-C11-C12-C13
26	O	303	PSC	C9-C10-C11-C12
20	N	607	PGV	C7-C8-C9-C10
22	P	307	CHD	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
24	C	303	CDL	C32-C33-C34-C35
25	P	309	PEK	C32-C33-C34-C35
26	O	303	PSC	C5-C6-C7-C8
19	N	609	TGL	CA4-CA5-CA6-CA7
19	D	201	TGL	CC1-CC2-CC3-CC4
24	G	103	CDL	CB7-C71-C72-C73
20	P	302	PGV	C12-C13-C14-C15
25	C	306	PEK	C1-C2-C3-C4
19	N	610	TGL	CC5-CC6-CC7-CC8
19	Q	201	TGL	C10-C11-C12-C13
25	C	306	PEK	C30-C31-C32-C33
15	A	602	HEA	C19-C20-C21-C22
25	G	102	PEK	C3-C4-C5-C6
25	P	304	PEK	C3-C4-C5-C6
25	P	304	PEK	C17-C18-C19-C20
25	P	304	PEK	C2-C1-O01-C02
19	N	609	TGL	CC5-CC6-CC7-CC8
26	O	303	PSC	C23-C24-C25-C26
19	Q	201	TGL	CA5-CA6-CA7-CA8
26	O	303	PSC	C4-C5-C6-C7
26	O	303	PSC	C31-C32-C33-C34
24	P	306	CDL	OB5-CB3-CB4-CB6
25	G	104	PEK	C01-C02-C03-O11
25	T	101	PEK	C01-C02-C03-O11
20	C	307	PGV	C24-C25-C26-C27
26	O	303	PSC	C21-C22-C23-C24
20	C	307	PGV	C31-C32-C33-C34
25	C	306	PEK	C34-C35-C36-C37
24	T	102	CDL	OB9-CB7-OB8-CB6
24	C	303	CDL	C75-C76-C77-C78
19	L	101	TGL	C11-C10-CB9-CB8
19	Q	201	TGL	CA4-CA5-CA6-CA7
28	G	101	DMU	C25-C28-C31-C34
26	O	303	PSC	C03-C02-O01-C1
25	T	101	PEK	C16-C17-C18-C19
20	A	609	PGV	C12-C13-C14-C15
20	N	608	PGV	C12-C13-C14-C15
24	T	102	CDL	C37-C38-C39-C40
20	A	609	PGV	C25-C26-C27-C28
20	A	609	PGV	C31-C32-C33-C34
20	N	607	PGV	O01-C02-C03-O11
24	C	303	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
24	G	103	CDL	OA5-CA3-CA4-OA6
26	E	201	PSC	O01-C02-C03-O11
25	G	102	PEK	C35-C36-C37-C38
24	C	303	CDL	CA3-CA4-CA6-OA8
24	P	306	CDL	CA3-CA4-CA6-OA8
24	P	306	CDL	CB3-CB4-CB6-OB8
25	T	101	PEK	O03-C01-C02-C03
24	C	303	CDL	C40-C41-C42-C43
20	P	302	PGV	C9-C10-C11-C12
19	D	201	TGL	CC5-CC6-CC7-CC8
19	D	201	TGL	CA9-C20-C21-C22
24	C	303	CDL	C34-C35-C36-C37
19	Q	201	TGL	C18-C19-C33-C34
24	P	306	CDL	C76-C77-C78-C79
26	O	303	PSC	C05-C04-O12-P
24	G	103	CDL	C40-C41-C42-C43
24	C	303	CDL	C74-C75-C76-C77
19	L	101	TGL	OG2-CG2-CG3-OG3
19	N	610	TGL	OG2-CG2-CG3-OG3
24	C	303	CDL	OA6-CA4-CA6-OA8
19	D	201	TGL	C14-C29-C30-C31
25	P	309	PEK	C22-C21-O03-C01
25	P	309	PEK	O04-C21-O03-C01
19	A	607	TGL	CA4-CA5-CA6-CA7
25	P	309	PEK	C29-C30-C31-C32
19	D	201	TGL	C16-C15-CC9-CC8
26	E	201	PSC	O12-C04-C05-N
19	N	609	TGL	C18-C19-C33-C34
24	T	102	CDL	C14-C15-C16-C17
20	C	302	PGV	C13-C14-C15-C16
25	C	306	PEK	C7-C8-C9-C10
28	P	301	DMU	C25-C28-C31-C34
20	A	609	PGV	C28-C29-C30-C31
24	G	103	CDL	C13-C14-C15-C16
19	A	607	TGL	C13-C14-C29-C30
25	C	306	PEK	C15-C16-C17-C18
24	C	303	CDL	OB5-CB3-CB4-CB6
26	E	201	PSC	C01-C02-C03-O11
19	D	201	TGL	CC3-CC4-CC5-CC6
24	C	303	CDL	C35-C36-C37-C38
19	N	609	TGL	C24-C25-C26-C27
24	G	103	CDL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
19	N	609	TGL	CB6-CB7-CB8-CB9
19	A	607	TGL	CC7-CC8-CC9-C15
20	C	302	PGV	C26-C27-C28-C29
20	A	609	PGV	C05-C04-O12-P
25	P	304	PEK	O02-C1-O01-C02
24	C	303	CDL	OB5-CB3-CB4-OB6
25	G	104	PEK	O01-C02-C03-O11
25	C	306	PEK	C28-C29-C30-C31
19	N	609	TGL	C23-C24-C25-C26
25	P	304	PEK	C24-C25-C26-C27
15	A	603	HEA	C4A-C3A-CMA-OMA
15	N	602	HEA	C4A-C3A-CMA-OMA
15	N	603	HEA	C4A-C3A-CMA-OMA
19	Q	201	TGL	C11-C10-CB9-CB8
20	C	307	PGV	C27-C28-C29-C30
19	Q	201	TGL	OG1-CG1-CG2-OG2
20	A	609	PGV	O03-C01-C02-O01
24	P	306	CDL	OA6-CA4-CA6-OA8
25	P	304	PEK	O03-C01-C02-O01
19	L	101	TGL	C24-C25-C26-C27
20	N	607	PGV	C14-C15-C16-C17
19	L	101	TGL	CG1-CG2-CG3-OG3
19	N	610	TGL	CG1-CG2-CG3-OG3
24	T	102	CDL	C64-C65-C66-C67
25	G	102	PEK	C28-C29-C30-C31
26	E	201	PSC	C31-C32-C33-C34
25	T	101	PEK	C3-C4-C5-C6
20	C	302	PGV	C15-C16-C17-C18
19	L	101	TGL	CA6-CA7-CA8-CA9
20	C	302	PGV	C20-C21-C22-C23
24	C	303	CDL	C57-C58-C59-C60
20	N	607	PGV	C03-O11-P-O13
20	N	607	PGV	C04-O12-P-O13
20	P	302	PGV	C03-O11-P-O12
24	C	303	CDL	CA3-OA5-PA1-OA3
24	P	306	CDL	CB2-OB2-PB2-OB3
26	E	201	PSC	C03-O11-P-O12
26	E	201	PSC	C03-O11-P-O13
26	E	201	PSC	C04-O12-P-O13
20	N	608	PGV	C25-C26-C27-C28
20	N	607	PGV	C21-C22-C23-C24
24	G	103	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	OG2-CB1-CB2-CB3
24	C	303	CDL	CB5-C51-C52-C53
20	C	302	PGV	C02-C03-O11-P
24	C	303	CDL	CA4-CA3-OA5-PA1
24	P	306	CDL	C1-CA2-OA2-PA1
24	T	102	CDL	CA4-CA3-OA5-PA1
19	Q	201	TGL	CC3-CC4-CC5-CC6
22	P	307	CHD	C13-C17-C20-C22
25	C	306	PEK	O04-C21-O03-C01
20	P	305	PGV	C28-C29-C30-C31
28	M	101	DMU	C28-C31-C34-C37
19	N	609	TGL	CG1-CG2-OG2-CB1
20	A	609	PGV	C03-C02-O01-C1
20	P	305	PGV	C21-C22-C23-C24
24	P	306	CDL	C44-C45-C46-C47
20	P	302	PGV	C01-C02-C03-O11
25	C	306	PEK	C01-C02-C03-O11
24	P	306	CDL	CA7-C31-C32-C33
19	L	101	TGL	CA3-CA4-CA5-CA6
24	T	102	CDL	C40-C41-C42-C43
24	C	303	CDL	C38-C39-C40-C41
22	P	307	CHD	C16-C17-C20-C21
19	D	201	TGL	C16-C17-C18-C19
24	C	303	CDL	OB6-CB4-CB6-OB8
19	L	101	TGL	OG1-CA1-CA2-CA3
20	P	302	PGV	C4-C5-C6-C7
25	C	306	PEK	C22-C21-O03-C01
20	N	608	PGV	C29-C30-C31-C32
24	G	103	CDL	C17-C18-C19-C20
24	P	306	CDL	C43-C44-C45-C46
20	A	608	PGV	C10-C11-C12-C13
26	O	303	PSC	O03-C19-C20-C21
19	A	607	TGL	CA6-CA7-CA8-CA9
25	P	309	PEK	C15-C16-C17-C18
20	A	609	PGV	O03-C19-C20-C21
19	D	201	TGL	OG1-CG1-CG2-CG3
24	G	103	CDL	CB3-CB4-CB6-OB8
24	T	102	CDL	CB3-CB4-CB6-OB8
19	Q	201	TGL	CC7-CC8-CC9-C15
19	N	610	TGL	C12-C13-C14-C29
20	N	607	PGV	C5-C6-C7-C8
20	A	608	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	G	103	CDL	C55-C56-C57-C58
20	N	607	PGV	C20-C21-C22-C23
25	C	306	PEK	C32-C33-C34-C35
25	G	104	PEK	C14-C15-C16-C17
19	N	610	TGL	CC7-CC8-CC9-C15
19	A	607	TGL	C24-C25-C26-C27
19	N	610	TGL	CA7-CA8-CA9-C20
24	G	103	CDL	C34-C35-C36-C37
20	C	302	PGV	C23-C24-C25-C26
24	P	306	CDL	C19-C20-C21-C22
24	P	306	CDL	C35-C36-C37-C38
24	G	103	CDL	C16-C17-C18-C19
24	P	306	CDL	C41-C42-C43-C44
25	P	309	PEK	C23-C24-C25-C26
20	A	608	PGV	C23-C24-C25-C26
19	D	201	TGL	OG2-CB1-CB2-CB3
24	G	103	CDL	C35-C36-C37-C38
25	G	104	PEK	C29-C30-C31-C32
24	G	103	CDL	C75-C76-C77-C78
20	A	609	PGV	C11-C12-C13-C14
25	T	101	PEK	C2-C3-C4-C5
26	E	201	PSC	O02-C1-O01-C02
24	G	103	CDL	C79-C80-C81-C82
22	O	302	CHD	C22-C23-C24-O25
20	P	305	PGV	C30-C31-C32-C33
24	C	303	CDL	C20-C21-C22-C23
19	Q	201	TGL	CG3-CG2-OG2-CB1
19	L	101	TGL	CC9-C15-C16-C17
24	T	102	CDL	CB7-C71-C72-C73
19	D	201	TGL	OG1-CA1-CA2-CA3
19	N	610	TGL	OG2-CB1-CB2-CB3
28	M	101	DMU	C18-C19-C22-C25
24	G	103	CDL	C71-CB7-OB8-CB6
24	C	303	CDL	C23-C24-C25-C26
15	A	603	HEA	CAD-CBD-CGD-O1D
20	C	302	PGV	C05-C04-O12-P
24	P	306	CDL	CA4-CA3-OA5-PA1
19	A	607	TGL	C18-C19-C33-C34
20	C	307	PGV	C14-C15-C16-C17
22	B	302	CHD	C22-C23-C24-O25
19	A	607	TGL	C25-C26-C27-C28
19	D	201	TGL	CB4-CB5-CB6-CB7

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	C15-C16-C17-C18
25	C	306	PEK	C5-C6-C7-C8
25	C	306	PEK	C6-C7-C8-C9
25	G	104	PEK	C5-C6-C7-C8
25	P	304	PEK	C11-C12-C13-C14
25	P	309	PEK	C5-C6-C7-C8
24	G	103	CDL	C80-C81-C82-C83
19	N	609	TGL	CA6-CA7-CA8-CA9
24	P	306	CDL	C18-C19-C20-C21
15	A	603	HEA	CAA-CBA-CGA-O2A
22	O	302	CHD	C22-C23-C24-O26
20	P	305	PGV	C05-C04-O12-P
24	G	103	CDL	CB4-CB3-OB5-PB2
19	L	101	TGL	C23-C24-C25-C26
19	N	610	TGL	C21-C20-CA9-CA8
15	A	603	HEA	CAA-CBA-CGA-O1A
24	G	103	CDL	OB9-CB7-OB8-CB6
26	E	201	PSC	O01-C1-C2-C3
24	T	102	CDL	CA3-CA4-CA6-OA8
22	B	302	CHD	C22-C23-C24-O26
20	C	307	PGV	C29-C30-C31-C32
20	A	608	PGV	O03-C19-C20-C21
24	P	306	CDL	OB5-CB3-CB4-OB6
15	N	602	HEA	C27-C19-C20-C21
22	C	305	CHD	C22-C23-C24-O26
24	G	103	CDL	C37-C38-C39-C40
26	O	303	PSC	C27-C28-C29-C30
20	A	609	PGV	C9-C10-C11-C12
20	N	608	PGV	O03-C19-C20-C21
25	C	306	PEK	C13-C14-C15-C16
25	C	306	PEK	O03-C01-C02-O01
15	N	603	HEA	CAD-CBD-CGD-O2D
25	P	304	PEK	C14-C15-C16-C17
24	C	303	CDL	C43-C44-C45-C46
20	P	305	PGV	C7-C8-C9-C10
25	P	309	PEK	C26-C27-C28-C29
15	N	603	HEA	CAD-CBD-CGD-O1D
25	P	304	PEK	C34-C35-C36-C37
15	A	603	HEA	CAD-CBD-CGD-O2D
22	P	307	CHD	C22-C23-C24-O26
20	C	307	PGV	C11-C12-C13-C14
25	G	102	PEK	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	G	102	PEK	C34-C35-C36-C37
24	G	103	CDL	C84-C85-C86-C87
26	E	201	PSC	C7-C8-C9-C10
22	P	308	CHD	C22-C23-C24-O25
24	P	306	CDL	C11-C12-C13-C14
15	N	603	HEA	C2A-C3A-CMA-OMA
22	C	304	CHD	C22-C23-C24-O25
25	P	304	PEK	C35-C36-C37-C38
15	N	602	HEA	C26-C15-C16-C17
19	L	101	TGL	CB7-CB8-CB9-C10
25	G	104	PEK	C21-C22-C23-C24
26	E	201	PSC	C30-C31-C32-C33
26	O	303	PSC	C7-C8-C9-C10
24	P	306	CDL	C23-C24-C25-C26
20	C	307	PGV	O04-C19-O03-C01
19	L	101	TGL	CB3-CB4-CB5-CB6
20	A	609	PGV	C22-C23-C24-C25
20	C	302	PGV	C9-C10-C11-C12
19	Q	201	TGL	C20-C21-C22-C23
25	P	304	PEK	C05-C04-O12-P
26	E	201	PSC	C05-C04-O12-P
25	G	104	PEK	C28-C29-C30-C31
25	P	309	PEK	C14-C15-C16-C17
19	N	609	TGL	CB3-CB4-CB5-CB6
19	N	609	TGL	OG1-CA1-CA2-CA3
19	L	101	TGL	OB1-CB1-CB2-CB3
24	P	306	CDL	C57-C58-C59-C60
22	P	307	CHD	C22-C23-C24-O25
24	C	303	CDL	C80-C81-C82-C83
20	N	608	PGV	C11-C12-C13-C14
20	C	302	PGV	C12-C13-C14-C15
20	N	607	PGV	C15-C16-C17-C18
25	T	101	PEK	O01-C1-C2-C3
15	N	602	HEA	CAD-CBD-CGD-O1D
20	P	305	PGV	C23-C24-C25-C26
22	C	304	CHD	C22-C23-C24-O26
26	E	201	PSC	C2-C1-O01-C02
20	P	302	PGV	O01-C1-C2-C3
26	E	201	PSC	O03-C19-C20-C21
20	C	307	PGV	C23-C24-C25-C26
20	N	608	PGV	C7-C8-C9-C10
24	P	306	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
24	P	306	CDL	C32-C33-C34-C35
15	A	602	HEA	CAD-CBD-CGD-O1D
25	G	102	PEK	O01-C1-C2-C3
15	N	602	HEA	CAD-CBD-CGD-O2D
19	A	607	TGL	OA1-CA1-OG1-CG1
24	G	103	CDL	C82-C83-C84-C85
15	N	603	HEA	CAA-CBA-CGA-O1A
15	A	603	HEA	C26-C15-C16-C17
24	P	306	CDL	C12-C11-CA5-OA6
20	N	607	PGV	O03-C01-C02-O01
15	N	603	HEA	CAA-CBA-CGA-O2A
20	C	307	PGV	C20-C19-O03-C01
22	P	307	CHD	C13-C17-C20-C21
19	Q	201	TGL	OG3-CC1-CC2-CC3
25	C	306	PEK	O01-C1-C2-C3
26	O	303	PSC	O01-C1-C2-C3
25	T	101	PEK	C24-C25-C26-C27
15	A	602	HEA	CAD-CBD-CGD-O2D
19	A	607	TGL	CB2-CB3-CB4-CB5
19	N	610	TGL	CB7-CB8-CB9-C10
20	P	305	PGV	C13-C14-C15-C16
24	T	102	CDL	C52-C53-C54-C55
25	G	102	PEK	C30-C31-C32-C33
15	N	602	HEA	CAA-CBA-CGA-O1A
19	Q	201	TGL	OG1-CA1-CA2-CA3
24	C	303	CDL	C51-C52-C53-C54
24	P	306	CDL	C52-C53-C54-C55
22	C	304	CHD	C20-C22-C23-C24
20	P	302	PGV	C2-C3-C4-C5
19	D	201	TGL	OG3-CC1-CC2-CC3
15	A	602	HEA	CAA-CBA-CGA-O1A
24	T	102	CDL	C78-C79-C80-C81
24	P	306	CDL	C52-C51-CB5-OB7
26	E	201	PSC	O04-C19-C20-C21
19	A	607	TGL	CC1-CC2-CC3-CC4
28	G	101	DMU	C5-C10-O7-C3
25	T	101	PEK	O02-C1-C2-C3
20	P	305	PGV	C25-C26-C27-C28
19	N	609	TGL	OA1-CA1-CA2-CA3
24	P	306	CDL	C12-C11-CA5-OA7
25	G	102	PEK	O02-C1-C2-C3
20	P	302	PGV	O02-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	P	309	PEK	C13-C14-C15-C16
20	N	608	PGV	C4-C5-C6-C7
24	T	102	CDL	C20-C21-C22-C23
26	O	303	PSC	O02-C1-C2-C3
25	T	101	PEK	C35-C36-C37-C38
24	P	306	CDL	C55-C56-C57-C58
19	D	201	TGL	CB2-CB3-CB4-CB5
25	P	309	PEK	C17-C18-C19-C20
19	L	101	TGL	CC2-CC3-CC4-CC5
24	C	303	CDL	C12-C11-CA5-OA6
25	P	304	PEK	O01-C1-C2-C3
19	N	610	TGL	CB3-CB4-CB5-CB6
24	G	103	CDL	C60-C61-C62-C63
15	N	602	HEA	CAA-CBA-CGA-O2A
24	C	303	CDL	C12-C11-CA5-OA7
25	C	306	PEK	O02-C1-C2-C3

There are no ring outliers.

36 monomers are involved in 281 short contacts:

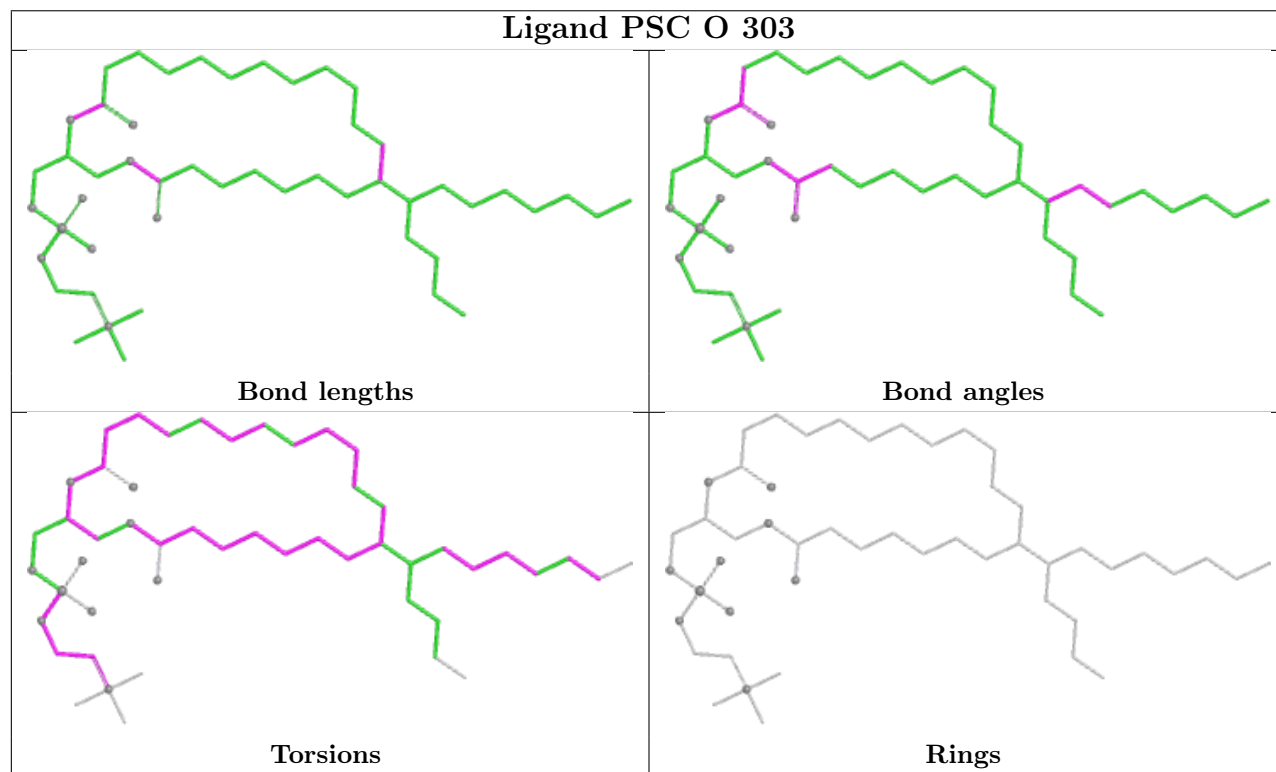
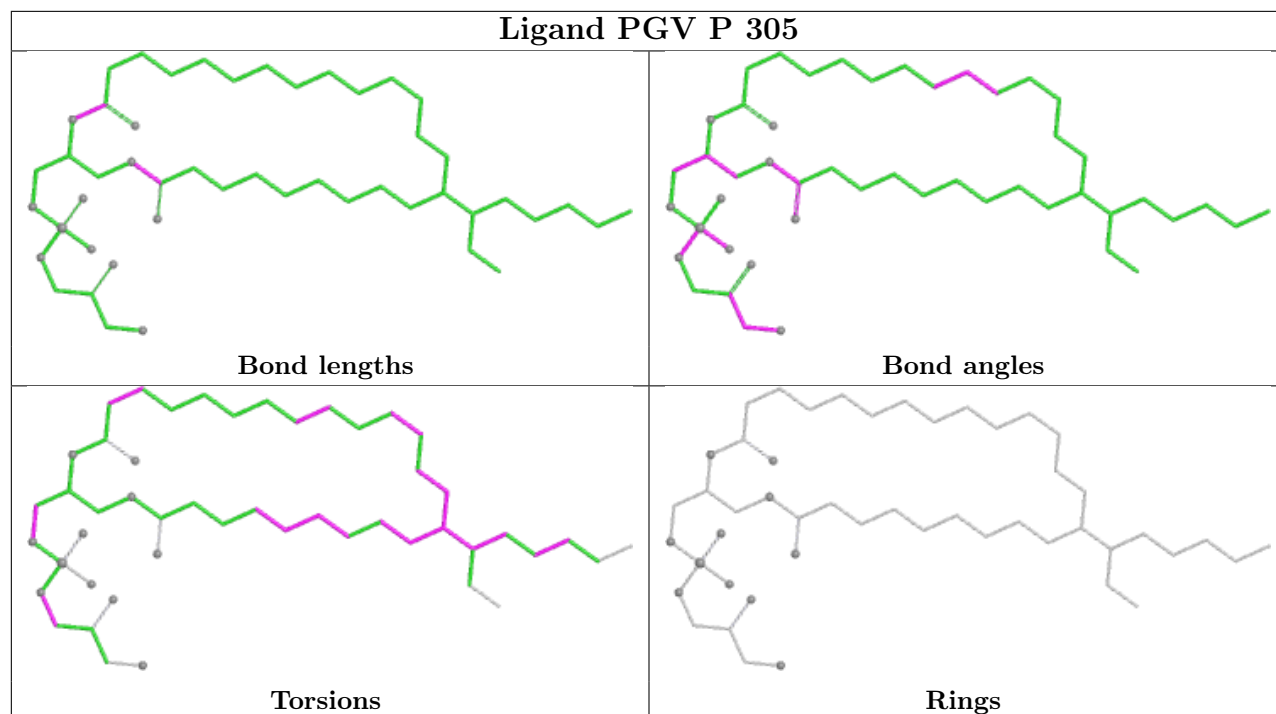
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	P	305	PGV	3	0
26	O	303	PSC	17	0
22	C	305	CHD	1	0
20	P	302	PGV	2	0
28	G	101	DMU	4	0
22	C	304	CHD	5	0
25	P	309	PEK	8	0
15	N	602	HEA	6	0
25	C	306	PEK	6	0
24	P	306	CDL	21	0
19	L	101	TGL	14	0
24	G	103	CDL	26	0
24	C	303	CDL	16	0
19	N	610	TGL	14	0
25	P	304	PEK	5	0
20	N	608	PGV	1	0
24	T	102	CDL	26	0
22	O	302	CHD	1	0
25	G	104	PEK	11	0
20	N	607	PGV	9	0
20	A	609	PGV	8	0

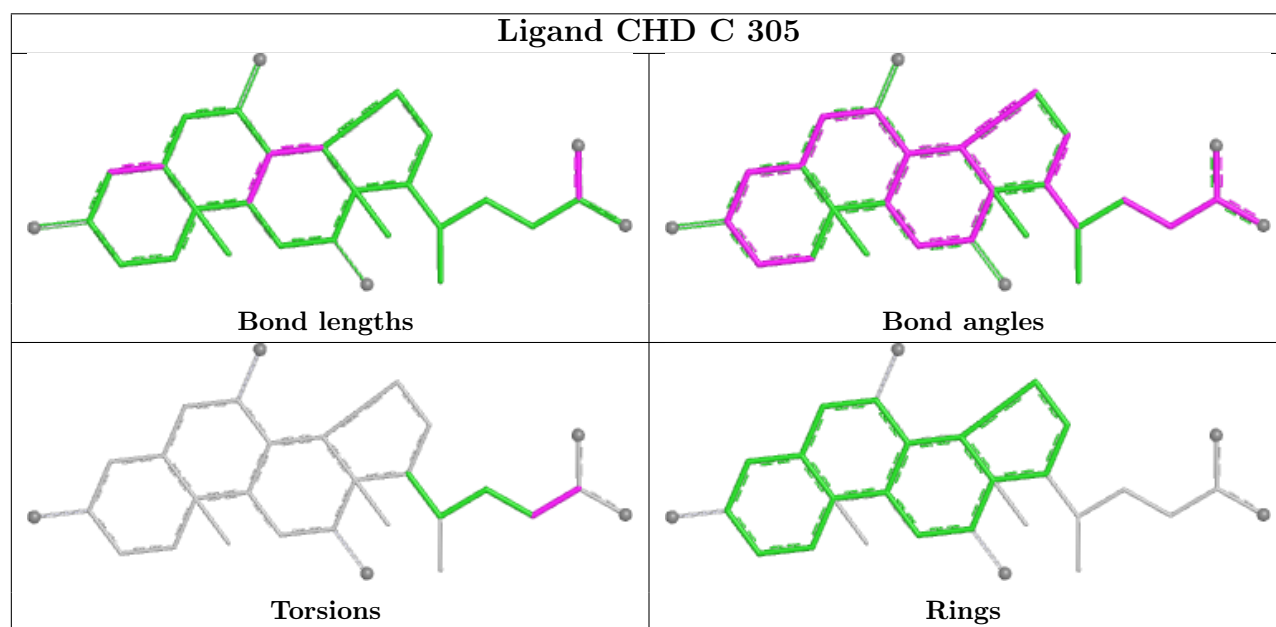
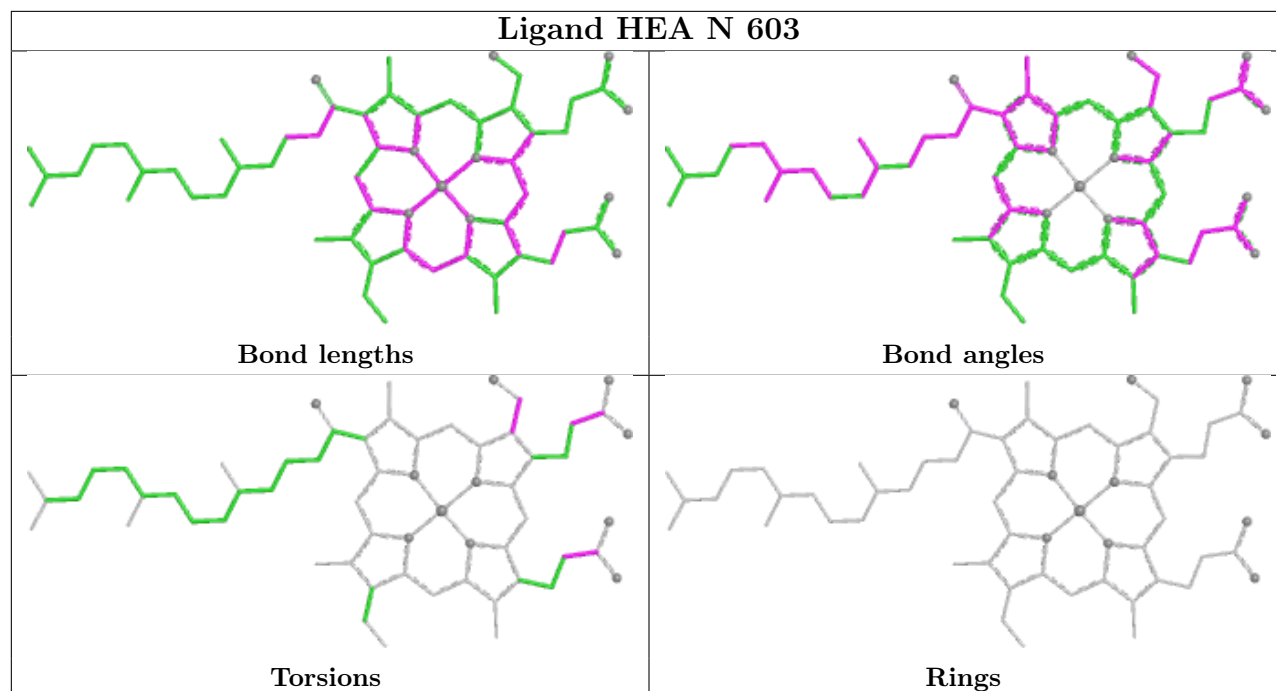
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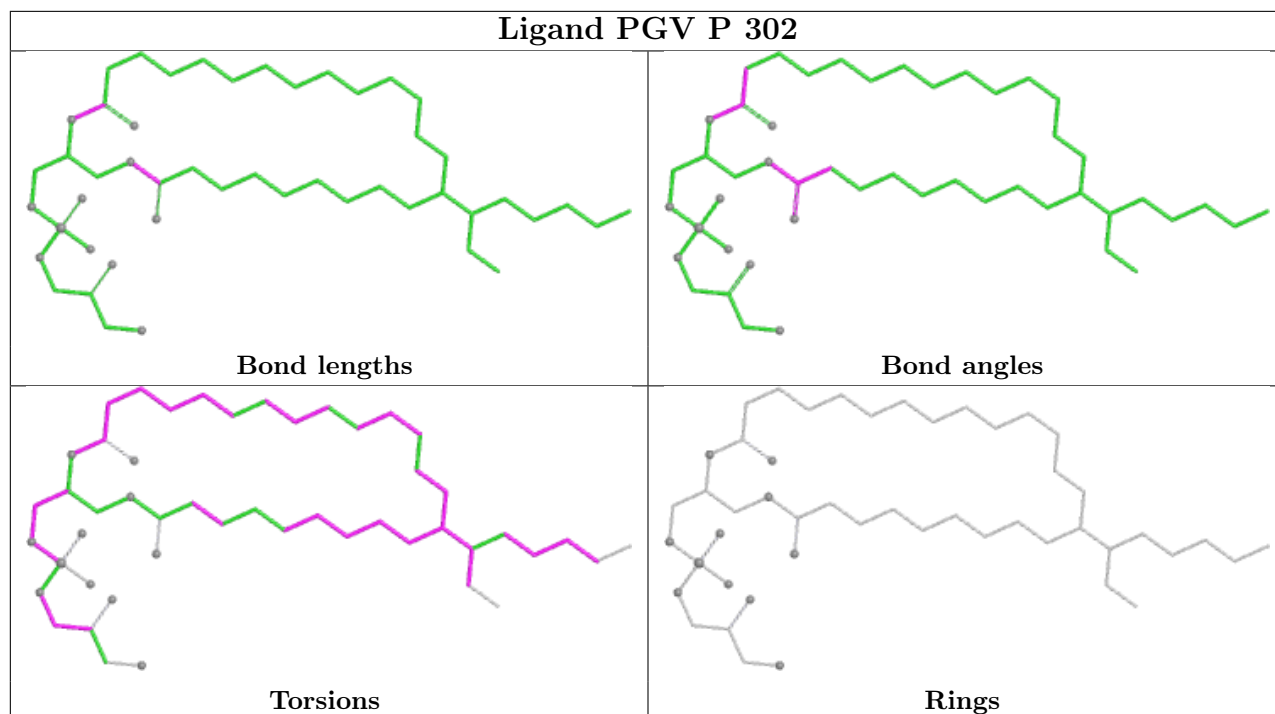
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	P	308	CHD	1	0
25	T	101	PEK	22	0
28	P	301	DMU	3	0
26	E	201	PSC	16	0
19	A	607	TGL	6	0
19	Q	201	TGL	2	0
22	B	302	CHD	2	0
20	C	302	PGV	2	0
15	A	603	HEA	1	0
25	G	102	PEK	2	0
15	A	602	HEA	6	0
20	C	307	PGV	3	0
19	D	201	TGL	12	0
22	P	307	CHD	7	0
19	N	609	TGL	8	0

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

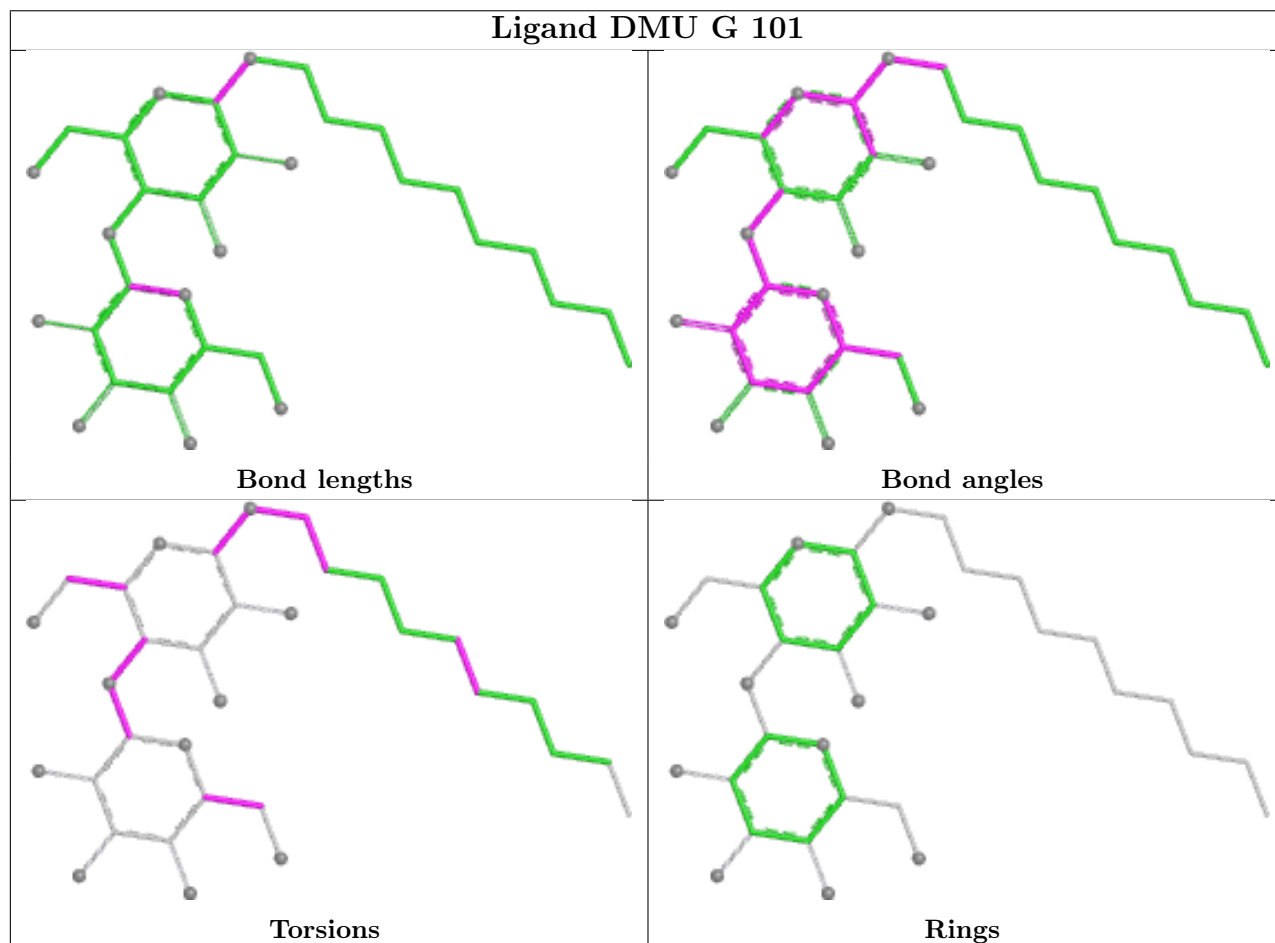


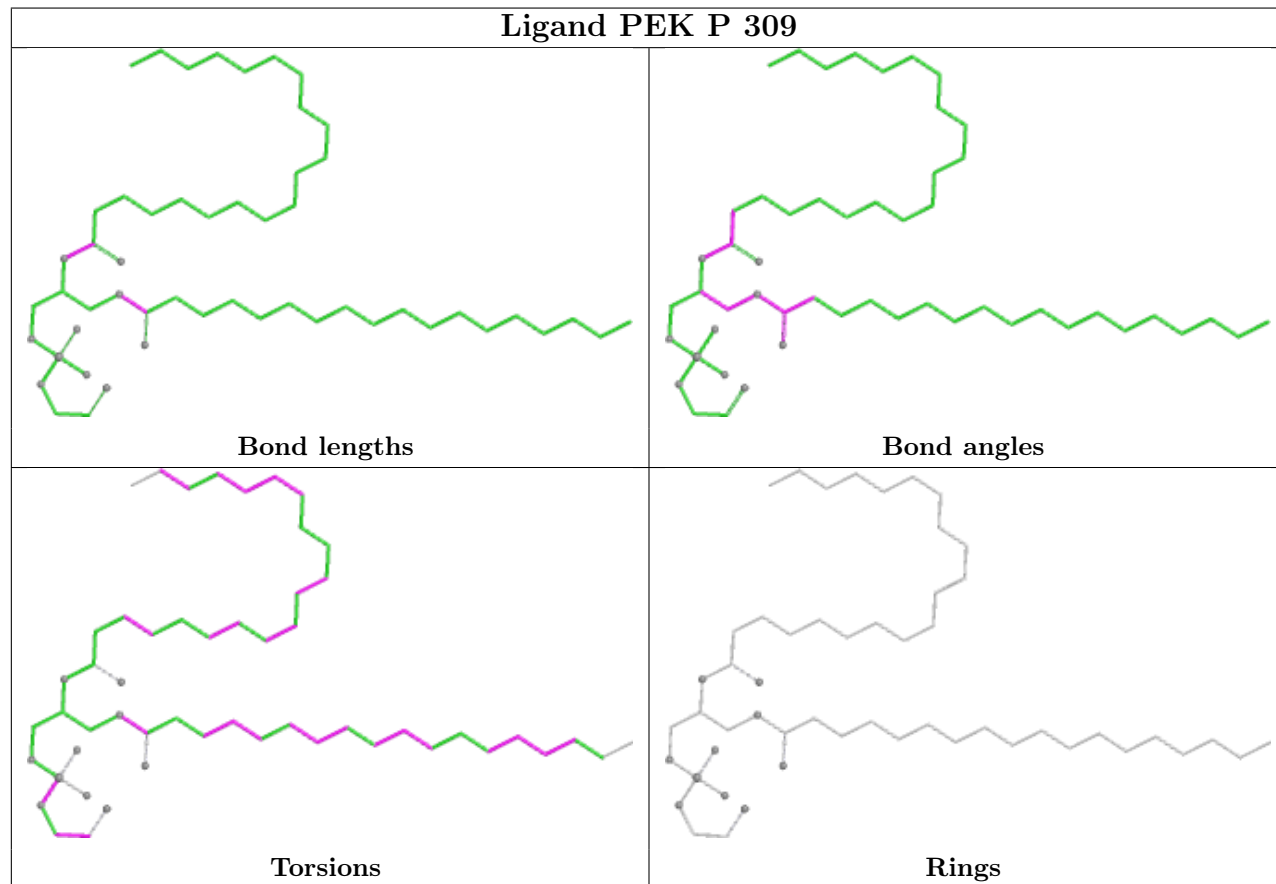
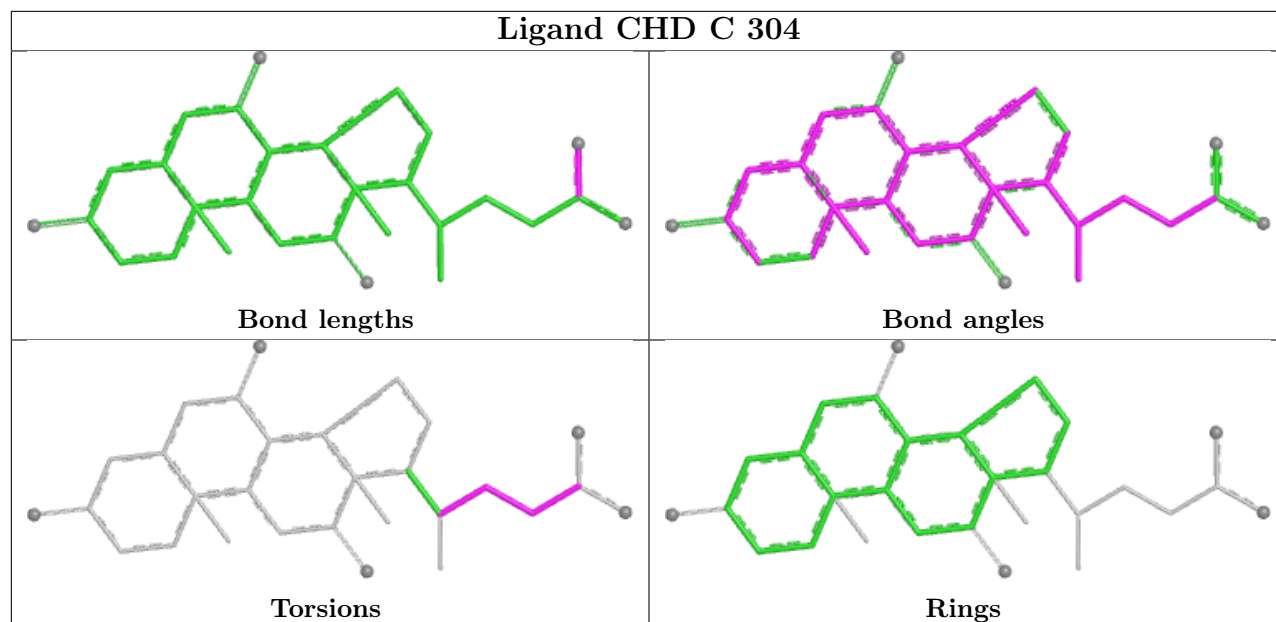


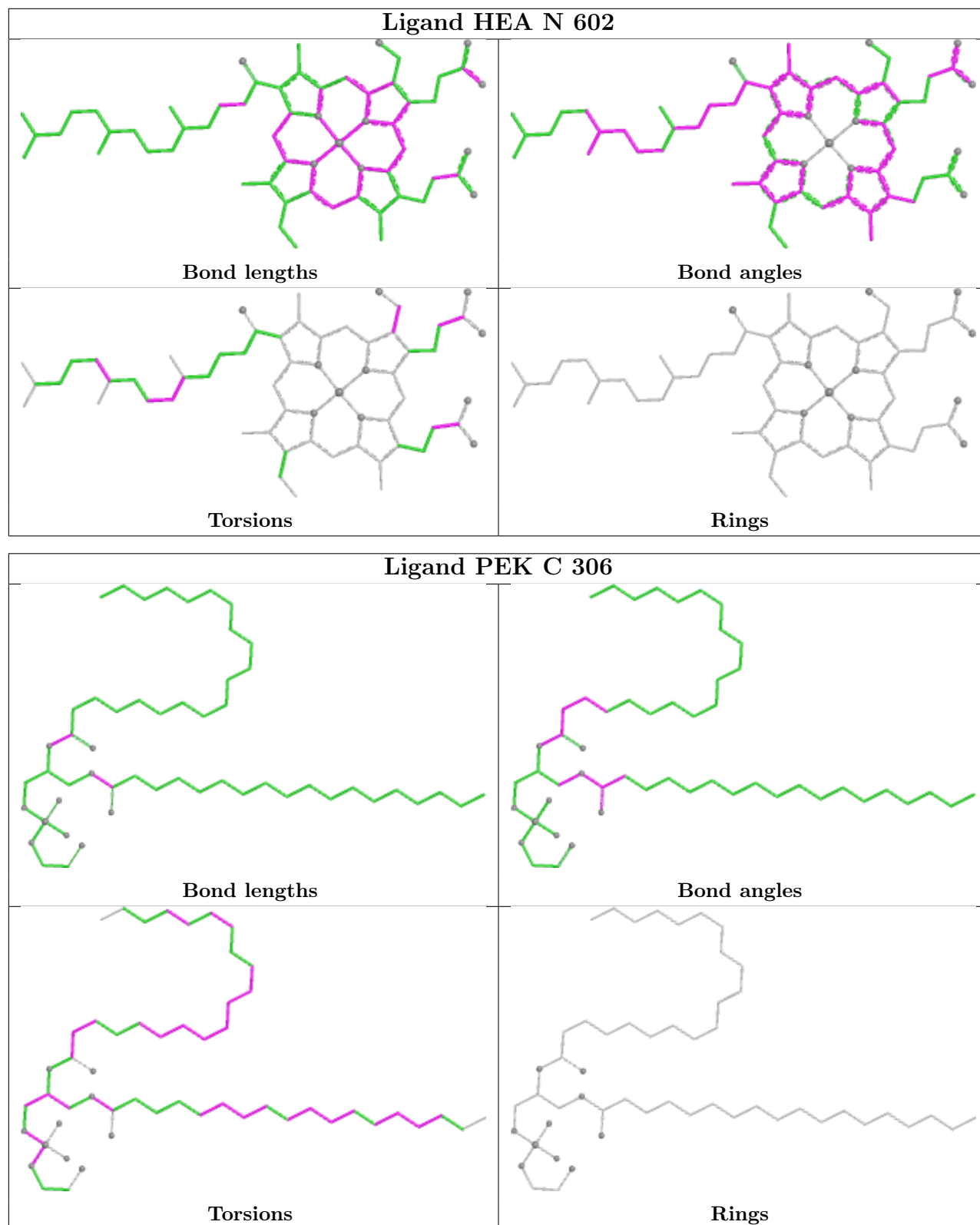
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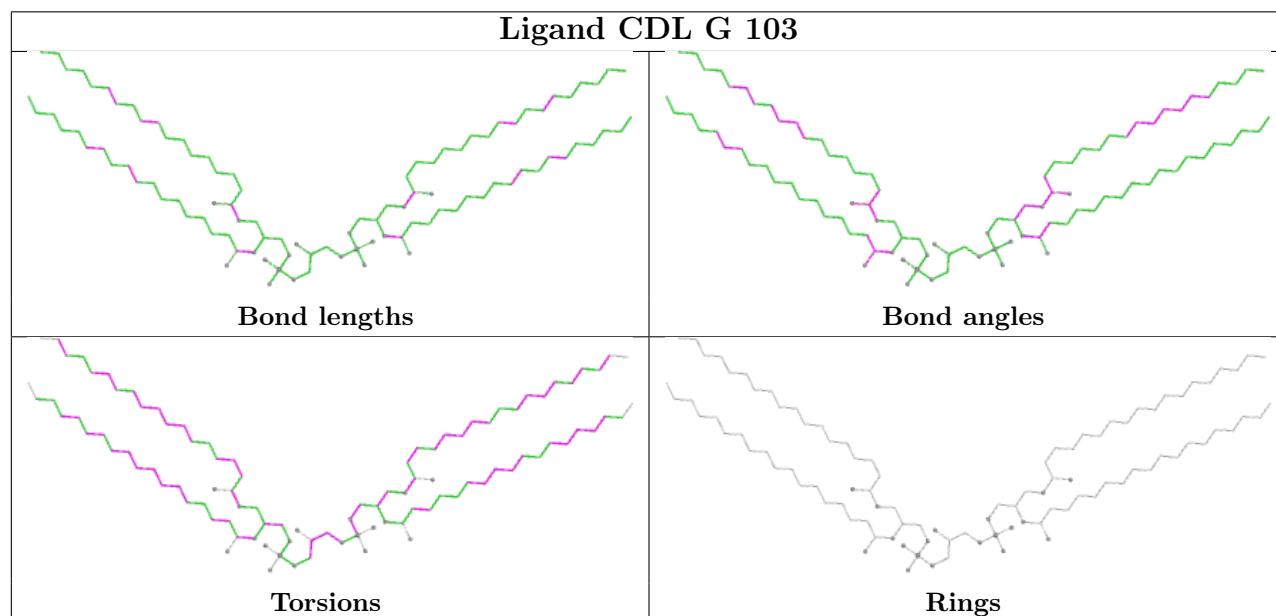
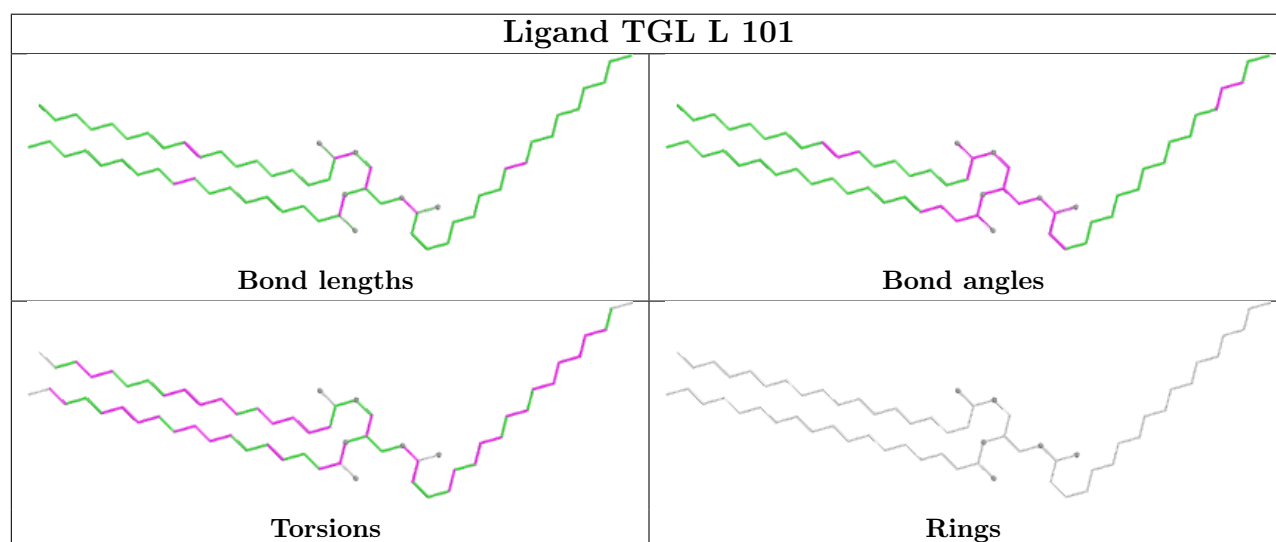
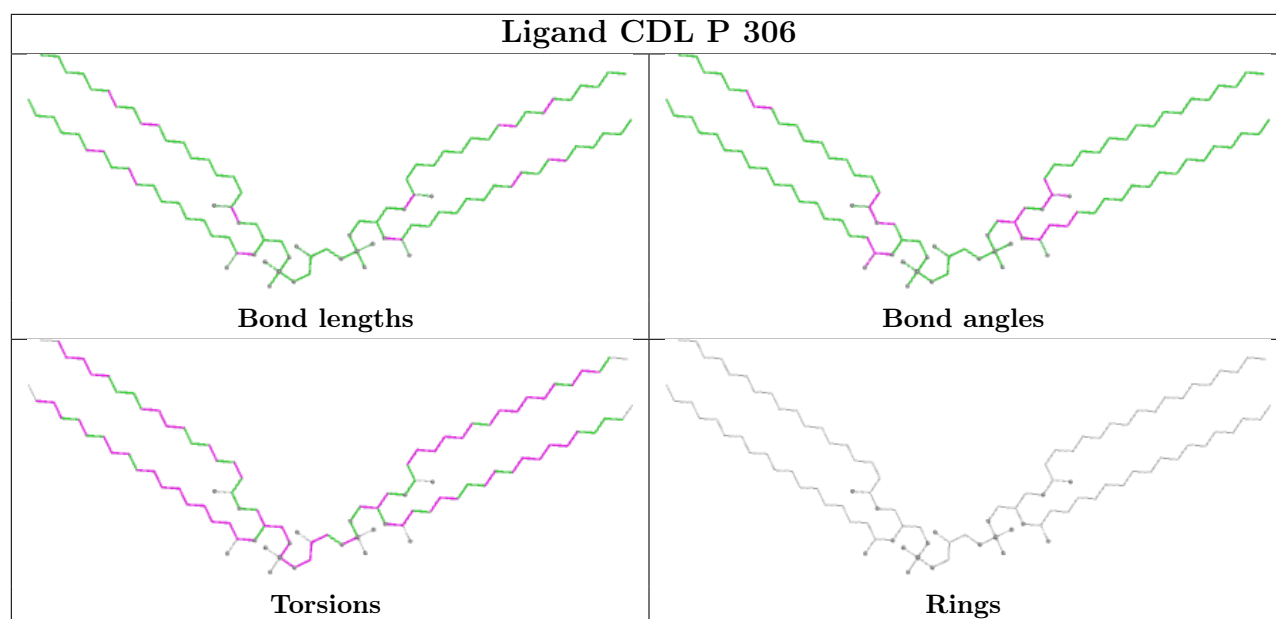


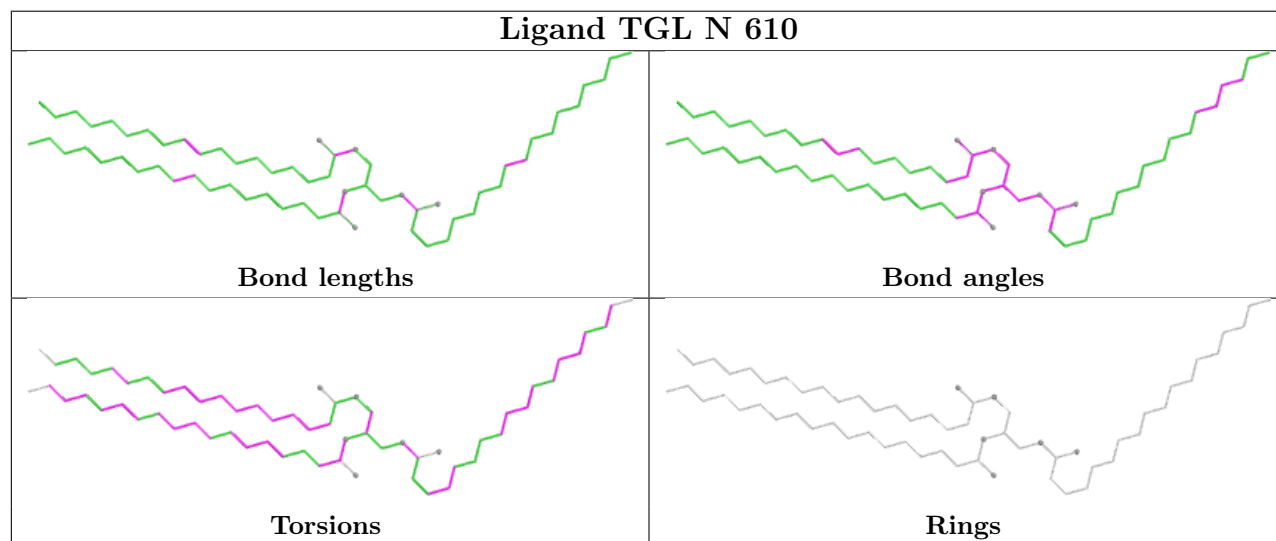
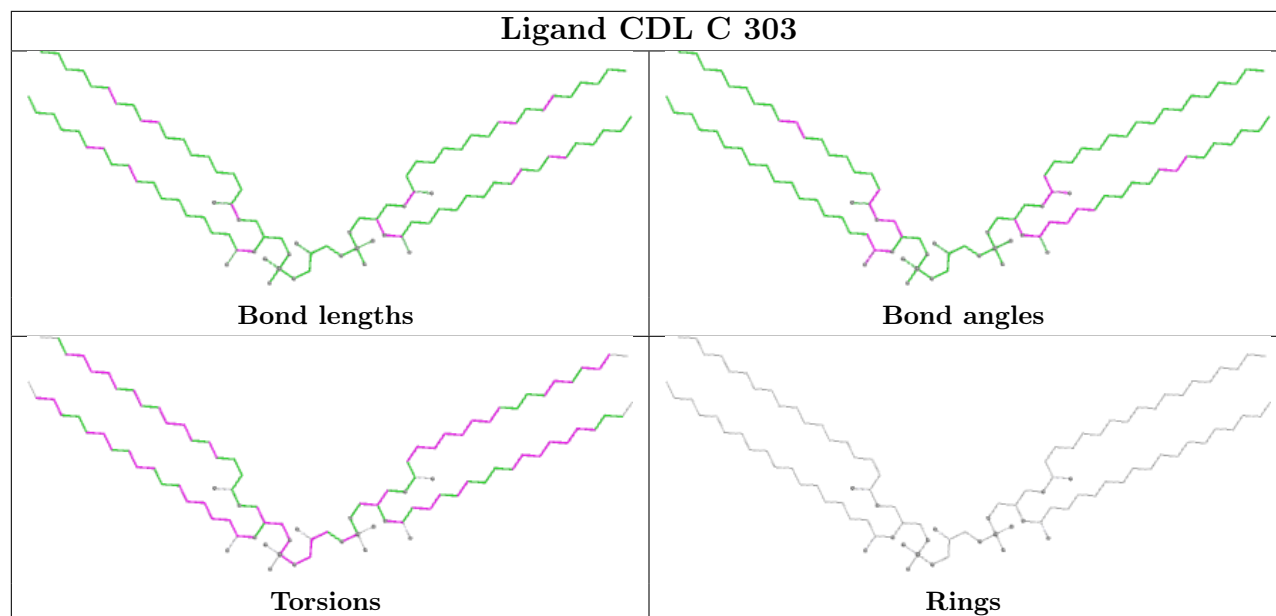
Ligand DMU G 101

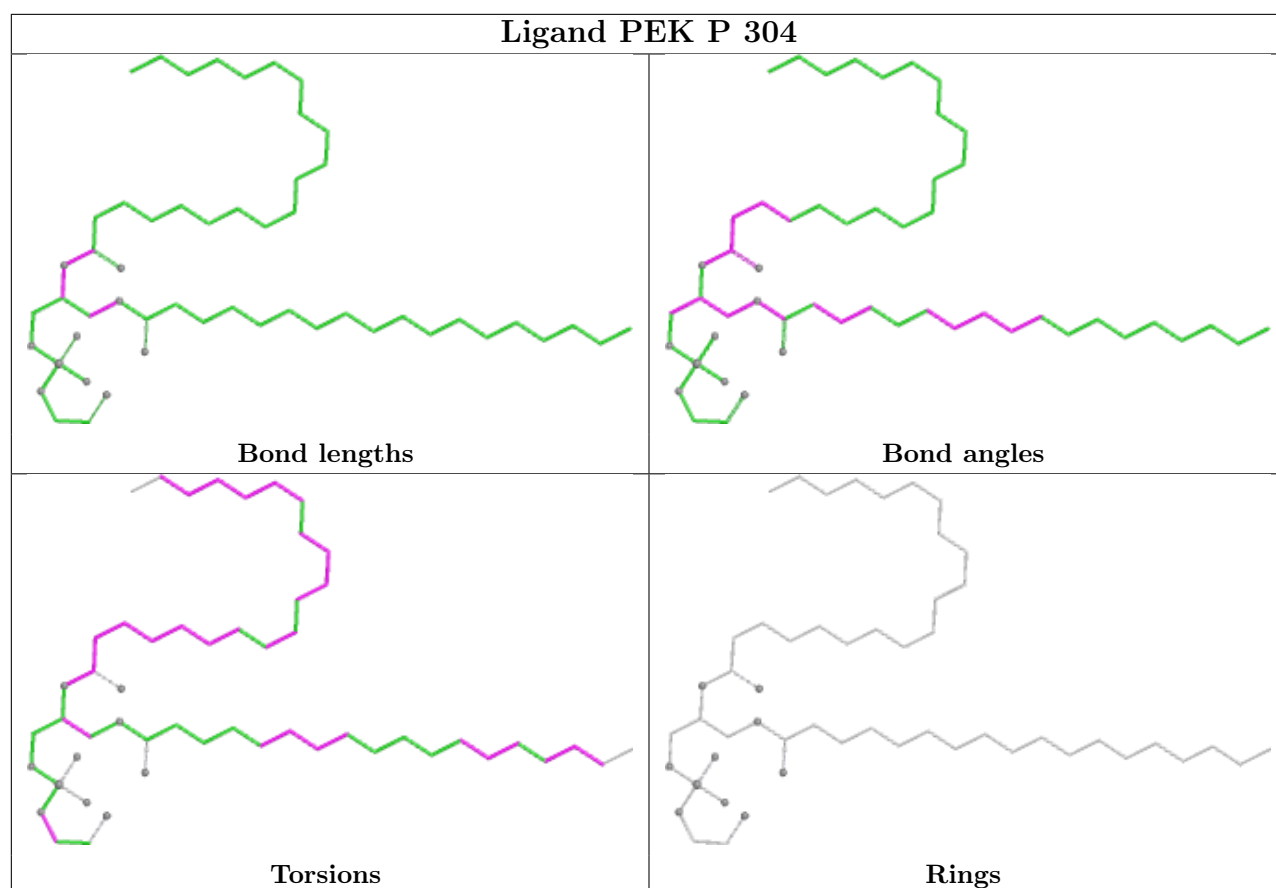


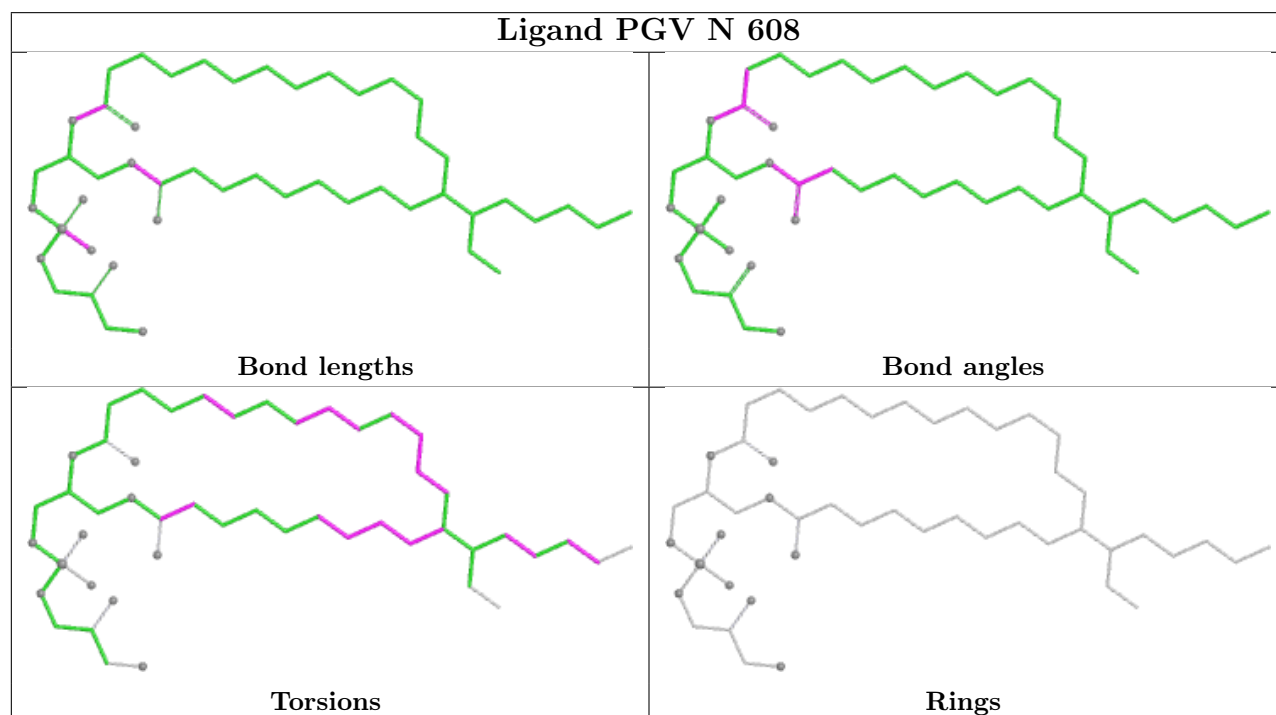
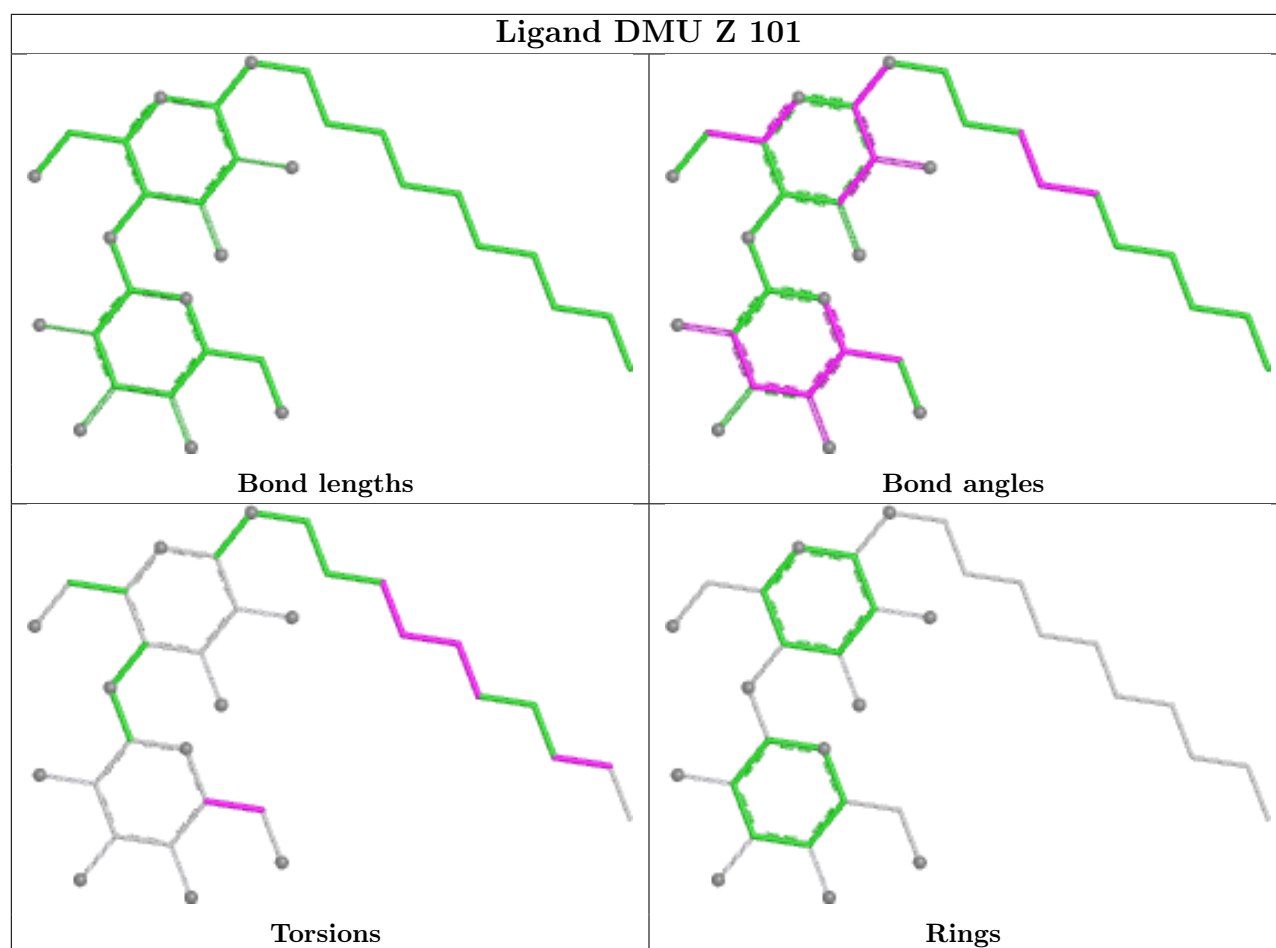


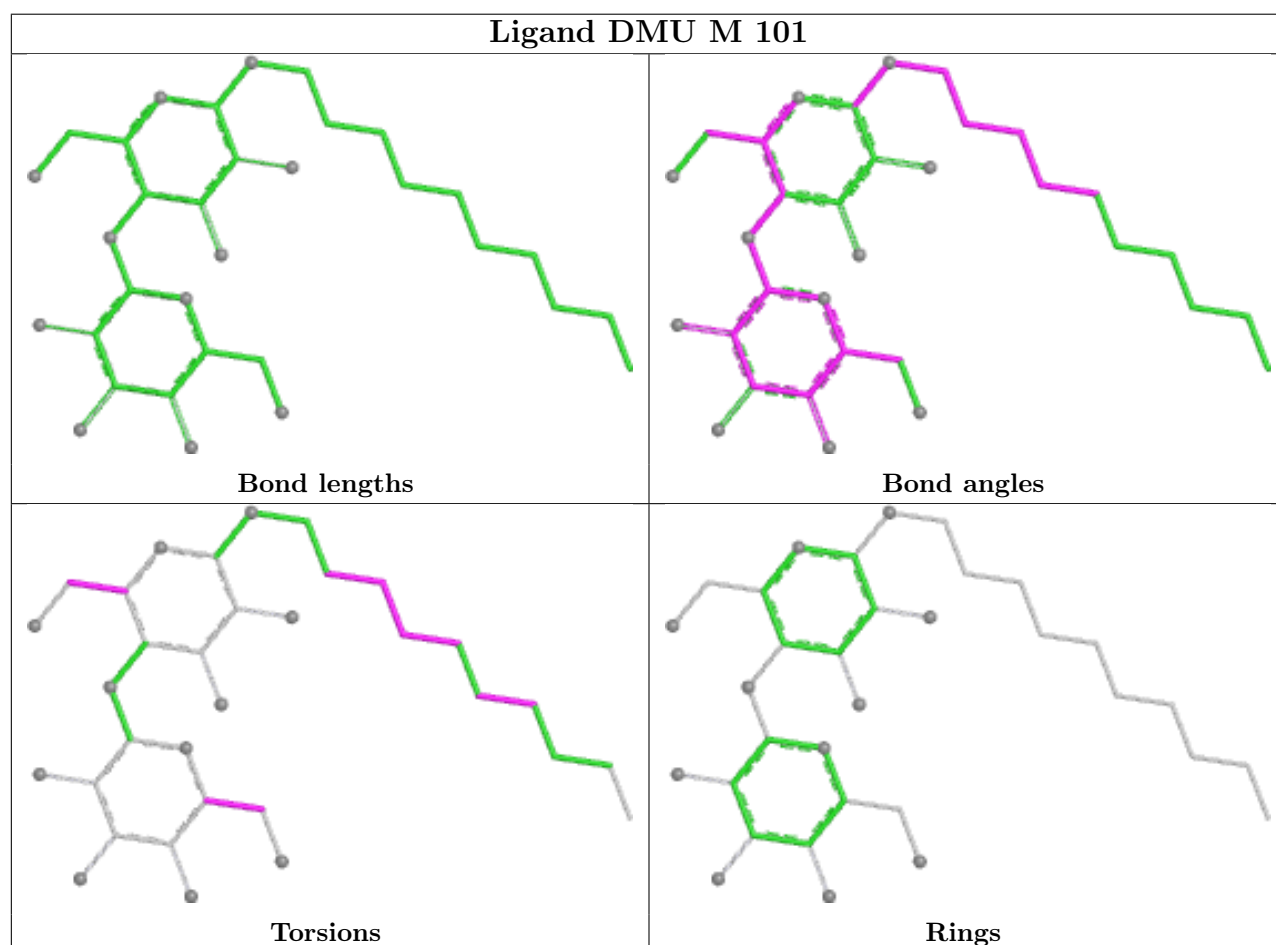
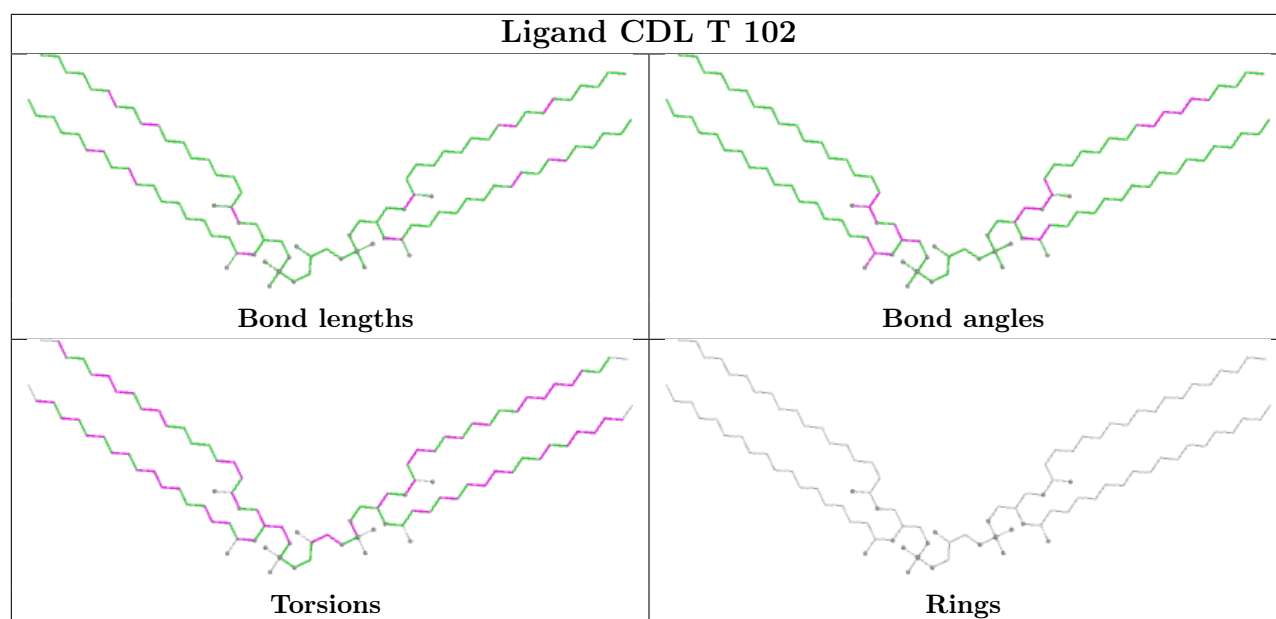


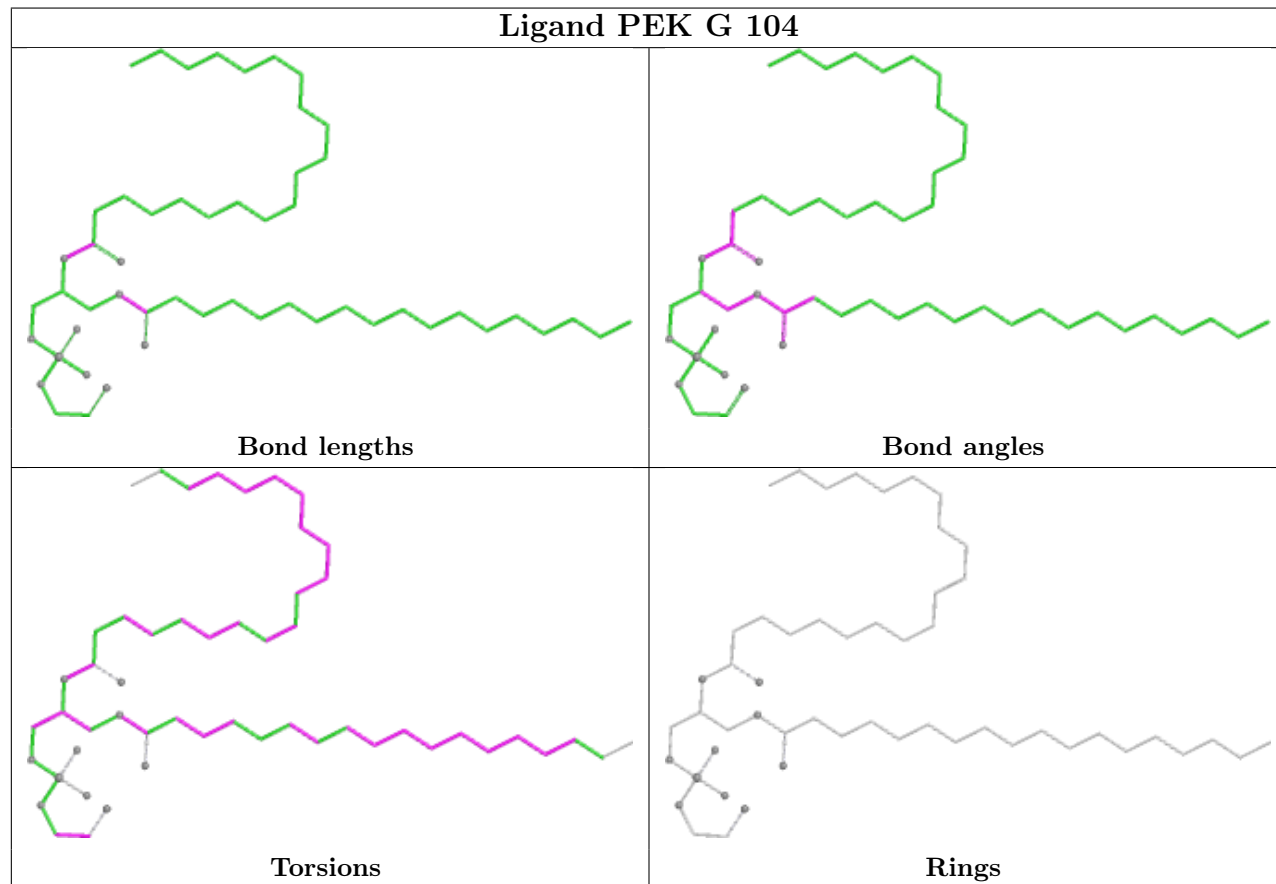
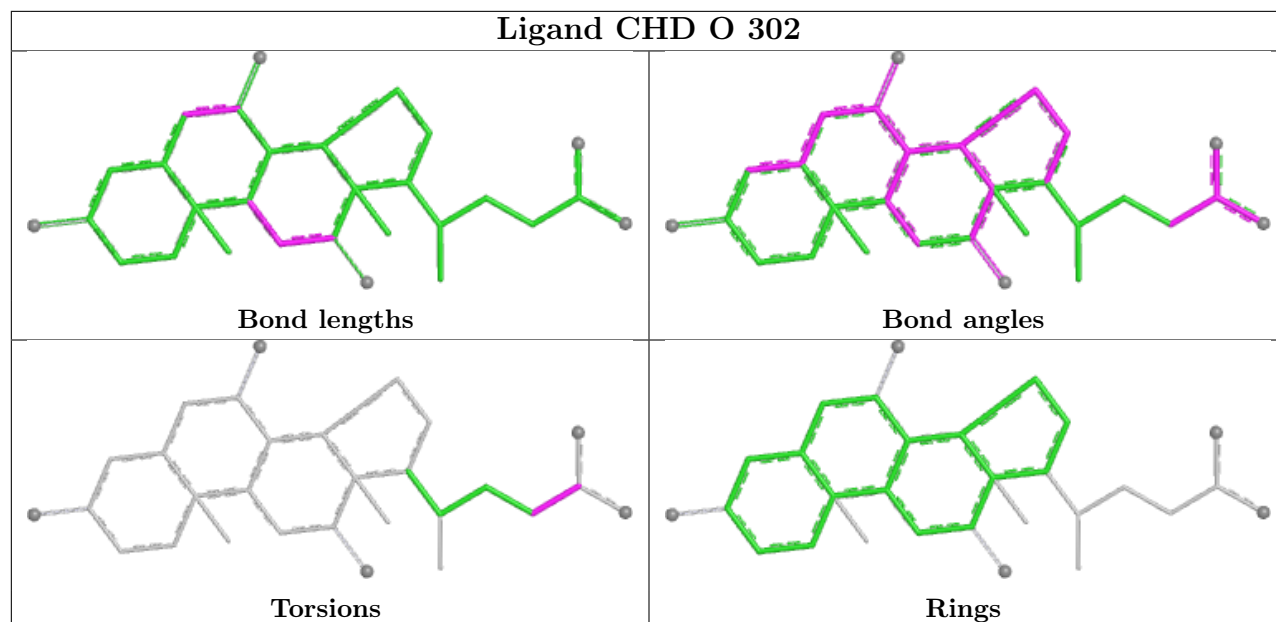


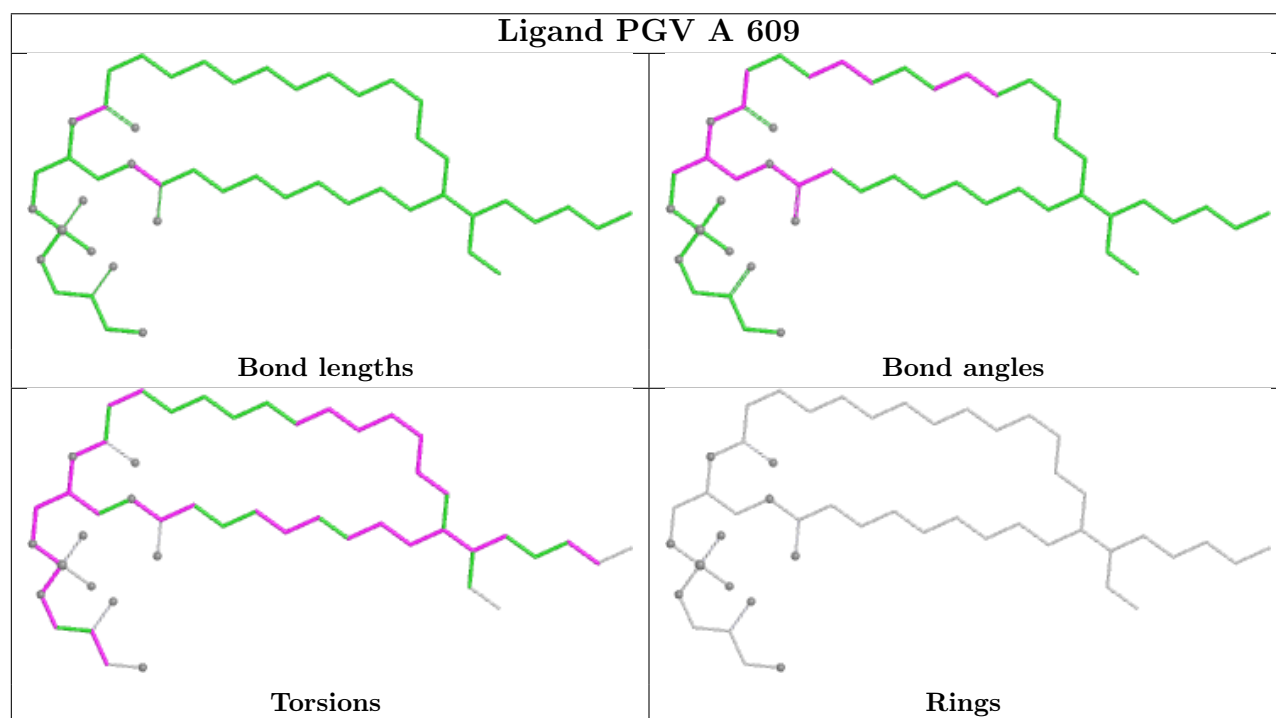
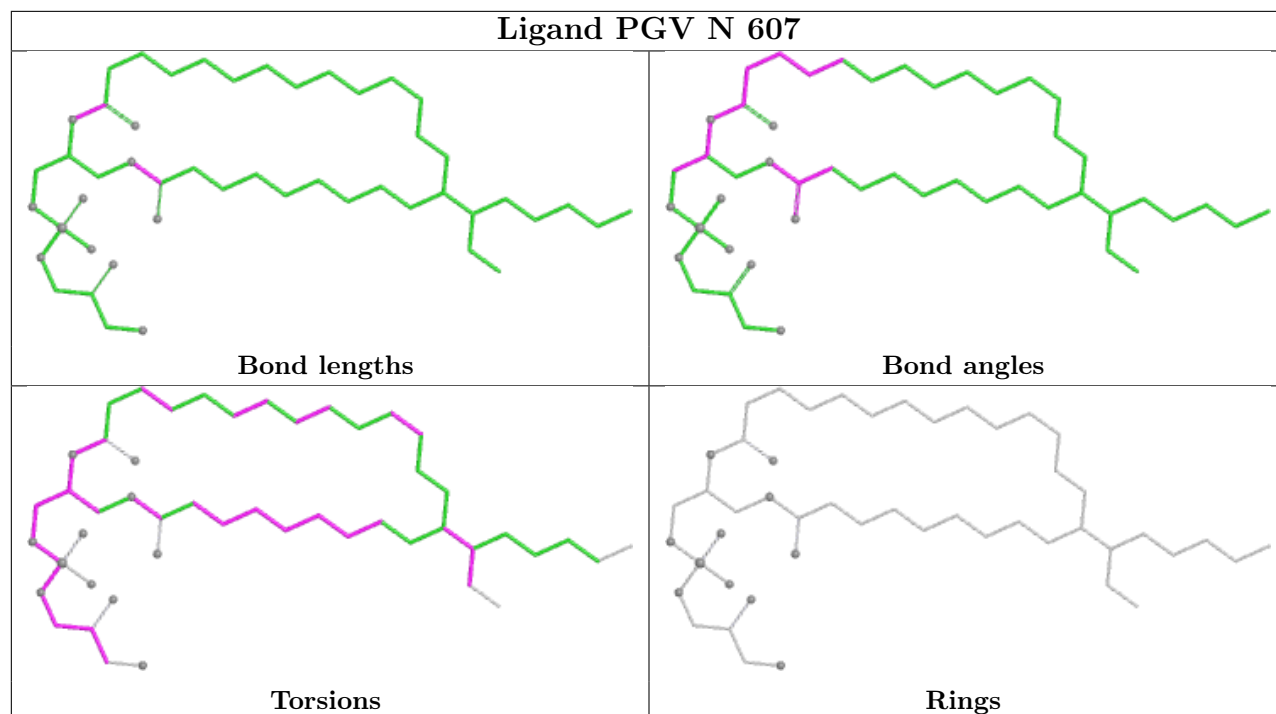


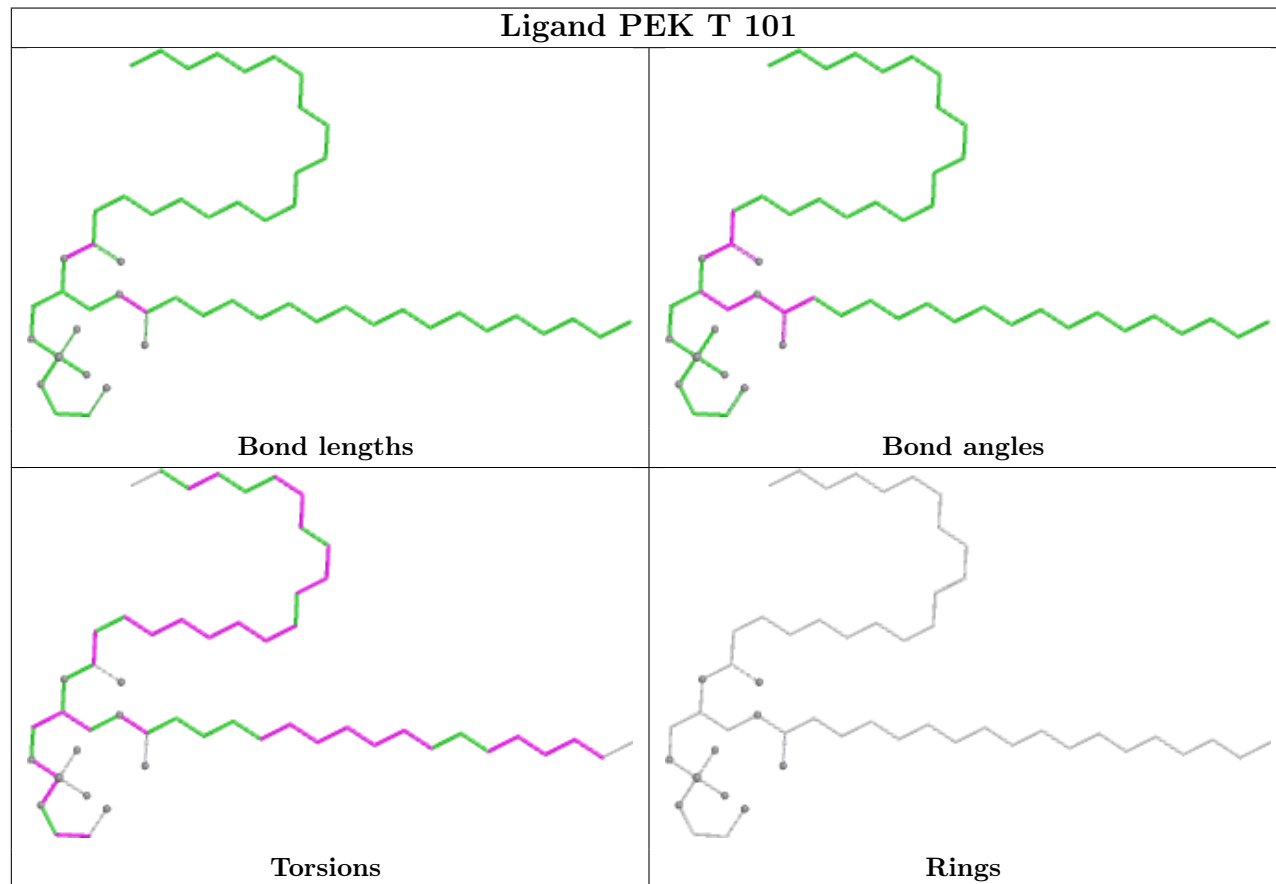
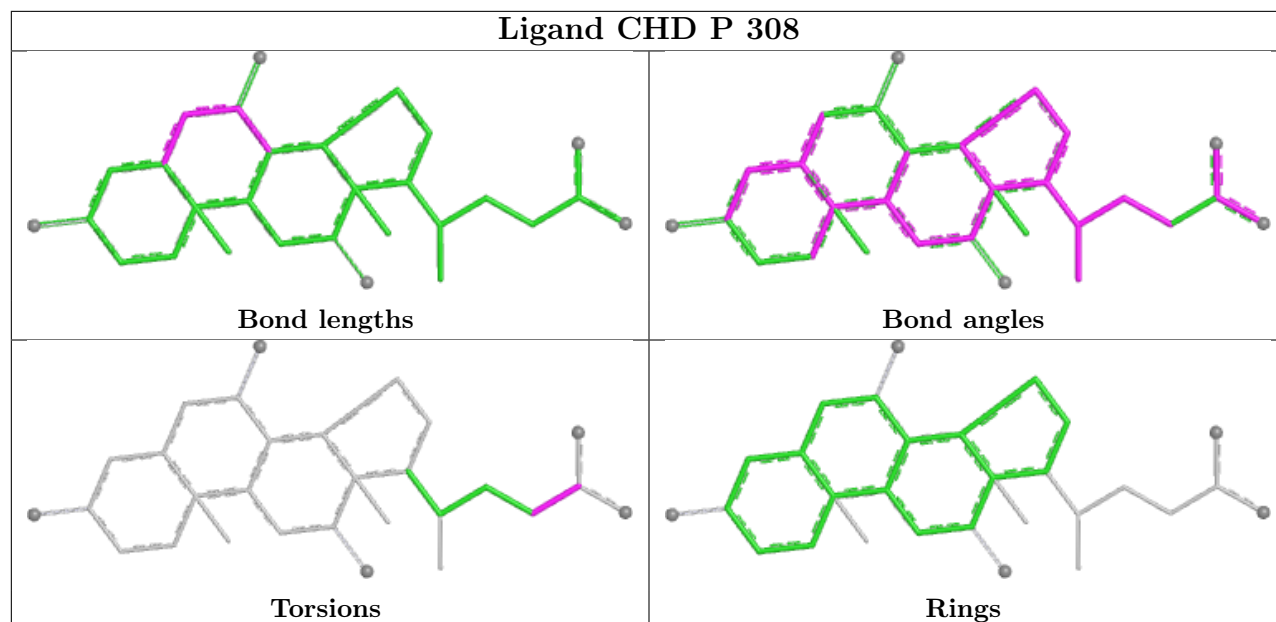


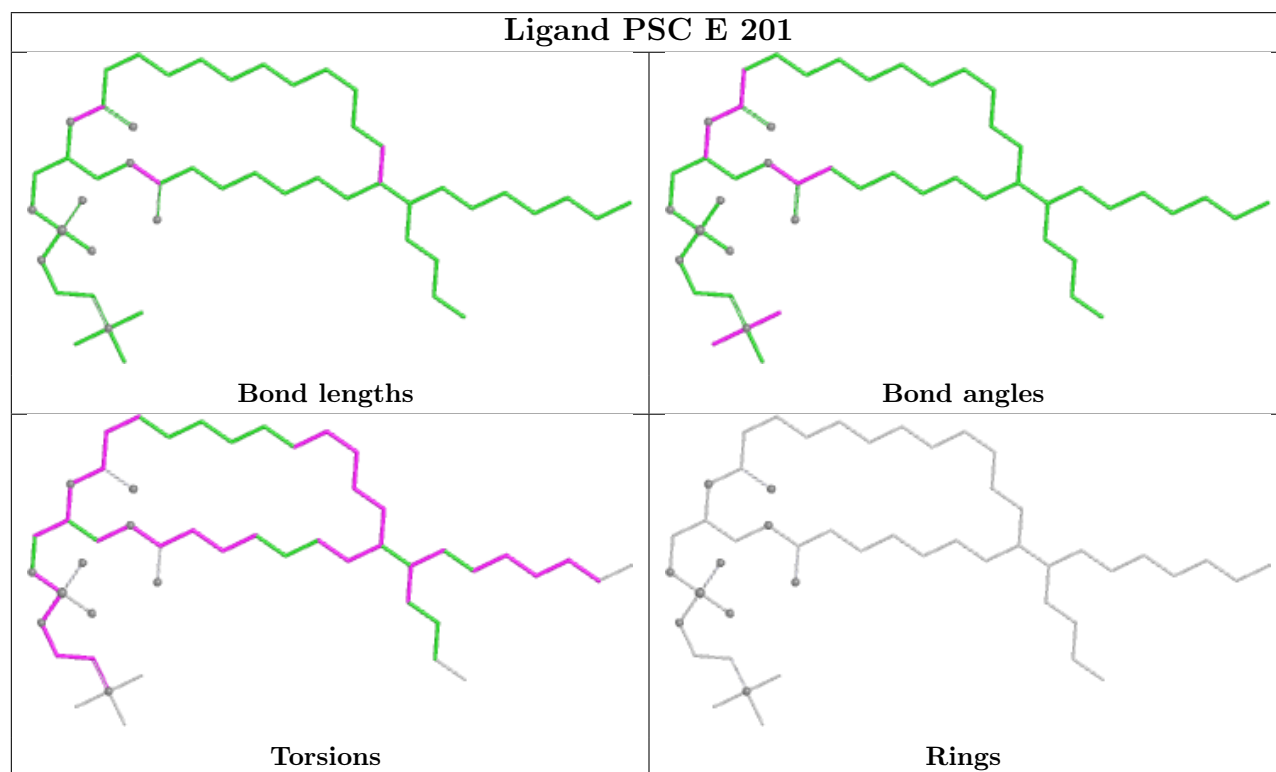
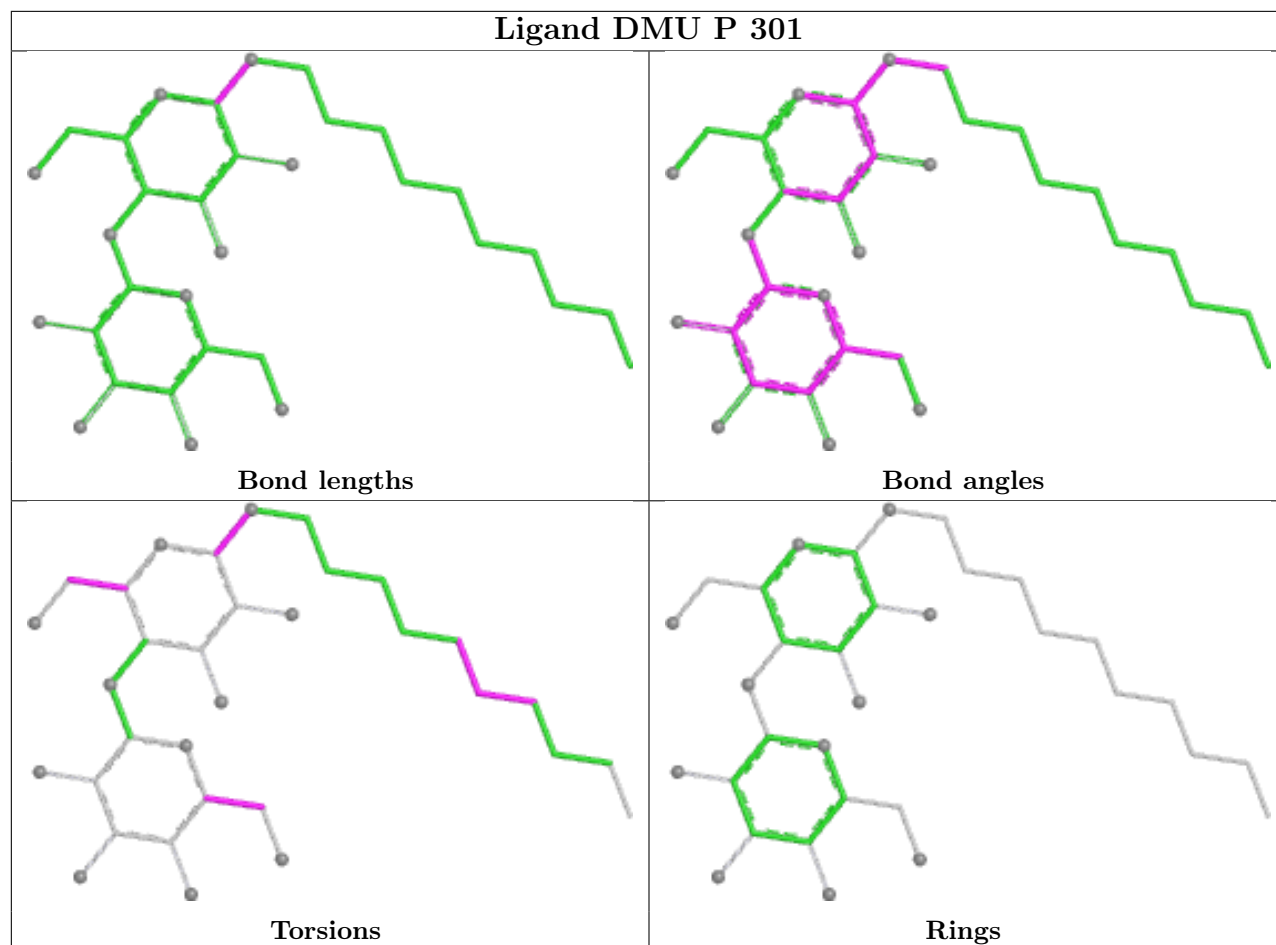


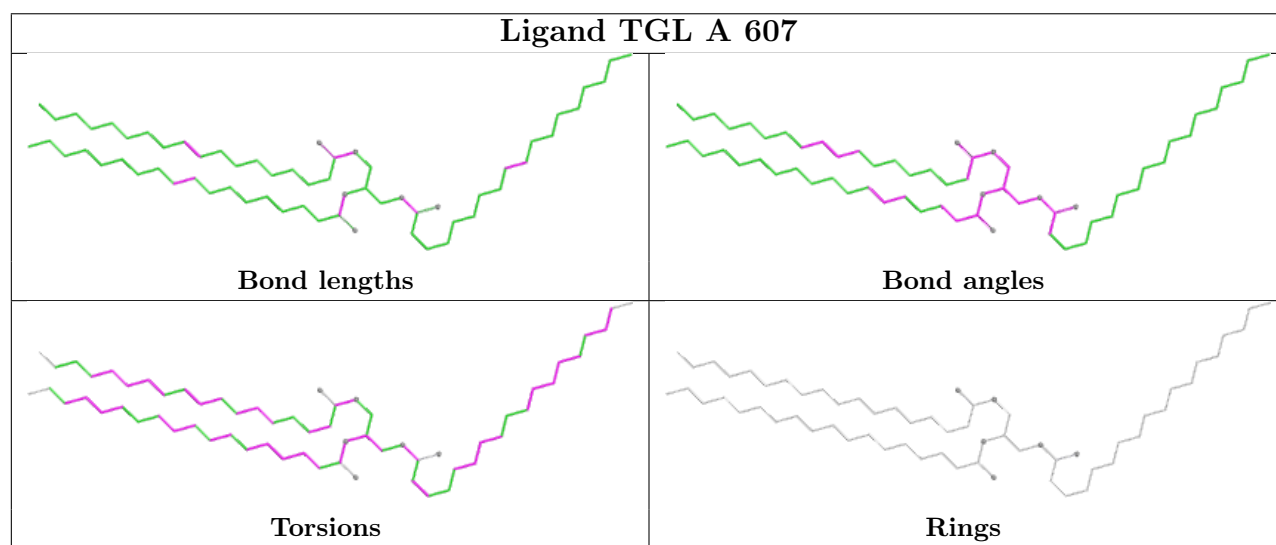
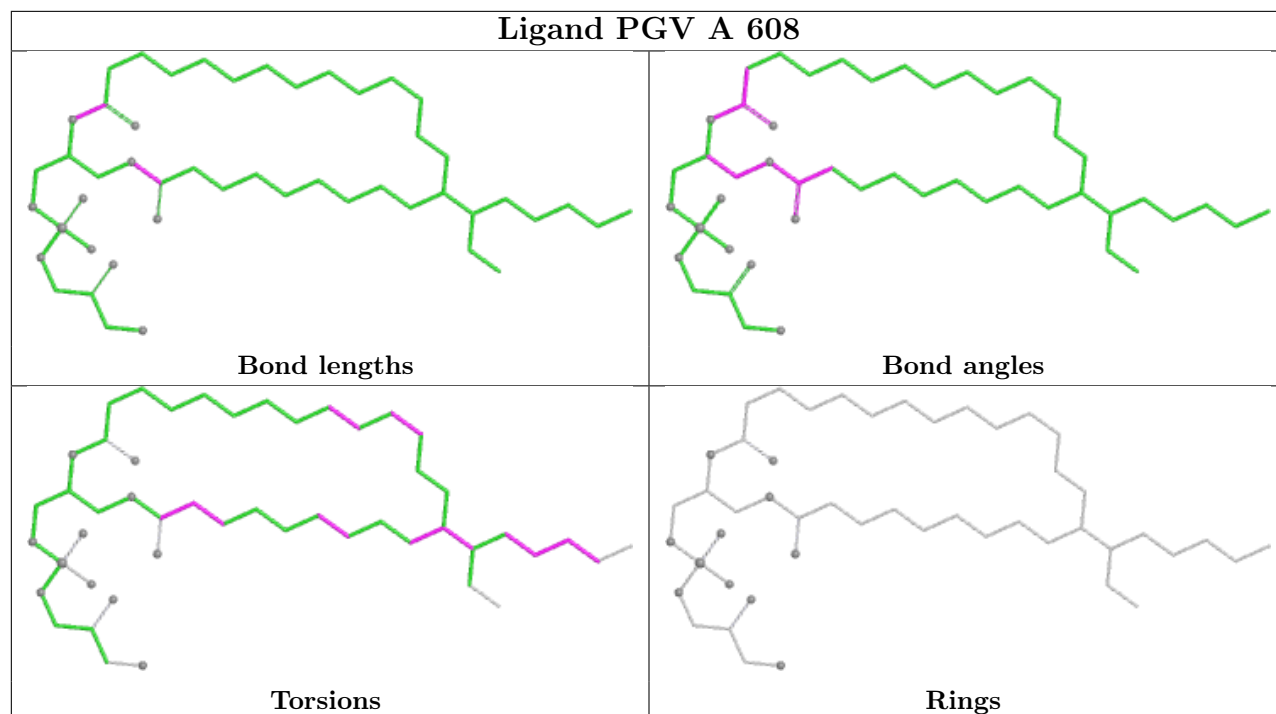




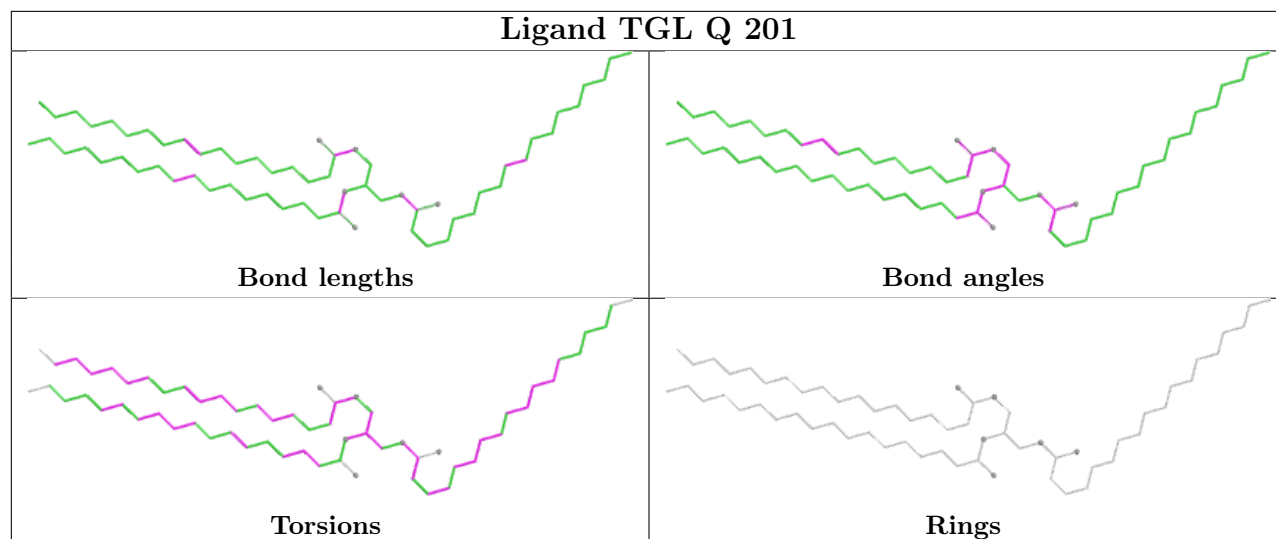




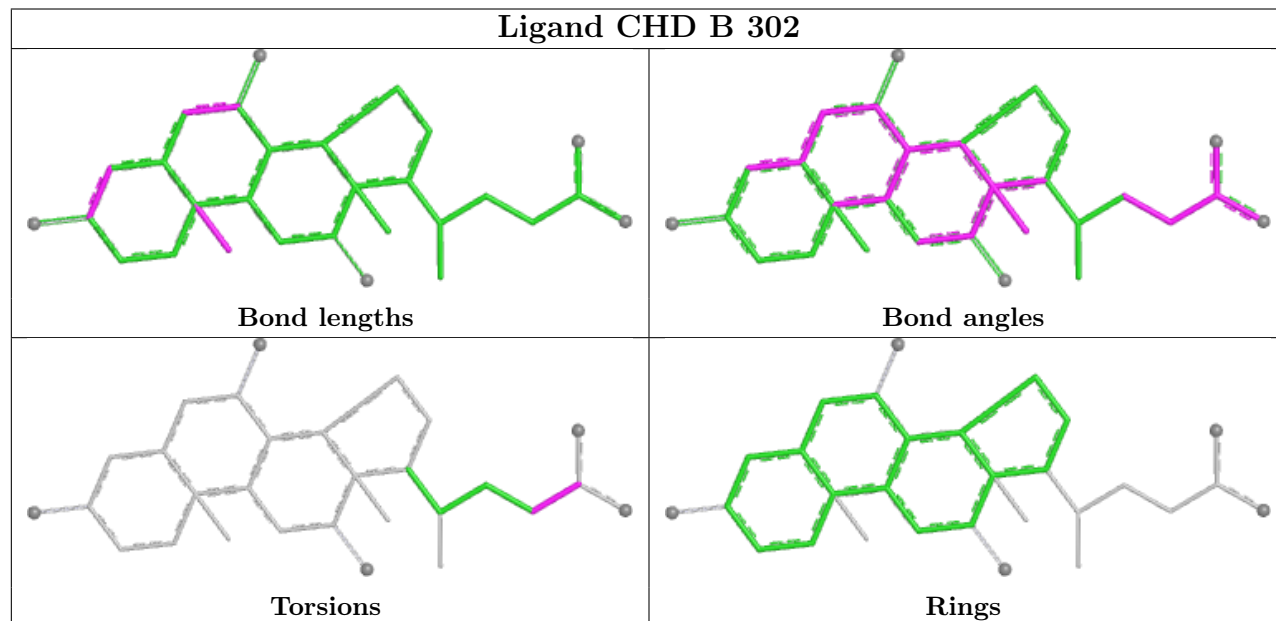


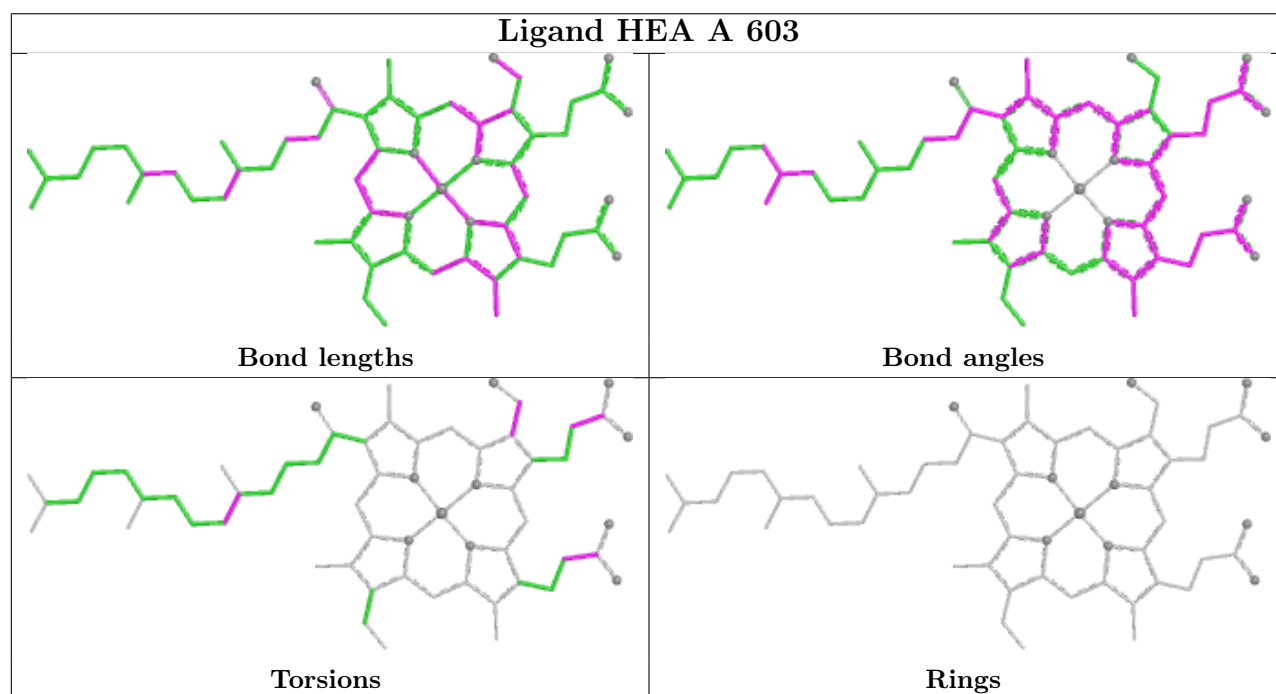
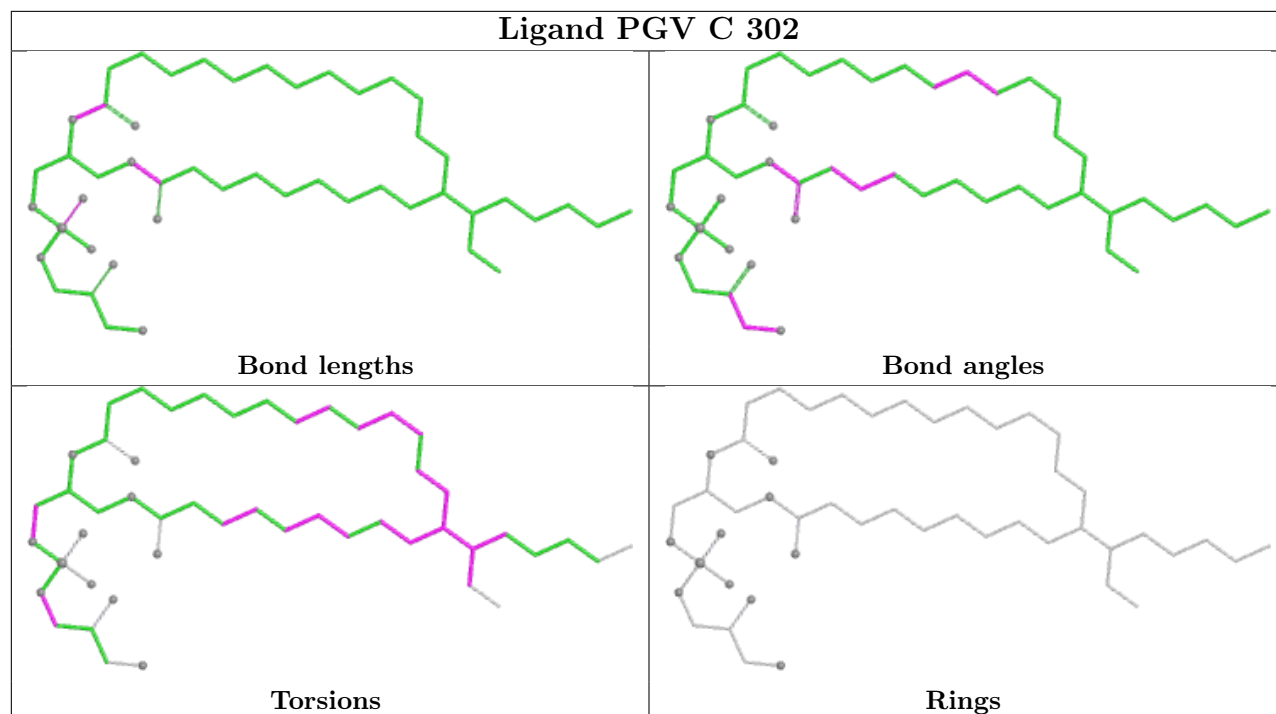


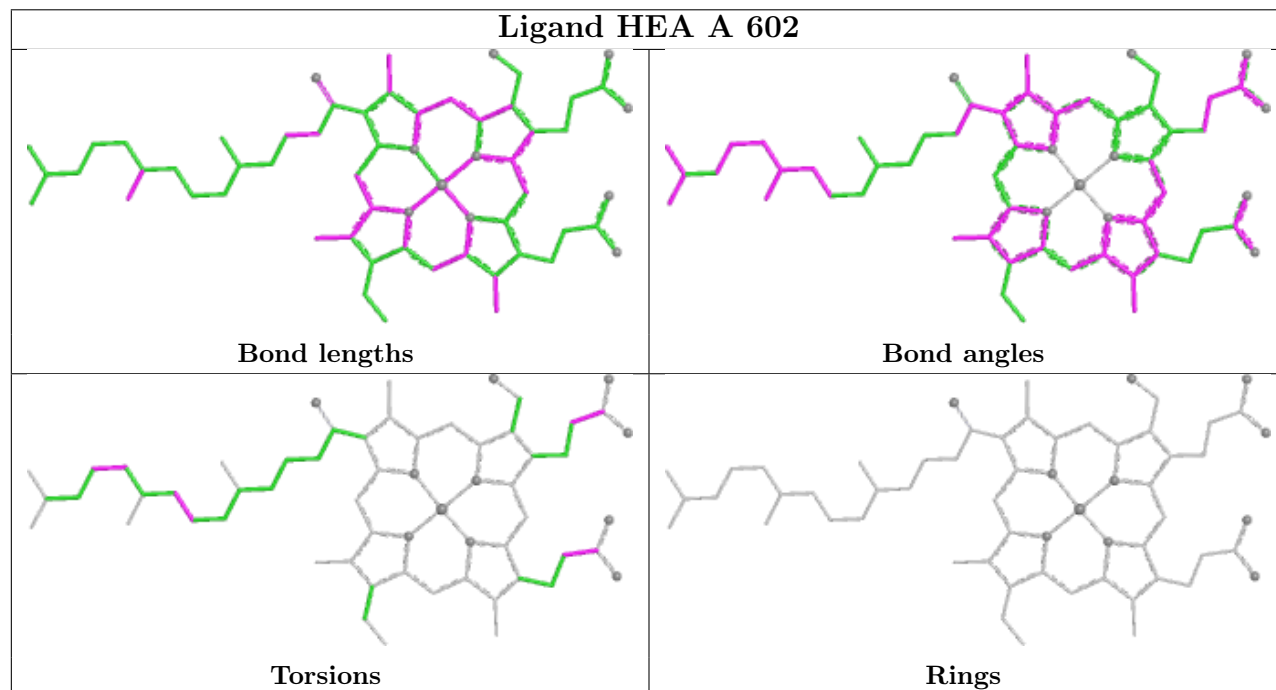
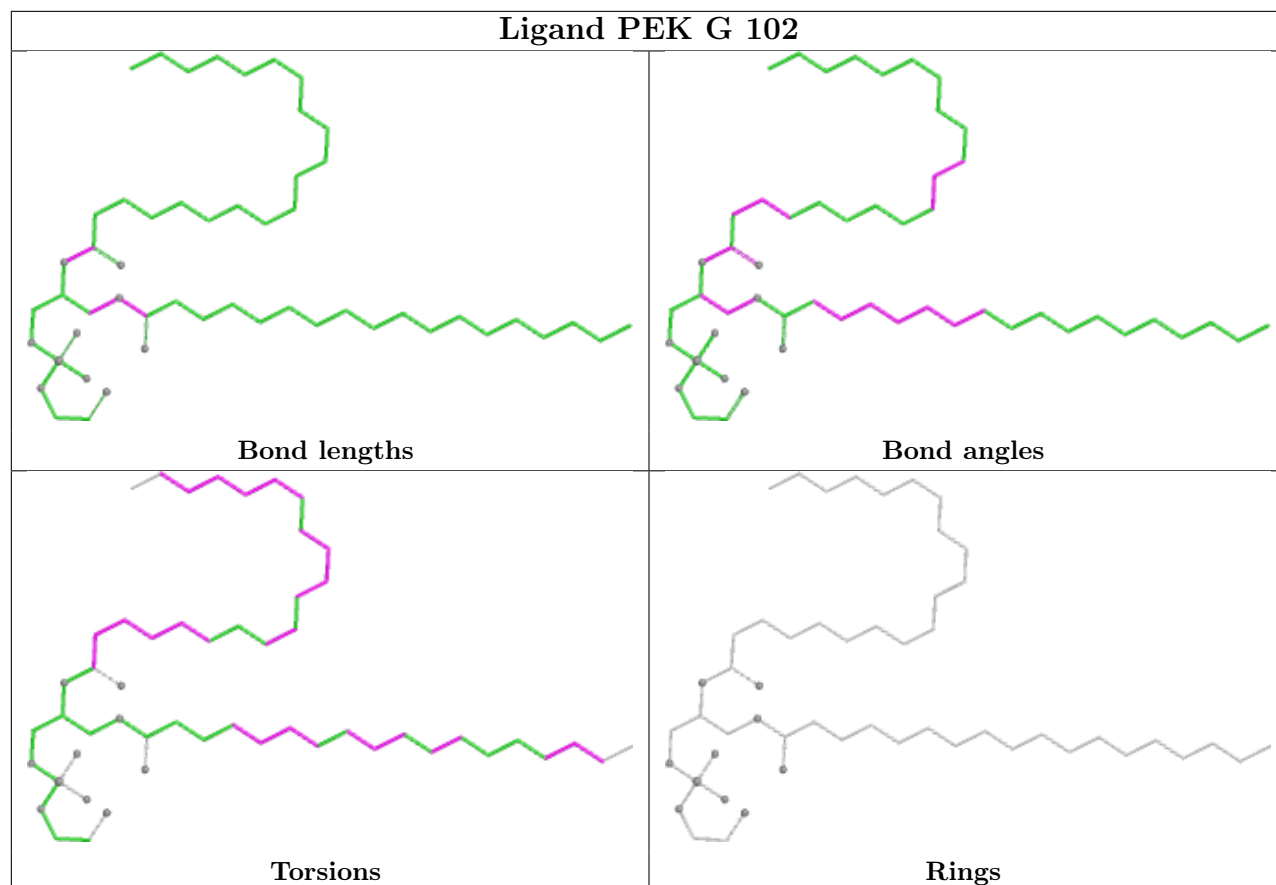
Ligand TGL Q 201

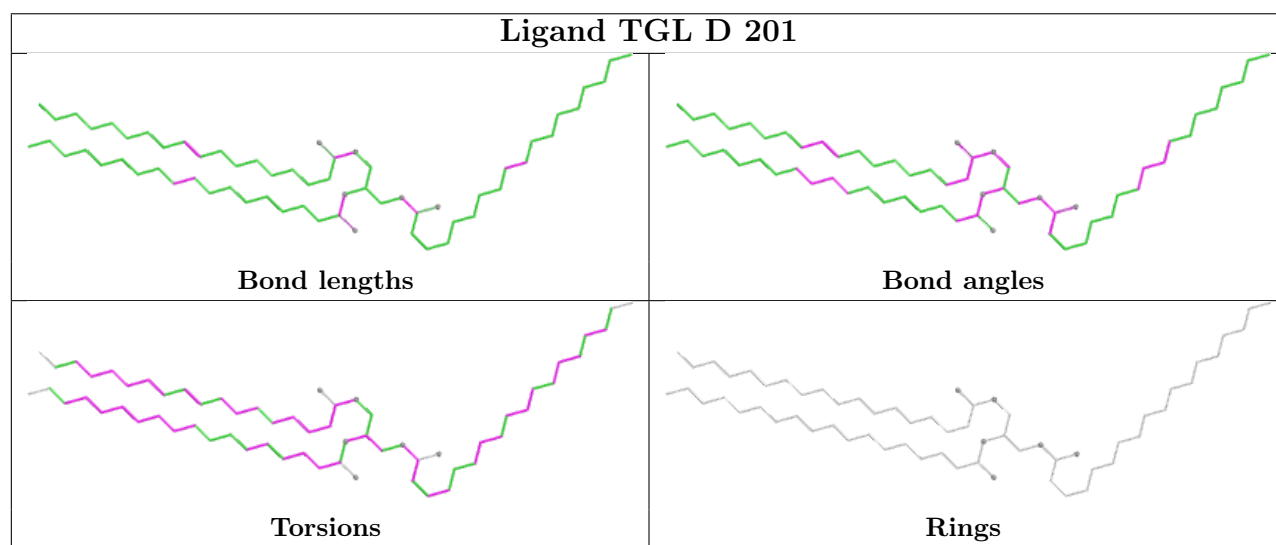
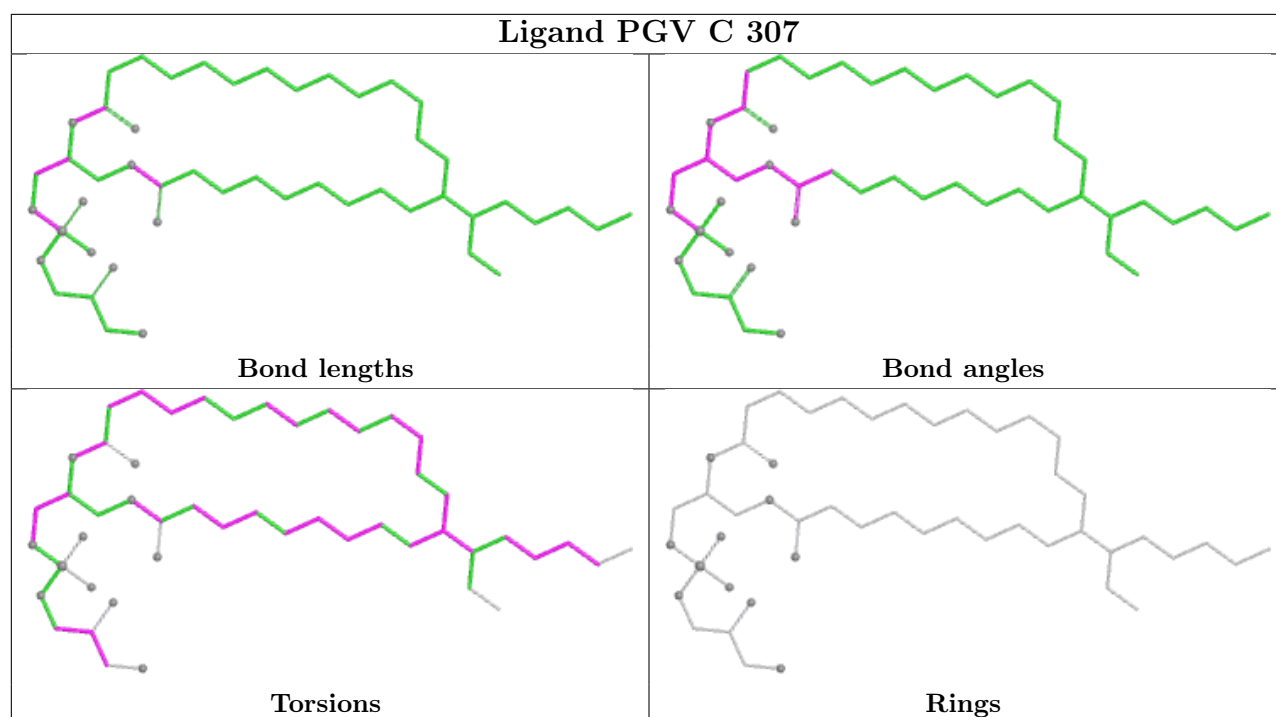


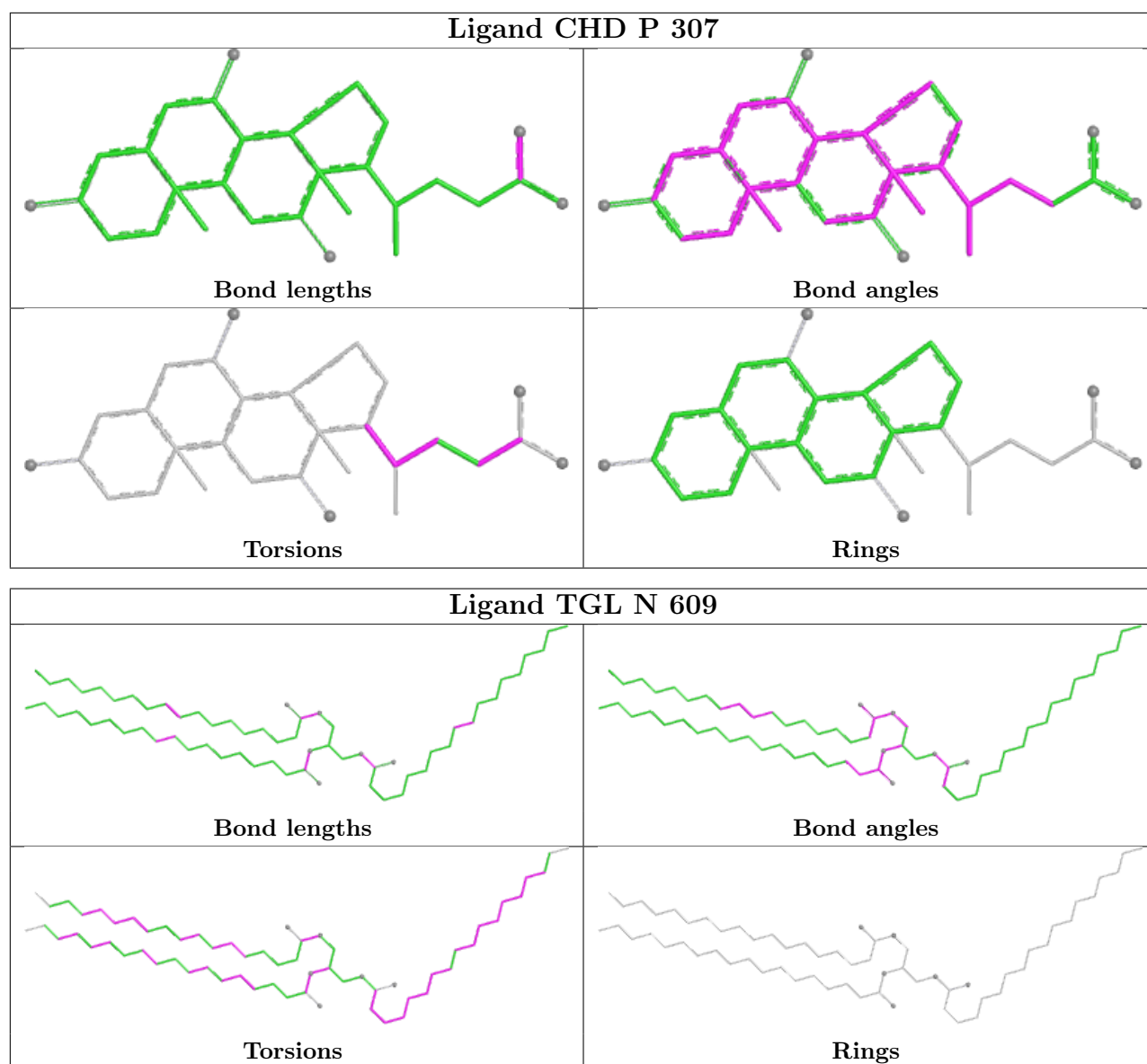
Ligand CHD B 302











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%)	-0.65	2 (0%) 88 88	13, 27, 35, 67	3 (0%)
1	N	513/514 (99%)	-0.25	5 (0%) 79 79	16, 35, 47, 76	3 (0%)
2	B	226/227 (99%)	-0.18	11 (4%) 35 34	24, 33, 55, 80	0
2	O	226/227 (99%)	0.26	11 (4%) 35 34	34, 45, 69, 94	0
3	C	259/261 (99%)	-0.33	2 (0%) 82 82	18, 32, 44, 64	3 (1%)
3	P	259/261 (99%)	-0.16	3 (1%) 76 76	22, 37, 48, 69	3 (1%)
4	D	144/147 (97%)	-0.18	2 (1%) 73 73	28, 36, 52, 69	0
4	Q	144/147 (97%)	0.95	19 (13%) 7 6	41, 58, 83, 130	0
5	E	105/109 (96%)	-0.21	2 (1%) 66 66	28, 36, 59, 99	0
5	R	105/109 (96%)	0.06	4 (3%) 44 43	36, 47, 66, 104	0
6	F	98/98 (100%)	0.46	9 (9%) 14 13	29, 39, 97, 134	0
6	S	98/98 (100%)	0.92	14 (14%) 6 5	31, 45, 103, 128	0
7	G	83/85 (97%)	0.97	18 (21%) 2 2	31, 39, 110, 123	0
7	T	83/85 (97%)	1.10	20 (24%) 2 2	32, 47, 104, 119	0
8	H	79/85 (92%)	0.47	11 (13%) 6 5	30, 40, 88, 113	0
8	U	79/85 (92%)	0.83	12 (15%) 5 5	39, 50, 97, 125	0
9	I	73/74 (98%)	0.35	3 (4%) 41 40	34, 44, 67, 71	0
9	V	73/74 (98%)	0.83	6 (8%) 17 16	35, 60, 77, 116	0
10	J	58/59 (98%)	0.38	3 (5%) 33 31	33, 43, 72, 103	0
10	W	58/59 (98%)	0.64	6 (10%) 12 11	41, 52, 85, 125	0
11	K	49/56 (87%)	0.12	1 (2%) 65 64	34, 40, 52, 57	0
11	X	49/56 (87%)	0.90	5 (10%) 12 11	47, 59, 76, 84	0
12	L	46/47 (97%)	-0.12	2 (4%) 40 39	28, 33, 55, 83	0
12	Y	46/47 (97%)	0.60	4 (8%) 16 15	38, 50, 74, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.30	5 (11%) 9 8	29, 34, 90, 114	0
13	Z	43/46 (93%)	0.86	7 (16%) 4 4	46, 54, 122, 136	0
All	All	3552/3616 (98%)	0.06	187 (5%) 32 31	13, 38, 72, 136	12 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	15.2
6	S	97	ALA	12.5
4	Q	6	VAL	11.4
4	Q	5	VAL	9.5
6	S	1	ALA	9.0
6	S	94	HIS	8.3
6	F	96	LEU	8.2
6	S	93	PRO	8.1
6	S	96	LEU	7.8
8	U	8	ILE	7.8
7	G	5	LYS	7.4
7	G	2	SER	7.4
8	H	8	ILE	7.2
6	F	97	ALA	7.0
7	G	3	ALA	7.0
7	T	3	ALA	6.9
7	T	36	TRP	6.9
7	G	4	ALA	6.8
7	T	4	ALA	6.8
10	J	1	PHE	6.8
7	T	5	LYS	6.7
7	G	9	GLY	6.5
6	F	3	GLY	6.1
7	G	36	TRP	6.1
7	T	1	ALA	5.9
6	S	3	GLY	5.8
7	T	9	GLY	5.7
6	S	95	GLN	5.6
10	W	1	PHE	5.6
6	S	98	HIS	5.6
13	Z	41	LYS	5.5
7	T	2	SER	5.4
2	B	59	GLN	5.3
7	G	7	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
4	Q	8	SER	5.1
8	U	45	ALA	5.1
4	Q	7	LYS	5.1
7	G	1	ALA	5.1
6	F	2	SER	5.0
2	O	113	TYR	5.0
2	O	226	MET	5.0
4	Q	4	SER	4.8
7	G	10	GLY	4.8
1	N	136[A]	LEU	4.7
7	T	12	GLY	4.7
2	O	90	ILE	4.7
7	T	37	LEU	4.6
7	G	6	GLY	4.6
13	Z	40	TYR	4.5
6	F	94	HIS	4.5
6	S	2	SER	4.4
2	O	227	LEU	4.2
7	T	84	LYS	4.2
9	V	2	THR	4.2
7	G	12	GLY	4.1
7	G	8	HIS	4.1
5	E	5	HIS	4.0
13	M	42	LYS	4.0
13	M	40	TYR	4.0
6	F	98	HIS	4.0
11	X	6	ALA	3.9
13	M	41	LYS	3.9
2	B	60	GLU	3.9
2	B	58	ALA	3.9
7	G	37	LEU	3.9
8	H	9	LYS	3.9
8	H	45	ALA	3.9
5	E	109	VAL	3.8
4	D	4	SER	3.8
10	W	58	LYS	3.8
9	V	3	ALA	3.8
8	U	47	GLY	3.8
8	U	46	LYS	3.7
13	Z	42	LYS	3.7
10	J	48	TYR	3.7
7	T	7	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
13	M	43	SER	3.6
12	Y	20	ARG	3.5
4	Q	9	GLU	3.5
5	R	109	VAL	3.5
6	F	95	GLN	3.4
5	R	5	HIS	3.4
8	U	10	ASN	3.4
5	R	80	GLU	3.4
10	J	58	LYS	3.4
9	V	37	PHE	3.3
2	O	65	TRP	3.2
7	T	6	GLY	3.2
7	T	8	HIS	3.2
7	G	84	LYS	3.2
1	N	514	LYS	3.2
12	L	2	HIS	3.1
9	V	1	SER	3.1
9	V	26	MET	3.1
7	T	10	GLY	3.1
12	Y	2	HIS	3.0
8	U	44	THR	3.0
11	X	23	THR	2.9
3	P	3	HIS	2.9
4	Q	58	GLU	2.9
7	T	39	SER	2.9
8	U	9	LYS	2.9
4	Q	10	ASP	2.8
4	Q	35	ALA	2.8
1	N	48	LEU	2.8
7	T	38	HIS	2.8
2	O	58	ALA	2.8
10	W	48	TYR	2.8
2	B	65	TRP	2.8
6	S	43	LYS	2.7
11	K	47	ARG	2.7
8	H	10	ASN	2.7
13	Z	43	SER	2.7
6	S	4	GLY	2.7
2	B	113	TYR	2.7
2	O	91	ASN	2.7
2	O	126	SER	2.7
7	T	42	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
7	T	41	HIS	2.7
7	T	40	GLY	2.7
8	H	44	THR	2.6
3	C	3	HIS	2.6
1	N	49	GLY	2.6
11	X	52	GLU	2.6
2	B	57	ASP	2.6
8	H	46	LYS	2.6
8	U	50	VAL	2.6
3	C	38	ASN	2.6
13	Z	35	TYR	2.6
2	B	90	ILE	2.5
8	U	7	LYS	2.5
8	U	42	ALA	2.5
2	B	61	VAL	2.5
11	X	48	VAL	2.5
13	Z	37	LEU	2.5
2	B	91	ASN	2.5
12	Y	45	LEU	2.5
1	N	513	LEU	2.4
4	Q	33	LEU	2.4
7	G	40	GLY	2.4
9	V	25	PHE	2.4
2	O	92	ASN	2.4
4	Q	39	ALA	2.4
13	M	39	ASN	2.4
9	I	37	PHE	2.4
4	Q	53	ILE	2.4
6	F	93	PRO	2.4
7	G	41	HIS	2.4
5	R	108	LYS	2.3
2	O	57	ASP	2.3
4	Q	11	TYR	2.3
6	S	26	LYS	2.3
8	H	7	LYS	2.3
12	L	47	LYS	2.3
7	T	33	LEU	2.3
8	U	55	TRP	2.3
10	W	52	TRP	2.3
7	G	38	HIS	2.2
3	P	261	SER	2.2
12	Y	21	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	32	PHE	2.2
4	Q	94	LEU	2.2
7	G	39	SER	2.2
6	S	22	LEU	2.2
8	H	50	VAL	2.1
2	B	82	ARG	2.1
9	I	26	MET	2.1
4	Q	87	PHE	2.1
4	Q	105	GLY	2.1
10	W	57	HIS	2.1
4	Q	95	LEU	2.1
4	Q	107	ILE	2.1
8	H	47	GLY	2.1
6	S	92	VAL	2.1
11	X	13	TYR	2.1
9	I	30	GLY	2.1
2	O	221	LYS	2.1
4	D	5	VAL	2.1
4	Q	17	VAL	2.1
3	P	40	MET	2.0
1	A	514	LYS	2.0
1	A	45	GLY	2.0
13	Z	1	ILE	2.0
10	W	55	PHE	2.0
8	H	43	MET	2.0
8	H	42	ALA	2.0
8	U	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	0.47	0.28	87,95,113,113	0
7	TPO	G	11	11/12	0.62	0.35	83,91,111,114	0
1	FME	A	1	10/11	0.86	0.14	44,53,74,81	0
1	FME	N	1	10/11	0.88	0.15	52,58,75,76	0
2	FME	B	1	10/11	0.95	0.09	32,34,43,59	0
2	FME	O	1	10/11	0.97	0.08	45,47,58,65	0

6.3 Carbohydrates ⓘ

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
18	NA	A	606	1/1	0.58	0.28	45,45,45,45	0
28	DMU	P	301	33/33	0.70	0.32	132,165,171,171	0
25	PEK	T	101	53/53	0.73	0.30	62,105,129,130	0
25	PEK	C	306	53/53	0.73	0.30	53,92,130,133	0
25	PEK	G	104	53/53	0.74	0.30	60,112,135,137	0
26	PSC	O	303	52/52	0.75	0.30	57,105,133,136	0
28	DMU	G	101	33/33	0.75	0.27	103,146,153,154	0
20	PGV	C	307	51/51	0.75	0.29	62,90,111,112	0
22	CHD	C	304	29/29	0.76	0.26	92,125,126,127	0
22	CHD	P	307	29/29	0.76	0.23	91,121,122,124	0
19	TGL	N	610	63/63	0.76	0.27	57,80,98,100	0
18	NA	N	606	1/1	0.76	0.24	53,53,53,53	0
20	PGV	P	302	51/51	0.77	0.27	74,105,119,121	0
25	PEK	P	309	53/53	0.77	0.28	47,97,125,127	0
24	CDL	G	103	100/100	0.78	0.28	73,101,133,138	0
20	PGV	A	609	51/51	0.78	0.26	34,78,100,106	0
19	TGL	Q	201	63/63	0.79	0.29	64,87,97,100	0
24	CDL	P	306	100/100	0.79	0.26	57,103,125,132	0
26	PSC	E	201	52/52	0.79	0.22	53,106,127,129	0
24	CDL	T	102	100/100	0.79	0.27	68,101,133,137	0
19	TGL	D	201	63/63	0.79	0.24	46,69,82,83	0
19	TGL	A	607	63/63	0.79	0.26	49,77,97,100	0
24	CDL	C	303	100/100	0.80	0.24	44,96,128,130	0
20	PGV	N	607	51/51	0.80	0.25	54,92,119,123	0
19	TGL	L	101	63/63	0.80	0.24	38,61,82,85	0
19	TGL	N	609	63/63	0.83	0.24	57,84,100,103	0
28	DMU	Z	101	33/33	0.87	0.14	57,70,87,91	0
23	UNX	C	301	1/1	0.90	0.23	38,38,38,38	0
22	CHD	C	305	29/29	0.90	0.11	37,44,47,48	0
22	CHD	P	308	29/29	0.91	0.10	41,47,50,50	0
23	UNX	P	303	1/1	0.92	0.27	35,35,35,35	0
28	DMU	M	101	33/33	0.92	0.11	43,49,68,70	0

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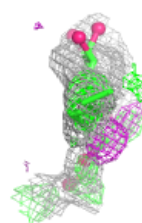
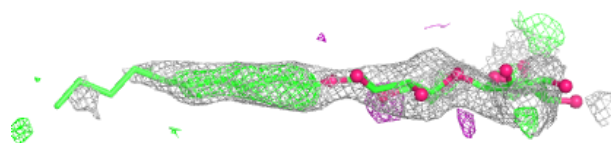
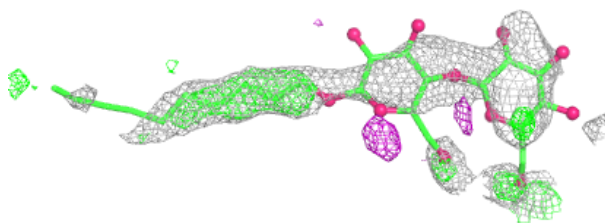
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	PEK	P	304	53/53	0.93	0.16	38,60,93,95	0
17	MG	N	605	1/1	0.94	0.08	39,39,39,39	0
25	PEK	G	102	53/53	0.95	0.13	29,50,79,81	0
20	PGV	N	608	51/51	0.96	0.11	30,49,74,76	0
20	PGV	C	302	51/51	0.96	0.11	26,37,79,82	0
22	CHD	B	302	29/29	0.96	0.07	33,37,42,53	0
20	PGV	A	608	51/51	0.96	0.10	24,41,65,70	0
17	MG	A	605	1/1	0.96	0.04	27,27,27,27	0
20	PGV	P	305	51/51	0.97	0.10	31,47,86,89	0
22	CHD	O	302	29/29	0.97	0.06	33,37,43,45	0
15	HEA	A	602	60/60	0.98	0.06	17,23,51,55	0
15	HEA	N	602	60/60	0.98	0.09	15,31,57,63	0
14	CYN	N	601	2/2	0.99	0.06	30,30,30,31	0
15	HEA	N	603	60/60	0.99	0.06	25,30,39,42	0
27	ZN	S	101	1/1	0.99	0.03	40,40,40,40	0
14	CYN	A	601	2/2	0.99	0.04	20,20,20,24	0
15	HEA	A	603	60/60	0.99	0.05	18,23,33,35	0
21	CUA	B	301	2/2	0.99	0.03	26,26,26,27	0
21	CUA	O	301	2/2	0.99	0.02	38,38,38,38	0
27	ZN	F	101	1/1	1.00	0.01	35,35,35,35	0
16	CU	A	604	1/1	1.00	0.01	25,25,25,25	0
16	CU	N	604	1/1	1.00	0.01	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.

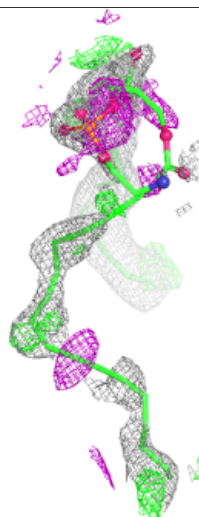
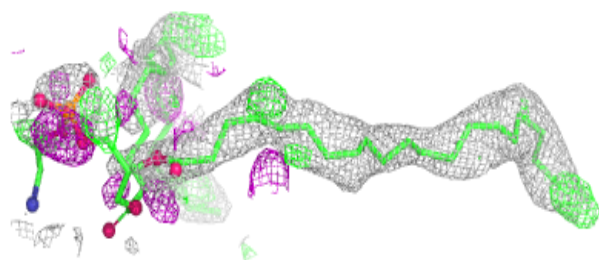
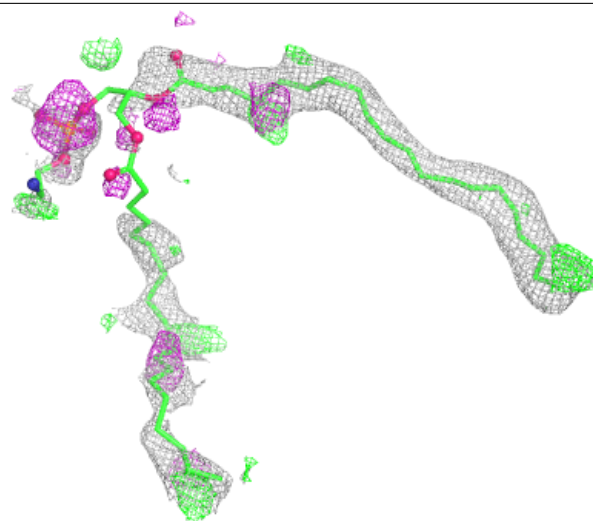
Electron density around DMU P 301:

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



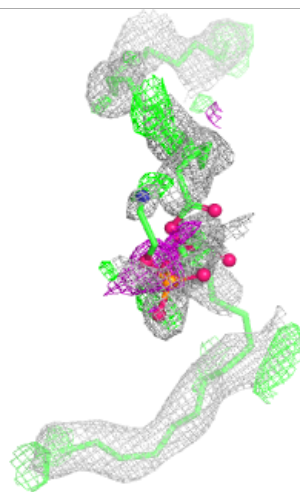
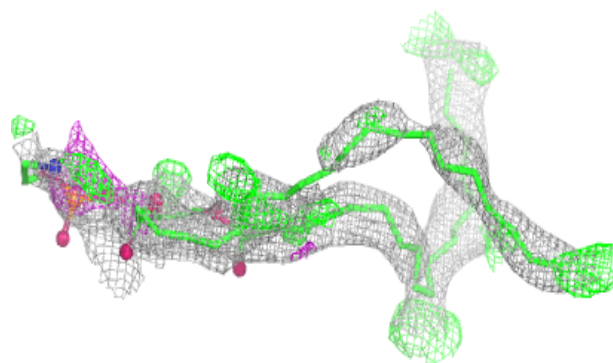
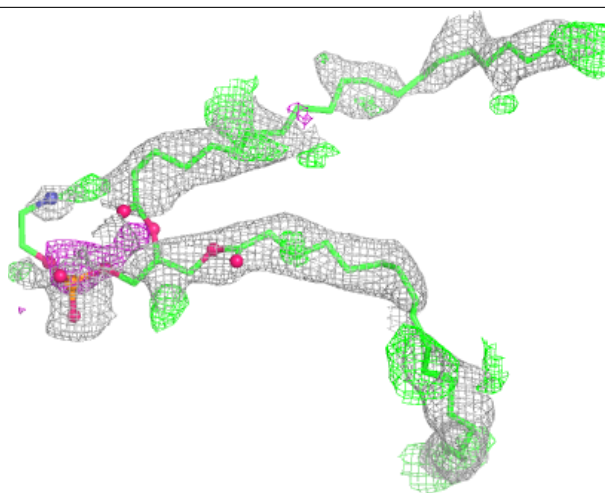
Electron density around PEK T 101:

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



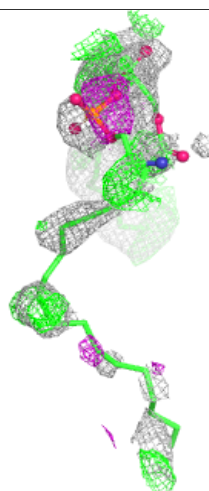
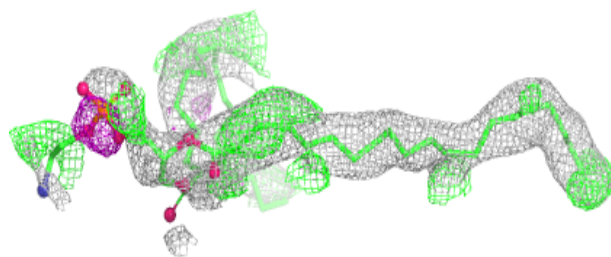
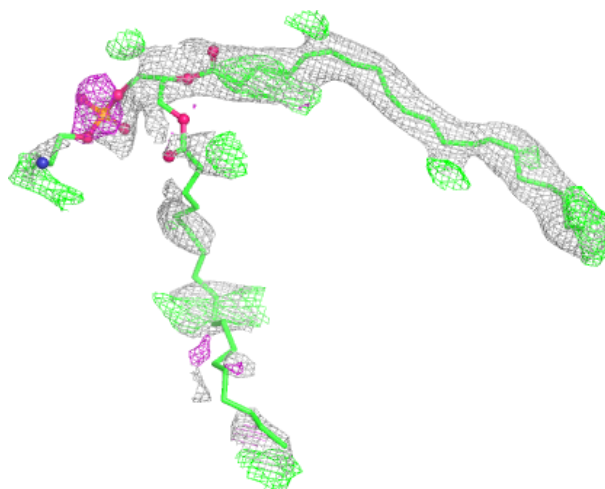
Electron density around PEK C 306:

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



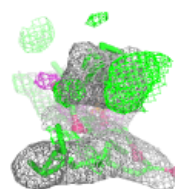
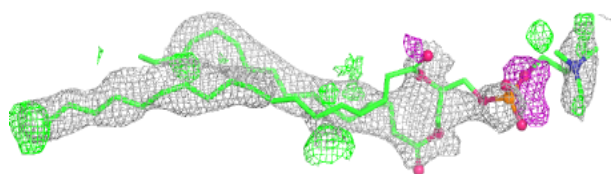
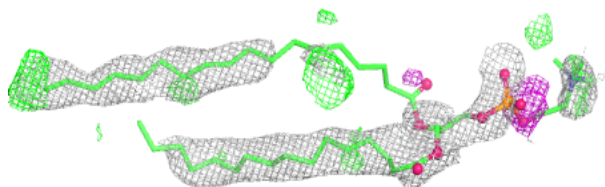
Electron density around PEK G 104:

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

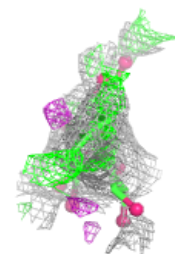
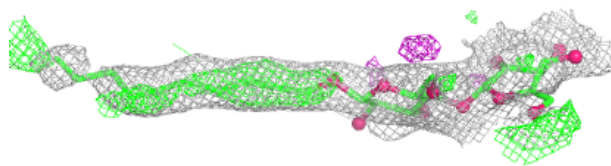
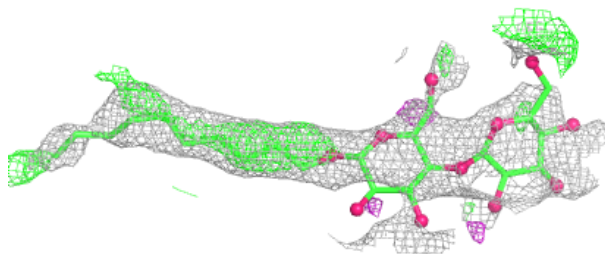


Electron density around PSC O 303:

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

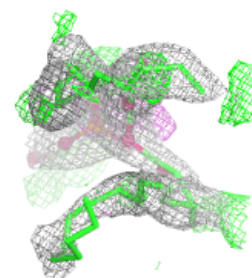
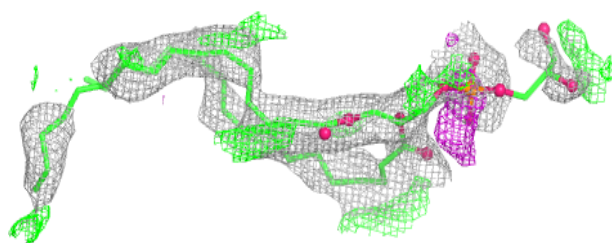
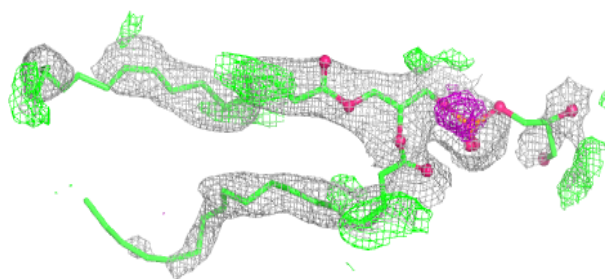
**Electron density around DMU G 101:**

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

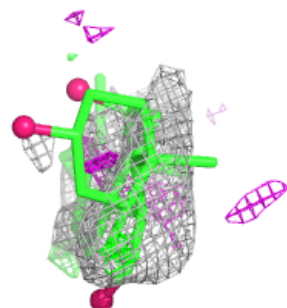
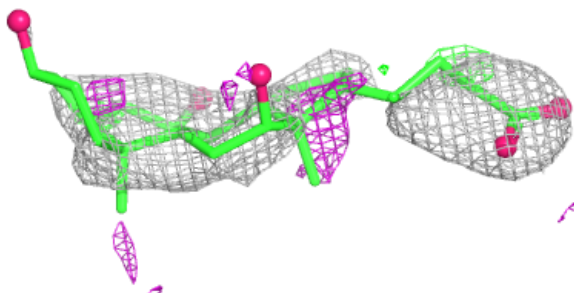
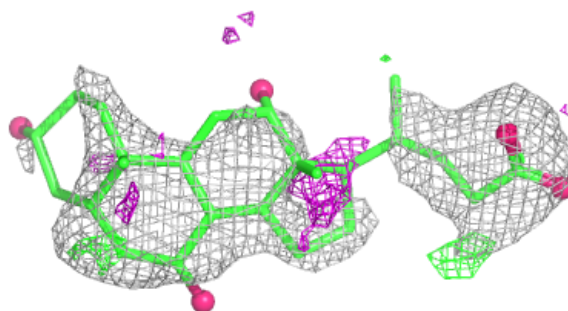


Electron density around PGV C 307:

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

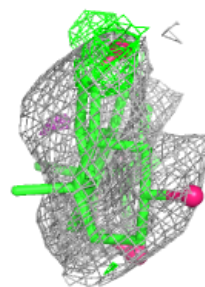
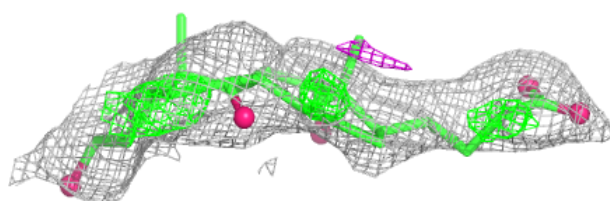
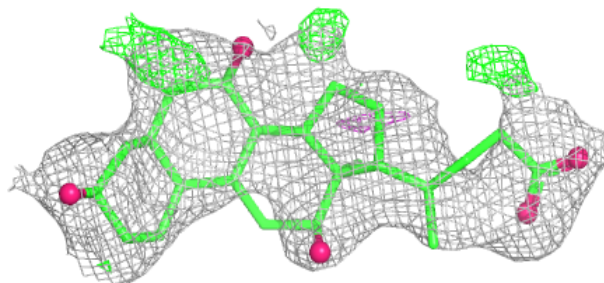
**Electron density around CHD C 304:**

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

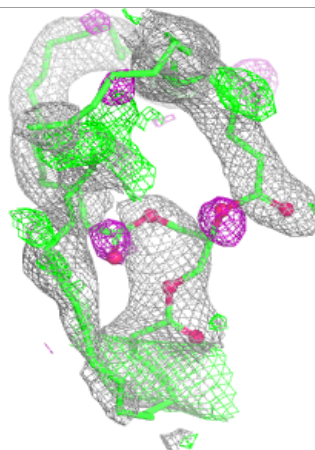
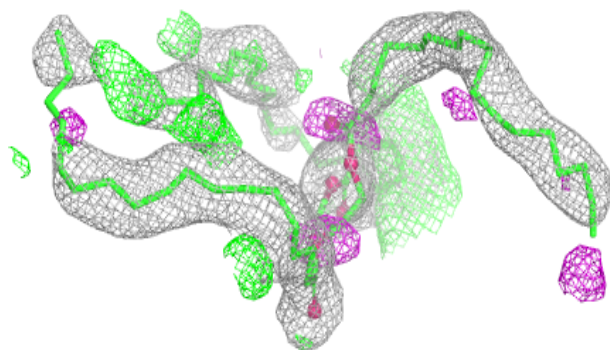
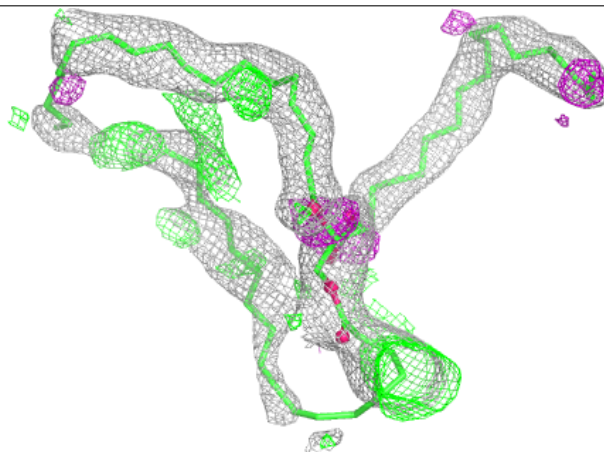


Electron density around CHD P 307:

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

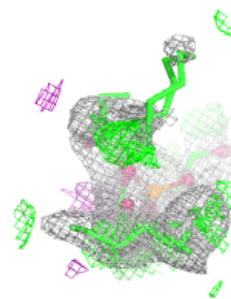
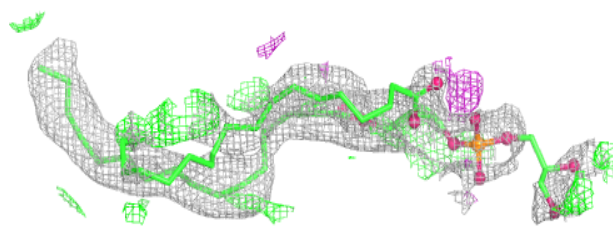
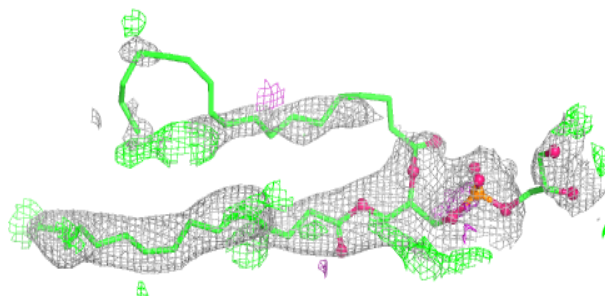
**Electron density around TGL N 610:**

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



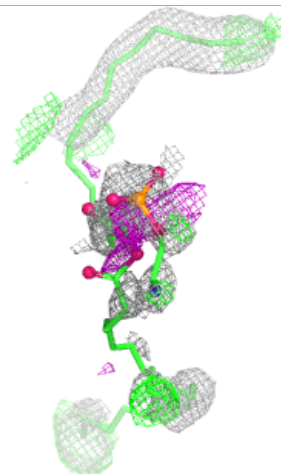
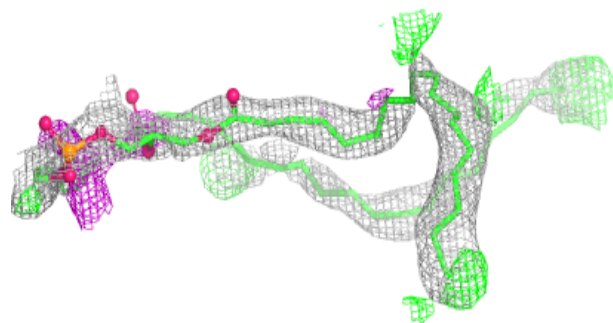
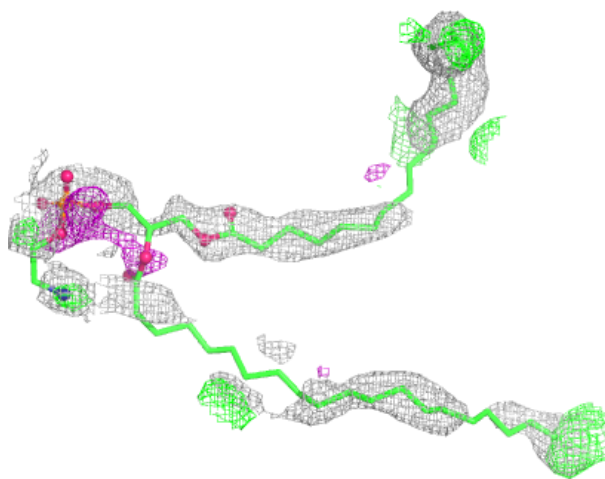
Electron density around PGV P 302:

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



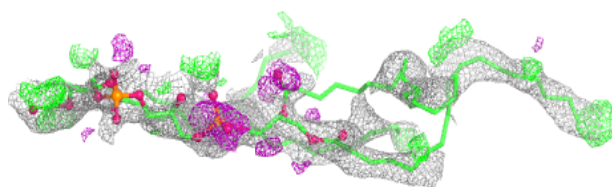
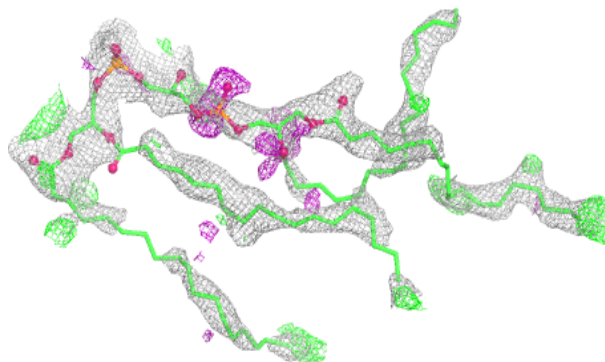
Electron density around PEK P 309:

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

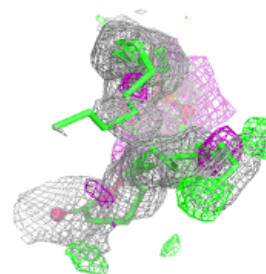
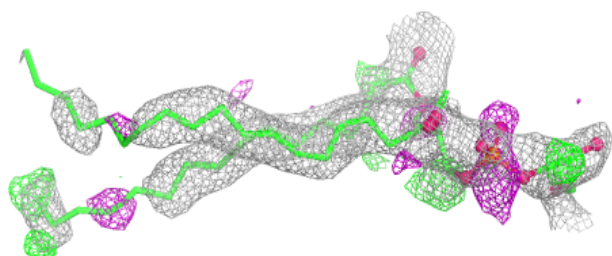
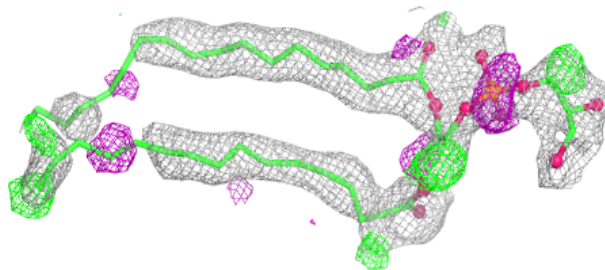


Electron density around CDL G 103:

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

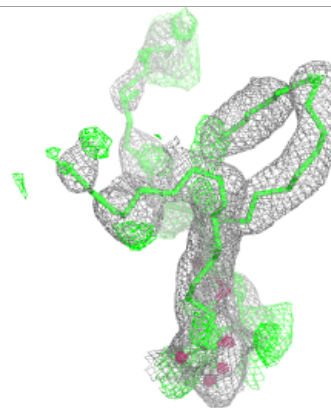
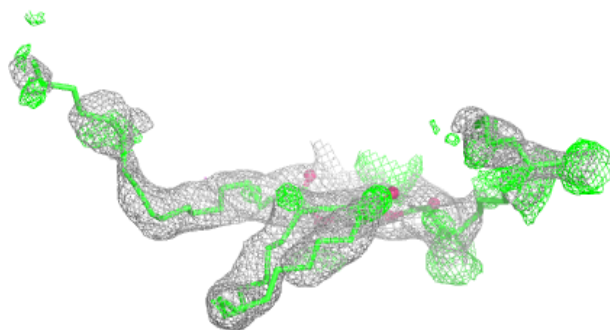
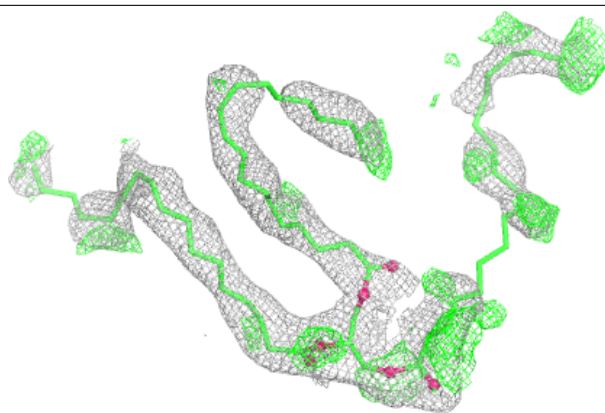
**Electron density around PGV A 609:**

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



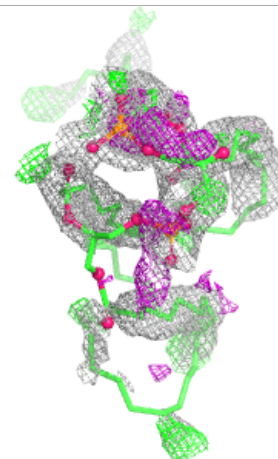
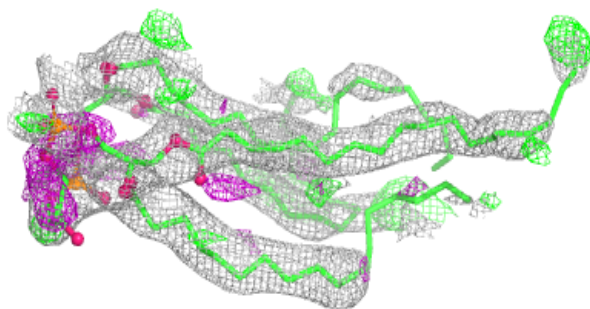
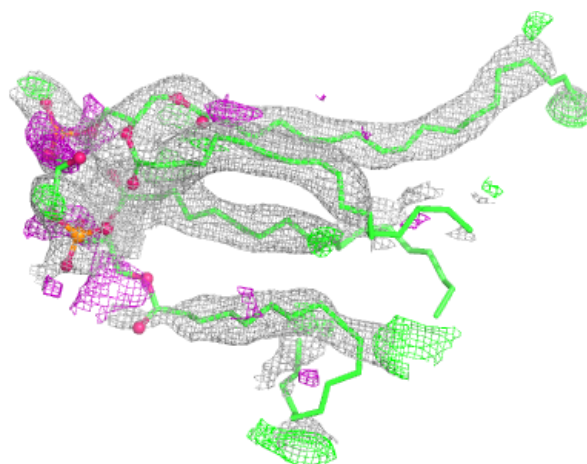
Electron density around TGL Q 201:

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



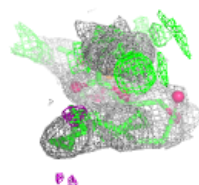
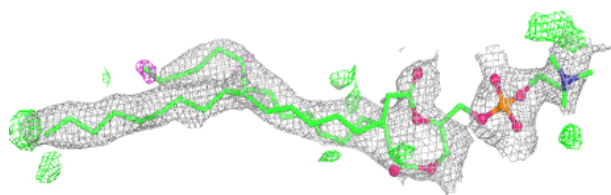
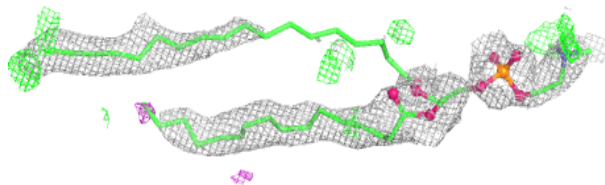
Electron density around CDL P 306:

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

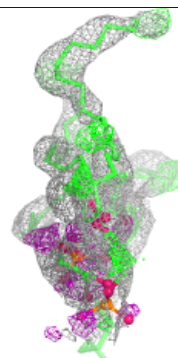
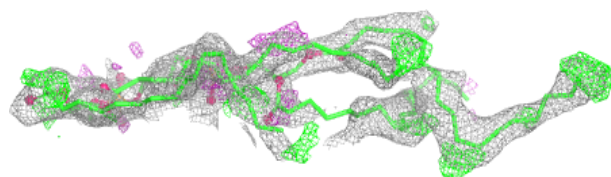
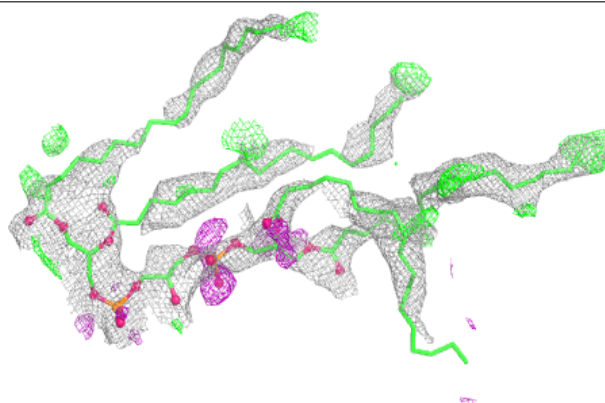


Electron density around PSC E 201:

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

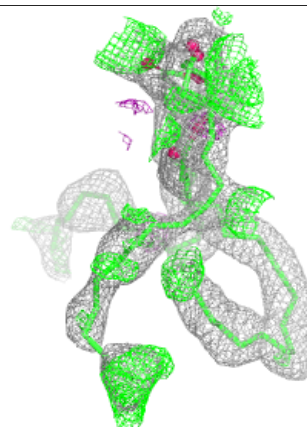
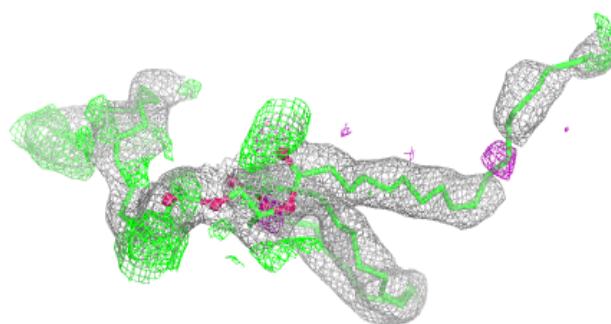
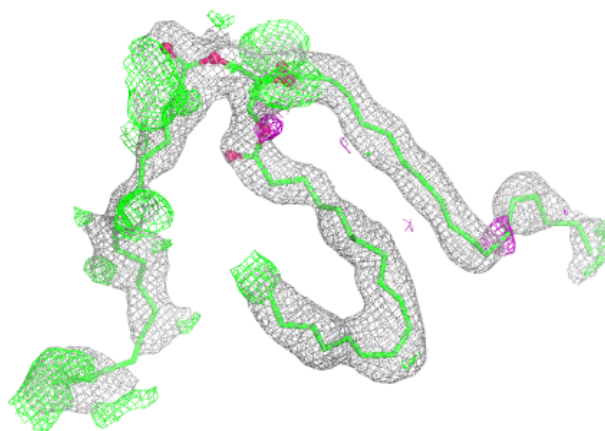
**Electron density around CDL T 102:**

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



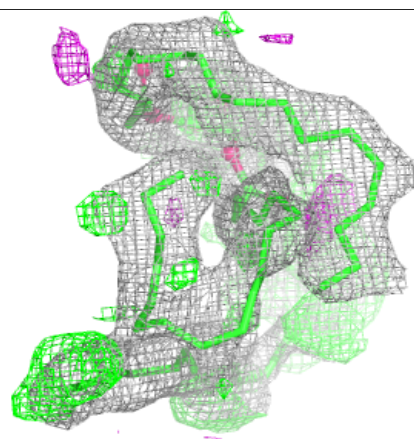
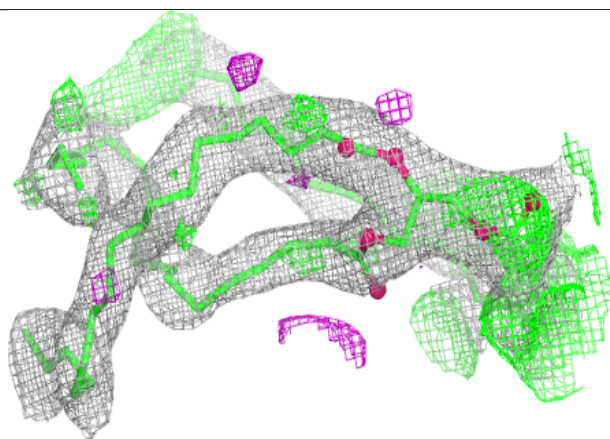
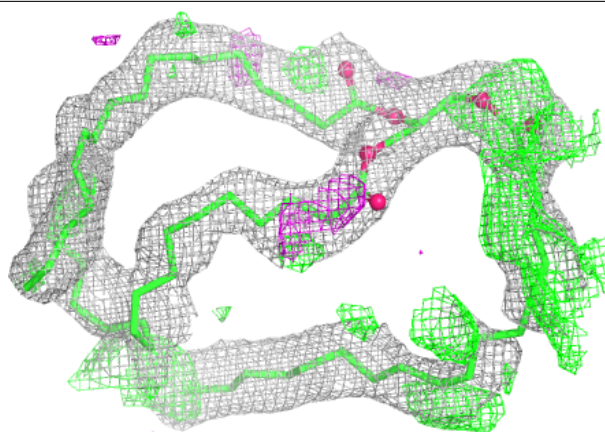
Electron density around TGL D 201:

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



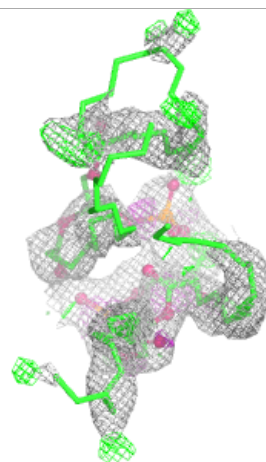
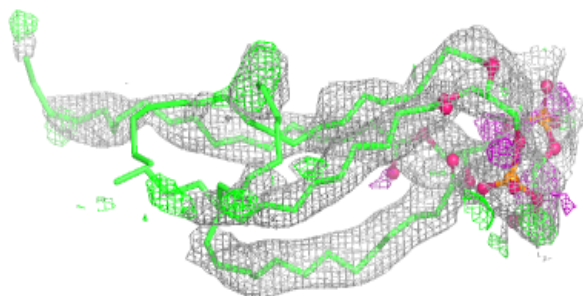
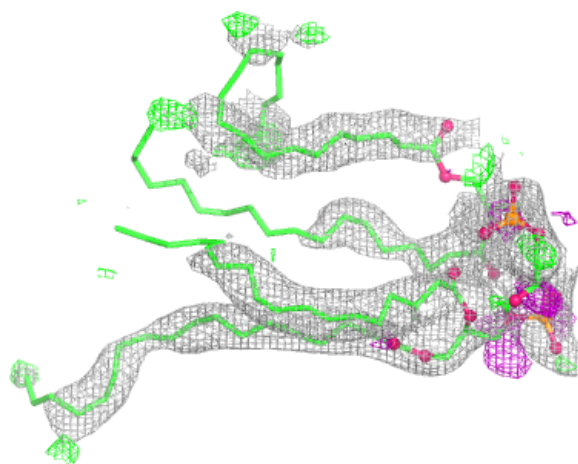
Electron density around TGL A 607:

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



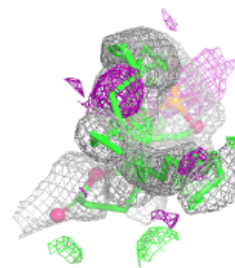
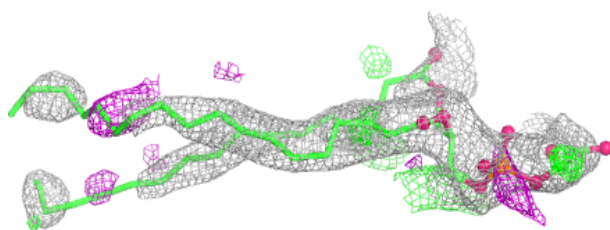
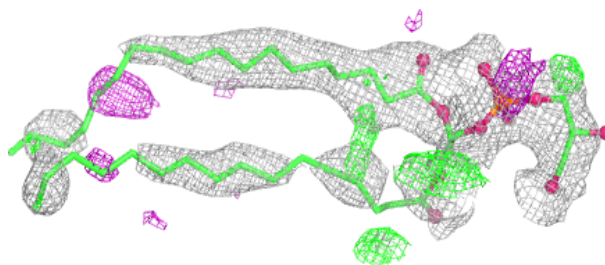
Electron density around CDL C 303:

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



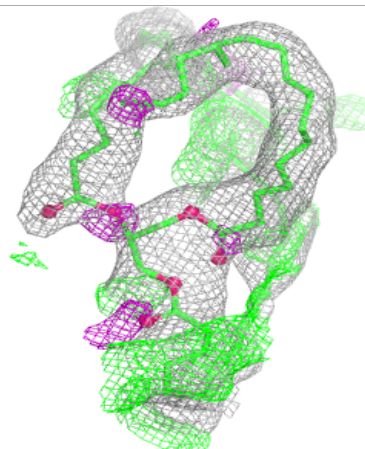
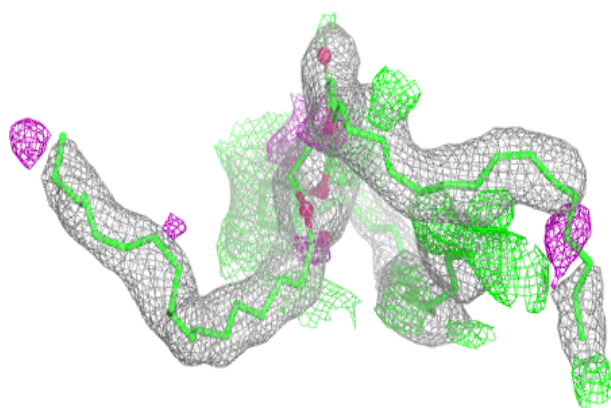
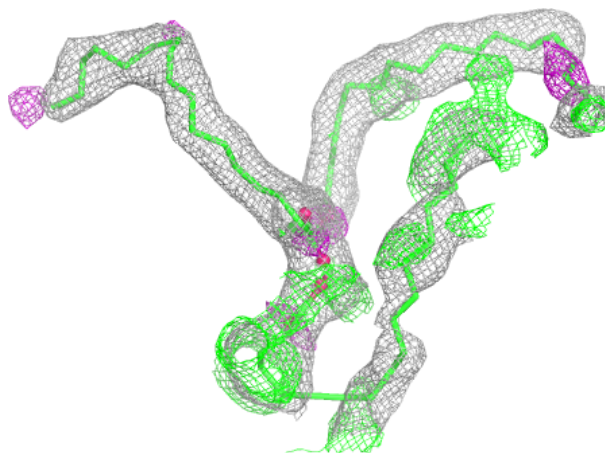
Electron density around PGV N 607:

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



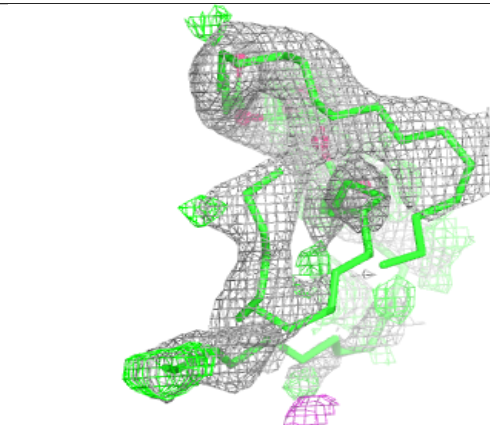
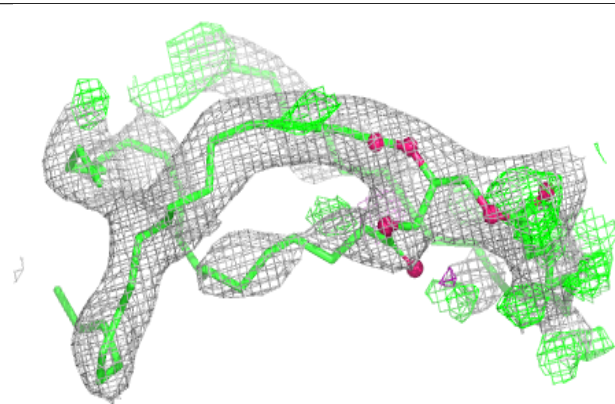
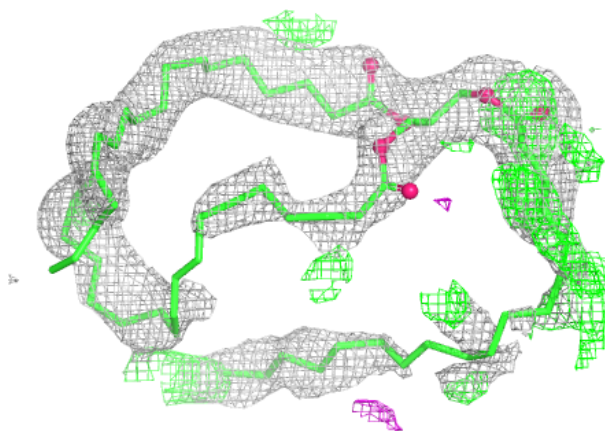
Electron density around TGL L 101:

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

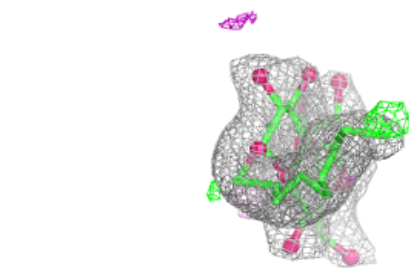
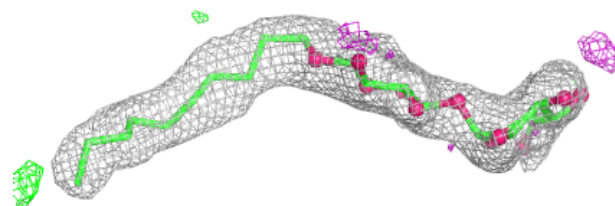
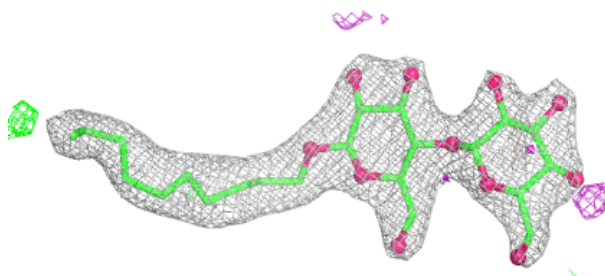


Electron density around TGL N 609:

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

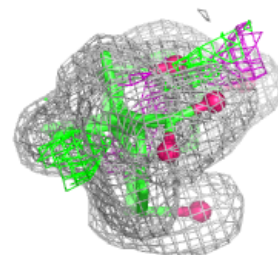
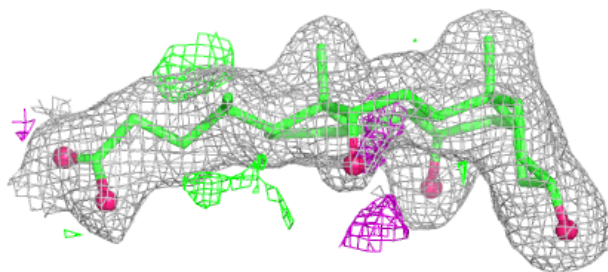
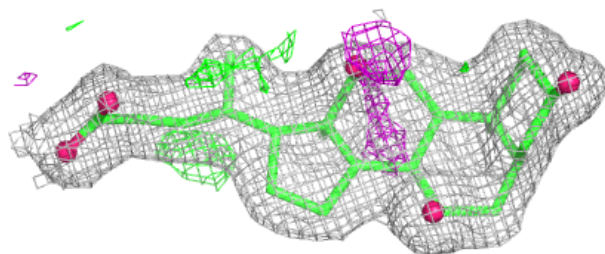
**Electron density around DMU Z 101:**

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

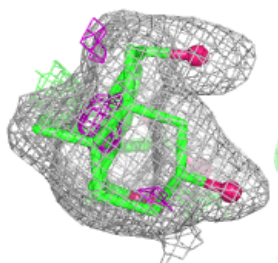
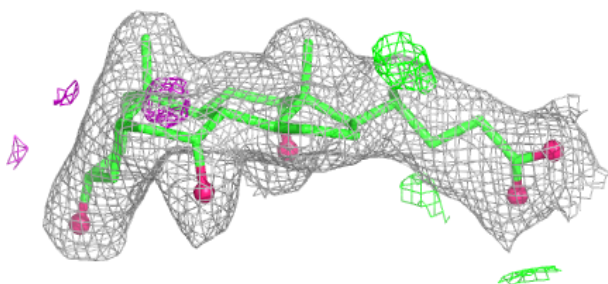
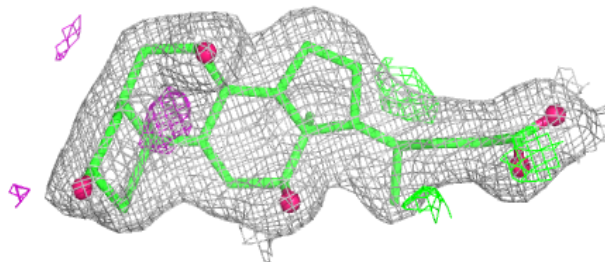


Electron density around CHD C 305:

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

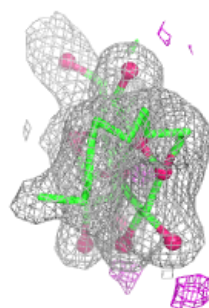
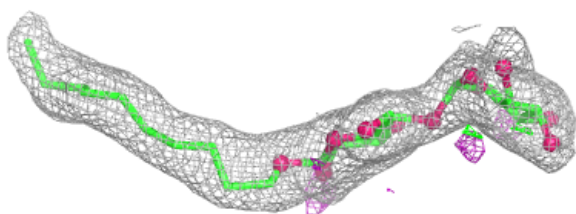
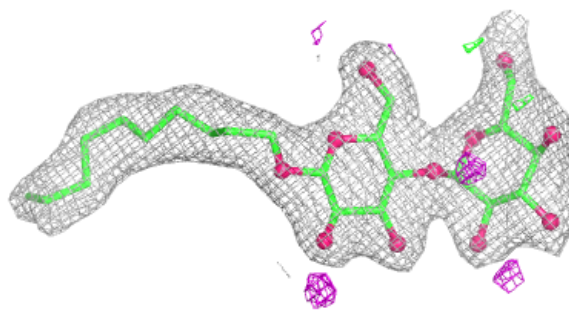
**Electron density around CHD P 308:**

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

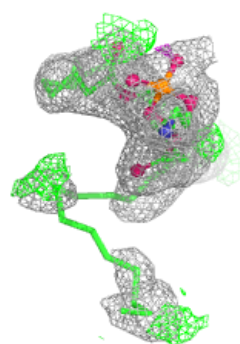
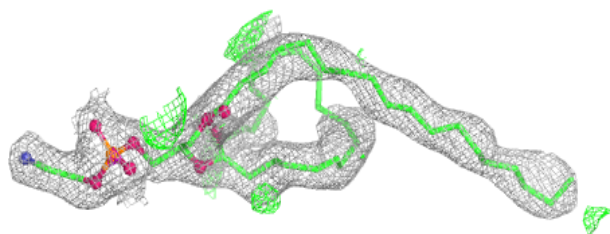
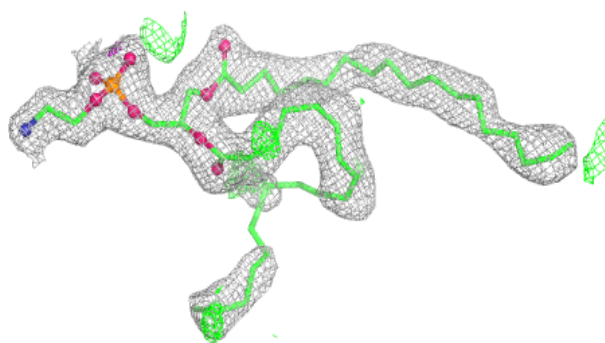


Electron density around DMU M 101:

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

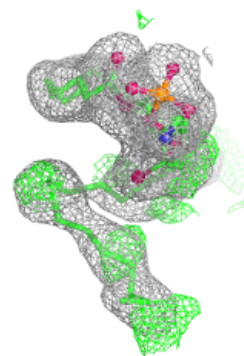
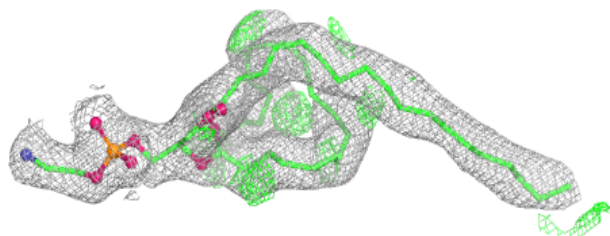
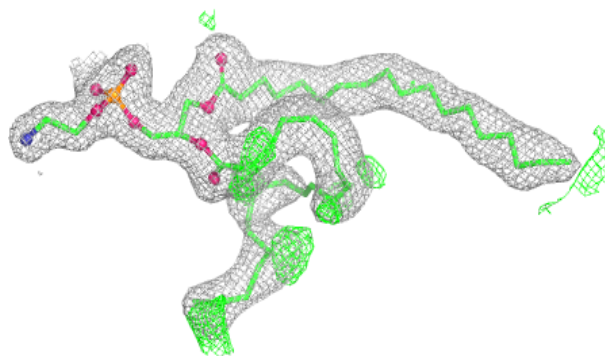
**Electron density around PEK P 304:**

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

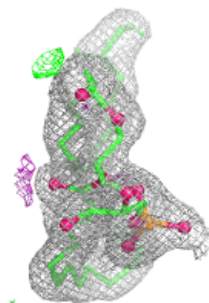
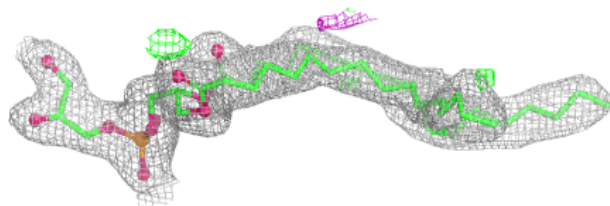
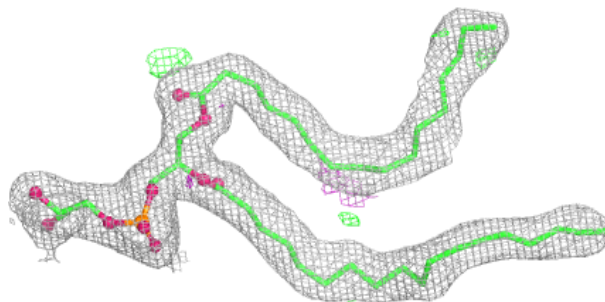


Electron density around PEK G 102:

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

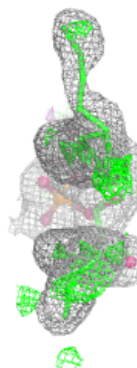
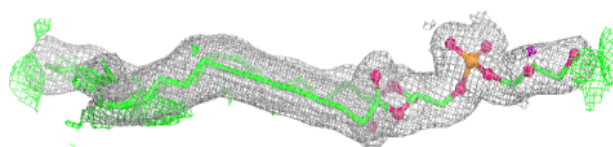
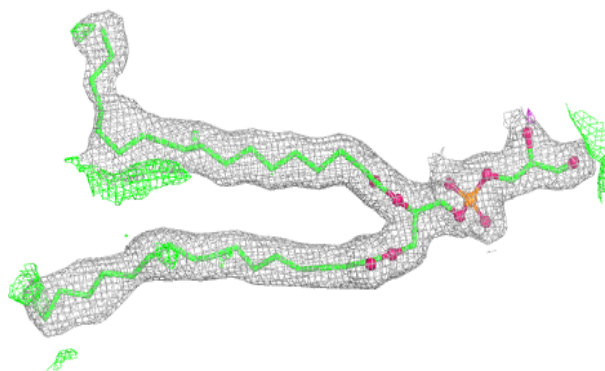
**Electron density around PGV N 608:**

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

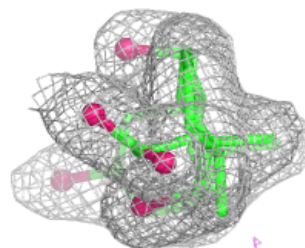
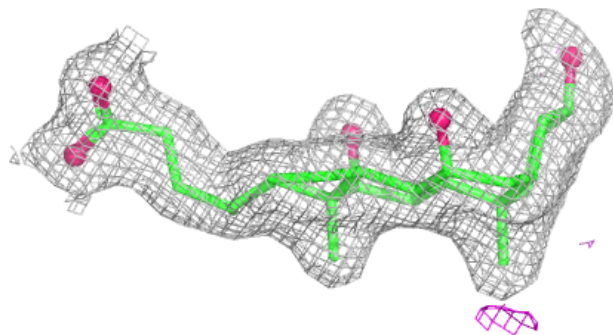
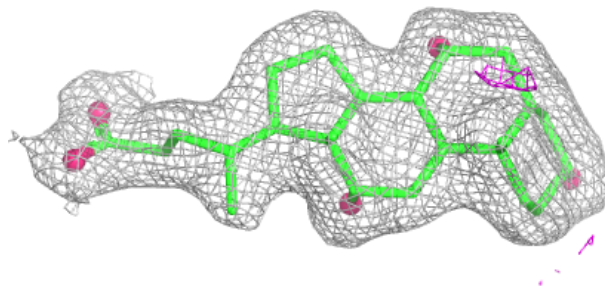


Electron density around PGV C 302:

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

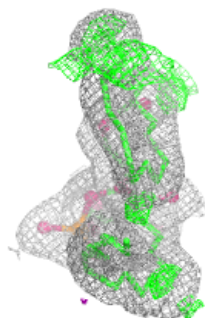
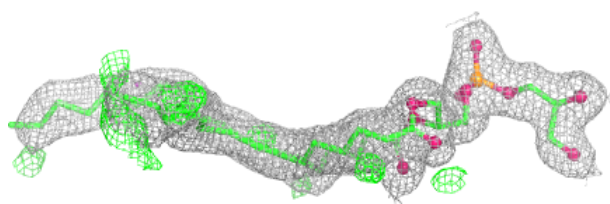
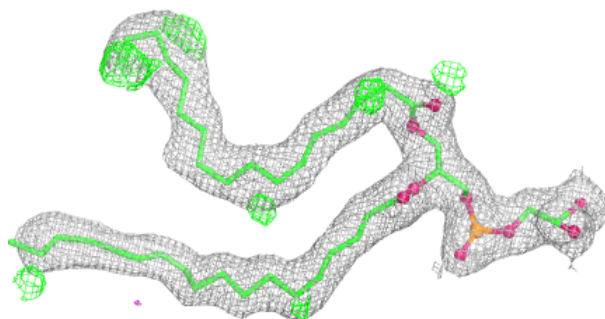
**Electron density around CHD B 302:**

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

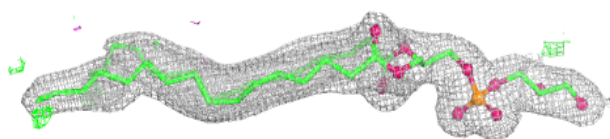
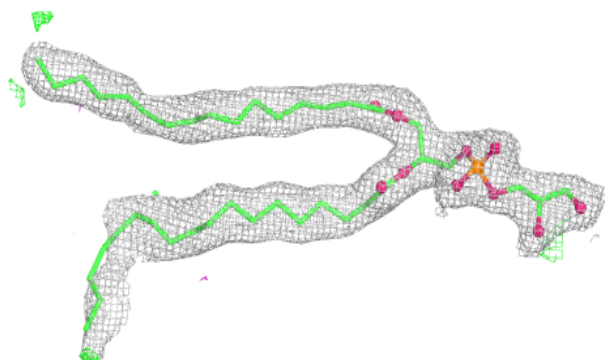


Electron density around PGV A 608:

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

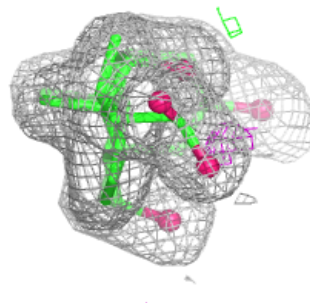
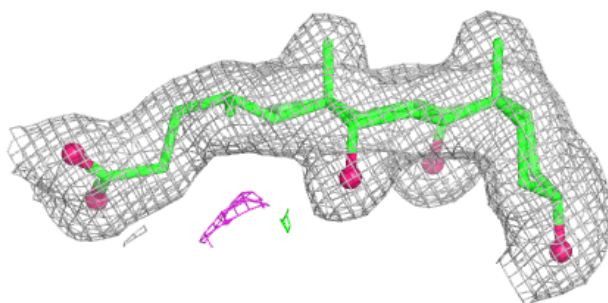
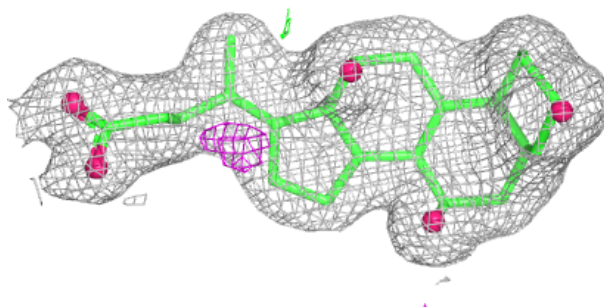
**Electron density around PGV P 305:**

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

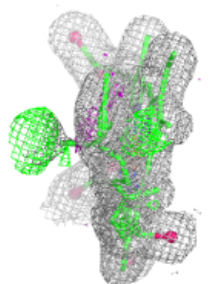
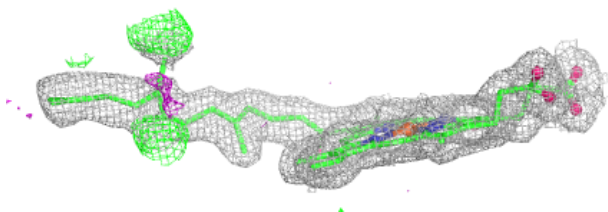
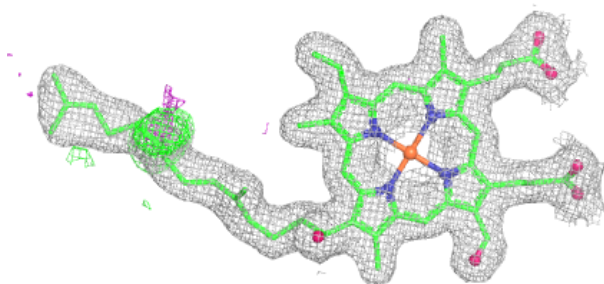


Electron density around CHD O 302:

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

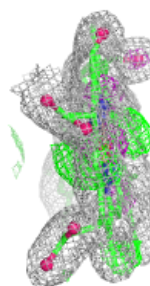
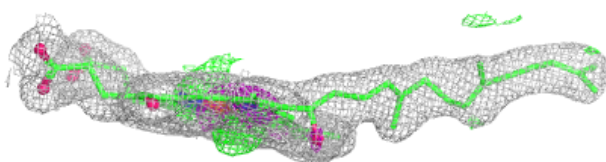
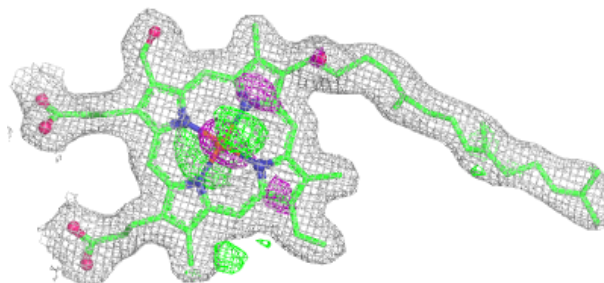
**Electron density around HEA A 602:**

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

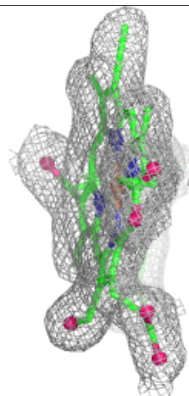
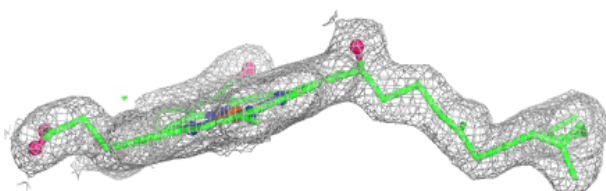
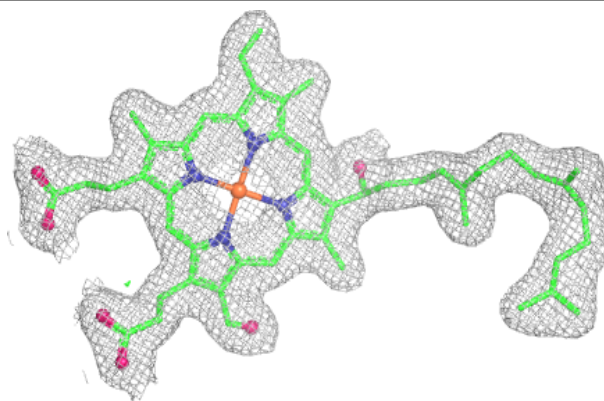


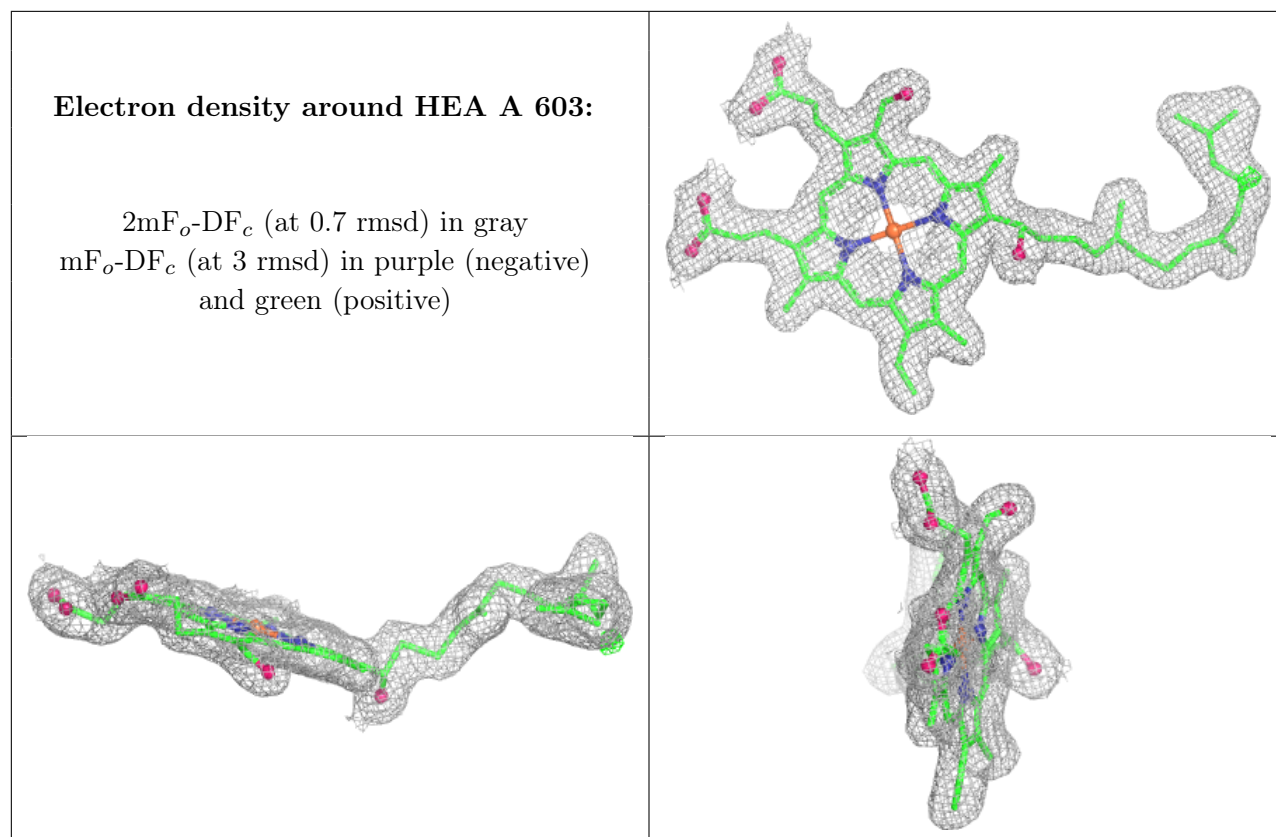
Electron density around HEA N 602:

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

**Electron density around HEA N 603:**

$2mF_o-DF_c$ (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.